On Asymptotic Properties of Hyperparameter Estimators for Kernel-based Regularization Methods

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Abstract

The kernel-based regularization method has two core issues: kernel design and hyperparameter estimation. In this paper, we focus on the second issue and study the properties of several hyperparameter estimators including the empirical Bayes (EB) estimator, two Stein’s unbiased risk estimators (SURE) and their corresponding Oracle counterparts, with an emphasis on the asymptotic properties of these hyperparameter estimators. To this goal, we first derive and then rewrite the first order optimality conditions of these hyperparameter estimators, leading to several insights on these hyperparameter estimators. Then we show that as the number of data goes to infinity, the two SUREs converge to the best hyperparameter minimizing the corresponding mean square error, respectively, while the more widely used EB estimator converges to another best hyperparameter minimizing the expectation of the EB estimation criterion. This indicates that the two SUREs are asymptotically optimal but the EB estimator is not. Surprisingly, the convergence rate of two SUREs is slower than that of the EB estimator, and moreover, unlike the two SUREs, the EB estimator is independent of the convergence rate of $\Phi^T\Phi/N$ to its limit, where $\Phi$ is the regression matrix and $N$ is the number of data. A Monte Carlo simulation is provided to demonstrate the theoretical results.

Key words: Linear system identification, Gaussian process regression, Kernel-based regularization, Empirical Bayes, Stein’s unbiased risk estimators, Oracle estimators, Asymptotic analysis

1 Introduction

The kernel-based regularization methods (KRM) from machine learning and statistics were first introduced to the system identification community in Pillonetto & De Nicolao (2010) and then further developed in Chen et al. (2014, 2012); Pillonetto et al. (2011). These methods attract increasing attention in the community and have become a complement to the classical maximum likelihood/prediction error methods (ML/PEM) (Chen et al., 2012; Ljung et al., 2015; Pillonetto & Chiuso, 2015). In particular, KRM may have better average accuracy and robustness than ML/PEM when the data is short and/or has low signal-to-noise ratio (SNR).

There are two core issues for KRM: kernel design and hyperparameter estimation. The former is regarding how to parameterize the kernel matrix with a parameter vector, called hyperparameter, to embed the prior knowledge of the system to be identified, and the latter is regarding how to estimate the hyperparameter based on the data such that the resulting model estimator achieves a good bias-variance tradeoff or equivalently, suitably balances the adherence to the data and the model complexity.

The kernel design plays a similar role as the model structure design for ML/PEM and determines the underlying model structure for KRM. In the past few years, many efforts have been spent on this issue and several kernels have been invented to embed various types of prior knowledge, e.g., Carli et al. (2017); Chen et al. (2014, 2016, 2012); Dinuzzo (2015); Marconato et al. (2016); Pillonetto et al. (2016, 2011); Pillonetto & De Nicolao (2010); Zorzi & Chiuso (2017). In particular, two systematic kernel design methods (one is from a machine learning perspective and the other one is from a system theory perspective) were developed in Chen & Ljung (2016) by embedding the corresponding type of prior knowledge.

The hyperparameter estimation plays a similar role as the model order selection in ML/PEM and its essence is to determine a suitable model complexity based on the data. As mentioned in the survey of KRM Pillonetto et al. (2014), many methods can be used for hyperparameter estimation, such as the cross-validation (CV),
empirical Bayes (EB), $C_p$ statistics and Stein’s unbiased risk estimator (SURE) and etc. In contrast with the numerous results on kernel design, there are however few results on hyperparameter estimation except Aravkin et al. (2012a,b, 2014); Chen et al. (2014); Pillonetto & Chiuso (2015). In Aravkin et al. (2012a,b, 2014), two types of diagonal kernel matrices are considered. When $\Phi^T \Phi / N$ is an identity matrix, where $\Phi$ is the regression matrix and $N$ is the number of data, the optimal hyperparameter estimate of the EB estimator has explicit form and is shown to be consistent in terms of the mean square error (MSE). When $\Phi^T \Phi / N$ is not an identity matrix, the EB estimator is shown to asymptotically minimize a weighted MSE. In Chen et al. (2014), the EB with linear multiple kernel is shown to be a difference of convex programming problem and moreover, the optimal hyperparameter estimate is sparse. In Pillonetto & Chiuso (2015), an unbiased estimator of MSE was introduced and used as a measure to evaluate the performance of the EB estimator and two SUREs: one for impulse response reconstruction and the other one for output prediction, and the robustness issue by introducing the so-called excess degree of freedom was considered.

In this paper, we study the properties of the EB estimator and two SUREs in Pillonetto & Chiuso (2015) with an emphasis on the asymptotic properties of these hyperparameter estimators. In particular, we are interested in the following questions: When the number of data goes to infinity,

1) what will be the best kernel matrix, or equivalently, the best value of the hyperparameter?

2) which estimator (method) shall be chosen such that the hyperparameter estimate tends to this best value in the given sense?

3) what will be the convergence rate of that the hyperparameter estimate tends to this best value? and what factors does this rate depend on?

In order to answer these questions, we employ the regularized least squares method for FIR model estimation in Chen et al. (2012). As a motivation, we first show that the regularized least squares estimate can have smaller MSE than the least squares estimate for any data length, if the kernel matrix is chosen carefully. We then derive the first order optimality conditions of these hyperparameter estimators and their corresponding Oracle counterparts (relying on the true impulse response, see Section 3.2 for details). These first order optimality conditions are then rewritten in a way to better expose their relations, leading to several insights on these hyperparameter estimators. For instance, one insight is that for the Oracle estimators, for any data length, and without structure constraints on the kernel matrix, the optimal kernel matrices are same as the one in Chen et al. (2012) and equal to the outer product of the vector of the true impulse response and its transpose. Moreover, explicit solutions of the optimal hyperparameter estimate for two special cases are derived accordingly. Then we turn to the asymptotic analysis of these hyperparameter estimators. Regardless of the parameterization of the kernel matrix, we first show that the two SUREs actually converge to the best hyperparameter minimizing the corresponding MSE, respectively, as the number of data goes to infinity, while the more widely used EB estimator converges to the best hyperparameter minimizing the expectation of the EB estimation criterion. In general, these best hyperparameters are different from each other except for some special cases. This means that the two SUREs are asymptotically optimal but the EB estimator is not. We then show that the convergence rate of two SUREs is slower than that of the EB estimator, and moreover, unlike the two SUREs, the EB estimator is independent of the convergence rate of $\Phi^T \Phi / N$ to its limit.

The remaining parts of the paper is organized as follows. In Section 2, we recap the regularized least squares method for FIR model estimation and introduce two types of MSE. In Section 3, we introduce a couple of widely used parameterizations of kernel matrix and six hyperparameter estimators, including the EB estimator, two SUREs, and their corresponding Oracle counterparts. In Section 4, we derive the first order optimal conditions of these hyperparameter estimators and put them in a form that clearly shows their relation, leading to several insights. In Section 5, we give the asymptotic analysis of these hyperparameter estimators, including the asymptotic convergence and the corresponding convergence rate. In Section 6, we illustrate our theoretical results with a Monte Carlo simulation. Finally, we conclude this paper in Section 7. All proofs of the theoretical results (propositions, corollaries and theorems) are postponed to the Appendix.

## 2 Regularized Least Squares Approach for FIR Model Estimation

Consider a single-input single-output linear discrete-time invariant, stable and causal system

$$y(t) = G_0(q^{-1})u(t) + v(t), \quad t = 1, \ldots, N$$

where $t$ is the time index, $y(t), u(t), v(t)$ are the output, input and disturbance of the system at time $t$, respectively, $G_0(q^{-1})$ is the transfer function of the system and $q^{-1}$ is the backshift operator: $q^{-1}u(t) = u(t - 1)$. Assume that the input $u(t)$ is known (deterministic) and the input-output data are collected at time instants $t = 1, \ldots, N$, and moreover, the disturbance $v(t)$ is a zero mean white noise with variance $\sigma^2 > 0$. The problem is to estimate a model for $G_0(q^{-1})$ as well as possible based on the the available data $\{u(t - 1), y(t)\}_{t=1}^N$.

The transfer function $G_0(q^{-1})$ can be written as

$$G_0(q^{-1}) = \sum_{k=1}^{\infty} g_k^0 q^{-k},$$

where $g_k^0, k = 1, \ldots, \infty$ form the impulse response of the system. Since the impulse response of a stable linear system decays exponentially, it is possible to truncate the infinite impulse response at a sufficiently high order,
leading to the finite impulse response (FIR) model:
\[
G(q^{-1}) = \sum_{k=1}^{n} g_k q^{-k}, \quad \theta = [g_1, \ldots, g_n]^T \in \mathbb{R}^n. \tag{3}
\]
With the FIR model (3), system (1) is now written as
\[
y(t) = \phi^T(t)\theta + v(t), \quad t = 1, \ldots, N
\]
where \(\phi(t) = [u(t-1), \ldots, u(t-n)]^T \in \mathbb{R}^n\), and its matrix-vector form is
\[
Y = \Phi\theta + V, \quad \text{where}
\]
\[
Y = [y(1), y(n+2), \ldots, y(N)]^T
\]
\[
\Phi = [\phi(1), \phi(n+2), \ldots, \phi(N)]^T
\]
\[
V = [v(1), v(n+2), \ldots, v(N)]^T.
\]

The well-known least squares (LS) estimator
\[
\hat{\theta}_{LS} = \arg\min_{\theta \in \mathbb{R}^n} \|Y - \Phi\theta\|^2 \tag{5a}
\]
\[
= (\Phi^T \Phi)^{-1} \Phi^T Y, \tag{5b}
\]
where \(\cdot \| \cdot \) is the Euclidean norm, is unbiased but may have large variance and mean square error (MSE) (e.g., when the input is low-pass filtered white noise). The large variance can be mitigated if some bias is allowed and traded for smaller variance and smaller MSE.

One possible way to achieve this goal is to add a regularization term \(\sigma^2 \theta^T P^{-1} \theta\) in the LS criterion (5a), leading to the regularized least squares (RLS) estimator:
\[
\hat{\theta}^R = \arg\min_{\theta \in \mathbb{R}^n} \|Y - \Phi\theta\|^2 + \sigma^2 \theta^T P^{-1} \theta \tag{6a}
\]
\[
= P\Phi^T (P\Phi P^T + \sigma^2 I_N)^{-1} Y \tag{6b}
\]
where \(P\) is positive semidefinite and is called the kernel matrix (\(\sigma^2 P^{-1}\) is often called the regularization matrix), and \(I_N\) is the \(N\)-dimensional identity matrix.

**Remark 1** As well known, the RLS estimator (6b) has a Bayesian interpretation. Specifically, assume that \(\theta\) and \(v(t)\) are independent and Gaussian distributed with
\[
\theta \sim \mathcal{N}(0, P), \quad v(t) \sim \mathcal{N}(0, \sigma^2), \tag{7}
\]
where \(P\) is the prior covariance matrix. Then \(\theta\) and \(Y\) are jointly Gaussian distributed and moreover, the posterior distribution of \(\theta\) given \(Y\) is
\[
\theta|Y \sim \mathcal{N}(\hat{\theta}^R, \hat{\theta}^R)
\]
\[
\hat{\theta}^R = P\Phi^T (P\Phi P^T + \sigma^2 I_N)^{-1} Y
\]
\[
\hat{\theta}^R = P - P\Phi^T (P\Phi P^T + \sigma^2 I_N)^{-1} \Phi P.
\]

Two types of MSE could be used to evaluate the performance of the RLS estimator (6b). The first one is the MSE related to the impulse response reconstruction, see e.g., Chen et al. (2012); Pillonetto & Chiuso (2015),
\[
\text{MSE}_g(P) = E(\|\hat{\theta}^R - \theta_0\|^2), \tag{8}
\]
where \(E(\cdot)\) is the mathematical expectation and \(\theta_0 = [g_1^0, \ldots, g_n^0]^T\) with \(g_i^0, i = 1, \ldots, n\), defined in (2). The second one is the MSE related to output prediction, see e.g., Pillonetto & Chiuso (2015),
\[
\text{MSE}_y(P) = E \left[ \sum_{t=1}^{N} (\phi^T(t)(\theta_0 + v^*(t) - \hat{y}(t)))^2 \right], \tag{9}
\]
where \(\hat{y}(t) = \phi^T(t)\hat{\theta}^R(P)\) and \(v^*(t)\) is an independent copy of the noise \(v(t)\). Interestinly, the two MSEs (8) and (9) are related with each other through
\[
\text{MSE}_y(P) = \text{Tr}(E(\hat{\theta}^R - \theta_0)(\hat{\theta}^R - \theta_0)^T \Phi^T \Phi) + N\sigma^2, \tag{10}
\]
where \(\text{Tr}(\cdot)\) is the trace of a square matrix. Moreover, they have explicit expressions, which are given in the following proposition.

