ASYMPTOTIC THEORY AND APPLICATIONS OF RANDOM FUNCTIONS

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ABSTRACT

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Random functions is the central component in many statistical and probabilistic problems. This dissertation presents theoretical analysis and computation for random functions and its applications in statistics.

This dissertation consists of two parts. The first part is on the topic of classic continuous random fields. We present asymptotic analysis and computation for three non-linear functionals of random fields. In Chapter 2, we propose an efficient Monte Carlo algorithm for computing $\mathbb{P}\{\sup_T f(t) > b\}$ when b is large, and f is a Gaussian random field living on a compact subset T. For each pre-specified relative error ε, the proposed algorithm runs in a constant time for an arbitrarily large b and computes the probability with the relative error ε. In Chapter 3, we present the asymptotic analysis for the tail probability of $\int_T e^{\sigma f(t)+\mu(t)}dt$ under the asymptotic regime that σ tends to zero. In Chapter 4, we consider partial differential equations (PDE) with random coefficients, and we develop an unbiased Monte Carlo estimator with finite variance for computing expectations of the solution to random PDEs. Moreover, the expected computational cost of generating one such estimator is finite. In this analysis, we employ a quadratic approximation to solve random PDEs and perform precise error analysis of this numerical solver.

The second part of this dissertation focuses on topics in statistics. The random functions of interest are likelihood functions, whose maximum plays a key role in statistical inference. We present asymptotic analysis for likelihood based hypothesis tests and sequential analysis. In Chapter 5, we derive an analytical form for the exponential decay rate of error probabilities of the generalized likelihood ratio test for testing two general families of hypotheses. In Chapter 6, we study the asymptotic property of the generalized sequential probability ratio test, the stopping rule of which is the first boundary crossing time of the generalized likelihood ratio statistic. We show that this sequential test is asymptotically optimal in the sense that it achieves asymptotically the shortest expected sample size as the maximal type I and type II error probabilities tend to zero. These results have important theoretical implications in hypothesis testing, model selection, and other areas where maximum likelihood is employed.

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To my family

Chapter 1

Introduction

Random functions is the central component in many statistical and probabilistic problems. This dissertation presents theoretical analysis and computation for random functions and its applications in statistics.

This dissertation consists of two parts. The the first part (Chapter 2, Chapter 3 and Chapter 4) falls into the category of applied probability, where the random functions are classic continuous random fields such as Gaussian random fields. Under different problem settings, three types of functionals of random fields are studied.

In Chapter 2, we consider the supremum of a Hölder continuous Gaussian random field $\{f(t) : t \in T\}$ living on a compact set $T \subset \mathbb{R}^d$. A classic problem in applied probability is the asymptotic analysis and simulation of the tail probability $\mathbb{P}(\sup_{t\in T} f(t) > b)$ as $b \to \infty$, which have a wide range of applications including, but not limited to, physical oceanography, cosmology, quantum chaos, and brain mapping [Adler *et al.*, 1996; Bardeen *et al.*, 1986; Dennis, 2007; Friston *et al.*, 1994]. For simulating such small probabilities with a reasonable relative accuracy, standard Monte Carlo method requires computational cost that grows exponentially fast in b^2. We design efficient computational method that runs in *constant* time that is independent with b for achieving the same level of relative accuracy. Besides computation, the change of measure and its analysis techniques have several theoretical indications in the asymptotic analysis of general random functions, which will be presented in Chapter 5 and Chapter 6.

In Chapter 3, we consider the integral $\int_T e^{\sigma f(t)+\mu(t)}dt$, where σ is a scale factor and $\mu(t)$ is a deterministic function living on T. Such integral of lognormal random fields plays a key role in many probabilistic models in portfolio risk analysis, spatial point processes, etc. [Liu and Xu, 2012]. We present asymptotic analysis for the tail probability of $\int_T e^{\sigma f(t)+\mu(t)}dt$ under the asymptotic regime that the scale factor σ tends to zero. This analysis has implications in risk analysis of short-term behavior of a large size portfolio under high correlations, for which the variances of log-returns could be as small as a few percent.

In Chapter 4, we consider functionals that are more complicated than those described in Chapter 2 and 3. In particular, we consider an elliptic partial differential equation (PDE)

$$-\nabla \cdot (a(x)\nabla u(x)) = f(x) \text{ for } x \in U,$$

where $U \subset \mathbb{R}^d$ is a connected domain and the functions $a(\cdot)$ and $f(\cdot)$ are random fields living on the domain U. Such random PDE is a powerful tool to characterizing various physical systems which are microscopic heterogeneous or contain measurement errors of parameters [De Marsily *et al.*, 2005; Delhomme, 1979]. Let $C(U)$ be the set of continuous functions on U and $\mathcal{Q} : C(U) \to \mathbb{R}$ be a real valued functional. We are interested in computing the expectation $\mathbb{E}\mathcal{Q}(u)$. For simulating this quantity, standard Monte Carlo is computationally intensive and has bias due to the inaccuracy of numerical solutions of PDEs. We develop an unbiased Monte Carlo estimator with finite variance for computing expectations of the solution of random PDEs. Moreover, the expected computational cost of generating one such estimator is also finite.

The second part (Chapter 5 and 6) of the this dissertation focuses on topics in statistics. The random functions of interest are likelihood functions indexed by model parameters (Chapter 5) and possibly sample size as well (Chapter 6), whose maximum is a key component in statistical inference.

In Chapter 5, we consider the generalized likelihood ratio test and derive an analytical form for the exponential decay rate of error probabilities. The study on generalized likelihood ratio test was initiated by Neyman and Pearson [1933a]. Cox [1961, 1962, 2013] discussed the case where the null hypothesis and alternative hypothesis are separate parametric families. In the context of testing a simple null hypothesis against a fixed simple alternative hypothesis, Chernoff [1952] introduced a measure of asymptotic efficiency for tests based on sum of independent and identically distributed observations, a special case of which is the likelihood ratio test. This dissertation present an extension of results in Chernoff [1952] to the generalized likelihood ratio test for testing composite null against a composite alternative hypothesis. The technical challenges of this extension mainly lie in the fact that the generalized likelihood ratio statistic is the ratio of two maximized likelihood functions. Usual techniques such as large deviation theory for independent and identically distributed random variables are no longer applicable. We resort to similar change of measure technique discussed in Chapter 2 and provide a definitive conclusion of the asymptotic efficiency of generalized likelihood ratio test under Chernoff's asymptotic regime. This result has important theoretical implications in hypothesis testing, model selection, and other areas where maximum likelihood is employed.

In Chapter 6, we present asymptotic analysis for generalized likelihood ratio test in the context of sequential analysis. The central goal of sequential analysis is to reduce the sample size required to achieve a certain level of error probabilities compared to its fixed-sample-size counterpart, by means of constructing appropriate early stopping rules. In the literature of composite sequential hypothesis testing, a univariate or multivariate exponential family is usually assumed, and asymptotic analysis of error probabilities are discussed in Bartroff and Lai [2008]; Shih *et al.* [2010]. We present asymptotic analysis for non-exponential families with the aid of an extension of the technique discussed in Chapter 5. In particular, we consider the case where the stopping rule is the first boundary crossing time of the generalized likelihood ratio statistic. We show that this sequential test is asymptotically optimal in the sense that it achieves asymptotically the shortest expected sample size as the maximal type I and type II error probabilities tend to zero.

Chapter 2

Rare-event Simulation and Efficient Discretization for the Supremum of Gaussian Random Fields[1]

2.1 Introduction

In this chapter, we consider the design and the analysis of efficient Monte Carlo methods for the high excursion events of Gaussian random fields. Consider a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and a Gaussian random field

$$f : T \times \Omega \to \mathbb{R}$$

living on a d-dimensional compact subset $T \subset \mathbb{R}^d$. Most of the time, we omit the second argument and write $f(t)$. Let $M = \sup_{t \in T} f(t)$. In this chapter, we are

[1]This chapter is based on an accepted manuscript of an article published in *Advances in Applied Probability*, Volume 47, Issue 03, September 2015, available online: http://journals.cambridge.org/abstract_S0001867800048837.

interested in the efficient computation of the high excursion probabilities, that is,

$$w(b) \triangleq \mathbb{P}(M > b) \tag{2.1}$$

as $b \to \infty$. On computing small probabilities converging to zero, it is sensible to consider relative accuracy that is defined as follows.

Definition 1. *For some positive ε and δ, a Monte Carlo estimator Z of w is said to admit $\varepsilon - \delta$ relative accuracy if*

$$\mathbb{P}(|Z - w| < \varepsilon w) > 1 - \delta. \tag{2.2}$$

We propose a Monte Carlo estimator admitting $\varepsilon - \delta$ relative accuracy for computing the tail probabilities $w(b)$. One notable feature of this estimator is that *the total computational complexity to generate one such estimator is bounded by a constant $C(\varepsilon, \delta)$ that is independent of the excursion level b.* Thus, to compute $w(b)$ with any prescribed relative accuracy as in (2.2), the total computational complexity remains bounded as the event becomes arbitrarily rare. With such an algorithm, the computation of rare event probabilities is at the same level of complexity as the computation of regular probabilities. This efficiency result is applicable to a large class of Hölder continuous Gaussian random fields and thus is very generally applicable.

The analysis mainly consists of two components. First, we consider a change of measure on the continuous sample path space (denoted by Q_b). The corresponding importance sampling estimator given in (2.16) is unbiased. The first step of the analysis is to show that this estimator admits a standard deviations on the order $O(w(b))$. Such estimators are said to be *strongly efficient*, which is a common efficiency concept in the rare-event simulation literature (Asmussen and Glynn [2007]; Bucklew [2004]).

The second part of the analysis concerns the implementation. The simulation of the estimators in the previous paragraph requires the generation of the entire sample path of f. In that context, the process f is a continuous function. A computer can only generate finite-dimensional objects, so we need to seek for an appropriate discretization scheme to perform the simulations. For instance, a natural approach is to choose a subset

$$T_m = (t_1, ..., t_m) \subset T \tag{2.3}$$

and to use the discrete field on T_m to approximate the continuous field. Thanks to continuity and under certain regularity conditions of T_m, one can show that $\mathbb{P}(\sup_{T_m} f(t) > b)/w(b) \to 1$ as $m \to \infty$, i.e., the bias vanishes as the size of the discretization increases. However, it is well understood that this convergence is not uniform in b. The smaller $w(b)$ is, the slower it converges. Thus, the set T_m needs to grow in order to maintain a prefixed relative bias. In fact, as discussed in Adler *et al.* [2012], for any deterministic subset T_m, the size m *must increase* at least polynomially with b to ensure a given relative accuracy. In this chapter, we introduce a random discretization scheme adapted to (correlated with) the random field f. This adaptive scheme substantially reduces the computation complexity to a constant level.

The high level excursion of Gaussian random fields is a classic topic in probability. There is a wealth of literature that contains general bounds on $\mathbb{P}(\sup f(t) > b)$ as well as sharp asymptotic approximations as $b \to \infty$. An incomplete list of references is Berman [1985]; Borell [1975a, 2003]; Landau and Shepp [1970]; Ledoux and Talagrand [1991]; Marcus and Shepp [1970]; Sudakov and Tsirelson [1974]; Talagrand [1996]. Several methods have been introduced to obtain bounds and asymptotic approximations, each of which imposes different regularity conditions on the random fields. General upper bound for the tail of $\max f(t)$ is developed in Borell [1975a]; Tsirelson *et al.* [1976], which is known as the Borel–TIS lemma. For asymptotic results, there are several methods. The double sum method (Piterbarg [1996]) requires an expansion of the covariance function around its global maximum and also locally stationary structure. The Euler–Poincaré Characteristics of the excursion set approximation (denoted by $\chi(A_b)$, where A_b is the excursion set) uses the fact $\mathbb{P}(M > b) \approx \mathbb{E}(\chi(A_b))$ and requires the random field to be at least twice differentiable (Adler and Taylor [2007]; Adler [1981]; Taylor and Adler [2003]; Taylor *et al.* [2005]).

The tube method (Sun [1993]) uses the Karhunen-Loève expansion and imposes differentiability assumptions on the covariance function (fast decaying eigenvalues) and regularity conditions on the random field. The Rice method (Azais and Wschebor [2008, 2009]) represents the distribution of M (density function) in an implicit form. For other convex functionals, the exact tail approximation of integrals of exponential functions of Gaussian random fields is developed by Liu and Xu [2012]; Liu [2012]. Recently, Adler *et al.* [2009] studied the geometric properties of high level excursion set for infinitely divisible non-Gaussian fields as well as the conditional distributions of such properties given the high excursion. The recent paper Adler *et al.* [2012] studies numerical methods and proposes importance sampling estimators of $w(b)$. In particular, the authors show that the proposed estimator is a fully polynomial randomized approximation scheme (FPRAS), that is, to achieve the $\varepsilon - \delta$ relative accuracy, the total computation complexity is of order $O(\varepsilon^{-q_1}\delta^{-q_2}|\log w(b)|^q)$ (Mitzenmacher and Upfal. [2005]; Traub *et al.* [1988]; Wozniakowski [1996]). When $w(b)$ is very small, the complexity $O(|\log w(b)|^q)$ could be computationally heavy.

The algorithm in this chapter is built upon a change of measure initially introduced in Adler *et al.* [2012]. Nevertheless, the results are nontrivial and substantial generalizations of Adler *et al.* [2012]. The contributions are as follows. First, we show that the continuous importance sampling estimator proposed in Adler *et al.* [2012] given as in (2.16) is strongly efficient to compute $w(b)$ for Hölder continuous fields and under mild regularity conditions. This generalizes the results in Adler *et al.* [2012] who establishes that their relative error grows polynomially fast with b unless the process is twice differentiable for which the exact Slepian model is available. Second, we introduce an adaptive discretization scheme that reduces the overall computational cost to a constant level. This is a substantial improvement of Adler *et al.* [2012] who requires the discretization size grow polynomially in b for both differentiable and non-differentiable fields.

The rest of this chapter is organized as follows. In Section 2.2, we present the problem settings and some existing results that we will refer to in the later analysis. Section 2.3 presents the Monte Carlo methods and their efficiency results. Numerical implementations are included in Section 2.4. Sections 2.5 and 2.6 include the proofs of the theorems.

2.2 Preliminaries: Gaussian random fields and rare-event simulation

2.2.1 Gaussian random fields

Throughout this chapter, we consider a Gaussian random field living on a d-dimensional compact subset $T \subset \mathbb{R}^d$, that is, for any finite subset $(t_1, ..., t_n) \subset T$, $(f(t_1), ..., f(t_n))$ is a multivariate Gaussian random vector. For each $s, t \in T$, we define the following functions,

$$\mu(t) = \mathbb{E}(f(t)), \qquad C(s,t) = Cov(f(s), f(t)), \qquad \mu_T = \sup_{t\in T} |\mu(t)|,$$
$$\sigma^2(t) = C(t,t), \qquad \sigma_T^2 = \sup_{t\in T} \sigma^2(t), \qquad r(s,t) = \frac{C(s,t)}{\sigma(s)\sigma(t)}.$$

Let A_γ be the excursion set over the level γ

$$A_\gamma = \{t \in T : f(t) > \gamma\} \tag{2.4}$$

and thus $w(b) = \mathbb{P}(A_b \neq \emptyset)$. Furthermore, we define the concept of slowly varying function.

Definition 2. *A function L is said to be slowly varying at zero if $\lim_{x\to 0} \frac{L(tx)}{L(x)} = 1$, for all $t \in (0,1)$.*

Throughout this chapter, we impose the following technical conditions.

A1 The process $f(t)$ is almost surely continuous in t.

A2 For some $\alpha_1 \in (0,2]$, the correlation function satisfies the following local expansion

$$1 - r(s,t) \sim \Delta_s L_1(|t-s|)|t-s|^{\alpha_1}, \quad \text{as } t \to s \tag{2.5}$$

where $\Delta_s \in (0,\infty)$ is continuous in s and L_1 is a slowly varying function at zero. Furthermore, there exist nonnegative constants κ_r, β_0, and positive constant $\beta_1 > 0$ satisfying $\beta_0 + \beta_1 \geq \alpha_1$ such that

$$|r(t,t+s_1) - r(t,t+s_2)| \leq \kappa_r L_1(|s_1|)|s_1|^{\beta_0}|s_1 - s_2|^{\beta_1} \qquad \text{for } |s_1| \leq |s_2|. \tag{2.6}$$

A3 The correlation function is non-degenerate, that is, $r(s,t) < 1$ for all $s \neq t$.

A4 The standard deviation $\sigma(t)$ belongs to either of the following two types.

Type 1 $\sigma(t) = 1$ for all $t \in T$.

Type 2 $\sigma(t)$ has a unique maximum attained at t^* satisfies the following conditions

$$\begin{aligned} |\sigma(t) - \sigma(s)| &\leq \kappa_\sigma \times L_2(|t-s|) \times |t-s|^{\alpha_2} \qquad \text{for all } s,t \in T, &(2.7)\\ \sigma(t^*) - \sigma(t) &\sim \Lambda \times L_2(|t^*-t|) \times |t^*-t|^{\alpha_2} \qquad \text{as } t \to t^*, &(2.8)\end{aligned}$$

where $\alpha_2 \in (0,1]$, $\Lambda > 0$, and L_2 is a slowly varying function at zero such that the limit $\lim_{x\to 0+} \frac{L_1(x)}{L_2(x)}$ exists.

A5 There exists $\kappa_\mu > 0$ such that if $\sigma(t)$ is of Type 1 then $|\mu(s) - \mu(s+t)| \leq \kappa_\mu \sqrt{L_1(|t|)}|t|^{\alpha_1/2}$; if $\sigma(t)$ is of Type 2 then $|\mu(s) - \mu(s+t)| \leq \kappa_\mu \sqrt{L_2(|t|)}|t|^{\alpha_2/2}$.

A6 There exist κ_m and ϵ small enough, such that $mes(B(t,\epsilon) \cap T) \geq \kappa_m \epsilon^d \omega_d$, for any $t \in T$, where $B(t,\epsilon)$ is the ϵ-ball centered around t and ω_d is the volume of the $d-$dimensional unit ball.

Condition A2 ensures that the normalized process $\frac{f(t)-\mu(t)}{\sigma(t)}$ is Hölder continuous with coefficient $\alpha_1/2$. The bound in (2.6) imposes slightly more conditions. For instance, in case when $1 - r(s,t) = |t-s|^{\alpha_1}$, we can choose that $\beta_0 = \alpha_1 - 1$ and

$\beta_1 = 1$ if $\alpha_1 \geq 1$; $\beta_0 = 0$ and $\beta_1 = \alpha_1$ if $0 < \alpha_1 < 1$. Condition A3 excludes the degenerated case that is not essential and it makes the technical development more concise. Conditions A4 and A5 require that the mean and the standard deviation functions are also Hölder continuous. In Condition A4, we can adjust the constant Λ such that the limit $\lim_{x \to 0+} L_1(x)/L_2(x)$ belongs to the set $\{0, 1, \infty\}$. Condition A5 ensures that the variation of the mean function is bounded by those of $f(t)$ and $\sigma(t)$. In the later technical developments, the analysis is divided into two cases: $\alpha_1 < \alpha_2$ and $\alpha_1 \geq \alpha_2$.

Throughout this chapter, we use the following notations for the asymptotics. We write $h(b) = o(g(b))$ if $h(b)/g(b) \to 0$ as $b \to \infty$; $h(b) = O(g(b))$ if $h(b) \leq \kappa g(b)$ for some $\kappa > 0$; $h(b) = \Theta(g(b))$ if $h(b) = O(g(b))$ and $g(b) = O(h(b))$; $h(b) \sim g(b)$ if $h(b)/g(b) \to 1$ as $b \to \infty$.

2.2.2 Rare-event simulation and importance sampling

2.2.2.1 Rare-event simulation

The research focus of rare-event simulation is on estimating $w = \mathbb{P}(B)$, where $\mathbb{P}(B) \approx 0$. It is customary to introduce a parameter, say $b > 0$, with a meaningful interpretation from an applied standpoint such that $w(b) \to 0$ as $b \to \infty$. Consider an estimator Z_b such that $\mathbb{E}Z_b = w(b)$. A popular efficiency concept in the rare-event simulation literature is the so-called strong efficiency that is defined as follows (c.f. Asmussen and Glynn [2007]; Bucklew [2004]; Juneja and Shahabuddin [2006]).

Definition 3. *A Monte Carlo estimator Z_b is said to be* strongly efficient *in estimating $w(b)$ if $\mathbb{E}(Z_b) = w(b)$ and there exists a $\kappa_0 \in (0, \infty)$ such that*

$$\sup_{b>0} \frac{Var(Z_b)}{w^2(b)} < \kappa_0.$$

Strong efficiency measures mean squared error in relative terms for an unbiased estimator. Suppose that a strongly efficient estimator of $w(b)$ has been constructed, denoted by Z_b, and n i.i.d. replicates of Z_b are generated $Z_b^{(1)}, ..., Z_b^{(n)}$. Let $\bar{Z}_{b,n} \triangleq \frac{1}{n}\sum_{i=1}^{n} Z_b^{(i)}$ be the averaged estimator that has variance $\frac{Var(Z_b)}{n}$. By means of the Chebyshev's inequality, we obtain that

$$\mathbb{P}\left(|\bar{Z}_{b,n} - w(b)| > \varepsilon w(b)\right) \leq \frac{Var(Z_b)}{n\varepsilon^2 w^2(b)}.$$

For any $\delta > 0$, to achieve the $\varepsilon - \delta$ accuracy, we need to generate

$$n = \frac{Var(Z_b)}{\delta\varepsilon^2 w^2(b)} \leq \frac{\kappa_0}{\delta\varepsilon^2}$$

replicates of Z_b. This choice of n is uniform in the rarity parameter b. We will later show that the proposed continuous importance sampling estimator is strongly efficient.

2.2.2.2 Importance sampling and variance reduction

Importance sampling is based on the basic identity,

$$\mathbb{P}(B) = \int I(\omega \in B)\, d\mathbb{P}(\omega) = \int I(\omega \in B) \frac{d\mathbb{P}}{dQ}(\omega)\, dQ(\omega) \quad \text{for a measurable set } B, \tag{2.9}$$

where we assume that the probability measure Q is such that $Q(\cdot \cap B)$ is absolutely continuous with respect to the measure $\mathbb{P}(\cdot \cap B)$. If we use $\mathbb{E}^Q$ to denote expectation under Q, then (2.9) trivially yields that the random variable $Z(\omega) = I(\omega \in B)\frac{d\mathbb{P}}{dQ}(\omega)$ is an unbiased estimator of $\mathbb{P}(B) > 0$ under the measure Q, or symbolically, $\mathbb{E}^Q Z = \mathbb{P}(B)$.

A central component lies in the selection of Q in order to minimize the variance of Z. It is easy to verify that if we choose $\mathcal{Q}^*(\cdot) = \mathbb{P}(\cdot|B) = \mathbb{P}(\cdot \cap B)/\mathbb{P}(B)$ then the corresponding estimator has zero variance and thus it is usually referred to as the the *zero-variance change of measure*. However, $\mathcal{Q}^*$ is clearly a change of measure that is of no practical value, since $\mathbb{P}(B)$ – the quantity that we are attempting to evaluate in the first place – is unknown. Nevertheless, when constructing a good importance sampling distribution for a family of sets $\{B_b : b \geq b_0\}$ for which $0 < \mathbb{P}(B_b) \to 0$ as

$b \to \infty$, it is often useful to analyze the asymptotic behavior of $\mathcal{Q}^*$ as $\mathbb{P}(B_b) \to 0$ in order to guide the construction of a useful Q.

2.2.2.3 The change of measure

We now present a change of measure defined on the continuous sample path space denoted by Q_b. This measure was initially proposed by Adler *et al.* [2012]. We should be able to compute the Radon-Nikodym derivative and also be able to simulate the process f under Q_b. We describe the measure Q_b from two aspects. First, we present its Radon-Nikokym derivative with respect to $\mathbb{P}$

$$\frac{dQ_b}{d\mathbb{P}}(f) = \int_T h_b(t) \frac{q_{b,t}(f(t))}{\varphi_t(f(t))} dt, \tag{2.10}$$

where $h_b(t)$ is a density function on the set T, $q_{b,t}(x)$ is a density function on the real line, and $\varphi_t(x)$ is the density function of $f(t)$ under the measure $\mathbb{P}$ evaluated at $f(t) = x$. We will need to choose $h_b(t)$ and $q_{b,t}(x)$ such that the measure Q_b satisfies the absolute continuity condition to guarantee the unbiasedness.

We will present the specific forms of $h_b(t)$ and $q_{b,t}(x)$ momentarily. Before that, we would like to complete the description of Q_b by presenting the simulation method of f under Q_b.

Algorithm 1 Continuous simulation

To generate a random sample path under the measure Q_b, we need a three-step procedure.

1: Generate a random index $\tau \in T$ following the density $h_b(t)$.

2: Conditional on the realization of τ, sample $f(\tau)$ from the density $q_{b,\tau}(x)$.

3: Conditional on the realization of $(\tau, f(\tau))$, generate $\{f(t) : t \neq \tau\}$ from the original conditional distribution $\mathbb{P}(f \in \cdot\, | f(\tau))$.

It is not difficult to verify that the above three-step procedure is consistent with the Randon-Nikodym derivative given as in (2.10). The process $f(t)$ mostly follows the distribution under $\mathbb{P}$ except at one random location τ where $f(\tau)$ follows an alternative distribution $q_{b,\tau}(x)$. The overall Randon-Nikodym derivative is an average of the likelihood ratio $q_{b,t}(f(t))/\varphi_t(f(t))$ with respect to the density $h_b(t)$.

Now, we present the specific forms of $h_b(t)$ and $q_{b,t}(x)$ for the computation of $w(b)$. For some positive constant a, let γ be

$$\gamma = b - a/b. \tag{2.11}$$

We choose

$$q_{b,t}(x) = \varphi_t(x)\frac{I(f(t) > \gamma)}{\mathbb{P}(f(t) > \gamma)} \tag{2.12}$$

that is the conditional distribution of $f(t)$ given that $f(t) > \gamma$. The distribution of τ is chosen as

$$h_b(t) = \frac{\mathbb{P}(f(t) > \gamma)}{\int_T \mathbb{P}(f(s) > \gamma)ds}. \tag{2.13}$$

The choice of a in (2.11) does not affect the efficiency results, nor the complexity analysis. To simplify the discussion, we fix a to be unity, that is,

$$\gamma = b - 1/b. \tag{2.14}$$

The random index τ indicates the location where the distribution of the random field is changed. Furthermore, $q_{b,t}(x)$ is chosen to be the conditional distribution given a high excursion. The index τ basically localizes the maximum of $f(t)$. Thus, as an approximation of the zero-variance change of measure, the distribution $h_b(t)$ should be chosen close to the conditional distribution of the maximum $t_* \triangleq \arg\sup_t f(t)$ given that $f(t_*) > b$. This is our guideline to choose $h_b(t)$. For each $t \in T$, the conditional probability that $f(t) > b$ given $M > b$ is

$$\mathbb{P}(f(t) > b | M > b) = \frac{\mathbb{P}(f(t) > b)}{\mathbb{P}(M > b)}.$$

The denominator $\mathbb{P}(M > b)$ is free of t and thus $\mathbb{P}(f(t) > b|M > b) \propto \mathbb{P}(f(t) > b)$. Our choice of $h_b(t) \propto \mathbb{P}(f(t) > \gamma)$ approximates $\mathbb{P}(f(t) > b|M > b)$ by replacing b

with γ mostly for technical convenience. With such choices of $h_b(t)$ and $q_{b,t}(x)$, the Radon-Nikodym takes the following form

$$\frac{dQ_b}{d\mathbb{P}} = \frac{\int_T I(f(t) > \gamma)dt}{\int_T \mathbb{P}(f(t) > \gamma)dt} = \frac{mes(A_\gamma)}{\int_T \mathbb{P}(f(t) > \gamma)dt}, \tag{2.15}$$

where

$$mes(A_\gamma) = \int I(t \in A_\gamma)dt$$

is the Lebesgue measure of A_γ. According to Fubini's theorem, the denominator of (2.15) is

$$\int_T P(f(t) > \gamma)dt = \mathbb{E}[mes(A_\gamma)].$$

Remark 1. *For different problems, we may choose different $h_b(t)$ and $q_{b,t}(x)$ to approximate various conditional distributions. For instance, $q_{b,t}(x)$ was chosen to be in the exponential family of $\varphi_t(x)$ in Liu and Xu [To appear] for the derivation of tail approximations of $\int e^{f(t)}dt$.*

2.2.3 The bias control

In addition to the variance control, one also needs to account for the computational effort required to generate Z_b. This issue is especially important for the current study. The random objects in this analysis are continuous processes. For the implementation, we need to use a discrete object to approximate the continuous process. Inevitably, discretization induces bias, though it vanishes as the discretization mesh increases. To ensure the $\varepsilon - \delta$ relative accuracy, the bias needs to be controlled to a level less than $\varepsilon w(b)$.

In Adler *et al.* [2012], it is established that, to ensure a bias of order $\varepsilon w(b)$, the size of the discretization must grow at a polynomial rate of b for both differentiable and non-differentiable fields. The authors also provide an optimality result. For twice differentiable and homogeneous fields, the size of a prefixed/deterministic set T_m must be at least of order $O(b^d)$ so that the bias can be controlled to the level $\varepsilon w(b)$. In this chapter, we adopt an adaptive discretization that substantially reduces the necessary size of T_m to constant.

2.3 Main results

The main results of this chapter consist of a random discretization scheme of T associated with the change of measure Q_b and the efficiency results of the importance sampling estimators and the overall complexity.

2.3.1 An adaptive discretization scheme and the algorithms

2.3.1.1 The continuous estimator and the challenges

Based on the change of measure Q_b, an unbiased estimator for $w(b)$ is given by

$$Z_b \triangleq I(M > b)\frac{d\mathbb{P}}{dQ_b} = I(M > b)\frac{\int_T \mathbb{P}(f(t) > \gamma)dt}{mes(A_\gamma)}. \tag{2.16}$$

We call Z_b the *continuous estimator*. It is straightforward to obtain that $E_b(Z_b) = w(b)$, where we use $E_b(\cdot)$ to denote the expectation under the measure Q_b. The second moment of Z_b is

$$\mathbb{E}_b(Z_b^2) = E_b\Big[\frac{\{\int_T \mathbb{P}(f(t) > \gamma)dt\}^2}{mes^2(A_\gamma)}; M > b\Big],$$

where $f(t)$ is generated from Algorithm 1. We will later show that Z_b (under regularity conditions) is strongly efficient, that is, $E_b(Z_b^2) = O(w^2(b))$.

For the implementation, we are not able to simulate the continuous field f and therefore have to adopt a simulatable estimator, $\hat{Z}_b$, that approximates the continuous estimator Z_b. A natural approach is to consider the random field on a finite set $T_m = \{t_1, ..., t_m\} \subset T$ and to use $\mathbb{P}(\max_{T_m} f(t_i) > b)$ as an approximation of $w(b) = \mathbb{P}(\sup_T f(t) > b)$. The bias is given by

$$\mathbb{P}(\sup_T f(t) > b) - \mathbb{P}(\max_{T_m} f(t) > b) = \mathbb{P}(T_m \cap A_b = \emptyset, M > b).$$

We explain without rigorous derivation that the above scheme usually induces a heavy computational overhead. To simplify the discussion, we consider that f is a stationary process and its covariance function satisfies the local expansion (slightly abusing the notation)

$$C(t) \triangleq Cov(f(s), f(s+t)) = 1 - |t|^{\alpha} + o(|t|^{\alpha}) \tag{2.17}$$

Then, the process is Hölder continuous with coefficient $\alpha/2$. Under this setting, standard results yield an estimate of the excursion set $\mathbb{E}(mes(A_b)|M > b) = \Theta(b^{-2d/\alpha})$. Thanks to stationarity, A_b is approximately uniformly distributed over the domain T.

Notice that the bias term $\mathbb{P}(T_m \cap A_b = \emptyset, M > b)$ is the probability that T_m does not intersect with A_b. Therefore, if $m \ll b^{2d/\alpha}$, T_m is too sparse such that it is not able to catch the set A_b no matter how T_m is distributed over T. It is necessary to have a lattice of size at least of order $O(b^{2d/\alpha})$. This heuristic calculation was made rigorous for smooth fields in Adler *et al.* [2012]. Thus, the computational complexity to generate the process f on the set T_m grows at a polynomial rate with b. In this chapter, we aim at further reduction of the discretization size to a constant level while still maintaining the ε-relative bias. For this sake, we propose to randomly sample an appropriate discrete set that is correlated with f.

2.3.1.2 A closer look at the excursion set A_γ

The proposed adaptive discretization scheme is closely associated with the three-step simulation procedure. Among the three steps in Algorithm 1, Step 1 and Step 2 are implementable. It is Step 3, generating $\{f(t) : t \neq \tau\}$ conditional on $(\tau, f(\tau))$, that requires discretization. In order to estimate $w(b)$ and to generate the estimator Z_b, we only need to simulate the random indicator $I(M > b)$ and the volume of the excursion set $mes(A_\gamma)$ conditional on $(\tau, f(\tau))$. The term $\int_T \mathbb{P}(f(t) > \gamma)dt$ is a deterministic number that can be computed via routine numerical methods.

In what follows, we focus on the simulation and approximation of $I(M > b)$ and $mes(A_\gamma)$. For illustration purpose, we discuss the stationary case with covariance function satisfying the expansion (2.17). We define $\zeta = b^{2/\alpha}$ and the normalized process

$$g(t) = b(f(\tau + t/\zeta) - b). \tag{2.18}$$

Note that $b \times (f(\tau) - \gamma)$ asymptotically follows an exponential distribution. Conditional on $f(\tau) = \gamma + z/b$ the g process has expectation $\mathbb{E}_b[g(t)|f(\tau) = \gamma + z/b] = z - 1 - (1 + o(1))|t/\zeta|^\alpha[b^2 + (z - 1)]$. For all $z = o(b^2)$, we have that

$$\mathbb{E}_b[g(t)|f(\tau) = \gamma + z/b] = z - 1 - (1 + o(1))|t|^\alpha \qquad \text{as } b \to \infty.$$

In addition, the covariance of $g(t)$ is $Cov(g(s), g(t)) = (|s|^\alpha + |t|^\alpha - |s - t|^\alpha) + o(1)$ where $o(1) \to 0$ as $b \to \infty$. Therefore, $g(t)$ converges in distribution to a Gaussian process with the above mean and covariance function. In addition, $f(\tau + t/\zeta) \geq \gamma$ if and only if $g(t) > -1$. The excursion set A_γ can be written as

$$A_\gamma = \tau + \zeta^{-1} \cdot A^g_{-1} \triangleq \{\tau + \zeta^{-1}t : t \in A^g_{-1}\},$$

where $A^g_{-1} = \{t : g(t) > -1\}$. Note that the process $g(t)$ is a Gaussian process with standard deviation $O(|t|^{\alpha/2})$ and a negative drift of order $O(-|t|^\alpha)$. Therefore, in expectation, $g(t)$ goes below -1 when $z \ll |t|^\alpha$ where z is asymptotically an exponential random variable. Thus, the excursion set A^g_{-1} is of order $O(1)$. Furthermore, A_γ is a random set within $O(\zeta^{-1})$ distance from the random index τ. The volume $mes(A_\gamma)$ is of order $O(\zeta^{-d})$. This heuristic calculation is well understood; see Aldous [1989]; Berman and others [1972]. The above discussion quantifies the intuition that τ localizes the global maximum of f. It also localizes the excursion set A_γ. Therefore, upon considering approximating/computing $mes(A_\gamma)$ and $I(M > b)$, we should focus on the region around τ.

Conditional on a specific realization of the process f, we formulate the approximation of $mes(A_\gamma)$ as an estimation problem. The ratio $mes(A_\gamma)/mes(T) \in [0, 1]$

corresponds to the following probability

$$\frac{mes(A_\gamma)}{mes(T)} = \mathbb{P}(U \in A_\gamma)$$

where U is a uniform random variable on the set T with respect to the Lebesgue measure. Estimating $mes(A_\gamma)$ constitutes another rare-event simulation problem.

2.3.1.3 An adaptive discretization scheme

Based on the understanding of the excursion set A_γ, we set up a discretization scheme adaptive to the realization of τ. To proceed, we provide the general form of ζ in presence of slowly varying functions

$$\zeta \triangleq \max\left\{|s|^{-1} : L_1(|s|)|s|^{\alpha_1} \geq b^{-2} \text{ or } L_2(|s|)|s|^{\alpha_2} \geq b^{-2}\right\}. \tag{2.19}$$

In the case of constant variance, we formally define $\alpha_2 = \infty$ and thus ζ is defined as $\zeta \triangleq \max\{|s|^{-1} : L_1(|s|)|s|^{\alpha_1} \geq b^{-2}\}$. We further define two other scale factors

$$\zeta_i \triangleq \max\left\{|s|^{-1} : L_i(|s|)|s|^{\alpha_i} \geq b^{-2}\right\}, \quad i = 1, 2. \tag{2.20}$$

It is straightforward to verify that

$$\zeta = \max(\zeta_1, \zeta_2).$$

Consider an isotropic distribution (centered around zero) with density $k(t)$, that is, $k(t) = k(s)$ if $|s| = |t|$. We choose $k(t)$ to be reasonably heavy-tailed such that for some $\varepsilon_1 > 0$

$$k(t) \sim |t|^{-d-\varepsilon_1}, \qquad \text{as } t \to \infty.$$

In addition there exists a $\kappa_1 > 0$ such that $k(t) \leq \kappa_1$ for all t. For instance, we can choose $k(t)$ to be, but not necessarily restricted to, the multivariate t-distribution. Furthermore, conditional on τ, we define the rescaled density

$$k_{\tau,\zeta}(t) = \zeta^d \times k(\zeta(t - \tau)) \tag{2.21}$$

that centers around τ and has scale ζ^{-1}. We construct a τ-adapted random subset of T by generating i.i.d. random variables from the density $k_{\tau,\zeta}(t)$, denoted by $t_1, ..., t_m$. Then, define

$$\widehat{mes}(A_\gamma) \triangleq \frac{1}{m} \sum_{i=1}^{m} \frac{I(f(t_i) > \gamma)}{k_{\tau,\zeta}(t_i)} \tag{2.22}$$

that is an unbiased estimator of $mes(A_\gamma)$ in the sense that for each realization of f

$$E_{\tau,\zeta}[\widehat{mes}(A_\gamma)|f] = mes(A_\gamma)$$

where $E_{\tau,\zeta}(\cdot|f)$ is the expectation with respect to $t_1, ..., t_m$ under the density $k_{\tau,\zeta}$ for a particular realization of f. Notationally, if $t_i \notin T$, then $I(f(t_i) > \gamma) = 0$.

Similar to the approximation of $mes(A_\gamma)$, we use the same τ-adapted random subset to approximate $I(M > b)$, that is,

$$I(\max_{i=1}^{m} f(t_i) > b) \approx I(M > b).$$

Based on the above discussions, we present the final algorithm.

Algorithm 2 Discrete estimator

1: Generate a random index $\tau \in T$ following the density $h_b(t)$ in (2.13).

2: Conditional on the realization of τ, sample $f(\tau)$ from $q_{b,t}(x)$ in (2.12).

3: Conditional on the realization of τ, generate i.i.d. random indices $t_1, ..., t_m$ following density $k_{\tau,\zeta}(t)$.

4: Conditional on the realization of $(\tau, f(\tau))$, generate multivariate normal random vector $(f(t_1), ..., f(t_m))$ from the original/nominal conditional distribution of $\mathbb{P}(\cdot|f(\tau))$.

5: **return**

$$\hat{Z}_b = \frac{I(\max_{i=1}^{m} f(t_i) > b)}{\widehat{mes}(A_\gamma)} \int_T \mathbb{P}(f(t) > \gamma) dt,$$

where $\widehat{mes}(A_\gamma)$ is given as in (2.22).

We will call $\hat{Z}_b$ the *discrete estimator*.

2.3.2 The main results

We present the efficiency results of the proposed algorithms.

Theorem 1. *Consider a Gaussian random field f that satisfies Conditions A1-6. Let Z_b be given as in* (2.16) *and Algorithm 1. Then, Z_b is strongly efficient in estimating $w(b)$, that is, there exists κ_0 such that*

$$E_b(Z_b^2) \leq \kappa_0 w^2(b), \text{ for all } b > 0.$$

Theorem 2. *Consider a Gaussian random field f that satisfies Conditions A1-6. Let $\hat{Z}_b$ be the estimator given by Algorithm 2. There exists $\lambda > 0$ such that for any $\varepsilon > 0$ if we choose $m = \lambda \varepsilon^{-d(2/\min(\alpha_1,\alpha_2)+2/\beta_1)}$, then*

$$|E_b(\hat{Z}_b) - w(b)| \leq \varepsilon w(b)$$

for all $b > 0$. Furthermore, there exists κ_0 such that

$$E_b(\hat{Z}_b^2) \leq \kappa_0 w^2(b).$$

With the above results, we generate n i.i.d. replicates of $\hat{Z}_b$, denoted by $\hat{Z}_b^{(1)}$, ...,$\hat{Z}_b^{(n)}$, with m chosen as in the theorem such that the averaged estimator, $\frac{1}{n}\sum_{i=1}^{n} \hat{Z}_b^{(i)}$, has its bias bounded by $\varepsilon w(b)/2$ and its variance is bounded by $\kappa_0 w^2(b)/n$. To achieve ε relative error with at $(1-\delta)$ confidence, we need to choose $n = \frac{4\kappa_0}{\varepsilon^2 \delta}$, that is,

$$\mathbb{P}\Big(\Big|\frac{1}{m}\sum_{i=1}^{n} \hat{Z}_b^{(i)} - w(b)\Big| > \varepsilon w(b)\Big) < \delta.$$

The total computational complexity is of order $O(m^3 \varepsilon^{-2} \delta^{-1})$, where m^3 is the complexity of Cholesky decomposition of the covariance matrix for the generation of an m-dimensional Gaussian random vector.

2.4 Numerical analysis

We present four numerical examples to show the performance of our algorithm. First, we consider a one-dimensional Gaussian field whose tail probability is known in a closed form. For the discretization, we deploy $m = 20$ points when $d = 1$ and 40 points when $d = 2$. To make sure that the bias is small enough, we have run the simulations with 10 times more points and the results didn't change substantially. We only report the results with fewer points to illustrate the efficiency.

Example 1. *Consider $f(t) = X\cos t + Y\sin t$, $T = [0, 3/4]$, where X and Y are independent standard Gaussian variables. The probability $\mathbb{P}(\sup_{t\in T} f(t) > b)$ is known in closed form (Adler [1981]),*

$$\mathbb{P}(\sup_{0\leq t\leq 3/4} f(t) > b) = 1 - \Phi(b) + \frac{3}{8\pi}e^{-b^2/2}. \tag{2.23}$$

Table 1 shows the simulation results.

b	true value	est	std dev	coefficient of variation
3	2.68E-03	2.55E-03	1.09E-04	1.35
4	7.17E-05	7.17E-05	3.22E-06	1.42
5	7.31E-07	7.33E-07	3.41E-08	1.47
6	2.80E-09	2.84E-09	1.35E-10	1.51
7	4.01E-12	4.07E-12	1.98E-13	1.54

Table 2.1: Simulation results for the cosine process where $n = 1000$, $m = 20$, $k(t)$ is chosen to be the density function of $t-$distribution with degrees of freedom 3. The "true value" is calculated from (2.23), the "std dev" is the standard deviation of the averaged Monte Carlo estimator over n i.i.d. samples, and the "coefficient of variation" is the ratio between the standard deviation of a single Monte Carlo estimator and its expectation.

The following three examples consider random fields over a two-dimensional square.

Example 2. *Consider a mean zero, unit variance, stationary and smooth Gaussian field over $T = [0, 1]^2$, with covariance function*

$$C(t) = e^{-|t|^2}.$$

Table 2 shows the simulation results.

b	est	std dev	coefficient of variation
3	9.32E-03	3.63E-04	1.23
4	3.39E-04	1.51E-05	1.41
5	4.20E-06	1.71E-07	1.28
6	1.93E-08	8.15E-10	1.33
7	3.25E-11	1.27E-12	1.23
8	1.87E-14	7.11E-16	1.20

Table 2.2: Simulation results for Example 2, where $n = 1000$, $m = 40$, $k(t) = \frac{25}{32\pi}(1 + 0.64|t|^2)^{-3}$.

Example 3. *Consider a continuous inhomogenous Gaussian field on* $T = [0, 1]^2$ *with mean and covariance function*

$$\mu(t) = 0.1t_1 + 0.1t_2 \quad C(s, t) = e^{-|t-s|^2}.$$

Table 3 shows the simulation results.

b	est	std dev	coefficient of variation
3	1.25E-02	5.61E-04	1.42
4	4.95E-04	1.95E-05	1.24
5	7.16E-06	2.80E-07	1.24
6	3.51E-08	1.36E-09	1.22
7	6.69E-11	2.72E-12	1.29
8	4.50E-14	1.91E-15	1.34

Table 2.3: Simulation results for Example 3, where $n = 1000$, $m = 40$, $k(t)$ is the same as that of Example 2.

Example 4. *Consider the continuous Gaussian field living on $T = [0,1]^2$ with mean and covariance function*

$$\mu(t) = 0.1t_1 + 0.1t_2 \quad C(s,t) = e^{-|t-s|/4}.$$

Table 4 shows the simulation results.

b	est	std dev	coefficient of variation
3	1.35E-02	6.63E-04	1.55
4	7.40E-04	4.36E-05	1.86
5	1.54E-05	7.53E-07	1.55
6	9.93E-08	5.23E-09	1.66
7	2.87E-10	1.33E-11	1.47
8	2.60E-13	1.41E-14	1.71

Table 2.4: Simulation results for Example 4, where $n = 1000$, $m = 40$, $k(t) = \frac{1}{8\pi}(1+|t|^2)^{-3}$.

For all the examples, the ratios of standard error over the estimated value do not increase as b increase. This is consistent with our theoretical analysis. Also note that m does not increase as the level increases, which reduces the computational complexity significantly. Overall, the numerical estimates are very accurate.

2.5 Proof of Theorem 1

Throughout the proof, we will use κ as a generic notation to denote large and not-so-important constants whose value may vary from place to place. Similarly, we use ε_0 as a generic notation for small positive constants.

The first result we cite is the Borel-TIS (Borel-Tsirelson-Ibragimov-Sudakov) inequality Adler and Taylor [2007]; Borell [1975b]; Tsirelson *et al.* [1976] that will be used very often in our technical development.

Proposition 1. *Let $f(t)$ be a centered Gaussian process almost surely bounded in T. Then,* $\mathbb{E}[\sup_{t\in T} f(t)] < \infty$ *and*

$$\mathbb{P}\Big(\sup_{t\in T} f(t) - \mathbb{E}[\sup_{t\in T} f(t)] \geq b\Big) \leq \exp\left(-b^2/(2\sigma_T^2)\right).$$

In order to show strong efficiency, we need to establish a lower bound of the probability

$$w(b) = E_b\Big[\frac{1}{mes(A_\gamma)}; M > b\Big] \int_T \mathbb{P}(f(t) > \gamma)dt$$

and an upper bound of the second moment

$$\mathbb{E}_b(Z_b^2) = E_b\Big[\frac{1}{mes^2(A_\gamma)}; M > b\Big]\Big[\int_T \mathbb{P}(f(t) > \gamma)dt\Big]^2$$

The central analysis lies in the following two quantities:

$$I_1 = E_b\Big[\frac{1}{mes(A_\gamma)}; M > b\Big], \qquad I_2 = E_b\Big[\frac{1}{mes^2(A_\gamma)}; M > b\Big]. \tag{2.24}$$

We will show that there exist constants κ and ε_0 such that

$$I_1 \geq \varepsilon_0 \zeta^d, \qquad I_2 \leq \kappa \zeta^{2d}. \tag{2.25}$$

If these inequalities are proved, then $\limsup_{b\to\infty} \frac{I_2}{I_1^2} < \infty$ is in place and we finish our proof for Theorem 1. For the rest of the proof, we establish these two inequalities.

To proceed, we describe the conditional Gaussian random field given $f(\tau)$. First, if we write $f(\tau) = \gamma + z/b$, then (conditional on τ) z asymptotically follows an exponential distribution with expectation $\sigma^2(\tau)$. Conditional on $f(\tau) = \gamma + z/b$, let

$$f(t+\tau) = \mathbb{E}[f(t+\tau)|f(\tau) = \gamma + z/b] + f_0(t), \tag{2.26}$$

where $f_0(t)$ is a zero-mean Gaussian process. By means of conditional Gaussian calculation, the conditional mean and conditional covariance function are given by

$$\begin{aligned} \mu_\tau(t) &= \mathbb{E}(f(t+\tau)|f(\tau) = \gamma + z/b) \qquad (2.27)\\ &= \mu(t+\tau) + \frac{\sigma(\tau+t)}{\sigma(\tau)} r(\tau+t,\tau)(\gamma + z/b - \mu(\tau)) \\ C_0(s,t) &= Cov(f_0(s), f_0(t)) \\ &= \sigma(\tau+s)\sigma(\tau+t)[r(s+\tau,t+\tau) - r(\tau+t,\tau)r(\tau+s,\tau)]. \end{aligned}$$

The next lemma controls the conditional variance.

Lemma 1. *Under condition A1-6, there exists a constant $\lambda_1 > 0$ such that, for all $\tau \in T$ and b large enough, the following statements hold.*

(i) For all $t + \tau \in T$,

$$C_0(t,t) \le \lambda_1 L_1(|t|)|t|^{\alpha_1};$$

(ii) for $s, t \in T$,

$$Var(f_0(s) - f_0(t)) \le \lambda_1 \max(L_1(|t-s|)|t-s|^{\alpha_1}, L_2(|t-s|)|t-s|^{\alpha_2});$$

(iii) for any $\varepsilon > 0$, there exists $\delta > 0$ (independent of b) such that for each t

$$\mathbb{E}(\sup_{|s-t|\le\delta\zeta^{-1}} f_0(s)) \le \frac{\varepsilon}{b}.$$

The proofs for (i) and (ii) are an application of Conditions A2, A3 and A6 and elementary calculations. (iii) is a direct corollary of (ii) and Dudley's entropy bound (Theorem 1.1 of Dudley [2010]). We omit the detailed derivations. We proceed to the analysis of I_1 and I_2 by considering the Type 1 and Type 2 standard deviation function (Condition A4) separately.

In the main text, we only provide the proof when $\sigma(t)$ is of Type 1 in Condition A4, that is, a constant variance. The proof of the non-constant case is similar. We present it in the Supplemental Material available on arXiv (http://arxiv.org/abs/1309.7365). The constant variance case corresponds to $\alpha_2 = \infty$. The scaling factor is given by

$$\zeta = \zeta_1.$$

We aim at showing that $I_2 \le \kappa\zeta_1^{2d}$ and $I_1 \ge \varepsilon_0\zeta_1^d$.

2.5.1 The I_2 term

For some $y_0 > 0$ chosen to be sufficiently small (independent of b) and to be determined in the later analysis, the I_2 term is bounded by

$$\mathbb{E}_b\Big[\frac{1}{mes^2(A_\gamma)}; M > b\Big] \le y_0^{-2d}\zeta_1^{2d} + E_b\Big(\frac{1}{mes^2(A_\gamma)}; mes(A_\gamma) < y_0^d\zeta_1^d, M > b\Big). \quad (2.28)$$

To control the second term of the above inequality, we need to provide a bound on the following tail probability for $0 < y < y_0$

$$\begin{aligned} & Q_b(mes(A_\gamma) < y^d \zeta_1^{-d}, M > b) \\ = & \int \mathbb{P}(mes(A_\gamma) < y^d \zeta_1^{-d}, M > b | f(\tau) = \gamma + z/b) h_b(\tau) \frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz. \end{aligned} \tag{2.29}$$

The probability inside the integral is with respect to the original measure $\mathbb{P}$ because, conditional on $f(\tau)$, $f(t)$ follows the original conditional distribution. We develop bounds for $\mathbb{P}(mes(A_\gamma) < y^d \zeta_1^{-d}, M > b | f(\tau) = \gamma + z/b)$ under two situations: $z > 1$ and $0 < z \leq 1$.

Situation 1: $z > 1$**.**

Define constant $c_d = \omega_d^{-1/d}$ where ω_d is the volume of the d-dimensional unit ball. The event $\{mes(A_\gamma) < y^d \zeta_1^{-d}\}$ implies the event $\{\inf_{|t-\tau| \leq c_d y \zeta_1^{-1}} f(t) \leq \gamma\}$. Otherwise, if $\{\inf_{|t-\tau| \leq c_d y \zeta_1^{-1}} f(t) > \gamma\}$, then $\{|t - \tau| \leq c_d y \zeta_1^{-1}\} \subseteq A_\gamma$ and $mes(A_\gamma) \geq y^d \zeta_1^{-d}$. Thus, we have the bound

$$\begin{aligned} & \mathbb{P}\Big(mes(A_\gamma) \leq y^d \zeta_1^{-d}, M > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\ \leq \; & \mathbb{P}\Big(\inf_{|t-\tau| \leq c_d y \zeta_1^{-1}} f(t) \leq \gamma | f(\tau) = \gamma + \frac{z}{b}\Big). \end{aligned}$$

Using the representation in (2.26), the right-hand side of the above probability is

$$= \mathbb{P}\Big(\inf_{|t| \leq c_d y \zeta_1^{-1}} f_0(t) + \mu_\tau(t) \leq \gamma\Big). \tag{2.30}$$

Notice that $\mu_\tau(0) = \gamma + z/b > \gamma + 1/b$. For the constant variance case, expression (2.27) can be written as

$$\mu_\tau(t) = \mu(t + \tau) + r(\tau + t, \tau)(\gamma + z/b - \mu(\tau)). \tag{2.31}$$

According to the Condition A5, we have that $|\mu_\tau(t) - \mu_\tau(0)| = O(bL_1(t)|t|^{\alpha_1}) + O(\sqrt{L_t(t)|t|^{\alpha_1}})$. According to the choice of ζ_1 in (2.20), we have that for $|t| \leq c_d y \zeta_1^{-1}$,

$$bL_1(t)|t|^{\alpha_1} \leq \kappa b L_1(c_d y \zeta_1^{-1}) y^{\alpha_1} \zeta_1^{-\alpha_1} = \kappa b^{-1} \frac{L_1(c_d y \zeta_1^{-1})}{L_1(\zeta_1^{-1})} y^{\alpha_1}.$$

According to Lemma 5 (i) in the Supplemental Material, the ratio $L_1(c_d y\zeta_1^{-1})/L_1(\zeta_1^{-1})$ varies slower than any polynomial of y. Thus, we have

$$|\mu_\tau(t) - \mu_\tau(0)| \leq y^{\alpha_1/2} b^{-1}. \tag{2.32}$$

By choosing y small, we have

$$\mu_\tau(t) \geq \gamma + \frac{1}{2b} \text{ for } |t| \leq c_d y \zeta_1^{-1}. \tag{2.33}$$

Furthermore, by Lemma 1(i) the conditional variance is $C_0(t,t) \leq \lambda_1 L_1(c_d y \zeta_1^{-1}) c_d^{\alpha_1} y^{\alpha_1} \zeta_1^{-\alpha_1}$. With the same argument as that of (2.32), we obtain

$$C_0(t,t) = O(y^{\alpha_1/2} b^{-2}) \text{ for } |t| \leq c_d y \zeta_1^{-1}. \tag{2.34}$$

By Lemma 1(iii), $\mathbb{E}(\sup_{|t|\leq c_d y_0 \zeta_1^{-1}} b \times f_0(t)) = o(1)$ as $y_0 \to 0$. So we can pick y_0 small enough such that

$$\mathbb{E}(\sup_{|t|\leq c_d y_0 \zeta_1^{-1}} f_0(t)) \leq \frac{1}{4b}\ . \tag{2.35}$$

By the Borel-TIS inequality (Proposition 1), (2.30), (2.33), (2.34), and (2.35), there exists a positive constant ε_0, such that

$$\begin{aligned} & \mathbb{P}(mes(A_\gamma) \leq y^d \zeta_1^{-d}, M > b | f(\tau) = \gamma + z/b) \\ \leq\ & \mathbb{P}(\inf_{|t|\leq c_d y \zeta_1^{-1}} |f_0(t)| > \frac{1}{2b}) \\ \leq\ & \exp(-\varepsilon_0 y^{-\alpha_1/2}). \end{aligned}$$

Situation 2: $0 < z \leq 1$.

We now proceed to the case where $0 < z \leq 1$. With y_0 defined to satisfy (2.33) and (2.35), we let $c = c_d y_0$ and define a finite subset $\tilde{T} = \{t_1, ..., t_N\} \subset T$ such that

1. For $i \neq j$, $|t_i - t_j| \geq \frac{c}{2\zeta_1}$.

2. For any $t \in T$, there exists i, such that $|t - t_i| \leq \frac{c}{\zeta_1}$.

Furthermore, let

$$B_i = \{t \in T : |t - t_i| \le c\zeta_1^{-1}\} \qquad \text{for } i \in \{1, 2, ..., N\}.$$

and thus $\cup_i B_i = T$. Note that

$$\mathbb{P}\left(mes(A_\gamma) \le y^d \zeta_1^{-d}, M > b | f(\tau) = \gamma + \frac{z}{b}\right) \le \sum_{i=1}^{N} \mathbb{P}\Big(mes(A_\gamma) \le y^d \zeta_1^{-d}, \sup_{t \in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big).$$

With c_d as previously chosen, each of the summands in the above display is bounded by

$$\begin{aligned} & \mathbb{P}\left(mes(A_\gamma) \le y^d \zeta_1^{-d}, \sup_{t \in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\right) \\ \le\ & \mathbb{P}\Big(\sup_{t \in B_i, |s-t| \le c_d y \zeta_1^{-1}} |f(t) - f(s)| > \frac{1}{b}, \sup_{t \in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big). \end{aligned} \tag{2.36}$$

The above inequality is derived from the following argument. Suppose that $f(t_0) > b$. In order to have $mes(A_\gamma) \le y^d \zeta_1^{-d}$, with the same argument as that of (2.30), one must have $\inf_{|s-t_0| \le c_d y \zeta_1^{-1}} f(s) \le b - 1/b$. Thus, there exists $|s_0 - t_0| \le c_d y \zeta_1^{-1}$ and $|f(s_0) - f(t_0)| > \frac{1}{b}$. Therefore, the event $\{mes(A_\gamma) > y^d \zeta_1^{-d}, \sup_{t \in B_i} f(t) > b\}$ is a subset of $\{\sup_{t \in B_i, |s-t| \le c_d y \zeta_1^{-1}} |f(t) - f(s)| > \frac{1}{b}, \sup_{t \in B_i} f(t) > b\}$, which yields (2.36).

Select $\delta_0, \delta_1 > 0$ small enough and λ large enough, We provide a bound for (2.36) under the following four cases:

Case 1. $0 < |t_i - \tau| < y^{-\delta_0} \zeta_1^{-1}$;

Case 2. $y^{-\delta_0} \zeta_1^{-1} < |t_i - \tau| < \delta_1$;

Case 3. $|t_i - \tau| \ge \delta_1$, $y < b^{-\lambda}$;

Case 4. $|t_i - \tau| \ge \delta_1$, $y \ge b^{-\lambda}$.

To facilitate the discussion, define

$$x_i \triangleq \zeta_1 \times |t_i - \tau|.$$

Case 1: $0 < |t_i - \tau| < y^{-\delta_0}\zeta_1^{-1}$. We provide a bound for (2.36) via the conditional representation (2.26) and the calculation in (2.27). According to Conditions A2 and A5, for $|t-s| \leq c_d y \zeta_1^{-1}$ and $t \in B_i$, we have

$$|\mu_\tau(t) - \mu_\tau(s)| \leq \kappa_\mu \zeta_1^{-\alpha_1/2}\sqrt{L_1(y/\zeta_1)}y^{\alpha_1/2} + \kappa_r(x_i+1)^{\beta_0}L_1((x_i+1)\zeta_1^{-1})y^{\beta_1}\zeta_1^{-\alpha_1}b.$$

According the definition of ζ_1 in (2.20) and Lemma 5(i), the above display can be bounded by

$$|\mu_\tau(t) - \mu_\tau(s)| \leq \frac{2\kappa_\mu y^{\alpha_1/4} + 2\kappa_r y^{-\delta_0\beta_0+\beta_1-\varepsilon_0}}{b}.$$

We choose δ_0 small such that it is further bounded by

$$|\mu_\tau(t) - \mu_\tau(s)| \leq \kappa y^{\varepsilon_0} b^{-1} \qquad \text{for some possibly different } \varepsilon_0 > 0.$$

Furthermore, we pick $y_0 > 0$ small enough such that for $0 < y < y_0$ and $|s-t| < c_d y \zeta_1^{-1}$

$$|\mu_\tau(s) - \mu_\tau(t)| \leq \frac{1}{2b}. \tag{2.37}$$

The above inequality provides a bound on the variation of the mean function over the set B_i when t_i is within $y^{-\delta_0}\zeta_1^{-1}$ distance close to τ. The probability in (2.36) can be bounded by

$$(2.36) \leq \mathbb{P}(\sup_{t\in B_i, |t-s|\leq c_d y\zeta_1^{-1}} |f_0(t) - f_0(s)| > \frac{1}{2b}).$$

Note that by Lemma 1(ii), for $|s-t| < c_d y \zeta_1^{-1}$ and for $y < y_0$, we have that

$$Var(f_0(s) - f_0(t)) \leq \lambda_1 \frac{L_1(c_d y \zeta_1^{-1})}{L_1(\zeta_1^{-1})} y^{\alpha_1} b^{-2} = O(y^{\alpha_1/2} b^{-2}). \tag{2.38}$$

We apply the Borel-TIS inequality (Proposition 1) to the double-indexed Gaussian field $\xi(s,t) \triangleq f_0(s) - f_0(t)$ and obtain that there exists a positive constant ε_0 such that

$$\begin{aligned}
&\mathbb{P}\left(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, \sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\right) \\
\leq\ & \mathbb{P}(\sup_{t\in B_i, |t-s|\leq c_d y\zeta_1^{-1}} |f_0(t) - f_0(s)| > \frac{1}{2b}) \\
\leq\ & \exp(-\varepsilon_0 y^{-\alpha_1/2}). \qquad (2.39)
\end{aligned}$$

We put together all the B_i's such that $|t_i - \tau| < y^{-\delta_0}\zeta_1^{-1}$ and obtain that

$$\begin{aligned}
&\mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, \sup_{|t-\tau|\le y^{-\delta_0}\zeta_1^{-1}} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\
= \ & O(y^{-\delta_0 d}\exp(-\varepsilon_0 y^{-\alpha_1/2})) \le \exp(-y^{-\varepsilon_0})
\end{aligned}$$

possibly redefining ε_0.

Case 2: $y^{-\delta_0}\zeta_1^{-1} < |t_i - \tau| < \delta_1$. For this case, we implicitly require that $y^{-\delta_0}\zeta_1^{-1} < \delta_1$. For $t \in B_i$ and y small enough, we have that

$$\begin{aligned}
&\mathbb{P}(\sup_{t\in B_i, |s-t|\le c_d y\zeta_1^{-1}} |f(t) - f(s)| > \frac{1}{b}, \sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}) \\
\le \ & \mathbb{P}(\sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}).
\end{aligned}$$

According to Condition A2 and expression (2.31), we have the bound

$$\mu_\tau(t) \ \le \ b - \frac{\Delta_\tau}{2}\frac{L_1(x_i\zeta_1^{-1})}{L_1(\zeta_1^{-1})}x_i^{\alpha_1}b^{-1}, \text{ for } \tau + t \in B_i. \tag{2.40}$$

According to Lemma 1 and definition of ζ_1, the variance of $f_0(t)$ is controlled by

$$C_0(t,t) \le 2\lambda_1 \frac{L_1(x_i\zeta_1^{-1})}{L_1(\zeta_1^{-1})}x_i^{\alpha_1}b^{-2}. \tag{2.41}$$

According to Proposition 1 and Lemma 5(ii) in the Supplemental Material, we have $\frac{L_1(x_i\zeta_1^{-1})}{L_1(\zeta_1^{-1})}x_i^{\alpha_1} > x_i^{\alpha_1/2}$ for $y^{-\delta_0} < x_i < \delta_1\zeta_1$. We continue the calculations

$$\begin{aligned}
\mathbb{P}(\sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}) \ &\le \ \mathbb{P}(\sup_{t+\tau\in B_i} f_0(t) > \frac{\Delta_\tau}{2}\frac{L_1(x_i\zeta_1^{-1})}{L_1(\zeta_1^{-1})}x_i^{\alpha_1}b^{-1}) \\
&\le \ \exp\Big(-\frac{\Delta_\tau^2}{8\lambda_1}\frac{L_1(x_i\zeta_1^{-1})}{L_1(\zeta_1^{-1})}x_i^{\alpha_1}\Big) \\
&\le \ \exp(-\frac{\Delta_\tau^2}{8\lambda_1}x_i^{\alpha_1/2}).
\end{aligned}$$

Putting together all the B_i's such that $y^{-\delta_0} < x_i < \delta_1\zeta_1$, we have that

$$\begin{aligned}
&\mathbb{P}(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, \sup_{y^{-\delta_0}\zeta_1^{-1} < |t-\tau| < \delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}) \\
\le \ & \sum_{k=0}^\infty \kappa(y^{-\delta_0} + k)^{d-1}\exp[-\frac{\Delta_\tau^2}{8\lambda_1}(y^{-\delta_0} + k)^{\alpha_1/2}] \\
\le \ & \exp(-y^{-\varepsilon_0})
\end{aligned}$$

for some constant $\varepsilon_0 > 0$.

Case 3: $|t_i - \tau| \geq \delta_1$ **and** $y < b^{-\lambda}$**.** Since $C(s,t)$ is uniformly Hölder continuous, we can always choose λ large such that for $|s-t| \leq c_d y \zeta_1^{-1} \leq c_d b^{-\lambda}\zeta_1^{-1}$,

$$|\mu_\tau(t) - \mu_\tau(s)| \;\leq\; \frac{1}{4b}. \tag{2.42}$$

By Lemma 1(ii) and Lemma 5(i), for $|s-t| \leq c_d y \zeta_1^{-1}$, the conditional variance $Var(f_0(s) - f_0(t))$ is bounded by

$$Var(f_0(s) - f_0(t)) \;\leq\; \lambda_1 \frac{L_1(c_d y \zeta_1^{-1})}{L_1(\zeta_1^{-1})} y^{\alpha_1} b^{-2} = O(y^{\alpha_1/2} b^{-2}).$$

Thus, there exist a constant $\varepsilon_0 > 0$ such that

$$\begin{aligned}
& \mathbb{P}\Big(\sup_{t\in B_i, |s-t|\leq c_d y \zeta_1^{-1}} |f(t) - f(s)| > \frac{1}{b}, \sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\
\leq\; & \mathbb{P}\Big(\sup_{t\in B_i, |s-t|\leq c_d y \zeta_1^{-1}} |f_0(t) - f_0(s)| > \frac{1}{2b}\Big) \\
\leq\; & 2\exp(-\varepsilon_0 y^{-\alpha_1}).
\end{aligned}$$

Note that $\zeta_1 \ll b^{4/\alpha_1}$, so for $y < b^{-\lambda}$, we have

$$\begin{aligned}
& \mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, \sup_{|t-\tau|>\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\
\leq\; & O(\zeta_1^d) \sup_i \mathbb{P}\Big(\sup_{t\in B_i, |s-t|\leq c_d y \zeta_1^{-1}} |f(t) - f(s)| > \frac{1}{b}, \sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\
\leq\; & O(b^{4d/\alpha_1}) \exp(-\varepsilon_0 y^{-\alpha_1/2}) \\
\leq\; & O(y^{-\frac{4d}{\alpha_1 \lambda}}) \exp(-\varepsilon_0 y^{-\alpha_1/2}) \\
\leq\; & \exp(-y^{-\varepsilon_0})
\end{aligned} \tag{2.43}$$

for some possibly different constant ε_0.

Case 4: $|t_i - \tau| \geq \delta_1$ **and** $y \geq b^{-\lambda}$**.** Note that Condition A3 implies that for any $\delta_1 > 0$, there exists $\varepsilon > 0$ such that for $|s-t| > \delta_1$ one has $r(s,t) < 1 - \varepsilon$.

Thus according to expression (2.31), there exists $\varepsilon > 0$ such that $\mu_\tau(t) \le (1-\varepsilon)b$. According to Proposition 1 , we have that for b large enough and some $\varepsilon > 0$,

$$\begin{aligned}
& \mathbb{P}(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, \sup_{|t-\tau|\ge\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}) \\
\le\ & \mathbb{P}(\sup_{|t|\ge\delta_1} f_0(t) + \mu_\tau(t) > b) \\
\le\ & \mathbb{P}(\sup_{|t|\ge\delta_1} f_0(t) > \varepsilon b) \le \exp(-\frac{\varepsilon^2 b^2}{2\sigma_T^2}) \le \exp(-y^{-\varepsilon_0}).
\end{aligned}$$

Combining Cases 1-4, for some constants ε_0 and y_0 chosen to be small, we have that for $y \in (0, y_0]$

$$\mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, M > b \Big| f(\tau) = \gamma + \frac{z}{b}\Big) \le \exp(-y^{-\varepsilon_0}). \tag{2.44}$$

Together with (2.29), we have

$$Q_b\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, M > b\Big) \le \exp(-y^{-\varepsilon_0}). \tag{2.45}$$

Thus, according to (2.28), for some $\kappa > 0$, we have

$$\mathbb{E}^Q\Big[\frac{1}{mes(A_\gamma)^2}; M > b\Big] \le (\kappa + y_0^{-2d})\zeta_1^{2d}. \tag{2.46}$$

2.5.2 The I_1 term

To provide a lower bound of

$$I_1 = \mathbb{E}^{Q_b}\Big[\frac{1}{mes(A_\gamma)}; M > b\Big],$$

we basically need to prove that $mes(A_\gamma)$ cannot be always very large. Thus, it is sufficient to show that $f(t)$ drops below γ when t is reasonably far away from τ. The next lemma shows that for any $\delta > 0$, the process $f(t)$ drops below γ almost all the time when $|t-\tau| > \delta$.

Lemma 2. *Under conditions A1-6, for standard deviation of Type 1, we have that*

$$Q_b(\sup_{|t-\tau|>\delta} f(t) \ge \gamma) \le e^{-\varepsilon_0 b^2} \qquad \textit{for some } \varepsilon_0 > 0. \tag{2.47}$$

Lemma 3. *Under conditions A1-6, there exists δ small and κ large (independent of b), such that for $x > \kappa$ we have*

$$Q_b\Big(\sup_{x\zeta^{-1}\leq|t-\tau|\leq\delta} f(t) \geq \gamma\Big) < e^{-\varepsilon_0 x^{\alpha_1/4}}. \tag{2.48}$$

The proof of these two Lemmas are provided in the Supplemental Material. We proceed to developing a lower bound for I_1. First, notice that the event $\{M > b\}$ is a regular event under Q_b, that is,

$$Q_b(M > b) \geq Q_b(f(\tau) > b) > \frac{1}{2}e^{-1}.$$

The last step is based on an asymptotic calculation of the overshoot distribution of a standard Gaussian random variable. According to Lemma 2 and 3, we choose x such that

$$Q_b(\sup_{|t-\tau|>x\zeta_1^{-1}} f(t) \geq \gamma) < \frac{1}{2}e^{-2}.$$

Let ω_d be the volume of the d-dimensional unit ball. Thus, we have

$$\begin{aligned}
I_1 &\geq \mathbb{E}^{Q_b}(\frac{1}{mes(A_\gamma)}; M > b, mes(A_\gamma) < \omega_d x^d \zeta_1^{-d}) \\
&\geq \omega_d^{-1} x^{-d} \zeta_1^d Q_b(mes(A_\gamma) < \omega_d x^d \zeta_1^{-d}, M > b) \\
&\geq \omega_d^{-1} x^{-d} \zeta_1^d \big[Q_b(M > b) - Q_b(mes(A_\gamma) \geq \omega_d x^d \zeta_1^{-d})\big] \\
&\geq \omega_d^{-1} x^{-d} \zeta_1^d \big[Q_b(M > b) - Q_b(\sup_{|t-\tau|>x\zeta_1^{-1}} f(t) \geq \gamma)\big] \\
&\geq \frac{1}{2}\omega_d^{-1} x^{-d} \zeta_1^d (e^{-1} - e^{-2}).
\end{aligned} \tag{2.49}$$

Summarizing the results in (2.46) and (2.49), we have that

$$E_b(Z_b^2) \leq \kappa \zeta_1^{2d}\Big(\int \mathbb{P}(f(t) > \gamma)dt\Big)^2, \quad \mathbb{P}(M > b) > \varepsilon_0 \zeta_1^d \int \mathbb{P}(f(t) > \gamma)dt,$$

and therefore

$$\sup_b \frac{\mathbb{E}^{Q_b} Z_b^2}{\mathbb{P}^2(M > b)} < \infty.$$

2.6 Proof of Theorem 2

Let $T_m = \{t_1, ..., t_m\}$ be generated in the Step 3 of Algorithm 2. We start the analysis with the following decomposition

$$\begin{aligned}
\hat{Z}_b - Z_b &= \left[\frac{I(\sup f(t) > b)}{mes(A_\gamma)} - \frac{I(\max_{i=1}^m f(t_i) > b)}{\widehat{mes}(A_\gamma)}\right]\mathbb{E}(mes(A_\gamma)) \\
&= \mathbb{E}(mes(A_\gamma)) \\
&\quad \times \Big[\frac{I(\sup f(t) > b)}{mes(A_\gamma)} - \frac{I(\max_{i=1}^m f(t_i) > b)}{mes(A_\gamma)} \\
&\qquad + \frac{I(\max_{i=1}^m f(t_i) > b)}{mes(A_\gamma)} - \frac{I(\max_{i=1}^m f(t_i) > b)}{\widehat{mes}(A_\gamma)}\Big],
\end{aligned}$$

where $\widehat{mes}(A_\gamma)$ is defined as in (2.22). According to the result in Theorem 1, it is sufficient to show that $|\mathbb{E}^{Q_b}(\hat{Z}_b - Z_b)| \leq \varepsilon \mathbb{P}(M > b)$ and $Var(\hat{Z}_b - Z_b) = O(\mathbb{P}^2(M > b))$. We define notation

$$\begin{aligned}
J_1 &= \frac{I(\sup f(t) > b)}{mes(A_\gamma)} - \frac{I(\max_{i=1}^m f(t_i) > b)}{mes(A_\gamma)} \\
J_2 &= \frac{I(\max_{i=1}^m f(t_i) > b)}{mes(A_\gamma)} - \frac{I(\max_{i=1}^m f(t_i) > b)}{\widehat{mes}(A_\gamma)}.
\end{aligned}$$

We control each of the two terms respectively.

2.6.1 The J_1 term

Note that J_1 is non-negative and

$$\mathbb{E}_b(J_1) = E_b\left(\frac{1}{mes(A_\gamma)}; M > b; \max_{i=1}^m f(t_i) \leq b\right). \tag{2.50}$$

The proof of Theorem 1, in particular (2.45), shows that $\frac{I(M>b)}{\zeta^d mes(A_\gamma)}$ is uniformly integrable in the parameter b where

$$\zeta = \max(\zeta_1, \zeta_2).$$

Thus, for any δ small enough, we have that

$$\sup_{Q_b(B)\leq\delta} E_b\left(\frac{1}{mes(A_\gamma)}; M > b; B\right) \leq (-\log\delta)^{1/\varepsilon_0}\delta\zeta^d. \tag{2.51}$$

Therefore, it is sufficient to derive a bound for

$$Q_b(M > b; \max_{i=1}^{m} f(t_i) \leq b).$$

Let x be large and δ' be small and we have the following split

$$\begin{aligned}
& Q_b\Big(M > b; \max_{i=1}^{m} f(t_i) \leq b\Big) \\
\leq\ & Q_b\Big(\sup_{x\zeta^{-1}<|t-\tau|<\delta'} f(t) > b; \max_{i=1}^{m} f(t_i) \leq b\Big) \\
+\ & Q_b\Big(\sup_{|t-\tau|<x\zeta^{-1}} f(t) > b, \sup_{|t-\tau|>x\zeta^{-1}} f(t) \leq b; \max_{i=1}^{m} f(t_i) \leq b\Big) \\
+\ & Q_b\Big(\sup_{|t-\tau|\geq\delta'} f(t) > b; \max_{i=1}^{m} f(t_i) \leq b\Big).
\end{aligned} \tag{2.52}$$

We will provide a specific choice of m such that

$$Q_b\left(\sup f(t) > b; \max_{i=1}^{m} f(t_i) \leq b\right) \leq \delta \triangleq \varepsilon^{1+\varepsilon_0},$$

where ε is the relative bias preset in the statement of the theorem. We consider each of the three terms in (2.52).

2.6.1.1 The first term in (2.52).

We choose

$$x = \min\{(-\log\delta)^{4/\alpha}, \delta'\zeta\}, \qquad \text{where } \alpha = \min\{\alpha_1, \alpha_2\}.$$

According to Lemma 3, the first term in (2.52) is bounded by

$$Q_b\Big(\sup_{x\zeta^{-1}<|t-\tau|<\delta'} f(t) > b; \max_{i=1}^{m} f(t_i) \leq b\Big) \leq Q_b\Big(\sup_{x\zeta^{-1}<|t-\tau|<\delta'} f(t) > b\Big) \leq \delta.$$

Notationally, we define that $\sup_{t\in\emptyset} f(t) = -\infty$. Thus, when $x = \delta'\zeta$, the above probability is zero.

2.6.1.2 The second term in (2.52).

Simple derivations yield that

$$\begin{aligned} & Q_b\Big(\sup_{|t-\tau|<x\zeta^{-1}} f(t) > b, \sup_{|t-\tau|>x\zeta^{-1}} f(t) \le b, \max_{i=1}^{m} f(t_i) \le b\Big) \\ = \;& E_b\Big[Q_b(\max_{i=1}^{m} f(t_i) \le b|f); \sup_{|t-\tau|<x\zeta^{-1}} f(t) > b, \sup_{|t-\tau|>x\zeta^{-1}} f(t) \le b\Big] \\ \le \;& E_b\Big[(1-\beta(A_b))^m; \sup_{|t-\tau|<x\zeta^{-1}} f(t) > b\Big] \end{aligned} \tag{2.53}$$

where

$$\beta(A_b) = \zeta^d \times mes(A_b \cap B(\tau, x/\zeta)) \times \inf_{|t|\le x} k(t)$$

is a lower bound of the probability that $Q_b(t_i \in A_b|f)$ and $B(\tau, x)$ is the ball centered around τ with radius x. In what follows, we need to show that $mes(A_b)$ cannot be too small on the set $\{\sup_{|t-\tau|<x\zeta^{-1}} f(t) > b\}$ and therefore $\beta(A_b)$ cannot be too small. We write

$$\mathcal{E}_1 = \{\sup_{|t-\tau|<x\zeta^{-1}} f(t) > b\}$$

and write (2.53) as

$$\mathbb{E}_b[(1-\beta(A_b))^m; \mathcal{E}_1] = E_b[(1-\beta(A_b))^m; \mathcal{E}_1, D^c_{\lambda_3,\delta_1}] + E_b[(1-\beta(A_b))^m; \mathcal{E}_1, D_{\lambda_3,\delta_1}]$$

where, for some λ_3 and δ_1 positive, we define

$$D_{\lambda_3,\delta_1} = \{\sup_{\substack{|s-t|\le\lambda_3\zeta^{-1} \\ s,t\in B(\tau, x\zeta^{-1})}} |f(s) - f(t)| \le \delta_1 b^{-1}\}.$$

For some ε_0 small, we choose $\delta_1 = \varepsilon_0\delta$ and $\lambda_3 = \varepsilon_0\delta_1^{2/\alpha+1/\beta_1+\varepsilon_0}$. We apply the Borel-TIS lemma to the double-indexed process $\xi(s,t) = f(s) - f(t)$ whose variance is bounded by Lemma 1 (ii). Thus, we obtain the following bound

$$E_b\Big[(1-\beta(A_b))^m; \mathcal{E}_1, D^c_{\lambda_3,\delta_1}\Big] \le Q_b(D^c_{\lambda_3,\delta_1}) \le \delta.$$

Therefore, (2.53) is bounded by

$$\delta + E_b\Big[(1-\beta(A_b))^m; \mathcal{E}_1, D_{\lambda_3,\delta_1}\Big].$$

We further split the expectation

$$\begin{aligned} & \mathbb{E}_b\Big[(1-\beta(A_b))^m; \mathcal{E}_1, D_{\lambda_3,\delta_1}\Big] \\ \leq\ & E_b\Big[(1-\beta(A_b))^m; D_{\lambda_3,\delta_1}; \sup_{|t-\tau|<x\zeta^{-1}} f(t) > b + \delta_1 b^{-1}, \mathcal{E}_1\Big] \\ & + Q_b\Big[D_{\lambda_3,\delta_1}; b < \sup_{|t-\tau|<x\zeta^{-1}} f(t) \leq b + \delta_1 b^{-1}, \mathcal{E}_1\Big]. \end{aligned}$$

We derive a bound of the second term by considering the standardized process $g(t) = b(f(\tau + t/\zeta) - b)$ conditional on $f(\tau) = \gamma + \frac{z}{b}$. $g(t)$ can be written as

$$g(t) = \frac{C(t/\zeta + \tau, \tau)}{C(\tau, \tau)} z + l(t), \tag{2.54}$$

where $l(t)$ is a random field whose distribution is independent of z. So we have

$$\begin{aligned} Q_b(b < \sup_{|t-\tau|<x\zeta^{-1}} f(t) < b + \delta_1 b^{-1}) &= Q_b\Big(\sup_{|t|\leq x} \frac{C(t/\zeta+\tau)}{C(\tau,\tau)} z + l(t) \in (0, \delta_1)\Big) \\ &= O(\delta_1). \end{aligned}$$

The last equality holds because z has a density bounded everywhere (asymptotically exponential), and $\frac{1}{2} < \frac{C(t/\zeta+\tau)}{C(\tau,\tau)} < \frac{\sigma_T^2}{\sigma^2(\tau)}$. Given a realization of $l(t)$, $\sup_{|t|\leq x} \frac{C(t/\zeta+\tau)}{C(\tau,\tau)} z + l(t) \in (0, \delta_1)$ implies that z has to fall in an interval with length less than $2\delta_1$. Thus, if we choose ε_0 small and $\delta_1 = \varepsilon_0 \delta$, then

$$Q_b(b < \sup_{|t-\tau|<x\zeta^{-1}} f(t) < b + \delta_1 \zeta^{-1}) < \delta.$$

Therefore, we have that (2.53) is bounded by

$$2\delta + \mathbb{E}^{Q_b}[(1-\beta(A_b))^m; D_{\lambda_3,\delta_1}; \sup_{|t-\tau|<x\zeta^{-1}} f(t) > b + \delta_1 b^{-1}, \mathcal{E}_1].$$

Note that, on the set D_{λ_3,δ_1}, $mes(A_b \cap B(\tau, x\zeta^{-1}))$ is controlled by the overshoot $\sup_{|t-\tau|<x\zeta^{-1}} f(t) - b$, that is, if $\sup_{|t-\tau|<x\zeta^{-1}} f(t) > b + \delta_1/b$, then $mes(A_b \cap B(\tau, x\zeta^{-1})) \geq \varepsilon_0 \lambda_3^d \zeta^{-d}$. In addition, the density $k_{\tau,\zeta}(t)$ is bounded from below by $x^{-d-\varepsilon_1}$ for $t \in B(\tau, x\zeta^{-1})$. Thus, the probability $\beta(A_b)$ has a lower bound

$$\beta(A_b) \geq \varepsilon_0 x^{-d-\varepsilon_1} \lambda_3^d \geq \varepsilon_0 \delta^{2d/\alpha + d/\beta_1 + 2\varepsilon_0}.$$

The last step of the above inequality follows from that $x = \min\{(-\log\delta)^{4/\alpha}, \delta'\zeta\}$. Thus, we have that (2.53) is bounded by

$$2\delta + (1 - \varepsilon_0 \delta^{2d/\alpha + d/\beta_1 + 2\varepsilon_0})^m.$$

For some κ large,

$$m = \kappa\delta^{-2d/\alpha - d/\beta_1 - 3\varepsilon_0}$$

and therefore

$$Q_b\Big(\sup_{|t-\tau|<x\zeta^{-1}} f(t) > b, \sup_{|t-\tau|>x\zeta^{-1}} f(t) \le b; \max_{i=1}^m f(t_i) \le b\Big) \le 4\delta.$$

2.6.1.3 The last term in (2.52).

According to the result in Lemma 2, we can choose ε_0 and δ' such that

$$Q_b(\sup_{|t-\tau|\ge\delta'} f(t) \ge \gamma) \le e^{-\varepsilon_0 b^2}.$$

There are two cases: $\delta > e^{-\varepsilon_0 b^2}$ and $\delta \le e^{-\varepsilon_0 b^2}$.

Case 1: $\delta > e^{-\varepsilon_0 b^2}$**.** In this case, The last term in (2.52) is bounded trivially by

$$Q_b\Big(\sup_{|t-\tau|\ge\delta'} f(t) > b; \max_{i=1}^m f(t_i) \le b\Big) \le Q_b(\sup_{|t-\tau|\ge\delta'} f(t) \ge \gamma) \le \delta.$$

Case 2: $\delta < e^{-\varepsilon_0 b^2}$**.** We need a similar analysis to that of the second term. We now split the probability for $\delta_2 = \delta^{1+\varepsilon_0}$

$$\begin{aligned} &Q_b\Big(\sup_{|t-\tau|\ge\delta'} f(t) > b; \max_{i=1}^m f(t_i) \le b\Big) \\ &\quad \le Q_b\Big(\sup_{|t-\tau|\ge\delta'} f(t) \in [b, \delta_2 b^{-\lambda}]\Big) + Q_b\Big(\sup_{|t-\tau|\ge\delta'} f(t) > b + \delta_2 b^{-\lambda}; \max_{i=1}^m f(t_i) \le b\Big). \end{aligned}$$

We now consider the first term split the set $\{t : |t-\tau| > \delta'\}$ into two parts. Define the set $F = \{t : \frac{C(t,\tau)}{C(\tau,\tau)} > \frac{1}{(-\log\delta_2)^2}\}$, We start with the small overshoot probability on the set F

$$Q_b\Big(b < \sup_{|t-\tau|>\delta', t\in F} f(t) \le b + \delta_2/b\Big).$$

Using the representation (2.54), applying similar analysis as that of the second term, we have that

$$
\begin{aligned}
& Q_b\Big(b < \sup_{|t-\tau|\geq\delta', t\in F} f(t) < b+\delta_2 b^{-1}\Big) \\
\leq\ & Q_b\Big(\sup_{|\frac{t}{\zeta}|>\delta', \frac{t}{\zeta}+\tau\in F} \frac{C(t/\zeta+\tau)}{C(\tau,\tau)} z + l(t) \in (0,\delta_2)\Big) \\
=\ & O((-\log\delta_2)^2\delta_2) \leq \delta. \qquad (2.55)
\end{aligned}
$$

The last two steps are based on the fact that z is a random variable independent of $l(t)$ and has bounded density. Thus, the above probability is bounded by

$$
\sup_x \mathbb{P}(x < z < x + (\log\delta_2)^2\delta_2) = O((\log\delta_2)^2\delta_2).
$$

We will return to this estimate soon.

We now consider t in F^c. For some κ_0 large, we have that $Q_b(z > -\kappa_0\log\delta_2) < \delta_2$. Thus, we only consider $z < -\kappa_0\log\delta_2$. Conditional on $f(\tau) = \gamma + z/b$, the conditional mean is $\sup_{t\in F^c}\mu_\tau(t-\tau) \leq C > 0$. In addition, the conditional variance of $f(t)$ on the set F^c is almost $\sigma^2(t)$. Thus, we can apply classic results on the density estimation of the $\sup f(t)$ (c.f. Theorem 2 of Tsirel'son [1975]). That is, conditional on $f(\tau) = \gamma + \frac{z}{b}$, $\sup_{|t-\tau|\geq\delta', F^c} f(t)$ has a bounded density over $[b, b+\delta_2 b^{-\lambda}]$ for some $\lambda \geq 1$ and thus

$$
Q_b(\sup_{|t-\tau|\geq\delta', t\in F^c} f(t) \in [b, b+\delta_2 b^{-\lambda}] | f(\tau) = \gamma + \frac{z}{b}) = O(\delta_2).
$$

Summarizing the above results, we have that

$$
\begin{aligned}
& Q_b(\sup_{|t-\tau|\geq\delta'} f(t) \in [b, b+\delta_2 b^{-\lambda}]) \\
\leq\ & Q_b(\sup_{|t-\tau|\geq\delta', t\in F} f(t) \in [b, b+\delta_2 b^{-\lambda}]) \\
& + Q_b(z \geq -\kappa_0\log\delta_2) + Q_b(\sup_{|t-\tau|\geq\delta', t\in F^c} f(t) \in [b, b+\delta_2 b^{-\lambda}], z \leq -\kappa_0\log\delta_2) \\
\leq\ & 3\delta.
\end{aligned}
$$

The last term in (2.52) is bounded by

$$
\begin{aligned}
& Q_b\Big(\sup_{|t-\tau|\geq\delta'} f(t) > b; \max_{i=1}^m f(t_i) \leq b\Big) \leq 3\delta + Q_b\Big(\sup_{|t-\tau|\geq\delta'} f(t) > b \\
& + \delta_2 b^{-\lambda}; \max_{i=1}^m f(t_i) \leq b\Big).
\end{aligned}
$$

For the second term, we apply the old trick by choosing $\lambda_4 = \delta_2^{2/\alpha+1/\beta_1+\varepsilon_0} b^{-2\lambda/\alpha-\lambda/\beta_1}$, and thus

$$Q_b(\sup_{|s-t|<\lambda_4} |f(s) - f(t)| > \delta_2 b^{-\lambda}) < \delta_2. \tag{2.56}$$

Note that $b^2 \leq -\varepsilon_0^{-1} \log \delta_2$, we can choose a different ε_0 such that λ_4 can be simplified to

$$\lambda_4 = \delta_2^{2/\alpha+1/\beta_1+\varepsilon_0}.$$

If $\sup_{|s-t|<\lambda_4} |f(s) - f(t)| < \delta_2 b^{-\lambda}$ and $\sup_{|t-\tau|\geq\delta'} f(t) > b + \delta_2 b^{-\lambda}$, we have that $\beta(A_b) \geq \varepsilon_0 \lambda_4^d \zeta^{-d-\varepsilon_1}$. With a different choice of ε_0, we choose

$$m = -2\lambda_4^{-d} \zeta^{d+\varepsilon_1} \log \delta = O(\delta^{-d(2/\alpha+1/\beta_1)-\varepsilon_0}), \tag{2.57}$$

then we have

$$\mathbb{E}_b[(1 - \beta(A_b))^m; \sup_{|s-t|<\lambda_4} b < |f(s) - f(t)| < \delta_2 b^{-\lambda}, f(t) > b + \delta_2 b^{-\lambda}] \leq \delta. \tag{2.58}$$

Therefore, combining the bounds in (2.55), (2.56), and (2.58), if $\varepsilon < e^{-\varepsilon_0 b^2}$ and we choose m as in (2.57) and, then

$$Q_b\Big(\sup_{|t-\tau|>\delta'} f(t) > b; \max_{i=1}^{m} f(t_i) \leq b\Big) \leq 5\delta.$$

Putting together the bounds for all the three terms in (2.52), we have that

$$Q_b\Big(M > b; \max_{i=1}^{m} f(t_i) \leq b\Big) \leq 5\delta.$$

If we choose $\delta = \varepsilon^{1+\varepsilon_0}$ and

$$m = O(\delta^{-d(2/\alpha+1/\beta_1+\varepsilon_0)}) = O(\varepsilon^{-d(2/\alpha+1/\beta_1)-2d\varepsilon_0})$$

then according to the bound in (2.51), we have that

$$\mathbb{E}^{Q_b} J_1 \leq \zeta^d \varepsilon.$$

Similarly, according to the uniform integrability of $\zeta^{-2d}/mes^2(A_\gamma)$, by choosing the same m, there exists a κ_0 such that

$$\mathbb{E}^{Q_b}(J_1^2) \leq \kappa_0 \zeta^{2d}.$$

2.6.2 The J_2 term

We now proceed to

$$J_2 = I(\max_{i=1}^{m} f(t_i) > b)\left[\frac{1}{mes(A_\gamma)} - \frac{1}{\widehat{mes}(A_\gamma)}\right].$$

We study the behavior of J_2 by means of the scaled process $g(t)$ defined as in (2.18). For the analysis of J_2, we translate everything to the scale of $g(t)$. Recall the process $g(t)$ given by (2.18) is

$$g(t) = b(f(\tau + t/\zeta) - b), \tag{2.59}$$

For each t, $f(\tau + t/\zeta) > \gamma$ if and only if $g(t) > -1$.

Conditional on τ, $t_1, ..., t_m$ are i.i.d. with density $k_{\tau,\zeta}(t)$ defined as in (2.21). Let $s_i = (t_i - \tau)\zeta$ and thus $s_1, ..., s_m$ are i.i.d. following density $k(s)$. We can then rewrite the estimator in (2.22) as

$$\widehat{mes}(A_\gamma) = \frac{\zeta^{-d}}{m}\sum_{i=1}^{m}\frac{I(g(s_i) > -1)}{k(s_i)}.$$

Thus, $\widehat{mes}(A_\gamma)$ is an unbiased estimator of $mes(A_\gamma)$, that is, $\mathbb{E}(\widehat{mes}(A_\gamma)|f) = mes(A_\gamma)$. Conditional on a particular realization of $f(t)$ (or equivalently, g(t)), the variance of $\widehat{mes}(A_\gamma)$ is

$$Var(\widehat{mes}(A_\gamma)|f) = \frac{\kappa_f \zeta^{-2d}}{m},$$

where

$$\kappa_f = Var\Big[\frac{I(g(S) > -1)}{k(S)}\Big| f\Big] \le k^{-2}(t_f) \tag{2.60}$$

and

$$t_f = \max(|t| : g(t) > -1). \tag{2.61}$$

By means of the inequality $\frac{1}{1+x} - 1 \ge -x$, we have $\frac{1}{mes(A_\gamma)} - \frac{1}{\widehat{mes}(A_\gamma)} \le \frac{\widehat{mes}(A_\gamma) - mes(A_\gamma)}{mes^2(A_\gamma)}$. Therefore,

$$\mathbb{E}\Big[\Big(\frac{1}{mes(A_\gamma)} - \frac{1}{\widehat{mes}(A_\gamma)}\Big)^2; \widehat{mes}(A_\gamma) > mes(A_\gamma)\ \Big|\ f\Big] \le \frac{\kappa_f \zeta^{-2d}}{m \times mes^4(A_\gamma)}.$$

It is the expectation on the set $\{\widehat{mes}(A_\gamma) < mes(A_\gamma)\}$ that induces complications in that the factor $\frac{1}{\widehat{mes}(A_\gamma)}$ can be very large when there are not many t_i's in the excursion set A_γ. We now proceed to this case. Conditional on a particular realization of f (and equivalently the process $g(t)$), the analysis consists of three steps.

Step 1. Define the f-dependent probability

$$p_f \triangleq Q_b(t_i \in A_\gamma | f) = \int_{A_\gamma} k_{\tau,\zeta}(t)dt = \int_{A_{-1}^g} k(t)dt. \tag{2.62}$$

Using standard exponential change of measure techniques for large deviations Dembo and Zeitouni [2009], we obtain that

$$Q_b\left[\sum_{i=1}^m I(t_i \in A_\gamma) \le p_f(1-\delta_3)m \Big| f\right] \le e^{-mI(\delta_3, p_f)} \tag{2.63}$$

for all $\delta_3 \in (0,1)$, where the rate function $I(\delta_3, p_f) = \theta_* p_f(1-\delta_3) - \varphi(\theta_*)$, $\varphi(\theta) = \log(1-p_f+p_f e^\theta)$, and $\theta_* = \log\left(1 - \frac{\delta_3}{1-p_f(1-\delta_3)}\right)$. By elementary calculus, if we choose $\delta_3 = \frac{1}{2}$, then we have that for some $\varepsilon_0 > 0$

$$I(\delta_3, p_f) \ge \varepsilon_0 p_f \quad \text{for all } p_f > 0.$$

We further have

$$\begin{aligned}
&\mathbb{E}\Big[\Big(\frac{1}{mes(A_\gamma)} - \frac{1}{\widehat{mes}(A_\gamma)}\Big)^2; \\
&\widehat{mes}(A_\gamma) \le mes(A_\gamma), \max_{i=1}^m f(t_i) > b, \sum_{i=1}^m I(t_i \in A_\gamma) \le \frac{p_f m}{2} \ \Big| \ f\Big] \\
\le\ & \mathbb{E}\Big[\frac{4}{\widehat{mes}^2(A_\gamma)}; \widehat{mes}(A_\gamma) \le mes(A_\gamma), \max_{i=1}^m f(t_i) > b, \sum_{i=1}^m I(t_i \in A_\gamma) \le \frac{p_f m}{2} \ \Big| \ f\Big].
\end{aligned}$$

There is at least one t_i in the excursion set A_γ. Therefore, the estimator $\widehat{mes}(A_\gamma) \ge m^{-1}\zeta^{-d}k^{-1}(t_f)$. Thus, the above expectation is upper bounded by

$$\le \kappa k^{-2}(t_f) m^2 \zeta^{2d} e^{-\varepsilon_0 m p_f}.$$

Step 2. We consider the situation that $\sum I(t_i \in A_\gamma) > \frac{p_f m}{2}$. The unbiasedness of $\widehat{mes}(A_\gamma)$ suggests that

$$mes(A_\gamma) = \mathbb{E}\Big(\frac{1}{\zeta^d k(S)} \mid S \in A_{-1}^g\Big) p_f,$$

where S is a random index following density $k(s)$. Note that on the set A_{-1}^g, $k(t_f) \leq k(S) \leq \kappa_1$. Thus, if we let $\lambda_f = \kappa_1^{-1} k(t_f)$, then on the set $\{\sum I(t_i \in A_\gamma) > \frac{p_f m}{2}\}$ we have

$$\widehat{mes}(A_\gamma) \geq \frac{\lambda_f mes(A_\gamma)}{2}.$$

Thus, using Taylor expansion, we have that

$$\begin{aligned}
& E_b\Big[\Big(\frac{1}{mes(A_\gamma)} - \frac{1}{\widehat{mes}(A_\gamma)}\Big)^2; \widehat{mes}(A_\gamma) < mes(A_\gamma); \sum I(t_i \in A_\gamma) > \frac{p_f m}{2}\Big| f\Big] \\
\leq \;& E_b\left[\frac{2^4\left(mes(A_\gamma) - \widehat{mes}(A_\gamma)\right)^2}{\lambda_f^4 mes^4(A_\gamma)}; \widehat{mes}(A_\gamma) < mes(A_\gamma); \sum I(t_i \in A_\gamma) > \frac{p_f m}{2} \;\Big|\; f\right] \\
\leq \;& \frac{2^4 \kappa_f \zeta^{-2d}}{m\lambda_f^4 mes^4(A_\gamma)}.
\end{aligned}$$

Step 3. We combine the previous analysis and have that

$$\mathbb{E}_b(J_2^2|f) \leq \frac{2^4\zeta^{-2d}}{mes^4(A_\gamma)}\frac{\kappa_1^2}{k^2(t_f)m} + \frac{\kappa_f \zeta^{-2d}}{m \times mes^4(A_\gamma)} + k(t_f)^{-2} m^2 \zeta^{2d} e^{-\varepsilon_0 m p_f}. \tag{2.64}$$

The density $k(t)$ has a heavy tail that is $k(t) \sim \frac{1}{|t|^{d+\varepsilon_1}}$ and $k(t) \leq \kappa_1$ for all t. In Step 3, we provide a bound on the distributions of t_f and p_f.

We start with t_f. For each $s > 0$, $t_f > s$ if and only if $\sup_{|t-\tau|>s} g(t) > -1$. According to the results in Lemmas 2 and 3, for s sufficiently large, there exists some $\varepsilon_0 > 0$ such that

$$Q_b(t_f > s) = Q_b(\sup_{|t-\tau|>s} g(t) > -1) \leq \exp\{-s^{\varepsilon_0}\}, \qquad \text{for } s < \delta'\zeta \tag{2.65}$$

and

$$Q_b(t_f > s) \leq \exp(-\varepsilon_0 b^2), \qquad \text{for } s > \delta'\zeta.$$

Therefore, all moments of $k^{-1}(t_f)$ is bounded.

$$E_b[k^{-l}(t_f)] \leq E_b[t_f^{(d+\varepsilon_1)l}] \leq \kappa_l$$

for some constant κ_l possibly depending on l. Thus, by Cauchy-Schwarz inequality, the expectation of the first two terms in (2.64) can be bounded as follows

$$\begin{aligned}\mathbb{E}\Big[\frac{2^4\zeta^{-2d}}{mes^4(A_\gamma)}\frac{\kappa_1^2}{k^2(t_f)m}; M > b\Big] &\leq \frac{O(1)}{m}\sqrt{\mathbb{E}\Big[\frac{\zeta^{-4d}}{mes^8(A_\gamma)}\Big]\mathbb{E}(k^{-4}(t_f))} \leq \frac{\kappa\zeta^{2d}}{m} \\ \mathbb{E}\Big[\frac{\kappa_f\zeta^{-2d}}{m\times mes^4(A_\gamma)}\Big] &\leq \frac{O(1)}{m}\sqrt{\mathbb{E}\Big[\frac{\zeta^{-4d}}{mes^8(A_\gamma)}\Big]\mathbb{E}(k^{-4}(t_f))} \leq \frac{\kappa\zeta^{2d}}{m}.\end{aligned}$$

We now proceed to the third term in (2.64) concerning p_f. The expectation of this term is bounded by

$$\mathbb{E}_b(m^2k(t_f)^{-2}e^{-m\varepsilon_0 p_f}; M > b) \leq \sqrt{E_b(m^4e^{-2m\varepsilon_0 p_f}; M > b)}\sqrt{E_b(k^{-4}(t_f))}.$$

The second term $\sqrt{E_b(k^{-4}(t_f))}$ is $O(1)$. We proceed to the first term

$$\begin{aligned}\mathbb{E}_b(m^4e^{-2m\varepsilon_0 p_f}; M > b) &= E_b(m^4e^{-2m\varepsilon_0 p_f}; p_f \geq m^{-1/2}) \\ &\quad + E_b(m^4e^{-2m\varepsilon_0 p_f}; p_f \leq m^{-1/2}, M > b) \\ &\leq m^4e^{-2\varepsilon_0\sqrt{m}} + m^4Q_b(p_f \leq m^{-1/2}, M > b).\end{aligned}$$

We now proceeding to controlling $Q_b(p_f \leq m^{-1/2}, M > b)$. Note that $p_f \geq k(t_f)mes(A^g_{-1})$. For each $x > 0$,

$$\begin{aligned}Q_b(p_f < x, M > b) &\leq Q_b\Big(k(t_f) < \sqrt{x} \quad \text{or} \quad mes(A^g_{-1}) < \sqrt{x}, M > b\Big) \\ &\leq Q_b(t_f > x^{-\frac{1}{2(d+\varepsilon_1)}}) + Q_b(mes(A^g_{-1}) < \sqrt{x}, M > b).\end{aligned}$$

According to the bounds in (2.44), for some $\delta_0 > 0$ and $\varepsilon_0 > 0$, we have that

$$Q_b(mes(A^g_{-1}) < \sqrt{x}, M > b) = Q_b(mes(A_\gamma) < \zeta^{-d}\sqrt{x}, M > b) \leq e^{-x^{-\varepsilon_0/d}}$$

for x sufficiently small. According to the previous result, we have that

$$Q_b(t_f > x^{-\frac{1}{2(d+\varepsilon_1)}}) \leq e^{-x^{-\varepsilon_0}}, \quad \text{for } x^{-\frac{1}{2(d+\varepsilon_1)}} < \delta'\zeta$$

and

$$Q_b(t_f > x^{-\frac{1}{2(d+\varepsilon_1)}}) \leq e^{-\varepsilon_0 b^2}, \quad \text{for } x^{-\frac{1}{2(d+\varepsilon_1)}} \geq \delta'\zeta.$$

Thus, for some λ large enough and ε_0 small enough, we have that

$$Q_b(p_f \leq m^{-1/2}, M > b) \leq e^{-m^{\varepsilon_0}}, \quad \text{for } m < b^{\lambda};$$

for $m > b^{\lambda}$ (with λ sufficiently large), $t_f > m^{\frac{1}{4(d+\varepsilon_1)}}$ implies that $\tau + t_f/\zeta \notin T$, that is, $m^{\frac{1}{4(d+\varepsilon_1)}}$ is too large and thus

$$Q_b(p_f < m^{-1/2}) = 0, \qquad \text{for } m > b^{\lambda}.$$

Therefore, we have $m^4 Q_b(p_f \leq m^{-1/2}, M > b) \leq \kappa m^4 e^{-m^{\varepsilon_0}}$ for m sufficiently large and furthermore

$$E_b(m^4 k(t_f)^{-2} e^{-m\varepsilon_0 p_f}; M > b) \leq \kappa m^4 e^{-m^{\varepsilon_0}/2}.$$

Summarizing the results in all the three steps, we have that $E_b(J_2^2) \leq \frac{\kappa\zeta^{-2d}}{m}$. If we choose $m = \kappa \max\{\varepsilon^{-2}, \varepsilon^{-d(2/\alpha+1/\beta_1+3\varepsilon_0)}\} = O(\varepsilon^{-d(2/\alpha+2/\beta_1)})$, then

$$E_b|\hat{Z}_b - Z_b| = E_b|J_1 + J_2| \int_T \mathbb{P}(f(t) > \gamma)dt \leq \varepsilon\zeta^d \int_T \mathbb{P}(f(t) > \gamma)dt$$

and

$$E_b(\hat{Z}_b - Z_b)^2 \leq \kappa\zeta^{2d}\Big(\int_T \mathbb{P}(f(t) > \gamma)dt\Big)^2.$$

2.7 Appendix to Chapter 2

2.7.1 Efficient simulation and efficient discretization for conditional expectations

In this section, we develop an efficient algorithm to compute conditional expectations given a high excursion

$$v(b) \triangleq \mathbb{E}(\Gamma(f)|M > b) \tag{2.66}$$

in the asymptotic regime that b tends to infinity, where $\Gamma(\cdot)$ is a functional (possibly a random functional) mapping from the space of continuous functions to the real line.

It turns out that the computations of $w(b)$ and $v(b)$ are closely related, which will be discussed in details later in this section. We define integral

$$\alpha(b) = \int_{A_b} \xi(t)dt. \tag{2.67}$$

where $\xi(t)$ is another random field living on T and A_b is the excursion set $\{t \in T : f(t) > b\}$. Then we are interested in computing conditional expectation

$$v(b) = \mathbb{E}(\alpha(b)|M > b).$$

In Section 2.2.2.2, we introduced importance sampling for the probability of a family of rare event $\{B_b : b \geq b_0\}$ for which $0 < \mathbb{P}(B_b) \to 0$. We now describe briefly how an efficient importance sampling estimator for $\mathbb{P}(B_b)$ can also be used to estimate a large class of conditional expectations given B_b. Suppose that an importance sampling estimator has been constructed

$$Z_b \ \triangleq\ I(\omega \in B_b)\frac{d\mathbb{P}}{dQ},$$

such that $Var\left(Z_b\right) = O\left(\mathbb{P}(B_b)^2\right)$. Then, by noting that

$$\frac{\mathbb{E}^Q\left(XZ_b\right)}{\mathbb{E}^Q\left(Z_b\right)} = \frac{\mathbb{E}[X; B_b]}{\mathbb{P}(B_b)} = \mathbb{E}[X|\, B_b], \tag{2.68}$$

it follows easily that an estimator can be naturally obtained; i.e. the ratio of the corresponding averaged importance sampling estimators suggested by the ratio in the left of (2.68). Of course, when X is difficult to simulate exactly, one must assume that the bias in estimating $\mathbb{E}[X; B_b]$ can be reduced with certain computational costs.

Similar to (2.16), a natural estimator for the numerator $\mathbb{E}(\alpha(b); M > b)$ in (2.68) is

$$Y_b \triangleq \frac{\alpha(b)}{mes(A_\gamma)} \int_T \mathbb{P}(f(t) > \gamma) dt, \tag{2.69}$$

which, under regularity conditions, will be shown to estimate $\mathbb{E}(\alpha(b); M > b)$ with strong efficiency.

For the discrete version of the estimator Y_b as in (2.69), we approximate it in the same way as in Algorithm 2 except for Step 4. In Step 4 of Algorithm 2, we simulate $\{(f(t_i), \xi(t_i)) : i = 1, ..., m\}$ jointly conditional on $(\tau, f(\tau))$. Then, we output the estimator

$$\hat{Y}_b = \frac{\hat{\alpha}(A_b)}{\widehat{mes}(A_\gamma)} \int_T \mathbb{P}(f(t) > \gamma) dt$$

where

$$\hat{\alpha}(A_b) \triangleq \frac{1}{m} \sum_{i=1}^{m} \frac{\xi(t_i)}{k_{\tau,\zeta}(t_i)} I(f(t_i) > b). \tag{2.70}$$

Theorem 3. *Consider a Gaussian random field f that satisfies Conditions A1-6. There exists $0 < a_1 < a_2 < \infty$, such that $\xi(t) \in [a_1, a_2]$ almost surely. We have the following results*

1. *Then, there exists κ_0 such that for all $b > 0$*

   $$\mathbb{E}_b(Y_b^2) \le \kappa_0 u^2(b)$$

   where $u(b) = \mathbb{E}(\alpha(b); M > b)$.

2. *There exists λ such that for each $\varepsilon > 0$ if we choose $m = \lambda \varepsilon^{-d(2/\min(\alpha_1,\alpha_2)+2/\beta_1)}$ then*

   $$|E_b(\hat{Y}_b) - u(b)| \le \varepsilon u(b)$$

   and

   $$E_b(\hat{Y}_b^2) \le \kappa_0 u^2(b).$$

In the previous theorem, we require that the process $\xi(t)$ take values in a positive interval $[a_1, a_2]$. This constraint is imposed for technical convenience. There are several ways in which we can relax this condition. If $\xi(t)$ is independent of $f(t)$, then, we can relax the interval to be $(0, \infty)$. In the case when $\xi(t) \in (0, \infty)$ and $\xi(t)$ and $f(t)$ are dependent, we may need to modify the algorithm. This is because $\xi(t)$ could be very close to zero on the excursion set A_b and therefore the estimator (2.70) may not be strongly efficient in estimating $\alpha(t)$. In this case, we may further change the sampling distribution of $\{(f(t_i), \xi(t_i)) : i = 1, ..., m\}$ to reduce the variance of $\hat{\alpha}(t)$. These modifications have to be case-by-case and they can be handled by routine variance reduction techniques that we do not pursue in this chapter.

2.7.2 Proof of Theorem 3

2.7.2.1 The asymptotic lower bound and the continuous estimator

We start the analysis by first establishing an asymptotic lower bound of $v(b)$. Note that

$$v(b) = \mathbb{E}(mes(A_\gamma))E_b\left[\frac{1}{mes(A_\gamma)}\int_{A_b}\xi(t)dt\right].$$

Since $\xi(t)$ is bounded by a_2, then $v(b) \leq a_2\mathbb{E}(mes(A_\gamma))$. In addition, a lower bound can be given by

$$\mathbb{E}\Big(\int_{A_b}\xi(t)dt\Big) \geq a_1\mathbb{E}(mes(A_b))$$

Thus

$$v(b) = \Theta(1)\mathbb{E}(mes(A_\gamma)).$$

The second moment of the estimator is

$$\mathbb{E}_b(Y_b^2) = \mathbb{E}^2(mes(A_\gamma))E_b\left[\frac{\alpha^2(b)}{mes^2(A_\gamma)}; M > b\right] \leq a_2^2\mathbb{E}^2(mes(A_\gamma)) \leq \frac{a_2^2}{a_1^2}v(b).$$

2.7.2.2 Analysis of the discrete estimator

We start the analysis by the following decomposition

$$\begin{aligned}
\hat{Y}_b - Y_b &= \left[\frac{\alpha(b)}{mes(A_\gamma)} I(\sup f(t) > b) - \frac{\hat{\alpha}(b)}{\widehat{mes}(A_\gamma)} I(\max_{i=1}^{m} f(t_i) > b)\right] \mathbb{E}(mes(A_\gamma)) \\
&= \mathbb{E}(mes(A_\gamma)) \\
&\quad \times \Big[\frac{\alpha(b) I(\sup f(t) > b)}{mes(A_\gamma)} - \frac{\alpha(b) I(\max_{i=1}^{m} f(t_i) > b)}{mes(A_\gamma)} \\
&\quad + \frac{\alpha(b) I(\max_{i=1}^{m} f(t_i) > b)}{mes(A_\gamma)} - \frac{\hat{\alpha}(b) I(\max_{i=1}^{m} f(t_i) > b)}{\widehat{mes}(A_\gamma)}\Big].
\end{aligned}$$

We redefine the terms

$$\begin{aligned}
J_1 &= \frac{\alpha(b) I(\sup f(t) > b)}{mes(A_\gamma)} - \frac{\alpha(b) I(\max_{i=1}^{m} f(t_i) > b)}{mes(A_\gamma)} \\
J_2 &= \frac{\alpha(b) I(\max_{i=1}^{m} f(t_i) > b)}{mes(A_\gamma)} - \frac{\hat{\alpha}(b) I(\max_{i=1}^{m} f(t_i) > b)}{\widehat{mes}(A_\gamma)}.
\end{aligned}$$

Note that the factor $\alpha(b)/mes(A_\gamma)$ is bounded by a_2, so we have

$$\mathbb{E}_b|J_1| \leq a_2 Q_b(\sup f(t) > b, \max_{i=1}^{m} f(t_i) > b),\ E_b(J_1^2) \leq a_2^2 Q_b(\sup f(t) > b, \max_{i=1}^{m} f(t_i) > b)$$

According to the previous analysis, for each ε, there exists an $m = O(\varepsilon^{-d(2/\alpha + 1/\beta_1) - \varepsilon_0})$ such that

$$\mathbb{E}_b(|J_1| \ \mid f) \leq a_2 \varepsilon, \quad E_b(J_1^2 | f) = a_2^2 \varepsilon.$$

For the second term, we apply similar analysis as the proof for Theorem 2. Note that $\alpha(b) \leq a_2 mes(A_\gamma)$, so by rearranging terms in J_2, we have

$$|J_2| \leq \left[\frac{|\alpha(b) - \hat{\alpha}(b)|}{mes(A_\gamma)} + a_2 \frac{|mes(A_\gamma) - \widehat{mes}(A_\gamma)|}{mes(A_\gamma)}\right] I(M > b).$$

Because $\hat{\alpha}(b)$ is an unbiased estimator for $\alpha(b)$ conditional on f, we have

$$\mathbb{E}_b\Big[(\hat{\alpha}(b) - \alpha(b))^2 | f\Big] \leq m^{-1} a_2^2 k^{-2}(t_f) \zeta^{-2d}.$$

Thus,

$$\begin{aligned}
& E_b\Big[(\hat{a}(b) - \alpha(b))^2 + a_2(mes(A_\gamma) - \widehat{mes}(A_\gamma))^2 \Big| f\Big] \\
\leq\ & 2E_b\Big[(\hat{\alpha}(b) - \alpha(b))^2 | f\Big] + 2a_2^2 E_b\Big[(mes(A_\gamma) - \widehat{mes}(A_\gamma)) | f\Big] \\
\leq\ & 4a_2^2 m^{-1} k^{-2}(t_f) \zeta^{-2d}.
\end{aligned}$$

Therefore,

$$\begin{aligned} \mathbb{E}_b\Big(|J_2|^2|f\Big) &\leq \frac{4a_2^2}{\lambda_f^2 mes(A_\gamma)^2\zeta^{2d}mk^2(t_f)} \\ \mathbb{E}_b\Big(|J_2||f\Big) &\leq \frac{2a_2}{\lambda_f mes(A_\gamma)\zeta^d\sqrt{m}k(t_f)} \end{aligned}$$

According the proof in Section 2.6, there exists a $\kappa > 0$ such that

$$\mathbb{E}(|J_2|) \leq \frac{\kappa}{\sqrt{m}}.$$

With a similar argument, we have that

$$\mathbb{E}(J_2^2) \leq \kappa.$$

Summarizing the result for J_1 and J_2, we can choose
$m = O(\max(\varepsilon^{-d(2/\alpha+1/\beta_1+\varepsilon_0)}, \varepsilon^{-2})) = O(\varepsilon^{-d(2/\alpha+2/\beta_1)})$, such that

$$\mathbb{E}_b(\hat{Y}_b - v(b)) \leq \varepsilon v(b), \qquad Var(\hat{Y}_b) = O(1).$$

2.7.3 Proof of Theorem 1 when $\sigma(t)$ is of Type 2 in Assumption A4

In our proof for Type 2 standard deviation, we use similar methods as that for Type 1. We are going to establish similar results as in (2.44) and Lemmas 2 and 3 hold for Gaussian random field with type 2 standard deviation. To proceed, we provide some bounds on the distribution of τ. The next lemma suggests that τ is close to

$$t^* = \arg\sup_{t\in T}\sigma(t).$$

Lemma 4. *There exists constants $\delta,\ \varepsilon_0 > 0$ small enough and $\kappa > 0$ large enough (but independent of b), such that for $x > \kappa$ the following bounds hold*

(i) $\int_{|t-t^*|\leq\zeta_2^{-1}} h_b(t)dt > \varepsilon_0$,

(ii) $\int_{\delta>|t-t^*|>x\zeta_2^{-1}} h_b(t)dt < \exp(-x^{\alpha_2/2})$,

(iii) $\int_{|t-t^*|>\delta} h_b(t)dt < \exp(-\varepsilon_0 b^2)$.