**Proposition 1** For a given kernel matrix \(P\), the two MSEs (8) and (9) take the following form
\[
\text{MSE}_g(P) = \|P\Phi^T Q^{-1} \theta_0 - \theta_0\|^2 + \sigma^2 \text{Tr}(P\Phi^T Q^{-1} Q^{-T} \Phi P^T) \tag{11}
\]
\[
\text{MSE}_y(P) = \|\Phi P\Phi^T Q^{-1} \theta_0 - \theta_0\|^2 + N\sigma^2 + \sigma^2 \text{Tr}(\Phi P\Phi^T Q^{-1} Q^{-T} \Phi P^T) \tag{12}
\]
\[
Q = \Phi P\Phi^T + \sigma^2 I_N. \tag{13}
\]

2.1 RLS estimator can outperform LS estimator

It is interesting to investigate whether the RLS estimator (6b) with a suitable choice of the kernel matrix \(P\) can have smaller MSEs (8) and (9) than the LS estimator (5b). The answer is affirmative for MSEg (8) and for the ridge regression case, where \(P^{-1} = (\beta/\sigma^2)I_n\) with \(\beta > 0\), Hoerl & Kennard (1970); Theobald (1974). In what follows, we further show that this property also holds for more general \(P\) for MSEg (8) and MSEy (9).

**Proposition 2** Consider the RLS estimator (6b) and the LS estimator (5b). Suppose that \(P^{-1} = \beta A/\sigma^2\), where \(\beta > 0\) and \(A\) is positive semidefinite. Then for a given \(A\), there exits \(\beta > 0\) such that (6b) has a smaller MSEg (8) and MSEy (9) than (5b). Moreover, if \(A\) is positive definite, then (6b) has a smaller MSEg (8) and MSEy (9) than (5b) whenever \(0 < \beta < 2\sigma^2/(\theta_0^T A \theta_0)\).

Proposition 2 shows that for any data length \(N\), the RLS estimator (6b) can have smaller MSEg (8) and MSEy (9) than the LS estimator (5b) with a sufficiently small regularization “in any direction” and this merit motivates to further explore the potential of the RLS estimator (6b) by careful design of the kernel matrix \(P\).
3 Design of Kernel Matrix and Hyperparameter Estimation

The regularization method has two core issues: kernel matrix design, namely parameterization of the kernel matrix by a parameter vector, called hyperparameter, and the hyperparameter estimation.

3.1 Parametrization of Kernel Matrix

For efficient regularization, the kernel matrix $P$ has to be chosen carefully. It is typically done by postulating a parameterized family of matrices

$$P(\eta), \quad \eta \in \Omega \subseteq \mathbb{R}^p,$$

where $\eta$ is called the hyperparameter and the feasible set $\Omega$ of $\eta$ is assumed to be compact. The choice of parameterization is a trade-off of the same kind as the choice of model class in identification: On one hand it should be a large and flexible class to allow as much benefits from regularization as possible. On the other hand, a large set requires larger dimensions of $\eta$, and the estimation of these comes with their own penalties (much in the spirit of the Akaike’s criterion). Since $P$ is the prior covariance of the true impulse response, the prior knowledge of the underlying system to be identified, e.g., exponential stability and smoothness, should be embedded in the parameterized matrix $P(\eta)$.

A popular way to achieve this goal is through a parameterized positive semidefinite kernel function. So far, several kernels have been invented, such as the stable spline (SS) kernel (Pillonetto & D’Oriol, 2010), the diagonal correlated (DC) kernel and the tuned-correlated (TC) kernel (Chen et al., 2012), which are defined as follows:

**SS:** $P_{kj}(\eta) = c \left( \frac{\alpha^{k+j+\max(k,j)}}{2} - \frac{\alpha^{3\max(k,j)}}{6} \right)^2$,

$$\eta = [c, \alpha] \in \Omega = \{c \geq 0, 0 \leq \alpha \leq 1\};$$

**DC:** $P_{kj}(\eta) = c \alpha^{(k+j)/2} \rho^{j-k}$,

$$\eta = [c, \alpha, \rho] \in \Omega = \{c \geq 0, 0 \leq \alpha \leq 1, |\rho| \leq 1\};$$

**TC:** $P_{kj}(\eta) = c \alpha^{\max(k,j)}$,

$$\eta = [c, \alpha] \in \Omega = \{c \geq 0, 0 \leq \alpha \leq 1\}.$$

3.2 Hyperparameter Estimation

Once a parameterized family of the kernel matrix $P(\eta)$ has been chosen, the task is to estimate, or “tune”, the hyperparameter $\eta$ based on the data.

Several methods are suggested in the literature, see e.g., Section 14 of Pillonetto et al. (2014), including the empirical Bayes (EB) and SURE methods. The EB method uses the Bayesian interpretation in Remark 1. Under the assumption (7), it follows that $Y$ is Gaussian with mean zero and covariance matrix $\Phi^T P(\eta) \Phi + \sigma^2 I_N$. As a result, it is possible to estimate the hyperparameter $\eta$ by maximizing the (marginal) likelihood of $Y$, i.e.,

$$\hat{\eta}_{EB} = \arg \min_{\eta \in \Omega} \mathcal{F}_{EB}(P(\eta)),$$

$$\mathcal{F}_{EB}(P) = Y^T Q^{-1}Y + \log \det(Q).$$
is ill-conditioned, SUREg (23) should be avoided for hyperparameter estimation. One may also note that $(\Phi^T \Phi)^{-1}$ in the second term is independent of $P$ and thus can actually be removed in the calculation.

**Remark 3** It is interesting to note that the first terms of $F_{Sy}(P)$, $F_{Sy}(P)$, and $F_{EB}(P)$ given in (20), (21), and (19) contain the same factors $Y$ and $Q^{-1}$. Moreover, similar to (10), $F_{Sy}(P)$ and $F_{Sy}(P)$ are related with each other through
\begin{equation}
F_{Sy}(P) = \text{Tr} \left\{ \left[ (\theta_{LS} - \hat{\theta}_{LS}(P)) (\frac{\partial}{\partial P} \theta_{LS} - \hat{\theta}_{LS}(P)) \right]^T \right. \\
+ \sigma^2 (2R^{-1} - (\Phi^T \Phi)^{-1}) \Phi^T \Phi \\
+ Y^T \Phi (\Phi^T \Phi)^{-1} \Phi^TY - Y^TY - n \sigma^2 \left. \right\} \text{ independent of the kernel matrix } P 
\end{equation}

In what follows, we will investigate the properties of the hyperparameter estimators EB, SUREg, and SUREy and their corresponding Oracle estimators EEB, MSEg and MSEy. Before proceeding to the details, we make, without loss of generality, the following assumption.

**Assumption 1** The optimal hyperparameter estimates $\hat{\eta}_{EB}$, $\hat{\eta}_{Sy}$, $\hat{\eta}_{EB}$, $\hat{\eta}_{MSEg}$, $\hat{\eta}_{MSEy}$, and $\hat{\eta}_{EEB}$ are interior points of $\Omega$.

**Remark 4** To justify Assumption 1, we take the DC kernel as an example. For the case where either $c = 0$ or $\alpha = 0$, $P(\eta) = 0$ and thus (6b) is trivially 0. For the case where $\alpha = 1$, this violates the stability of the system. For the case where $|\rho| = 1$, the coefficients of the impulse response is perfectly positive or negative correlated, but this is impossible for a stable system. In fact, more formal justification regarding this assumption can be found on Pillonetto & Chiuso, 2015, p. 115), which shows that the measure of the set containing all optimal estimates lying on the boundary of $\Omega$ is zero and thus can be neglected when making almost sure convergence statement.

### 4 Properties of Hyperparameter Estimators: Finite Data Case

In this section, focusing on the finite data case we first give the first order optimality conditions of the hyperparameter estimators and then we consider two special cases for which closed-form expressions of the optimal hyperparameter estimates are available.

#### 4.1 First Order Optimality Conditions

The optimal hyperparameter estimates $\hat{\eta}_{EB}$, $\hat{\eta}_{Sy}$, and $\hat{\eta}_{EB}$ in (23), (24), and (18) should satisfy the first order optimality conditions if they are interior points of $\Omega$. For convenience, we let $\mathcal{C}$ to denote one of the following estimation criteria $F_{Sy}$, $F_{Sy}$, $F_{EB}$, MSEg, MSEy or EEB. Then the corresponding optimal hyperparameter estimates are a root of the system of equations:
\begin{equation}
\frac{\partial \mathcal{C}(P(\eta))}{\partial \eta} = 0. \quad (30)
\end{equation}

By the chain rule of compound functions, we have
\begin{equation}
\text{Tr} \left( \frac{\partial \mathcal{C}(P)}{\partial P} \left( \frac{\partial P(\eta)}{\partial \eta} \right)^T \right) = 0, \quad 1 \leq i \leq p. \quad (31)
\end{equation}

where the symmetry of $P$ is not considered, that is, the elements of $P$ are treated independently. Clearly, the term $\frac{\partial \mathcal{C}(P)}{\partial P}$ is irrespective of the parameterization of $P$ and its explicit expressions for the estimation criteria (20), (21), and (19) are available.

**Proposition 3** The first order partial derivatives of (20), (21), and (19) with respect to $P$ are, respectively,
\begin{align*}
&\frac{\partial F_{Sy}(P)}{\partial P} = -2\sigma^4 \Phi^T Q^{-T} \Phi (\Phi^T \Phi)^{-2} \Phi^T Q^{-1} YY^T Q^{-T} \Phi \\
&+ 2\sigma^4 H^{-1} \Phi^T \\
&\frac{\partial F_{Sy}(P)}{\partial P} = -2\sigma^4 \Phi^T Q^{-T} Q^{-1} YY^T Q^{-T} \Phi \\
&+ 2\sigma^4 \Phi^T Q^{-T} Q^{-T} \Phi \\
&\frac{\partial F_{EB}(P)}{\partial P} = -\Phi^T Q^{-T} YY^T Q^{-T} \Phi + \Phi^T Q^{-T} \Phi \\
&H = P\Phi^T \Phi + \sigma^2 I_n, \quad \Phi = P\Phi^T \Phi + \sigma^2 I_n. \quad (32)\end{align*}

Similarly, the partial derivatives of MSEg($P$), MSEy($P$), and EEB($P$) with respect to $P$ are also available.

**Proposition 4** The first order partial derivatives of (11), (12), and (28) with respect to $P$ are, respectively,
\begin{align*}
&\frac{\partial \text{MSyg} (P)}{\partial P} = -2\sigma^4 H^{-1} \theta_0 \theta_0^T \Phi^T Q^{-T} \Phi \\
&+ 2\sigma^4 H^{-1} P \Phi^T Q^{-T} \Phi \quad (33) \\
&\frac{\partial \text{MSEy} (P)}{\partial P} = -2\sigma^4 \Phi^T Q^{-T} Q^{-1} \Phi \theta_0 \theta_0^T \Phi^T Q^{-T} \Phi \\
&+ 2\sigma^4 \Phi^T Q^{-T} Q^{-1} \Phi P \Phi^T Q^{-T} \Phi \\
&\frac{\partial \text{EEB} (P)}{\partial P} = -\Phi^T Q^{-T} \Phi \theta_0 \theta_0^T \Phi^T Q^{-T} \Phi \\
&+ \Phi^T Q^{-T} \Phi P \Phi^T Q^{-T} \Phi. \quad (34) \end{align*}

where $H$ is defined in (35).

In order to better expose the relation among the partial derivatives derived in Propositions 3 and 4, we define
\begin{equation}
S = P + \sigma^2 (\Phi^T \Phi)^{-1}. \quad (35)
\end{equation}

With the use of (35) and the identities (B.49)–(B.51) in the appendix, we rewrite the partial derivatives derived in Propositions 3 and 4 as follows.

**Corollary 1** The partial derivatives derived in Propositions 3 and 4 can be rewritten as follows:
\begin{equation}
\frac{\partial \text{MSE} (P)}{\partial P} = 2\sigma^4 S^{-T}(\Phi^T \Phi)^{-2} S^{-1} (P - \theta_0 \theta_0^T) S^{-T} \quad (36)
\end{equation}
\[
\frac{\partial F_{\theta_0}(P)}{\partial P} = 2\sigma^4 S^{-T}(\Phi^T \Phi)^{-2} S^{-1}(S - \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T) S^{-T} \\
\frac{\partial MSE_y(P)}{\partial P} = 2\sigma^4 S^{-T}(\Phi^T \Phi)^{-1} S^{-1}(P - \theta_0 \theta_0^T) S^{-T} \\
\frac{\partial F_{\theta_0}(P)}{\partial P} = 2\sigma^4 S^{-T}(\Phi^T \Phi)^{-1} S^{-1}(S - \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T) S^{-T} \\
\frac{\partial EE\beta(P)}{\partial P} = S^{-T}(P^T - \theta_0 \theta_0^T) S^{-T} \\
\frac{\partial F_{\theta_0}(P)}{\partial P} = S^{-T}(S^T - \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T) S^{-T}.
\] (41) (42) (43) (44) (45)

It follows from Corollary 1 that the difference between the partial derivatives of \( F_{\theta_0}(P), F_{\theta_0}(P), F_{\theta_0}(P) \) and that of their Oracle counterparts is that the factor \( S - \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T \) is replaced by \( P - \theta_0 \theta_0^T \). Moreover, the difference between the partial derivative of \( F_{\theta_0}(P) \) and that of \( F_{\theta_0}(P) \) is that there is one extra factor \((\Phi^T \Phi)^{-1}\). The difference between the first order derivative of \( F_{\theta_0}(P) \) and that of \( F_{\theta_0}(P) \) is that there is one extra factor \( 2\sigma^4 (\Phi^T \Phi)^{-1} S^{-1} = 2\sigma^4 H^{-1} \). The above relations extend to the partial derivatives of their Oracle counterparts.

**Remark 5** It is important to note from Propositions 3 and 4 that only the first term of \( \frac{\partial F_{\theta_0}(P)}{\partial P} \) depends on the possibly ill-conditioned \((\Phi^T \Phi)^{-1}\). With the use of \( S \) in (39), all partial derivatives of the hyperparameter estimators seemingly depend on the possibly ill-conditioned term \( (\Phi^T \Phi)^{-1} \). However, it should be stressed that the partial derivatives derived in Corollary 1 are not intended for numerical calculation but for theoretical analysis and for better exposition of the relation among the partial derivatives derived in Propositions 3 and 4.

**Remark 6** The kernel matrix \( P \) is in general assumed to be symmetric. In this case, we have \( S^T = S \) and thus the partial derivatives derived in Corollary 1 can be simplified accordingly.

Setting \( \frac{\partial MSE_y(P)}{\partial P} = 0, \frac{\partial MSE_y(P)}{\partial P} = 0, \) and \( \frac{\partial EE\beta(P)}{\partial P} = 0 \) in Corollary 1 leads to the next proposition.

**Proposition 5** The optimal kernel matrix that minimizes MSE\( g(P), MSE_y(P), \) and EEB\( (P) \) without structure constraints on \( P \) is

\[
P = \theta_0 \theta_0^T.
\] (46)

It was found in Chen et al. (2012) that (46) minimizes the MSE matrix \( E(\hat{\theta}_L^R - \theta_0)(\hat{\theta}_L^R - \theta_0)^T \) in the matrix sense. Here we further find that (46) is optimal for MSE\( g(P), MSE_y(P), \) and EEB\( (P), \) and for any data length \( N \).

**Remark 7** It seems that \( S - \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T = 0 \), i.e., \( P = \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T - \sigma^2(\Phi^T \Phi)^{-1} \) is a possible candidate for the optimal matrix minimizing SURE\( g(P), SURE_y(P), \) and \( EEB(P) \). However, this is not true, since this kernel matrix would make \( S = \hat{\theta}_{L^S}(\hat{\theta}_{L^S})^T \) singular and SURE\( g(P), SURE_y(P), \) and \( EEB(P) \) take the value of \(-\infty\).

In general, there is no explicit expression of these hyper-parameter estimators. However, there exist some specific cases, for which it is possible to derive the explicit solution based on Corollary 1. In the following, we consider two special cases.

### 4.2 Ridge Regression with \( \Phi^T \Phi = NI_n \)

We let \( P(\eta) = \eta I_n \) with \( \eta \geq 0 \) and assume \( \Phi^T \Phi = NI_n \). Then we have the following result.

**Proposition 6** Consider \( P(\eta) = \eta I_n \) with \( \eta \geq 0 \). Further assume that \( \Phi^T \Phi = NI_n \). Then we have

\[
\hat{\eta}_{Sg} = \hat{\eta}_{Sy} = \hat{\eta}_{EB} = \max\left(0, \frac{\hat{\theta}_{L^S}^T \hat{\theta}_{L^S}}{n} - \frac{\sigma^2}{N}\right).
\] (47)

Moreover,

\[
\hat{\eta}_{MSEg} = \hat{\eta}_{MSEy} = \hat{\eta}_{EEB} = \theta_0^T \theta_0/n.
\] (48)

**Remark 8** It is worth noting that the optimal hyperparameter \( \theta_0^T \theta_0/n \) holds for any \( N \). Moreover, one has

\[
MSE_g(\theta_0^T \theta_0/n I_n) = \frac{n\sigma^2}{N + n\sigma^2/(\theta_0^T \theta_0)} < \frac{n \sigma^2}{N},
\]

where \( n\sigma^2/N \) is equal to the MSE of the LS estimator (5b). This means that the ridge regression with \( P = \theta_0^T \theta_0/n I_n \) has a smaller MSE than the LS estimator (5b) when \( \Phi^T \Phi = NI_n \). Finally, (47) is a consistent estimator of \( \theta_0^T \theta_0/n \) if \( \hat{\theta}_{L^S} \to \theta_0 \) as \( N \to \infty \).

### 4.3 Diagonal Kernel Matrix with \( \Phi^T \Phi = NI_n \)

We let \( P(\eta) \) be a diagonal kernel matrix (in this case we have \( p = n \)), i.e.,

\[
P(\eta) = \text{diag}[\eta_1, \ldots, \eta_n] \quad \text{with} \quad \eta_i \geq 0, \quad 1 \leq i \leq n.
\] (49)

where \( \eta_1, \ldots, \eta_n \) are the main diagonal elements of the diagonal matrix diag\( [\eta_1, \ldots, \eta_n] \). Then under the assumption \( \Phi^T \Phi = NI_n \), we have the following result.

**Proposition 7** Consider \( P(\eta) \) in (49). Further assume that \( \Phi^T \Phi = NI_n \). Then we have

\[
\hat{\eta}_{Sg} = \hat{\eta}_{Sy} = \hat{\eta}_{EB} = \left[\max\{0, \hat{\eta}_1^2 - \sigma^2/N\}, \ldots, \max\{0, \hat{\eta}_n^2 - \sigma^2/N\}\right]^T
\] (50)

where \( \hat{\eta}_i \) is the \( i \)-th element of the LS estimate (5b), \( i = 1, \ldots, n \). Moreover,

\[
\hat{\eta}_{MSEg} = \hat{\eta}_{MSEy} = \hat{\eta}_{EEB} = \left[\eta_1^0, \ldots, \eta_n^0\right]^T.
\] (51)
Remark 9 In the papers (Arauskien et al., 2012b, 2014), the linear model (4) but with a slightly different setting is considered, where the parameter \( \theta \) is partitioned into \( m \) sub-vectors \( \theta = [\theta^{(1)^T}, \cdots, \theta^{(m)^T}]^T \) and the dimension of \( \theta^{(i)} \) is \( n_i \) so that \( n = \sum_{i=1}^m n_i \). In addition, the prior distribution of \( \theta^{(i)} \) is set to be \( \mathcal{N}(0, \eta_i n_i) \) and \( \eta_i \) is an independent and identically distributed exponential random variable with probability density \( p_\lambda(\eta_i) = \gamma \exp(-\gamma \eta_i) \chi(\eta_i) \) where \( \gamma \) is a positive scalar and \( \chi(t) = 1 \) for \( t \geq 0 \) and 0 otherwise. Under the setting given above, the solution maximizing the marginal posterior density of \( \eta \) given the data and the optimal solution of the MSEg are derived in Arauskien et al. (2012b, 2014) where \( \Phi^T \Phi = NI_n \). When \( n_i = 1 \) for \( i = 1, \ldots, m \) and \( \gamma = 0 \), their solutions become (50) and (51), respectively. In contrast, we study here the SUREg, SUREy, MSEy, and EEB estimators other than the EB and MSEg estimators and find their solutions are the same under the simplified setting, respectively. Clearly, \( \max \{0, \sigma^2 - \sigma^2/N\} \) is a consistent estimator of \( (\theta_0^0)^2 \), \( i = 1, \ldots, n \).

5 Properties of Hyperparameter Estimators: Infinite Data Case

In this section, we investigate the asymptotic properties of these hyperparameter estimators. For this purpose, it is useful to first consider the asymptotic property of the partial derivatives derived in Corollary 1. Noting the finding of Corollary 1 under (45) and that \( S - \hat{\theta}^S \hat{\theta}_0^S \) converges to \( P - \theta_0^0 \theta_0^0 \) under proper conditions, we can derive the following Proposition.

Proposition 8 Consider the partial derivatives derived in Corollary 1. Assume that \( P \) is nonsingular and \( \Phi^T \Phi/N \to \Sigma \) almost surely as \( N \to \infty \), where \( \Sigma \) is positive definite. Then we have as \( N \to \infty \)

\[
N^2 \frac{\partial \text{MSEg}(P)}{\partial P} \to 2\sigma^4 P^{-T} \Sigma^{-2} P^{-1} (P - \theta_0^0 \theta_0^0)^T P^{-T} \tag{52}
\]

\[
N^2 \frac{\partial \mathcal{F}_{\text{SE}}(P)}{\partial P} \to 2\sigma^4 P^{-T} \Sigma^{-2} P^{-1} (P - \theta_0^0 \theta_0^0)^T P^{-T} \tag{53}
\]

\[
N \frac{\partial \text{MSEy}(P)}{\partial P} \to 2\sigma^4 P^{-T} \Sigma^{-1} P^{-1} (P - \theta_0^0 \theta_0^0)^T P^{-T} \tag{54}
\]

\[
N \frac{\partial \mathcal{F}_{\text{Sy}}(P)}{\partial P} \to 2\sigma^4 P^{-T} \Sigma^{-1} P^{-1} (P - \theta_0^0 \theta_0^0)^T P^{-T} \tag{55}
\]

\[
\frac{\partial \text{EEB}(P)}{\partial P} \to P^{-T} (P - \theta_0^0 \theta_0^0) P^{-T} \tag{56}
\]

\[
\frac{\partial \mathcal{F}_{\text{EB}}(P)}{\partial P} \to P^{-T} (P - \theta_0^0 \theta_0^0) P^{-T} \tag{57}
\]

almost surely.