To continue the analysis of I_2 and I_1, we discuss two different scenarios:

1. $\alpha_1 > \alpha_2$, or $\alpha_1 = \alpha_2$ and $\lim_{x\to 0} \frac{L_1(x)}{L_2(x)} \in \{0,1\}$; that is, as $x \to 0$, $L_1(x)x^{\alpha_1} \leq (1+o(1))L_2(x)x^{\alpha_2}$.

2. $\alpha_1 < \alpha_2$, or $\alpha_1 = \alpha_2$ and $\lim_{x\to 0} \frac{L_1(x)}{L_2(x)} = \infty$; that is, as $x \to 0$, $L_2(x)x^{\alpha_2} = o(1)L_1(x)x^{\alpha_1}$.

The proof of this lemma is provided in the Supplemental Material B.

2.7.4 Proof for scenario 1: $\alpha_1 > \alpha_2$, or $\alpha_1 = \alpha_2$ and $\lim_{x\to 0} \frac{L_1(x)}{L_2(x)} \in \{0,1\}$.

For the proof of this scenario, the variation of $\sigma(t)$ is the dominating term. According to A2, there exists a constant Δ such that

$$1 - r(s,t) \leq \Delta L_2(|s-t|)|s-t|^{\alpha_2} \tag{2.71}$$

In addition, we can further replace the slowly varying function L_1 in (2.6) by L_2 and the inequality still holds, that is,

$$|r(t,t+s_1) - r(t,t+s_2)| \leq \kappa_r \max(L_2(|s_1|)|s_1|^{\beta_0}, L_2(|s_2|)|s_2|^{\beta_0})|s_1-s_2|^{\beta_1}. \tag{2.72}$$

For the proof of this scenario, we work under the above two inequalities instead of A2. The proof follows a similar idea as that of the constant variance case by providing bounds for I_2 and I_1.

The I_2 term. For a given τ and z, we adopt a similar conditional representation as in (2.26). We start with establishing similar results as in Lemma 1. Since $L_1(x)x^{\alpha_1} \leq (1+o(1))L_2(x)x^{\alpha_2}$, we can replace α_1 and L_1 in the statement of Lemma 1 by α_2 and

L_2 and the statement still holds. Now we proceed to prove (2.44).According to the expression (2.29), we proceed by deriving an upper bound of

$$\int_T \mathbb{P}\left(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_2^{-1}, M > b | f(\tau) = \gamma + \frac{z}{b}\right) h_b(\tau) \frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz, \qquad (2.73)$$

for y small enough. We discuss two situation: $z > 1$ and $0 < z \leq 1$.

Situation 1: $z > 1$**.** From condition A2, A4, A5, (2.72) and Lemma 5(i), for $|t| < c_d y \zeta_2^{-1}$, we have that

$$|\mu_\tau(t) - \mu_\tau(0)| \leq \kappa_\mu \sqrt{L_2(|t|)}|t|^{\alpha_2/2} + \kappa b L_2(|t|)|t|^{\alpha_2} = O(y^{\alpha_2/4} b^{-1})$$

Note that $\mu_\tau(0) = \gamma + z/b > \gamma + 1/b$. Thus, by picking y_0 small enough, we have that

$$\mu_\tau(t) \geq \gamma + \frac{1}{2b} \qquad \text{for } |t| \leq c_d y \zeta_2^{-1}.$$

With a similar development as in (2.30) and the conditional variance calculation for $f_0(t)$ as in (2.34), that is,

$$C_0(t,t) = O(y^{\alpha_2/2} b^{-2}),$$

we conclude that for some small $\varepsilon_0 > 0$

$$\begin{aligned} Q_b\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_2^{-1}, M > b\Big) &\leq \mathbb{P}\Big(\inf_{|t| \leq c_d y \zeta_2^{-1}} (f_0(t) + \mu_\tau(t)) \leq \gamma\Big) \\ &\leq \mathbb{P}(\inf_{|t| \leq c_d y \zeta_2^{-1}} |f_0(t)| > \frac{1}{2b}) \\ &\leq \exp(-y^{-\varepsilon_0}). \end{aligned}$$

Situation 2: $0 < z \leq 1$**.** For $0 < z < 1$, we choose δ_0, δ_1 to be small enough and λ to be large enough and develop bounds for the above probability under four cases (same as in the proof of constant variance case):

Case 1. $t \in C_1 \triangleq \{t : 0 < |t - \tau| < y^{-\delta_0}\zeta_2^{-1}\}$,

Case 2. $t \in C_2 \triangleq \{t : y^{-\delta_0}\zeta_2^{-1} < |t - \tau| < \delta_1\}$, Case 3. $t \in C_3 \triangleq \{t : |t-\tau| \geq \delta_1\}$ and $y < b^{-\lambda}$,

Case 4. $t \in C_3$ and $y \geq b^{-\lambda}$.

With these notation, we have the following bound

$$
\begin{aligned}
& Q_b\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_2^{-1}, M > b\Big) \\
\leq \ & \sum_{i=1}^{3}\int_T \mathbb{P}\left(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta^d, \sup_{t\in C_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\right) h_b(\tau)\frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz.
\end{aligned}
$$

With the same argument for (2.36), each of the summands on the right-hand-side is further bounded by

$$
\begin{aligned}
& \int_T \mathbb{P}\left(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_2^d, \sup_{t\in C_i} f(t) > b \Big| f(\tau) = \gamma + \frac{z}{b}\right) h_b(\tau)\frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz \\
\leq \ & \int_T \mathbb{P}\Big(\sup_{t\in C_i, |s-t|\leq c_d y\zeta_2^{-1}} |f(t) - f(s)| > \frac{1}{b}, \sup_{t\in C_i} f(t) > b \Big| f(\tau) = \gamma + \frac{z}{b}\Big) \\
& \times h_b(\tau)\frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz. \qquad (2.74)
\end{aligned}
$$

Similarly, we define

$$
x_i \triangleq \zeta_2 \times |t_i - \tau|.
$$

Case 1: $0 < |t-\tau| < y^{-\delta_0}\zeta_2^{-1}$. We adopt the same lattice and cover sets, $\tilde{T}$, and B_i, defined on page 29 for the proof of the constant variance case, with ζ_1 replaced by ζ_2. For this case, we bound the right-hand-side of (2.74) by

$$
\sum_{B_i\cap C_1\neq\emptyset}\int_T \mathbb{P}\Big(\sup_{t\in B_i, |s-t|\leq c_d y\zeta_2^{-1}} |f(t) - f(s)| > \frac{1}{b}\Big| f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau)\frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz
$$

and take advantage of the conditional representation $f(t) = \mu_\tau(t) + f_0(t)$. We proceed to investigating the variation of $\mu_\tau(t)$ and $f_0(t)$. For $f_0(t)$ and $|s-t| \leq c_d y\zeta_2^{-1}$, with the same argument as in (2.38), we have that $Var(f_0(t) - f_0(s)) \leq \kappa y^{\alpha_2/2}b^{-2}$. For the conditional mean, by means of the representation (2.27),

$$
\begin{aligned}
|\mu_\tau(t) - \mu_\tau(s)| \ \leq \ & \kappa\zeta_2^{-\alpha_2/2}\sqrt{L_2(y/\zeta_2)}y^{\alpha_2/2} \\
& +\kappa b L_2(c_d y/\zeta_2)y^{\alpha_2}\zeta_2^{-\alpha_2} + \kappa(x_i+1)^{\beta_0} b L_2((x_i+1)/\zeta_2)y^{\beta_1}\zeta_2^{-\alpha_2} \\
\leq \ & \kappa b^{-1}y^{\varepsilon_0}
\end{aligned}
$$

for some small positive constant ε_0. Now we pick y_0 small enough. For $0 < y < y_0$ and $|\mu_\tau(t) - \mu_\tau(s)| < \frac{1}{2b}$, together with the variance control of $f_0(t) - f_0(s)$, we have that

$$\begin{aligned}
&\int_T \mathbb{P}\Big(\sup_{t\in B_i, |s-t|\leq c_d y \zeta_2^{-1}} |f(t) - f(s)| > \frac{1}{b} \Big| f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau) d\tau \\
&\qquad \leq \int_T \mathbb{P}\Big(\sup_{t\in B_i, |s-t|\leq c_d y \zeta_2^{-1}} |f_0(t) - f_0(s)| > \frac{1}{2b} \Big| f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau) d\tau \\
&\qquad \leq \exp(-y^{-\varepsilon_0})
\end{aligned}$$

for some $\varepsilon_0 > 0$. We sum up all the B_i's such that $0 < |t_i - \tau| < y^{-\delta_0}\zeta_2^{-1}$ and obtain that

$$\mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_1^d, \sup_{t\in C_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \leq \exp(-y^{-\varepsilon_0})$$

for which we may need to choose a smaller ε_0.

Case 2: $y^{-\delta_0}\zeta_2^{-1} < |t-\tau| < \delta_1$. We split (2.74) as follows

$$\begin{aligned}
(2.74) \quad \leq \quad & \sum_{B_i \cap C_2 \neq \emptyset} \int_{|\tau - t^*| \leq \frac{1}{3} y^{-\delta_0}\zeta_2^{-1}} \mathbb{P}\Big(\sup_{t\in B_i} f(t) > b \Big| f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau) d\tau \\
& + \int_{|\tau - t^*| > \frac{1}{3} y^{-\delta_0}\zeta_2^{-1}} h_b(\tau) d\tau. \qquad (2.75)
\end{aligned}$$

For this case, we implicitly requires that $y^{-\delta_0} < \delta_1 \zeta_2$. Thus, Lemma 4 (ii) and (iii) provide an upper bound of the second term in the above display

$$\int_{|\tau - t^*| > \frac{1}{3} y^{-\delta_0}\zeta_2^{-1}} h_b(\tau) d\tau \leq \exp(-y^{-\varepsilon_0})$$

for ε_0 and y sufficiently small and $y^{-\delta_0} < \delta_1\zeta_2$.

For the first term on the right-hand-side of (2.75), we bound it in a similar way as in constant variance case. In particular, each summand is bounded by

$$\sup_{|\tau - t^*| \leq \frac{1}{3} y^{-\delta_0}\zeta_2^{-1}} \mathbb{P}(\sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b})$$

For $y^{-\delta_0}\zeta_2^{-1} < |t-\tau| < \delta_1$ and $|\tau - t^*| \leq \frac{1}{3}y^{-\delta_0}\zeta_2^{-1}$ we have that $|t-t^*| > \frac{2}{3}y^{-\delta_0}\zeta_2^{-1}$. Using the expansion $\sigma(t^*) - \sigma(t) \sim \Lambda L_2(|t-t^*|)|t-t^*|^{\alpha_2}$, we have that

$$\frac{\sigma(t)}{\sigma(\tau)} \leq 1 - \varepsilon_0 \frac{L_2(x_i\zeta_2^{-1})}{L_2(\zeta_2^{-1})}\frac{(\zeta_2|t_i-\tau|)^{\alpha_2}}{b^2}, \quad \text{for some small } \varepsilon_0 > 0 \text{ and } . \tag{2.76}$$

From the expression of (2.27) and the inequality (2.76), for $t \in B_i \cap C_2 \neq \emptyset$ and $x_i = \zeta_2|t_i - \tau|$, we have that

$$\mu_\tau(t) \leq b + \kappa\sqrt{\frac{L_2(x_i\zeta_2^{-1})}{L_2(\zeta_2^{-1})}}\frac{x_i^{\alpha_2/2}}{b} - \varepsilon_0\frac{L_2(x_i\zeta_2^{-1})}{L_2(\zeta_2^{-1})}\frac{x_i^{\alpha_2}}{b} \leq b - \frac{\varepsilon_0}{2}x_i^{\alpha_2}\frac{L_2(x_i\zeta_2^{-1})}{L_2(\zeta_2^{-1})}b^{-1}.$$

Furthermore, Lemma 1(i) implies that

$$Var(f_0(t)) = C_0(t,t) \leq 2\lambda_2\frac{L_2(x_i\zeta_1^{-1})}{L_2(\zeta_1^{-1})}x_i^{\alpha_2}b^{-2}. \tag{2.77}$$

Thus, the Borel-TIS inequality suggests that

$$\sup_{|\tau-t^*|\leq\frac{1}{3}y^{-\delta_0}\zeta_2^{-1}} \mathbb{P}(\sup_{t\in B_i} f(t) > b | f(\tau) = \gamma + \frac{z}{b}) \leq \exp(-x_i^{-\varepsilon_0}),$$

for some small constant ε_0.

Combining the upper bound for the two term on the right side of (2.75), and putting together all B_i's such that $y^{-\delta_0} < x_i < \delta_1$, we have that

$$\begin{aligned}
&\int_T \mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_2^d, \sup_{t\in C_2} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau)\frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz \\
\leq\ & \exp(-y^{-\varepsilon_0}) + \sum_{k=0}^{\infty}\kappa(y^{-\delta_0}+k)^{d-1}\exp(-(y^{-\delta_0}+k)^{\varepsilon_0}) \\
\leq\ & \exp(-y^{-\varepsilon_0/2})
\end{aligned}$$

for some large constant $\kappa > 0$ and possible a different choice of ε_0.

Case 3: $|t-\tau| \geq \delta_1$ **and** $y < b^{-\lambda}$**.** The analysis is completely analogous to the Case 3 on Page 32. The only difference is that the variance function $\sigma^2(t)$ is non-constant. Given that $\sigma(t)$ is Hölder continuous, all the calculations remain. Therefore, we omit the details and directly reach the bound that

$$\int_T \mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta^d, \sup_{|t-\tau|>\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau) \frac{q_{b,\tau}(\gamma + z/b)}{b} d\tau dz$$
$$\leq \exp(-y^{-\varepsilon_0})$$

for all $y < b^{-\lambda}$.

Case 4: $|t-\tau| \geq \delta_1, y \geq b^{-\lambda}$. We split the bound (2.74) into two parts.

$$\begin{aligned} &\int_T \mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta^d, \sup_{|t-\tau|>\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) h_b(\tau) d\tau \\ \leq\ & \sup_{|\tau-t^*|\leq\delta_1/3} \mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta^d, \sup_{|t-\tau|>\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\ & + \int_{|\tau-t^*|>\delta_1/3} h_b(\tau) d\tau. \end{aligned} \tag{2.78}$$

From Lemma 4 (iii), the second term on the right side of last inequality can be bound by $\exp(-b^{\varepsilon_0})$ for some $\varepsilon_0 > 0$. Note that in Case 4, $y > b^{-\lambda}$, so this expression can be further bounded by

$$\int_{|\tau-t^*|>\delta_1/3} h_b(\tau) d\tau \leq \exp(-\varepsilon_0 b^2) \leq \exp(-y^{-\varepsilon_0/\lambda}).$$

Now we consider the first term on the right side of (2.78). On the set $|\tau - t^*| < \delta_1/3$ and $|t-\tau| > \delta_1$, there exists some ε_0 such that the conditional mean can be bounded from below by

$$\mu_\tau(t) \leq (1 - \frac{\varepsilon_0}{2}) b. \tag{2.79}$$

This is because from condition A4, $\sigma(\tau) \geq \sigma(t^*) - \Lambda L(\delta_1/3)(\delta_1/3)^\alpha$, for $|\tau - t^*| \leq 1/3\delta_1$; while $\sigma(t) \leq \sigma(t^*) - \Lambda L(2\delta_1/3)(2\delta_1/3)^{\alpha_2}$, for $|t-t^*| \geq 2\delta_1/3$. As a result, there exists a constant $\varepsilon_0 > 0$ such that $\frac{\sigma(t)}{\sigma(\tau)} \leq 1 - \varepsilon_0$. In addition, the correlation function also drops.

For the rest of case 4, we follow the same analysis as that of Case 4 on page 32 and derive an upper bound for the first term on the right side of (2.78).

$$\begin{aligned}
&\mathbb{P}\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta^d, \sup_{|t-\tau|\geq\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\
\leq\ & \mathbb{P}\Big(\sup_{|t-\tau|\geq\delta_1} f(t) > b | f(\tau) = \gamma + \frac{z}{b}\Big) \\
\leq\ & \mathbb{P}\Big(\sup_{|t-\tau|\geq\delta_1} f_0(t) + \mu_\tau(t) > b\Big) \\
\leq\ & \mathbb{P}\Big(\sup_{|t-\tau|\geq\delta_1} f_0(t) > \varepsilon_0 b/2\Big) \\
\leq\ & \exp(-\frac{\varepsilon_0^2}{8\sigma_T^2} b^2) \qquad (2.80) \\
\leq\ & \exp(-y^{-\varepsilon_0'}).
\end{aligned}$$

for some $\varepsilon_0, \varepsilon_0' > 0$. Combining our result for the first and second term of (2.78), and for $C_i = C_3$ for $y \geq b^{-\lambda}$

$$(2.74) \leq \exp(-y^{-\varepsilon_0}), \qquad \text{for some possibly smaller } \varepsilon_0 > 0.$$

Summary of the analysis for I_2. Putting all the results in Cases 1-4 together, we have that there exists a $y_0 > 0$ such that

$$Q_b\Big(\frac{1}{mes(A_\gamma)} > y^{-d}\zeta_2^{-1}, M > b\Big) \leq \exp(-y^{-\varepsilon_0}), \tag{2.81}$$

for $0 < y < y_0$. Thus, for some $\kappa > 0$, we have

$$I_2 = \mathbb{E}^{Q_b}\Big(\frac{1}{mes(A_\gamma)^2}; M > b\Big) \leq (\kappa + y_0^{-d})\zeta_2{}^{2d}.$$

The I_1 term. We are going to derive a lower bound for I_1 by showing that Lemma 2 and Lemma 3 are valid. Following the same calculation for (2.78), we reach the result of Lemma 2 (on page 33) that

$$Q_b(\sup_{|t-\tau|\geq\delta'} f(t) \geq \gamma) \leq Q_b(|t^* - \tau| \geq \delta'/3) + Q_b(\sup_{|t-\tau|\geq\delta'} f(t) \geq \gamma, |t^* - \tau| < \delta'/3)$$

The first term on the right-hand-side is controlled by Lemma 4 (iii). The second term can be bounded by a similar analysis as in (2.80). Thus, we have that

$$Q_b(\sup_{|t-\tau|\geq\delta'} f(t) \geq \gamma) \leq e^{-\varepsilon_0 b^2} \tag{2.82}$$

for some ε_0 small.

Now, we proceed to proving a similar result as in Lemma 3 (page 34). Note that for $x{\zeta_2}^{-1} < \delta'$

$$
\begin{aligned}
Q_b\Big(\sup_{x{\zeta_2}^{-1}\le|t-\tau|\le\delta'} f(t)\ge\gamma\Big) \;&\le\; Q_b\Big(\sup_{x{\zeta_2}^{-1}\le|t-\tau|\le\delta'} f(t)\ge\gamma, |\tau-t^*|<x\zeta_2^{-1}/3\Big)\\
&\quad + Q_b\Big(|\tau-t^*|>x\zeta_2^{-1}/3\Big).
\end{aligned}
$$

Thanks to Lemma 4, the second term on the right-hand-side is bounded by $e^{-x^{\varepsilon_0}}$. For the first term, we follow a similar analysis as in Lemma 3. In particular, we can establish a bound for the conditional mean $\mu_\tau(t) = \mathbb{E}(f(\tau+t)|\tau, z)$ in the following form

$$
\mu_\tau(t) \le \gamma + \frac{z}{b} - \varepsilon_0\frac{x^{\alpha_2}}{b}
$$

for all $x\zeta_2^{-1} < |t| < \delta'$ and $|\tau - t^*| < x\zeta_2^{-1}/3$. With this bound, we follow exactly the same analysis as in Lemma 3 and obtain that

$$
Q_b\Big(\sup_{x{\zeta_2}^{-1}\le|t-\tau|\le\delta'} f(t)\ge\gamma\Big) \le e^{-x^{\alpha_2/4}} \tag{2.83}
$$

and thus a similar result in Lemma 3 has been proved. With these results, we use the same analysis as that in (2.49) and obtain that for some x sufficiently large

$$
I_1 \;\ge\; \varepsilon_0 x^{-d}\zeta_2^d.
$$

Combining our upper bound for I_2 and lower bound for I_1, we conclude the proof for scenario 1.

$$
\sup_b \frac{\mathbb{E}^{Q_b} Z_b^2}{\mathbb{P}^2(M>b)} = \sup_b \frac{I_2}{I_1^2} < \infty.
$$

2.7.4.1 Proof for scenario 2: $\alpha_1 < \alpha_2$, or $\alpha_1 = \alpha_2$ and $\lim_{x\to 0}\frac{L_1(x)}{L_2(x)} = \infty$

In scenario 2, we first consider the covariance function $C(s,t) = cov(f(s), f(t))$. It satisfies the following conditions:

B1 There exists $\beta_0 \ge 0$, $\beta_1 > 0$, such that $\beta_0 + \beta_1 \ge \alpha_1$, and

$$
|C(\tau, t+s_1) - C(\tau, t+s_2)| \le \kappa \max(L_2(|s_1|)|s_1|^{\beta_0}, L_2(|s_2|)|s_2|^{\beta_0})|s_1-s_2|^{\beta_1}
$$

B2 As $|t-s| \to 0$,

$$C(s,s) - C(s,t) \sim \sigma(s)^2 \Delta_s L_1(|s-t|)|s-t|^{\alpha_1}$$

B3 There exists $\varepsilon'', \delta'' > 0$ such that for $|s-t^*| < \delta''$, $|t-s| > 2\delta''$, we have

$$C(s,s) - C(s,t) > \varepsilon''.$$

Therefore, we can basically replicate the analysis in Section 2.5 for the constant mean by replacing the correlation function $r(s,t)$ with the covariance function $C(s,t)$ and all the derivations are exactly the same except for one place. In the analysis of Case 4 (Page 32), for which we need to provide a bound for

$$Q_b\Big(mes(A_\gamma)^{-1} > y^{-d}\zeta_1^d, \sup_{|t-\tau|>\delta_1} f(t) > b\Big).$$

For this part, we need to following the analysis of Case 4 for scenario 1 (page 57). Other analyses are all the same and therefore are omitted.

2.7.5 Proof of Lemmas

Throughout the proof, we use several properties of slowly varying functions. They are stated in the next Lemma.

Lemma 5. *Suppose $L(x), x > 0$ is a positive continuous slowly varying function, then it has the following properties.*

(i) $\forall \beta > 0, \exists \delta_\beta > 0, \kappa_s$, *s.t. for* ζ *satisfying* $\zeta^{-1} < \delta_\beta$, $x \le 1$ *we have*

$$\frac{L(x\zeta^{-1})}{L(\zeta^{-1})} x^\beta \le \kappa_s$$

(ii) $\forall \beta > 0, \exists \delta_\beta > 0, \kappa_s > 0$, *s.t. for* ζ *satisfying* $\zeta^{-1}x < \delta_\beta, x \ge 1$, *we have*

$$\frac{L(\zeta^{-1}x)x^\beta}{L(\zeta^{-1})} \ge \kappa_s^{-1}$$

This lemma is a direct application of Theorem 1.5.3, and Theorem 1.5.4 in Bingham *et al.* [1989]. We now continue to providing proofs of other lemmas.

Proof of Lemma 2. For $|t-\tau| \geq \delta$, according to condition A3, there exits $\varepsilon > 0$, such that $r(t,\tau) < 1-\varepsilon$. For b large enough, and $0 < z < \frac{\varepsilon}{4}b^2$, we have

$$\begin{aligned}\mu_\tau(t) &= \mu(t+\tau) + \frac{r(t+\tau,\tau)}{r(\tau,\tau)}(\gamma + \frac{z}{b} - \mu(\tau)) \\ &\leq 2\mu_T + (1-\varepsilon)(\gamma + \frac{z}{b}) \\ &\leq (1-\varepsilon/2)b\end{aligned}$$

and the conditional variance $C_0(t,t) = C(t+\tau, t+\tau) - C(t+\tau,\tau)^2 C(\tau,\tau)^{-1}$ is bounded by σ_T^2. Then by the Borel-TIS inequality (Proposition 1), we have that

$$\mathbb{P}(\sup_{|t-\tau|\geq\delta} f(t) \geq \gamma | f(\tau) = \gamma + \frac{z}{b}) \leq e^{-\frac{\varepsilon^2}{8\sigma_T^2}b^2} \tag{2.84}$$

Since z is asymptotically exponentially distributed with mean $\sigma(\tau)^2$ and τ is asymptotically uniformly distributed, we have

$$Q_b(\sup_{|t-\tau|>\delta} f(t) \geq \gamma) \leq \sup_{z<\frac{\varepsilon b^2}{4}} \mathbb{P}(\sup_{|t-\tau|\geq\delta} f(t) \geq \gamma | f(\tau) = \gamma + \frac{z}{b}) + Q_b(z > \varepsilon b^2/4) \leq e^{-\varepsilon_0 b^2}.$$

□

Proof of Lemma 3. According to conditional Gaussian calculation, we have that

$$Q_b(b \times (f(\tau) - \gamma) \geq x^{\alpha_1/2}) \leq e^{-\varepsilon_0 x^{\alpha_1/2}}.$$

Therefore, we only need to consider that $f(\tau) = \gamma + \frac{z}{b}$ for $z < x^{\alpha_1/2}$. Let $\tilde{T} = \{t_1, ..., t_N\}$ such that:

1. For $i \neq j$, $i,j \in \{1,...,N\}$, $|t_i - t_j| > \zeta_1^{-1}$
2. For any $t \in T$, there exists $i \in \{1,...,N\}$, such that $|t - t_i| \leq 2\zeta_1^{-1}$.

Furthermore, let $B_i = \{t : |t - t_i| \le 2\zeta_1^{-1}\}$, $i \in \{1, 2, ..., N\}$. First calculate the upper bound for conditional mean and variance. For $k/\zeta_1 \le |t_i - \tau| \le (k+1)/\zeta_1$, $t \in B_i$, and $z < x^{\alpha_1/2}$ according to condition A2 and A5, we have that

$$\begin{aligned}\mu_\tau(t) &\le b + \frac{z}{b} + \kappa_\mu \sqrt{L_1(|t|)}|t|^{\alpha_1/2} - \Delta_\tau b L_1(|t|)|t|^{\alpha_1} \\ &\le b - \frac{\Delta_\tau}{2}\frac{L_1(k\zeta_1^{-1})}{L_1(\zeta_1^{-1})}k^{\alpha_1}b^{-1}. \qquad (2.85)\end{aligned}$$

For the conditional variance, by Lemma 1(i), when $t \in B_i$ and k large enough, we have

$$\begin{aligned}C_0(t,t) &\le \lambda_1 L_1((k+3)\zeta_1^{-1})(k+3)^{\alpha_1}\zeta_1^{-\alpha_1} \\ &\le 2\lambda_1 \frac{L_1(k\zeta_1^{-1})}{L_1(\zeta_1^{-1})}k^{\alpha_1}b^{-2} \qquad (2.86)\end{aligned}$$

According to Lemma 1 (iii), $\mathbb{E}(\sup_{|t+\tau-t_i|\le 2\zeta_1^{-1}} f_0(t)) = O(b^{-1})$ as $b \to \infty$. So for k large enough, we have

$$\mathbb{E}\Big[\sup_{t\in B_i} f_0(t)\Big] \le \frac{\Delta_\tau}{4}\frac{L_1(k\zeta_1^{-1})}{L_1(\zeta_1^{-1})}k^{\alpha_1}b^{-1}. \qquad (2.87)$$

By Proposition 1, (2.85), (2.86), and (2.87), we have

$$\begin{aligned}&\mathbb{P}(\sup_{|t-t_i|\le 2\zeta_1^{-1}} f(t) \ge \gamma | f(\tau) = \gamma + \frac{z}{b}) \qquad (2.88)\\ \le\ &\exp(-\frac{\Delta_\tau^2 L_1(k\zeta_1^{-1})k^{\alpha_1}}{64 L_1(\zeta_1^{-1})\lambda_1}) \le \exp(-\frac{\Delta_\tau^2 k^{\alpha_1/2}}{64\lambda_1}). \qquad (2.89)\end{aligned}$$

The last inequality of the above display is due to Lemma 5(ii). Note that

$$\mathbb{P}(\sup_{x\zeta_1^{-1}<|t-\tau|<\delta} f(t) > \gamma | f(\tau) = \gamma + \frac{z}{b}) \le \sum_{x\zeta_1^{-1}<|t_i-\tau|<\delta'} \mathbb{P}(\sup_{t\in B_i} f(t) \ge \gamma | f(\tau) = \gamma + \frac{z}{b}).$$

According to (2.89), we further bound the above probability by

$$\begin{aligned}\sum_{x\zeta_1^{-1}<|t_i-\tau|<\delta} \mathbb{P}(\sup_{t\in B_i} f(t) \ge \gamma | f(\tau) = \gamma + \frac{z}{b}) &\le O(1)\sum_{k=\lfloor x\rfloor}^{\delta\zeta_1} k^{d-1}\exp(-\frac{\Delta_\tau k^{\alpha_1/2}}{64\lambda_1}) \\ &\le e^{-x^{\alpha_1/2-\varepsilon_0}}\end{aligned}$$

for x sufficiently large and ε_0 small. We integrate the above bound with respect to (z, τ) under the measure Q_b and conclude the proof. $\square$

Proof of Lemma 4. The proof of this lemma is based on the fact that $\mathbb{P}(f(t) > \gamma)$ has the approximation

$$\mathbb{P}(f(t) > \gamma) = \frac{1}{\sqrt{2\pi}} \frac{\sigma(t)}{\gamma - \mu(t)} \exp\left(-\frac{\gamma - \mu(t)}{2\sigma(t)}\right)(1 + o(1)),$$

combined with the expansion of $\sigma(t)^2$ around t^*,

$$\sigma(t)^2 = \sigma(t^*)^2 - 2\sigma(t^*)\Lambda L_2(|t - t^*|)|t - t^*|^{\alpha_2}(1 + o(1)).$$

After basic calculation of expansion and integration, we can prove that there exist $\varepsilon_0, \kappa > 0$, such that for $x > \kappa$, we have

$$\begin{aligned}
\int_{|t-t^*|\le\zeta_2^{-1}} \mathbb{P}(f(t) > \gamma)dt &\ge \frac{1}{\sqrt{2\pi}} \frac{\sigma(t^*)/2}{\gamma + \mu_T} \zeta_2^{-d} \exp\left(-\frac{(\gamma - \mu(t^*))^2}{2\sigma(t^*)^2}\right) \cdot \varepsilon_0 \\
\int_{x\zeta_2^{-1}<|t-t^*|<\delta} \mathbb{P}(f(t) > \gamma)dt &\le \frac{1}{\sqrt{2\pi}} \frac{\sigma(t^*)}{\gamma - \mu_T} \zeta_2^{-d} \exp\left(-\frac{(\gamma - \mu(t^*))^2}{2\sigma(t^*)^2}\right) \exp\left(-x^{\alpha_2/2}\right) \\
\int_{|t-t^*|>\delta} \mathbb{P}(f(t) > \gamma)dt &\le \frac{1}{\sqrt{2\pi}} \frac{\sigma(t^*)}{\gamma - \mu_T} \exp\left(-\frac{(\gamma - \mu(t^*))^2}{2\sigma(t^*)^2}\right) \exp(-\varepsilon_0 b^2)
\end{aligned}$$

Combining the three inequalities above, and noticing that $h_b(t) = \frac{\mathbb{P}(f(t)>\gamma)}{\int_{t\in T}\mathbb{P}(f(t)>\gamma)dt}$, we have the result in this lemma. $\square$

Chapter 3

Tail Probabilities of Aggregated Lognormal Random Fields with Small Noise[1]

3.1 Introduction

Let $\{f(t) : t \in T\}$ be a zero-mean continuous Gaussian random field living on a compact set $T \subset R^d$. For a continuous and deterministic function $\mu(t)$ and a finite positive measure $m(\cdot)$ on T, we are interested in the probability

$$v(\sigma) = \mathbb{P}\Big(\int_T e^{\sigma f(t)+\mu(t)} m(dt) > b\Big), \quad \text{as } \sigma \to 0, \tag{3.1}$$

where

$$b = \int_T e^{\mu(t)} m(dt) + \kappa\sigma^\alpha \tag{3.2}$$

for some constants $\kappa > 0$ and $0 < \alpha < 1$. We consider two cases: m is a discrete measure with finitely many point masses and m is the Lebesgue measure.

[1]This chapter is based on an accepted manuscript of an article published in *Mathematics of Operations Research*, Volume 41, Issue 01, February 2016, available online: http://pubsonline.informs.org/doi/10.1287/moor.2015.0724.

Motivation. The integral of lognormal random fields is the central quantity of many probabilistic models in portfolio risk analysis, spatial point processes, etc. (see, e.g., Liu and Xu [2012, 2014]). The current analysis is of interest particularly for risk analysis of short-term behavior of a large size portfolio under high correlations. We elaborate more on this application. Consider a portfolio consisting of n assets denoted by S_1, ..., S_n, each of which is associated to a weight, denoted by w_1, ..., w_n. The total value is $S = \sum_{i=1}^n w_i S_i$. Of interest is the tail behavior of S. A stylized model assumes that S_i's are lognormal random variables. Then, the total value is the sum of n correlated lognormal random variables (Ahsan [1978]; Basak and Shapiro [2001]; Deutsch [2004]; Duffie and Pan [1997]; Glasserman *et al.* [2000]). Under such a setting, one may employ a latent space approach by embedding S_1, ..., S_n in a Gaussian process. More precisely, we construct a Gaussian process $f(t)$ and a deterministic function $w(t)$. For each $1 \leq i \leq n$ there exists $t_i \in T$ such that $S_i = e^{f(t_i)}$ and $w_i = w(t_i)$. An interesting situation is that the portfolio size is large and the asset prices become highly correlated. Then the set $\{t_1, ..., t_n\}$ becomes dense in T. Ultimately, as the portfolio size tends to infinity, the limiting value of the unit share price becomes

$$\frac{1}{n}\sum_{i=1}^{n} w(t_i) S_i \to \int_T w(t) e^{f(t)} m(dt)$$

where $m(\cdot)$ is the limiting distribution of $\{t_1, ..., t_n\}$.

Upon considering the short-term behavior of the portfolio, the variance of each asset S_i is usually small. For instance, the variance of the daily log-return of a liquid stock is usually on the order of a few percent that corresponds to the variance of f. Thus, we introduce an additional overall volatility parameter σ and consider

$$\int_T w(t) e^{\sigma f(t)} m(dt).$$

Sending σ to zero is equivalently to considering a very short-term return of the portfolio. We are interested in that $\int_T w(t)e^{\sigma f(t)}m(dt)$ deviates from its limiting value, $\int_T w(t)m(dt)$, by an amount $\kappa\sigma^\alpha$ that is slightly larger than σ, i.e., the target probability in (3.1) with $e^{\mu(t)} = w(t)$. For instance, if σ is on the order of a few percent, then $\kappa\sigma^\alpha$ is of a larger order such as ten percent. In order to have the probability $v(\sigma)$ eventually converging to zero, it is necessary to keep α strictly less than one.

Related works. The tail probabilities of integrals of lognormal fields have been studied both intensively and extensively in the literature, most of which focuses on the asymptotic regime that b tends to infinity and σ is fixed. Asmussen and Rojas-Nandayapa [2008] and Gao *et al.* [2009] study tail probabilities and the density functions for summations of lognormal random variables. The distributions of integrals of geometric Brownian motions are studied in Yor [1992] and Dufresne [2001]. For more general continuous Gaussian random fields, Liu [2012] and Liu and Xu [2012] derive the asymptotic approximations of $\mathbb{P}(\int_T e^{f(t)}dt > b)$ as $b \to \infty$ when $f(t)$ is a three-time differentiable Gaussian random field. Under similar conditions, Liu and X-u [2014] characterize the conditional probabilities $\mathbb{P}(\ \cdot \mid \int_T e^{\sigma f(t)+\mu(t)}dt > b)$ as $b \to \infty$ and efficient Monte Carlo estimators of $v(\sigma)$ are then constructed. The corresponding density function is studied in Liu and Xu [2013].

We the asymptotic regime that σ tends to zero and develop asymptotic approximations of the tail probabilities under very weak regularity conditions. The tail behaviors under small noise are different from the cases when b tends to infinity and σ is fixed. For the latter case the most likely sample paths typically admit the so-called *one-big-jump principle*, that is, the high value of the exponential integral is due to the high excursion of $f(t)$ at one location and the integral in a small region around the maximum of $f(t)$ is dominating. For case that σ converges to zero, there is not a small dominating region and the integral on every piece of the region has a contribution. This feature is often observed in the portfolio risk analysis. Suppose that a large portfolio has a 10% downturn in one day. It is very likely to observe that most stocks in the portfolio has a substantial negative return lead by a few (or sector of) names whose returns are the most negative among all.

In addition to the right tail, with completely analogous analysis, we provide approximations of the left tail probabilities

$$v_l(\sigma) = \mathbb{P}\Big(\int_T e^{\sigma f(t)+\mu(t)} m(dt) < b\Big), \quad \text{for } b = \int_T e^{\mu(t)} m(dt) - \kappa\sigma^\alpha. \tag{3.3}$$

The rest of the paper is organized as follows. The main approximation results are presented in Section 3.2. Section 3.3 includes the proofs of the theorems presented in Section 3.2.

3.2 Main results

3.2.1 Asymptotic approximations

We start the discussion with the case when $m(\cdot)$ is the Lebesgue measure. Let

$$C(s,t) = \mathbb{E}(f(s)f(t))$$

be the covariance function of the Gaussian random field $f(t)$ and assume that $C(s,t)$ is positive definite. Let $\mathcal{C}(T)$ denote the set of continuous functions on T. Define a map $K : \mathcal{C}(T) \mapsto [0,\infty]$ as follows: for each $x(\cdot) \in \mathcal{C}(T)$,

$$K(x) = \int_T \int_T x(s)C(s,t)x(t)dsdt \tag{3.4}$$

that is the squared Mahalanobis distance induced by C. Define a linear map $\mathbf{C}$: $\mathcal{C}(T) \mapsto \mathcal{C}(T)$

$$\mathbf{C}(x)(t) = \int_T C(s,t)x(s)ds.$$

We consider the optimization problem

$$K^*_\sigma = \min_{x\in\mathcal{C}(T)} K(x) \quad \text{such that} \quad \int_T e^{\sigma\mathbf{C}(x)(t)+\mu(t)}dt \geq b \text{ and } \sup_{t\in T}|x(t)| \leq \sigma^{\alpha-1-\varepsilon}, \tag{3.5}$$

for some $\varepsilon \in (0, \min(\alpha, 1-\alpha))$. For σ sufficiently small, the above optimization problem has a unique solution and it does not depend on the choice of ε. The properties of the solution will be discussed later in this section. Now we present the first result.

Theorem 4. *For $0 < \alpha < 1$, suppose that the covariance function $C(s,t)$ is positive definite and m is the Lebesgue measure. Let K_σ^* be defined as in (3.5). We have the following approximation of $v(\sigma)$*

$$v(\sigma) = (c_1 + o(1))\sigma^{1-\alpha} \exp\Big(-\frac{1}{2}K_\sigma^*\Big), \quad \text{as } \sigma \to 0, \tag{3.6}$$

where

$$c_1 = \kappa^{-1}\{(2\pi)^{-1}K(e^{\mu(\cdot)})\}^{1/2} \tag{3.7}$$

and the constant κ appears initially in (3.2).

The above theorem provides an almost explicit approximation of $v(\sigma)$. The implicitly part lies in K_σ^* that is unfortunately not in a closed form. We will later present an iterative algorithm to compute K_σ^* numerically. To maintain the approximation accuracy in Theorem 4, we need to have the computational error reduced to the level of $o(1)$. Due to the technical complication and also to smooth the discussion, we delay this topic to the following subsection. In the meantime, we provide the first order approximation of K_σ^* in the following proposition. This approximation is sufficient to provide an exponential decay rate of $v(\sigma)$.

Proposition 2. *Under the conditions of Theorem 4, for σ sufficiently small, we have the following results.*

(i) For $0 < \alpha < 1$, the optimization problem (3.5) has a unique solution, denoted by $x^*(t)$.

(ii) We have the following approximations as $\sigma \to 0$

$$\begin{aligned} x^*(t) &= (1+o(1))\kappa\sigma^{\alpha-1}\frac{e^{\mu(t)}}{\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt}, \\ K_\sigma^* &= (1+o(1))\kappa^2\sigma^{2\alpha-2}K(e^{\mu(\cdot)})^{-1}. \end{aligned} \tag{3.8}$$

The first $o(1)$ term is uniform in $t \in T$ as $\sigma \to 0$.

The approximations in Proposition 2(ii) are obtained via the first order expansion of the integral $\int_T e^{\sigma f(t)+\mu(t)}dt$. Better approximations of x^* and K_σ^* can be obtained by expanding higher orders. As mentioned previously, to maintain an accurate approximation, we need to reduce the accuracy to the level $o(1)$. The necessary order of expansions in fact depends on α and the derivation is doable but very tedious. Thus, we seek for alternative numerical methods presented in the sequel. Combining Theorem 4 and Proposition 2 we have the following approximation of $\log v(\sigma)$.

Corollary 1. *Under the conditions of Theorem 4, for $0 < \alpha < 1$, as $\sigma \to 0$,*

$$\log v(\sigma) = -(1 + o(1))\frac{1}{2}\kappa^2\sigma^{2\alpha-2}K(e^{\mu(\cdot)})^{-1}.$$

Remark 2. *An intuitive understanding of the above approximation result is given as follows. As $\sigma \to 0$, we approximate the interval by Taylor expansion $\int_T e^{\sigma f(t)+\mu(t)}dt \approx \int_T e^{\mu(t)}(1 + \sigma f(t))dt$. This suggests that $v(\sigma) \approx \mathbb{P}(\int_T e^{\mu(t)} f(t)dt > \kappa\sigma^{\alpha-1})$. Since $\int_T e^{\mu(t)} f(t)dt$ is a Gaussian random variable with zero mean and finite variance, we have approximation $v(\sigma) \approx \exp\{-O(\kappa^2\sigma^{2\alpha-2})\}$. This gives the order of the leading term in Theorem 4.*

We now consider that $m(\cdot)$ is a discrete measure on T with finitely many point masses. For simplicity, we write the random field in terms of a random vector $X = (X_1, .., X_n)^T$ that has a positive definite covariance matrix Σ. Furthermore, we replace the function $\mu(t)$ with a vector $\mu = (\mu_1, .., \mu_n)^T$. The probability $v(\sigma)$ becomes

$$v(\sigma) = \mathbb{P}\Big(\sum_{i=1}^{n} e^{\sigma X_i+\mu_i} > b\Big). \tag{3.9}$$

Similarly to the continuous case, we define the squared Mahalanobis distance for $x \in R^n$,

$$\tilde{K}(x) = x^T\Sigma x.$$

We further define $\tilde{K}_\sigma^*$ through the optimization problem

$$\tilde{K}_\sigma^* = \min_x \tilde{K}(x) \quad \text{subject to the constraint} \quad \sum_{i=1}^{n} e^{\sigma(\Sigma x)_i+\mu_i} \geq b, \tag{3.10}$$

where $(\Sigma x)_i$ is the ith element of Σx. The next theorem presents an approximation of $v(\sigma)$ for $0 < \alpha < 1$, which is the discrete analogue of Theorem 4.

Theorem 5. *The covariance matrix* Σ *is positive definite. Let* $\tilde{K}_\sigma^*$ *be defined as in* (3.10) *and* b *be defined as in* (3.2)*. For* $0 < \alpha < 1$*, we have*

$$v(\sigma) = (c_2 + o(1))\sigma^{1-\alpha} \exp\Big(-\frac{\tilde{K}_\sigma^*}{2}\Big), \quad \textit{as } \sigma \to 0, \tag{3.11}$$

where $c_2 = \kappa^{-1}\sqrt{(2\pi)^{-1} y^{*T}\Sigma y^*}$ *and*

$$y^* = (e^{\mu_1}, ..., e^{\mu_n})^T. \tag{3.12}$$

We have the following discrete analogue of Proposition 2.

Proposition 3. *Under the conditions of Theorem 5, for* $0 < \alpha < 1$*, we have the following results.*

(i) The optimization problem (3.10) *has a unique solution* $x^* \in R^n$*.*

(ii) We have the following approximation

$$\begin{aligned} x^* &= (1 + o(1))\kappa\sigma^{\alpha-1}(y^{*T}\Sigma y^*)^{-1} y^*, \\ \tilde{K}_\sigma^* &= (1 + o(1))\kappa^2\sigma^{2\alpha-2}(y^{*T}\Sigma y^*)^{-1}, \end{aligned}$$

where y^* *is given as in* (3.12)*.*

Combining the above proposition and Theorem 5, we have the following approximation of $\log v(\sigma)$.

Corollary 2. *Under the conditions of Theorem 5, for* $0 < \alpha < 1$*, we have as* $\sigma \to 0$

$$\log(v(\sigma)) = -(1 + o(1))\frac{1}{2}\kappa^2(y^{*T}\Sigma y^*)^{-1}\sigma^{2\alpha-2}.$$

The approximations of the left-tail probabilities can be derived similarly as those of the right tail. Therefore, we present the results as corollaries and omit the proof. For the case when $m(\cdot)$ is the Lebesgue measure, we redefine K_σ^* through the optimization problem

$$\begin{aligned} K_\sigma^* = \quad & \min_{x\in\mathcal{C}(T)} K(x) \text{ subject to the constraints} \\ & \int_T e^{\sigma\mathbf{C}(x)(t)+\mu(t)}dt \le \int_T e^{\mu(t)}dt - \kappa\sigma^\alpha \text{ and } \sup_{t\in T}|x(t)| \le \sigma^{\alpha-1-\varepsilon}. \end{aligned} \tag{3.13}$$

Corollary 3. *With K_σ^* defined in* (3.13)*, we have*

$$\mathbb{P}\Big(\int_T e^{\sigma f(t)+\mu(t)}dt < \int_T e^{\mu(t)}dt - \kappa\sigma^\alpha\Big) = (c_1+o(1))\sigma^{1-\alpha}\exp\Big(-\frac{1}{2}K_\sigma^*\Big), \quad \text{as } \sigma\to 0,$$

where c_1 is given as in (3.7)*.*

When $m(\cdot)$ is a discrete measure with finitely many point masses, we redefine the optimization problem as

$$\tilde{K}_\sigma^* = \min_x \tilde{K}(x) \quad \text{subject to} \quad \sum_{i=1}^n e^{\sigma(\Sigma x)_i+\mu_i} \le \sum_{i=1}^n e^{\mu_i} - \kappa\sigma^\sigma. \tag{3.14}$$

Corollary 4. *With $\tilde{K}_\sigma^*$ defined in* (3.14)*, we have*

$$\mathbb{P}\Big(\sum_{i=1}^n e^{\sigma X_i+\mu_i} < \sum_{i=1}^n e^{\mu_i} - \kappa\sigma^\alpha\Big) = (c_2+o(1))\sigma^{1-\alpha}\exp\Big(-\frac{\tilde{K}_\sigma^*}{2}\Big), \quad \text{as } \sigma\to 0,$$

where $c_2 = \kappa^{-1}\sqrt{(2\pi)^{-1}y^{*T}\Sigma y^*}$.

3.2.2 Numerical approximation for K_σ^*

As discussed previously, K_σ^* is not a closed form expression. In this section, we present an iterative algorithm to solve (3.5) and m is the Lebesgue measure. The case of discrete measure is similar and therefore is omitted. Let

$$\mathcal{B} = \{x\in\mathcal{C}(T) : \|x\|_\infty \le \sigma^{\alpha-1-\varepsilon}\},$$

where $\|x\|_\infty = \sup_{t\in T}|x(t)|$. Define the function $\Lambda(\cdot):\mathcal{B}\to[0,+\infty)$ such that, for each $x\in\mathcal{B}$, $\lambda=\Lambda(x)$ solves the following equation

$$\int_T \exp\Big\{\sigma\lambda\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t)+\mu(t)\Big\}dt = b. \tag{3.15}$$

The next proposition ensures that $\Lambda(\cdot)$ is well defined.

Proposition 4. *For each $x \in \mathcal{B}$, there is a unique solution $\Lambda(x)$ satisfying equation* (3.15). *Moreover, $0 \leq \Lambda(x) \leq \kappa_c \sigma^{\alpha-1}$, where κ_c is a positive constant depending only on the covariance function C and the mean function μ.*

We further define the operator $\mathbf{S} : \mathcal{B} \to \mathcal{B}$ by

$$\mathbf{S}(x)(t) = \Lambda(x) e^{\sigma \mathbf{C}(x)(t) + \mu(t)}. \tag{3.16}$$

Our algorithm to compute K_σ^* is based on the following proposition.

Proposition 5. $\mathbf{S}$ *is a contraction mapping over $\mathcal{B}$, that is, for $x, y \in \mathcal{B}$,*

$$\|\mathbf{S}(x) - \mathbf{S}(y)\|_\infty \leq \kappa_0 \sigma^\alpha \|x - y\|_\infty, \tag{3.17}$$

where κ_0 is a positive constant depending only on the covariance function C and the mean function μ. Furthermore, the solution $x^*(\cdot)$ to the optimization problem (3.5) *is the unique fixed point of $\mathbf{S}$, that is, $x^* = \mathbf{S}(x^*)$.*

With the above proposition, we present an iterative algorithm to compute x^* using the above contraction mapping theorem.

1. Let
$$\hat{x}_0^* = \kappa \sigma^{\alpha-1} \frac{e^{\mu(t)}}{\int_T \int_T C(s,t) e^{\mu(s)+\mu(t)} ds dt}.$$
2. For each k, compute $\hat{x}_k^*$ according to
$$\hat{x}_k^* = \mathbf{S}(\hat{x}_{k-1}^*).$$

We iterate step 2 until convergence. According to the contraction mapping theorem, the rate of convergence is

$$\|\hat{x}_k^* - x^*\|_\infty \leq (\kappa_0 \sigma^\alpha)^k \|\hat{x}_0^* - x^*\|_\infty = O(\sigma^{\alpha k + \alpha - 1}).$$

If we run the algorithm for $k > 2(1-\alpha)/\alpha$ iterations, then $\|\hat{x}_k^* - x^*\|_\infty = O(\sigma^{\alpha k + \alpha - 1}) = o(\sigma^{1-\alpha})$. We obtain that $|K(\hat{x}_k^*) - K_\sigma^*| = o(\sigma^{1-\alpha})$ and the asymptotic results in the previous theorems still hold by replacing K_σ^* with $K(\hat{x}_k^*)$.

3.3 Proof

In this section, we present the proofs of Theorem 4 and Propositions 2, 4, and 5. The proofs for Theorem 5 and Proposition 3 are completely analogous to those of Theorem 4 and Proposition 2 and therefore are omitted.

We begin with some useful lemmas. The following lemma is known as the Borell-TIS lemma, which is proved independently by Borell [1975a] and Tsirelson *et al.* [1976].

Lemma 6 (Borell-TIS)**.** *Let $f(t)$, $t \in \mathcal{U}$, $\mathcal{U}$ is a parameter set, be a mean zero Gaussian random field. f is almost surely bounded on $\mathcal{U}$. Then,* $\mathbb{E}[\sup_{\mathcal{U}} f(t)] < \infty$*, and*

$$\mathbb{P}\left(\sup_{t\in\mathcal{U}} f\left(t\right) - \mathbb{E}[\sup_{t\in\mathcal{U}} f\left(t\right)] \geq b\right) \leq \exp\left(-\frac{b^2}{2\sigma_{\mathcal{U}}^2}\right),$$

where $\sigma_{\mathcal{U}}^2 = \sup_{t\in\mathcal{U}} Var[f(t)]$.

The Borell-TIS lemma provides a general bound of the tail probabilities of $\sup_t f(t)$. In most cases, $\mathbb{E}[\sup_t f(t)]$ is much smaller than b. Thus, for b that is sufficiently large, the tail probability can be further bounded by:

$$\mathbb{P}\Big(\sup_{t\in T} f(t) > b\Big) \leq \exp\left(-\frac{b^2}{4\sigma_T^2}\right). \tag{3.18}$$

To prove Theorem 4, the following lemma shows that $f(t)$ can be localized to the event

$$\mathcal{L} = \Big\{f(t) : \sup_{t\in T} |f(t)| \leq \kappa_f \sigma^{\alpha-1}\Big\},$$

and we only need to focus on $\mathcal{L}$ for our analysis.

Lemma 7. *There exists a positive constant κ_f sufficiently large such that*

$$\mathbb{P}\Big(\sup_{t\in T} |f(t)| > \kappa_f \sigma^{\alpha-1}\Big) = o(1)\sigma^{1-\alpha} \exp\Big(-\frac{1}{2}K_\sigma^*\Big).$$

Proof of Lemma 7. According to Proposition 2, whose proof is independent of the current one, $K_\sigma^* = (1 + o(1))\kappa^2\sigma^{2\alpha-2}K(e^{\mu(\cdot)})^{-1}$. We choose the constant $\kappa_f >$

$2\sigma_T\kappa\sqrt{K(e^{\mu(\cdot)})^{-1}}$, then inequality (3.18) implies that

$$\mathbb{P}\Big(\sup_{t\in T}|f(t)| > \kappa_f\sigma^{\alpha-1}\Big) \leq 2\exp\big(-\kappa^2\sigma^{2\alpha-2}K(e^{\mu(\cdot)})^{-1}\big) = o(1)\sigma^{1-\alpha}\exp\Big(-\frac{1}{2}K_\sigma^*\Big),$$

which yields the desired result. $\square$

We proceed to the proof of Theorem 4. We use a change of measure technique to derive the asymptotic approximation. The change of measure is constructed such that it focuses on the most likely sample path corresponding to the solution to the optimization problem (3.5). The theoretical properties of the optimization problem (3.5) are established in Propositions 2, 4 and 5. These three propositions are the key elements of the proof.

Proof of Theorem 4. Let $x^*(t)$ be the solution to (3.5). We define the exponential change of measure

$$\frac{dQ}{dP} = \exp\Big(\int_T x^*(t)f(t)dt - \frac{1}{2}\int_T\int_T x^*(s)C(s,t)x^*(t)dsdt\Big).$$

The introduced change of measure Q defines a translation of the original Gaussian random field $f(t)$. We state this result in the next lemma, whose proof is delayed after the proof of Theorem 4.

Lemma 8. *Under measure Q, $f(t)$ is a Gaussian random field with mean function $\mathbf{C}(x^*)(t)$ and covariance function $C(s,t)$.*

According to Lemma 7,

$$\mathbb{P}\left(\int_T e^{\sigma f(t)+\mu(t)} > b, \mathcal{L}^c\right) = o(1)\sigma^{1-\alpha}\exp\Big(-\frac{1}{2}K_\sigma^*\Big).$$

Therefore, we only need to consider $\mathbb{P}(\int_T e^{\sigma f(t)+\mu(t)} > b, \mathcal{L})$. By means of the change of measure Q, we have

$$\begin{aligned}
& \mathbb{P}\left(\int_T e^{\sigma f(t)+\mu(t)} > b, \mathcal{L}\right) \\
= \ & \mathbb{E}^Q\left[\frac{dP}{dQ}; \ \int_T e^{\sigma f(t)+\mu(t)} > b, \ \mathcal{L}\right] \\
= \ & \exp\left(\frac{1}{2}\int_{T\times T} x^*(s)C(s,t)x^*(t)dsdt\right) && (3.19) \\
& \times \mathbb{E}^Q\left[e^{-\int_T x^*(t)f(t)dt}; \int_T e^{\sigma f(t)+\mu(t)}dt > b, \mathcal{L}\right], && (3.20)
\end{aligned}$$

where $\mathbb{E}^Q$ denotes the expectation with respect to the measure Q. Let

$$f^* = \mathbf{C}(x^*).$$

With this notation, we have

$$\int_T e^{\sigma f^*(t)+\mu(t)}dt = b, \quad \int_T f^*(t)x^*(t)dt = \int_{T\times T} x^*(s)C(s,t)x^*(t)dsdt.$$

The random field $f^*(t) + f(t)$ under $\mathbb{P}$ has the same distribution as $f(t)$ under Q. Thus, we replace the probability measure Q and f with $\mathbb{P}$ and $f^* + f$ in (3.19) and obtain

$$\begin{aligned}
& \mathbb{P}\left(\int_T e^{\sigma f(t)+\mu(t)} > b, \mathcal{L}\right) \\
= \ & \exp\left(\frac{1}{2}\int_{T\times T} x^*(s)C(s,t)x^*(t)dsdt\right) \\
& \times \mathbb{E}\left[e^{-\int_T x^*(t)(f^*(t)+f(t))dt}; \int_T e^{\sigma(f^*(t)+f(t))+\mu(t)}dt > b, \mathcal{L}\right] \\
= \ & \exp\left(-\frac{1}{2}\int_{T\times T} x^*(s)C(s,t)x^*(t)dsdt\right) \\
& \times \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; \int_T (e^{\sigma f(t)} - 1)w(dt) > 0, \mathcal{L}\right], && (3.21)
\end{aligned}$$

where

$$w(dt) = \frac{y^*(t)dt}{\int_T y^*(s)ds} \text{ and } y^*(t) = e^{\sigma f^*(t)+\mu(t)}.$$

We define

$$F = \left\{\int_T (e^{\sigma f(t)} - 1)w(dt) > 0\right\}.$$

By the fact that $e^x - 1 \geq x$, we have

$$\int_T (e^{\sigma f(t)} - 1)w(dt) \geq \int_T \sigma f(t)w(dt).$$

Thus, F can be written as the union of two disjoint sets, $F = F_1 \cup F_2$, where

$$F_1 = \left\{\int_T f(t)w(dt) > 0\right\} \text{ and } F_2 = \left\{\int_T f(t)w(dt) < 0, \int_T (e^{\sigma f(t)} - 1)w(dt) > 0\right\}.$$

Thus, the expectation in (3.21) can be written as

$$\begin{aligned}\mathbb{E}&\left[e^{-\int_T x^*(t)f(t)dt}; \int_T (e^{\sigma f(t)} - 1)w(dt) > 0, \mathcal{L}\right] \\ &= \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; F_1, \mathcal{L}\right] + \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; F_2, \mathcal{L}\right]. \quad (3.22)\end{aligned}$$

We calculate each of the two terms on the right-hand side of the above equation separately. First, we compute

$$\mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; \int_T f(t)w(dt) > 0, \mathcal{L}\right]. \quad (3.23)$$

According to Proposition 5, whose proof is independent of the current one, x^* is the fixed point of the contraction map $\mathbf{S}$ and thus

$$x^*(t) = \mathbf{S}(x^*)(t) = \Lambda(x^*)e^{\sigma\mathbf{C}(x^*)(t)+\mu(t)} = \Lambda(x^*)y^*(t).$$

Therefore, $x^*(t)$ and $y^*(t)$ are different by a factor $\Lambda(x^*)$. Thus, $\int_T x^*(t)f(t)dt$ and $\int_T f(t)w(dt)$ are different by a factor $\int_T x^*(t)dt$. Thanks to Proposition 2(ii), we have

$$\int_T x^*(t)dt = (1 + o(1))\frac{\kappa\sigma^{\alpha-1}\int_T e^{\mu(t)}dt}{\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt}.$$

As the result, we have

$$\begin{aligned}\int_T x^*(t)f(t)dt &= \int_T x^*(t)dt \int_T f(t)w(dt) \\ &= (1 + o(1))\frac{\kappa\sigma^{\alpha-1}\int_T e^{\mu(t)}dt}{\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt}\int_T f(t)w(dt). \quad (3.24)\end{aligned}$$

Define

$$\Delta = \frac{\kappa\sigma^{\alpha-1}\int_T e^{\mu(t)}dt}{\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt}.$$

The expectation (3.23) can be computed as follows

$$
\begin{aligned}
& \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; \int_T f(t)w(dt) > 0, \mathcal{L}\right] \\
= & \ \mathbb{E}\left[e^{-(1+o(1))\Delta\int_T f(t)w(dt)}; \int_T f(t)w(dt) > 0, \mathcal{L}\right] \\
= & \ (1+o(1))\mathbb{E}\left[e^{-(1+o(1))\Delta\int_T f(t)w(dt)}; \int_T f(t)w(dt) > 0\right] \\
= & \ (1+o(1))\frac{1}{\Delta\sqrt{2\pi Var(\int_T f(t)w(dt))}}.
\end{aligned}
$$

The second step in the above derivation is due to the fact that $\mathbb{P}(\mathcal{L}) \to 1$ for κ_f chosen sufficiently large. Furthermore, notice that $w(t) = (1+o(1))e^{\mu(t)}/\int e^{\mu(s)}ds$. Then,

$$
Var\left(\int_T f(t)w(dt)\right) = (1+o(1))\frac{\int_{T\times T} e^{\mu(s)+\mu(t)}C(s,t)dsdt}{(\int_T e^{\mu(t)}dt)^2}
$$

and

$$
\begin{aligned}
& \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; \int_T f(t)w(dt) > 0, \mathcal{L}\right] \\
& \qquad = (1+o(1))\kappa^{-1}\sigma^{1-\alpha}\sqrt{(2\pi)^{-1}\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt}. \qquad (3.25)
\end{aligned}
$$

Thus, we conclude the derivation of the first expectation on the right-hand side of (3.22).

Now we proceed to the second expectation term. On the set $\mathcal{L}$, by Taylor's expansion, we have that $e^{\sigma f(t)} - 1 \leq \sigma f(t) + \sigma^2 f^2(t)$ and thus

$$
\int_T (e^{\sigma f(t)} - 1)w(dt) \leq \int_T \sigma f(t)w(dt) + \int_T \sigma^2 f^2(t)w(dt).
$$

So the event $\{\int_T (e^{\sigma f(t)} - 1)w(dt) \geq 0\}$ is a subset of $\{\int_T [f(t) + \sigma f^2(t)]w(dt) \geq 0\}$. This gives an upper bound of the expectation

$$
\begin{aligned}
& \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; F_2, \mathcal{L}\right] \\
& \qquad \leq \mathbb{E}\left[e^{-\int_T x^*(t)f(t)dt}; \int_T [f(t) + \sigma f^2(t)]w(dt) \geq 0, \int_T f(t)w(dt) < 0, \mathcal{L}\right].
\end{aligned}
$$

We write

$$Z_1 = -\int_T f(t)w(dt) \text{ and } Z_2 = \int_T f^2(t)w(dt).$$

From (3.24), the right-hand side of the above inequality can be written as

$$\mathbb{E}[e^{\Delta Z_1}; Z_1 > 0, Z_2 \geq Z_1/\sigma, \mathcal{L}].$$

On the set $\{0 < Z_1 \leq \sigma^{1-\alpha+\varepsilon}\}$, this expectation is negligible as $\Delta = O(\sigma^{\alpha-1})$, that is,

$$\mathbb{E}[e^{\Delta Z_1}; 0 < Z_1 < \sigma^{1-\alpha+\varepsilon}] = O(\mathbb{P}(0 < Z_1 < \sigma^{1-\alpha+\varepsilon})) = o(1). \tag{3.26}$$

Furthermore, on the set $\mathcal{L}$, we have $\sup_t |f(t)| \leq \kappa_f \sigma^{\alpha-1}$ and thus $Z_1 < \sigma^{\alpha-1-\varepsilon}$ for ε and σ sufficiently small. Therefore, we only need to focus on the expectation

$$\begin{aligned} &\mathbb{E}\left[e^{\Delta Z_1}; \sigma^{1-\alpha+\varepsilon} < Z_1 < \sigma^{\alpha-1-\varepsilon}, Z_2 > Z_1/\sigma\right] \\ &\qquad = \int_{\sigma^{1-\alpha+\varepsilon}}^{\sigma^{\alpha-1-\varepsilon}} e^{\Delta z}\mathbb{P}(Z_2 > z/\sigma | Z_1 = z) p_{Z_1}(z)dz, \end{aligned} \tag{3.27}$$

where $p_{Z_1}(z)$ is the density function of Z_1. We need the following lemma.

Lemma 9. *For $z \in [\sigma^{1-\alpha+\varepsilon}, \sigma^{\alpha-1-\varepsilon}]$, there exists a constant $\varepsilon_0 > 0$ such that*

$$\mathbb{P}(Z_2 > z/\sigma | Z_1 = z) \leq e^{-\varepsilon_0 z/\sigma}. \tag{3.28}$$

Lemma 9 implies that the expectation (3.27) is bounded by

$$\begin{aligned} (3.27) &\leq \int_{\sigma^{1-\alpha+\varepsilon}}^{\sigma^{\alpha-1-\varepsilon}} e^{-(\varepsilon_0/\sigma - \Delta)z} p_{Z_1}(z)dz \\ &= \int_{\sigma^{1-\alpha+\varepsilon}}^{\sigma^{\alpha-1-\varepsilon}} e^{-(1+o(1))\varepsilon_0 z/\sigma} p_{Z_1}(z)dz \\ &= O(\sigma). \end{aligned} \tag{3.29}$$

Combining the results in (3.26) and (3.29), we have $\mathbb{E}[e^{-\int_T x^*(t)f(t)dt}; F_2, \mathcal{L}] = o(1)$ and Theorem 4 is proved. □

Proof of Lemma 3.3. It is sufficient to show that, for any finite subset $\{t_1, \ldots, t_k\} \in T$, the moment generating function of $(f(t_1), \ldots, f(t_k))$ under the measure Q is the same as that of the multivariate normal distribution with mean $(\mathbf{C}(x^*)(t_1), \ldots, \mathbf{C}(x^*)(t_k))$ and covariance matrix $\{C(t_i, t_j)\}_{i,j=1,\ldots,k}$. For any $(\lambda_1, ..., \lambda_k) \in \mathbb{R}^k$, we have

$$\begin{aligned}
& \mathbb{E}^Q\Big[\exp\{\lambda_1 f(t_1) + \cdots + \lambda_k f(t_k)\}\Big] \\
= \ & \mathbb{E}\left[\frac{dQ}{dP}\exp\{\lambda_1 f(t_1) + \cdots + \lambda_k f(t_k)\}\right] \\
= \ & \exp\left\{\sum_{i=1}^k \lambda_i \mathbf{C}(x^*)(t_i) + \frac{1}{2}\sum_{i}^k \sum_{j=1}^k \lambda_i\lambda_j C(t_i, t_j)\right\},
\end{aligned}$$

which is the moment generating function of the target multivariate normal distribution. This completes the proof. □

Proof of Lemma 9. Conditional on $Z_1 = z$, $\{f(t) : t \in T\}$ is still a Gaussian random field, with the mean and variance given as follows:

$$\tilde{\mu}(t) = \mathbb{E}(f(t)|Z_1 = z) = -\frac{\int_T C(s,t)w(ds)}{\int_{T\times T} C(s,t)w(ds)w(dt)} \cdot z, \tag{3.30}$$

$$Var(f(t)|Z_1 = z) = C(t,t) - \left(\int_{T\times T} C(s,t)w(ds)w(dt)\right)^{-1}\left(\int_T C(s,t)w(ds)\right)^2.$$

We write the conditional random field as $f(t) = \tilde{\mu}(t) + g(t)$, then the probability in (3.28) is bounded by

$$\mathbb{P}\left(\int_T \{\tilde{\mu}(t) + g(t)\}^2 w(dt) > z/\sigma\right) \le \mathbb{P}\left(\sup_{t\in T}|\tilde{\mu}(t)| + \sup_T |g(t)| > \sqrt{z/\sigma}\right).$$

According to (3.30), for $z \in [\sigma^{1-\alpha+\varepsilon}, \sigma^{\alpha-1-\varepsilon}]$,
we have $\sup_{t\in T}|\tilde{\mu}(t)| = O(z) = o(1)\sqrt{z/\sigma}$. So the above probability can be further bounded by

$$\mathbb{P}\left(\sup_T |g(t)| > (1 + o(1))\sqrt{z/\sigma}\right).$$

We obtain (3.28) by applying Lemma 6. This concludes our proof. □

The proof of Proposition 2 needs the results of Propositions 4 and 5. Thus, we present the proofs of these two propositions first.

Proof of Proposition 4. For $x \in \mathcal{B}$, we define

$$h(\lambda) = \int_T \exp\Big(\sigma\lambda\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t) + \mu(t)\Big)dt.$$

We have

$$\begin{aligned} h(\lambda) &\geq \int_T e^{\mu(t)}(1 + \sigma\lambda\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t))dt \qquad (3.31) \\ &= \int_T e^{\mu(t)}dt + \sigma\lambda\int_T e^{\mu(t)}\mathbf{C}(e^{\mu}(1+o(1)))(t)dt \\ &= \int_T e^{\mu(t)}dt + (1+o(1))\sigma\lambda\int_{T\times T} e^{\mu(s)}C(s,t)e^{\mu(t)}dsdt. \end{aligned}$$

The second equality holds because $\sigma\mathbf{C}(x) = O(\sigma^{\alpha-\varepsilon}) = o(1)$. If $h(\lambda) = b$, then, together with the fact that $b = \int_T e^{\mu(t)}dt + \kappa\sigma^{\alpha}$, the above display suggests that

$$\lambda \leq (1+o(1))\kappa\sigma^{\alpha-1}(\int_T\int_T e^{\mu(s)}C(s,t)e^{\mu(t)}dsdt)^{-1}.$$

This means that the equation $h(\lambda) = b$ has no solution outside $[0, \kappa_c\sigma^{\alpha-1}]$ for some constant κ_c large.

For $\lambda \in [0, \kappa_c\sigma^{\alpha-1}]$, we obtain the following approximation by Taylor's expansion

$$h(\lambda) = \int_T e^{\mu(t)}dt + \sigma\lambda(1+o(1))\int_T\int_T e^{\mu(s)}C(s,t)e^{\mu(t)}dsdt$$

and $h(\lambda)$ is approximately linear in λ as σ tends to 0. Because $h(0) < b$ and $h(\kappa_c\sigma^{\alpha-1}) > b$ for κ_c sufficiently large, there exists $\lambda \in [0, \kappa_c\sigma^{\alpha-1}]$ such that $h(\lambda) = b$. Moreover, for $\lambda \in [0, \kappa_c\sigma^{\alpha-1}]$,

$$h'(\lambda) = (1+o(1))\sigma\int_T\int_T e^{\mu(s)}C(s,t)e^{\mu(t)}dsdt > 0,$$

so the solution is unique. □

Proof for Proposition 5. We first show that $\mathbf{S}$ is a contraction mapping. According to the definition of $\mathbf{S}(x)$ in (3.16) we have that for $x, y \in \mathcal{B}$

$$\|\mathbf{S}(x) - \mathbf{S}(y)\|_\infty \leq |\Lambda(x) - \Lambda(y)| \cdot \|e^{\sigma \mathbf{C}(x)+\mu}\|_\infty + \Lambda(y)\|e^{\sigma \mathbf{C}(x)+\mu} - e^{\sigma \mathbf{C}(y)+\mu}\|_\infty. \quad (3.32)$$

We give upper bounds for $|\Lambda(x) - \Lambda(y)|$ and $\|e^{\sigma \mathbf{C}(x)+\mu} - e^{\sigma \mathbf{C}(y)+\mu}\|_\infty$ separately. According to (3.15), we have

$$\int_T \exp\Big(\sigma\Lambda(x)\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t) + \mu(t)\Big)dt - \int_T \exp\Big(\sigma\Lambda(y)\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t) + \mu(t)\Big)dt \quad (3.33)$$

$$= \int_T \exp\Big(\sigma\Lambda(y)\mathbf{C}(e^{\sigma\mathbf{C}(y)+\mu})(t) + \mu(t)\Big)dt - \int_T \exp\Big(\sigma\Lambda(y)\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t) + \mu(t)\Big)dt. \quad (3.34)$$

We provide a bound for $|\Lambda(x) - \Lambda(y)|$ by deriving approximations for both sides of the above identity. Without loss of generality, we assume $\Lambda(x) > \Lambda(y)$. By exchanging the integration and derivative, the left-hand side is

$$(3.33) = \int_{\Lambda(y)}^{\Lambda(x)} \int_T \sigma\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t) \exp\Big(\sigma\lambda\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t) + \mu(t)\Big)dtd\lambda.$$

Thus, we have

$$(3.33) = (1 + o(1))\sigma|\Lambda(x) - \Lambda(y)| \times \int_T \mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu})(t)e^{\mu(t)}dt.$$

Similarly, we have the right-hand side is

$$(3.34) \leq (1 + o(1))\sigma\Lambda(y) \int_T e^{\mu(t)}\mathbf{C}(e^{\sigma\mathbf{C}(x)+\mu} - e^{\sigma\mathbf{C}(y)+\mu})(t)dt.$$

Notice that $\|e^{\sigma\mathbf{C}(x)+\mu} - e^{\sigma\mathbf{C}(y)+\mu}\|_\infty \leq O(\sigma)\|x - y\|_\infty$. Thus,

$$(3.34) = O(\sigma^2)\Lambda(y)\|x - y\|_\infty = O(\sigma^{\alpha+1})\|x - y\|_\infty.$$

By equating (3.33) and (3.34), we have

$$|\Lambda(x) - \Lambda(y)| = O(\sigma^\alpha)\|x - y\|_\infty. \quad (3.35)$$

Thus, the first term in (3.32) is bounded from the above by

$$|\Lambda(x) - \Lambda(y)| \cdot \|e^{\sigma \mathbf{C}(x)+\mu}\|_\infty = O(\sigma^\alpha)\|x-y\|_\infty.$$

We proceed to the second term on the right side of (3.32). By Taylor's expansion, we have

$$\|e^{\sigma \mathbf{C}(x)+\mu} - e^{\sigma \mathbf{C}(y)+\mu}\|_\infty \leq O(\sigma)\|x-y\|_\infty. \tag{3.36}$$

Thus we obtain (3.17) by combining (3.32), (3.35), (3.36), and the fact that $\Lambda(x) \leq \kappa_c \sigma^{\alpha-1}$.

We proceed to the proof that the fixed point of $\mathbf{S}$ is the solution to (3.5). We define set

$$\mathcal{M} = \left\{ x \in \mathcal{C}(T) : \int_T e^{\sigma \mathbf{C}(x)(t)+\mu(t)} dt \geq b \text{ and } \|x\|_\infty \leq \sigma^{\alpha-1-\varepsilon} \right\}.$$

For $x \in \mathcal{M}$, define function $l(\eta) = \int_T e^{\sigma\eta \mathbf{C}(x)(t)+\mu(t)} dt$ that is monotonic increasing in η, so all solutions to the optimization problem (3.5) lie on the boundary set

$$\partial\mathcal{M} = \left\{ x \in \mathcal{C}(T) : \int_T e^{\sigma \mathbf{C}(x)(t)+\mu(t)} dt = b \text{ and } \|x\|_\infty \leq \sigma^{\alpha-1-\varepsilon} \right\}.$$

We use arguments in calculus of variation to show the conclusion. Let g be an arbitrary continuous function on T and s be a scalar close to 0. We compute the derivative of the function

$$h(s) = K(x^* + sg) - \frac{2\lambda}{\sigma} \times \left(\int_T e^{\sigma \mathbf{C}(x^*+sg)(t)+\mu(t)} dt - b \right),$$

where $2\lambda/\sigma$ is the Lagrange multiplier. We take derivative with respect to s

$$h'(0) = 2\int_T x^*(t)\mathbf{C}(g)(t)dt - 2\lambda \int_T e^{\sigma \mathbf{C}(x^*)(t)+\mu(t)} \mathbf{C}(g)(t)dt. \tag{3.37}$$

The solution x^* satisfies $h'(0) = 0$. Since g is arbitrary, we have that x^* is a solution to (3.5) is equivalent to the following conditions

$$x^*(t) = \lambda e^{\sigma \mathbf{C}(x^*)(t)+\mu(t)} \text{ and } \int_T e^{\sigma \mathbf{C}(x^*)(t)+\mu(t)} dt = b. \tag{3.38}$$

We plug the formula of x^* in the first identity into the second identity and obtain that $\lambda = \Lambda(x^*)$ and thus x^* is a fixed point of $\mathbf{S}$. This concludes the proof. $\square$

Proof of Proposition 2. According to the contraction mapping theorem, the operator $\mathbf{S}$ has a unique fixed point. According to Proposition 5 whose proof is independent of the current one, this fixed point x^* is the solution to optimization problem (3.5). This implies that (3.5) has a unique solution in $\mathcal{B}$.

To prove (ii), we expand the exponents in (3.38) and have that

$$x^*(t) = \lambda e^{\mu(t)}(1 + O(\sigma^{\alpha-\varepsilon})) \text{ and } \int_T e^{\mu(t)}[1 + \sigma \mathbf{C}(x^*)(t)]dt + O(\sigma^{2(\alpha-\varepsilon)}) = b.$$

Based on the above two identities, we solve

$$\lambda = \frac{(1 + o(1))\kappa\sigma^{\alpha-1}}{\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt}.$$

This yields

$$x^*(t) = (1 + o(1))\kappa\sigma^{\alpha-1}\frac{e^{\mu(t)}}{\int_{T\times T} C(s,t)e^{\mu(s)+\mu(t)}dsdt} \tag{3.39}$$

and

$$K_\sigma^* = (1 + o(1))\kappa^2\sigma^{2\alpha-2}\Big(\int_T \int_T C(s,t)e^{\mu(s)+\mu(t)}dsdt\Big)^{-1}.$$

$\square$

Chapter 4

Unbiased Sampling of Random Elliptic Partial Differential Equations

4.1 Introduction

Elliptic partial differential equation is a classic equation that are employed to describe various static physics systems. In practical life, such systems are usually not described precisely. For instance, imprecision could be due to microscopic heterogeneity or measurement errors of parameters. To account for this, we introduce uncertainty to the system by letting certain coefficients contain randomness. To be precise, let $U \subset R^d$ be a simply connected domain. We consider the following differential equation concerning $u : U \to R$

$$-\nabla \cdot (a(x)\nabla u(x)) = f(x) \text{ for } x \in U, \tag{4.1}$$

where $f(x)$ is a real-valued function and $a(x)$ is a strictly positive function. Just to clarify the notation, $\nabla u(x)$ is the gradient of $u(x)$ and "$\nabla \cdot$" is the divergence of a vector field. For each a and f, one solves u subject to certain boundary conditions that are necessary for the uniqueness of the solution. This will be discussed in the sequel. The randomness is introduced to the system through $a(x)$ and $f(x)$. Thus, the solution u as an implicit functional of a and f is a real-valued stochastic process living on U. Throughout this chapter, we consider $d \leq 3$ that is sufficient for most physics applications.

Of interest is the distributional characteristics of $\{u(x) : x \in U\}$. The solution is typically not in an analytic form of a and f and thus closed form characterizations are often infeasible. In this dissertation, we study the distribution of u via Monte Carlo. Let $C(U)$ be the set of continuous functions on U. For a real-valued functional

$$\mathcal{Q} : C(U) \to R$$

satisfying certain regularity conditions, we are interested in computing

$$w_{\mathcal{Q}} = \mathbb{E}\{\mathcal{Q}(u)\}.$$

Such problems appear often in the studies of physics systems; see, for instance, De Marsily *et al.* [2005]; Delhomme [1979].

The contribution of the current work is the development of an unbiased Monte Carlo estimator of $w_{\mathcal{Q}}$ with finite variance. Furthermore, the expected computational cost of generating one such estimator is finite. The analysis strategy is a combination of multilevel Monte Carlo and a randomization scheme. Multilevel Monte Carlo is a recent advance in simulation and approximation of continuous processes Cliffe *et al.* [2011]; Giles [2008]; Graham *et al.* [2011]. The randomization scheme is developed by Rhee and Glynn [2012, 2013]. Under the current setting, a direct application of these two methods leads to either an estimator with infinite variance or infinite expected computational cost. This is mostly due to the fact that the accuracy of regular numerical methods of the partial differential equations is insufficient. More precisely, the mean squared error of a discretized Monte Carlo estimator is proportional to the square of mesh size Charrier *et al.* [2013]; Teckentrup *et al.* [2013]. The technical contribution of this chapter is to employ quadratic approximation to solve PDE under certain smoothness conditions of $a(x)$ and $f(x)$ and to perform careful analysis of the numerical solver for equation (4.1).

Physics applications. Equation (4.1) has been widely used in many disciplines to describe time-independent physical problems. The well-known Poisson equation or Laplace equation is a special case when $a(x)$ is a constant. In different disciplines, the solution $u(x)$ and the coefficients $a(x)$ and $f(x)$ have their specific physics meanings. When the elliptic PDE is used to describe the steady-state distribution of heat (as temperature), $u(x)$ carries the meaning of temperature at x and the coefficient $a(x)$ is the heat conductivity. In the study of electrostatics, u is the potential (or voltage) induced by electronic charges, ∇u is the electric field, and $a(x)$ is the permittivity (or resistance) of the medium. In groundwater hydraulics, the meaning of $u(x)$ is the hydraulic head (water level elevation) and $a(x)$ is the hydraulic conductivity (or permeability). The physics laws for the above three different problems to derive the same type of elliptic PDE are called Fourier's law, Gauss's law, and Darcy's law, respectively. In classical continuum mechanics, equation (4.1) is known as the generalized Hook's law where u describes the material deformation under the external force f. The coefficient $a(x)$ is known as the elasticity tensor.

In this chapter, we consider that both $a(x)$ and $f(x)$ possibly contain randomness. We elaborate its physics interpretation in the context of material deformation application. In the model of classical continuum mechanics, the domain U is a smooth manifold denoting the physical location of the piece of material. The displacement $u(x)$ depends on the external force $f(x)$, boundary conditions, and the elasticity tensor $\{a(x) : x \in U\}$. The elasticity coefficient $a(x)$ is modeled as a spatially varying random field to characterize the inherent heterogeneity and uncertainties in the physical properties of the material (such as the modulus of elasticity, c.f. Ostoja-Starzewski [2007]; Sobczyk and Kirkner [2001]). For example, metals, which lend themselves most readily to the analysis by means of the classical elasticity theory, are actually polycrystals, i.e., aggregates of an immense number of anisotropic crystals randomly oriented in space. Soils, rocks, concretes, and ceramics provide further examples of materials with very complicated structures. Thus, incorporating randomness in $a(x)$ is necessary to take into account of the heterogeneities and the uncertainties under many situations. Furthermore, there may also be uncertainty contained in the external force $f(x)$.

The rest of the paper is organized as follows. In Section 4.2, we present the problem settings and some preliminary materials for the main results. Section 4.3 presents the construction of the unbiased Monte Carlo estimator for $w_{\mathcal{Q}}$ and rigorous complexity analysis. Numerical implementations are included in Section 4.4. Technical proofs are included in the appendix.

4.2 Preliminary analysis

Throughout this chapter, we consider equation (4.1) living on a bounded domain $U \subset R^d$ with twice differentiable boundary denoted by ∂U. To ensure the uniqueness of the solution, we consider the Dirichlet boundary condition

$$u(x) = 0, \quad \text{for } x \in \partial U. \tag{4.2}$$

We let both exogenous functions $f(x)$ and $a(x)$ be random processes, that is,

$$f(x,\omega) : U \times \Omega \to R \quad \text{and} \quad a(x,\omega) : U \times \Omega \to R$$

where $(\Omega, \mathcal{F}, \mathbb{P})$ is a probability space. To simplify notation, we omit the second argument and write $a(x)$ and $f(x)$. As an implicit function of the input processes $a(x)$ and $f(x)$, the solution $u(x)$ is also a stochastic process living on U. We are interested in computing the distribution of $u(x)$ via Monte Carlo. In particular, for some functional

$$\mathcal{Q} : C(\bar{U}) \to R$$

satisfying certain regularity conditions that will be specified in the sequel, we compute the expectation

$$w_{\mathcal{Q}} = \mathbb{E}[\mathcal{Q}(u)] \tag{4.3}$$

by Monte Carlo. The notation $\bar{U}$ is the closure of domain U and $C(\bar{U})$ is the set of real-valued continuous functions on $\bar{U}$.

Let $\hat{Z}$ be an estimator (possibly biased) of $\mathbb{E}\mathcal{Q}(u)$. The mean square error (MSE)

$$\mathbb{E}(\hat{Z} - w_{\mathcal{Q}})^2 = Var(\hat{Z}) + \{\mathbb{E}(\hat{Z}) - w_{\mathcal{Q}}\}^2. \tag{4.4}$$

consists of a bias term and a variance term. For the Monte Carlo estimator in this chapter, the bias is removed via a randomization scheme combined with multilevel Monte Carlo. To start with, we present the basics of multilevel Monte Carlo and the randomization scheme.

4.2.1 Multilevel Monte Carlo

Consider a biased estimator of $w_{\mathcal{Q}}$ denote by Z_n. In the current context, Z_n is the estimator corresponding to some numerical solution based on certain discretization scheme, for instance, $Z_n = \mathcal{Q}(u_n)$ where u_n is the solution of the finite element method. The subscript n is a generic index of the discretization size. The detailed construction of Z_n will be provided in the sequel. As $n \to \infty$, the estimator becomes unbiased, that is,

$$\mathbb{E}(Z_n) \to w_{\mathcal{Q}}.$$

Multilevel Monte Carlo is based on the following telescope sum

$$w_{\mathcal{Q}} = \mathbb{E}(Z_0) + \sum_{i=0}^{\infty} \mathbb{E}(Z_{i+1} - Z_i). \tag{4.5}$$

One may choose Z_0 to be some simple constant. Without loss of generality, we choose $Z_0 \equiv 0$ and thus the first term vanishes. The advantage of writing $w_{\mathcal{Q}}$ as the telescope sum is that one is often able to construct Z_i and Z_{i+1} carefully such that they are appropriately coupled and the variance of $Y_i = Z_{i+1} - Z_i$ decreases fast as i tends infinity. Let

$$\Delta_i = \mathbb{E}(Z_{i+1} - Z_i) \tag{4.6}$$

be estimated by

$$\hat{\Delta}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} Y_i^{(j)}$$

where $Y_i^{(j)}$, $j = 1, ..., n_i$ are independent replicates of Y_i. The multilevel Monte Carlo estimator is

$$\hat{Z} = \sum_{i=1}^{I} \hat{\Delta}_i \tag{4.7}$$

where I is a large integer truncating the infinite sum (4.5).

4.2.2 An unbiased estimator via a randomization scheme

In the construction of the multilevel Monte Carlo estimator (4.7), the truncation level I is always finite and therefore the estimator is always biased. In what follows, we present an estimator with the bias removed. It is constructed based on the telescope sum of the multilevel Monte Carlo estimator and a randomization scheme that is originally proposed by Rhee and Glynn [2012, 2013].

Let N be a positive-integer-valued random variable that is independent of $\{Z_i\}_{i=1,2,...}$. Let $p_n = \mathbb{P}(N = n)$ be the probability mass function of N such that $p_n > 0$ for all $n > 0$. The following identity holds trivially

$$w_{\mathcal{Q}} = \sum_{i=1}^{\infty} \mathbb{E}(Z_n - Z_{n-1}) = \sum_{n=1}^{\infty} \frac{\mathbb{E}[Z_n - Z_{n-1}; N = n]}{p_n} = \mathbb{E}\Big(\frac{Z_N - Z_{N-1}}{p_N}\Big).$$

Therefore, an unbiased estimator of $w_{\mathcal{Q}}$ is given by

$$\tilde{Z} = \frac{Z_N - Z_{N-1}}{p_N}. \tag{4.8}$$

Let $\tilde{Z}_i, i = 1, ..., M$ be independent copies of $\tilde{Z}$. The averaged estimator

$$\tilde{Z}_M = \frac{1}{M} \sum_{i=1}^{M} \tilde{Z}_i$$

is unbiased for $w_{\mathcal{Q}}$ with variance $Var(\tilde{Z})/M$ if finite.

We provide a complexity analysis of the estimator $\tilde{Z}$. This consists of the calculation of the variance of $\tilde{Z}$ and of the computational cost to generate $\tilde{Z}$. We start with the second moment

$$\mathbb{E}(\tilde{Z}^2) = \mathbb{E}\Big[\frac{(Z_N - Z_{N-1})^2}{p_N^2}\Big] = \sum_{n=1}^{\infty} \frac{\mathbb{E}(Z_n - Z_{n-1})^2}{p_n}. \tag{4.9}$$

In order to have finite second moment, it is almost necessary to choose the random variable N such that

$$p_n > n\mathbb{E}(Z_n - Z_{n-1})^2 \text{ for all } n \text{ sufficiently large.} \tag{4.10}$$

Furthermore, p_n must also satisfy the natural constraint that

$$\sum_{n=1}^{\infty} p_n = 1,$$

which suggests $p_n < n^{-1}$ for sufficiently large n. Combining with (4.10), we have

$$n^{-1} > p_n > n\mathbb{E}(Z_n - Z_{n-1})^2 \tag{4.11}$$

Notice that we have not yet specified a discretization method, thus (4.11) can typically be met by appropriately indexing the mesh size. For instance, in the context of solving PDE numerically, one may choose the mesh size converging to 0 at a super exponential rate with n (such as e^{-n^2}) and thus $\mathbb{E}(Z_n - Z_{n-1})^2$ decreases sufficiently fast that allows quite some flexibility in choosing p_n. Thus, constraint (4.11) alone can always be satisfied and it is not intrinsic to the problem. It is the combination with the following constraint that forms the key issue.

We now compute the expected computational cost for generating $\tilde{Z}$. Let c_n be the computational cost for generating $Z_n - Z_{n-1}$. Then, the expected cost is

$$C = \sum_{i=1}^{n} p_n c_n. \tag{4.12}$$

In order to have C finite, it is almost necessary that

$$p_n < n^{-1} c_n^{-1}. \tag{4.13}$$

Based on the above calculation, if the estimator $\tilde{Z}$ has a finite variance and a finite expected computation time, then p_n must satisfy both (4.11) and (4.13), which suggests

$$\mathbb{E}(Z_n - Z_{n-1})^2 < n^{-2}c_n^{-1}. \tag{4.14}$$

That is, one must be able to construct a coupling between Z_n and Z_{n-1} such that (4.14) is in place. In Section 4.3, we provide detailed complexity analysis for the random elliptic PDE illustrating the challenges and presenting the solution.

4.2.3 Function spaces and norms

In this section, we present a list of notation that will be frequently used in later discussion. Let $U \subset R^d$ be a bounded open set. We define the following spaces of functions.

$$\begin{aligned}
C^k(\bar{U}) &= \{u : \bar{U} \to R | u \text{ is } k\text{-time continuously differentiable}\} \\
L^p(U) &= \{u : U \to R | \int_U |u(x)|^p dx < \infty\} \\
L^p_{loc}(U) &= \{u : U \to R | u \in L^p(K) \text{ for any compact subset } K \subset U\} \\
C^\infty_c(U) &= \{u : U \to R | u \text{ is infinitely differentiable} \\
&\qquad \text{with a compact support that is a subset of } U\}.
\end{aligned}$$

Definition 4. *For $u, w \in L^1_{loc}(U)$ and a multiple index α, we say w is the α-weak derivative of u, and write*

$$D^\alpha u = w$$

if

$$\int_U u D^\alpha \phi dx = (-1)^{|\alpha|} \int_U w \phi dx \text{ for all } \phi \in C^\infty_c(U),$$

where $D^\alpha \phi$ in the above expression denote the usual α-partial derivative of ϕ.

If $u \in C^k(\bar{U})$ and $|\alpha| \leq k$, then the α-weak derivative and the usual partial derivative are the same. Therefore, we can write $D^\alpha \phi$ for both continuously differentiable and weakly differentiable functions without ambiguous.

We further define norms $\|\cdot\|_{C^k(\bar{U})}$ and $\|\cdot\|_{L^p(U)}$ on $C^k(\bar{U})$ and $L^p(U)$ respectively as follows.

$$\|u\|_{C^k(\bar{U})} = \sup_{|\alpha|\le k, x\in\bar{U}} |D^\alpha u(x)|, \tag{4.15}$$

and

$$\|u\|_{L^p(U)} = \Big(\int_U |u|^p dx\Big)^{1/p}. \tag{4.16}$$

We proceed to the definition of Sobolev space $H^k(U)$ and $H^k_{loc}(U)$

$$H^k(U) = \{u : U \to R | D^\alpha u \in L^2(U) \text{ for all multiple index } \alpha \text{ such that } |\alpha| \le k\}, \tag{4.17}$$

and

$$H^k_{loc}(U) = \{u : U \to R|\ u|_V \in H^k(V) \text{ for all } V \subsetneq U\}$$

For $u \in H^k(U)$, the norm $\|u\|_{H^k(U)}$ and semi-norm $|u|_{H^k(U)}$ are defined as

$$\|u\|_{H^k(U)} = \Big(\sum_{|\alpha|\le k} \|D^\alpha u\|^2_{L^2(U)}\Big)^{1/2}, \tag{4.18}$$

and

$$|u|_{H^k(U)} = \Big(\sum_{|\alpha|=k} \|D^\alpha u\|^2_{L^2(U)}\Big)^{1/2}. \tag{4.19}$$

We define the space $H^1_0(U)$ as

$$H^1_0(U) = \{u \in H^1(U) : u(x) = 0 \text{ for } x \in \partial U\}. \tag{4.20}$$

On the space $H^1_0(U)$ the norm $\|\cdot\|_{H^1(U)}$ and the semi-norm $|\cdot|_{H^1(U)}$ are equivalent.

4.2.4 Finite element method for partial differential equation

We briefly describe the finite element method for partial differential equations. The weak solution $u \in H^1_0(U)$ to (4.1) under the Dirichlet boundary condition (4.2) is defined through the following variational form

$$b(u, v) = L(v) \text{ for all } v \in H^1_0(U), \tag{4.21}$$

where we define the bilinear and linear forms

$$b(u,v)=\int_U a(x)\nabla u(x)\cdot\nabla v(x)dx \quad \text{and} \quad L(v)=\int_U f(x)v(x)dx,$$

and "$\cdot$" is the vector inner product. When the coefficients a and f are sufficiently smooth, say, infinitely differentiable, the weak solution u becomes a strong solution. The key step of the finite element method is to approximate the infinite dimensional space $H_0^1(U)$ by some finite dimensional linear space $V_n = \text{span}\{\phi_1, ..., \phi_{L_n}\}$, where L_n is the dimension of V_n. The approximate solution $u_n \in V_n$ is defined through the set of equations

$$b(u_n, v) = L(v) \text{ for all } v \in V_n. \tag{4.22}$$

Both sides of the above equations are linear in v. Then, (4.22) is equivalent to

$$b(u_n, \phi_i) = L(\phi_i) \text{ for } i = 1, ..., L_n.$$

We further write $u_n = \sum_{i=1}^{L_n} d_i\phi_i$ as a linear combination of the basis functions. Then, (4.22) is equivalent to solving linear equations

$$\sum_{j=1}^{L_n} d_j b(\phi_j, \phi_i) = L(\phi_i) \text{ for } i = 1, ..., L_n. \tag{4.23}$$

The basis functions $\phi_1, ..., \phi_{L_n}$ are often chosen such that (4.23) is a sparse linear system. Solving a sparse linear system requires a computational cost of order $O(L_n \log(L_n))$ as $L_n \to \infty$.

4.3 Main results

In this section, we present the construction of $\tilde{Z}$ and its complexity analysis. We use finite element method to solve the PDE numerically and then construct Z_n. To illustrate the challenge, we start with the complexity analysis of $\tilde{Z}$ based on usual finite element method with linear basis functions, with which we show that (4.11) and (4.13) cannot be satisfied simultaneously. Thus, $\tilde{Z}$ either has infinite variance or has infinite expected computational cost. We improve upon this by means of quadratic approximation under smoothness assumptions on a and f. The estimator $\tilde{Z}$ thus can be generated in constant time and has a finite variance.

4.3.1 Error analysis of finite element method

Piecewise linear basis functions. A popular choice of V_n is the space of piecewise linear functions defined on a triangularization $\mathcal{T}_n$ of U. In particular, $\mathcal{T}_n$ is a partition of U that is each element of $\mathcal{T}_n$ is a triangle partitioning U. The maximum edge length of triangles is proportional to 2^{-n} and V_n is the space of all the piecewise linear functions over $\mathcal{T}_n$ that vanish on the boundary ∂U. The dimension of $\mathcal{T}_n$ is $L_n = O(2^{dn})$. Detailed construction of $\mathcal{T}_n$ and piecewise linear basis functions is provided in Appendix 4.5.3 and Example 5 therein.

Once a set of basis functions has been chosen, the coefficients d_i's are solved according to the linear equations (4.23) and the numerical solution is given by

$$u_n(x) = \sum_{i=1}^{L_n} d_i \phi_i(x).$$

For each functional $\mathcal{Q}$, the biased estimator is

$$Z_n = \mathcal{Q}(u_n).$$

It is important to notice that, for different n, u_n are computed based on the same realizations of a and f. Thus, Z_n and Z_{n-1} are coupled.

We now proceed to verifying (4.14) for linear basis functions. The dimension of V_n is of order $L_n = O(2^{dn})$ where $d = dim(U)$. We consider the case when $\mathcal{Q}$ is a functional that involves weak derivatives of u. For instance, $\mathcal{Q}$ could be in the form $q(|\cdot|_{H^1(U)})$ for some smooth function q and $Z = \mathcal{Q}(u)$, where $|\cdot|_{H^1(U)}$ is defined as in (4.19).

According to Proposition 4.2 of Charrier *et al.* [2013], under the conditions that $\mathbb{E}[\frac{1}{\min_{x\in U} a^p(x)}] < \infty$, $\mathbb{E}(\|a\|^p_{C^1(\bar{U})}) < \infty$, and $\mathbb{E}(\|f\|^p_{L^2(U)}) < \infty$ for all $p > 0$, $\mathbb{E}(Z_n -$

$Z_{n-1})^2 = O(2^{-2n})$ if u_n and u_{n-1} are computed using the same sample of a and f. The condition (4.14) becomes

$$n2^{-2(n-1)} < n^{-1}2^{-dn}|\log 2^{-nd}|^{-1}.$$

A simple calculation yields that the above inequality holds only if $d = 1$. Therefore, *it is impossible to pick p_n such that the estimator $\tilde{Z}$ has a finite variance and a finite expected computational cost using the finite element method with linear basis functions if $d \geq 2$.* The one-dimensional case is not of great interest given that u can be solved explicitly. To establish (4.14) for higher dimensions, we need a faster convergence rate of the PDE numerical solver.

Quadratic basis functions. We improve accuracy of the finite element method by means of piecewise polynomial basis functions under smoothness conditions on $a(x)$ and $f(x)$. Classical results (e.g. Knabner and Angermann [2003]) show that finite element method with polynomial basis functions provides more accurate results than that with piecewise linear basis functions. We obtain similar results for random coefficients. Define the minimum and maximum of $a(x)$ as

$$a_{\min} = \min_{x\in\bar{U}} a(x) \text{ and } a_{\max} = \max_{x\in\bar{U}} a(x).$$

We make the following assumptions on the random coefficients $a(x)$ and $f(x)$.

A1. $a_{\min} > 0$ almost surely and $\mathbb{E}(1/a_{\min}^p) < \infty$, for all $p \in (0, \infty)$.

A2. a is almost surely continuously twice differentiable and $\mathbb{E}(\|a\|_{C^2(\bar{U})}^p) < \infty$ for all $p \in (0, \infty)$.

A3. $f \in H^1(U)$ almost surely and $\mathbb{E}(\|f\|_{H^1(U)}^p) < \infty$ for all $p \in (0, \infty)$.

A4. There exist non-negative constants p' and κ_q such that for all $w_1, w_2 \in H_0^1(U)$,

$$|\mathcal{Q}(w_1) - \mathcal{Q}(w_2)| \leq \kappa_q \max\{\|w_1\|_{H^1(U)}^{p'}, \|w_2\|_{H^1}^{p'}\}\|w_1 - w_2\|_{H^1(U)}.$$

With the assumptions A1-A4, we are able to construct an unbiased estimator for $w_{\mathcal{Q}} = \mathbb{E}[\mathcal{Q}(u)]$ with both finite variance and finite expected computational time.

Let k be a positive interger and $\mathcal{T}_n$ be a regular triangularization of the domain U with mesh size $\sup_{K\in\mathcal{T}_n} diam(K) = O(2^{-n})$, whose detailed definition is provided in Appendix 4.5.3 and let $V_n^{(k)}$ be the set of piecewise continuous polynomials on $\mathcal{T}_n$ that have degrees no more than k and vanish on the boundary of U. To be more specific, $V_n^{(k)}$ is defined as follows

$$V_n^{(k)} = \Big\{v \in C(\bar{U}) : v|_K \text{ is a polynomial with degree no more than } k, \\ \text{for each } K \in \mathcal{T}_n \text{ and } v|_{\bar{U}\setminus D_n} = 0\Big\},$$

where $D_n = int(\cup_{K\in\mathcal{T}_n, K\subset\bar{U}} K)$ and $int(A)$ denotes the interior of the set A. An approximate solution $u_n^{(k)}$ is obtained by solving (4.22) with $V_n = V_n^{(k)}$, that is,

$$u_n^{(k)} \in V_h^{(k)} \text{ such that } b(u_n^{(k)}, v) = L(v), \text{ for all } v \in V_n^{(k)}. \tag{4.24}$$

In what follows, we present a bound of the convergence rate of $\|u_n^{(k)} - u\|_{H^1(U)}$, where u is the solution to (4.21) and $u_n^{(k)}$ is the solution to (4.24).

We start with the existence and the uniqueness of the solution. Notice that $a(x)$ is bounded below by positive random variables $a_{\min}$ and above by $a_{\max}$. According to Lax-Milgram Lemma, (4.21) has a unique solution almost surely.

Lemma 10 (Charrier *et al.* [2013], Lemma 2.1.)**.** *Under assumptions A1-A3,* (4.21) *has a unique solution $u \in H_0^1(U)$ almost surely and*

$$\|u\|_{H^1(U)} \leq \kappa \frac{\|f\|_{L^2(U)}}{a_{\min}}.$$

The next theorem establishes the convergence rate of the approximate solution $u_n^{(k)}$ to the exact solution u.

Theorem 6. *Let $u_n^{(k)}$ be the solution to* (4.24)*. For* $\dim(U) \leq 3$ *with a* $(k+1)$*-time differentiable boundary ∂U, if $a(x) \in C^k(\bar{U})$ and $f(x) \in H^{k-1}(U)$ for some positive* *integer k, then we have*

$$\|u - u_n^{(k)}\|_{H^1(U)} = O\Big(\kappa(a,k)\|f\|_{H^{k-1}(U)} 2^{-kn}\Big), \tag{4.25}$$

where the constant $\kappa(a,k)$ is defined as

$$\kappa(a,k) = \frac{\max(\|a\|_{C^k(\bar{U})}, 1)^{\frac{k^2}{2}+\frac{9}{2}k-\frac{1}{2}}}{\min(a_{\min}, 1)^{\frac{k^2}{2}+\frac{7}{2}k+\frac{3}{2}}}.$$

The proof of Theorem 6 is given in Appendix 4.5.1. In our analysis, we focus on the case $k = 2$ that is sufficient for our analysis. We state the results for this special case.

Corollary 5. *For $dim(U) \leq 3$, if $a(x) \in C^2(\bar{U})$ and $f(x) \in H^1(U)$, then*

$$\|u - u_n^{(2)}\|_{H^1(U)} = O\Big(\frac{\max(\|a\|_{C^2(\bar{U})}, 1)^{10.5}}{\min(a_{\min}, 1)^{10.5}}\|f\|_{H^1(U)} 2^{-2n}\Big).$$

Quadrature Error Analysis. The numerical solution $u_n^{(k)}$ in (4.24) requires the evaluation of the integrals $b(w,v) = \sum_{K\in\mathcal{T}_n}\int_K a(x)\nabla w(x)\cdot\nabla v(x)dx$ and $L(v) = \sum_{K\in\mathcal{T}_n}\int_K f(x)v(x)dx$. This requires generating the entire continuous random fields $a(x)$ and $f(x)$. For the evaluation of these integrals we apply quadrature approximation.

In our analysis, we use linear approximation to $a(\cdot)$ and $f(\cdot)$ on each simplex $K \in \mathcal{T}_n$, then the integrals can be calculated analytically. We will give a careful analysis for the quadrature error of $b(w,v)$. The analysis for $L(v)$ is similar and thus is omitted.

Let $\tilde{a}(\cdot)$ be the linear interpolation of $a(\cdot)$ given its values on vertices such that for all simplex $K \in \mathcal{T}_n$, $\tilde{a}(x) = a(x)$ if x is a vertice of K, and $\tilde{a}|_K$ is linear. Such interpolation is easy to obtain using piecewise linear basis functions discussed in Section 4.3.1. We define the bilinear form induced by $\tilde{a}(\cdot)$ as

$$\tilde{b}_n(w,v) = \sum_{K\in\mathcal{T}_n}\int_K \tilde{a}(x)\nabla w(x)\cdot\nabla v(x)dx,$$

and denote by $\tilde{u}_n \in V_n^{(2)}$ the solution to

$$\tilde{b}_n(\tilde{u}_n, v) = L(v), \text{ for all } v \in V_n^{(2)}. \tag{4.26}$$

The next theorem establishes the convergence rate for $\tilde{u}_n$ to the solution u. The proof for Theorem 7 is given in Appendix 4.5.1.

Theorem 7. *For dim$(U) \leq 3$, if $a(x) \in C^2(\bar{U})$ and $f(x) \in H^1(U)$, then*

$$\|u - \tilde{u}_n\|_{H^1(U)} = O\Big(\frac{\min(\|a\|_{C^2(\bar{U})}, 1)^{11.5}}{\min(a_{\min}, 1)^{11.5}}\|f\|_{H^1(U)}2^{-2n}\Big).$$

This accuracy is sufficient for the unbiased estimator to have finite variance and finite expected stopping time. Similarly, we let $\tilde{f}$ be the linear interpolation of f on $\mathcal{T}_n$ and define $\tilde{L}(v) = \sum_{K\in\mathcal{T}_n}\int_K \tilde{f}(x)v(x)dx$. We redefine $\tilde{u}_n$ such that

$$\tilde{b}_n(\tilde{u}_n, v) = \tilde{L}(v), \text{ for all } v \in V_n^{(2)}. \tag{4.27}$$

Similar approximation results as that of Theorem 7 can be obtained. We omit the repetitive details.

4.3.2 Construction of the unbiased estimator

In this section, we apply the results obtained in Section 4.3.1 to construct an unbiased estimator with both finite variance and finite expected computational cost through (4.8). We start with providing an upper bound of $\mathbb{E}[\mathcal{Q}(u) - \mathcal{Q}(\tilde{u}_n)]^2$.

Proposition 6. *Under assumptions A1-A4, we have*

$$\mathbb{E}[\mathcal{Q}(u) - \mathcal{Q}(\tilde{u}_n)]^2 = O(\kappa_q 2^{-4n}), \tag{4.28}$$

where u is the solution to (4.21) *and $\tilde{u}_n$ is the solution to* (4.27)*, and κ_q the Lipschitz constant appeared in condition A4.*

Proof. The proof is a direct application of Lemma 10, Theorem 7 and A4 and therefore is omitted. □

We proceed to the construction of the unbiased estimator $\tilde{Z}$ via (4.8). Choose

$$\mathbb{P}(N = n) = p_n \propto 2^{-\frac{4+d}{2}n}.$$

For each n, let $\tilde{u}_{n-1}$ and $\tilde{u}_n$ be defined as in (4.27) with respect to the same a and f. Notice that the computation of $\tilde{u}_n$ requires the values of a and f only on the vertices of $\mathcal{T}_n$. Then, Z_{n-1} and Z_n are given by $Z_{n-1} = \mathcal{Q}(\tilde{u}_{n-1})$ and $Z_n = \mathcal{Q}(\tilde{u}_n)$. With this coupling, according to Proposition 6, we have that

$$\mathbb{E}(Z_n - Z_{n-1})^2 \leq 2\mathbb{E}[\mathcal{Q}(\tilde{u}_n) - \mathcal{Q}(u)]^2 + 2\mathbb{E}[\mathcal{Q}(\tilde{u}_{n-1}) - \mathcal{Q}(u)]^2 = O(2^{-4n}).$$

According to equation (4.9), for $d = \dim(U) \leq 3$, we have

$$\mathbb{E}(\tilde{Z}^2) \leq \sum_{n=1}^{\infty} 2^{-4n}/2^{-(4+d)n/2} < \infty.$$

Furthermore, (4.27) requires solving $O(2^{dn})$ sparse linear equations. The computational cost of obtaining u_n is $O(n2^{dn})$. According to (4.12), the expected cost of generating a single copy of $\tilde{Z}$ is

$$\mathbb{E}(C) = \sum_{n=1}^{\infty} p_n c_n \leq \sum_{i=1}^{\infty} n2^{dn} \cdot 2^{-(4+d)n/2} < \infty.$$

This guarantees that the unbiased estimator $\tilde{Z}$ has a finite variance and can be generated in finite expected time.

4.4 Simulation Study

4.4.1 An illustrating example

We start with a simple example for which closed form solution is available and therefore we are able to check the accuracy of the simulation. Let $U = (0,1)^2$, $f(x) = \sin(\pi x_1)\sin(\pi x_2)$ and $a(x) = e^W$, where W is a standard normal distributed random variable. In this example, the exact solution to (4.1) is

$$u(x_1, x_2) = (2\pi^2)^{-1} e^{-W} \sin(\pi x_1)\sin(\pi x_2). \tag{4.29}$$

We are interested in the output functional $\mathcal{Q}(u) = |u|^2_{H^1(U)}$ whose expectation is in a closed form.

$$\mathbb{E}|u|^2_{H^1(U)} = \mathbb{E}[(8\pi^2)^{-1}e^{-2W}] = (8\pi^2)^{-1}e^2 \approx 0.0936.$$

Let $p_n = 0.875 \times 0.125^n$ and $Z_n = \mathcal{Q}(\tilde{u}_n)$ for $n > 0$. Here Z_0 is not a constant and we estimate $\mathbb{E}(Z_0)$ and $\mathbb{E}(Z - Z_0)$ separately. To be more precise, we first estimate $\mathbb{E}(Z_0)$ using the usual Monte Carlo estimate with 10000 replicates and obtain $\hat{Z}_0 = 0.036$ with standard error 0.0024. The estimator according to (4.8) is

$$\tilde{Z} = \hat{Z}_0 + \frac{Z_N - Z_{N-1}}{p_N}. \tag{4.30}$$

We perform Monte Carlo simulation with $M = 10000$ replications. The averaged estimator is 0.0939 with the standard deviation 0.0036. Figure 4.1 shows the histogram of samples of $\tilde{Z}$ and $\log \tilde{Z}$.

In order to conform our analytical results, we simulate the expectation for $\mathbb{E}(Z_n - Z)^2$ and c_n for $n = 0, .., 5$, using 1000 Monte Carlo sample for each of them. The scatter plot of n and $\log_2(\mathbb{E}(Z_n - Z)^2)$ is shown in Figure 4.2. The slope of the regression line in this graph is -3.85, which is close to the theoretical value -4. The scatter plot of n and $\log_2 c_n$ is shown in Figure 4.3. The slope of the regression line in this graph is 2.031, which is close to the theoretical value 2.

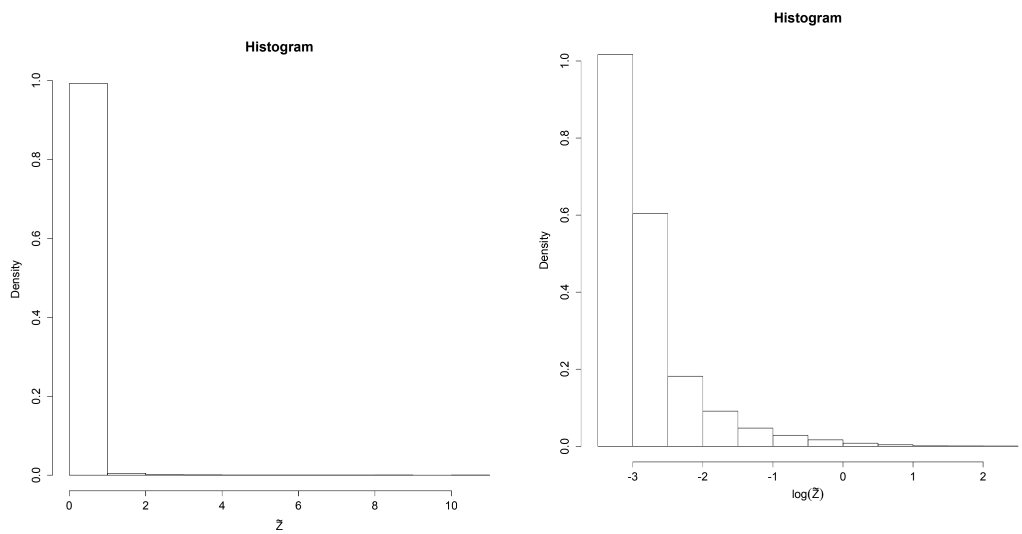
4.4.2 Log-normal random field with Gaussian covariance kernel

Here we let $U = (0,1)^2$, $f = 1$, and $\log a$ be modeled as a Gaussian random field with the covariance function

$$Cov(\log(a(x)), \log(a(y))) = \exp(-|x - y|^2/\lambda).$$

with $\lambda = 0.03$. Such a log-normal random field is infinitely differentiable and satisfies assumptions A1 and A2. We use the circulant embedding method (see Dietrich and Newsam [1997]) to generate the random field $\log a$ exactly. We use the same estimator

Figure 4.1: Histogram of Monte Carlo sample of $\tilde{Z}$ and $\log \tilde{Z}$ that are defined in Section 4.4.1.



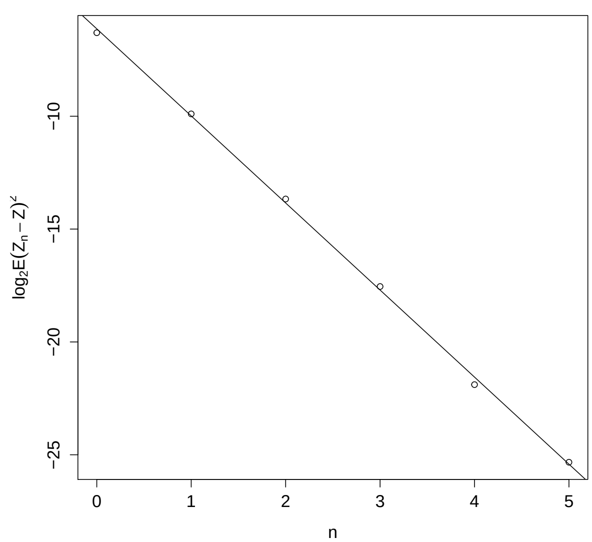


Figure 4.2: Scatter plots for n against $\log(\mathbb{E}(Z - Z_n)^2)$ in the example in Section 4.4.1.

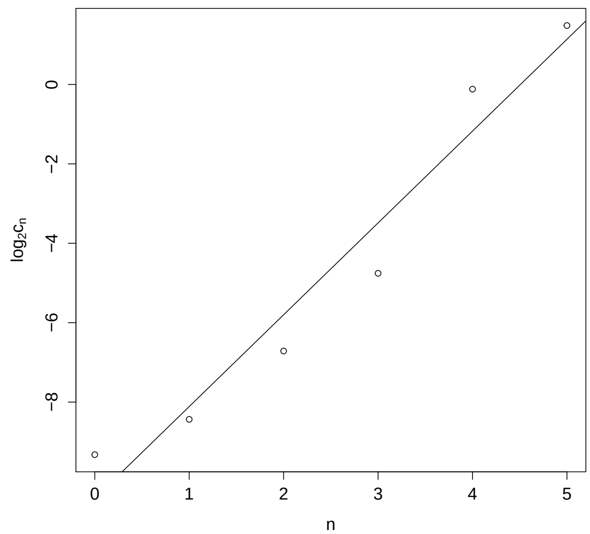


Figure 4.3: Scatter plots for n against $\log(c_n)$ in the example in Section 4.4.1.

as in (4.30) and consider $\mathcal{Q}(u) = |u|^2_{H^1(U)}$. We perform Monte Carlo simulation for $M = 100000$ replications. The averaged estimator for the expectation $\mathbb{E}\mathcal{Q}(u)$ is 0.0428 and the standard deviation is 0.0032 for the averaged estimator. Figure 4.4 shows the histogram of the Monte Carlo sample.

4.5 Appendix to Chapter 4

4.5.1 Proof of the Theorems

In this section, we provide technical proofs of Theorem 6 and Theorem 7. Throughout the proof we will use κ as a generic notation to denote large and not-so-important constants whose value may vary from place to place. Similarly, we use ε as a generic notation for small positive constants.

Proof of Theorem 6. Using Céa's lemma (Theorem 2.17 of Knabner and Angermann [2003]), the convergence rate of finite element method can be bounded according to

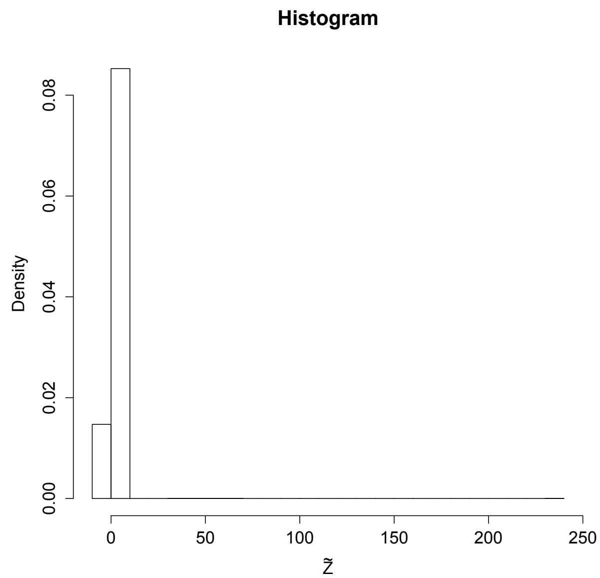


Figure 4.4: Histogram of Monte Carlo sample of $\tilde{Z}$ when $\log a$ has a Gaussian covariance.

the regularity property of u.

$$\|u - u_n^{(k)}\|_{H^1(U)} \leq (\frac{a_{\max}}{a_{\min}})^{1/2} \inf_{v \in V_n^{(k)}} \|u - v\|_{H^1(U)}. \tag{4.31}$$

Furthermore, if $u \in H^{k+1}(U)$, standard interpolation result (See Theorem 3.29 of Knabner and Angermann [2003]) gives an upper bound of the right-hand side of the inequality (4.31)

$$\inf_{v \in V_n^{(k)}} \|u - v\|_{H^1(U)} = O\Big(2^{-kn} \|u\|_{H^{k+1}(U)}\Big). \tag{4.32}$$

According to (4.31) and (4.32), it is sufficient to derive an upper bound of $\|u\|_{H^{k+1}(U)}$, which is given in the following proposition.