Proposition 8 shows that the three pairs, \( N^2 \frac{\partial \text{MSEg}(P)}{\partial P} \) and \( N^2 \frac{\partial \mathcal{F}_{\text{SE}}(P)}{\partial P} \), \( N \frac{\partial \text{MSEy}(P)}{\partial P} \) and \( N \frac{\partial \mathcal{F}_{\text{Sy}}(P)}{\partial P} \), and \( \frac{\partial \text{EEB}(P)}{\partial P} \) and \( \frac{\partial \mathcal{F}_{\text{EB}}(P)}{\partial P} \), have respectively the same limit as \( N \) goes to \( \infty \). This observation motivates to explore if this property also holds for the estimation criteria of these hyperparameter estimators. The answer is affirmative and we have the following result.

Proposition 9 Consider the hyperparameter estimation criteria SUREg (20), SUREy (21), and their corresponding Oracle counterparts MSEg (11), MSEy (12), and EEB (28). Assume that \( P \) is nonsingular and \( \Phi^T \Phi/N \to \Sigma \) almost surely as \( N \to \infty \), where \( \Sigma \) is positive definite. Then we have as \( N \to \infty \)

\[
N^2 (\text{MSEg}(P) - \sigma^2 \text{Tr}((\Phi^T \Phi)^{-1})) \to W_g(P, \Sigma, \theta_0) \tag{58}
\]

\[
N^2 (\mathcal{F}_{\text{SE}}(P) - \sigma^2 \text{Tr}((\Phi^T \Phi)^{-1})) \to W_g(P, \Sigma, \theta_0), \tag{59}
\]

\[
N (\text{MSEy}(P) - n + N) \sigma^2 \to W_g(P, \Sigma, \theta_0), \tag{60}
\]

\[
N (\mathcal{F}_{\text{Sy}}(P) + Y^T \Phi (\Phi^T \Phi)^{-1} \Phi^T Y - 2n \sigma^2) \to W_g(P, \Sigma, \theta_0), \tag{61}
\]

\[
\text{EEB}(P) - (N - n) - (N - n) \log \sigma^2 - \log \det(\Phi^T \Phi) \to W_B(P, \theta_0), \tag{62}
\]

\[
\mathcal{F}_{\text{EB}}(P) + Y^T \Phi (\Phi^T \Phi)^{-1} \Phi^T Y/\sigma^2 - Y^T Y/\sigma^2 \to (N - n) \log \sigma^2 - \log \det(\Phi^T \Phi) \to W_B(P, \theta_0), \tag{63}
\]

almost surely, where

\[
W_g(P, \Sigma, \theta_0) = \sigma^4 \theta_0^T P^{-T} \Sigma^{-2} P^{-1} \theta_0 - 2\sigma^4 \text{Tr}(\Sigma^{-1} P^{-1} \Sigma^{-1}), \tag{64}
\]

\[
W_g(P, \Sigma, \theta_0) = \sigma^4 \theta_0^T P^{-T} \Sigma^{-1} P^{-1} \theta_0 - 2\sigma^4 \text{Tr}(\Sigma^{-1} P^{-1}), \tag{65}
\]

\[
W_B(P, \theta_0) = \theta_0^T P^{-1} \theta_0 + \log \det(P). \tag{66}
\]

Remark 10 For these hyperparameter estimation criteria, \( W_g(P, \Sigma, \theta_0), W_g(P, \Sigma, \theta_0) \) and \( W_B(P, \theta_0) \) contain all information about the asymptotic benefits of regularization: how it depends on any kernel matrix \( P \), any true impulse response vector \( \theta_0 \) and any stationary properties of the input covariance matrix \( \Sigma \).

Proposition 9 enable us to derive asymptotic properties of these hyperparameters estimator for any parameterization \( P(\eta) \) of the kernel matrix. Moreover, it also implies that the estimators \( \hat{\eta}_{\text{SE}}, \hat{\eta}_{\text{Sy}}, \) and \( \hat{\eta}_{\text{EB}} \) possibly share the same limits with their corresponding Oracle counterparts \( \hat{\eta}_{\text{MSEg}}, \hat{\eta}_{\text{MSEy}}, \) and \( \hat{\eta}_{\text{EEB}} \), respectively.

To state the result, we need an extra assumption. It is worth to note that the limit functions \( W_g(P(\eta), \Sigma, \theta_0) \) and \( W_B(P(\eta), \theta_0) \) may not have a unique global minimum, respectively. In this case, the analysis of how minimizing elements of a sequence of functions \( M_N(\eta) \) converge to the minimizing element of the limit function \( \lim M_N(\eta) \), i.e.,

\[
\lim \min_{\eta \in \Omega} M_N(\eta) = \arg \min_{\eta \in \Omega} M_N(\eta), \tag{67}
\]

where \( M_N(\eta) \) denotes any function on the left hand-side of “\( \to \)” in (58) to (63), follows the same idea as for prediction error identification methods, see, e.g. Lemma 8.2 and Theorem 8.2 in Ljung (1999). Accordingly, it is useful in this context to let \( \arg \min \) denote the set of minimizing arguments in case where \( W_g(P(\eta), \Sigma, \theta_0) \) and \( W_B(P(\eta), \theta_0) \) do not have a unique global minimum, respectively:

\[
\arg \min_{\eta \in \Omega} M(\eta) = \{\eta | \eta \in \Omega, M(\eta) = \min_{\eta' \in \Omega} M(\eta')\}, \tag{68}
\]
Theorem 1 Assume that $P(\eta)$ is any parameterization of the kernel matrix such that $P(\eta)$ is positive definite and moreover, $\Phi^T\Phi/N \to \Sigma$ almost surely as $N \to \infty$, where $\Sigma$ is positive definite. Then we have as $N \to \infty$

$$\hat{\eta}_{\text{MSE}g} \to \eta^*_g, \quad \hat{\eta}_{\text{MSk}g} \to \eta^*_g,$$

$$\hat{\eta}_{\text{MSE}y} \to \eta^*_y, \quad \hat{\eta}_{\text{MSky}} \to \eta^*_y,$$

$$\hat{\eta}_{\text{EB}} \to \eta^*_g, \quad \hat{\eta}_{\text{EB}} \to \eta^*_y.$$ 

Remark 11 In contrast with $W_g(P, \Sigma, \theta_0)$ and $W_y(P, \Sigma, \theta_0)$, a unique property of $W_{\text{EB}}(P, \theta_0)$ is that it does not depend on the limit $\Sigma$ of $\Phi^T\Phi/N$. This can to some extent explain why the EB estimator is more robust than the SUREg and SUREy, when $\Phi^T\Phi$ is ill-conditioned. Interested readers can find experimental evidence for this in Pilonetto & Chiuso (2015). However, in contrast with the SUREg and SUREy, the EB estimator is not asymptotically optimal.

Remark 12 The different expressions of the limit functions $W_g(P(\eta), \Sigma, \theta_0), W_y(P(\eta), \Sigma, \theta_0)$, and $W_{\text{EB}}(P(\eta), \theta_0)$ imply that the optimal hyperparameters $\eta^*_g, \eta^*_y, \eta^*_{\text{EB}}$ may be different. To check this, we consider the ridge regression case, where $P = \eta I_n$ with $\eta > 0$. In this case, (69), (70) and (71) become

$$\eta^*_g = \arg \min_{\eta > 0} \frac{\sigma^4}{\eta^2} \sigma^2 \Sigma^2 \theta_0 - 2\sigma^4 \eta - \text{Tr}(\Sigma^{-2}) = \frac{\theta_0^* \Sigma^{-1} \theta_0}{\text{Tr}(\Sigma^{-1})},$$

$$\eta^*_y = \arg \min_{\eta > 0} \frac{\sigma^4}{\eta^2} \sigma^2 \Sigma^2 \theta_0 - 2\sigma^4 \eta - \text{Tr}(\Sigma^{-1}) = \frac{\theta_0^* \Sigma^{-1} \theta_0}{\text{Tr}(\Sigma^{-1})},$$

$$\eta^*_{\text{EB}} = \arg \min_{\eta > 0} \frac{\sigma^4}{\eta^2} \sigma^2 \Sigma^2 \theta_0 - 2\sigma^4 \eta - \text{Tr}(\Sigma^{-1}) = \frac{\theta_0^* \Sigma^{-1} \theta_0}{\text{Tr}(\Sigma^{-1})},$$

which shows that $\eta^*_g, \eta^*_y$ and $\eta^*_{\text{EB}}$ can be different. Clearly, when $\Sigma = dI_n$ with $d > 0$, $\eta^*_g = \eta^*_y = \eta^*_{\text{EB}}$. 

Corollary 2 Assume that $\Phi^T\Phi/N \to dI_n$ almost surely with $d > 0$ and $P(\eta)$ is any positive definite parameterization of the kernel matrix. Then we have

$$\eta^*_g = \eta^*_y = \eta^*_{\text{EB}} = \arg \min_{\eta > 0} \frac{\sigma^4}{\eta^2} \sigma^2 \Sigma^2 \theta_0 - 2\sigma^4 \eta - \text{Tr}(P(\eta)^{-1}) = \text{Tr}(P(\eta)^{-1}),$$

and further $\eta^*_g$ and $\eta^*_y$ are roots of the following system of equations, respectively:

$$\text{Tr}\left(P(\eta)^{-2} (P(\eta) - \theta_0 \theta_0^T) P(\eta)^{-1} \frac{\partial P(\eta)}{\partial \eta_i}\right) = 0, \quad i = 1, \ldots, p,$$

$$\text{Tr}\left(P(\eta)^{-2} (P(\eta) - \theta_0 \theta_0^T) P(\eta)^{-1} \frac{\partial P(\eta)}{\partial \eta_i}\right) = 0, \quad i = 1, \ldots, p.$$
Assume that $\|\Phi^T\Phi/N - \Sigma\| = O_p(\delta_N)$, where $\delta_N \to 0$ as $N \to \infty$ and $P(\eta)$ is any positive definite parameterization of the kernel matrix. Then

$$\|\hat{\eta}_{EEB} - \eta_*^B\| = O_p(1/N), \quad \|\hat{\eta}_{EEB} - \eta_*^B\| = O_p(1/\sqrt{N}),$$

$$\sigma_N = \max \left( O_p(\sigma_N), O_p(1/N) \right),$$

$$\mu_N = \max \left( O_p(\sigma_N), O_p(1/\sqrt{N}) \right).$$

Theorem 2 has the following corollary.

**Corollary 3** Assume that $\|\Phi^T\Phi/N - \Sigma\| = O_p(\delta_N)$, where $\delta_N \to 0$ as $N \to \infty$ and $P(\eta)$ is any positive definite parameterization of the kernel matrix. Then

$$\|\hat{\eta}_{MSEg} - \hat{\eta}_{Sg}\| = O_p(\mu_N).$$

$$\|\hat{\eta}_{MSEy} - \hat{\eta}_{Sy}\| = O_p(\mu_N),$$

$$\|\hat{\eta}_{EEB} - \hat{\eta}_{EEB}\| = O_p(1/\sqrt{N}),$$

where $\mu_N$ is defined in (79).

This corollary shows that the convergence rate of $\|\hat{\eta}_{EEB} - \hat{\eta}_{EEB}\|$ to zero is faster than that of $\|\hat{\eta}_{MSEg} - \hat{\eta}_{Sg}\|$ and $\|\hat{\eta}_{MSEy} - \hat{\eta}_{Sy}\|$ to zero.

### 6 Numerical Simulation

In this section, we illustrate the theoretical results with numerical simulation.

#### 6.1 Test data-bank

The method in Chen et al. (2012); Pillonetto & Chiuso (2015) is used to generate 1000 30th order test systems.
Then for each test system, we consider four different test inputs:

- The first two test inputs are implemented by the MATLAB command `idinput` choosing the bandlimited white Gaussian noise with normalized bands $[0, 0.6]$ and $[0, 1]$, respectively, and denoted by IT1 and IT2, respectively.
- The third and fourth test inputs are the white Gaussian noise of unit variance filtered by a second order rational transfer function $1/(1 - aq^{-1})^2$ with $a$ chosen to be 0.95 and 0.05, respectively, and denoted by IT3 and IT4, respectively.

To generate the data set, we simulate each system with one of the four test inputs to get the output, which is then corrupted by an additive white Gaussian noise. The signal-to-noise ratio (SNR), i.e., the ratio between the variance of the noise-free output and the noise, is uniformly distributed over $[1, 10]$, and is kept same for the four test inputs.

Finally, in order to test the finite sample and asymptotic behavior of the hyperparameter estimators, we consider data sets with different data lengths $N = 500$ and 8000, respectively.

### 6.2 Simulation Setup

The performance of the RLS estimator (6b) is evaluated by the measure of fit (Ljung, 2012) defined as follows:

$$
\text{Fit} = 100 \times \left( 1 - \frac{\|\hat{\theta} - \theta_0\|}{\|\theta_0 - \theta_0\|} \right), \quad \hat{\theta}_0 = \frac{1}{n} \sum_{k=1}^{n} g_k^0
$$

where $n$ is set to 200. This fit is actually to evaluate the RLS estimator in the MSe$g$ sense.

The TC kernel (17) is considered and its hyperparameter $\eta = [c, \alpha]^{T}$ is estimated by using the estimators SUREg (23), SUREy (24), and EB (18), respectively. For reference, we also consider their corresponding Oracle counterparts, i.e., the estimators MSe$g$ (25), MSEy (26), and EEB (27), respectively. The notations $Sg$, $Sy$, $EB$, $MSeg$, $MSEy$, and $EEB$ are used to denote the corresponding simulation results, respectively.

### 6.3 Simulation results

The average fits are given in Table 1. The boxplots of the 1000 fits for IT1 and IT2 are displayed in Figs. 1–2, respectively. The boxplots for IT3 and IT4 are skipped because of their similarity with IT1 and IT2.

### 6.4 Findings

Firstly, for all tested cases and in terms of average accuracy and robustness, the Oracle estimators MSe$g$ and MSEy (not implementable in practice) are better than $Sg$ and $Sy$, respectively, while $EB$ is just a little bit worse than but very close to its Oracle estimator EEB.

| $N$ | MSe$g$ | S$g$ | MSEy | S$y$ | EEB | EB |
|-----|-------|-----|------|-----|-----|----|
| 500 | 86.78 | 83.89 | 86.69 | 85.66 | 86.24 | 85.84 |
| 8000 | 96.57 | 96.49 | 96.56 | 96.49 | 96.38 | 96.35 |

Secondly, we consider the cases with input IT1, where $\Phi^T \Phi$ is very ill-conditioned for both $N = 500$ and $N = 8000$. In this case and in terms of average accuracy and robustness, $Sg$ performs badly because it depends on $(\Phi^T \Phi)^{-1}$. Moreover, $Sy$ is better than $Sg$, but worse than $EB$.

Thirdly, we consider the case with input IT2 and $N = 500$, where $\Phi^T \Phi$ is much better conditioned than the cases with input IT1. In this case and in terms of average accuracy and robustness, $Sg$ behaves much better in contrast with the cases with input IT1. Moreover, $EB$ and $Sy$ are quite close though $EB$ is a little bit better, and they are all better than $Sg$.

Lastly, we consider the case with input IT2 and $N = 8000$, where $\Phi^T \Phi$ is very well-conditioned and in terms of average accuracy and robustness, $Sg$ behaves much better in contrast with all the other cases, and performs as well as $Sy$ and better than $EB$. Moreover, $Sg$ and $Sy$ are very close to the corresponding Oracle estimators MSe$g$ and MSEy. These observations coincide with the results found in Theorem 1 and Corollary 2. Namely, $Sg$ and $Sy$ are asymptotically optimal but $EB$ is not in the MSe$g$/MSEy senses and moreover, $Sg$ and $Sy$ give the same optimal hyperparameter estimate as their Oracle counterparts MSe$g$ and MSEy, because the limit $\Sigma = I_n$ of $\Phi^T \Phi / N$ as $N \to \infty$. It can also be seen from Figs. 1 and 2 that the boxplots of EEB and $EB$ are closer than that of MSe$g$ and S$g$ and that of MSEy and S$y$. This observation coincides with the result found in Corollary 3, that is, the convergence rate of $\|\tilde{\eta}_{EB} - \tilde{\eta}_{EB} \|$ to zero is faster than that of $\|\tilde{\eta}_{MSeg} - \tilde{\eta}_{Sg} \|$ and $\|\tilde{\eta}_{MSEy} - \tilde{\eta}_{Sy} \|$ to zero.

### 7 Conclusions

Kernel matrix design and hyperparameter estimation are two core issues for the kernel based regularization methods. In contrast with the former issue, there are few results reported for the latter issue. In this paper, we focused on the latter issue and studied the properties of
several hyperparameter estimators including the empirical Bayes (EB) estimator, two Stein’s unbiased risk estimators (SURE) and their corresponding Oracle counterparts, with an emphasis on the asymptotic properties of these hyperparameter estimators. Our major results are the following:

- The first order optimality conditions of these hyperparameter estimators are put in similar forms that better expose their relation and lead to several insights on these hyperparameter estimators.
- As the number of data goes to infinity, the two SUREs converge to the best hyperparameter minimizing the corresponding mean square error, respectively, while the widely more used EB estimator converges to another best hyperparameter minimizing the expectation of the EB estimation criterion. This indicates that the two SUREs are asymptotically optimal but the EB estimator is not.
- The convergence rate of two SUREs is slower than that of the EB estimator, and moreover, unlike the two SUREs, the EB estimator is independent of the convergence rate of $\Phi^T\Phi/N$ to its limit, where $\Phi$ is the regression matrix and $N$ is the number of data.

The results enhance our understanding about these hyperparameter estimators and is one step forward towards the goal of building a theory of the hyperparameter estimation for the kernel-based regularization methods.

**Appendix A**

Appendix A contains the proof of the results in the paper, for which the technical lemmas are placed in Appendix B. The proofs of Propositions 1, 5, 6, 7, and 8 and Corollaries 1, 2, and 3 are straightforward and thus omitted.

### A.1 Proof of Proposition 2

Under the setting $P^{-1} = \beta A/\sigma^2$, the MSEg (11) of the RLS estimator (6b) is a function of $\beta$ for a given $A$:

$$\text{MSEg}(\beta) = \text{Bias}(\beta) + \text{Var}(\beta)$$

where the formula $\frac{dC^{-1}(\beta)}{d\beta} = -C^{-1}(\beta)\frac{dC(\beta)}{d\beta}C^{-1}(\beta)$ for an invertible matrix $C(\beta)$ is used. Then we have

$$\left.\frac{dBias(\beta)}{d\beta}\right|_{\beta \to 0^+} = 0$$

$$\left.\frac{dVar(\beta)}{d\beta}\right|_{\beta \to 0^+} = -2\sigma^2\text{Tr}((\Phi^T\Phi)^{-1}A(\Phi^T\Phi)^{-1}) < 0$$

where Lemma B2 in Appendix B is used. Therefore, we have $\frac{d\text{MSEg}(\beta)}{d\beta}\bigg|_{\beta \to 0^+} < 0$. This means that $\text{MSEg}(\beta) < \text{MSEg}(0)$ in some small right neighborhood of the origin $\beta = 0$.

Under the assumption that $A$ is positive definite, denote

$$M(\beta) \triangleq E(\hat{\theta}^R - \theta_0)(\hat{\theta}^R - \theta_0)^T.$$  

We first prove $M(0) - M(\beta) > 0$ for $0 < \beta < 2\sigma^2/(\theta_0^T A \theta_0)$. A straightforward calculation gives

$$M(0) - M(\beta) = \sigma^2(\Phi^T\Phi)^{-1} - \sigma^2(\Phi^T\Phi + \beta A)^{-1}\Phi^T(\Phi^T\Phi + \beta A)^{-1}$$

$$- \beta^2(\Phi^T\Phi + \beta A)^{-1}A\theta_0\theta_0^T A(\Phi^T\Phi + \beta A)^{-1}$$

$$= \beta(\Phi^T\Phi + \beta A)^{-1}(\sigma^2[2A + \beta A(\Phi^T\Phi)^{-1}A] - \beta A\theta_0\theta_0^T A \times (\Phi^T\Phi + \beta A)^{-1}.$$

As a result, to prove $M(0) - M(\beta) > 0$, it suffices to show

$$\sigma^2[2A + \beta A(\Phi^T\Phi)^{-1}A] - \beta A\theta_0\theta_0^T A > 0 \quad (A.4)$$

which is true if $2\sigma^2I_n - \beta A^{1/2}\theta_0\theta_0^T A^{1/2} > 0$ due to

$$\sigma^2[2A + \beta A(\Phi^T\Phi)^{-1}A] - \beta A\theta_0\theta_0^T A$$

$$> 2\sigma^2 A - \beta A\theta_0\theta_0^T A$$

$$= A^{1/2}(2\sigma^2 I_n - \beta A^{1/2}\theta_0\theta_0^T A^{1/2})A^{1/2} > 0.$$  

In addition, the eigenvalues of $A^{1/2}\theta_0\theta_0^T A^{1/2}$ are $\theta_0^T A \theta_0$ and zero (with multiplicity $n-1$). This shows $2\sigma^2 I_n - \beta A^{1/2}\theta_0\theta_0^T A^{1/2} > 0$ for $0 < \beta < 2\sigma^2/(\theta_0^T A \theta_0)$.

Note that $\text{MSEg}(\beta) = \text{Tr}(M(\beta))$. One has proved that $M(0) - M(\beta)$ is positive definite if $0 < \beta < 2\sigma^2/(\theta_0^T A \theta_0)$, so we have $\text{MSEg}(0) - \text{MSEg}(\beta) = \text{Tr}(M(0) - M(\beta)) > 0$.

The proof for the MSEy (12) is similar to that for the MSEg (11) by using the connection (10).

**Remark 13** When $\beta \to \infty$, from the MSEg (A.1) we have

1. $\text{Bias}(\beta) \to \theta_0^T \theta_0$ and $\left.\frac{dBias(\beta)}{d\beta}\right|_{\beta \to 0^+} = 0,$
2. $\text{Var}(\beta) \to 0$ and $\left.\frac{dVar(\beta)}{d\beta}\right|_{\beta \to 0^+} = 0,$
3. $\text{MSEg}(\beta) \to \theta_0^T \theta_0$ and $\left.\frac{d\text{MSEg}(\beta)}{d\beta}\right|_{\beta \to 0^+} = 0.$
A.2 Proof of Proposition 3

We first prove (34). Using the formulas (B.40) and (B.41) derives that

\[
\frac{\partial \mathcal{F}_{EB}(P)}{\partial P} = \sum_{i,j} \left( - Q^{-T} Y Y^T Q^{-T} + Q^{-T} \right)_{ij} \frac{\partial Q_{ij}}{\partial P} = - \Phi^T Q^{-T} Y Y^T Q^{-T} \Phi + \Phi^T Q^{-T} \Phi.
\]

To prove (32), let us set

\[
\mathcal{F}_{S_1}(P) = \sigma^4 Y^T Q^{-T} \Phi (\Phi^T \Phi)^{-2} \Phi^T Q^{-1} Y
\]

\[
\mathcal{F}_{S_2}(P) = \sigma^2 \text{Tr}(2R^{-1} - (\Phi^T \Phi)^{-1}).
\]

By (B.39) and (B.42), the derivative of \( \mathcal{F}_{S_1}(P) \) is

\[
\frac{\partial \mathcal{F}_{S_1}(P)}{\partial P} = \sigma^4 \sum_{i,j} \left( 2i \Phi (\Phi^T \Phi)^{-2} \Phi^T Q^{-1} Y Y^T \right)_{ij} \frac{\partial (Q^{-1})_{ij}}{\partial P} = -2\sigma^4 \sum_{i,j} (\Phi(\Phi^T \Phi)^{-2} \Phi^T Q^{-1} Y Y^T)_{ij} \Phi^T Q^{-T} J_{ij} Q^{-T} \Phi
\]

\[= -2\sigma^4 \Phi^T Q^{-T} \Phi (\Phi^T \Phi)^{-2} \Phi^T Q^{-1} Y Y^T Q^{-T} \Phi. \tag{A.5} \]

and using (B.54) implies the derivative of \( \mathcal{F}_{S_2}(P) \)

\[
\frac{\partial \mathcal{F}_{S_2}(P)}{\partial P} = 2\sigma^2 \sum_{i=1}^{n} \frac{\partial (R^{-1})_{ii}}{\partial P} = 2\sigma^4 P^{-T} R^{-T} R^{-T} P^{-T} = 2\sigma^4 H^{-T} H^{-T}. \tag{A.6} \]

Combining (A.5) with (A.6) derives (32).