Proposition 7. *Under the setting of Theorem 6, we have*

$$\|u\|_{H^{k+1}(U)} \leq \kappa \frac{\max(\|a\|_{C^k(\bar{U})}, 1)^{\frac{k^2}{2} + \frac{9}{2}k - 1}}{\min(a_{\min}, 1)^{\frac{k^2}{2} + \frac{7}{2}k}} \Big(\|f\|_{H^{k-1}(U)} + \|u\|_{L^2(U)}\Big).$$

Combining (4.32) and Proposition 7 we have

$$\inf_{v\in V_n^{(k)}} \|u-v\|_{H^1(U)} \le 2^{-kn}\kappa \frac{\max(\|a\|_{C^k(\bar{U})},1)^{\frac{k^2}{2}+\frac{9}{2}k-\frac{1}{2}}}{\min(a_{\min},1)^{\frac{k^2}{2}+\frac{7}{2}k+\frac{1}{2}}}\Big(\|f\|_{H^{k-1}(U)}+\|u\|_{L^2(U)}\Big). \quad (4.33)$$

According to the Poincaré's lemma (Theorem 2.18 of Knabner and Angermann [2003])

$$\|u\|_{L^2(U)} \le \kappa\|u\|_{H^1(U)}.$$

Thanks to Lemma 10, the above display can be further bounded by

$$\|u\|_{L^2(U)} \le \kappa\frac{\|f\|_{L^2(U)}}{a_{\min}}.$$

We complete the proof by combining the above expression and (4.33). □

Proof of Theorem 7. According to Lemma 3.12 of Knabner and Angermann [2003],

$$\|u-\tilde{u}_n\|_{H^1(U)} \le \inf_{v\in V_n^{(k)}} \Big\{(1+\frac{a_{\max}}{a_{\min}})\|u-v\|_{H^1(U)} + \frac{1}{a_{\min}}\sup_{w\in V_n^{(k)}}\frac{|b(v,w)-\tilde{b}(v,w)|}{\|w\|_{H^1(U)}}\Big\}. \quad (4.34)$$

Notice that $\tilde{a}$ is a linear interpolation of a with $O(2^{-n})$ mesh size, so the difference between $\tilde{a}$ and a is $O(\|a\|_{C^2(\bar{U})}2^{-2n})$ and

$$\begin{aligned} |b(v,w)-\tilde{b}(v,w)| &= |\sum_{K\in\mathcal{T}_n}\int_K(\tilde{a}(x)-a(x))\nabla v\cdot\nabla w dx| \\ &\le \kappa\|a\|_{C^2(\bar{U})}2^{-2n}\sum_{K\in\mathcal{T}_n}\int_K|\nabla v|\cdot|\nabla w|dx. \end{aligned}$$

Therefore, for all $v\in V_n^{(k)}$, we have

$$\|u-\tilde{u}_n\|_{H^1(U)} \le \kappa(1+\frac{a_{\max}}{a_{\min}})\|u-v\|_{H^1(U)} + \frac{\|a\|_{C^2(\bar{U})}}{a_{\min}}\|v\|_{H^1(U)}2^{-2n}.$$

Let $v=u_n^{(2)}$. According to Lemma 10, Theorem 6, and the above display, we complete the proof. □

For the rest of the section, we provide the proof for Proposition 7. Proposition 7 is similar to Theorem 5 in Chapter 6.3 of Evans [1998] but we provide explicitly the dependence of constants on a and f.

Proof of Proposition 7. We prove Proposition 7 by proving the following result for the weak solution $w \in H_0^1(U)$ to a more general PDE,

$$\begin{cases} -\nabla \cdot (A\nabla w) &= f \text{ in } U \\ w &= 0 \text{ on } \partial U, \end{cases} \tag{4.35}$$

where $A(x) = (A_{ij}(x))_{1\le i,j\le d}$ is a symmetric positive definite matrix function in the sense that there exist $A_{\min} > 0$ satisfying

$$\xi^T A(x)\xi \ge A_{\min}|\xi|^2 \tag{4.36}$$

for all $x \in \bar{U}$ and $\xi \in R^d$. Assume that $A_{ij}(x) \in C^k(\bar{U})$ for all $i, j = 1, ..., d$. Then, it is sufficient to show that

$$\|w\|_{H^{k+1}(U)} \le \kappa_r(A,k)\Big(\|f\|_{H^{k-1}(U)} + \|w\|_{L^2(U)}\Big), \tag{4.37}$$

where $\kappa_r(A,k) = \kappa\frac{\max(\|A\|_{C^k(\bar{U})},1)^{\frac{k^2}{2}+\frac{9}{2}k-1}}{\min(A_{\min},1)^{\frac{k^2}{2}+\frac{7}{2}k}}$, and $\|A\|_{C^k(\bar{U})} = \max_{1\le i,j\le d}\|A_{ij}\|_{C^k(\bar{U})}$.

Let $B^0(0,r)$ denote the open ball $\{x : |x| < r\}$ and $R^d_+ = \{x \in R^d : x_d > 0\}$. We will first prove that if $U = B^0(0,r) \cap R^d_+$ and $V = B^0(0,t) \cap R^d_+$, then for all t and r such that and $0 < t < r$,

$$\|w\|_{H^{m+2}(V)} \le \kappa_{r,t,m+1}\frac{\max(\|A\|_{C^k(\bar{U})},1)^{\frac{(m+1)^2}{2}+\frac{9}{2}(m+1)-1}}{\min(A_{\min},1)^{\frac{(m+1)^2}{2}+\frac{7}{2}(m+1)}}\Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)}\Big), \tag{4.38}$$

where $\kappa_{r,t,m+1}$ is a constant depending only on r, t, and $m+1$. The following lemma establish (4.38) for $m = 0$.

Lemma 11 (Boundary H^2-regularity)**.** *Assume ∂U is twice differentiable and $A(x)$ satisfies* (4.36)*. Assume that $A_{ij}(x) \in C^1(\bar{U})$ for all $i, j = 1, ..., d$. Suppose furthermore $w \in H_0^1(U)$ is a weak solution to the elliptic PDE with boundary condition*

(4.35). *Then* $w \in H^2(U)$ *and*

$$\|w\|_{H^2(U)} \leq \kappa \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^4}{\min(A_{\min}, 1)^4} \Big(\|f\|_{L^2(U)} + \|w\|_{L^2(U)} \Big).$$

We establish (4.38) by induction. Suppose for some m

$$\|w\|_{H^{m+1}(W)} \leq \kappa_{t,s,m} \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{\frac{m^2}{2}+\frac{9}{2}m-1}}{\min(A_{\min}, 1)^{\frac{m^2}{2}+\frac{7}{2}m}} (\|f\|_{H^{m-1}(U)} + \|w\|_{L^2(U)}), \tag{4.39}$$

where

$$W = B^0(0, s) \cap R^d_+, \text{ and } s = \frac{t+1}{2}. \tag{4.40}$$

Since w is a weak solution to (4.35), it satisfies the integration equation

$$\int_D \nabla w(x)^T A(x) \nabla v(x) dx = \int_D f(x) v(x) dx, \text{ for all } v \in H^1_0(U). \tag{4.41}$$

Let $\alpha = (\alpha_1, ..., \alpha_d)$ be a multiple index with such that $\alpha_d = 0$ and $|\alpha| = m$. We consider the multiple weak derivative $\bar{w} = D^\alpha w$ and investigate the PDE that $\bar{w}$ satisfies. For any $\bar{v} \in C_c^\infty(W)$, where $C_c^\infty(W)$ is the space of infinitely differentiable functions that have compact support in W, we plug $v = (-1)^{|\alpha|} D^\alpha \bar{v}$ into (4.41). With some calculations, we have

$$\int_W (\nabla \bar{w}(x))^T A(x) \nabla \bar{v}(x) = \int_W \bar{f}(x) \bar{v}(x) dx,$$

where

$$\bar{f} = D^\alpha f - \sum_{\beta \leq \alpha, \beta \neq \alpha} \binom{\alpha}{\beta} \Big[-\nabla \cdot (D^{\alpha-\beta} A \nabla D^\beta w) \Big]. \tag{4.42}$$

Consequently, $\bar{w}$ is a weak solution to the PDE

$$-\nabla \cdot (A \nabla \bar{w}) = \bar{f} \quad \text{ for } x \text{ in } W. \tag{4.43}$$

Furthermore, we have the boundary condition $\bar{w}(x) = 0$ for $x \in \partial W \cap \{x_d = 0\}$. By the induction assumption (4.39) and (4.42), we have

$$\|\bar{f}\|_{L^2(W)} \leq \|f\|_{H^m(U)} + \kappa_{t,s,m} \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{\frac{m^2}{2}+\frac{9}{2}m-1}}{\min(A_{\min}, 1)^{\frac{m^2}{2}+\frac{7}{2}m}} \times \|A\|_{C^{m+1}(\bar{U})} \Big(\|f\|_{H^{m-1}(U)} + \|w\|_{L^2(U)} \Big). \tag{4.44}$$

According to the definition of $\bar{w}$, we have

$$\|\bar{w}\|_{L^2(W)} \leq \|w\|_{H^m(W)}. \tag{4.45}$$

Applying Lemma 11 to $\bar{w}$ with (4.44) and (4.45), we have

$$\begin{aligned}
&\|D^\alpha w\|_{H^2(V)} \\
&\leq \kappa_{t,s,m}\kappa \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^4}{\min(A_{\min}, 1)^4} \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{\frac{m^2}{2}+\frac{9}{2}m-1}}{\min(A_{\min}, 1)^{\frac{m^2}{2}+\frac{7}{2}m}} \\
&\qquad \times \|A\|_{C^{m+1}(\bar{U})}\Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)}\Big).
\end{aligned} \tag{4.46}$$

Because α is an arbitrary multi-index such that $\alpha_d = 0$, and $|\alpha| = m$, (4.46) implies that $D^\beta w \in L^2(W)$ for any multiple index β such that $|\beta| \leq m+2$ and $\beta_d = 0, 1, 2$. We now extend this result to multiple index β whose last component is greater than 2. Suppose for all β such that $|\beta| \leq m+2$ and $\beta_d \leq j$, we have

$$\|D^\beta w\|_{H^2(V)} \leq \kappa_r^{(j)}\Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)}\Big), \tag{4.47}$$

where $\kappa_r^{(j)}$ is a constant depending on A, m and j that we are going to determine later. We establish the relationship between $\kappa_r^{(j)}$ and $\kappa_r^{(j+1)}$. For any γ that is a multiple index such that $|\gamma| = m+2$ and $\gamma_d = j+1$, we use (4.47) to develop an upper bound for $\|D^\gamma w\|_{H^2(V)}$. In particular, let $\beta = (\gamma_1, .., \gamma_{d-1}, j-1)$. According to the remark (ii) after Theorem 1 of Chapter 6.3 in Evans [1998], we have that

$$-\nabla \cdot (A\nabla(D^\beta w)) = f^\dagger \text{ in } W \text{ a.e}, \tag{4.48}$$

where

$$f^\dagger = D^\beta f - \sum_{\delta\leq\beta,\delta\neq\beta} \binom{\beta}{\delta}\Big[-\nabla\cdot(D^{\beta-\delta}A\nabla D^\delta w)\Big]. \tag{4.49}$$

Notice that

$$\begin{aligned}
&-\nabla\cdot(A\nabla(D^\beta w)) \\
=\ &-A_{dd}D^\gamma w \\
&+ \text{sum of terms involves at most } j \text{ times weak derivatives of } w \\
&\ \text{with respect to } x_d \text{ and at most } m+2 \text{ times derivatives in total.}
\end{aligned}$$

According to (4.47), (4.48), (4.49), and the above display, we have

$$\|D^\gamma w\|_{L^2(U)} \leq \kappa \frac{1}{\min(A_{\min}, 1)} \Big\{ \|A\|_{C^{m+1}(\bar{U})} \kappa_r^{(j)} \Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)} \Big) + \|f\|_{H^m(U)} \Big\}.$$

Therefore,

$$\|D^\gamma w\|_{L^2(U)} \leq \kappa_r^{(j+1)} \Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)} \Big),$$

where

$$\kappa_r^{(j+1)} = \kappa_r^{(j)} \frac{\max(\|A\|_{C^{m+1}(\bar{U})}, 1)}{\min(A_{\min}, 1)}. \tag{4.50}$$

The above expression provides a relationship for $\kappa_r^{(j+1)}$ and $\kappa_r^{(j)}$. According to (4.46),

$$\kappa_r^{(2)} = \kappa_{t,s,m} \kappa \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^4}{\min(A_{\min}, 1)^4} \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{\frac{m^2}{2} + \frac{9}{2}m - 1}}{\min(A_{\min}, 1)^{\frac{m^2}{2} + \frac{7}{2}m}} \max(\|A\|_{C^{m+1}(\bar{U})}, 1).$$

Using (4.50) and the above initial value for the iteration, we have

$$\begin{aligned}\kappa_r^{(m+2)} = \kappa_{t,s,m} \kappa &\frac{\max(\|A\|_{C^1(\bar{U})}, 1)^4}{\min(A_{\min}, 1)^4} \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{\frac{m^2}{2} + \frac{9}{2}m - 1}}{\min(A_{\min}, 1)^{\frac{m^2}{2} + \frac{7}{2}m}} \\ &\times \max(\|A\|_{C^{m+1}(\bar{U})}, 1) \Big\{ \frac{\max(\|A\|_{C^{m+1}(\bar{U})}, 1)}{\min(A_{\min}, 1)} \Big\}^m. \end{aligned} \tag{4.51}$$

Consequently,

$$\|w\|_{H^{m+2}(V)} \leq \kappa_{t,s,m} \kappa \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{\frac{m^2}{2} + \frac{11}{2}m + 4}}{\min(A_{\min}, 1)^{\frac{m^2}{2} + \frac{9}{2}m + 4}} \Big(\|f\|_{H^m(U)} + \|w\|_{L^2(V)} \Big).$$

Using induction, we complete the proof of (4.37) for the case where U is a half ball.

Now we extend the result to the case that U has a C^{k+1} boundary ∂U. We first prove the theorem locally for any point $x^0 \in \partial U$. Because ∂U is $(k+1)$-time differentiable, with possibly relabeling, the coordinates of x there exist a function $\gamma : R^{d-1} \to R$ and $r > 0$ such that,

$$B(x^0, r) \cap U = \{x \in B(x^0, r) : x_d > \gamma(x_1, ..., x_{d-1})\}.$$

Let $\Phi = (\Phi_1, ..., \Phi_d)^T : R^d \to R^d$ be a function such that

$$\Phi_i(x) = x_i \text{ for } i = 1, ..., d-1 \text{ and } \Phi_d(x) = x_d - \gamma(x_1, ..., x_{d-1}).$$

Let $y = \Phi(x)$ and choose $s > 0$ sufficiently small such that

$$U^* = B^0(0, s) \cap \{y_d > 0\} \subset \Phi(U \cap B(x^0, r)).$$

Furthermore, we let $V^* = B^0(0, \frac{s}{2}) \cap \{y_d > 0\}$ and set

$$w^*(y) = w(x) = w(\Phi^{-1}(y)).$$

With some calculation, we have that w^* is a weak solution to the PDE

$$-\nabla \cdot \Big(A^*(y)\nabla w^*(y)\Big) = f^*(y),$$

where $A^*(y) = J(y)A(\Phi^{-1}(y))J^T(y)$ and $J(y)$ is the Jacobian matrix for Φ with $J_{ij}(y) = \frac{\partial \Phi_i(x)}{\partial x_j}|_{x=\Phi^{-1}(y)}$, and $f^*(y) = f(\Phi^{-1}(y))$. In addition, $w^* \in H^1(U^*)$ and $w^*(y) = 0$ for $y \in \partial U^* \cap \{y_d = 0\}$. It is easy to check A^* is symmetric and $A^*_{ij} \in C^k(\bar{U})$ for all $1 \leq i, j \leq d$. Furthermore, according to the definition of J and Φ, all the eigenvalues of $J(y)$ are 1 and thus $\zeta^T A^*(y)\xi \geq A_{\min}|J^T(y)\xi|^2 \geq \varepsilon A_{\min}|\xi|^2$ for all $\xi \in R^d$. By substituting U, V, A, f with U^*, V^*, A^* and f^* in (4.38) we have

$$\|w^*\|_{H^2(V^*)} \leq \kappa_r(A, k)\Big(\|w^*\|_{L^2(U^*)} + \|f^*\|_{H^{k-1}(U^*)}\Big).$$

According to the definitions of w^* and f^*, the above display implies

$$\|w\|_{H^2(\Phi^{-1}(V^*))} \leq \kappa_r(A, k)\Big(\|w\|_{L^2(U)} + \|f\|_{H^{k-1}(U)}\Big).$$

Because U is bounded, ∂U is compact and thus can be covered by finitely many sets $\Phi^{-1}(V_1^*), .., \Phi^{-1}(V_K^*)$ that are constructed similarly as $\Phi^{-1}(V^*)$. We finish the proof by combining the result for points around ∂U and the following Lemma 12 for interior points.

Lemma 12 (Higher order interior regularity)**.** *Under the setting of Lemma 11, we assume that ∂U is C^{k+1}, $A_{ij}(x) \in C^k(U)$ for all $i, j = 1, ..., d$, and $f \in H^{k-1}(U)$, and that $w \in H^1(U)$ is one of the weak solutions to the PDE* (4.35) *without boundary condition. Then, $w \in H^{k+1}_{loc}(U)$. For each open set $V \subsetneq U$*

$$\|w\|_{H^{k+1}(V)} \leq \kappa_i(A, k)\Big(\|f\|_{H^{k-1}(U)} + \|w\|_{L^2(U)}\Big),$$

where $\kappa_i(A, k) = \frac{\max(\|A\|_{C^k(\bar{U})}, 1)^{3k-1}}{\min(A_{\min}, 1)^{2k}}\kappa$, and κ is a constant depending on V.

□

4.5.2 Proof of supporting lemmas

In this section, we provide the proofs for lemmas that are necessary for the proof of Proposition 7. We start with a useful lemma showing $w \in H^2_{loc}(U)$ which will be used in the proof of Lemma 11

Lemma 13 (Interior H^2-regularity)**.** *Under the setting of Lemma 11, we further assume that $A_{ij}(x) \in C^1(\bar{U})$ for all $i, j = 1, ..., d$, and $f \in L^2(U)$, and that $w \in H^1(U)$ is one of the weak solutions to the PDE* (4.35) *without boundary condition. Then, $w \in H^2_{loc}(U)$. For each open subset $V \subsetneqq U$, there exist κ depending on V such that*

$$\|w\|_{H^2(V)} \leq \kappa \frac{\max(\|A\|_{C^1(U)}, 1)^2}{\min(A_{\min}, 1)^2} \Big(\|f\|_{L^2(U)} + \|w\|_{L^2(U)}\Big),$$

where we define the norm $\|A\|_{C^1(\bar{U})} = \max_{1\leq i,j\leq d} \|A_{ij}\|_{C^1(\bar{U})}$.

Proof of Lemma 13. Let h be a real number whose absolute value is sufficiently small, we define the difference quotient operator

$$D^h_k w(x) = \frac{w(x + he_k) - w(x)}{h},$$

where e_k is the kth unit vector in R^d. According to Theorem 3 in Chapter 5.8 of Evans [1998], if there exist a positive constant κ such that $\|D^h_k w\|_{L^2(U)} \leq \kappa$ for all h, then $\frac{\partial w}{\partial x_k} \in L^2(U)$ and $\|\frac{\partial w}{\partial x_k}\|_{L^2(U)} \leq \kappa$. We use this theorem and seek for an upper bound of

$$\int_V |U^h_k \nabla w|^2 dx, \tag{4.52}$$

for $k = 1, ..., d$ for the rest of the proof.

We derive a bound of (4.52) by plugging an appropriate v in (4.41). Let W be an open set such that $V \subsetneqq W \subsetneqq U$. We select a smooth function ζ such that

$$\zeta = 1 \text{ on } V, \qquad \zeta = 0 \text{ on } W^c, \qquad \text{and } 0 \leq \zeta \leq 1.$$

We plug

$$v = -D_k^{-h}(\zeta^2 D_k^h w)$$

into (4.41), and have

$$-\int_D \nabla w^T A \nabla [D_k^{-h}(\zeta^2 D_k^h w)] dx = -\int_D f D_k^{-h}(\zeta^2 D_k^h w) dx. \tag{4.53}$$

We give a lower bound of the left-hand side of (4.53) and an upper bound of the right-hand. We use two basic formulas that are similar to integration by part and derivative of product respectively. For any functions $w_1, w_2 \in L^2(U)$, such that $w_2(x) = 0$ if $dist(x, \partial U) < h$, we have

$$\int_D w_1 D_k^{-h} w_2 dx = -\int_D D_k^h w_1 w_2 dx \text{ and } D_k^h(w_1 w_2) = w_1^h D_k^h w_2 + w_2 D_k^h w_1,$$

where we define $w_1^h(x) = w_1(x + he_k)$. Similarly, we define the matrix function $A^h = A(x + he_k)$. Applying the above formulas to the left hand side of (4.53), we have

$$\begin{aligned}
& -\int_D \nabla w^T A \nabla [D_k^{-h}(\zeta D_k^h w)] dx \\
= & \int_D D_k^h(\nabla w^T A) \nabla(\zeta^2 D_k^h w) dx \\
= & \int_D D_k^h(\nabla w^T) A^h \nabla(\zeta^2 D_k^h w) + \nabla w^T D_k^h A \nabla(\zeta^2 D_k^h w) dx \\
= & \underbrace{\int_D \zeta^2 D_k^h \nabla w^T A^h D_k^h \nabla w dx}_{J_1} \\
& + \underbrace{\int_D 2\zeta(D_k^h \nabla w^T A^h \nabla\zeta) D_k^h w + 2\zeta(\nabla w^T D_k^h A \nabla\zeta) D_k^h w + \zeta^2 \nabla w^T D_k^h A D_k^h \nabla w dx}_{J_2}.
\end{aligned}$$

J_1 in the above expression has a lower bound

$$J_1 \geq A_{\min} \int_D \zeta^2 |D_k^h \nabla w|^2 dx$$

due to the positively definitiveness of $A(x)$. $|J_2|$ is bounded above by

$$|J_2| \leq \kappa \|A\|_{C^1(\bar{U})} \Big(\int_D \zeta |D_k^h \nabla w| |D_k^h w| + \zeta |\nabla w| |D_k^h w| + \zeta |\nabla w| |D_k^h \nabla w| dx \Big). \tag{4.54}$$

The expression (4.54) can be further bounded by

$$|J_2| \leq \frac{A_{\min}}{2}\int_D \zeta^2 |D_k^h \nabla w|^2 dx + \kappa \|A\|_{C^1(\bar{U})} \times (1 + \frac{\|A\|_{C^1(\bar{U})}}{A_{\min}}) \int_W |\nabla w|^2 + |D_k^h w|^2 dx. \tag{4.55}$$

thanks to Cauchy-Schwarz inequality. According to Theorem 3 in Chapter 5.8 of Evans [1998],

$$\int_W |D_k^h w|^2 dx \leq \kappa \int_W |\nabla w|^2 dx. \tag{4.56}$$

Therefore, (4.55) is bounded above by

$$|J_2| \leq \frac{A_{\min}}{2}\int_D \zeta^2 |D_k^h \nabla w|^2 dx + \kappa^2 \|A\|_{C^1(\bar{U})} \times (1 + \frac{\|A\|_{C^1(\bar{U})}}{A_{\min}}) \int_W |\nabla w|^2 dx. \tag{4.57}$$

Combining (4.54) and (4.57), we have

$$\begin{aligned} & \text{LHS of (4.53)} \\ = \ & J_1 + J_2 \geq J_1 - |J_2| \\ \geq \ & \frac{A_{\min}}{2}\int_D \zeta^2 |D_k^h \nabla w|^2 dx - \kappa^2 \|A\|_{C^1(\bar{U})} \times (1 + \frac{\|A\|_{C^1(\bar{U})}}{A_{\min}}) \int_W |\nabla w|^2 dx. \end{aligned} \tag{4.58}$$

We proceed to an upper bound of the right hand side of (4.53). According to (4.56), we have

$$\begin{aligned} & \int_D |D_k^{-h}(\zeta^2 D_k^h w)|^2 dx \\ \leq \ & \kappa \int_D |\nabla(\zeta^2 D_k^h w)|^2 dx \\ \leq \ & \kappa \int_W 4|D_k^h w|^2 |\nabla \zeta|^2 \zeta^2 + \zeta^2 |D_k^h \nabla w|^2 dx \\ \leq \ & \kappa^3 \int_W |\nabla w|^2 + \zeta^2 |D_k^h \nabla w|^2 dx. \end{aligned} \tag{4.59}$$

Apply Cauchy's inequality to the right-hand side of (4.53), we have

$$\begin{aligned} & \text{RHS of (4.53)} \\ \leq & \int_D |f||D_k^{-h}(\zeta^2 D_k^h w)| dx \leq \frac{2\kappa^3}{A_{\min}}\int_D |f|^2 dx + \frac{A_{\min}}{4\kappa^3}\int_D |D_k^{-h}(\zeta^2 D_k^h w)|^2 dx. \end{aligned} \tag{4.60}$$

We combine (4.59) and (4.60),

$$\text{RHS of (4.53)} \leq \frac{A_{\min}}{4}\int_W \zeta^2|D_k^h\nabla w|^2dx + \frac{A_{\min}}{4}\int_W |\nabla w|^2dx + \frac{2\kappa^3}{A_{\min}}\int_W |f|^2dx. \tag{4.61}$$

Combining (4.58) and (4.61), we have

$$\int_D \zeta^2|D_k^h\nabla w|^2dx \leq \frac{8\kappa^3}{A_{\min}^2}\int_W |f|^2dx+\Big[1+4\kappa^2\|A\|_{C^1(\bar{U})}\frac{\|A\|_{C^1(\bar{U})}+A_{\min}}{A_{\min}^2}\Big]\int_W |\nabla w|^2dx. \tag{4.62}$$

Therefore,

$$\int_D \zeta^2|D_k^h\nabla w|^2dx \leq \kappa\frac{\max(\|A\|_{C^1(\bar{U})},1)^2}{\min(A_{\min},1)^2}\Big(\int_W |f|^2dx + \int_W |\nabla w|^2\Big). \tag{4.63}$$

Now we give an upper bound of $\int_D |\nabla w|$ by taking $v = \tilde{\zeta}^2 w$ in (4.41), where we choose $\tilde{\zeta}$ to be a smooth function such that $\tilde{\zeta} = 1$ on W and $\tilde{\zeta} = 0$ on U^c. Using similar arguments as that for (4.63), we have

$$\int_W |\nabla w|^2dx \leq \kappa\frac{\max(\|A\|_{C^1(\bar{U})},1)^2}{\min(A_{\min},1)^2}\Big(\int_W |f|^2dx + \int_W |\nabla w|^2\Big). \tag{4.64}$$

(4.63) and (4.64) together give

$$\int_D \zeta^2|D_k^h\nabla w|^2dx \leq \kappa\frac{\max(\|A\|_{C^1(\bar{U})},1)^4}{\min(A_{\min},1)^4}\int_D |f|^2 + |w|^2dx. \tag{4.65}$$

We complete our proof by combining (4.65) for all $k = 1, ..., d$. $\square$

Proof of Lemma 11. We first consider a special case when U is a half ball

$$U = B^0(0,1)\cap R_+^d.$$

Let $V = B^0(0,\frac{1}{2})\cap R_+^d$, and select a smooth function ζ such that

$$\zeta = 1 \text{ on } B(0,\frac{1}{2}), \zeta = 0 \text{ on } B(0,1)^c, \text{ and } 0 \leq \zeta \leq 1.$$

For $k = 1, ..., d-1$, we plug

$$v = -D_k^{-h}(\zeta^2 D_k^h w)$$

into (4.41). Using the same arguments for deriving (4.62) as in the proof for Lemma 13, we obtain that

$$\int_V |D_k^h \nabla w|^2 dx \leq \kappa \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^2}{\min(A_{\min}, 1)^2} \int_W |f|^2 + |\nabla w|^2 dx.$$

The above display holds for arbitrary h, so we have

$$\sum_{i,j=1, i+j<2d}^{d} \int_V |\frac{\partial^2 w}{\partial x_i \partial x_j}|^2 dx \leq \kappa \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^2}{\min(A_{\min}, 1)^2} \int_W |f|^2 + |\nabla w|^2 dx. \tag{4.66}$$

We proceed to an upper bound for

$$\int_V |\frac{\partial^2 w}{\partial x_d \partial x_d}|^2 dx.$$

According to the remark (ii) after Theorem 1 in Chapter 6.3 of Evans [1998], with the interior regularity obtained by Lemma 13, w solves (4.35) almost everywhere in U. Consequently,

$$A_{dd} \frac{\partial^2 w}{\partial x_d \partial x_d} = - \sum_{i,j=1, i+j<2d}^{d} A_{ij} \frac{\partial^2 w}{\partial x_i \partial x_j} - \sum_{i,j=1}^{d} \frac{\partial A_{ij}}{\partial x_j} \frac{\partial w}{\partial x_i} - f \text{ a.e.}$$

Note that $A_{dd} \geq A_{\min}$, so the above display implies that

$$|\frac{\partial^2 w}{\partial x_d \partial x_d}| \leq \kappa \frac{\|A\|_{C^1(\bar{U})}}{A_{\min}} \Big(\sum_{i,j=1, i+j<2d}^{d} |\frac{\partial^2 w}{\partial x_i \partial x_j}| + |\nabla w| + |f| \Big).$$

Combining the above display with (4.66), we have

$$\|w\|_{H^2(V)} \leq \kappa \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^2}{\min(A_{\min}, 1)^2} \Big(\||\nabla w|\|_{L^2(U)} + \|f\|_{L^2(U)} \Big).$$

According to (4.64), the above display implies

$$\|w\|_{H^2(V)} \leq \frac{\max(\|A\|_{C^1(\bar{U})}, 1)^4}{\min(A_{\min}, 1)^4} \Big(\|w\|_{L^2(U)} + \|f\|_{L^2(U)} \Big).$$

Similar to the proof for Proposition 7, this result can be extended to the case where U has a twice differentiable boundary. We omit the details. □

Proof of Lemma 12. We use induction to prove Lemma 12. When $k = 1$, Lemma 13 gives

$$\|w\|_{H^2(V)} \leq \kappa_i(A, 1)\Big(\|f\|_{L^2(U)} + \|w\|_{L^2(U)}\Big).$$

Suppose for $k = 1, ..., m$, Lemma 12 holds. We intend to prove that for $k = m + 1$,

$$\|w\|_{H^{m+2}}(V) \leq \kappa_i(A, m + 1)\Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)}\Big).$$

By induction assumption, we have $w \in H^{m+1}_{loc}(U)$ and for any W such that $V \subsetneq W \subsetneq U$

$$\|w\|_{H^{m+1}(W)} \leq \kappa_i(A, m)\Big(\|f\|_{H^{m-1}(U)} + \|w\|_{L^2(U)}\Big). \tag{4.67}$$

Denote by $\alpha = (\alpha_1, .., \alpha_d)^T$ a multiple index with $|\alpha| = \alpha_1 + ... + \alpha_d = m$. With similar arguments as for (4.43), we have that $\bar{w} = D^\alpha w$ is a weak solution to the PDE (4.43) without boundary condition. Similar to the derivation for (4.46), $w \in H^{m+2}(V)$ and

$$\|w\|_{H^{m+2}(V)} \leq \kappa_i(A, 1)\kappa_i(A, m) \max(\|A\|_{C^{m+1}(\bar{U})}, 1)\Big(\|f\|_{H^m(U)} + \|w\|_{L^2(U)}\Big).$$

We complete the proof by induction. □

4.5.3 Triangularization

The triangularization $\mathcal{T}_n$ is a partition of U into triangles parametrized with the mesh size $\max_{K\in\mathcal{T}_h} \operatorname{diam}(K) = O(2^{-n})$, and satisfies the following properties,

(1) $\bar{U} \subset \cup_{K\in\mathcal{T}_n} K$;

(2) For any $K \in \mathcal{T}_n$, the vertices of K lie either all in $\bar{U}$ or all in U^c;

(3) For $K, K' \in \mathcal{T}_n$, $K \neq K'$, $int(K) \cap int(K') = \emptyset$ where $int(K)$ denote the interior of the triangle K;

(4) If $K \neq K'$ but $K \cap K' \neq \emptyset$, then $K \cap K'$ is either a point or a common edge of K and K'.

Example 5. *Here we provide an example of V_n and $\mathcal{T}_n$ defined over the region $U = (0,1)^2$. The detailed definition of $\mathcal{T}_n$ and the finite dimensional subspace V_n is given in Appendix 4.5.3. In Figure 4.5, $\mathcal{T}_n$ is the set of triangles that partitions $(0,1)^2$. The shaded area is the support for the basis function ϕ_1 of the space V_2. In particular, ϕ_1 is a piecewise linear function on each triangle (and is constant if the triangle is outside the support) and $\phi_1(0.25, 0.25) = 1$, $\phi_1(0.25, 0) = \phi_1(0.5, 0) = \phi_1(0.5, 0.25) = \phi_1(0.25, 0.5) = \phi_1(0, 0.5) = 0$. Similar basis functions $\phi_2, ..., \phi_9$ can be constructed corresponding to the nine inner nodes (circled points in Figure 4.5).*

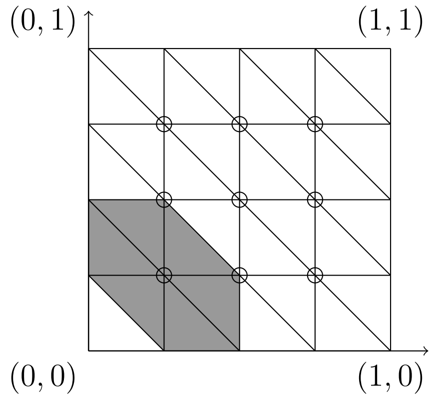


Figure 4.5: Triangularization $\mathcal{T}_2$ on $(0,1)^2$.

Chapter 5

Chernoff Index for the Generalized Likelihood Ratio Test

5.1 Introduction

Cox [1961, 1962] introduced the problem of testing two separate parametric families. Let $X_1, \ldots, X_n$ be independent and identically distributed real-valued observations from a population with density f with respect to some baseline measure μ. Let $\{g_\theta,\ \theta \in \Theta\}$ and $\{h_\gamma,\ \gamma \in \Gamma\}$ denote two separate parametric families of density functions with respect to the same measure μ. Consider testing H_0: $f \in \{g_\theta,\ \theta \in \Theta\}$ against H_1: $f \in \{h_\gamma,\ \gamma \in \Gamma\}$. To avoid singularity, we assume that all the distributions in the families g_θ and h_γ are mutually absolutely continuous so that the likelihood ratio stays away from zero and infinity. Furthermore, we assume that the model is correctly specified, that is, f belongs to either the g-family or the h-family.

Recently revisiting this problem, Cox [2013] mentioned several applications such as the one-hit and two-hit models of binary dose-response and testing of interactions in a balanced 2^k factorial experiment. Furthermore, this problem has been studied in econometrics [Davidson and MacKinnon, 1981; Pesaran and Deaton, 1978; Pesaran, 1974; Vuong, 1989; White, 1982a,b]. For more applications of testing separate families of hypotheses, see Berrington de González and Cox [2007] and Braganca Pereira [2005], and the references therein. Furthermore, there is a discussion of model misspecification, that is, f belongs to neither the g-family nor the h-family, which is beyond the current discussion. For semiparametric models, Fine [2002] proposed a similar test for non-nested hypotheses under the Cox proportional hazards model assumption.

In the discussion of Cox [1962], the test statistic $l = l_g(\hat{\theta}) - l_h(\hat{\gamma}) - E_{g_{\hat{\theta}}}\{l_g(\hat{\theta}) - l_h(\hat{\gamma})\}$ is considered. The functions $l_g(\theta)$ and $l_h(\gamma)$ are the log-likelihood functions under the g-family and the h-family and $\hat{\theta}$ and $\hat{\gamma}$ are the corresponding maximum likelihood estimators. Rigorous distributional discussions of statistic l can be found in Huber [1967] and White [1982a,b]. In the current chapter and Chapter 6, we consider the generalized likelihood ratio statistic

$$LR_n = \frac{\max_{\gamma \in \Gamma} \prod_{i=1}^n h_\gamma(X_i)}{\max_{\theta \in \Theta} \prod_{i=1}^n g_\theta(X_i)} = e^{l_h(\hat{\gamma}) - l_g(\hat{\theta})} \tag{5.1}$$

that is slightly different from Cox's approach. We are interested in the Chernoff efficiency, whose definition is provided in Section 5.2.1, of the generalized likelihood ratio test.

In the hypothesis testing literature, there are several measures of asymptotic relative efficiency for simple null hypothesis against simple alternative hypothesis. Let n_1 and n_2 be the necessary sample sizes for each of two testing procedures to perform equivalently in the sense that they admit the same type I and type II error probabilities. Then, the limit of ratio n_1/n_2 in the regime that both sample sizes tend to infinity represents the asymptotic relative efficiency between these two procedures.

Relative efficiency depends on the asymptotic manner of the two types of error probabilities with large samples. Under different asymptotic regimes, several asymptotic efficiency measures are proposed and they are summarized in Chapter 10 of Serfling [1980]. Under the regime of Pitman efficiency, several asymptotically equivalent tests to Cox test exist. Furthermore, Pesaran [1984] and Rukhin [1993] applied Bahadur's criterion of asymptotic comparison [Bahadur, 1960, 1967] to tests for separate families and compared different tests for lognormal against exponential distribution and for non-nested linear regressions. There are other efficiency measures that are frequently considered, such as Kallenberg efficiency [Kallenberg, 1983].

In the context of testing a simple null hypothesis against a fixed simple alternative hypothesis, Chernoff [1952] introduces a measure of asymptotic efficiency for tests based on sum of independent and identically distributed observations, a special case of which is the likelihood ratio test. This efficiency is introduced by showing no preference between the null hypothesis and the alternative hypothesis. The rejection region is setup such that the two types of error probabilities decay at the same exponential rate ρ. The rate ρ is later known as the Chernoff index. A brief summary of the Chernoff index is provided in Section 5.2.1.

The basic strategy of Chernoff [1952] is applying large deviations techniques to the log-likelihood ratio statistic and computes/approximates the probabilities of the two types of errors. Under the situation when either the null hypothesis or the alternative hypothesis is composite, one naturally considers the generalized likelihood ratio test. To the authors' best knowledge, the asymptotic behavior of the generalized likelihood ratio test under the Chernoff's regime remains an open problem. This is mostly because large deviations results are not directly applicable as the test statistic is the ratio of the supremums of two random functions. This paper fills in this void and provides a definitive conclusion of the asymptotic efficiency of the generalized likelihood ratio test under Chernoff's asymptotic regime. We define the Chernoff index via the asymptotic decay rate of the maximal type I and type II error probabilities that is also the minimax risk corresponding to the zero-one loss function.

We compute the generalized Chernoff index of the generalized likelihood ratio test for two separate parametric families that keep a certain distance away from each other. That is, the Kullback-Leibler distance between g_θ and h_γ are bounded away from zero for all $\theta \in \Theta$ and $\gamma \in \Gamma$. We use $\rho_{\theta\gamma}$ to denote the Chernoff index of the likelihood ratio test for the simple null $H_0: \ f = g_\theta$ against simple alternative $H_1: \ f = h_\gamma$. Under mild moment conditions, we show that the exponential decay rate of the maximal error probabilities is simply the minimum of the one-to-one Chernoff index $\rho_{\theta\gamma}$ over the parameter space, that is, $\rho = \min_{\theta,\gamma} \rho_{\theta\gamma}$. This result suggests that the generalized likelihood ratio test is asymptotically the minimax strategy in the sense that with the same sample size it achieves the optimal exponential decay rate of the maximal type I and type II error probabilities when they decay equally fast. The present result can also be generalized to asymptotic analysis of Bayesian model selection among two or more families of distributions. A key technical component is to deal with the excursion probabilities of the likelihood functions, for which random field and non-exponential change of measure techniques are applied. This paper also in part corresponds to the conjecture in Cox [2013] "formal discussion of possible optimality properties of the test statistics would, I think, require large deviation theory" though we consider a slightly different statistic.

We further extend the analysis to the cases when the two families may not be completely separate, that is, one may find two sequences of distributions in each family and the two sequences converge to each other. For this case, the Chernoff index is zero. We provide asymptotic decay rate of the type I error probability under a given distribution g_{θ_0} in H_0. To have the problem well-posed, the minimum Kullback-Leibler divergence between g_{θ_0} and all distributions in H_1 has to be bounded away from zero. The result is applicable to both separated and non-separated families and thus *it provides a means to approximate the error probabilities of the generalized likelihood ratio test for general parametric families.* This result has important theoretical implications in hypothesis testing, model selection, and other areas where maximum likelihood is employed. We provide a discussion concerning variable selection for regression models.

The rest of this chapter is organized as follows. We present our main results for separate families of hypotheses in Section 5.2. Further extension to more than two families and Bayesian model selection is discussed in Section 5.3. Results for possibly non-separate families are presented in Section 5.4. Numerical examples are provided in Section 5.5. Lastly a concluding remark is give in Section 5.6.

5.2 Main results

5.2.1 Simple null against simple alternative – a review of Chernoff index

In this section we state the main results and their implications. To start with, we provide a brief review of Chernoff index for simple null versus simple alternative; then, we proceed to the case of simple null versus composite alternative; furthermore, we present the generalized Chernoff index for the composite null versus composite alternative.

Under the context of simple null hypothesis versus simple alternative hypothesis, we have the null hypothesis $H_0 : f = g$ and the alternative hypothesis $H_1 : f = h$. We write the log-likelihood ratio of each observation as $l^i = \log h(X_i) - \log g(X_i)$. Then, the likelihood ratio is $LR_n = \exp(\sum_{i=1}^n l^i)$. We use l to denote the generic random variable equal in distribution to l^i. We define the moment generating function of l under distribution g as $M_g(z) = E_g(e^{zl}) = \int \{h(x)/g(x)\}^z g(x)\mu(dx)$, which must be finite for $z \in [0, 1]$ by the Hölder inequality. Furthermore, define the rate function

$$m_g(t) = \max_z [zt - \log\{M_g(z)\}].$$

The following large deviations result is established by Chernoff (1952).

Proposition 8. *If* $-\infty < t < E_g(l)$, *then* $\log \mathbb{P}_g(LR_n < e^{nt}) \sim -n \times m_g(t)$; *if* $E_g(l) < t < \infty$, *then* $\log \mathbb{P}_g(LR_n > e^{nt}) \sim -n \times m_g(t)$.

We write $a_n \sim b_n$ if $a_n/b_n \to 1$ as $n \to \infty$. The above proposition provides an asymptotic decay rate of the type I error probability: for any $t > E_g(l)$

$$\mathbb{P}_g(LR_n > e^{nt}) = e^{-\{1+o(1)\}n\times m_g(t)} \quad \text{as } n \to \infty.$$

Similarly, we switch the roles of g and h and define $M_h(z)$ and $m_h(t)$ by flipping the sign of the log-likelihood ratio $l = \log g(X) - \log h(X)$ and computing the expectations under h. One further defines $\rho(t) = \min\{m_g(t), m_h(-t)\}$ that is the slower rate among the type I and type II error probabilities. A measure of efficiency is given by

$$\rho = \max_{E_g(l)<t<E_h(l)} \rho(t) \tag{5.2}$$

that is known as the Chernoff index between g and h.

In the decision framework, we consider the zero-one loss function

$$L(C, f, X_1, ..., X_n) = \begin{cases} 1 & \text{if } f = g \text{ and } (X_1, ..., X_n) \in C \\ 1 & \text{if } f = h \text{ and } (X_1, ..., X_n) \notin C \\ 0 & \text{otherwise} \end{cases} \tag{5.3}$$

where $C \subset R^n$ and f is a density function. Then, the risk function is

$$R(C, f) = E_f\{L(C, f, X_1, ..., X_n)\} = \begin{cases} \mathbb{P}_g(C) & \text{if } f = g \\ \mathbb{P}_h(C^c) & \text{if } f = h \end{cases}. \tag{5.4}$$

The Chernoff index is the asymptotic exponential decay rate of the minimax risk $\min_C \max_f R(C, f)$ within the family of tests. In the following section, we will generalize the Chernoff efficiency following the minimaxity definition.

Using the fact that $M_g(z) = M_h(1 - z)$, one can show that the optimization in (5.2) is solved at $t = 0$ and

$$\rho = \rho(0). \tag{5.5}$$

Both $m_g(t)$ and $m_h(-t)$ are monotone functions of t and (5.5) suggests that $\rho = m_g(0) = m_h(0)$. To achieve the Chernoff index, we reject the null hypothesis if the likelihood ratio statistic is greater than 1 and the type I and type II error probabilities have identical exponential decay rate ρ.

To have a more concrete idea of the above calculations, Figure 5.1 shows one particular $-\log\{M_g(z)\}$ as a function of z where $g(x)$ is a lognormal distribution and $h(x)$ is an exponential distribution. There are several useful facts. First, $-\log\{M_g(z)\}$ is

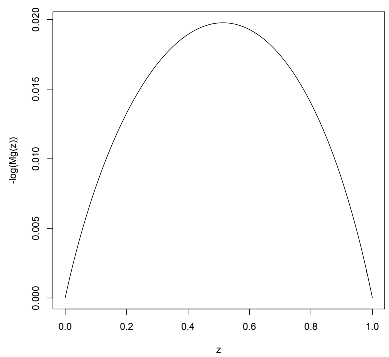


Figure 5.1: Plot of $-\log\{M_g(z)\}$ (y-coordinate) against z (x-coordinate) for the example of lognormal distribution versus exponential distribution

a concave function of z and $-\log\{M_g(0)\} = -\log\{M_g(1)\} = 0$. The maximization $\max_z[zt - \log\{M_g(z)\}]$ is solved at $d\log\{M_g(z)\}/dz = t$. Furthermore, the Chernoff index is achieved at $t = 0$. We insert $t = 0$ into the maximization and the Chernoff index is $\rho = \max_z[-\log\{M_g(z)\}]$.

5.2.2 Generalized Chernoff index for testing composite hypothesis

In this subsection, we develop the corresponding results for testing composite hypotheses. Some technical conditions are required as follows.

A1 Complete separation: $\min_{\theta\in\Theta,\gamma\in\Gamma} E_{g_\theta}\{\log g_\theta(X) - \log h_\gamma(X)\} > 0$.

A2 The parameter spaces Θ and Γ are compact subsets of R^{d_g} and R^{d_h} with continuously differentiable boundary $\partial\Theta$ and $\partial\Gamma$, respectively.

A3 Define $l_{\theta\gamma} = \log h_\gamma(X) - \log g_\theta(X)$, $S_1 = \sup_{\theta,\gamma} |\nabla_\theta l_{\theta\gamma}|$, and $S_2 = \sup_{\theta,\gamma} |\nabla_\gamma l_{\theta\gamma}|$. There exists some $\eta, x_0 > 0$, that are independent with θ and γ, such that for

$x > x_0$

$$\sup_{\theta\in\Theta,\gamma\in\Gamma} \max\{\mathbb{P}_{g_\theta}(S_i > x), \mathbb{P}_{h_\gamma}(S_i > x)\} \le e^{-(\log x)^{1+\eta}}, \quad (i = 1, 2). \tag{5.6}$$

Remark 3. *Condition A3 requires certain tail conditions of S_i. It excludes some singularity cases. This condition is satisfied by most parametric families. For instance, if $g_\theta(x) = g_0(x)e^{\theta x - \varphi_g(\theta)}$ and $h_\gamma = h_0(x)e^{\gamma x - \varphi_h(\gamma)}$ are exponential families, then*

$$|\nabla_\theta l_{\theta\gamma}| = |x - \varphi_g'(\theta)| \le |x| + O(1).$$

Thus (5.6) *is satisfied if $|x|$ has a finite moment generating function.*

If $g_\theta = g(x-\theta)$ is the scale family, then

$$|\nabla_\theta l_{\theta\gamma}| = \Big|\frac{g'(x-\theta)}{g(x-\theta)}\Big|$$

that usually has finite moment generating function for light-tailed distributions (Gaussian, exponential, etc) and is usually bounded for heavy-tailed distributions (e.g. t-distribution). Similarly, one may verify (5.6) *for scale families. Thus, A3 is a weak condition and is applicable to most parametric families practically in use.*

We start the discussion for a simple null hypothesis against a composite alternative hypothesis

$$H_0: \ f = g \quad \text{and} \quad H_1: \ f \in \{h_\gamma : \gamma \in \Gamma\}. \tag{5.7}$$

In this case, the likelihood ratio takes the following form

$$LR_n = \frac{\max_{\gamma\in\Gamma} \prod_{i=1}^n h_\gamma(X_i)}{\prod_{i=1}^n g(X_i)}. \tag{5.8}$$

For each distribution h_γ in the alternative family, we define ρ_γ to be the Chernoff index of the likelihood ratio test for $H_0: \ f = g$ against $H_1: \ f = h_\gamma$, whose form is given as in (5.2). The first result is given as follows.

Lemma 14. *Consider the hypothesis testing problem given as in* (5.7) *and the generalized likelihood ratio test with rejection region $C_\lambda = \{(x_1, ..., x_n) : LR_n > \lambda\}$ where*

LR_n is given by (5.8). *If conditions A1-3 are satisfied and we choose $\lambda = 1$, then the asymptotic decay rate of the type I and maximal type II error probabilities are identical, more precisely,*

$$\log \mathbb{P}_g(C_1) \sim \sup_{\gamma\in\Gamma} \log \mathbb{P}_{h_\gamma}(C_1^c) \sim -n \times \min_\gamma \rho_\gamma.$$

For composite null versus composite alternative

$$H_0 : \ f \in \{g_\theta : \theta \in \Theta\} \quad \text{against} \quad H_1 : \ f \in \{h_\gamma : \gamma \in \Gamma\} \tag{5.9}$$

similar results can be obtained. The generalized likelihood ratio statistic is given by (5.1). For each single pair (g_θ, h_γ), we let $\rho_{\theta\gamma}$ denote the corresponding Chernoff index of the likelihood ratio test for $H_0 : f = g_\theta$ and $H_1 : f = h_\gamma$. The following theorem states the main result.

Theorem 8. *Consider a composite null hypothesis against a composite alternative hypothesis given as in* (5.9) *and the generalized likelihood ratio test with rejection region $C_\lambda = \{(x_1, ..., x_n) : LR_n > \lambda\}$ where LR_n is given by* (5.1). *If conditions A1-3 are satisfied and we choose $\lambda = 1$, then the asymptotic decay rate of the maximal type I and type II error probabilities are identical, more precisely,*

$$\sup_{\theta\in\Theta} \log \mathbb{P}_{g_\theta}(C_1) \sim \sup_{\gamma\in\Gamma} \log \mathbb{P}_{h_\gamma}(C_1^c) \sim -n \times \min_{\theta\in\Theta,\gamma\in\Gamma} \rho_{\theta\gamma}. \tag{5.10}$$

We call

$$\rho = \min_{\theta,\gamma} \rho_{\theta\gamma}$$

the generalized Chernoff index between the two families $\{g_\theta\}$ and $\{h_\gamma\}$ that is the exponential decay rate of the maximal type I and type II error probabilities for the generalized likelihood ratio test. We would like to make a few remarks. Suppose that $\rho_{\theta\gamma}$ is minimized at θ_* and γ_*. The maximal type I and type II error probabilities of C_1 have identical exponential decay rate as that of the error probabilities of the likelihood ratio test for the simple null $H_0 : f = g_{\theta_*}$ versus simple alternative $H_1 : f = h_{\gamma_*}$ problem. Then, according to the Neyman-Pearson lemma, we have the following statement. Among all the tests for (5.9) that admit maximal type I error probabilities that decays exponentially at least at rate ρ, their maximal type II error probabilities decay at most at rate ρ. This asymptotic efficiency can only be obtained at the particular threshold $\lambda = 1$, at which the maximal type I and the type II error probabilities decay exponentially equally fast. Consider the loss function as in (5.3) and the risk function is

$$R(C, f) = \begin{cases} \mathbb{P}_f(C) & \text{if } f \in \{g_\theta : \theta \in \Theta\} \\ \mathbb{P}_f(C^c) & \text{if } f \in \{h_\gamma : \gamma \in \Gamma\} \end{cases} . \tag{5.11}$$

According to the above discussion, the maximum risk of the rejection region $C_1 = \{LR_n > 1\}$ achieves the same asymptotic decay rate as that of the minimax risk that is

$$\min_{C \subset R^n} \max_{f \in \{g_\theta\} \cup \{h_\gamma\}} \frac{\log\{R(C, f)\}}{n} \to -\rho.$$

Upon considering the exponential decay rate of the two types of error probabilities, one can simply reduce the problem to testing $H_0 : f = g_{\theta_*}$ against $H_1 : f = h_{\gamma_*}$. Each of these two distributions can be viewed as the least favorable distribution if its own family is chosen to be the null family. The results in Lemma 14 and Theorem 8 along with their proofs suggest that the maximal type I and type II error probabilities are achieved at $f = g_{\theta_*}$ and $f = h_{\gamma_*}$. In addition, under the distribution g_{θ_*} and conditional on the event C_1, in which H_0 is rejected, the maximum likelihood estimator $\hat{\gamma}$ converges to γ_*; vice versa, under the distribution $f = h_{\gamma_*}$, if H_0 is not rejected, the maximum likelihood estimator $\hat{\theta}$ converges to θ_*.

5.2.3 Relaxation of the technical conditions

The results of Lemma 14 and Theorem 8 require three technical conditions. Condition A1 ensures that the two families are separated and it is crucial for the exponential decay of the error probabilities. Condition A2, though important for the proof, can be relaxed for most parametric families. They can be replaced by certain localization conditions for the maximum likelihood estimator. We present one as follows.

A4 There exist parameter-dependent compact sets $A_\theta, \tilde{A}_\gamma \subset \Gamma$ and $B_\gamma, \tilde{B}_\theta \subset \Theta$ such that for all θ and γ

$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}_{g_\theta}(\hat{\theta} \in \tilde{B}_\theta^c \text{ or } \hat{\gamma} \in A_\theta^c) < -\rho, \tag{5.12}$$
$$\liminf_{n\to\infty} \frac{1}{n} \log \mathbb{P}_{h_\gamma}(\hat{\theta} \in B_\gamma^c \text{ or } \hat{\gamma} \in \tilde{A}_\gamma^c) < -\rho$$

where $\hat{\theta}$ and $\hat{\gamma}$ are the maximum likelihood estimators under the two families. Condition A3 is satisfied if the maximization in the definition of S_i is taken on the set A_θ and $\tilde{B}_\theta$ when the tail is computed under g_θ and is taken on the set $\tilde{A}_\gamma$ and B_γ when the tail is computed under h_γ.

Remark 4. *Assumption A4 can be verified by means of large deviations of the maximum likelihood estimator; see Arcones [2006]. Under regularity conditions, the probability that the maximum likelihood estimator deviates from the true parameter by a constant decreases exponentially. One can choose the constant large enough so that it decays at a faster rate than ρ and thus Assumption 4 is satisfied.*

Consider the first probability in (5.12) under g_θ. We typically choose $\tilde{B}_\theta$ to be a reasonably large compact set containing θ and thus $\mathbb{P}_{g_\theta}(\hat{\theta} \in \tilde{B}_\theta^c)$ decays exponentially fast at a higher rate than ρ. For the choice of A_θ, we first define

$$\gamma_\theta = \arg\max_{\gamma\in\Gamma} E_{g_\theta}\{\log h_\gamma(X)\}$$

that is the limit of $\hat{\gamma}$ under g_θ. Then, we choose A_θ be a sufficiently large compact set containing γ_θ so that the decay rate of $\mathbb{P}_{g_\theta}(\hat{\gamma} \in A_\theta^c)$ is higher than ρ. Similarly, we can choose B_γ and $\tilde{A}_\gamma$. Furthermore, the maximum score function for a single observation over a compact set usually has a sufficiently light tail to satisfy condition A4, for instance, $\mathbb{P}_{g_\theta}(\sup_{\theta\in\tilde{B}_\theta,\gamma\in A_\theta} |\nabla_\theta l_{\theta\gamma}| > x) \leq e^{-(\log x)^{1+\eta}}$.

Corollary 6. *Consider a composite null hypothesis against composite alternative hypothesis given as in* (5.9)*. Suppose that conditions A1 and A4 are satisfied. Then,* *the asymptotic decay rates of the maximal type I and type II error probabilities are identical, more precisely,*

$$\sup_{\theta\in\Theta}\log\mathbb{P}_{g_\theta}(C_1)\sim\sup_{\gamma\in\Gamma}\log\mathbb{P}_{h_\gamma}(C_1^c)\sim -n\times\min_{\theta,\gamma}\rho_{\theta\gamma}.$$

5.3 Extensions

5.3.1 On the asymptotic behavior of Bayes factor

The result in Theorem 8 can be further extended to the study of Bayesian model selection. Consider the two families in (5.9) each of which is endowed with a prior distribution on its own parameter space, denoted by $\phi(\theta)$ and $\varphi(\gamma)$. We use $\mathcal{M}$ to denote the family membership: $\mathcal{M}=0$ for the g-family and $\mathcal{M}=1$ for the h-family. Then, the Bayes factor is

$$BF=\frac{p(X_1,...,X_n|\mathcal{M}=1)}{p(X_1,...,X_n|\mathcal{M}=0)}=\frac{\int_{\gamma\in\Gamma}\varphi(\gamma)\prod_{i=1}^n h_\gamma(X_i)d\gamma}{\int_{\theta\in\Theta}\phi(\theta)\prod_{i=1}^n g_\theta(X_i)d\theta}. \tag{5.13}$$

With a similar derivation as that of Bayesian information criterion [Schwarz, 1978], the marginalized likelihood $p(X_1,...,X_n|\mathcal{M}=i)$ is the maximized likelihood multiplied by a polynomial prefactor depending on the dimension of the parameter space. Therefore, we can approximate the Bayesian factor by the generalized likelihood ratio statistic as follows

$$\kappa^{-1}n^{-\beta}\le\frac{BF}{LR_n}\le\kappa n^{\beta} \tag{5.14}$$

for some κ and β sufficiently large. Therefore, $\log BF=\log LR_n+O(\log n)$. Since the expectation of $\log LR_n$ is of order n, the $O(\log n)$ term does not affect the exponential rate. Therefore, we have the following result.