Finally, let us prove (33). Similarly, by using (B.52), we write (21) as

\[
\mathcal{F}_{Sy}(P) = \sigma^4 Y^T Q^{-T} Q^{-1} Y + (2\sigma^2 N - 2\sigma^4 \text{Tr}(Q^{-1})) = \mathcal{F}_{Sy_1}(P) + \mathcal{F}_{Sy_2}(P).
\]

By (B.39) and (B.53), the derivative of \( \mathcal{F}_{Sy_1}(P) \) is

\[
\frac{\partial \mathcal{F}_{Sy_1}(P)}{\partial P} = \sigma^4 \sum_{i,j} \left( 2Q^{-1} Y Y^T \right)_{ij} \frac{\partial (Q^{-1})_{ij}}{\partial P} = -2\sigma^4 \sum_{i,j} (Q^{-1} Y Y^T)_{ij} \Phi^T Q^{-T} J_{ij} Q^{-T} \Phi
\]

\[= -2\sigma^4 \Phi^T Q^{-T} Q^{-1} Y Y^T Q^{-T} \Phi. \tag{A.7} \]

and by using (B.43) the derivative of \( \mathcal{F}_{Sy_2}(P) \) is

\[
\frac{\partial \mathcal{F}_{Sy_2}(P)}{\partial P} = -2\sigma^4 \sum_{i=1}^{n} \frac{\partial (Q^{-1})_{ii}}{\partial P} = 2\sigma^4 \Phi^T Q^{-T} Q^{-T} \Phi. \tag{A.8} \]

The equations (A.7) and (A.8) implies (33).

A.3 Proof of Proposition 4:

It follows from (6b) that

\[
\tilde{\theta}^T - \theta_0 = R^{-1} \Phi^T Y - \theta_0 = -\sigma^2 R^{-1} P^{-1} \theta_0 + R^{-1} \Phi^T V
\]

\[= -\sigma^2 H^{-1} \theta_0 + R^{-1} \Phi^T V,
\]

which derives

\[
\text{MSE}_g(P) = \sigma^4 \theta_0^T H^{-T} H^{-1} \theta_0 + \sigma^2 \text{Tr}(R^{-1} \Phi^T \Phi R^{-T}) = \text{MSE}_g1(P) + \text{MSE}_g2(P).
\]

For the term \( \text{MSE}_g1(P) \), using the formulas (B.39) and (B.42) gives

\[
\frac{\partial \text{MSE}_g1(P)}{\partial P} = \sigma^4 \sum_{i,j} \left( 2H^{-1} \theta_0 \theta_0^T \right)_{ij} \frac{\partial (R^{-1})_{ij}}{\partial P} = \sigma^4 \sum_{i,j} \left( 2H^{-1} \theta_0 \theta_0^T \right)_{ij} (-H^{-1} J_{ij} H^{-1} \Phi^T \Phi)
\]

\[= -2\sigma^4 H^{-1} H^{-1} \theta_0 \theta_0^T H^{-T} \Phi^T \Phi = -2\sigma^4 H^{-1} H^{-1} \theta_0 \theta_0^T H^{-T} \Phi^T Q^{-T} \Phi. \tag{A.9} \]

By using the formulas (B.44) and (B.54), one derives

\[
\frac{\partial \text{MSE}_g2(P)}{\partial P} = \sigma^2 \sum_{i,j} \left( 2R^{-1} \Phi^T \Phi \right)_{ij} \frac{\partial (R^{-1})_{ij}}{\partial P} = \sigma^2 \sum_{i,j} \left( 2R^{-1} \Phi^T \Phi \right)_{ij} (\sigma^2 P^{-T} R^{-T} J_{ij} R^{-T} P^{-T})
\]

\[= 2\sigma^4 P^{-T} R^{-T} R^{-T} P^{-T} = 2\sigma^4 H^{-T} H^{-1} P \Phi^T Q^{-T} \Phi. \tag{A.10} \]

Combining (A.9) with (A.10) implies the conclusion (36).

In the following, we intend to prove (37). Let us set

\[
\text{MSE}_{\gamma_1}(P) = \| \Phi P \Phi^T Q^{-1} \Phi \theta_0 - \Phi \theta_0 \|^2 + 2N \sigma^2
\]

\[= \sigma^4 \theta_0^T \Phi^T Q^{-1} \Phi^T \Phi \theta_0 + 2N \sigma^2
\]

\[
\text{MSE}_{\gamma_2}(P) = \sigma^2 \text{Tr}(\Phi P \Phi^T Q^{-1} \Phi^T \Phi P \Phi^T \Phi)
\]

\[= \sigma^2 \text{Tr}((I_N - \sigma^2 Q^{-1})(I_N - \sigma^2 Q^{-T})).
\]

By using (B.39) and (B.53), one obtains

\[
\frac{\partial \text{MSE}_{\gamma_1}(P)}{\partial P} = \sigma^4 \sum_{i,j} \left( 2Q^{-1} \Phi \theta_0 \theta_0^T \Phi^T \right)_{ij} \frac{\partial (Q^{-1})_{ij}}{\partial P}
\]

\[= 2\sigma^4 Q^{-1} \Phi \theta_0 \theta_0^T \Phi^T (\Phi^T Q^{-T} J_{ij} Q^{-T} \Phi)
\]

\[= -2\sigma^4 \Phi^T Q^{-T} Q^{-1} \Phi \theta_0 \theta_0^T \Phi^T Q^{-T} \Phi. \tag{A.11} \]

For the term \( \text{MSE}_{\gamma_2}(P) \), using the formulas (B.44) and (B.54) derives

\[
\frac{\partial \text{MSE}_{\gamma_2}(P)}{\partial P} = \sigma^2 \sum_{i,j} \left( 2(I_N - \sigma^2 Q^{-1}) \right)_{ij} \frac{\partial (-\sigma^2 Q^{-1})_{ij}}{\partial P}
\]
\[ = 2\sigma^2 \sum_{i,j} (I_N - \sigma^2 Q^{-1})_{ij} (\sigma^2 \Phi^T Q^{-T} J_{ij} Q^{-T} \Phi) \]
\[ = 2\sigma^4 \Phi^T Q^{-T} (I_N - \sigma^2 Q^{-1}) Q^{-T} \Phi \]
\[ = 2\sigma^4 \Phi^T Q^{-T} Q^{-1} \Phi P \Phi^T Q^{-T} \Phi. \]  
(A.12)

Combining (A.11) with (A.12) implies the assertion (37).

At last, we prove (38), which is derived by

\[
\frac{\partial \text{EEB}(P)}{\partial P} = \sum_{i,j} \left( -Q^{-T} \Phi_0 \theta_0^T \Phi^T Q^{-T} - \sigma^2 Q^{-T} \right)
\]
\[ + \frac{\partial Q_{ij}}{\partial P} \]
\[ = -\Phi^T Q^{-T} \Phi_0 \theta_0^T \Phi^T Q^{-T} \Phi + \Phi^T Q^{-T} (I_N - \sigma^2 Q^{-T}) \Phi \]
\[ = -\Phi^T Q^{-T} \Phi_0 \theta_0^T \Phi^T Q^{-T} \Phi + \Phi^T Q^{-T} \Phi P \Phi^T Q^{-T} \Phi \]

in terms of (B.40), (B.41), (B.43) and (B.52).

### A.4 Proof of Proposition 9

Under the assumptions that \( \Phi^T \Phi / N \to \Sigma > 0 \) and the white noise \( v(t) \), we have \( (\Phi^T \Phi)^{-1} = O_p(1/N) \to 0 \), \( S^{-1} \to P^{-1}, NR^{-1} \to \Sigma^{-1}, R^{-1} \Phi^T \Phi \to I_n \), and \( \hat{\theta} \to \theta_0 \) almost surely as \( N \to \infty \).

Let us first prove (58). Using (39), we rewrite \( \text{MSE}_g(P) \) in (11) as follows:

\[
\text{MSE}_g(P) = \sigma^4 \theta_0^T S^{-T} (\Phi^T \Phi)^{-2} S^{-1} \theta_0
\]
\[ + \sigma^2 \text{Tr}(R^{-1} \Phi^T \Phi R^{-T}). \]

Noting \( \text{Tr}(\Sigma^{-1} P^{-1} \Sigma^{-1}) = \text{Tr}(\Sigma^{-1} P^{-1} \Sigma^{-1}) \) and

\[
N^2(R^{-1} \Phi^T \Phi R^{-T} - (\Phi^T \Phi)^{-1})
\]
\[ = -\sigma^2 N^2 R^{-1}(P^{-1} + P^{-T} + \sigma^2 P^{-1} (\Phi^T \Phi)^{-1} P^{-T}) R^{-T}
\]
\[ \to -\sigma^2 \Sigma^{-1}(P^{-1} + P^{-T}) \Sigma^{-1} \]  
(A.13)
yields that

\[
N^2(\text{MSE}_g(P) - \sigma^2 \text{Tr}((\Phi^T \Phi)^{-1}))
\]
\[ = \sigma^4 \theta_0^T S^{-T} (N^2 (\Phi^T \Phi)^{-2}) S^{-1} \theta_0
\]
\[ + \sigma^2 N^2 \text{Tr}(R^{-1} \Phi^T \Phi R^{-T} - (\Phi^T \Phi)^{-1})
\]
\[ \to \sigma^4 \theta_0^T P^{-T} \Sigma^{-2} P^{-1} \theta_0 - 2 \sigma^4 \text{Tr}(\Sigma^{-1} P^{-1} \Sigma^{-1})
\]
\[ = W_g(P, \Sigma, \theta_0). \]  
(A.14)

To prove (59), note that the first term of \( \mathcal{F}_g(P) \) can be rewritten as \( \sigma^4(\hat{\theta} \Sigma^{LS})^T S^{-T} (\Phi^T \Phi)^{-2} S^{-1} \hat{\theta} \Sigma^{LS} \). Thus one derives

\[
N^2(\mathcal{F}_g(P) - \sigma^2 \text{Tr}((\Phi^T \Phi)^{-1}))
\]
\[ = \sigma^4(\hat{\theta} \Sigma^{LS})^T S^{-T} N^2 (\Phi^T \Phi)^{-2} S^{-1} \hat{\theta} \Sigma^{LS}
\]
\[ + 2 \sigma^2 N^2 \text{Tr}(R^{-1} \Phi^T \Phi R^{-T} - (\Phi^T \Phi)^{-1})
\]
\[ \to W_g(P, \Sigma, \theta_0) \]  
(A.15)

where we use the limit

\[
N^2(R^{-1} - (\Phi^T \Phi)^{-1}) = -\sigma^2 N R^{-1} P^{-1} N(\Phi^T \Phi)^{-1}
\]
\[ \to -\sigma^2 \Sigma^{-1} P^{-1} \Sigma^{-1}. \]

Similarly, we can rewrite \( \text{MSE}_y(P) \) as

\[
\text{MSE}_y(P) = \sigma^4 \theta_0^T S^{-T} (\Phi^T \Phi)^{-1} S^{-1} \theta_0 + N \sigma^2
\]
\[ + \text{Tr}(R^{-1} \Phi^T \Phi R^{-T} \Phi^T \Phi - I_n) \]
\[ \to W_g(P, \Sigma, \theta_0) \]  
(A.16)

and hence the assertion (60) is proved by

\[
N(\text{MSE}_y(P) - (n + N) \sigma^2)
\]
\[ = \sigma^4 \theta_0^T S^{-T} N(\Phi^T \Phi)^{-1} S^{-1} \theta_0
\]
\[ + \sigma^2 N \text{Tr}(R^{-1} \Phi^T \Phi R^{-T} \Phi^T \Phi - I_n) \]  
(A.17)

where we use the formulas

\[
N(R^{-1} \Phi^T \Phi R^{-T} \Phi^T \Phi - I_n)
\]
\[ = -\sigma^2 N R^{-1}[P^{-1} + P^{-T} + \sigma^2 P^{-1} (\Phi^T \Phi)^{-1} P^{-T}] R^{-T} \Phi^T \Phi
\]
\[ \to -\sigma^2 \Sigma^{-1}(P^{-1} + P^{-T}) \]
\[ \text{and } \text{Tr}(\Sigma^{-1} P^{-1}) = \text{Tr}(P^{-T} \Sigma^{-1}) = \text{Tr}(\Sigma^{-1} P^{-T}). \]