Theorem 9. *Consider two families of distributions given as in* (5.9) *satisfying conditions A1-3. The prior densities φ and ϕ are positive and Lipschitz continuous. We select $\mathcal{M}=1$ if $BF>1$ and $\mathcal{M}=0$ otherwise where BF is given by* (5.13). *Then,* *the asymptotic decay rate of selecting the wrong model are identical under each of the two families. More precisely,*

$$\log \int_{\theta\in\Theta} \mathbb{P}_{g_\theta}(BF > 1)\phi(\theta)d\theta \sim \sup_{\theta\in\Theta} \log \mathbb{P}_{g_\theta}(BF > 1)$$
$$\sim \log \int_{\gamma\in\Gamma} \mathbb{P}_{h_\gamma}(BF \leq 1)\varphi(\gamma)d\gamma \sim \sup_{\gamma\in\Gamma} \log \mathbb{P}_{h_\gamma}(BF \leq 1) \sim -n \times \min_{\theta,\gamma} \rho_{\theta\gamma}.$$

The proof of the above theorem is an application of Theorem 8 and (5.14) and thus we omit it. The above result does not rely on the validity of the prior distributions. Therefore, model selection based on Bayes factor is asymptotically efficient even if the prior distribution is misspecified. That is, the Bayes factor is calculated based on the probability measures with density functions φ and ϕ that are different from the true prior probability measures under which θ and γ are generated.

5.3.2 Extensions to more than two families

Suppose that there are K non-overlapping families $\{g_{k,\theta_k} : \theta_k \in \Theta_k\}$ for $k = 1, ..., K$, among which we would like to select the true family to which the distribution f belongs. Let

$$L_k(\theta_k) = \prod_{i=1}^{n} g_{k,\theta_k}(X_i)$$

be the likelihood of family k. A natural decision is to select the family that has the highest likelihood, that is,

$$\hat{k} = \arg\max_{k=1,\ldots,K} \sup_{\theta_k} L_k(\theta_k).$$

According to the results in Theorem 8, we obtain that

$$\sup_{k,\theta_k} \log \mathbb{P}_{g_{k,\theta_k}}(\hat{k} \neq k) \sim -n\rho$$

where ρ is the smallest generalized Chernoff indices, defined as in Theorem 8, among all the $(K-1)K/2$ pairs of families. To obtain the above limit, one simply considers each family k as the null hypothesis and the union of the rest $K-1$ altogether as the alternative hypothesis.

With the same argument as in Section 5.3.1, we consider Bayesian model selection among the K families each of which is endowed with a prior $\phi_k(\theta_k)$. Consider the marginalized maximum likelihood estimator

$$\hat{k}_B = \arg\max_k \int L_k(\theta_k)\phi_k(\theta_k)d\theta_k$$

that admits the same misclassification rate

$$\sup_{k,\theta_k} \log \mathbb{P}_{g_{k,\theta_k}}(\hat{k}_B \neq k) \sim \sup_k \log \int \mathbb{P}_{g_{k,\theta_k}}(\hat{k}_B \neq k)\phi_k(\theta_k)d\theta_k \sim -n\rho.$$

5.4 Results for possibly non-separated families

5.4.1 The asymptotic approximation of error probabilities

In this section we extend the results to the cases when the g-family and the h-family are not necessarily separated, that is,

$$\min_{\theta\in\Theta,\gamma\in\Gamma} E_{g_\theta}\{\log g_\theta(X) - \log h_\gamma(X)\} = 0. \tag{5.15}$$

In the case of (5.15), the Chernoff index is trivially zero. We instead derive the asymptotic decay rate of the following error probabilities. For some $\theta_0 \in \Theta$ such that

$$\min_\gamma E_{g_{\theta_0}}\{\log g_{\theta_0}(X) - \log h_\gamma(X)\} > 0,$$

we consider the type I error probability

$$\mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb}) \quad \text{as } n \to \infty \tag{5.16}$$

where LR_n is the generalized likelihood ratio statistic as in (5.1). For b, we require that

$$\sup_{\gamma\in\Gamma} \mathbb{E}_{g_{\theta_0}}\{\log h_\gamma(X) - \log g_{\theta_0}(X)\} < b \tag{5.17}$$

ensuring that $\mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb})$ eventually converges to zero.

The statement of the theorem requires the following construction. For each θ and γ, we first define the moment generating function of $\log h_\gamma(X) - \log g_\theta(X) - b$

$$M_{g_{\theta_0}}(\theta,\gamma,\lambda) = \mathbb{E}_{g_{\theta_0}}\Big[\exp\{\lambda(\log h_\gamma(X) - \log g_\theta(X) - b)\}\Big] \tag{5.18}$$

and consider the optimization problem

$$M^\dagger_{g_{\theta_0}} \triangleq \inf_{\theta\in\Theta}\sup_{\gamma\in\Gamma}\inf_{\lambda\in R} M_{g_{\theta_0}}(\theta,\gamma,\lambda). \tag{5.19}$$

Under Assumption A2, there exists at least one solution to the above optimization we assume one of the solutions is

$$(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) = \arg\inf_{\theta\in\Theta}\sup_{\gamma\in\Gamma}\inf_{\lambda\in R} M_{g_{\theta_0}}(\theta,\gamma,\lambda).$$

Furthermore, we define a measure $Q^\dagger$ that is absolutely continuous with respect to $\mathbb{P}_{g_{\theta_0}}$

$$\frac{dQ^\dagger}{d\mathbb{P}_{g_{\theta_0}}} = \exp\Big\{\lambda^\dagger(\log h_{\gamma^\dagger}(X) - \log g_{\theta^\dagger}(X) - b)\Big\}/M^\dagger_{g_{\theta_0}}. \tag{5.20}$$

Definition 5 (Solid tangent cone)**.** *For a set $A \subset R^d$ and $x \in A$, the solid tangent cone T_xA is defined as the set*

$$\{y \in R^d : \exists\, y_m \text{ and } \lambda_m \text{ such that } y_m \to y,\ \lambda_m \to 0 \text{ as } m \to \infty, \text{ and } x + \lambda_m y_m \in A\}.$$

If A has continuously differentiable boundary and $x \in \partial A$, then T_xA consists of all the vectors in R^d that have negative inner products with the normal vector to ∂A at x pointing outside of A; if x is in the interior of A, then $T_xA = R^d$. We consider the following technical conditions for the main theorem in this section.

A5 The moment generating function $M_{g_{\theta_0}}$ is twice differentiable at $(\theta^\dagger,\gamma^\dagger,\lambda^\dagger)$.

A6 Under $Q^\dagger$, the the solution to the Euler condition is unique, that is, the equation with respect to θ and γ

$$\mathbb{E}^{Q^\dagger}\{y^\top \nabla_\theta \log g_\theta(X)\} \le 0 \text{ for all } y \in T_\theta\Theta \tag{5.21}$$
$$\mathbb{E}^{Q^\dagger}\{y^\top \nabla_\gamma h_\gamma(X)\} \le 0 \text{ for all } y \in T_\gamma\Gamma$$

has a unique solution $(\bar{\theta}, \bar{\gamma})$. In addition,

$$\mathbb{E}^{Q^\dagger}\{\sup_{\theta\in\Theta} |\nabla^2_\theta \log g_\theta(X)|\} < \infty \text{ and } \mathbb{E}^{Q^\dagger}\{\sup_{\gamma\in\Gamma} |\nabla^2_\gamma \log h_\gamma(X)|\} < \infty.$$

We also assume that under measure $Q^\dagger$ as $n \to \infty$,

$$\sqrt{n}(\hat{\theta} - \bar{\theta}) = O_{Q^\dagger}(1) \text{ and } \sqrt{n}(\hat{\gamma} - \bar{\gamma}) = O_{Q^\dagger}(1),$$

where $\hat{\theta}$ and $\hat{\gamma}$ are the maximum likelihood estimators

$$\hat{\theta} = \arg\sup_\theta \sum_{i=1}^n \log g_\theta(X_i) \text{ and } \hat{\gamma} = \arg\sup_\gamma \sum_{i=1}^n \log h_\gamma(X_i),$$

and a random sequence $a_n = O_{Q^\dagger}(1)$ means it is tight under measure $Q^\dagger$.

A7 We assume that g_{θ_0} does not belong to the closure of the family of distributions $\{h_\gamma : \gamma \in \Gamma\}$, that is, $\inf_{\gamma\in\Gamma} D(g_{\theta_0}\|h_\gamma) > 0$.

Assumption A6 requires $n^{-1/2}$ convergence of $\hat{\theta}$ and $\hat{\gamma}$ under $Q^\dagger$. It also requires the local maximum of the function $\mathbb{E}^{Q\dagger} \log g_\theta(X)$ and $\mathbb{E}^{Q\dagger} \log h_\gamma(X)$ to be unique. We elaborate the Euler condition for $\theta \in int(\Theta)$ and $\theta \in \partial\Theta$ separately. If $\theta \in int(\Theta)$, then $T_\theta\Theta = R^{d_g}$. The Euler condition is equivalent to $\mathbb{E}^{Q^\dagger}\nabla_\theta \log g_\theta(X) = 0$, which is the usual first order condition for a local maximum. If $\theta \in \partial\Theta$, then the Euler condition requires that the directional derivative of $\mathbb{E}^{Q^\dagger}\{\log g_\theta(X)\}$ along a vector pointing towards inside Θ is non-positive. Assumption A7 guarantees that the probability $\lim_{n\to\infty} \mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb}) = 0$ for some b.

Theorem 10. *Under Assumptions A2-A3 and A5-A7, for each b satisfying* (5.17)*, we have*

$$\log \mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb}) \sim -n \times \rho^\dagger_{g_{\theta_0}},$$

where $\rho^\dagger_{g_{\theta_0}} = -\log M^\dagger_{g_{\theta_0}}$ and $M^\dagger_{g_{\theta_0}}$ is defined in (5.19).

This theorem provides a means to approximate the type I and type II error probabilities for general parametric families. The above results are applicable to the both cases that the two families are separated or not separated. According to standard large deviations calculation for random walk, we have that for each $\theta \in \Theta$ and $\gamma \in \Gamma$,

$$\log \mathbb{P}_{g_{\theta_0}}\Big(\sum_{i=1}^{n} \log h_\gamma(X_i) - \log g_\theta(X_i) - nb > 0\Big) \sim \inf_\lambda \log M_{g_{\theta_0}}(\theta, \gamma, \lambda).$$

Theorem 10 together with the above display implies that

$$\begin{aligned}\log \mathbb{P}_{g_{\theta_0}}(LR_n > 1) &\sim \inf_\theta \sup_\gamma \log \mathbb{P}_{g_{\theta_0}}\Big(\sum_{i=1}^{n} \log h_\gamma(X_i) - \log g_\theta(X_i) > nb\Big)\\ &\sim \log \mathbb{P}_{g_{\theta_0}}\Big(\sum_{i=1}^{n} \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) > nb\Big)\end{aligned}$$

The exponential decay rate of the error probabilities under g_{θ_0} is the same as the exponential decay rate of the probability that $h_{\gamma^\dagger}$ is preferred to $g_{\theta^\dagger}$.

One application of Theorem 10 is to compute the power function asymptotically. Consider the fixed type I error α and the critical region of the generalized likelihood ratio test is determined by the quantile of a χ^2 distribution, that is $\{LR_n > e^{\lambda_\alpha}\}$ where $2\lambda_\alpha$ is the $(1-\alpha)$th quantile of the χ^2 distribution. This correspond to choosing $b = o(1)$. For a given alternative distribution h_γ, one can compute the type II error probability asymptotically by means of Theorem 10 switching the role of the null and the alternative families. Thus, the power function can be computed asymptotically.

5.4.2 Application to model selection in generlized linear models

We discuss the application of Theorem 10 on model selection for generalized linear models [McCullagh and Nelder, 1989]. Let Y_i be the response of the ith observation and $X^{(i)} = (X_{i1}, ..., X_{ip})^T$ and $Z^{(i)} = (Z_{i1}, ..., Z_{iq})^T$ be two sets of predictors, $i = 1, ..., n$. Consider a generalized linear model with canonical link function and the true conditional distribution of Y_i is

$$g_i(y_i, \beta^0) = \exp\Big\{(\beta^0)^T X^{(i)} y_i - b((\beta^0)^T X^{(i)}) + c(y_i)\Big\}, \qquad i = 1, 2, ..., n, \tag{5.22}$$

where $f(y) = e^{c(y)}$ is the base-line density, $b(\cdot)$ is the logarithm of the moment generating function, $\beta^0 = (\beta_1^0, ..., \beta_p^0)^T$ is the vector of true regression coefficients, and X is the set of true predictors. Let the null hypothesis be

$$H_0 : g_i(y_i, \beta) = \exp\Big\{\beta^T X^{(i)} y_i - b(\beta^T X^{(i)}) + c(y_i)\Big\}, \qquad i = 1, 2, ..., n; \tag{5.23}$$

the alternative hypothesis is

$$H_1 : h_i(y_i, \gamma) = \exp\Big\{\gamma^T Z^{(i)} y_i - b(\gamma^T Z^{(i)}) + c(y_i)\Big\}, \qquad i = 1, 2, ..., n. \tag{5.24}$$

We further assume that H_1 does not contain (5.22). Conditional on the covariates X and Z, we consider the asymptotic decay rate of the type I error probability

$$\mathbb{P}_{\beta^0}(LR_n \geq 1),$$

where $LR_n = \frac{\sup_\gamma \prod_{i=1}^n h_i(Y_i,\gamma)}{\sup_\beta \prod_{i=1}^n g_i(Y_i,\beta)}$ is the generalized likelihood ratio.

We present the construction of the rate function as follows. For each $\beta \in R^p$, $\gamma \in R^q$ and $\lambda \in R$, define

$$\begin{aligned}&\widetilde{\rho}_n(\beta, \gamma, \lambda)\\ &= \frac{1}{n}\sum_{i=1}^n \Big\{\lambda\Big[b(\gamma^T Z^{(i)}) - b(\beta^T X^{(i)})\Big] + b((\beta^0)^T X^{(i)}) - b\Big((\beta^0)^T X^{(i)} + \lambda(\gamma^T Z^{(i)} - \beta^T X^{(i)})\Big)\Big\}.\end{aligned} \tag{5.25}$$

Taking derivative with respect to λ, we have

$$\begin{aligned}&\frac{\partial}{\partial\lambda}\widetilde{\rho}_n(\beta, \gamma, \lambda)\\ &= \frac{1}{n}\sum_{i=1}^n \Big\{b(\gamma^T Z^{(i)}) - b(\beta^T X^{(i)}) - b'\Big((\beta^0)^T X^{(i)} + \lambda(\gamma^T Z^{(i)} - \beta^T X^{(i)})\Big)(\gamma^T Z^{(i)} - \beta^T X^{(i)})\Big\}.\end{aligned} \tag{5.26}$$

According to fact that $b(\cdot)$ is a convex function, we have

$$\limsup_{\lambda \to +\infty} \frac{\partial}{\partial\lambda}\widetilde{\rho}_n(\beta, \gamma, \lambda) < 0,$$

if $\beta^T X^{(i)} \neq \gamma^T Z^{(i)}$ for some i. Define the set $B_n \subset R^p$ such that

$$B_n = \{\beta : \inf_{\gamma} \frac{\partial}{\partial\lambda}\widetilde{\rho}_n(\beta,\gamma,0) \geq 0\}.$$

Then for each $\beta \in B_n$ and $\gamma \in R^q$, there is a $\lambda \geq 0$ such that $\frac{\partial}{\partial\lambda}\widetilde{\rho}_n(\beta,\gamma,0) = 0$. Thanks to the convexity of b, $\beta^0 \in B_n$ and thus B_n is never empty. The second derivative is

$$\frac{\partial^2}{(\partial\lambda)^2}\widetilde{\rho}_n(\beta,\gamma,\lambda) = -\frac{1}{n}\sum_{i=1}^{n} b''\Big((\beta^0)^T X^{(i)} + \lambda(\gamma^T Z^{(i)} - \beta^T X^{(i)})\Big)(\gamma^T Z^{(i)} - \beta^T X^{(i)})^2 < 0,$$

if $\beta^T X^{(i)} \neq \gamma^T Z^{(i)}$ for some i. Therefore, there is a unique solution to the maximization $\sup_\lambda \widetilde{\rho}_n(\beta,\gamma,\lambda)$. We further consider the optimization

$$\widetilde{\rho}_n^{\dagger} = \sup_{\beta\in B_n} \inf_{\gamma} \sup_{\lambda} \widetilde{\rho}_n(\beta,\gamma,\lambda). \tag{5.27}$$

We consider the following technical conditions.

A8 For each n, the solution to (5.27) exists, denoted by $(\beta_n^\dagger, \gamma_n^\dagger, \lambda_n^\dagger)$. There exists a constant κ_1 such that

$$\|\beta_n^\dagger\| \leq \kappa_1,\ \|\gamma_n^\dagger\| \leq \kappa_1 \text{ and } \lambda_n^\dagger \leq \kappa_1 \text{ for all } n.$$

Here, $\|\cdot\|$ is the Euclidean norm.

A9 There exists a constant $\delta_1 > 0$ such that $\inf_\gamma \sup_\lambda \widetilde{\rho}_n(\beta^0,\gamma,\lambda) > \delta_1$ for all n.

A10 There exists a constant κ_2 such that $\|X^{(i)}\| \leq \kappa_2$ and $\|Z^{(i)}\| \leq \kappa_2$ for all i. Additionally, there exits $\delta_2 > 0$ such that for all n the smallest eigenvalue of $\frac{1}{n}\sum_{i=1}^n X^{(i)} X^{(i)T}$ is bounded below by δ_2.

A11 For any compact set $K \subset R$, $\inf_{u\in K} b''(u) > 0$. In addition, $b(\cdot)$ is four-time continuously differentiable.

Assumption A8 requires that the solution of the optimization (5.27) does not tend to infinity as n increases, which is a mild condition. In particular, if the Kullback-Leibler divergence $D(g_i(\cdot,\beta^0)|g_i(\cdot,\beta))$ tend to infinity uniformly for all i as $\|\beta\|$ goes to infinity, then B_n is a bounded subset of R^p and $\|\beta_n^\dagger\|$ is also bounded. Similar checkable sufficient conditions can be obtained for $\gamma_n^\dagger$ and $\lambda_n^\dagger$.

Theorem 11. *Under Assumptions A8-A11, conditional on the covariates $X^{(i)}$ and $Z^{(i)}$, $i = 1, ..., n$, we have*

$$\log \mathbb{P}_{\beta^0}(LR_n \geq 1) \sim -n \times \widetilde{\rho}_n^\dagger,$$

where $\widetilde{\rho}_n^\dagger$ is defined in (5.27).

For generalized linear models, the moment generating function of likelihood ratio is

$$\mathbb{E}_{\beta^0}\Big\{\lambda \sum_{i=1}^{n} [\log h_i(Y_i, \gamma) - \log g_i(Y_i, \beta)]\Big\} = e^{-n\widetilde{\rho}_n(\beta,\gamma,\lambda)}.$$

Therefore, $\widetilde{\rho}_n^\dagger$ is a natural generalization of $\rho_{g_{\theta_0}}^\dagger$ for the nonidentical distribution case.

Theorem 11 provides the asymptotic rate of selecting the wrong model by maximizing the likelihood. The asymptotic rate as a function of the true regression coefficients β^0 quantifies the strength of the signals. The larger the rate is, the easier it is to select the correct variables. The rate also depends on covariates. If Z is highly correlated with X, then the rate is small. Overall, the rate serves as an efficiency measure of selecting the true model from families that mis-specifies the model.

5.5 Numerical examples

In this section, we present numerical examples to illustrate the asymptotic behavior of the maximal type I and type II error probabilities and the sample size tends to infinity. The first one is an example of continuous distributions and the second one is an example of discrete distributions. The third one is an example of linear regression models where the null hypotheses and alternative are not separated. In these examples, we compute the error probabilities using importance sampling corresponding to the change of measure in the proof with sufficiently large number of Monte Carlo replications to ensure that our estimates are sufficiently accurate.

Example 6. *Consider the lognormal distribution and exponential distribution. For* $x > 0$*, let*

$$g_\theta(x) = \frac{1}{x(2\pi\theta)^{1/2}} e^{-\frac{(\log x)^2}{2\theta}} \quad \Theta = (0, +\infty), \qquad h_\gamma(x) = \frac{1}{\gamma} e^{-\frac{x}{\gamma}} \quad \Gamma = (0, +\infty)$$

be the density functions of the lognormal distribution and the exponential distribution.

For each θ *and* γ*, we compute* $\rho_{\theta\gamma}$ *numerically. Figure 5.2 shows the contour plot of* $\rho_{\theta,\gamma}$*. The minimum of* $\rho_{\theta\gamma}$ *is* 0.020 *and is obtained at* $(\theta^*, \gamma^*) = (1.28, 1.72)$*. From the theoretical analysis, the maximal type I and type II error probabilities for the test decay at rate* $e^{-n\rho_{\theta^*\gamma^*}}$*.*

Figure 5.3 is the plot of the maximal type I and type II error probabilities as a function of the sample size for the composite versus composite test

$$H_0 : f \in \{g_\theta; \theta \in \Theta\} \quad \textit{against} \quad H_1 : f \in \{h_\gamma; \gamma \in \Gamma\}$$

and simple versus simple test

$$H_0 : f = g_{\theta_*} \quad \textit{against} \quad H_1 : f = h_{\gamma_*}.$$

We also fit a straight line to the logarithm of error probabilities against the sample sizes using least squares and the slope is -0.022*. This confirms the theoretical findings. The error probabilities shown in Figure 5.3 range from* 7×10^{-5} *to* 0.12 *and the range for sample size is from* 50 *to* 370*.*

Example 7. *We now proceed to the Poisson distribution versus the geometric distribution. Let*

$$g_\theta(x) = \frac{e^{-\theta}\theta^x}{x!} \quad \Theta = [1, +\infty), \qquad h_\gamma(x) = \frac{\gamma^x}{(1+\gamma)^{x+1}} \quad \Gamma = [0.5, +\infty),$$

for $x \in \mathbb{Z}^+$*. The parameter* γ *is the failure to success odds. The minimum Chernoff index without constraint is attained at* $\theta = \gamma = 0$ *and* $\rho_{00} = 0$*. Thus we truncate the parameter spaces away from zero to separate the two families.*

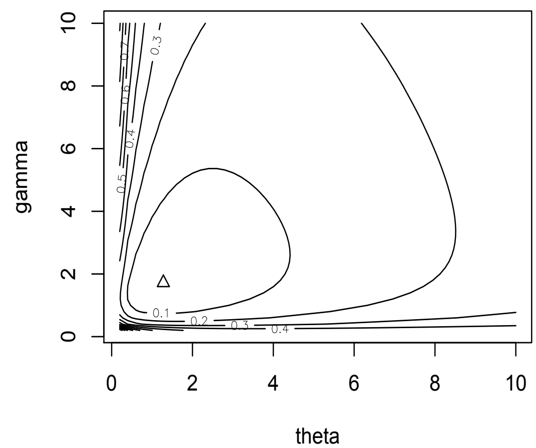


Figure 5.2: Contour plot for $\rho_{\gamma,\theta}$ in Example 6. The triangle point indicates the minimum.

The Chernoff index $\rho_{\theta,\gamma}$ can be computed numerically and is minimized at $(\theta^*, \gamma^*) = (1, 0.93)$, with $\rho_{\theta^*,\gamma^*} = 0.023$. Figure 5.4 shows the contour plot of $\rho_{\theta,\gamma}$. Same as in the previous example, we compute the maximal type I and type II error probabilities of the composite versus composite test and simple versus simple test. Figure 5.5 shows the maximal type I and type II error probabilities as a function of the sample size. The error probabilities appeared in Figure 5.5 range from 1.0×10^{-4} to 0.10 with the sample sizes range from 40 to 400. We also fit a straight line to the logarithm of error probabilities against the sample sizes and the slope is -0.025. This numerical analysis confirms our theorems.

Example 8. *We consider two regression models,*

$$H_0 : Y = \beta_1 X_1 + \beta_2 X_2 + \varepsilon_1 \ \textit{against} \ H_1 : Y = \beta_1 X_1 + \zeta_1 Z_1 + \varepsilon_2,$$

where (X_1, X_2, Z_1) jointly follows the multivariate Gaussian distribution with mean $(0, 0, 0)^T$ and the covariance matrix Σ. The random noises ε_1 and ε_2 follow the normal

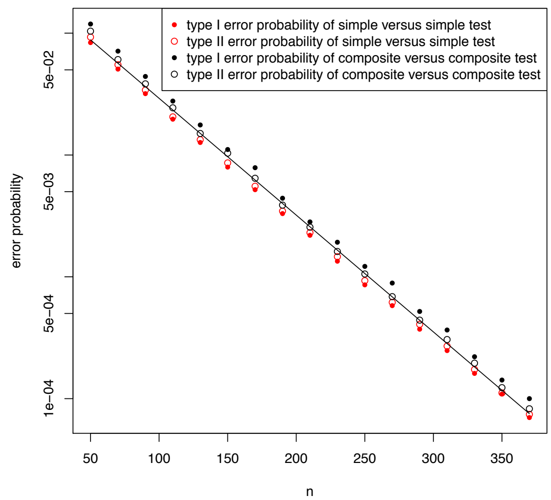


Figure 5.3: Decay rate of type I and type II error probabilities (y-coordinate) as a function of sample size (x-coordinate) in Example 6.

distributions $N(0,\sigma_1^2)$ *and* $N(0,\sigma_2^2)$ *respectively and are independent of* (X_1, X_2, Z_1). *We assume the true model to be*

$$Y = \beta_1^0 X_1 + \beta_2^0 X_2 + \varepsilon,$$

with the following parameters

$$\beta_1^0 = 1, \beta_2^0 = 2, \varepsilon \sim N(0,1), \text{ and } \Sigma = \begin{bmatrix} 1 & 0.1 & 0.1 \\ 0.1 & 1 & 0.1 \\ 0.1 & 0.1 & 1 \end{bmatrix}.$$

Let $(X_{i1}, X_{i2}, Z_{i1}, Y_i)^T$ *be i.i.d. copies of* (X_1, X_2, Z_1, Y) *generated under the true model, for* $i = 1, ..., n$. *Let* $\theta = (\beta_1, \beta_2)$ *and* $\gamma = (\beta_1, \zeta_1)$ *be the regression coefficients for the null and the alternative hypotheses respectively. The maximum likelihood estimators for* θ *and* γ *are the least square estimators*

$$\hat\theta = (\tilde X^\top \tilde X)^{-1} \tilde X^\top \tilde Y \text{ and } \hat\gamma = (\tilde Z^\top \tilde Z)^{-1} \tilde Z^\top \tilde Y,$$

where

$$\tilde{X} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \\ \cdots & \cdots \\ X_{n1} & X_{n2} \end{bmatrix}, \tilde{Z} = \begin{bmatrix} X_{11} & Z_{11} \\ X_{21} & Z_{21} \\ \cdots & \cdots \\ X_{n1} & Z_{n1} \end{bmatrix}, \text{ and } \tilde{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \cdots \\ Y_n \end{bmatrix}$$

are the design matrices for linear models under H_0 and H_1. We consider the error probability that the maximized log-likelihood of H_0 is smaller than that of H_1, equivalently, the residual sum of squares under H_0 is larger than that under H_1

$$\mathbb{P}_{\beta^0,\Sigma}\Big(\|\tilde{Y} - \tilde{X}\hat{\theta}\|^2 > \|\tilde{Y} - \tilde{Z}\hat{\gamma}\|^2\Big).$$

From the theoretical analysis, the above probability decays at rate $e^{-n\rho^\dagger_{g_{\theta_0}}}$ as $n \to \infty$, where the definition of $\rho^\dagger_{g_{\theta_0}}$ is given in Theorem 10. We solve the optimization problem (5.19) *numerically and obtain $\rho^\dagger_{g_{\theta_0}} = 0.45$. Figure 5.6a and Figure 5.6b are scatter plots of the error probability in the above display as a function of the sample size with different ranges for error probabilities. In Figure 5.6a, the range of the error probability is from 10^{-4} to 0.25 and the range of sample size is from 3 to 18. In Figure 5.6b, the range of error probabilities is from 1.2×10^{-8} to 4.0×10^{-6} with the sample size from 24 to 36. We fit straight lines for $\log \mathbb{P}_{\beta^0,\Sigma}\Big(\|\tilde{Y}-\tilde{X}\hat{\theta}\|^2 > \|\tilde{Y}-\tilde{Z}\hat{\gamma}\|^2\Big)$ against n using least square. The fitted slope in Figure 5.6a is -0.52 and the fitted slope in Figure 5.6b is -0.47. This confirms our theoretical results.*

5.6 Concluding remarks

The generalized likelihood ratio test of separate parametric families that was put forth by Cox in his two seminal papers has received a great deal of attention in the statistics and econometrics literature. The present investigation takes the viewpoint of an early work by Chernoff (1952) where testing a simple null versus a simple alternative is considered. By imposing that the two types of error probabilities decay at the same rate, we extend the Chernoff index to the case of the Cox test.

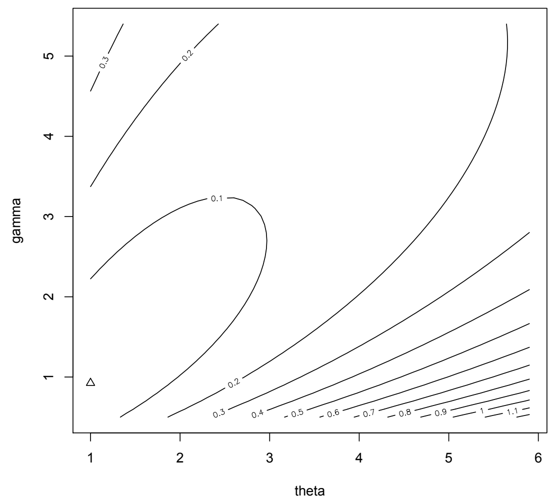


Figure 5.4: Contour plot for $\rho_{\gamma,\theta}$ in Example 7. The triangle point indicates the minimum.

Our results are under the basic assumption that the data come from one of the parametric families under consideration. It is often the case that none is the true model. It would be of interest to formulate error probabilities for this case and to see if similar exponential decay results continue to hold.

An initial motivation that led to the Cox formulation of the problem comes from the survival analysis where different models are used to fit failure time data. The econometrics literature also contains much subsequent development. Semiparametric models that contain infinite dimensional nuisance parameters are widely used in both econometrics and survival analysis. It would be of interest to develop parallel results for testing separate semiparametric models.

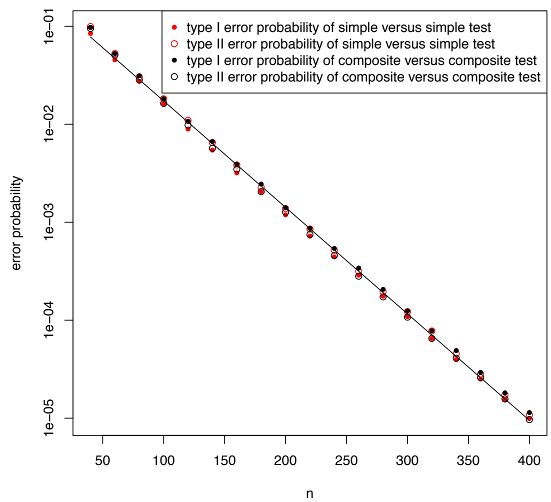


Figure 5.5: Maximal type I and type II error probabilities (y-coordinate) as a function of sample size (x-coordinate) in Example 7.

5.7 Appendix to Chapter 5

5.7.1 Proof of Lemma 14

Throughout the proof, we adopt the following notation $a_n \cong b_n$ if $\log a_n \sim \log b_n$. We define the log-likelihood ratio as

$$l_\gamma(x) = \log h_\gamma(x) - \log g(x).$$

The generalized log-likelihood ratio statistic is defined as

$$l = \sup_\gamma \sum_{i=1}^n l_\gamma^i$$

where $l_\gamma^i = l_\gamma(X_i)$. The generalized likelihood ratio test admits the rejection region

$$C_\lambda = \{e^l > \lambda\}.$$

We consider the case that $\lambda = 1$ and show that for this particular choice of λ the maximal type I and type II error probabilities decay exponentially fast with the same

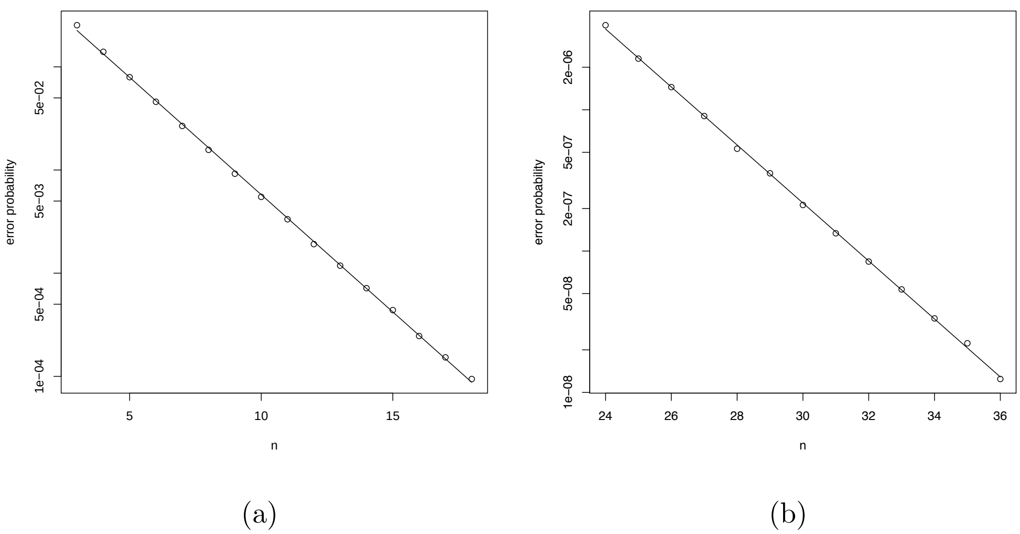


Figure 5.6: Error probability(y-coordinate) in Example 8 as a function of sample size(x-coordinate).

rate. We let $\gamma_* = \arg\inf \rho_\gamma$ and thus $\rho = \rho_{\gamma_*}$.

Based on Chernoff's calculation of large deviations for the log-likelihood ratio statistic, we proceed to the calculation of the type I error probability

$$\mathbb{P}_g(l > 0) = \mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l_\gamma^i > 0\Big).$$

We now provide an approximation of the right-hand side, which requires a lower bound and an upper bound. We start with the lower bound by noticing that

$$\mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l_\gamma^i > 0\Big) \geq \sup_\gamma \mathbb{P}_g\Big(\sum_{i=1}^n l_\gamma^i > 0\Big) \tag{5.28}$$

that is a simple lower bound. According to Proposition 8, the right-hand side is bounded from below by

$$\geq e^{-\{1+o(1)\}n\rho}$$

where $\rho = \min \rho_\gamma$. For the upper bound and with some $\beta > 0$, we split the probability

$$\begin{aligned}\mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l_\gamma^i > 0\Big) \quad \leq \quad & \mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l_\gamma^i > 0, \sup_\gamma \Big|\sum_{i=1}^n \nabla l_\gamma^i\Big| < e^{n^{1-\beta}}\Big) \\ & + \mathbb{P}_g\Big(\sup_\gamma \Big|\sum_{i=1}^n \nabla l_\gamma^i\Big| \geq e^{n^{1-\beta}}\Big). \qquad (5.29)\end{aligned}$$

The first term on the right-hand side is bounded by Lemma 15.

Lemma 15. *Consider a random function $\eta_n(\theta)$ living on a d-dimensional compact domain $\theta \in D$, where n is an asymptotic parameter that will be send to infinity. Suppose that $\eta_n(\theta)$ is almost surely differentiable with respect to θ and for each θ, there exists a rate $\rho(\theta)$ such that*

$$\mathbb{P}\{\eta_n(\theta) > \zeta_n\} \cong e^{-n\rho(\theta)} \quad \textit{for all } \zeta_n/n \to 0 \textit{ as } n \to \infty$$

where the above convergence is uniform in θ. Then, we have the following approximation

$$\liminf_{n\to\infty} -\frac{1}{n} \log \mathbb{P}\{\sup_{\theta \in D} \eta_n(\theta) > 0, \sup_{\theta\in D} |\nabla \eta_n(\theta)| < e^{n^{1-\beta}}\} \geq \min_\theta \rho(\theta)$$

for all $\beta > 0$.

With the aid of Proposition 8, we have that the random function $\sum_{i=1}^n l_\gamma^i$ satisfies the assumption in Lemma 15 with $\rho(\gamma) = \rho_{\theta\gamma}$. Then the first term in (5.29) is bounded from the above by $e^{-\{1+o(1)\}n\rho}$. For the second term in (5.29), according to condition A3, we choose β sufficiently small such that

$$\mathbb{P}_g\Big(\sup_\gamma \Big|\sum_{i=1}^n \nabla l_\gamma^i\Big| \geq e^{n^{1-\beta}}\Big) \leq n \times \mathbb{P}_g(\sup_\gamma |\nabla l_\gamma^i| > n^{-1} e^{n^{1-\beta}}) = o(e^{-n\rho}).$$

Thus, we obtain an upper bound

$$\mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l_\gamma^i > 0\Big) \leq e^{-n\{\rho+o(1)\}}.$$

Then, the type I error probability is approximated by

$$e^{-n\rho} \cong \sup_\gamma \mathbb{P}_g\Big(\sum_{i=1}^n l_\gamma^i > 0\Big) \leq \mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l_\gamma^i > 0\Big) \leq e^{-n\{\rho+o(1)\}}. \qquad (5.30)$$

We now consider the type II error probability $\alpha_2 = \sup_\gamma \mathbb{P}_{h_\gamma}(l < 0)$. For each γ, note that

$$\mathbb{P}_{h_\gamma}(l < 0) = \mathbb{P}_{h_\gamma}\Big(\sup_{\gamma_1} \sum_{i=1}^n l^i_{\gamma_1} < 0\Big) \le \mathbb{P}_{h_\gamma}\Big(\sum_{i=1}^n l^i_\gamma < 0\Big).$$

Note that the right-hand side is the type II error probability of the likelihood ratio test. According to Chernoff's calculation, we have that

$$\mathbb{P}_{h_\gamma}(l < 0) \le \mathbb{P}_{h_\gamma}\Big(\sum_{i=1}^n l^i_\gamma < 0\Big) \cong e^{-n\rho_\gamma}$$

for all γ. We take maximum with respect to γ on both sides and obtain that

$$\sup_\gamma \mathbb{P}_{h_\gamma}(l < 0) \le \sup_\gamma \mathbb{P}_g\Big(\sum_{i=1}^n l^i_\gamma > 0\Big) \cong e^{-n \min_\gamma \rho_\gamma}. \tag{5.31}$$

Thus, the maximal type II error probability has an asymptotic upper bound that decays at the rate of the Chernoff index.

In what follows, we show that this asymptotic upper bound is asymptotically achieved. We choose λ_n possibly depending on g such that

$$\mathbb{P}_g\Big(\sup_\gamma \sum_{i=1}^n l^i_\gamma > 0\Big) = \mathbb{P}_g\Big(\sum_{i=1}^n l^i_{\gamma_*} > n\lambda_n\Big).$$

Note that g is fixed and the probabilities on both sides of the above identity decay at the rate $e^{-n\rho}$. Together with the continuity of the large deviations rate function, it must be true that $\lambda_n \to 0-$. We apply Neyman-Pearson lemma to the simple null $H_0 : f = g$ versus simple alternative $H_1 : f = h_{\gamma_*}$. Note that $\{\sum_{i=1}^n l^i_{\gamma_*} > n\lambda_n\}$ is a uniformly most powerful test and $\{\sup_\gamma \sum_{i=1}^n l^i_\gamma > 0\}$ is a test with the same type I error probability. Then, we have that

$$\mathbb{P}_{h_{\gamma_*}}\Big(\sup_\gamma \sum_{i=1}^n l^i_\gamma < 0\Big) \ge \mathbb{P}_{h_{\gamma_*}}\Big(\sum_{i=1}^n l^i_{\gamma_*} < n\lambda_n\Big). \tag{5.32}$$

That is, the type II error probability of the generalized likelihood ratio test must be greater than that of the likelihood ratio test under the simple alternative h_{γ_*}. Note that $\lambda_n \to 0-$. Thanks to the the continuity of the large deviations rate function, we have that

$$\mathbb{P}_{h_{\gamma_*}}\Big(\sum_{i=1}^n l^i_{\gamma_*} < n\lambda_n\Big) \cong \mathbb{P}_{h_{\gamma_*}}\Big(\sum_{i=1}^n l^i_{\gamma_*} < 0\Big) \cong e^{-n\rho}. \tag{5.33}$$

Put together (5.31), (5.32), and (5.33), we have that

$$\sup_\gamma \mathbb{P}_{h_\gamma}(l < 0) \cong e^{-n\rho}.$$

Thus, we conclude the proof.

5.7.2 Proof of Theorem 8

The one-to-one log-likelihood ratio is

$$l_{\theta\gamma}(x) = \log h_\gamma(x) - \log g_\theta(x).$$

The generalized log-likelihood ratio statistic is

$$l = \sup_\gamma \sum_{i=1}^n \log h_\gamma(X_i) - \sup_\theta \sum_{i=1}^n \log g_\theta(X_i) = \inf_\theta \sup_\gamma \sum_{i=1}^n l^i_{\theta\gamma}$$

and the rejection region is

$$C_\lambda = \{e^l > \lambda\}.$$

We define that $\gamma(\theta) = \arg\inf_\gamma \rho_{\theta\gamma}$, and $\theta(\gamma) = \arg\inf_\theta \rho_{\theta\gamma}$, and $(\theta_*, \gamma_*) = \arg\inf_{\theta,\gamma} \rho_{\theta\gamma}$. Note that the null and the alternative are now symmetric, thus we only need to consider one of the two types of error probabilities. We consider the type II error probability. We now define

$$k_\theta = \sup_\gamma \sum_{i=1}^n l^i_{\theta\gamma}.$$

For each given θ and γ, we have a simple upper bound

$$\mathbb{P}_{h_\gamma}(k_\theta < 0) \le \mathbb{P}_{h_\gamma}\Big(\sum_{i=1}^n l^i_{\theta\gamma} < 0\Big) \cong e^{-n\rho_{\theta\gamma}}. \tag{5.34}$$

We now proceed to the type II error probability if h_γ is the true distribution, that is

$$\mathbb{P}_{h_\gamma}(\inf_\theta k_\theta < 0) \le \mathbb{P}_{h_\gamma}(\inf_\theta k_\theta < 0; \sup_\theta |\nabla k_\theta| < e^{n^{1-\beta}}) + \mathbb{P}_{h_\gamma}(\sup_\theta |\nabla k_\theta| \ge e^{n^{1-\beta}}).$$

The first term on the right-hand-side is bounded by Lemma 15 combined with (5.34)

$$\mathbb{P}_{h_\gamma}(\inf_\theta k_\theta < 0; \sup_\theta |\nabla k_\theta| < e^{n^{1-\beta}}) \le e^{-n\{\inf_\theta \rho_{\theta\gamma}+o(1)\}}.$$

For the second term, we have that

$$\begin{aligned}\mathbb{P}_{h_\gamma}\{\sup_\theta |\nabla(\sup_\gamma \sum_{i=1}^n l^i_{\theta\gamma})| \ge e^{n^{1-\beta}}\} &\le \mathbb{P}_{h_\gamma}(\sup_\theta \sup_\gamma \sum_{i=1}^n |\nabla l^i_{\theta\gamma}| \ge e^{n^{1-\beta}}) \\ &\le n\mathbb{P}_{h_\gamma}(\sup_\theta \sup_\gamma |\nabla l^i_{\theta\gamma}| \ge n^{-1}e^{n^{1-\beta}}) = o(e^{-n\rho}).\end{aligned}$$

Thus, we have that

$$\mathbb{P}_{h_\gamma}(\inf_\theta k_\theta < 0) = \mathbb{P}_{h_\gamma}(l < 0) \le e^{-n\{\inf_\theta \rho_{\theta\gamma}+o(1)\}},$$

which provides an upper bound for the type II error probability

$$\sup_\gamma \mathbb{P}_{h_\gamma}(l < 0) \le e^{-n\{\inf_{\theta,\gamma} \rho_{\theta\gamma}+o(1)\}}.$$

We now provide a lower bound. For a given θ and $\gamma(\theta) = \arg\inf_\gamma \rho_{\theta\gamma}$, applying proof of Lemma 14 for the type II error probability by considering $H_0 : f = g_\theta$ and $H_1 : f \in \{h_\gamma : \gamma \in \Gamma\}$, we have that

$$\mathbb{P}_{h_{\gamma(\theta)}}(k_\theta < 0) \cong e^{-n\rho_{\theta\gamma(\theta)}}.$$

and thus

$$\mathbb{P}_{h_{\gamma(\theta)}}(\inf_\theta k_\theta < 0) \ge \mathbb{P}_{h_{\gamma(\theta)}}(k_\theta < 0) \cong e^{-n\rho_{\theta\gamma(\theta)}}.$$

We set $\theta = \theta_*$ in the above asymptotic identity and conclude the proof.

5.7.3 Proof of Lemma 15

We consider a change of measure on the continuous sample path space Q_ζ that admits the following Radon-Nikodym derivative

$$\frac{dQ_\zeta}{d\mathbb{P}} = \frac{mes(A_\zeta)}{\int_D P\{\eta_n(\theta) > \zeta\}d\theta}, \tag{5.35}$$

where $A_\zeta = \{\theta \in D : \eta_n(\theta) > \zeta\}$ and $mes(\cdot)$ is the Lebesgue measure. Throughout the proof, we choose $\zeta = -1$. To better understand the measure Q_ζ, we provide another description of the sample path generation of η_n from Q_ζ, that requires the following three steps

1. Sample a random index $\tau \in D$ following the density function
$$h(\tau) = \frac{\mathbb{P}\{\eta_n(\tau) > \zeta\}}{\int_D \mathbb{P}\{\eta_n(\theta) > \zeta\} d\theta};$$

2. Sample $\eta_n(\tau)$ given that $\eta_n(\tau) > \zeta$;

3. Sample $\{\eta_n(\theta) : \theta \neq \tau\}$ from the original conditional distribution given the realized value of $\eta_n(\tau)$, that is, $\mathbb{P}\{\cdot|\eta_n(\tau)\}$.

To verify that the measure induced by the above sampling procedure is the same as that given by (5.35), see Adler *et al.* [2012] that provides a discrete analogue of the above change of measure.

With these constructions, the interesting probability is given by

$$\begin{aligned}
& \mathbb{P}\{\sup_{\theta\in D} \eta_n(\theta) > 0, \sup_{\theta \in D} |\nabla \eta_n(\theta)| < e^{n^{1-\beta}}\} \\
= \ & \mathbb{E}^{Q_\zeta}\Big\{\frac{d\mathbb{P}}{dQ_\zeta}; \sup_{\theta\in D} \eta_n(\theta) > 0, \sup_{\theta \in D} |\nabla \eta_n(\theta)| < e^{n^{1-\beta}}\Big\} \\
= \ & \mathbb{E}^{Q_\zeta}\Big\{\frac{1}{mes(A_\zeta)}; \sup_{\theta\in D} \eta_n(\theta) > 0, \sup_{\theta \in D} |\nabla \eta_n(\theta)| < e^{n^{1-\beta}}\Big\} \\
& \quad \times \int_D \mathbb{P}(\eta_n(\theta) > \zeta) d\theta
\end{aligned}$$

Via the condition of this lemma, we have that

$$\int_D \mathbb{P}(\eta_n(\theta) > \zeta) d\theta \cong e^{-n \min_\theta \rho(\theta)}.$$

Thus, it is sufficient to show that

$$\mathbb{E}^{Q_\zeta}\Big\{\frac{1}{mes(A_\zeta)}; \sup_{\theta\in D} \eta_n(\theta) > 0, \sup_{\theta \in D} |\nabla \eta_n(\theta)| < e^{n^{1-\beta}}\Big\}$$

cannot be too large. On the set $\{\sup_{\theta\in D}\eta_n(\theta) > 0, \sup_{\theta\in D}|\nabla\eta_n(\theta)| < n^{1-\beta}\}$, the volume $mes(A_\zeta)$ is in fact lower bounded. Let θ_* be the maximizer of $\eta_n(\theta)$ and thus $\eta_n(\theta_*) > 0$. On the other hand, the gradient of η_n is upper bounded by $e^{n^{1-\beta}}$. Therefore, there exists a small region of radius $e^{-n^{1-\beta}}$ in which η_n will be above $\zeta = -1$. Thus, $mes(A_\zeta)$ is lower bounded by $\varepsilon_0 e^{-dn^{1-\beta}}$. Thus, the bound

$$\mathbb{P}(\sup_{\theta\in D}\eta_n(\theta) > 0, \sup_{\theta\in D}|\nabla\eta_n(\theta)| < n^\beta) \leq \frac{e^{dn^{1-\beta}}}{\varepsilon_0}\int_D \mathbb{P}(\eta_n(\theta) > \zeta)d\theta \cong e^{-n\min_\theta\rho(\theta)}$$

concludes the proof.

5.7.4 Proof of Corollary 6

The proof is very similar to that of Theorem 8 and therefore we omit some repetitive steps. We first consider the type I error probability,

$$\sup_{\theta\in\Theta}\mathbb{P}_{g_\theta}(LR_n > 1).$$

For each $\theta\in\Theta$, we establish an upper bound for

$$\mathbb{P}_{g_\theta}(LR_n > 1) = \mathbb{P}_{g_\theta}\Big(\sup_{\gamma\in\Gamma}\log h_\gamma(X_i) - \sup_{\theta\in\Theta}\log g_\theta(X_i) > 0\Big). \tag{5.36}$$

The event

$$\{\sup_{\gamma\in\Gamma}\log h_\gamma(X_i) - \sup_{\theta\in\Theta}\log g_\theta(X_i) > 0\}$$

implies

$$\{\sup_{\gamma\in\Gamma}\log h_\gamma(X_i) - \log g_\theta(X_i) > 0\}.$$

Thus, we have

$$\mathbb{P}_{g_\theta}(LR_n > 1) \leq \mathbb{P}_{g_\theta}\Big(\sup_{\gamma\in\Gamma}\log h_\gamma(X_i) - \log g_\theta(X_i) > 0\Big).$$

We split the probability

$$\begin{aligned}
&\mathbb{P}_{g_\theta}\Big(\sup_{\gamma\in\Gamma}\log h_\gamma(X_i) - \log g_\theta(X_i) > 0\Big)\\
\leq\ &\mathbb{P}_{g_\theta}\Big(\sup_{\gamma\in\Gamma}\log h_\gamma(X_i) - \log g_\theta(X_i) > 0,\ \hat\gamma\in A_\theta\Big) + \mathbb{P}_{g_\theta}\Big(\hat\gamma\in A_\theta^c\Big)\\
\leq\ &\mathbb{P}_{g_\theta}\Big(\sup_{\gamma\in A_\theta}\log h_\gamma(X_i) - \log g_\theta(X_i) > 0\Big) + \mathbb{P}_{g_\theta}\Big(\hat\gamma\in A_\theta^c\Big).
\end{aligned} \tag{5.37}$$

According to Assumption A4, the second term is $o(e^{-n\rho})$. For the first term, notice that A_θ is a compact subset of R^{d_g}. The conditions for Lemma 14 are satisfied. According to Lemma 14, the first term in (5.37) is bounded above by

$$e^{-(1+o(1))n\times\min_{\gamma\in A_\theta}\rho_{\theta\gamma}} \le e^{-(1+o(1))n\times\min_{\gamma\in\Gamma}\rho_{\theta\gamma}} \le e^{-(1+o(1))n\times\min_{\theta,\gamma}\rho_{\theta\gamma}}.$$

Combining the upper bounds for the first and second terms in (5.37), we have

$$\mathbb{P}_{g_\theta}(LR_n > 1) \le e^{-(1+o(1))n\times\min_{\theta,\gamma}\rho_{\theta\gamma}}.$$

The above derivation is uniform in θ. We obtain an upper bound for the type I error

$$\sup_\theta \mathbb{P}_{g_\theta}(LR_n > 1) \le e^{-(1+o(1))n\times\min_{\theta,\gamma}\rho_{\theta\gamma}}.$$

Similarly, we obtain an upper bound for the type II error probability

$$\sup_\gamma \mathbb{P}_{h_\gamma}(LR_n \le 1) \le e^{-(1+o(1))n\times\min_{\theta,\gamma}\rho_{\theta\gamma}}.$$

Now we proceed to a lower bound for the type I error probability. Upon having the upper bounds for both type I and type II error probabilities, the lower bounds for type I and type II error probabilities can be derived using the same argument as that in the proof of Theorem 8. We omit the details.

5.7.4.1 Proof of Theorem 10

The proof of the theorem consists of establishing upper and lower bounds for the probability

$$\mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb}) = \mathbb{P}_{g_{\theta_0}}\Big(\sup_{\gamma\in\Gamma}\inf_{\theta\in\Theta}\sum_{i=1}^n[\log h_\gamma(X_i) - \log g_\theta(X_i)] > nb\Big).$$

Upper bound The event

$$\Big\{\sup_{\gamma\in\Gamma}\inf_{\theta\in\Theta}\sum_{i=1}^n \log h_\gamma(X_i) - \log g_\theta(X_i) > nb\Big\}$$

implies

$$\Big\{\sup_{\gamma\in\Gamma}\sum_{i=1}^{n}\log h_\gamma(X_i)-\log g_{\theta^\dagger}(X_i)>nb\Big\}.$$

Therefore, we have an upper bound

$$\mathbb{P}_{g_{\theta_0}}(LR_n>1)\le \mathbb{P}_{g_{\theta_0}}\Big(\sup_{\gamma}\sum_{i=1}^{n}\log h_\gamma(X_i)-\log g_{\theta^\dagger}(X_i)>nb\Big). \tag{5.38}$$

We split the probability

$$\begin{aligned} & \mathbb{P}_{g_{\theta_0}}\Big(\sup_{\gamma}\sum_{i=1}^{n}[\log h_\gamma(X_i)-\log g_{\theta^\dagger}(X_i)]>nb\Big) \qquad (5.39)\\ \le\ & \mathbb{P}_{g_{\theta_0}}\Big(\sup_{\gamma}\sum_{i=1}^{n}[\log h_\gamma(X_i)-\log g_{\theta^\dagger}(X_i)]>nb, \sup_{\gamma}\Big|\sum_{i=1}^{n}\nabla_\gamma\log h_\gamma(X_i)\Big|<e^{n^{1-\beta}}\Big)\\ & +\mathbb{P}_{g_{\theta_0}}\Big(\sup_{\gamma}\sum_{i=1}^{n}\Big|\nabla_\gamma\log h_\gamma(X_i)\Big|\ge e^{n^{1-\beta}}\Big). \end{aligned}$$

We establish upper bounds of the first and second terms in (5.39) separately. For the first term, let $\eta_n(\gamma)=\sum_{i=1}^{n}[\log h_\gamma(X_i)-\log g_{\theta^\dagger}(X_i)]-nb$. For each γ, the exponential decay rate of the probability

$$\log\mathbb{P}_{g_{\theta_0}}(\eta_n(\gamma)\ge 0)\le n\log\inf_{\lambda}M_{g_{\theta_0}}(\lambda,\gamma,\theta^\dagger). \tag{5.40}$$

is established through standard large deviation calculation. Thanks to Lemma 15 and (5.40), the first term in (5.39) is bounded above by

$$\sup_{\gamma}\inf_{\lambda}\{M_{g_{\theta_0}}(\theta^\dagger,\lambda,\gamma)\}^{(1+o(1))n}=e^{-(1+o(1))n\rho^\dagger_{g_{\theta_0}}}.$$

For the second term, according to the Assumption A3,

$$\mathbb{P}_{g_{\theta_0}}\Big(\sup_{\gamma}\sum_{i=1}^{n}\Big|\nabla_\gamma\log h_\gamma(X_i)\Big|\ge e^{n^{1-\beta}}\Big)\le n\mathbb{P}_{g_{\theta_0}}(\sup_{\gamma}|\nabla_\gamma\log h_\gamma(X_i)|>n^{-1}e^{n^{1-\beta}})=o(e^{-n\rho^\dagger_{g_{\theta_0}}}).$$

Combining the analyses for both the first and the second term, we arrive at an upper bound

$$\mathbb{P}_{g_{\theta_0}}(LR_n>e^{nb})\le e^{-(1+o(1))n\rho^\dagger_{g_{\theta_0}}}.$$

Lower bound Recall that

$$\frac{dQ^\dagger}{d\mathbb{P}_{g_{\theta_0}}} = \exp\Big\{\lambda^\dagger(\log h_{\gamma^\dagger}(X) - \log g_{\theta^\dagger}(X)) - nb\Big\}/M^\dagger_{g_{\theta_0}}.$$

Then, the probability can be written as

$$\mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb}) = \mathbb{E}^{Q^\dagger}\Big\{\frac{d\mathbb{P}_{g_{\theta_0}}}{dQ^\dagger}; \sum_{i=1}^n [\log h_{\hat\gamma}(X_i) - \log g_{\hat\theta}(X_i)] > nb\Big\},$$

where $\hat\gamma$ and $\hat\theta$ are the maximum likelihood estimators for the h-family and the g-family respectively. According to the definition of $Q^\dagger$, the above display is equal to

$$e^{-n\rho^\dagger_{g_{\theta_0}}}\mathbb{E}^{Q^\dagger}\Big\{e^{-\lambda^\dagger[\sum_{i=1}^n \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) - nb]}; \sum_{i=1}^n \log h_{\hat\gamma}(X_i) - \log g_{\hat\theta}(X_i) > nb\Big\}, \quad (5.41)$$

where $\rho^\dagger_{g_{\theta_0}} = -\log M^\dagger_{g_{\theta_0}}$. We now establish a lower bound for

$$I \triangleq \mathbb{E}^{Q^\dagger}\Big\{e^{-\lambda^\dagger[\sum_{i=1}^n \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) - nb]}; \sum_{i=1}^n \log h_{\hat\gamma}(X_i) - \log g_{\hat\theta}(X_i) > nb\Big\}.$$

Because $e^{-\lambda^\dagger[\sum_{i=1}^n \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) - nb]}$ is positive, we have

$$I \geq \mathbb{E}^{Q^\dagger}\Big\{e^{-\lambda^\dagger[\sum_{i=1}^n \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) - nb]}; \sum_{i=1}^n \log h_{\hat\gamma}(X_i) - \log g_{\hat\theta}(X_i) > nb, E_1\Big\}, \quad (5.42)$$

where

$$E_1 = \Big\{\Big|\sum_{i=1}^n \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) - nb\Big| \leq \sqrt{n}\Big|\Big\}.$$

On the set E_1, we have the following inequality of the integrand

$$e^{-\lambda^\dagger[\sum_{i=1}^n \log h_{\gamma^\dagger}(X_i) - \log g_{\theta^\dagger}(X_i) - nb]} \geq e^{-|\lambda^\dagger|\sqrt{n}}.$$

We plug the above inequality back to (5.42) and obtain a lower bound for

$$I \geq e^{-|\lambda^\dagger|\sqrt{n}} Q^\dagger\Big(\{\sum_{i=1}^n \log h_{\hat\gamma}(X_i) - \log g_{\hat\theta}(X_i) > nb\} \cap E_1\Big). \quad (5.43)$$

For the rest of the proof, we develop a lower bound for the probability

$$Q^{\dagger}\Big(\{\sum_{i=1}^{n}\log h_{\hat\gamma}(X_i)-\log g_{\hat\theta}(X_i)>nb\}\cap E_1\Big).$$

The maximum likelihood estimator $\hat\gamma$ satisfies the inequality

$$\sum_{i=1}^{n}\{\log h_{\hat\gamma}(X_i)-\log h_{\gamma^{\dagger}}(X_i)\}\geq 0. \tag{5.44}$$

Furthermore, with the aid of Rolle's Theorem, there exists $\tilde\theta$ such that

$$\begin{aligned}&\sum_{i=1}^{n}\{\log g_{\hat\theta}(X_i)-\log g_{\theta^{\dagger}}(X_i)\}\\ =\ &(\hat\theta-\theta^{\dagger})\cdot\sum_{i=1}^{n}\nabla_{\theta}\log g_{\theta^{\dagger}}(X_i)+\frac{1}{2}(\hat\theta-\theta^{\dagger})^{\top}\sum_{i=1}^{n}\nabla^2_{\theta}g_{\tilde\theta}(X_i)(\hat\theta-\theta^{\dagger}),\end{aligned} \tag{5.45}$$

where "∇^2_{θ}" denotes the Hessian matrices with respect to θ and "$\cdot$" denotes the inner product between vectors. (5.44) and (5.45) together give

$$\begin{aligned}&\sum_{i=1}^{n}\{\log h_{\hat\gamma}(X_i)-\log g_{\hat\theta}(X_i)\}-\sum_{i=1}^{n}\{\log h_{\gamma^{\dagger}}(X_i)-g_{\theta^{\dagger}}(X_i)\}\\ \geq\ &-(\hat\theta-\theta^{\dagger})\cdot\sum_{i=1}^{n}\nabla_{\theta}\log g_{\theta^{\dagger}}(X_i)-\frac{1}{2}(\hat\theta-\theta^{\dagger})^{\top}\sum_{i=1}^{n}\nabla^2_{\theta}g_{\tilde\theta}(X_i)(\hat\theta-\theta^{\dagger}).\end{aligned} \tag{5.46}$$

We define

$$E_2=\Big\{(\hat\theta-\theta^{\dagger})^{\top}\sum_{i=1}^{n}\nabla_{\theta}\log g_{\theta^{\dagger}}(X_i)\leq\frac{\sqrt{n}}{4}\Big\},$$

$$E_3=\Big\{\frac{1}{2}|\hat\theta-\theta^{\dagger}|^2\sup_{\theta}\sum_{i=1}^{n}|\nabla^2_{\theta}\log g_{\theta}(X_i)|\leq\frac{\sqrt{n}}{4}\Big\},$$

$$E_4=\Big\{\frac{\sqrt{n}}{2}<\sum_{i=1}^{n}[\log h_{\gamma^{\dagger}}(X_i)-\log g_{\theta^{\dagger}}(X_i)]-nb\leq\sqrt{n}\Big\}.$$

Based on (5.46), we have that

$$(E_2\cap E_3\cap E_4)\subset\{\sum_{i=1}^{n}\log h_{\hat\gamma}(X_i)-\log g_{\hat\theta}(X_i)>nb\}\cap E_1.$$

We insert this to (5.42), and obtain that

$$I\geq e^{-|\lambda^{\dagger}|\sqrt{n}}Q^{\dagger}(E_2\cap E_3\cap E_4)\geq e^{-|\lambda^{\dagger}|\sqrt{n}}\Big\{Q^{\dagger}(E_4)-Q^{\dagger}(E_2^c)-Q^{\dagger}(E_3^c)\Big\}. \tag{5.47}$$

For the rest of the proof, we develop upper bounds for $Q^\dagger(E_2^c)$ and $Q^\dagger(E_3^c)$ and a lower bound for $Q^\dagger(E_4)$. For $Q^\dagger(E_4)$, because $\lambda^\dagger = \arg\inf_\lambda M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda)$, we have

$$\frac{\partial}{\partial\lambda}M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger)=0.$$

Consequently,

$$\mathbb{E}^{Q^\dagger}(\log h_{\gamma^\dagger}(X)-\log g_{\theta^\dagger}(X)-b)=(M^\dagger_{g_{\theta_0}})^{-1}\frac{\partial}{\partial\lambda}M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger)=0.$$

According to the central limit theorem, there exists $\varepsilon_0>0$ such that

$$\liminf_{n\to\infty}Q^\dagger(E_4)>\varepsilon_0.$$

Thus a lower bound for $Q^\dagger(E_4)$ has been derived. Before we proceed to upper bounds for $Q^\dagger(E_2^c)$ and $Q^\dagger(E_3^c)$, we establish the following lemma, whose proof is provided in Appendix 5.7.5.1.