To prove (61), we need some identities. A straightforward calculation shows that

\[
Q^T(I_N - \Phi(\Phi^T \Phi)^{-1} \Phi^T) Q = \sigma^4(I_N - \Phi(\Phi^T \Phi)^{-1} \Phi^T).
\]

This means that

\[
\sigma^4 Q^{-T}(I_N - \Phi(\Phi^T \Phi)^{-1} \Phi^T) Q^{-1} = I_N - \Phi(\Phi^T \Phi)^{-1} \Phi^T
\]

and hence we derive

\[
\sigma^4 Y^T Q^{-T} Q^{-1} Y + Y^T \Phi(\Phi^T \Phi)^{-1} \Phi^T Y - Y^T Y
\]
\[ = \sigma^4 Y^T Q^{-T} (\Phi^T \Phi)^{-1} \Phi^T Q^{-1} Y. \]

It follows from (B.49) and (B.52) that

\[
N \left[ \mathcal{F}_g(P) + Y^T \Phi(\Phi^T \Phi)^{-1} \Phi^T Y - Y^T Y - 2n \sigma^2 \right]
\]
\[ = N \left[ \sigma^4 Y^T Q^{-T} (\Phi^T \Phi)^{-1} \Phi^T Q^{-1} Y + 2 \sigma^2 \text{Tr}(R^{-1} \Phi^T \Phi - I_n) \right]
\]
\[ = N \left[ \sigma^4 (\hat{\theta} \Sigma^{LS})^T S^{-T} (\Phi^T \Phi)^{-1} S^{-1} \hat{\theta} \Sigma^{LS} + 2 \sigma^2 \text{Tr}(R^{-1} \Phi^T \Phi - I_n) \right]
\]
\[ \to W_g(P, \Sigma, \theta_0) \]  
(A.18)

where we use the limit

\[
N(R^{-1} \Phi^T \Phi - I_n) = -\sigma^2 N R^{-1} P^{-1} \to -\sigma^2 \Sigma^{-1} P^{-1}. \]

Similarly, we need two identities to prove (62). Using the Sylvester’s determinant identity \( \det(I_N + AB) = \det(I_N + BA) \) derives

\[
\det(Q) = \sigma^2(N - n) \det(\Phi^T \Phi) \det(P + \sigma^2(\Phi^T \Phi)^{-1})
\]
which implies
\[
\log \det(Q) - (N - n) \log \sigma^2 - \log \det(\Phi^T \Phi) = \\
= \log \det(S) \to \log \det(P). \tag{A.19}
\]
Starting with the identity \( I_N = \sigma^2 Q^{-1} + \Phi P \Phi^T Q^{-1} \) gives
\[
\sigma^2 \text{Tr}(Q^{-1}) = N - \text{Tr}(\Phi P \Phi^T Q^{-1}) = \\
= N - \text{Tr}(R^{-1} \Phi^T \Phi) \to N - n.
\]
Therefore, the limit (62) is proved by
\[
\begin{align*}
\text{EEB}(P) - (N - n) \log \sigma^2 &- \log \det(\Phi^T \Phi) \\
= \theta_0^T S^{-1} \theta_0 + (\sigma^2 \text{Tr}(Q^{-1}) - (N - n)) \\
&+ \log \det(Q) - (N - n) \log \sigma^2 - \log \det(\Phi^T \Phi) \\
&\to \theta_0^T \sigma^2 P^{-1} \theta_0 + \log \det(P) = W_B(P, \theta_0).
\end{align*}
\tag{A.20}
\]
At last, we finish the proof by checking (63). The identity
\[
Q(I_N - \Phi (\Phi^T \Phi)^{-1} \Phi^T) / \sigma^2 = I_N - \Phi (\Phi^T \Phi)^{-1} \Phi^T
\]
implies that
\[
Y^T Q^{-1} Y + Y^T \Phi (\Phi^T \Phi)^{-1} \Phi^T Y / \sigma^2 - Y^T Y / \sigma^2 = \\
= Y^T Q^{-1} (\Phi^T \Phi)^{-1} \Phi^T Y. \tag{A.21}
\]
It follows from (A.19), (A.21), and (B.49) that
\[
\begin{align*}
\mathcal{F}_{\text{EEB}}(P) + Y^T \Phi (\Phi^T \Phi)^{-1} \Phi^T Y / \sigma^2 &- Y^T Y / \sigma^2 \\
= (N - n) \log \sigma^2 - \log \det(\Phi^T \Phi) \\
= Y^T Q^{-1} Y + Y^T \Phi (\Phi^T \Phi)^{-1} \Phi^T Y / \sigma^2 - Y^T Y / \sigma^2 \\
&+ \log \det(Q) - (N - n) \log \sigma^2 - \log \det(\Phi^T \Phi) \\
&\to W_B(P, \theta_0).
\end{align*}
\tag{A.22}
\]

### A.5 Proof of Theorem 1

Firstly, we prove \( \hat{\eta}_{\text{MSEg}} \to \eta^*_g \) as \( N \to \infty \). Define
\[
\underline{\text{MSEg}}_g(P) \triangleq N^2 \left( \text{MSEg}(P) - \sigma^2 \text{Tr}((\Phi^T \Phi)^{-1}) \right). \tag{A.23}
\]
Clearly, we have \( \hat{\eta}_{\text{MSEg}} \) also minimizes \( \underline{\text{MSEg}}_g(P(\eta)) \), i.e.,
\[
\hat{\eta}_{\text{MSEg}} = \arg\min_{\eta \in \Omega} \underline{\text{MSEg}}_g(P(\eta)).
\]
Under Assumption 1, there exists a compact set
\[
\Omega \subset \Omega \tag{A.24}
\]
containing \( \eta^*_g \) such that \( 0 < d_1 \leq \|P(\eta)\| \leq d_2 < \infty \) for all \( \eta \in \Omega \). Then by Lemma B4 in Appendix B, to prove \( \hat{\eta}_{\text{MSEg}} \to \eta^*_g \) as \( N \to \infty \), it suffices to show that \( \underline{\text{MSEg}}_g(P(\eta)) \) converges to \( W_g(P(\eta), \Sigma, \theta_0) \) almost surely and uniformly in \( \Omega \), as \( N \to \infty \).

It follows from (A.14) and (A.13) that
\[
\underline{\text{MSEg}}_g(P(\eta)) - W_g(P, \Sigma, \theta_0) = \sigma^4 Z_1 + 2 \sigma^4 \text{Tr}(Z_2),
\tag{A.25}
\]
where
\[
\begin{align*}
Z_1 &= \theta_0^T S^{-T} (N^2 (\Phi^T \Phi)^{-2}) S^{-1} \theta_0 \\
&- \theta_0^T P^{-T} \Sigma^{-2} P^{-1} \theta_0 \tag{A.26}
\end{align*}
\]
For the term \( Z_1 \), we have
\[
Z_1 = \theta_0^T (S^{-T} - P^{-T}) (N^2 (\Phi^T \Phi)^{-2}) S^{-1} \theta_0 \\
+ \theta_0^T P^{-T} (N^2 (\Phi^T \Phi)^{-2} - \Sigma^{-2}) S^{-1} \theta_0 \\
+ \theta_0^T P^{-T} \Sigma^{-2} (S^{-1} - P^{-1}) \theta_0
\tag{A.27}
\]
where
\[
\begin{align*}
S^{-1} - P^{-1} &= -\sigma^2 S^{-1} (\Phi^T \Phi)^{-1} P^{-1}.
\end{align*}
\tag{A.28}
\]
Note that \( \Phi^T \Phi / N \to \Sigma \) implies that \( \|N (\Phi^T \Phi)^{-1}\| = O_p(1) \). Then further noting that \( d_1 \leq \|P(\eta)\| \leq d_2 \) and \( \|N^{-1}\| < \|(P(\eta))^{-1}\| \leq 1/d_1 \) for \( \eta \in \Omega \), we have \( Z_1 \) converges to zero almost surely and uniformly in \( \Omega \). For the term \( Z_2 \), we have
\[
\Sigma^{-1} P^{-1} - N^2 R^{-1} P^{-1} R^{-T} \\
= (\Sigma^{-1} - N^2 R^{-1}) P^{-1} \Sigma^{-1} + N^2 R^{-1} P^{-1} (\Sigma^{-1} - N R^{-T}).
\]
Noting \( N R^{-1} \to \Sigma^{-1} \) and \( \|N R^{-1} - \Sigma^{-1}\| = O_p(1) \) yields that \( Z_2 \) converges to zero almost surely and uniformly in \( \Omega \). Finally, by noting \( (\Phi^T \Phi)^{-1} \to 0 \) as \( N \to \infty \), it is easy to see that \( Z_2 \) also converges to zero almost surely and uniformly. Making use of these facts shows that \( \underline{\text{MSEg}}_g(P(\eta)) \) converges to \( W_g(P(\eta), \Sigma, \theta_0) \) almost surely and uniformly in \( \Omega \) and hence, by Lemma B4, \( \hat{\eta}_{\text{MSEg}} \to \eta^*_g \) as \( N \to \infty \) almost surely.

Secondly, we prove that \( \hat{\eta}_g \to \eta^*_g \) as \( N \to \infty \) and the proof is similar to that of \( \hat{\eta}_{\text{MSEg}} \to \eta^*_g \) as \( N \to \infty \). Define
\[
\underline{\mathcal{F}}_g(P(\eta)) \triangleq N^2 (\underline{\mathcal{F}}_g(P(\eta)) - \sigma^2 \text{Tr}((\Phi^T \Phi)^{-1})).
\tag{A.29}
\]
Then, we have
\[
\hat{\eta}_g = \arg\min_{\eta \in \Omega} \underline{\mathcal{F}}_g(P(\eta)).
\tag{A.29}
\]
It follows from (A.15) that
\[
\begin{align*}
\underline{\mathcal{F}}_g(P(\eta)) - W_g(P, \Sigma, \theta_0) &= \sigma^4 Z'_1 + 2 \sigma^4 \text{Tr}(Z'_2), \\
Z'_1 &= (\hat{\theta}^L)^T S^{-T} N^2 (\Phi^T \Phi)^{-2} S^{-1} \hat{\theta}^L - \theta_0^T P^{-T} \Sigma^{-2} P^{-1} \theta_0 \\
Z'_2 &= \Sigma^{-1} P^{-1} \Sigma^{-1} - N^2 R^{-1} P^{-1} N (\Phi^T \Phi)^{-1}. \\
\end{align*}
\]
For the terms \( Z'_1 \) and \( Z'_2 \), we have
\[
\begin{align*}
Z'_1 &= (\hat{\theta}^L - \theta_0)^T S^{-T} N^2 (\Phi^T \Phi)^{-2} S^{-1} \hat{\theta}^L \\
&+ \theta_0^T (S^{-T} - P^{-T}) N^2 (\Phi^T \Phi)^{-2} S^{-1} \hat{\theta}^L
\end{align*}
\]
+ \theta_0^T P^{-T} (N^2(\Phi^T \Phi)^{-2} - \Sigma^{-2}) S^{-1} \delta \Theta
+ \theta_0^T P^{-T} \Sigma^{-2} (S^{-1} - P^{-1}) \delta \Theta
+ \theta_0^T P^{-T} \Sigma^{-2} - P^{-1} \delta \Theta
Z'_2 = (\Sigma^{-1} - NR^{-1}) P^{-1} \Sigma^{-1}
+ NR^{-1} P^{-1} (\Sigma^{-1} - N(\Phi^T \Phi)^{-1})
\tag{A.30}
\end{align*}

Then, noting that $\delta \Theta \to 0$, $S^{-1} \to P^{-1}$, $N(\Phi^T \Phi)^{-1} \to \Sigma^{-1}$, $NR^{-1} \to \Sigma^{-1}$ almost surely as $N \to \infty$, and

$$
||NR^{-1}|| = O_p(1), ||\delta \Theta|| = O_p(1), \text{ and } d_1 \leq ||P(\eta)|| \leq d_2, ||S(\eta)^{-1}|| < ||(P(\eta)^{-1}|| \leq 1/d_1, \text{ for } \eta \in \Omega, \text{ one can show that each term of } (A.30) \text{ and } (A.31), \text{ and thus both } Z'_1 \text{ and } Z'_2 \text{ converge to zero almost surely and uniformly in } \Omega. \text{ Therefore, } \mathcal{F}_{Sg}(P(\eta)) \text{ converges to } W_g(\Sigma, \theta_0) \text{ almost surely and uniformly in } \Omega. \text{ It then follows from Lemma B4 that } \hat{\eta}_{Sg} \to \eta^*_g \text{ almost surely as } N \to \infty.\label{eq:asymptotic}
$$

The proof of (73) and (74) can be done similarly and thus is omitted. The first order optimality conditions of $\eta^*_g, \eta^*_s$, and $\eta^*_g$ can be derived in a similar way as Proposition 4 and thus is omitted. This completes the proof.