Lemma 16. *Under the settings of Theorem 10, we have*

$$\gamma^\dagger=\bar\gamma \textit{ and } \theta^\dagger=\bar\theta.$$

We now proceed to an upper bound of $Q^\dagger(E_2^c)$. We split the sum

$$\begin{aligned}&(\hat\theta-\theta^\dagger)^\top\sum_{i=1}^n\nabla_\theta\log g_{\theta^\dagger}(X_i) \qquad (5.48)\\ &\quad=(\hat\theta-\theta^\dagger)^\top\sum_{i=1}^n[\nabla_\theta\log g_{\theta^\dagger}(X_i)-\mathbb{E}^{Q^\dagger}\nabla_\theta g_{\theta^\dagger}(X_i)]+n(\hat\theta-\theta^\dagger)^\top\mathbb{E}^{Q^\dagger}\nabla_\theta g_{\theta^\dagger}(X)\end{aligned}$$

Note that $\hat\theta\in T_{\theta^\dagger}\Theta$, according to Assumption A6 and Lemma 16, we have that $(\hat\theta-\theta^\dagger)^\top\mathbb{E}^{Q^\dagger}\nabla_\theta g_{\theta^\dagger}(X)\le 0$. Therefore, (5.48) implies

$$(\hat\theta-\theta^\dagger)^\top\sum_{i=1}^n\nabla_\theta\log g_{\theta^\dagger}(X_i)\le(\hat\theta-\theta^\dagger)^\top\sum_{i=1}^n[\nabla_\theta\log g_{\theta^\dagger}(X_i)-\mathbb{E}^{Q^\dagger}\nabla_\theta g_{\theta^\dagger}(X_i)]. \qquad (5.49)$$

Using Chebyshev's inequality and the fact $\mathbb{E}(|\nabla_\theta\log g_{\theta^\dagger}(X)|^2)<\infty$, we have

$$n^{-\frac{3}{4}}\sum_{i=1}^n[\nabla_\theta\log g_{\theta^\dagger}(X_i)-\mathbb{E}^{Q^\dagger}\nabla_\theta g_{\theta^\dagger}(X_i)]\to 0 \text{ in probability } Q^\dagger.$$

According to Slutsky's theorem and $\sqrt{n}(\hat{\theta}-\theta^\dagger) = O_{Q^\dagger}(1)$, we have

$$\sqrt{n}(\hat{\theta}-\theta^\dagger)^\top n^{-\frac{3}{4}} \sum_{i=1}^{n} \nabla_\theta \log g_{\theta^\dagger}(X_i) \to 0 \text{ in probability } Q^\dagger.$$

Consequently,

$$\lim_{n\to\infty} Q^\dagger\Big((\hat{\theta}-\theta^\dagger)^\top \sum_{i=1}^{n}[\nabla_\theta \log g_{\theta^\dagger}(X_i) - \mathbb{E}^{Q^\dagger}\nabla_\theta g_{\theta^\dagger}(X_i)] > \frac{\sqrt{n}}{4}\Big) = 0.$$

According to (5.49) and the above display, we have

$$\lim_{n\to\infty} Q^\dagger\Big((\hat{\theta}-\theta^\dagger)^\top \sum_{i=1}^{n} \nabla_\theta \log g_{\theta^\dagger}(X_i) > \frac{\sqrt{n}}{4}\Big) = 0.$$

Thus, $Q^\dagger(E_2^c) \to 0$ as $n \to \infty$. We provide an upper bound of $Q^\dagger(E_3^c)$ using a similar method. With the aid of Chebyshev's inequality, we have

$$n^{-\frac{5}{4}} \sum_{i=1}^{n} \sup_\theta |\nabla_\theta^2 \log g_\theta(X_i)| \to 0 \text{ in probability } Q^\dagger.$$

According to Slutsky's theorem and $\sqrt{n}(\hat{\theta}-\theta^\dagger) = O_{Q^\dagger}(1)$, we have

$$n|\hat{\theta}-\theta^\dagger|^2 \times n^{-\frac{5}{4}} \sum_{i=1}^{n} \sup_\theta |\nabla_\theta^2 \log g_\theta(X_i)| \xrightarrow{d} 0.$$

Consequently,

$$\begin{aligned} & \lim_{n\to\infty} Q^\dagger\Big(|\hat{\theta}-\theta^\dagger|^2 \sup_\theta \sum_{i=1}^{n} |\nabla_\theta^2 \log g_\theta(X_i)| > \frac{\sqrt{n}}{4}\Big) \\ \leq & \lim_{n\to\infty} Q^\dagger\Big(|\hat{\theta}-\theta^\dagger|^2 \sum_{i=1}^{n} \sup_\theta |\nabla_\theta^2 \log g_\theta(X_i)| > \frac{\sqrt{n}}{4}\Big) \\ = & \; 0. \end{aligned}$$

Therefore, $Q^\dagger(E_3) \to 0$ as $n \to \infty$. We combine the results for $Q^\dagger(E_2^c), Q^\dagger(E_3^c)$, $Q^\dagger(E_4)$, and (5.47),

$$I \geq \frac{\varepsilon_0}{2} e^{-|\lambda^\dagger|\sqrt{n}} \text{ for } n \text{ sufficiently large.}$$

Combining the above display with (5.41), we arrive at the lower bound

$$\mathbb{P}_{g_{\theta_0}}(LR_n > e^{nb}) \geq e^{-n(1+o(1))\rho^\dagger_{g_{\theta_0}}}.$$

We complete the proof by combining the lower bound and upper bound for the probability $\mathbb{P}_{g_{\theta_0}}(LR_n > 1)$.

5.7.5 Proof of Theorem 11

The proof is similar to that of Theorem 10. Throughout the proof, we will use κ as a generic notation to denote large and not-so-important constants whose value may vary from place to place. Similarly, we use ε as a generic notation for small positive constants. The proof of the theorem consists of establishing upper and lower bounds for the probability

$$\mathbb{P}_{\beta^0}(LR_n \geq 1) = \mathbb{P}_{\beta^0}\Big(\sup_{\gamma}\inf_{\beta}\sum_{i=1}^{n}[\log h_i(Y_i,\gamma) - \log g_i(Y_i,\beta)] \geq 0\Big).$$

Upper bound Similar to (5.38), we have

$$\mathbb{P}_{\beta^0}(LR_n \geq 1) \leq \mathbb{P}_{\beta^0}\Big(\sup_{\gamma}\sum_{i=1}^{n}[\log h_i(Y_i,\gamma) - \log g_i(Y_i,\beta_n^{\dagger})] \geq 0\Big)$$

According to the definition of $h_i(Y_i,\gamma)$ and $g_i(Y_i,\beta)$, we have

$$\begin{aligned}&\sum_{i=1}^{n}[\log h_i(Y_i,\gamma) - \log g_i(Y_i,\beta)]\\ =\ &\sum_{i=1}^{n}[\gamma^T Z^{(i)} Y_i - b(\gamma^T Z^{(i)})] - \sum_{i=1}^{n}[\beta_n^{\dagger T} X^{(i)} Y_i - b(\beta_n^{\dagger T} X^{(i)})].\end{aligned}$$

Consequently, we have

$$\mathbb{P}_{\beta^0}(LR_n \geq 1) \leq \mathbb{P}_{\beta^0}\Big((\frac{1}{n}\sum_{i=1}^{n} Z^{(i)} Y_i, \frac{1}{n}\sum_{i=1}^{n} X^{(i)} Y_i) \in A_n\Big), \tag{5.50}$$

where

$$\begin{aligned}A_n\ =\ &\Big\{(s_1,s_2) : s_1 \in R^p, s_2 \in R^q \text{and}\\ &\sup_{\gamma}[\gamma^T s_2 - \frac{1}{n}\sum_{i=1}^{n} b(\gamma^T Z^{(i)})] \geq [\beta_n^{\dagger T} s_1 - \frac{1}{n}\sum_{i=1}^{n} b(\beta_n^{\dagger T} X^{(i)})]\Big\}.\end{aligned}$$

We consider the change of measure

$$\frac{dQ^{\dagger}}{d\mathbb{P}} \tag{5.51}$$

$$= \exp\Big\{\lambda_n^{\dagger}\sum_{i=1}^{n}(\gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i) \tag{5.52}$$

$$-\sum_{i=1}^{n}[b((\beta^0)^T X^{(i)} + \lambda_n^{\dagger}\{\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}\}) - b((\beta^0)^T X^{(i)})]\Big\}. \tag{5.53}$$

According to (5.50), we have

$$\mathbb{P}_{\beta^0}(LR_n \geq 1) \leq \mathbb{E}^{Q^\dagger}\Big[\frac{d\mathbb{P}}{dQ^\dagger}; (\frac{1}{n}\sum_{i=1}^n Z^{(i)}Y_i, \frac{1}{n}\sum_{i=1}^n X^{(i)}Y_i) \in A_n.\Big]$$

The above display and (5.51) together gives

$$\begin{aligned}
&\mathbb{P}_{\beta^0}(LR_n \geq 1) \\
&\quad \leq \exp\Big\{\sum_{i=1}^n \Big[b\Big((\beta^0)^T X^{(i)} + \lambda_n^\dagger\{\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}\}\Big) - b\Big((\beta^0)^T X^{(i)}\Big)\Big]\Big\} \\
&\quad \times \mathbb{E}^{Q^\dagger}\Big[e^{-\lambda_n^\dagger \sum_{i=1}^n (\gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i)}; (\frac{1}{n}\sum_{i=1}^n Z^{(i)}Y_i, \frac{1}{n}\sum_{i=1}^n X^{(i)}Y_i) \in A_n\Big]. \quad (5.54)
\end{aligned}$$

The next lemma shows a property of $\beta_n^\dagger$ and A_n.

Lemma 17. *For all* $(s_1, s_2) \in A_n$,

$$[\gamma^{\dagger T} s_2 - \frac{1}{n}\sum_{i=1}^n b(\gamma^{\dagger T} Z^{(i)})] \geq [\beta_n^{\dagger T} s_1 - \frac{1}{n}\sum_{i=1}^n b(\beta_n^{\dagger T} X^{(i)})].$$

According to Lemma 17, the right-hand side of (5.54) is further bounded above by

$$\begin{aligned}
& \mathbb{P}_{\beta^0}(LR_n \geq 1) & (5.55)\\
\leq\ & \exp\Big\{\sum_{i=1}^n \Big[b\Big((\beta^0)^T X^{(i)} + \lambda_n^\dagger\{\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}\}\Big) - b((\beta^0)^T X^{(i)})\Big] & (5.56)\\
& -\lambda_n^\dagger \sum_{i=1}^n \Big[b\Big(\gamma_n^{\dagger T} Z^{(i)}\Big) - b\Big(\beta_n^{\dagger T} X^{(i)}\Big)\Big]\Big\} & (5.57)\\
& \times Q^\dagger\Big[(\frac{1}{n}\sum_{i=1}^n Z^{(i)}Y_i, \frac{1}{n}\sum_{i=1}^n X^{(i)}Y_i) \in A_n\Big]. & (5.58)
\end{aligned}$$

Because $Q^\dagger\Big[(\frac{1}{n}\sum_{i=1}^n Z^{(i)}Y_i, \frac{1}{n}\sum_{i=1}^n X^{(i)}Y_i) \in A_n\Big] \leq 1$, we arrive at

$$\begin{aligned}
& \mathbb{P}_{\beta^0}(LR_n \geq 1) \\
\leq\ & \exp\Big\{\sum_{i=1}^n [b((\beta^0)^T X^{(i)} + \lambda_n^\dagger\{\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}\}) - b((\beta^0)^T X^{(i)})] \\
& -\lambda_n^\dagger \sum_{i=1}^n [b(\gamma_n^{\dagger T} Z^{(i)}) - b(\beta_n^{\dagger T} X^{(i)})]\Big\}.
\end{aligned}$$

According to the definition of $\widetilde{\rho}_n^\dagger$, the right-hand side of the above inequality equals $e^{-n\widetilde{\rho}_n^\dagger}$. Therefore, we arrive at the upper bound

$$\mathbb{P}_{\beta^0}(LR_n \geq 1) \leq e^{-n\widetilde{\rho}_n^\dagger}.$$

Lower bound Notice that the event

$$\{\sum_{i=1}^n \log h_i(Y_i, \gamma_n^\dagger) - \sup_\beta \sum_{i=1}^n \log g_i(Y_i, \beta) \geq 0\}.$$

implies the event

$$\{\sup_\gamma \sum_{i=1}^n \log h_i(Y_i, \gamma) - \sup_\beta \sum_{i=1}^n \log g_i(Y_i, \beta) \geq 0\}.$$

Therefore, a lower bound for the probability $\mathbb{P}_{\beta^0}(LR_n \geq 1)$ is

$$\mathbb{P}_{\beta^0}\Big(\sum_{i=1}^n \log h_i(Y_i, \gamma_n^\dagger) - \sup_\beta \sum_{i=1}^n \log g_i(Y_i, \beta) \geq 0\Big).$$

According to the definition of $Q^\dagger$ in (5.51), the above probability equals

$$\exp\Big\{\sum_{i=1}^n [b((\beta^0)^T X^{(i)} + \lambda_n^\dagger\{\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}\}) - b((\beta^0)^T X^{(i)})]\Big\}$$
$$\times \mathbb{E}^{Q^\dagger}\Big[e^{-\lambda_n^\dagger \sum_{i=1}^n (\gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i)}; E\Big], \quad (5.59)$$

where the event

$$E = \Big\{\sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \hat{\beta}_n^T X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\hat{\beta}_n^T X^{(i)}) \geq 0\Big\},$$

and $\hat{\beta}_n$ is the maximum likelihood estimator

$$\hat{\beta}_n = \arg\sup_\beta \sum_{i=1}^n \beta^T X^{(i)} Y_i - b(\beta X^{(i)}).$$

Notice that

$$\begin{aligned} & e^{-n\widetilde{\rho}_n^\dagger} \\ = \quad & \exp\Big\{\sum_{i=1}^n [b((\beta^0)^T X^{(i)} + \lambda_n^\dagger\{\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}\}) - b((\beta^0)^T X^{(i)})] \\ & -\lambda_n^\dagger [b(\gamma_n^{\dagger T} Z^{(i)}) - b(\beta_n^{\dagger T} X^{(i)})]\Big\}. \end{aligned}$$

Therefore,

$$\mathbb{P}_{\beta^0}(LR_n \geq 1) \geq e^{-n\widetilde{\rho}_n} \times J, \tag{5.60}$$

where we define the quantity

$$J = \mathbb{E}^{Q^\dagger}\Big[e^{-\lambda_n^\dagger[\sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)})]}; E\Big].$$

We proceed to establishing a lower bound of J. We consider two events

$$E_1 = \Big\{\frac{\sqrt{n}}{2} < \sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)}) \leq \sqrt{n}\Big\}$$

and

$$E_2 = \Big\{\sum_{i=1}^n [\hat{\beta}_n^T X^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\hat{\beta}_n^T X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)})] \leq \frac{\sqrt{n}}{2}\Big\}.$$

Because E_1 together with E_2 implies E, we have $E \supset E_1 \cap E_2$. Consequently,

$$J \geq \mathbb{E}^{Q^\dagger}\Big[e^{-\lambda_n^\dagger[\sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)})]}; E_1 \cap E_2\Big].$$

Notice that on the set E_1,
$\sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)}) \leq \sqrt{n}$. Therefore,

$$J \geq e^{-\lambda_n^\dagger \sqrt{n}} Q^\dagger(E_1 \cap E_2) \geq e^{-\lambda_n^\dagger \sqrt{n}}\Big(Q^\dagger(E_1) - Q^\dagger(E_2^c)\Big). \tag{5.61}$$

We provide an upper bound for $Q^\dagger(E_1)$ and a lower bound for $Q^\dagger(E_2^c)$.

Lemma 18. *Let*

$$v_n = Var^{Q^\dagger}\Big(\sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)})\Big),$$

then $v_n = O(n)$ as $n \to \infty$. Furthermore, we have

$$\mathcal{L}\Big(v_n^{-\frac{1}{2}}\Big[\sum_{i=1}^n \gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)})\Big]\Big) \to N(0,1).$$

Here, $\mathcal{L}(\cdot)$ denotes the law of random variables and $N(0,1)$ is the distribution of standard normal.

According to Lemma 18, there exists a constant $\varepsilon > 0$ such that

$$Q^{\dagger}(E_1) \geq \varepsilon. \tag{5.62}$$

We proceed to a lower bound for $Q^{\dagger}(E_2)$. Define the function for $\mu \in R^p$

$$u(\mu, \beta) = (\beta - \beta_n^{\dagger})^T \mu - \sum_{i=1}^{n} [b(\beta^T X^{(i)}) - b(\beta_n^{\dagger} X^{(i)})].$$

We further define the function

$$v(\mu) = \sup_{\beta} u(\mu, \beta).$$

Lemma 19. *Let*

$$\mu^{\dagger} = \sum_{i=1}^{n} b'\Big(\lambda_n^{\dagger}(\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger} X^{(i)}) + (\beta^0)^T X^{(i)}\Big) X^{(i)},$$

then $v(\mu)$ *is twice continuous differentiable around* $\mu^{\dagger}$*, with* $v(\mu^{\dagger}) = 0$ *and* $\nabla v(\mu^{\dagger}) = 0$*. Moreover, we have*

$$\nabla^2 v(\mu) = \Big[\sum_{i=1}^{n} b''\Big(\beta(\mu)^T X^{(i)}\Big) X^{(i)} X^{(i)T}\Big]^{-1},$$

where $\beta(\mu) = \arg\sup_{\beta} u(\mu, \beta)$*.*

According to Lemma 19 and Taylor expansion of $v(\mu)$ around $\mu^{\dagger}$, we have

$$\Big\{v(\mu) \geq \frac{\sqrt{n}}{2}\Big\} \subset \Big\{\frac{1}{2}\|\mu - \mu^{\dagger}\|^2 \|\nabla^2 v(\mu^{\dagger})\|_2 \geq \frac{\sqrt{n}}{2}\Big\}, \tag{5.63}$$

where $\|\cdot\|_2$ is denotes the spectral norm of matrices. According to Lemma 19 and Assumptions A10 and A11, $\|\nabla^2 v(\mu^{\dagger})\|_2 = O(n)$. Therefore, (5.63) implies

$$\Big\{v(\mu) \geq \frac{\sqrt{n}}{2}\Big\} \subset \Big\{\|\mu - \mu^{\dagger}\| \geq \varepsilon n^{\frac{3}{4}}\Big\}.$$

Notice that the event $E_2^c = \{v(\sum_{i=1}^{n} X^{(i)} Y_i) \geq \frac{\sqrt{n}}{2}\}$, we have

$$Q^{\dagger}(E_2^c) \leq Q^{\dagger}\Big(\|\sum_{i=1}^{n} X^{(i)} Y_i - \mu^{\dagger}\| \geq \varepsilon n^{\frac{3}{4}}\Big).$$

With the aid of Chebyshev's inequality, the above display implies

$$Q^\dagger(E_2^c) \le (\varepsilon^{-2} n^{-\frac{3}{2}}) \mathbb{E}^{Q^\dagger} \| \sum_{i=1}^n X^{(i)} Y_i - \mu^\dagger \|^2$$

Because $\mathbb{E}^{Q^\dagger} \| \sum_{i=1}^n X^{(i)} Y_i - \mu^\dagger \|^2 = O(n)$, we have $Q^\dagger(E_2^c)$ tend to zero as n goes to infinity. Combining this result with (5.61) and (5.62), we arrive at a lower bound for J

$$J \ge \frac{\varepsilon}{2} e^{-\lambda_n^\dagger \sqrt{n}}.$$

The above inequality together with (5.60) gives a lower bound

$$\mathbb{P}(LR_n \ge 1) \ge \frac{\varepsilon}{2} e^{-n\widetilde{\rho}_n^\dagger - \lambda_n^\dagger \sqrt{n}}. \tag{5.64}$$

According to Assumption A9, $\widetilde{\rho}_n^\dagger \ge \inf_\gamma \sup_\lambda \widetilde{\rho}_n(\beta^0, \gamma, \lambda) \ge \delta_1$, so $\lambda_n^\dagger \sqrt{n} = o(1) n \widetilde{\rho}_n^\dagger$. Therefore, (5.64) implies $\mathbb{P}_{\beta^0}(LR_n \ge 1) \ge e^{-n\widetilde{\rho}_n^\dagger (1+o(1))}$. We complete the proof by combining the lower and upper bound for $\mathbb{P}_{\beta^0}(LR_n \ge 1)$

5.7.5.1 Proof of Lemma 16

Proof of Lemma 16. According to condition A6, it is sufficient to show that for all $y \in T_{\gamma^\dagger}\Gamma$,

$$\mathbb{E}^{Q^\dagger} y^\top \nabla_\gamma h_{\gamma^\dagger}(X) \le 0, \tag{5.65}$$

and for all $y \in T_{\theta^\dagger}\Theta$,

$$\mathbb{E}^{Q^\dagger} y^\top \nabla_\theta g_{\theta^\dagger}(X) \le 0. \tag{5.66}$$

We first prove (5.65). We discuss two cases: $\gamma^\dagger \in int(\Gamma)$ and $\gamma^\dagger \in \partial\Gamma$, where $int(\Gamma)$ denotes the interior of Γ.

Case 1: $\gamma^\dagger \in int(\Gamma)$ Because $\lambda^\dagger = \arg\inf_\lambda M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda)$, we have $\frac{\partial}{\partial\lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) = 0$. According to the definition of $\gamma^\dagger$, $(\gamma^\dagger, \lambda^\dagger)$ is a solution of the constrained optimization problem,

$$\max_{\gamma,\lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma, \lambda) \text{ such that } \frac{\partial}{\partial\lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma, \lambda) = 0, \tag{5.67}$$

and thus it satisfies the Karush-Kuhn-Tucker conditions. That is, there exists a constant μ such that

$$\begin{cases} \nabla_\gamma M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) & = & \mu\nabla_\gamma \frac{\partial}{\partial\lambda} M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) \\ \frac{\partial}{\partial\lambda} M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) & = & \mu\frac{\partial^2}{\partial^2\lambda} M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) \\ \frac{\partial}{\partial\lambda} M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) & = & 0 \end{cases}.$$

The second and third equations in the above display together imply that $\mu = 0$. We plug $\mu = 0$ to the first equation and obtain that

$$\nabla_\gamma M_{g_{\theta_0}}(\theta^\dagger,\gamma^\dagger,\lambda^\dagger) = 0. \tag{5.68}$$

According to the definition of $M_{g_{\theta_0}}(\theta,\gamma,\lambda)$, we have

$$\nabla_\gamma M_{g_{\theta_0}}(\theta,\gamma,\lambda) = \lambda\mathbb{E}_{g_{\theta_0}} \exp\{\lambda(\log h_\gamma(X) - \log g_\theta(X) - b)\}\nabla_\gamma \log h_\gamma(X)/M^\dagger_{g_{\theta_0}}. \tag{5.69}$$

We plug this in (5.68), and obtain

$$\mathbb{E}^{Q^\dagger}\nabla_\gamma \log h_{\gamma^\dagger}(X) = 0.$$

Consequently, for all $y \in R^{d_h}$, (5.65) holds.

Case 2: $\gamma^\dagger \in \partial\Gamma$ Because $\partial\Gamma$ is continuously differentiable, with possibly relabeling the coordinate of γ, there exists a continuously differentiable function $v : R^{d_h-1} \to R$ and $r > 0$ such that

$$B(\gamma^\dagger, r) \cap \Gamma = \{\gamma \in B(\gamma^\dagger, r) : \gamma_{d_h} \ge v(\gamma_1, ..., \gamma_{d_h-1})\}, \tag{5.70}$$

where $B(\gamma^\dagger, r) = \{\gamma : |\gamma - \gamma^\dagger| \le r\}$ is a closed ball centered around $\gamma^\dagger$. Similar to Case 1, we consider the constrained optimization problem (5.67) with the additional constraint

$$\gamma_{d_h} \ge v(\gamma_1, ..., \gamma_{d_h-1}).$$

The definition of $\gamma^\dagger$ implies that $(\gamma^\dagger, \lambda^\dagger)$ is a local maximum to this optimization problem. Again, it satisfies the Karush-Kuhn-Tucker conditions for optimization problem with inequality constraint. That is, there exists constant μ_1 and μ_2 such that $\mu_1 \geq 0$ and

$$\begin{cases} \frac{\partial}{\partial \gamma_i} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) &=& \mu_1 \frac{\partial}{\partial \gamma_i} v(\gamma_1^\dagger, ..., \gamma_{d_h-1}^\dagger) + \mu_2 \nabla_\gamma \frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger), i \leq d_h - 1 \\ \frac{\partial}{\partial \gamma_d} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) &=& -\mu_1 + \mu_2 \nabla_\gamma \frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) \\ \frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) &=& \mu_2 \frac{\partial^2}{\partial^2 \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) \\ \frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) &=& 0 \end{cases}.$$

Similar to the Case 1, the third and the fourth equalities together imply that $\mu_2 = 0$. We plug this in the first and the second equalities and obtain that

$$\nabla_\gamma M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) = \mu_1 (\nabla v(\gamma_1^\dagger, ..., \gamma_{d_h-1}^\dagger)^T, -1)^T. \tag{5.71}$$

We now prove that $\gamma^\dagger$ satisfies (5.65). Notice that $\partial \Gamma$ is continuously differentiable, therefore the tangent cone is

$$T_{\gamma^\dagger}\Gamma = \{y \in R^{d_h} : y \cdot (\nabla v(\gamma_1^\dagger, ..., \gamma_{d_h-1}^\dagger)^T, -1)^T \leq 0\}.$$

Consequently, for all $y \in T_{\gamma^\dagger}\Gamma$, (5.71) implies

$$\nabla_\gamma M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) \cdot y = \mu_1 y \cdot (\nabla v(\gamma_1^\dagger, ..., \gamma_{d_h-1}^\dagger)^T, -1)^T \leq 0. \tag{5.72}$$

Notice that

$$\frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, 0) = \mathbb{E}_{g_{\theta_0}}[\log h_{\gamma^\dagger}(X) - \log g_{\theta^\dagger}(X) - b] < 0,$$

and

$$\frac{\partial^2}{\partial^2 \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda) = \mathbb{E}_{g_{\theta_0}}\left\{ e^{\lambda[\log h_\gamma(X) - \log g_\theta(X) - b]} [\log h_{\gamma^\dagger}(X) - \log g_{\theta^\dagger}(X) - b]^2 \right\} > 0.$$

Thus $\lambda^\dagger > 0$. We prove (5.65) by plugging (5.69) in (5.72) and notice that $\lambda^\dagger > 0$. Now we proceed to the proof of (5.66). Again, we consider two cases: $\gamma^\dagger \in int(\Gamma)$ and $\gamma^\dagger \in \partial\Gamma$.

Case 1: $\gamma^\dagger \in int(\Gamma)$. According to the definition of $(\theta^\dagger, \gamma^\dagger, \lambda^\dagger)$ and (5.68), $(\theta^\dagger, \gamma^\dagger, \lambda^\dagger)$ is a local minimum of the optimization problem

$$\inf_{\theta,\gamma,\lambda} M_{g_{\theta_0}}(\theta, \gamma, \lambda) \text{ such that } \frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta, \gamma, \lambda) = 0, \text{ and } \nabla_\gamma M_{g_{\theta_0}}(\theta, \gamma, \lambda) = 0.$$

We prove (5.66) using a similar proof as that for (5.65) and treating $\theta^\dagger$ and $(\gamma^\dagger, \lambda^\dagger)$ as $\gamma^\dagger$ and $\lambda^\dagger$ respectively. The details are omitted.

Case 2: $\gamma^\dagger \in \partial\Gamma$. We will first transform the Case 2 to Case 1. Recall the definition of v and r in (5.70), for $\gamma \in B(\gamma^\dagger, r) \cap \partial\Gamma$, we have

$$\gamma_d = v(\gamma_1, ..., \gamma_{d_h-1}).$$

Let $\Phi : R^{d_h} \to R^{d_h-1}$ be a function such that $\Phi(\gamma) = (\gamma_1, ..., \gamma_{d_h-1})^T$. Let $\xi = \Phi(\gamma)$, and $\xi^\dagger = \Phi(\gamma^\dagger)$, then for $\gamma \in B(\gamma^\dagger, r) \cap \partial\Gamma$, $\gamma = (\xi^T, v(\xi))^T$. We abuse the notation a little and write

$$\widetilde{M}_{g_{\theta_0}}(\theta, \xi, \lambda) = M_{g_{\theta_0}}(\theta, \gamma, \lambda),$$

where $\gamma = (\xi^T, v(\xi))^T$. We further let $\Xi = \Phi(B(\gamma^\dagger, r) \cap \Gamma)$. We compute the partial derivatives of $\widetilde{M}_{g_{\theta_0}}(\theta, \xi, \lambda)$ at $(\theta^\dagger, \xi^\dagger, \lambda^\dagger)$,

$$\frac{\partial}{\partial \lambda} \widetilde{M}_{g_{\theta_0}}(\theta^\dagger, \xi^\dagger, \lambda^\dagger) = \frac{\partial}{\partial \lambda} M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger) = 0, \tag{5.73}$$

and

$$\nabla_\xi \widetilde{M}_{g_{\theta_0}}(\theta^\dagger, \xi^\dagger, \lambda^\dagger) = \frac{d\gamma}{d\xi}(\xi^\dagger)^T \nabla_\gamma M_{g_{\theta_0}}(\theta^\dagger, \gamma^\dagger, \lambda^\dagger), \tag{5.74}$$

where $\frac{d\gamma}{d\xi}$ is a $d_h \times (d_h - 1)$ Jacobian matrix

$$\frac{d\gamma}{d\xi} = \begin{bmatrix} I_{d_h-1} \\ \nabla v(\xi^\dagger)^T \end{bmatrix},$$

and I_{d_h-1} is the $(d_h - 1) \times (d_h - 1)$ identity matrix. We plug (5.71) and the above expression in (5.73), and obtain

$$\nabla_\xi \widetilde{M}_{g_{\theta_0}}(\theta^\dagger, \xi^\dagger, \lambda^\dagger) = \mu_1(\nabla v(\xi^\dagger) - \nabla v(\xi^\dagger))^T = 0.$$

Therefore, $(\theta^\dagger, \xi^\dagger, \lambda^\dagger)$ is a local minimum under the constrained optimization problem

$$\inf_{\theta,\xi,\lambda} \widetilde{M}_{g_{\theta_0}}(\theta,\xi,\lambda) \text{ such that } \nabla_\xi \widetilde{M}_{g_{\theta_0}}(\theta,\xi,\lambda) = 0 \text{ and } \frac{\partial}{\partial\lambda}\widetilde{M}_{g_{\theta_0}}(\theta,\xi,\lambda) = 0.$$

We complete the proof by replacing γ and Γ by ξ and Ξ respectively in the proof for Case 1. $\square$

5.7.6 Proof of Lemma 17

Define the function

$$w(s_1, s_2) = \sup_\gamma [\gamma^T s_2 - \frac{1}{n}\sum_{i=1}^n b(\gamma^T Z^{(i)})] - [\beta_n^{\dagger T} s_1 - \frac{1}{n}\sum_{i=1}^n b(\beta_n^{\dagger T} X^{(i)})].$$

Then $A_n = \{(s_1, s_2) : w(s_1, s_2) \geq 0\}$. Let

$$s_1^\dagger = \frac{1}{n}\sum_{i=1}^n b'\Big(\lambda_n^\dagger(\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}) + (\beta^0)^T X^{(i)}\Big) X^{(i)}$$

and

$$s_2^\dagger = \frac{1}{n}\sum_{i=1}^n b'\Big(\lambda_n^\dagger(\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}) + (\beta^0)^T X^{(i)}\Big) Z^{(i)}.$$

With similar proof as that for (5.65), we have that $\gamma_n^\dagger$ satisfies first order conditions

$$\begin{aligned} &\nabla_\gamma \widetilde{\rho}_n(\beta_n^\dagger, \gamma_n^\dagger, \lambda_n^\dagger) \\ &= \lambda_n^\dagger \frac{1}{n}\sum_{i=1}^n \Big[b'(\gamma_n^{\dagger T} Z^{(i)}) Z^{(i)} - b'\Big(\lambda_n^\dagger(\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}) + (\beta^0)^T X^{(i)}\Big) Z^{(i)}\Big] = 0_q. \end{aligned} \tag{5.75}$$

(5.75) is also the first order condition for the optimization problem

$$\sup_\gamma [\gamma^T s_2^\dagger - \frac{1}{n}\sum_{i=1}^n b(\gamma^T Z^{(i)})] - [\beta_n^{\dagger T} s_1^\dagger - \frac{1}{n}\sum_{i=1}^n b(\beta_n^{\dagger T} X^{(i)})].$$

Notice that this optimization is concave in γ. Therefore, $\gamma_n^\dagger$ is a solution of the above optimization problem, and

$$\begin{aligned} w(s_1^\dagger, s_2^\dagger) &= \sup_\gamma [\gamma^T s_2^\dagger - \frac{1}{n}\sum_{i=1}^n b(\gamma^T Z^{(i)})] - [\beta_n^{\dagger T} s_1^\dagger - \frac{1}{n}\sum_{i=1}^n b(\beta_n^{\dagger T} X^{(i)})] \\ &= \gamma_n^{\dagger T} s_2^\dagger - \frac{1}{n}\sum_{i=1}^n b(\gamma_n^{\dagger T} Z^{(i)}) - [\beta_n^{\dagger T} s_1^\dagger - \frac{1}{n}\sum_{i=1}^n b(\beta_n^{\dagger T} X^{(i)})]. \end{aligned} \tag{5.76}$$

Also notice that $\lambda_n^\dagger = \arg\sup_\lambda \widetilde{\rho}_n(\beta_n^\dagger, \gamma_n^\dagger, \lambda)$. Therefore, it satisfies the first order condition

$$\begin{aligned}
0 &= \frac{\partial}{\partial\lambda}\widetilde{\rho}_n(\beta_n^\dagger, \gamma_n^\dagger, \lambda_n^\dagger) \\
&= \frac{1}{n}\sum_{i=1}^n b(\gamma_n^\dagger Z^{(i)}) - b(\beta_n^\dagger X^{(i)}) \qquad (5.77)\\
&\quad -b'\Big(\lambda_n^\dagger(\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}) + (\beta^0)^T X^{(i)}\Big)[\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}].
\end{aligned}$$

(5.76) and (5.77) together gives

$$w(s_1^\dagger, s_2^\dagger) = 0.$$

Therefore, $(s_1^\dagger, s_2^\dagger)$ is a boundary point of A_n. Furthermore, we have

$$\nabla_{s_1} w(s_1^\dagger, s_2^\dagger) = 0_p \text{ and } \nabla_{s_2} w(s_1^\dagger, s_2^\dagger) = \beta_n^\dagger.$$

Consequently, the normal vector of A_n at $(s_1^\dagger, s_2^\dagger)$ is $-(\nabla_{s_1} w(s_1^\dagger, s_2^\dagger), \nabla_{s_2} w(s_1^\dagger, s_2^\dagger)) = -(0_p, \gamma_n^\dagger)$. Because A_n is a convex set, for all $(s_1, s_2) \in A_n$, we have

$$-(s_1 - s_1^\dagger, s_2 - s_2^\dagger) \cdot (0_p, \gamma_n^\dagger) \le 0.$$

We complete the proof by combining the above display and that $w(s_1^\dagger, s_2^\dagger) = 0$.

5.7.7 Proof of Lemma 18

Because Y_is are independent, we have

$$\begin{aligned}
v_n &= \sum_{i=1}^n (\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)})^2 Var^{Q^\dagger}(Y_i) \\
&= \sum_{i=1}^n (\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)})^2 b''\Big(\lambda_n^\dagger(\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}) + (\beta^0)^T X^{(i)}\Big).
\end{aligned}$$

According to Assumption A10 and A11, we have $v_n = O(n)$. We define a triangular array for $n, i \ge 1$

$$U_{n,i} = v_n^{-\frac{1}{2}}\Big[\gamma_n^{\dagger T} Z^{(i)} Y_i - \beta_n^{\dagger T} X^{(i)} Y_i - b(\gamma_n^{\dagger T} X^{(i)}) + b(\beta_n^{\dagger T} X^{(i)})\Big].$$

It is sufficient to show that $U_{n,i}$ satisfies conditions for the Lyapuvov central limit theorem [Billingsley, 1995, page 362] for triangular arrays. That is,

$$\lim_{n\to\infty}\sum_{i=1}^{n} E^{Q^\dagger}|U_{n,i}|^3 = 0. \tag{5.78}$$

According to Assumption A11, $b(\cdot)$ is four times continuously differentiable. This guarantees that

$$\sum_{i=1}^{n}\mathbb{E}^{Q^\dagger}\left[\gamma_n^{\dagger T}Z^{(i)}Y_i - \beta_n^{\dagger T}X^{(i)}Y_i - b(\gamma_n^{\dagger T}X^{(i)}) + b(\beta_n^{\dagger T}X^{(i)})\right]^3 = O(n).$$

Now we show that $v_n^{-1} = O(n^{-1})$. According to Assumptions A10 and A11 and (5.25), we have

$$|\widetilde{\rho}_n^\dagger| \leq \kappa\frac{1}{n}\sum_{i=1}^{n}|\gamma_n^{\dagger T}Z^{(i)} - \beta_n^{\dagger T}X^{(i)}| \leq \kappa\Big(\frac{1}{n}\sum_{i=1}^{n}(\gamma_n^{\dagger T}Z^{(i)} - \beta_n^{\dagger T}X^{(i)})^2\Big)^{\frac{1}{2}}.$$

On the other hand, Assumption A9 implies that

$$\widetilde{\rho}_n^\dagger \geq \inf_\gamma\sup_\lambda \widetilde{\rho}_n(\beta^0,\gamma,\lambda) \geq \delta_1.$$

Therefore,

$$\frac{1}{n}\sum_{i=1}^{n}(\gamma_n^{\dagger T}Z^{(i)} - \beta_n^{\dagger T}X^{(i)})^2 \geq \delta_1^2\kappa^{-2}.$$

According to Assumption A11 and (5.78), $v_n \geq \varepsilon\sum_{i=1}^{n}(\gamma_n^{\dagger T}Z^{(i)} - \beta_n^{\dagger T}X^{(i)})^2$. Together with the above display, we have $v_n^{-1} = O(n^{-1})$. Therefore,

$$\begin{aligned}&\sum_{i=1}^{n}E^{Q^\dagger}|U_{n,i}|^3\\ =&\lim_{n\to\infty}v_n^{-\frac{3}{2}}\sum_{i=1}^{n}E^{Q^\dagger}\left[\gamma_n^{\dagger T}Z^{(i)}Y_i - \beta_n^{\dagger T}X^{(i)}Y_i - b(\gamma_n^{\dagger T}X^{(i)}) + b(\beta_n^{\dagger T}X^{(i)})\right]^3 = O(n^{-\frac{1}{2}}),\end{aligned} \tag{5.79}$$

and (5.78) is proved.

5.7.8 Proof of Lemma 19

Let $\beta(\mu) = \arg\sup_\beta u(\mu, \beta)$, then $\beta(\mu)$ satisfies

$$\frac{\partial}{\partial \beta} u(\mu, \beta(\mu)) = 0. \tag{5.80}$$

We first show that $\beta(\mu^\dagger) = \beta_n^\dagger$. Similar to (5.66), we have

$$\begin{aligned}
&\nabla_\beta \widetilde{\rho}_n(\beta_n^\dagger, \gamma_n^\dagger, \lambda_n^\dagger) \\
&= \lambda_n^\dagger \frac{1}{n} \sum_{i=1}^n \Big[-b'(\beta_n^{\dagger T} X^{(i)}) X^{(i)} + b'\Big(\lambda_n^\dagger (\gamma_n^{\dagger T} Z^{(i)} - \beta_n^{\dagger T} X^{(i)}) + (\beta^0)^T X^{(i)}\Big) X^{(i)} \Big] = 0.
\end{aligned}$$

Therefore, we have

$$\frac{\partial}{\partial \beta} u(\mu^\dagger, \beta_n^\dagger) = \mu^\dagger - \sum_{i=1}^n b'(\beta_n^{\dagger T} X^{(i)}) X^{(i)} = 0.$$

Notice that $\sup_\beta u(\mu^\dagger, \beta)$ is a strictly concave optimization problem. Therefore, $\beta_n^\dagger$ is its unique solution $\beta(\mu)$. Now we compute $\nabla v(\mu)$.

$$\nabla v(\mu) = \nabla u(\mu, \beta(\mu)) = \frac{\partial}{\partial \mu} u(\mu, \beta(\mu)) + \frac{d}{d\mu} \beta(\mu) \frac{\partial}{\partial \beta} u(\mu, \beta(\mu)).$$

The above display together with (5.80) gives

$$\nabla v(\mu) = \frac{\partial}{\partial \mu} u(\mu, \beta(\mu)) = \beta(\mu) - \beta_n^\dagger. \tag{5.81}$$

Because $\beta(\mu^\dagger) = \beta_n^\dagger$, we have that $v(\mu)$ is continuously differentiable and $v(\mu^\dagger) = 0$ and $\nabla v(\mu^\dagger) = 0$. We proceed to the second derivatives of $v(\mu)$. Applying implicit function theorem to (5.80), we have

$$\nabla \beta(\mu) = -\frac{\partial^2}{(\partial \beta)^2} u(\mu, \beta)^{-1} \frac{\partial^2}{\partial \mu \partial \beta} u(\mu, \beta(\mu)) = -\frac{\partial^2}{(\partial \beta)^2} u(\mu, \beta)^{-1}.$$

According to (5.81) and the above equation, we complete the proof.

Chapter 6

Generalized Sequential Probability Ratio Test for Separate Families of Hypotheses[1]

6.1 Introduction

Sequential analysis starts with testing a simple null hypothesis against a simple alternative hypothesis. The fixed sample size problem of this classic test is solved by Neyman and Pearson [1933b] who lay down the theoretical foundation of likelihood-based hypothesis testing. The sequential probability ratio test (SPRT), formulated via the boundary crossing of the likelihood ratio statistic, is proved to be optimal in terms of minimal expected sample size for fixed type I and type II error probabilities [Wald and Wolfowitz, 1948; Wald, 1945]. In this chapter, we consider a natural extension of this classical problem to testing two families of composite hypotheses, that

[1] This chapter is based on an accepted manuscript of an article published in *Sequential Analysis* online, October 22, 2014, available online:
http://tandfonline.com/doi/full/10.1080/07474946.2014.961861.

is,

$$H_0 : f \in \{g_\theta : \theta \in \Theta\} \quad \text{against} \quad H_A : f \in \{h_\gamma : \gamma \in \Gamma\} \tag{6.1}$$

where the two families are completely separated from each other. Motivated by the optimality of the sequential probability ratio test, we consider a sequential test based on the generalized likelihood ratio statistic. The sampling stops after the nth observation if the generalized likelihood ratio crosses either of the two boundaries $L_n > e^A$ or $L_n < e^{-B}$ where

$$L_n = \frac{\sup_{\gamma\in\Gamma} \prod_{i=1}^n h_\gamma(X_i)}{\sup_{\theta\in\Theta} \prod_{i=1}^n g_\theta(X_i)}.$$

The null hypothesis is rejected if $L_n > e^A$ and is accepted otherwise where A and B are positive numbers determined by the type I and type II error probabilities. We call this procedure the generalized sequential probability ratio test (generalized SPRT).

The generalized sequential probability ratio test is a very natural generalization of the sequential probability ratio test both in terms of the problem formulation and the stopping rule. However, to the authors' best knowledge, there is no rigorous discussion on this sequential procedure in the literature. The results in this chapter fill in this void by providing asymptotic descriptions of the type I and type II error probabilities in terms of the levels A and B, the expected sample size (stopping time), and its asymptotic optimality in terms of expected sample size. As a corollary of these results, the generalized SPRT is asymptotically optimal in the following sense. As the maximal type I and type II error probabilities tend to zero possibly with different rates, the expected stopping time of the generalized SPRT achieves its asymptotic lower bound. For the test as general as (6.1) with a fixed sample size, the uniformly most powerful test usually does not exist. Therefore, we do not expect the optimal sequential test in terms of expected sample size (as optimal as SPRT) for (6.1) to exist. The asymptotic optimality is naturally the next level of optimality to consider. The current result for the generalized SPRT is parallel to the optimality result for SPRT.

From the technical point of view, the challenges mainly lie in the fact that the generalized likelihood ratio statistic is the ratio of two maximized likelihood functions. Usual techniques, such as large deviations theory for independently and identically distributed random variables, exponential tilting for random walks, and Bayesian arguments employed by Wald and Wolfowitz [1948], are no longer applicable. The technical contribution of this chapter is the proposal of a set of tools for the large deviations studies of the generalized likelihood ratio statistic. A key element is the construction of a change of measure for developing approximations of the type I and type II error probabilities. This change of measure is not of the traditional exponential tilting form and therefore is nonstandard. Similar change of measure techniques for the computation of small probabilities have been employed under various settings by Adler *et al.* [2012]; Naiman and Priebe [2001]; Shi *et al.* [2007].

Testing separate families of hypotheses, originally introduced by Cox [1961, 1962], is an important and fundamental problem in statistics. Cox recently revisited this problem in Cox [2013] that mentions several applications such as the one-hit and two-hit models of binary dose-response and testing of interactions in a balanced 2^k factorial experiment. Furthermore, this problem has been studied in econometrics [Vuong, 1989]. Another application is in psychometrics. Under the one-dimensional item response theory models, each examinee is assigned with a scalar θ indicating this person's ability. The so-called mastery test is interested in testing whether $\theta < \theta_-$ or $\theta > \theta_+$. Item response theory usually employs logistic models that fall into the exponential family for which there is a vast literature [Bartroff and Lai, 2008; Bartroff *et al.*, 2008; Lai and Shih, 2004; Shih *et al.*, 2010]. However, some more complicated models go beyond exponential family, for which existing results do not apply. For instance, the normal ogive model is not of the canonical form and the three-parameter logistic model includes a guessing parameter. The current results fill in this void. For more applications of testing separate families of hypotheses, see Berrington de González and Cox [2007], Braganca Pereira [2005], and the references therein.

There is a vast literature on sequential tests starting with seminal works Hoeffding [1960]; Kiefer and Weiss [1957]; Wald and Wolfowitz [1948]; Wald [1945] for testing simple null hypothesis against simple alternative hypothesis. An important generalization to SPRT is the 2-SPRT by Lorden [1976]. For composite hypotheses, a univariate or multivariate exponential family is usually assumed. Under such a setting, sequential testing procedures for two separate families of hypotheses are discussed by Lai and Zhang [1994]; Lai [1988]; Pollak and Siegmund [1975]. For testing non-exponential families, random walk based sequential procedures are discussed in the textbook Bartroff *et al.* [2013]. Another relevant work is given by Pavlov [1987, 1990] who considers testing/selecting among multiple composite hypotheses. The author establishes asymptotic efficiency of a different sequential procedure (similar to 2-SPRT). The efficiency results are similar to those in this chapter. Therefore, the generalized sequential probability ratio test admits the same asymptotic efficiency as that in Pavlov's papers. Recent applications of sequential tests are included in Bartroff *et al.* [2008]; Lai and Shih [2004]. Additional references can be found in the textbook Bartroff *et al.* [2013].

The rest of this chapter is organized as follows. The generalized sequential probability ratio test and its asymptotic properties are described in Section 6.2. Possible relaxation of some technical conditions are provided in Section 6.3. Numerical examples are given in Section 6.4. Proofs of the theorems are provided in Section 6.5.

6.2 Main Results

6.2.1 Generalized Sequential Probability Ratio Test

Let X_1,...,X_n,... be independently and identically distributed samples following a density f with respect to a baseline measure μ. We consider the problem of testing two separate families of hypotheses

$$H_0 : f \in \{g_\theta : \theta \in \Theta\} \quad \text{and} \quad H_A : f \in \{h_\gamma : \gamma \in \Gamma\}, \tag{6.2}$$

where g_θ and h_γ are density functions with respect to a common measure μ. To avoid singularity, we assume that g_θ and h_γ are mutually absolutely continuous for all θ and γ. The generalized sequential probability ratio test is based on the generalized likelihood ratio statistic

$$L_n = \frac{\sup_{\gamma\in\Gamma}\prod_{i=1}^n h_\gamma(X_i)}{\sup_{\theta\in\Theta}\prod_{i=1}^n g_\theta(X_i)}. \tag{6.3}$$

For two positive numbers A and B, we define stopping time

$$\tau = \inf\{n : L_n > e^A \text{ or } L_n < e^{-B}\}. \tag{6.4}$$

Under very mild conditions, τ is almost surely finite under all distributions in the two families. The null hypothesis is rejected if $L_\tau > e^A$ and is not rejected if $L_\tau < e^{-B}$. We further define the notation for the Kullback-Leibler divergence

$$D_g(\theta|\gamma) = \mathbb{E}_{g_\theta}\{\log g_\theta(X) - \log h_\gamma(X)\} \quad \textit{and} \quad D_h(\gamma|\theta) = \mathbb{E}_{h_\gamma}\{\log h_\gamma(X) - \log g_\theta(X)\},$$

where $\mathbb{E}_{g_\theta}$ and $\mathbb{E}_{h_\gamma}$ are expectations under the corresponding distributions. We present the following technical conditions.

A1 The two families are completely separate, that is, $\inf_{\theta,\gamma} D_g(\theta|\gamma) > \varepsilon_0$ and $\inf_{\theta,\gamma} D_h(\gamma|\theta) > \varepsilon_0$ for some $\varepsilon_0 > 0$. In addition, for each θ and γ, the solutions to the minimizations $\inf_\theta D_h(\gamma|\theta)$ and $\inf_\gamma D_g(\theta|\gamma)$ are unique. Lastly, both $D_g(\theta|\gamma)$ and $D_h(\gamma|\theta)$ are twice continuously differentiable with respect to θ and γ.

A2 The parameter spaces $\Theta \subset R^{d_1}$ and $\Gamma \subset R^{d_2}$ are compact.

A3 Let $\xi(\theta,\gamma) = \log h_\gamma(X) - \log g_\theta(X)$. There exists $\alpha > 1$ and x_0 such that for all θ, γ, and $x > x_0$

$$\mathbb{P}_{g_\theta}(\sup_{\gamma\in\Gamma} |\nabla_\gamma \xi(\theta,\gamma)| > x) \le e^{-|\log x|^\alpha} \quad \textit{and} \quad \mathbb{P}_{h_\gamma}(\sup_{\theta\in\Theta} |\nabla_\theta \xi(\theta,\gamma)| > x) \le e^{-|\log x|^\alpha}.$$

Condition A1 is important for the analysis that guarantees the exponential decay of error probabilities as a function of the expected sample size. A sufficient condition for the complete separation is that the Hellinger distances between any two distributions in the two families are strictly positive. Condition A2 can be further relaxed and replaced by some other conditions that will be discussed subsequently. Condition A3 imposes certain tail conditions on the score function that has a tail decaying faster than any polynomial.

6.2.2 The Main Theorems

We start the discussion with a simple null $H_0 : f = g_0$ against composite alternative $H_A : f \in \{h_\gamma : \gamma \in \Gamma\}$. In this case, the generalized likelihood ratio statistic is given by

$$L_n = \frac{\sup_{\gamma \in \Gamma} \prod_{i=1}^n h_\gamma(X_i)}{g_0(X_i)}. \tag{6.5}$$

The definition of the stopping time τ remains. The following theorem provides the asymptotic type I and type II error probabilities of the generalized sequential probability ratio test under this setting.

Theorem 12. *In the case of the simple null hypothesis against composite hypothesis, consider the generalized probability ratio test with stopping time* (6.4) *and the generalized likelihood ratio statistic given by* (6.5)*. Under Conditions A1-3, the type I and maximal type II error probabilities admit the following approximations*

$$\log \mathbb{P}_{g_0}(L_\tau > e^A) \sim -A, \quad \sup_{\gamma \in \Gamma} \log \mathbb{P}_{h_\gamma}(L_\tau < e^{-B}) \sim -B \quad \textit{as } A,\ B \to \infty.$$

The analysis technique of Theorem 12 and its intermediate results are central to all the analyses. For the general case of composite null hypothesis against composite alternative hypothesis, we establish similar asymptotic results that are given by the following theorem.

Theorem 13. *Consider the composite null hypothesis against composite alternative hypothesis given as in* (6.2)*. The generalized sequential probability ratio test admits* *stopping time* (6.4) *and the generalized likelihood ratio statistic* (6.3)*. Under Conditions A1-3, the maximal type I and type II error probabilities are approximated by*

$$\sup_{\theta\in\Theta} \log \mathbb{P}_{g_\theta}(L_\tau > e^A) \sim -A, \quad \sup_{\gamma\in\Gamma} \log \mathbb{P}_{h_\gamma}(L_\tau < e^{-B}) \sim -B \quad \text{as } A,\ B \to \infty. \tag{6.6}$$

In the power calculation of SPRT for the simple null hypothesis versus simple alternative hypothesis, if the likelihood ratio has zero overshoot, then we have the following equalities $A = \log\frac{1-\alpha_2}{\alpha_1}$ and $B = \log\frac{1-\alpha_1}{\alpha_2}$ where α_1 is the type I error probability and α_2 is the type II error probability. They have exactly the same asymptotic decay rate as (6.6). Lastly, we provide the asymptotic approximations of the expected stopping time.

Theorem 14. *Under the setting and the conditions of Theorem 13, the expected stopping time admits the following asymptotic approximation*

$$\mathbb{E}_{g_\theta}(\tau) \sim \frac{B}{\inf_{\gamma\in\Gamma} D_g(\theta|\gamma)}, \quad \mathbb{E}_{h_\gamma}(\tau) \sim \frac{A}{\inf_{\theta\in\Theta} D_h(\gamma|\theta)}, \quad \text{as } A,\ B \to \infty \text{ for all } \theta \text{ and } \gamma.$$

Based on the results of Theorems 13 and 14, we now discuss the asymptotic optimality of the generalized SPRT. Consider type I and type II error probabilities α_1 and α_2 that approach zero possibly with different rates. Theorem 13 suggests that we need to choose $A \sim -\log\alpha_1$ and $B \sim -\log\alpha_2$ for the generalized SPRT to achieve such levels of error probabilities. Then, the corresponding expected stopping time is given by Theorem 14. In what follows, we show that the expected stopping time in Theorem 14 is asymptotically the shortest. Consider an arbitrarily chosen sequential procedure testing between the g-family and the h-family with stopping time τ'. The two types of error probabilities of this test are less than or equal to α_1 and α_2 respectively. Then, its expected stopping time is bounded from below by

$$\mathbb{E}_{g_\theta}(\tau') \geq (1+o(1))\mathbb{E}_{g_\theta}(\tau) \quad \text{and} \quad \mathbb{E}_{h_\gamma}(\tau') \geq (1+o(1))\mathbb{E}_{h_\gamma}(\tau)$$

for all θ and γ.

We establish the above asymptotic inequalities via the optimality results of SPRT. For each θ and γ, we consider the testing problem of the simple null $H_0 : f = g_\theta$

against the simple alternative $H_A : f = h_\gamma$. We further consider SPRT for this test with stopping boundaries $e^{\tilde{A}}$ and $e^{-\tilde{B}}$. We choose $\tilde{A}$ and $\tilde{B}$ such that the type I error and type II error probabilities of SPRT for the simple (g_θ) versus simple (h_γ) test are (or slightly larger than, but of the same order as) α_1 and α_2 respectively. According to Theorem 13 and standard results of SPRT, we have that $A \sim \tilde{A} \sim -\log \alpha_1$ and $B \sim \tilde{B} \sim -\log \alpha_2$ if the overshoot is of order $O(1)$. Let $\tilde{\tau}$ be the stopping time of SPRT. According to classic results on random walks, we have that

$$\mathbb{E}_{g_\theta}(\tilde{\tau}) \sim B/D_g(\theta|\gamma) \quad \textit{and} \quad \mathbb{E}_{h_\gamma}(\tilde{\tau}) \sim A/D_h(\gamma|\theta).$$

Furthermore, we view the test with stopping time τ' in the previous paragraph as a testing procedure for the simple null (g_θ) versus simple alternative (h_γ) problem. According to the definition of α_1 and α_2, the type I and type II error probabilities of this test for the simple versus simple problem are bounded from the above by α_1 and α_2. Therefore, according to the optimality of SPRT we have that

$$\mathbb{E}_{g_\theta}(\tau') \geq \mathbb{E}_{g_\theta}(\tilde{\tau}) = (1+o(1))B/D_g(\theta|\gamma) \; \textit{and} \; \mathbb{E}_{h_\gamma}(\tau') \geq \mathbb{E}_{h_\gamma}(\tilde{\tau}) = (1+o(1))A/D_h(\gamma|\theta).$$

For the first inequality, the left-hand-side does not depend on γ and furthermore Γ is a compact set. Thus, the $o(1)$ is uniformly small for $\gamma \in \Gamma$. We maximize the right-hand-side with respect to γ and obtain that

$$\mathbb{E}_{g_\theta}(\tau') \geq (1+o(1)) \frac{B}{\inf_\gamma D_g(\theta|\gamma)}.$$

Note that the right-hand-side of the above inequality is precisely the asymptotic expected stopping time in Theorem 14. With the same argument, we have that

$$\mathbb{E}_{h_\gamma}(\tau') \geq (1+o(1)) \frac{A}{\inf_\theta D_h(\gamma|\theta)}.$$

Summarizing the above discussion, we have the following corollary

Corollary 7. *Let $\mathcal{T}(\alpha_1, \alpha_2)$ be the class of sequential tests with their type I and type II errors bounded above by α_1 and α_2, respectively. Each test in $\mathcal{T}(\alpha_1, \alpha_2)$ corresponds* *to a stopping time τ' and a decision function D'. Let $\alpha_1^{A,B} = \sup_\theta \mathbb{P}_{g_\theta}(L_\tau > e^A)$ and $\alpha_2^{A,B} = \sup_\gamma \mathbb{P}_{h_\gamma}(L_\tau < e^{-B})$. Then, under the setting of Theorem 13 and under Conditions A1-3, the generalized sequential probability test is asymptotically optimal in the sense that*

$$\mathbb{E}_{g_\theta}(\tau) \sim \inf_{(\tau',D')\in\mathcal{T}(\alpha_1^{A,B},\alpha_2^{A,B})} \mathbb{E}_{g_\theta}(\tau')$$

as $A \to \infty$ and $B \to \infty$.

6.3 Further Discussion on the Conditions

In this section, we provide further discussion on Condition A1, A2, and A3 and possible relaxations. Condition A1 requires that the two families of hypotheses are completely separate. This condition is crucial for the exponential decay of the error probabilities in Theorems 12 and 13. The uniqueness of the minimization of the Kullback-Leibler divergence ensures the convergence of the maximum likelihood estimators and validity of the stopping time analysis. Therefore, Condition A1 is necessary for the theorems. In what follows, we provide further discussions on Conditions A2 and A3.

6.3.1 Relaxing Condition A2 and Analysis for Non-compact Spaces

When the parameter spaces Θ and Γ are non-compact, the expected stopping time of the generalized sequential probability ratio test can usually be approximated similarly as that of Theorem 14 with mild regularity conditions such as almost sure convergence of the maximum likelihood estimators. For the asymptotic decay rate of the type I and type II error probabilities, the generalization to non-compact spaces is not straightforward and additional nontrivial conditions are necessary. We start the discussion with a counterexample in which Theorem 13 fails when the parameter spaces are non-compact.

Example 9. *Consider the null hypothesis being the lognormal distributions*

$$g_\theta(x) = x^{-1}(2\pi\theta)^{-1/2}e^{-\frac{(\log x)^2}{2\theta}}$$

and the alternative hypothesis being the exponential distributions

$$h_\gamma(x) = \gamma^{-1}e^{-x/\gamma}.$$

Both distributions live on the positive real line. The maximum likelihood estimators for the parameters based on n *observations are* $\hat{\theta}_n = \frac{1}{n}\sum_{i=1}^n(\log X_i)^2$ *and* $\hat{\gamma}_n = \frac{1}{n}\sum_{i=1}^n X_i$*. The generalized log-likelihood ratio statistic based on one sample is* $\log h_{\hat{\gamma}_1}(X_1) - \log g_{\hat{\theta}}(X_1) = \log|\log X_1| - \frac{1}{2} + \frac{1}{2}\log(2\pi)$ *and* $L_1 = \sqrt{2\pi/e} \times |\log(X_1)|$*. The type I error probability is bounded from below by*

$$\sup_{\theta\in\Theta}\mathbb{P}_{g_\theta}(L_\tau > e^A) \geq \sup_{\theta\in\Theta}\mathbb{P}_{g_\theta}(L_1 > e^A) \geq \lim_{\theta\to\infty}\mathbb{P}_{g_\theta}\{\sqrt{2\pi/e} \times |\log(X_1)| > e^A\} = 1$$

regardless of the choice of A*. The last equality holds because* $\log(X_1)$ *follows a normal distribution with mean* 0 *and variance* $2\pi\theta/e$*.*

Therefore, it is nontrivial and additional conditions are certainly needed to generalize the results of Theorem 13 to non-compact parameter spaces and to rule out cases such as Example 9. Let $\xi_i(\theta,\gamma)$, $i = 1, 2...$ be i.i.d. copies of $\xi(\theta,\gamma)$. The log-likelihood ratio based on n observations is defined as

$$S_n(\theta,\gamma) = \sum_{i=1}^n \xi_i(\theta,\gamma). \tag{6.7}$$

We further define $S_n = \sup_\gamma \inf_\theta \sum_{i=1}^n \xi_i(\theta,\gamma)$ and $\tau = \inf\{n : S_n < -B \text{ or } S_n > A\}$. To rule out the cases such as Example 9, we need to carefully go through the proof of Theorem 13 (Section 6.5) that consists of the development of an upper and a lower bound of the error probabilities. The lower bound does not require the compactness of the parameter spaces and is generally applicable. It is the development of the upper bound where the compactness plays an important role in the analysis. Define

$$H_{A,\theta} = \sum_{n=1}^\infty \int_\Gamma \mathbb{P}_{g_\theta}(S_n(\theta,\gamma) > A)d\gamma. \tag{6.8}$$

The condition for non-compact parameter spaces is

A2′ Let $H_{A,\theta}$ be defined as in (6.8) and $\limsup_{A\to\infty}\sup_{\theta\in\Theta}\frac{1}{A}\log H_{A,\theta}\leq -1$. Symmetrically, we define

$$G_{B,\gamma}=\sum_{n=1}^{\infty}\int_{\Theta}\mathbb{P}_{h_\gamma}(S_n(\theta,\gamma)<-B)d\theta$$

that satisfies $\limsup_{B\to\infty}\sup_{\theta\in\Theta}\frac{1}{B}\log G_{B,\theta}\leq -1$.

Condition A2′ is usually difficult to check. Therefore, we provide a set of sufficient conditions for A2′.

Lemma 20. *Assume that the following conditions hold.*

B1 For each θ, let $\gamma_\theta=\arg\inf_{\gamma\in\Gamma}D_h(\gamma|\theta)$. There exist ε and δ positive such that

$$D_h(\gamma|\theta)\geq D_h(\gamma_\theta|\theta)+\delta|\gamma-\gamma_\theta|^l,$$

for some $l>(d+1)/2$, all $\theta\in\Theta$, and all $|\gamma-\gamma_\theta|>\varepsilon$, where d is the dimension of Γ.

B2 The log-likelihood ratio $\xi(\theta,\gamma)$ has bounded variance under h_γ for all $\theta\in\Theta$ and $\gamma\in\Gamma$.

B3 There exists $\varepsilon>0$ such that $\varepsilon<D_g(\theta|\gamma)/D_h(\gamma|\theta)<\varepsilon^{-1}$ for all θ and γ.

Then, $\limsup_{A\to\infty}\sup_{\theta\in\Theta}\frac{1}{A}\log H_{A,\theta}\leq -1$.

For the two families of distributions in Example 9, Condition A2′ is not satisfied. With Condition A2′ in addition to Conditions A1 and A3, we expect to obtain similar approximation results as in Theorem 13. Given that the techniques are similar but substantially more tedious, we do not provide the details.

6.3.2 Relaxing Condition A3

We now consider the situation in which Condition A3 is violated. For instance, if the alternative hypothesis h_γ is the exponential distributions, then the partial derivative

$\partial_\gamma \xi(\theta,\gamma)$ is infinity when $\gamma \to 0$. For these types of families, we need to replace Condition A3 by some localization condition. Let $\hat{\gamma}_n$ be the maximum likelihood estimator based on n i.i.d. samples. The localization condition to replace A3 is as follows.

A3′ There exists a family of sets $\Gamma'_A \subset \Gamma$ indexed by A such that $\mathbb{P}_{g_\theta}(\hat{\gamma}_n \notin \Gamma'_A) \leq e^{-(n+1)A}$ and for some $\alpha > 1$, $\beta \in (\alpha^{-1}, 1)$ and all $\theta \in \Theta$

$$\mathbb{P}_{g_\theta}(\sup_{\gamma \in \Gamma'_A} |\partial_\gamma \xi(\theta,\gamma)| > e^{A^\beta} x) \leq e^{-|\log x|^\alpha}.$$

Similarly, there exists $\Theta'_B \subset \Theta$ such that $\mathbb{P}_{h_\gamma}(\hat{\theta}_n \notin \Theta'_B) \leq e^{-(n+1)B}$ and

$$\mathbb{P}_{h_\gamma}(\sup_{\theta \in \Theta'_b} |\partial_\theta \xi(\theta,\gamma)| > e^{A^\beta} x) \leq e^{-|\log x|^\alpha}.$$

For the two hypotheses in Example 9, we have $\alpha = 2$ and for some $1/2 < \beta < 1$ let

$$\Gamma' = [e^{-A^{\beta'}}, \infty) \quad \text{where } 1/2 < \beta' < \beta.$$

Then, we can verify that such the choice of Γ' satisfies Condition A3′. We summarize the discussion in this section as follows.

Theorem 15. *Under Conditions A1, A2′, and A3′, the approximations in* (6.6) *holds.*

Given that the proof of the above theorem is basically identical to that of Theorem 13 and therefore we do not provide the details.

6.4 Numerical Examples

6.4.1 Poisson Distribution against Geometric Distribution

In this section, we provide numerical examples to illustrate the results of the theorems. We start with the Poisson distribution against the geometric distribution. Let

$$g_\theta(x) = \frac{e^{-\theta}\theta^x}{x!} \quad \Theta = [0.5, 2], \qquad h_\gamma(x) = \frac{\gamma^x}{(1+\gamma)^{x+1}} \quad \Gamma = [0.5, 2]$$

where x is a non-negative integer and $1/(1+\gamma)$ is the success probability of the geometric trials. We truncate the parameter spaces from above for Condition A2 and from below to make these two families of distributions completely separated for Condition A1. The test statistic is

$$L_n = \frac{\prod_{i=1}^n h_{\hat{\gamma}}(X_i)}{\prod_{i=1}^n g_{\hat{\theta}}(X_i)} \qquad \text{where } \hat{\theta} = \hat{\gamma} = \max\{\min(\frac{1}{n}\sum_{i=1}^n X_i, 2), 0.5\}.$$

For B fixed to be 4, we compute the type I error probabilities for different values of A via Monte Carlo. Figure 6.1 plots the logarithm of the type I error probabilities against the boundary parameter A. For fixed $A = 4$, we compute the expected sample size under the distribution $g_{0.5}(x)$, $g_1(x)$, and $g_{1.5}(x)$ for different values of B as shown in Figure 6.2. Similarly, for fixed $B = 4$, we compute the expected sample size under the distribution $h_{0.5}(x)$, $h_1(x)$, and $h_{1.5}(x)$ for different values of A as shown in Figure 6.3.

The slope of the fitted line in Figure 6.1 is -1.02. The fitted slopes in Figure 6.2 are 35.50, 12.12, and 6.81. The fitted slopes in Figure 6.3 are 26.22, 8.22, and 4.61. From Theorems 2 and 3, the theoretical values of the slope in Figure 6.1 is -1, and the theoretical values of the slopes in Figure 6.2 are $\{\inf_\gamma D(g_{0.5}|h_\gamma)\}^{-1} = 36.85$, $\{\inf_\gamma D(g_1|h_\gamma)\}^{-1} = 12.28$, and $\{\inf_\gamma D(g_{1.5}|h_\gamma)\}^{-1} = 6.99$. The theoretical slopes in Figure 6.3 are $\{\inf_\theta D(g_\theta|h_{0.5})\}^{-1} = 26.97$, $\{\inf_\theta D(g_\theta|h_1)\}^{-1} = 8.23$, and $\{\inf_\theta D(g_\theta|h_{1.5})\}^{-1} = 4.30$. The numerical fitted values are close to the theoretical ones.

6.4.2 Gaussian Distribution against Laplace Distribution

We proceed to testing Gaussian distribution against Laplace distribution, for which the distributions are non-compact. Let

$$g_\theta(x) = (2\pi\theta)^{-1/2} e^{-x^2/(2\theta)} \quad \Theta = (0,\infty) \qquad h_\gamma(x) = (2\gamma)^{-1} e^{-|x|/\gamma} \quad \Gamma = (0,\infty)$$

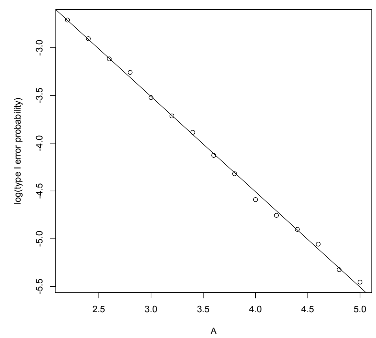


Figure 6.1: Logarithm of the type I error probabilities (y-coordinate) against boundary parameter A (x-coordinate) for Poisson distribution against geometric distribution with B fixed to be 4.

The generalized likelihood statistics is

$$L_n = \frac{\prod_{i=1}^n h_{\hat{\gamma}(X_i)}}{\prod_{i=1}^n g_{\hat{\theta}}(X_i)} \text{ where } \hat{\gamma} = \frac{1}{n}\sum_{i=1}^n |X_i| \text{ and } \hat{\theta} = \frac{1}{n}\sum_{i=1}^n X_i^2.$$

For B fixed to be 4 and different A values, we compute the type I error probabilities of the generalized sequential probability ratio test. Figure 6.4 is the plot for the logarithm of the type I error probabilities against the boundary parameter A. Furthermore, for fixed $A = 4$ and different B values, we calculate the expected sample size under probability g_1 and for fixed $B = 4$ with different A values we calculate the expeted sample size under h_2. Figure 6.5 is the plot for the expected sample size against B, and Figure 6.6 is the plot for expected sample size against A. We fit straight lines to each of the three plots via least square. The slopes of the fitted line in Figure 6.4, 6.5, and 6.6 are -1.00, 20.60, and 14.42 respectively. The theoretical values of these three slopes should be -1, $\{\inf_{\gamma\in\Gamma} D(g_1|h_\gamma)\}^{-1} = 20.65$ and $\{\inf_{\theta\in\Theta} D(g_\theta|h_2)\}^{-1} = 13.82$ that are close to the numerically fitted values.

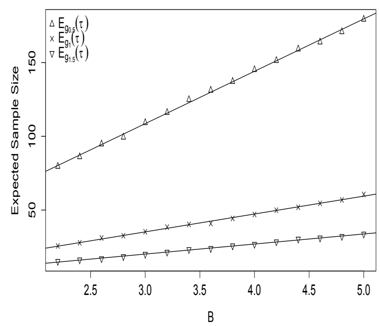


Figure 6.2: $\mathbb{E}_{g_{0.5}}(\tau)$, $\mathbb{E}_{g_1}(\tau)$ and $\mathbb{E}_{g_{1.5}}(\tau)$ (y-coordinate) against boundary parameter B (x-coordinate) for Poisson distribution against geometric distribution with A fixed to be 4.

6.4.3 Lognormal Distribution against Exponential Distribution

We proceed to the lognormal distribution against exponential distribution

$$g_\theta(x) = \frac{1}{x\sqrt{2\pi\theta}}e^{-\frac{(\log x)^2}{2\theta}} \quad \Theta = [0,1], \qquad h_\gamma(x) = \frac{1}{\gamma}e^{-\frac{x}{\gamma}} \quad \Gamma = [0,1]$$

As explained in Example 9, we consider θ and γ on compact sets for Condition A2. The generalized likelihood ratio statistic is

$$L_n = \frac{\prod_{i=1}^n h_{\hat{\gamma}}(X_i)}{\prod_{i=1}^n g_{\hat{\theta}}(X_i)} \qquad \text{where } \hat{\gamma} = \min(\frac{1}{n}\sum_{i=1}^n X_i, 1), \quad \hat{\theta} = \min\left\{\frac{1}{n}\sum_{i=1}^n (\log X_i)^2, 1\right\}$$

For a fixed B= 4 and different values of A, we compute the type I error probabilities of the generalized sequential probability ratio test under the distribution $g_1(x)$. Figure 6.7 is the scatter plot for the logarithm of the type I error probabilities against the boundary parameter A. Furthermore, for a fixed A and different B values, we compute the expected sample size under $g_{0.5}(x)$ and $g_1(x)$ via Monte Carlo. For a fixed B and different A, we also compute the expected sample size under probability measure $h_{0.5}$ and $h_1(x)$. Figure 6.8 is the scatter plot of expected sample size under

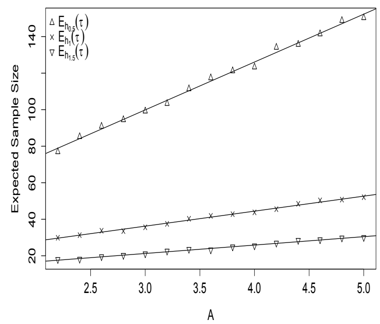


Figure 6.3: $\mathbb{E}_{h_{0.5}}(\tau)$, $\mathbb{E}_{h_1}(\tau)$ and $\mathbb{E}_{h_{1.5}}(\tau)$ (y-coordinate) against boundary parameter A (x-coordinate) for Poisson distribution against geometric distribution with B fixed to be 4.

probability measure $g_{0.5}$ and g_1 against B. Figure 6.9 is the scater plot of expected sample size under probability measure $h_{0.5}$ and h_1 against A. We fit straight lines to each of the three plots via least square. The slope of the fitted line in Figure 6.7 is -0.92. The slopes of the regression lines in Figure 6.8 are 4.67, and 4.75. . The slopes of the regression lines in Figure 6.9 are 1.08, and 3.28. From Theorems 13 and 14, the theoretical value of the slope in Figure 6.7 should be -1, and the slopes in Figure 6.8 are $\{\inf_{\gamma\in\Gamma} D(g_{0.5}|h_\gamma)\}^{-1} = 4.72$, and $\{\inf_{\gamma\in\Gamma} D(g_1|h_\gamma)\}^{-1} = 4.54$. The theoretical value of slopes in Figure 6.9 are $\{\inf_{\theta\in\Theta} D(g_\theta|h_{0.5})\}^{-1} = 1.03$ and $\{\inf_{\theta\in\Theta} D(g_\theta|h_1)\}^{-1} = 3.02$.

6.5 Technical Proofs

6.5.1 Proof of Theorem 12

We write $a_n \cong b_n$ if $\log a_n \sim \log b_n$ as $n \to \infty$. To make the discussion smooth, we delay the proof of the supporting lemmas to the appendix.

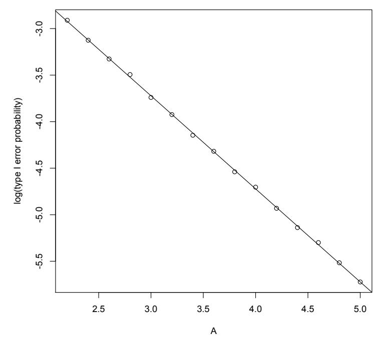


Figure 6.4: Logarithm of the type I error probabilities (y-coordinate) against boundary parameter A (x-coordinate) for Gaussian distribution against Laplace distribution with $B = 4$.

Proof of Theorem 12. Define the log-likelihood ratio of a single observation

$$\xi(\gamma) = \log h_\gamma(X) - \log g_0(X)$$

and $\xi_i(\gamma) = \log h_\gamma(X_i) - \log g_0(X_i)$ be i.i.d. copies of it. The log-likelihood ratio based on n i.i.d. samples is

$$S_n(\gamma) = \sum_{i=1}^{n} \xi_i(\gamma).$$

The generalized log-likelihood ratio statistic is $\log L_n = S_n = \sup_{\gamma\in\Gamma} S_n(\gamma)$. The stopping time can be equivalently written as $\tau = \inf\{n : S_n < -B \text{ or } S_n > A\}$. We reject the null hypothesis if $S_\tau > A$ and do not reject otherwise. Let $\gamma_* = \arg\sup_\gamma \mathbb{E}_{g_0}\{\xi(\gamma)\}$, $-\mu_g^\gamma = \mathbb{E}_{g_0}\{\xi(\gamma)\} = D_{g_0}(0|\gamma)$, and $\mu_h^\gamma = \mathbb{E}_{h_\gamma}\{\xi(\gamma)\} = -D_{h_\gamma}(\gamma|0)$. We now proceed to the computation of the type I and type II error probabilities. The decay rate of the type I error probability is given by the following lemmas that is the key result of the remaining derivations.

Lemma 21. *Under the setting and conditions of Theorem 12, the type I error probability is approximated by*

$$e^{-(1+o(1))A} \le \mathbb{P}_g(S_\tau > A) \le \mathbb{P}_g(\sup_n \sup_\gamma S_n(\gamma) > A) \le \kappa A^{\alpha_0} H_A$$

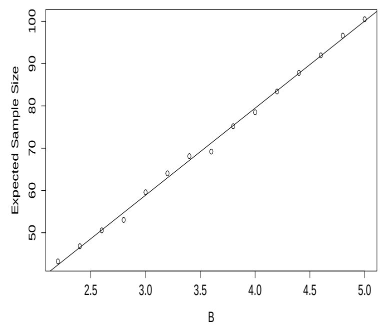


Figure 6.5: Expected sample size $\mathbb{E}_{g_1}(\tau)$ (y-coordinate) against boundary parameter B (x-coordinate) for Gaussian distribution against Laplace distribution with $A = 4$.

for some ε_0, α_0, and $\kappa > 0$ and

$$H_A = \sum_{n=1}^{\infty} \int_{\Gamma} \mathbb{P}(S_n(\gamma) > A - 1) d\gamma.$$

The constant κ depends on the dimension of Γ and α_0 depends on α in Condition A3.

Lemma 22. *Let $mes(\Gamma) = \int I(t \in \Gamma)dt$ be the Lebesgue measure of the parameter set Γ and let $D_h(\gamma|0) = \mathbb{E}_{h_\gamma}\{\log h_\gamma(X) - \log g_0(X)\}$ be the Kullback-Leibler divergence. Under the setting and conditions of Theorem 12, there exists some $\kappa_0 > 0$ such that for A sufficiently large H_A defined as in Lemma 21 admits the following bound*

$$H_A \leq \frac{\kappa_0 mes(\Gamma) A e^{-A}}{\min_\gamma D_h(\gamma|0)}.$$

Therefore, we finished the analysis of the type I error probability. We focus on the type II error computation $\alpha_2 = \sup_{\gamma \in \Gamma} \mathbb{P}_{h_\gamma}(S_\tau < -B)$. For each γ_0, notice that $S_n \geq S_n(\gamma_0)$ and thus

$$\mathbb{P}_{h_{\gamma_0}}(S_\tau < -B) < \mathbb{P}_{h_{\gamma_0}}(S_{\tau(\gamma_0)}(\gamma_0) < -B) \leq e^{-B}$$

where $\tau(\gamma_0) = \inf\{n : S_n(\gamma_0) < -B \text{ or } S_n(\gamma_0) > A\}$. The last step of the above display is a classical large deviations result of random walk. This provides an upper

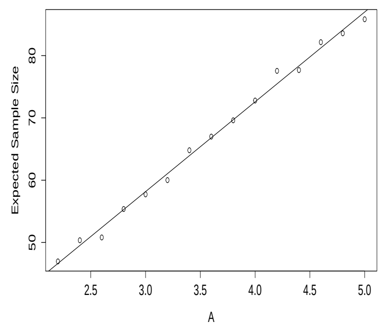


Figure 6.6: Expected sample size $\mathbb{E}_{h_2}(\tau)$ (y-coordinate) against boundary parameter A (x-coordinate) for Gaussian distribution against Laplace distribution with $B = 4$.

bound of α_2. We now show that this upper bound is achieved in the sense of "$\cong$". In particular, we wish to show that

$$\liminf_{A,B\to\infty} \frac{\log \mathbb{P}_{h_{\gamma_*}}(S_\tau < -B)}{B} \geq -1. \tag{6.9}$$

We establish the above inequality via contradiction. Suppose that (6.9) is not true, that is, there exist two sequences A_i, $B_i \to \infty$ as $i \to \infty$ and $\varepsilon_0 > 0$ such that

$$\frac{\log \mathbb{P}_{h_{\gamma_*}}(S_\tau < -B_i)}{B_i} < -1 - \varepsilon_0$$

and equivalently $\mathbb{P}_{h_{\gamma_*}}(S_\tau < -B_i) < e^{-(1+\varepsilon_0)B_i}$. Recall that, from the type I error computation, we have that $\mathbb{P}_{g_0}(S_\tau > A_i) \cong e^{-A_i}$.

Now we consider the simple null $f = g_0$ against the simple alternative $f = h_{\gamma_*}$ and SPRT with stopping time

$$\tilde{\tau}_i = \inf\{n : S_n(\gamma_*) < -\tilde{B}_i \text{ or } S_n(\gamma_*) > \tilde{A}_i\}.$$

The threshold $\tilde{A}_i$ and $\tilde{B}_i$ is chosen such that the SPRT has exactly the same (or slightly larger) type I and type II error probability as the generalized SPRT, that is,

$$e^{-\tilde{A}_i} \cong \mathbb{P}_{g_0}(S_{\tilde{\tau}_i}(\gamma_*) > \tilde{A}_i) \cong \mathbb{P}_{g_0}(S_\tau > A_i) \cong e^{-A_i}$$

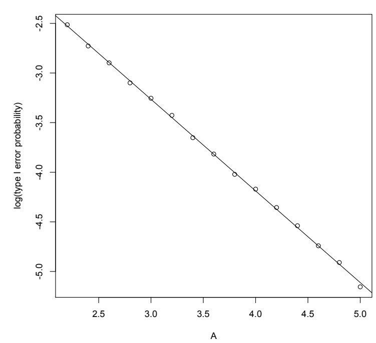


Figure 6.7: Logarithm of the type I error probabilities (y-coordinate) against boundary parameter A (x-coordinate) for lognormal distribution against exponential distribution where B is fixed to be 4

and

$$e^{-\tilde{B}_i} \cong \mathbb{P}_{h_{\gamma_*}}(S_{\tilde{\tau}_i}(\gamma_*) < -\tilde{B}_i) \cong \mathbb{P}_{h_{\gamma_*}}(S_\tau < -B_i) < e^{-(1+\varepsilon_0)B_i}.$$

Therefore, we have that $\tilde{A}_i \sim A_i$ and $\tilde{B}_i > (1+\varepsilon_0/2)B_i$. Furthermore, notice that the expected stopping time for SPRT is

$$\mathbb{E}_g(\tilde{\tau}_i) \sim \tilde{B}_i/\mu_g^{\gamma_*}, \quad \mathbb{E}_{h_{\gamma_*}}(\tilde{\tau}_i) \sim \tilde{A}_i/\mu_h^{\gamma_*}.$$

Note that $\mu_g^{\gamma_*} = \inf_{\gamma\in\Gamma} D_g(\theta|\gamma)$. According to Theorem 14 (whose proof is independent of the current one), we have that $\mathbb{E}_g(\tilde{\tau}_i) > \mathbb{E}_g(\tau) \sim B_i/\mu_g^{\gamma_*}$ that contradicts the optimality result of SPRT [Wald and Wolfowitz, 1948]. Thus, (6.9) must be true and we establish that

$$\alpha_2 = \sup_{\gamma\in\Gamma} \mathbb{P}_{h_\gamma}(S_\tau < -B) \cong e^{-B} \quad \text{as } A,\, B \to \infty.$$

$\square$

6.5.2 Proof of Theorem 13

With the above proof, Theorem 13 can be obtained rather easily. This proof also requires some intermediate results in the proof of Theorem 12.

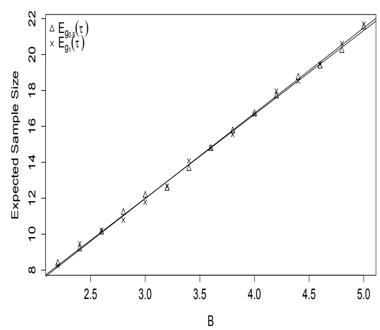


Figure 6.8: Expected sample size $\mathbb{E}_{g_{0.5}}(\tau)$ and $\mathbb{E}_{g_1}(\tau)$ (y-coordinate) against boundary parameter B (x-coordinate) for lognormal distribution against exponential distribution, where A is fixed to be 4.

Proof of Theorem 13. Let $S_n(\theta,\gamma)$ be defined as in (6.7). We define notation

$$S_n = \sup_\gamma \inf_\theta \sum_{i=1}^n \xi_i(\theta,\gamma), \quad \tau = \inf\{n : S_n < -B \text{ or } S_n > A\}.$$

As the two types of errors are completely symmetric, we only derive the type I error. We start with the upper bound. For each θ, by slightly abusing the notation, define

$$S_n(\theta) = \sup_\gamma S_n(\theta,\gamma), \quad \tau_1(\theta) = \inf\{n : S_n(\theta) < -B \textit{ or } S_n(\theta) > A\}.$$

Then, an upper bound is given by

$$\mathbb{P}_{g_\theta}(S_\tau > A) \le \mathbb{P}_{g_\theta}(S_{\tau_1(\theta)}(\theta) > A) \le \kappa A^{\alpha_0} \sum_{n=1}^\infty \int_\Gamma \mathbb{P}_{g_\theta}(S_n(\theta,\gamma) > A-1) d\gamma. \quad (6.10)$$

The last step follows from the fact that the right-hand-side is precisely the type I error probability of the simple null g_θ versus composite alternative $\{h_\gamma : \gamma \in \Gamma\}$. We now consider the lower bound. For each given γ and $\theta_* = \arg\inf_{\theta\in\Theta} D_h(\gamma|\theta)$, we have that

$$\mathbb{P}_{g_{\theta_*}}(\sup_{\gamma'} \inf_{\theta'} S_\tau(\theta',\gamma') > A) \ge \mathbb{P}_{g_{\theta_*}}(\inf_\theta S_{\tau_2(\gamma)}(\theta,\gamma) > A) \cong e^{-A}$$

where $\tau_2(\gamma) = \inf\{n : \inf_\theta S_n(\theta,\gamma) < -B \textit{ or } \sup_\gamma S_n(\theta,\gamma) > A\}$. Once again, the last step is thanks to the type II error proof in Theorem 12. $\square$

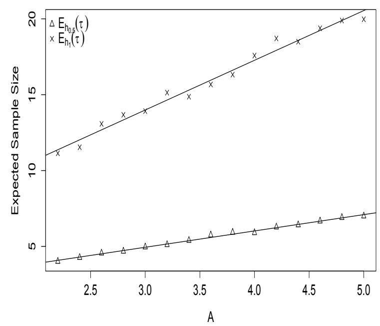


Figure 6.9: Expected sample size $\mathbb{E}_{h_{0.5}}(\tau)$ and $\mathbb{E}_{h_1}(\tau)$ (y-coordinate) against boundary parameter A (x-coordinate) for lognormal distribution against exponential distribution, where B is fixed to be 4.

6.5.3 Proof of Theorem 14

The proof of this theorem uses a change of measure. Suppose that $\xi(x)$ is a stochastic process living on some d-dimensional compact parameter space $x \in \mathcal{X} \subset R^d$. A generic probability measure is denoted by $\mathbb{P}$. The following change of measure helps to compute the tail probability of $\sup_x \xi(x)$. In particular, this change of measure is introduced in two ways. We first define it through the Radon-Nikodym derivative

$$\frac{dQ_b}{d\mathbb{P}} = H_b^{-1} \int_{\mathcal{X}} I(\xi(x) > b-1)\mu(dx)$$

where $I(\cdot)$ is the indicator function, μ is a positive measure, and

$$H_b = \int_{\mathcal{X}} \mathbb{P}(\xi(x) > b-1)\mu(dx).$$

To better understand this measure Q_b, we provide a procedure generating sample paths of $\xi(x)$ under Q_b. This provides an alternative distributional description of $\xi(x)$ under Q_b. The corresponding sample path generation is given as follows.

1. Sample a random index $x_* \in \mathcal{X}$ according to the density function (with respect to measure μ)

$$q_n(x_*) = \mathbb{P}(\xi(x_*) > b-1)/H_b.$$

2. Conditional on the realized x_*, sample $\xi(x_*)$ conditional on $\xi(x_*) > b-1$ under the measure $\mathbb{P}$.

3. Sample the rest of the process $\{\xi(x) : x \neq x_*\}$ conditional on the realization $\xi(x_*)$ under the original measure $\mathbb{P}$.

It is not hard to verify that the above three-step sample path generation is consistent with the Radnon-Nikodym derivative. Some variations of this change of measure will be used in the proof of other lemmas.

Proof of Theorem 14. Without loss of generality, we derive the approximation for $\mathbb{E}_{g_0}(\tau)$, that is, the true θ is 0. Using the notation in the proof of Theorem 13, we consider the limiting process of $S_n(\theta,\gamma)$. To start with, we consider a large constant $M > 0$ and split the expected stopping time

$$\mathbb{E}_{g_0}(\tau/B) = \mathbb{E}_{g_0}(\tau/B; \tau/B \le M) + \mathbb{E}_{g_0}(\tau/B; \tau/B > M). \tag{6.11}$$

Let $\hat\theta_n = \arg\inf_\theta S_n(\theta,\gamma)$ and $\hat\gamma_n = \arg\sup_\gamma S_n(\theta,\gamma)$. Then, as $n \to \infty$, we have the following almost sure convergence, $\hat\theta \to 0$ and $\hat\gamma \to \gamma_0 \triangleq \arg\inf_\gamma D_g(0|\gamma)$. Thus, we have the following weak convergence

$$\{S_{\lfloor Bt\rfloor}(\hat\theta_n, \hat\gamma_n)/B : t \in [0, M]\} \Rightarrow \{-t \times \inf_\gamma D_g(\theta|\gamma) : t \in [0, M]\}$$

where "$\Rightarrow$" is weak convergence. Thus, the first term is approximated by

$$\mathbb{E}_{g_0}(\tau/B; \tau/B \le M) \to 1/\mathbb{E}_{g_0}\{\xi(\gamma_0)\} = 1/\inf_\gamma D_g(0|\gamma) \quad \text{as } B \to \infty. \tag{6.12}$$

In what follows, we show that the second term $\mathbb{E}_{g_\theta}(\tau/B; \tau/B > M) \to 0$ as $B \to \infty$ for M sufficiently large. Let $\tau' = \inf\{n : \sup_\gamma S_n(0,\gamma) < -B\}$. We observe that $\tau' \ge \tau$ and thus it is sufficient to bound $\mathbb{E}_{g_\theta}(\tau'/B; \tau'/B > M)$. For each $\lambda > 0$, we consider the probability $\mathbb{P}_{g_0}(\tau' > \lambda B)$. Notice that $S_n(0,\gamma)$ has a negative drift that is bounded from the above by $-\varepsilon$ and thus $\sup_\gamma \mathbb{E}\{S_{\lambda B}(0,\gamma)\} < -\varepsilon\lambda B$. For

$\lambda > M$ with M sufficiently large, we have that $\sup_\gamma \mathbb{E}\{S_{\lambda B}(0,\gamma)\} < -B - \varepsilon\lambda B/2$. Note that

$$\mathbb{P}_{g_0}(\tau' > \lambda B) \leq \mathbb{P}_{g_0}(\sup_\gamma S_{\lambda B}(0,\gamma) \geq -B).$$

The last issue is to provide a bound of $\mathbb{P}_{g_0}(\sup_\gamma S_{\lambda B}(0,\gamma) \geq -B)$. We consider the change of measure

$$\frac{dQ_{-B}}{d\mathbb{P}_{g_0}} = H_{-B}^{-1}\int_\Gamma I(S_{\lambda B}(0,\gamma) \geq -B-1)d\gamma$$

where $H_{-B} = \int \mathbb{P}_{g_0}(S_{\lambda B}(0,\gamma) \geq -B-1)d\gamma$ and thus

$$\begin{aligned}\mathbb{P}_{g_0}\left(\sup_\gamma S_{\lambda B}(0,\gamma) \geq -B\right) &\leq \mathbb{P}_{g_0}\left(\sup_{k\leq\lambda B}|\partial\xi(0,\gamma)| \geq e^{(\lambda B)^\beta}\right)\\ &\quad + \mathbb{P}_{g_0}\left(S_{\lambda B}(0,\gamma) \geq -B; \sup_{k\leq\lambda B}|\partial\xi(0,\gamma)| < e^{(\lambda B)^\beta}\right).\end{aligned}$$

The first term is bounded by

$$\mathbb{P}_{g_0}\left(\sup_{k\leq\lambda B}|\partial\xi(0,\gamma)| \geq e^{(\lambda B)^\beta}\right) \leq \lambda B e^{-(\lambda B)^{\alpha\beta}}.$$

We use the change of measure for the second term

$$\begin{aligned}&\mathbb{P}_{g_0}\left(S_{\lambda B}(0,\gamma) < -B; \sup_{k\leq\lambda B}|\partial\xi(0,\gamma)| < e^{-(\lambda B)^\beta}\right)\\ = \quad & H_{-B}\mathbb{E}^{Q_{-B}}\left[\int_\Gamma I(S_{\lambda B}(0,\gamma) \geq -B-1)d\gamma; S_{\lambda B}(0,\gamma) \geq -B; \sup_{k\leq\lambda B}|\partial\xi(0,\gamma)| < e^{(\lambda B)^\beta}\right].\end{aligned}$$

By means of standard large deviations analysis,

$$H_{-B} \leq e^{-\varepsilon_0\lambda B}.$$

For the expectation, on the set $\{S_{\lambda B}(0,\gamma) \geq -B\}$, there exists at least one γ_0 such that $S_{\lambda B}(0,\gamma_0) \geq -B$. In addition, the derivative of $S_{\lambda B}(0,\gamma)$ is bounded by $\lambda B e^{(\lambda B)^\beta}$. Thus, we have a lower bound

$$\int_\Gamma I(S_{\lambda B}(0,\gamma) \geq -B-1)d\gamma \geq \delta_0\lambda^d B^d e^{d(\lambda B)^\beta}.$$

Plugging the above bound back, we have that

$$\mathbb{P}_{g_0}\left(S_{\lambda B}(0,\gamma) < -B; \sup_{k\leq\lambda B}|\partial\xi(0,\gamma)| < e^{-(\lambda B)^\beta}\right) \leq e^{-\varepsilon_0\lambda B/2}$$

and with λ sufficiently large

$$\mathbb{P}_{g_0}(\tau' > \lambda B) \leq e^{-\varepsilon_0 \lambda B/2}.$$

With the above bound, we have that

$$\mathbb{E}_{g_\theta}(\tau'/B; \tau'/B > M) = o(1)$$

as $B \to 0$. Together with the approximation in (6.12), we put this estimate back to (6.15) and conclude the proof. □

6.6 Conclusion

In this chapter, we study the asymptotic properties of the generalized sequential probability ratio test for the composite null hypothesis against composite alternative hypothesis. We derived the exponential decay rate of the maximal type I and type II error probabilities as the crossing levels tend to infinity. In particular, we show that these two probabilities decay to zero at rate e^{-A} and e^{-B}, respectively, which are the same as those of the classic sequential probability ratio test. With such approximations, we are able to establish the asymptotic optimality of the generalized SPRT, that is, it admits asymptotically the shortest expected sample size among all the sequential tests with the same maximal type I and type II error probabilities. These results serve as a natural extension to those of the classic optimality results for the sequential probability ratio test.

6.7 Appendix to Chapter 6

6.7.1 Other technical proofs

The proofs need some variations of the change of measure Q_b introduced in the previous section. Given that all the calculations for the rest of the proof are under the distribution g_0, we let $\mathbb{P} = \mathbb{P}_{g_0}$ through out this section. To start with, we introduce two measures that are special cases of the measure in the beginning of Section 6.5.3.

A change of measure. Define measure Q via the Radon-Nikodym

$$\frac{dQ}{d\mathbb{P}} = \frac{1}{H_A} \sum_{n=1}^{\infty} \int_{\Gamma} I(S_n(\gamma) > A - 1) d\gamma$$

where $I(\cdot)$ is the indicator function and

$$H_A = \sum_{n=1}^{\infty} \int_{\Gamma} \mathbb{P}(S_n(\gamma) > A - 1) d\gamma.$$

The measure Q depends on A. To simplify the notation, we omit the index A in notation Q. The sample path generation requires three steps.

1. Sample two random indices (n_*, γ_*) jointly according to the density/mass function

   $$q(n_*, \gamma_*) = \mathbb{P}(S_{n_*}(\gamma_*) > A - 1)/H_A.$$

   Note that n_* is integer-valued and q as a function of n_* is a probability mass function. Furthermore, γ_* is a continuous variable and q as a function of γ_* is a density function.

2. Conditional on the realized n_* and γ_*, sample $S_{n_*}(\gamma_*)$ conditional on $S_{n_*}(\gamma_*) > A - 1$ under the measure $\mathbb{P}$.

3. Sample the rest of the process $\{S_n(\gamma) : n \neq n_*, \gamma \neq \gamma_*\}$ conditional on the realization $S_{n_*}(\gamma_*)$ under the original measure $\mathbb{P}$.

A second change of measure. This change of measure is defined for $S_n(\gamma)$ with n fixed and $\gamma \in \Gamma$. Define measure Q_n via the Radon-Nikodym

$$\frac{dQ_n}{d\mathbb{P}} = H_n^{-1} \int_\Gamma I(S_n(\gamma) > -1) d\gamma$$

where $I(\cdot)$ is the indicator function and

$$H_n = \int_\Gamma \mathbb{P}(S_n(\gamma) > -1) d\gamma.$$

The corresponding sample path generation is given as follows.

1. Sample two random indices γ_* according to the density function

$$q_n(\gamma_*) = \mathbb{P}(S_n(\gamma_*) > -1)/H_n.$$

2. Conditional on the realized γ_*, sample $S_n(\gamma_*)$ conditional on $S_n(\gamma_*) > -1$ under the measure $\mathbb{P}$.

3. Sample the rest of the process $\{S_n(\gamma) : \gamma \neq \gamma_*\}$ conditional on the realization $S_n(\gamma_*)$ under the original measure $\mathbb{P}$.

Proof of Lemma 21. We start the proof by deriving a lower bound. Notice that $S_\tau \geq S_\tau(\gamma)$ for all γ. Thus, we have

$$\mathbb{P}(\sup_n \sup_\gamma S_n(\gamma) > A) \geq \mathbb{P}(S_\tau > A) \geq \mathbb{P}(S_{\tau(\gamma)} > A) \cong e^{-A}$$

where $\tau(\gamma) = \inf\{n : S_n(\gamma) < -B \text{ or } S_n(\gamma) > A\}$. The last step in the above display is a classic large deviations result. We now proceed to the derivation of an upper bound of $\mathbb{P}(\sup_n \sup_\gamma S_n(\gamma) > A)$ and start with a localization on the set

$$L_A = \cup_{n=1}^\infty \{\sup_\gamma |\partial \xi_n(\gamma)| > n^\zeta e^{A^\beta}\}$$

for some $\alpha^{-1} < \beta < 1$ and ζ sufficiently large. According to Condition A3, we have that

$$\mathbb{P}(L_A^c) \le \sum_{n=1}^{\infty} \mathbb{P}\{\sup_\gamma |\partial \xi_n(\gamma)| > n^\zeta e^{A^\beta}\} \le \sum_{n=1}^{\infty} n^{-(\alpha-1)\zeta A^\beta} e^{-A^{\alpha\beta}} = o(e^{-A}).$$

Define

$$\tau_A = \inf\{n : \sup_\gamma S_n(\gamma) > A\}$$

and thus $\sup_n \sup_\gamma S_n(\gamma) > A$ if $\tau_A < \infty$. We now derive an upper bound for $\mathbb{P}(\tau_A < \infty, L_A)$ via the change of measure Q as follows

$$\mathbb{P}(\sup_n \sup_\gamma S_n(\gamma) > A, L_A) = H_A \mathbb{E}^Q \left(\Big[\sum_{n=1}^{\infty} \int_\Gamma I\{S_n(\gamma) > A-1\} d\gamma \Big]^{-1}, \tau_A < \infty, L_A \right).$$

Note that on the set $\{\tau_A < \infty\}$, there exists at least one γ such that $S_{\tau_A}(\gamma) > A$. Furthermore, on the set L_A, the gradient $|\nabla S_{\tau_A}(\gamma)|$ is bound by $e^{A^\beta}\tau_A^{\zeta+1}$. Therefore, we have the following lower bound

$$\sum_{n=1}^{\infty} \int_\Gamma I\{S_n(\gamma) > A-1\} d\gamma \ge \int_\Gamma I\{S_{\tau_A}(\gamma) > A-1\} d\gamma \ge \{e^{dA^\beta} \tau_A^{(\zeta+1)d}\}^{-1}.$$

Thus,

$$\mathbb{P}(\sup_n \sup_\gamma S_n(\gamma) > A, L_A) \le e^{dA^\beta} H_A \mathbb{E}^Q(\tau_A^{(\zeta+1)d}; \tau_A < \infty).$$

The last step is to control the moment $\mathbb{E}^Q(\tau_A^{(\zeta+1)d})$. Let n_* and γ_* be the random indices generated from Step 1 of the three-step sample path generation from Q. Therefore, we split the expectation

$$\begin{aligned}
\mathbb{E}^Q(\tau_A^{(\zeta+1)d}; \tau_A < \infty) &\le \mathbb{E}^Q(\tau_A^{(\zeta+1)d}; \tau_A \le n_*) + \mathbb{E}^Q(\tau_A^{(\zeta+1)d}; \tau_A < \infty, n_* < \tau_A < \infty) \\
&\le \mathbb{E}^Q\{n_*^{(\zeta+1)d}\} + \mathbb{E}^Q(\tau_A^{(\zeta+1)d}; \tau_A < \infty, n_* < \tau_A < \infty) \\
&\le O(A^{(\zeta+1)d}) + \mathbb{E}^Q(\tau_A^{(\zeta+1)d}; n_* < \tau_A < \infty).
\end{aligned}$$

We now focus on the last term by starting with the probability

$$Q(\tau_A = n_* + k).$$

Note that $\tau_A > n_*$ implies that $A - 1 < S_{n_*}(\gamma_*) < A$ and $S_n(\gamma) < A$ for all $n \leq n_*$ and $\gamma \in \Gamma$. Therefore, we have

$$Q(\tau_A = n_* + k) \leq \mathbb{P}(\sup_\gamma S_k(\gamma) > 0).$$

To obtain an estimate of the above probability, we use the change of measure Q_n

$$\begin{aligned}
&\mathbb{P}\Big[\sup_\gamma S_k(\gamma) > 0; \cup_{n=1}^k \{\sup_\gamma |\partial \xi_n(\gamma)| > e^{k^\beta}\}\Big] \\
&= H_k \mathbb{E}^{Q_k}\left[(\int_\Gamma I(S_k(\gamma) > -1)d\gamma)^{-1}; \sup_\gamma S_k(\gamma) > 0, \cup_{n=1}^k \{\sup_\gamma |\partial \xi_n(\gamma)| > e^{k^\beta}\}\right]
\end{aligned}$$

and

$$\mathbb{P}(\cup_{n=1}^k \{\sup_\gamma |\partial \xi_n(\gamma)| > e^{k^\beta}\}) \leq k e^{-k^{\alpha\beta}}. \tag{6.13}$$

For the normalizing constant, we have that

$$H_k = O(e^{-\varepsilon_0 k}).$$

For the integral $\int_\Gamma I(S_k(\gamma) > -1)d\gamma$ inside the expectation, on the set $\{\sup_\gamma S_k(\gamma) > 0\}$, there exists at least one γ_0 such that $S_k(\gamma_0) > 0$. Furthermore, the derivative is bounded from the above by e^{k^β}. Thus, the integral is bounded from below by

$$\int_\Gamma I(S_k(\gamma) > -1)d\gamma \geq \delta_0 k^{-d} e^{-dk^\beta}.$$

Thus, we have

$$\mathbb{P}(\sup_\gamma S_k(\gamma) > 0; \cup_{n=1}^k \{\sup_\gamma |\partial \xi_n(\gamma)| > e^{k^\beta}\}) = O(e^{-\varepsilon_0 k/2}). \tag{6.14}$$

We put together (6.13) and (6.14) and obtain that

$$Q(\tau_A = n_* + k) \leq \mathbb{P}(\sup_\gamma S_k(\gamma) > 0) = O(k e^{-k^{\alpha\beta}} + e^{-\varepsilon_0 k/2}).$$

Therefore, we have that

$$\mathbb{E}^Q(\tau_A^{(\zeta+1)d}; n_* < \tau_A < \infty) = O(\mathbb{E}(n_*^{(\zeta+1)d})) = O\{A^{(\zeta+1)d}\}.$$

Thereby, we conclude the proof. □

Proof of Lemma 22. We now prove an important fact that $H_A \cong e^{-A}$. Recall the notation $\xi(\gamma) = \log h_\gamma(X) - \log g_0(X)$. For each pair (n, γ), we consider the probability $\mathbb{P}(S_n(\gamma) > A - 1)$. For each $\varepsilon > 0$ small enough but not changing with A, we approximate the tail probability via large deviations theory stated as follows. Let $\varphi_\gamma(\theta) = \log[\mathbb{E}\{e^{\theta\xi(\gamma)}\}]$ and the rate function is

$$\mathbb{P}\{S_n(\gamma) > A - 1\} \leq e^{-nI(n,\gamma)}$$

where the rate function is $I(n, \gamma) = \theta_* \frac{A-1}{n} - \varphi_\gamma(\theta_*)$ and θ_* solves identity $\varphi'_\gamma(\theta_*) = \frac{A-1}{n}$. For each given γ, $n \times I(n, \gamma)$ is minimized at $n(\gamma) = (A-1)/\mathbb{E}_{h_\gamma}\{\xi(\gamma)\}$ and $\min_n n \times I(n, \gamma) = A - 1$. Thus, we have that

$$\mathbb{P}\{S_{n(\gamma)}(\gamma) > A - 1\} \leq e^{-A+1}.$$

We switch the order of summation and integral by taking the sum with respect to n first. We derive the upper bound of H_A by splitting the summation (for some $M = \kappa_1 / \min_\gamma D_h(\gamma|0)$ and κ_1 large)

$$\sum_{n=1}^{\infty} \mathbb{P}(S_n(\gamma) > A - 1) = \sum_{n=1}^{MA} \mathbb{P}(S_n(\gamma) > A - 1) + \sum_{n=MA+1}^{\infty} \mathbb{P}(S_n(\gamma) > A - 1).$$

Therefore, the first term is bounded by

$$\sum_{n=1}^{MA} \mathbb{P}(S_n(\gamma) > A - 1) \leq MAe^{-A+1}.$$

Notice that, as $n/A \to \infty$, the rate function $I(n, \gamma) \to -\inf_\theta \varphi_\gamma(\theta) > 0$. Therefore, the large deviations approximation becomes

$$-\frac{1}{n} \log \mathbb{P}\{S_n(\gamma) > A - 1\} \to \inf_\theta \varphi_\gamma(\theta) > I(n(\gamma), \gamma)$$

as $n/A \to \infty$ and $A \to \infty$. Therefore, if we choose κ_1 sufficiently large depending and $M = \kappa_1 / \min_\gamma D_h(\gamma|0)$, then the second term is

$$\sum_{n=MA+1}^{\infty} \mathbb{P}(S_n(\gamma) > A - 1) \cong \sum_{n=MA+1}^{\infty} e^{-n \inf_\theta \varphi_\gamma(\theta)} = o(e^{-A})$$

and therefore $\sum_{n=1}^{\infty}\mathbb{P}(S_n(\gamma) > A-1) \leq (MA+1)e^{-A}$. Since Γ is a compact set, then with κ_0 sufficiently large

$$H_A = \int_{\gamma\in\Gamma}\sum_{n=1}^{\infty}\mathbb{P}(S_n(\gamma) > A-1)d\gamma \leq \kappa_0 mes(\Gamma)Ae^{-A}/\min_{\gamma} D_h(\gamma|0)$$

□

Proof of Lemma 20. We first switch the sum and integration

$$H_{A,\theta} = \int_{\Gamma}\sum_{n=1}^{\infty}\mathbb{P}_{g_\theta}\{S_n(\theta,\gamma) > A\}d\gamma.$$

Furthermore, notice the following approximation (for some κ large)

$$\mathbb{P}_{g_\theta}\{\sup_n S_n(\theta,\gamma) > A\} \leq \sum_{n=1}^{\infty}\mathbb{P}_{g_\theta}\{S_n(\theta,\gamma) > A\} \leq A^{\kappa}\mathbb{P}_{g_\theta}\{\sup_n S_n(\theta,\gamma) > A\}.$$

The first inequality is due to the inclusion and exclusion formula and the second step can be obtained by standard large deviations analysis, Condition B2 and B3. In addition, the choice of κ is independent of θ and γ. Then, it is sufficient to show that

$$\limsup_{A\to\infty}\sup_{\theta\in\Theta}\frac{1}{A}\log\Big[\int_{\Gamma}\mathbb{P}_{g_\theta}\{\sup_n S_n(\theta,\gamma) > A\}d\gamma\Big] \leq -1.$$

We now consider the tail probability $\mathbb{P}_{g_\theta}\{\sup_n S_n(\theta,\gamma) > A\}$ for each θ and γ. The tail probability has a universal upper bound

$$w(\theta,\gamma) \triangleq \mathbb{P}_{g_\theta}\{\sup_n S_n(\theta,\gamma) > A\} \leq e^{-A}$$

and the equality holds only when the overshoot is zero. Therefore, we have split the integral for M sufficiently large

$$\int_{|\gamma-\gamma_\theta|<MA^{1/l}} w(\theta,\gamma)d\gamma \leq \kappa_d A^{d/l}e^{-A} + \int_{|\gamma-\gamma_\theta|\geq MA^{1/l}} w(\theta,\gamma)d\gamma \qquad (6.15)$$

where κ_d is the volume of the d-dimensional unit ball. We now show that $w(\theta,\gamma)e^A \to 0$ as $|\gamma-\gamma_\theta| \to \infty$. Let $\tau_A = \inf\{n : S_n(\theta,\gamma) > A\}$. We choose M sufficiently large such that $\mathbb{E}_{h_\gamma}\{\xi(\theta,\gamma)\} = D_h(\gamma|\theta) > 3A$. Then, the tail probability has the following upper bound

$$\begin{aligned}
w(\theta,\gamma) &= \mathbb{E}_{h_\gamma}\{e^{-S_{\tau_A}(\theta,\gamma)}; S_{\tau_A}(\theta,\gamma) > A\} \\
&\leq e^{-A}\mathbb{P}_{h_\gamma}[\xi_1(\theta,\gamma) \\
&< \{D_h(\gamma|\theta)+1\}/2] + \mathbb{E}_{h_\gamma}[e^{-S_{\tau_A}(\theta,\gamma)}; \xi_1(\theta,\gamma) > \{D_h(\gamma|\theta)+1\}/2].
\end{aligned}$$

The second term of the above inequality is bounded from the above by

$$e^{-\{D_h(\gamma|\theta)+1\}/2} \leq e^{-\{1+D_h(\gamma_\theta|\theta)+\delta|\gamma-\gamma_\theta|^l\}/2} \leq e^{-A-\varepsilon_0|\gamma-\gamma_\theta|^l}.$$

For the first term, notice that $\xi_1(\theta,\gamma)$ has mean $D_h(\gamma|\theta)$ and bounded second moment. By Chebyshev's inequality (noting that $\mathbb{E}_{h_\gamma}\{\xi_1(\theta,\gamma)\} = D_h(\gamma|\theta)$), we have that

$$\mathbb{P}_{h_\gamma}[\xi_1(\theta,\gamma) < \{D_h(\gamma|\theta)+1\}/2] = O(1)A^{-2}D_h(\gamma|\theta)^{-2} \leq O(1)A^{-2}|\gamma-\gamma_\theta|^{-2l}$$

Therefore, the integral has an upper bound

$$\int_{|\gamma-\gamma_*|\geq MA^{1/l}} w(\theta,\gamma)d\gamma \leq \int_{|\gamma-\gamma_*|\geq MA^{1/l}} O(1)A^{-2}e^{-A}|\gamma-\gamma_\theta|^{-2l}d\gamma.$$

Since $l > (d+1)/2$, the above integral is $O(A^{-2}e^{-A})$. We insert this bound back to (6.15) and obtain that $\int_\Gamma w(\theta,\gamma)d\gamma = O(A^{d/l}e^{-A})$ and conclude the proof. $\square$

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