### A.6 Proof of Theorem 2

We first prove that $||\hat{\eta}_{\text{MSEg}} - \eta^*_g|| = O_p(\omega N)$.

Noting (A.14), the i-th elements of the gradient vectors of $	ext{MSEg}(P(\eta))$ and $W_g(\eta, \Sigma, \theta_0)$ with respect to $\eta$ are, respectively, for $1 \leq i \leq p$,

$$
\frac{\partial \text{MSEg}(P(\eta))}{\partial \eta_i} = 2\sigma^4 N^2 \theta_0^T S^{-T}(\Phi^T \Phi)^{-2} \frac{\partial S^{-1}}{\partial \eta_i} \theta_0
+ 2\sigma^2 N^2 Tr\left(\frac{\partial R^{-1}}{\partial \eta_i} (\Phi^T \Phi) R^{-T}\right)
\frac{\partial W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta_i} = 2\sigma^4 \theta_0^T P^{-T} \Sigma^{-2} \frac{\partial P^{-1}}{\partial \eta_i} \theta_0
- 2\sigma^4 Tr\left(\Sigma^{-1} \frac{\partial P^{-1}}{\partial \eta_i} \Sigma^{-1}\right).
\tag{A.32}
$$

Using the identity $\frac{\partial R^{-1}}{\partial \eta_i} = -R^{-1} \frac{\partial R}{\partial \eta_i} R^{-1} = -\sigma^2 R^{-1} \frac{\partial P^{-1}}{\partial \eta_i} R^{-1}$, we see their difference is

$$
\frac{\partial \text{MSEg}(P(\eta))}{\partial \eta_i} - \frac{\partial W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta_i} = 2\sigma^4 (\Upsilon_1 + \text{Tr}(\Upsilon_2)),
$$

where

$$
\Upsilon_1 = \theta_0^T S^{-T} (N^2(\Phi^T \Phi)^{-2}) \frac{\partial S^{-1}}{\partial \eta_i} \theta_0
- \theta_0^T P^{-T} \Sigma^{-2} \frac{\partial P^{-1}}{\partial \eta_i} \theta_0,
\Upsilon_2 = \Sigma^{-1} \frac{\partial P^{-1}}{\partial \eta_i} \Sigma^{-1} - NR^{-1} \frac{\partial P^{-1}}{\partial \eta_i} R^{-1} \Phi^T \Phi NR^{-T}.
$$

Noting $||N(\Phi^T \Phi)^{-1} - \Sigma^{-1}|| = O_p(\delta N)$, $||S^{-1} - P^{-1}|| = O_p(1/N)$, $||\frac{\partial S^{-1}}{\partial \eta_i} - \frac{\partial P^{-1}}{\partial \eta_i}|| = O_p(1/N)$, $||\frac{\partial \Phi^T \Phi}{\partial \eta_i}|| = O_p(1/N)$, $||\frac{\partial \Upsilon_1}{\partial \eta_i} - \frac{\partial \Upsilon_2}{\partial \eta_i}|| = O_p(1/N)$, $||\frac{\partial \Upsilon_1}{\partial \eta_i}|| = O_p(1/N)$, $||\frac{\partial \Upsilon_2}{\partial \eta_i}|| = O_p(1/N)$, $||\text{Tr}(\Upsilon_2)|| = O_p(1/N)$, and $d_1 \leq ||P(\eta)|| \leq d_2$ and $||S(\eta)^{-1}|| < ||(P(\eta)^{-1}|| \leq 1/d_1$ for $\eta \in \Omega$ yields

$$
||\Upsilon_1|| = O_p(\omega N), \text{ } ||\text{Tr}(\Upsilon_2)|| = O_p(\omega N)
\tag{A.33}
$$

uniformly in $\Omega$, where $\Omega$ is defined in (A.24). Therefore, we have

$$
\left| \frac{\partial \text{MSEg}(P(\eta))}{\partial \eta} - \frac{\partial W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta} \right| = O_p(\omega N)
$$

uniformly for any $\eta \in \Omega$. Since $\hat{\eta}_{\text{MSEg}}$ and $\eta^*_g$ minimize $\text{MSEg}(P)$ and $W_g(P, \Sigma, \theta_0)$, respectively, we have

$$
\frac{\partial \text{MSEg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \hat{\eta}_{\text{MSEg}}} = 0 \text{ and } \frac{\partial W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta} \bigg|_{\eta = \eta^*_g} = 0.
$$

It follows that

$$
\frac{\partial \text{MSEg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta^*_g} = O_p(\omega N).
$$

In addition, by using (A.32), the $(i, j)$-element of the Hessian matrix of $W_g(\eta, \Sigma, \theta_0)$ is

$$
\frac{\partial^2 W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta_i \partial \eta_j}
= 2\sigma^4 \theta_0^T P^{-T} \Sigma^{-2} \frac{\partial P^{-1}}{\partial \eta_i} \theta_0 + 2\sigma^4 \theta_0^T \frac{\partial P^{-T}}{\partial \eta_i} \Sigma^{-2} \frac{\partial P^{-1}}{\partial \eta_j} \theta_0
- 2\sigma^4 \text{Tr}(\Sigma^{-1} \frac{\partial P^{-1}}{\partial \eta_i} \Sigma^{-1})
\tag{A.34}
$$

The Hessian matrix $\frac{\partial^2 \text{MSEg}(P(\eta))}{\partial \eta_i \partial \eta_j}$ of $\text{MSEg}(P(\eta))$ is omitted here for simplicity. Then, it can be shown that

$$
\left| \frac{\partial^2 \text{MSEg}(P(\eta))}{\partial \eta_i \partial \eta_j} - \frac{\partial^2 W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta_i \partial \eta_j} \right| = O_p(1)
$$

uniformly for any $\eta \in \Omega$. Applying the Taylor expansion to $\frac{\partial \text{MSEg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta^*_g}$ yields

$$
0 = \frac{\partial \text{MSEg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \hat{\eta}_{\text{MSEg}}} = \frac{\partial \text{MSEg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta^*_g} + \frac{\partial^2 \text{MSEg}(P(\eta))}{\partial \eta \partial \eta^T} \bigg|_{\eta = \hat{\eta}_{\text{MSEg}} - \eta^*_g},
$$

where $\hat{\eta}$ lies between $\hat{\eta}_{\text{MSEg}}$ and $\eta^*_g$.

Clearly,

$$
\frac{\partial^2 W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta \partial \eta^T} \bigg|_{\eta = \eta^*_g} = O_p(1).
$$

Then under Assumption 2, we have $\frac{\partial^2 W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta \partial \eta^T} \bigg|_{\eta = \eta^*_g}$ is positive definite. For sufficiently large $N$, $\hat{\eta}$ would be close to $\eta^*_g$. In this case, we also have $\frac{\partial^2 W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta \partial \eta^T} \bigg|_{\eta = \hat{\eta}}$
is positive definite. Then it follows that
\[
\hat{\eta}_{\text{MSE}g} - \eta_g^* = -\left( \frac{\partial^2 \text{MSE}g(P(\eta))}{\partial \eta \partial \eta^T} \right)_{\eta = \hat{\eta}}^{-1} \frac{\partial \text{MSE}g(P(\eta))}{\partial \eta} \bigg|_{\eta = \hat{\eta}}^\prime = O_p(1) O_p(\varkappa_N) = O_p(\varkappa_N).
\]

Now, we prove \( \| \hat{\eta}_{\text{MSE}g} - \eta_g^* \| = O_p(\mu_N) \) and the proof is similar to that of \( \| \hat{\eta}_{\text{MSE}g} - \eta_g^* \| = O_p(\varkappa_N) \). By (A.15), the \( i \)-th element of gradient vector of \( \Phi_{sg}(P(\eta)) \) is
\[
\frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta_i} = 2\sigma^4 (\hat{\eta}^L S)^T S^{-T} N^2 (\Phi^T \Phi)^{-2} \frac{\partial S^{-1}}{\partial \eta_i} \hat{\eta} L S + 2\sigma^2 N^2 \text{Tr} \left( \frac{\partial R^{-1}}{\partial \eta_i} \right). \tag{A.35}
\]

Using the identity \( \frac{\partial R^{-1}}{\partial \eta} = -\sigma^2 R^{-1} \frac{\partial \sigma^{-1}}{\partial \eta} R^{-1} \), we see
\[
\frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta_i} = 2\sigma^4 \left[ (\hat{\eta}^LS)^T S^{-T} N^2 (\Phi^T \Phi)^{-2} \frac{\partial S^{-1}}{\partial \eta_i} \hat{\eta} L S \right] - \frac{\partial W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta_i} = 2\sigma^4 Y_1' + 2\sigma^4 \text{Tr}(Y_2)
\]
\[
\text{where } Y_1' = (\hat{\eta}^LS)^T S^{-T} N^2 (\Phi^T \Phi)^{-2} \frac{\partial S^{-1}}{\partial \eta_i} \hat{\eta} L S \quad \text{and } Y_2 = \Sigma^{-1} \frac{\partial P^{-1}}{\partial \eta_i} \Sigma^{-1} - NR^{-1} \frac{\partial P^{-1}}{\partial \eta_i} NR^{-1}.
\]

Since \( \Phi^T \Phi / N \rightarrow \Sigma \) and \( v(t) \) is a white noise, we have \( \| \hat{\eta}^LS / \eta_0 \| = O_p(1/\sqrt{N}) \). Then noting that \( \| N(\Phi^T \Phi)^{-1} - \Sigma^{-1} \| = O_p(\delta N), \| S^{-1} - P^{-1} \| = O_p(1/N), \| \frac{\partial S^{-1}}{\partial \eta} \Sigma^{-1} \| = O_p(\delta N), \| \Sigma^{-1} - NR^{-1} \| = O_p(1), \| S^{-1} \| = O_p(1), \) and \( d_1 \leq \| P(\eta) \| \leq d_2 \) and \( \| S(\eta^{-1}) \| < \| (P(\eta)^{-1}) \| \leq 1/d_1 \) for \( \eta \in \overline{\Theta} \), yields
\[
\| Y_1' \| = \max \left( O_p(1/\sqrt{N}), O_p(1/N), O_p(\delta N) \right) = O_p(\mu_N), \quad \| \text{Tr}(Y_2) \| = O_p(\delta N),
\]
uniformly in \( \overline{\Theta} \). It follows that
\[
\left\| \frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta} - \frac{\partial W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta} \right\| = O_p(\mu_N)
\]
is uniformly for any \( \eta \in \overline{\Theta} \). This implies
\[
\frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta_g^*} = O_p(\mu_N). \tag{A.37}
\]

Similarly, one can obtain the Hessian matrix of \( \Phi_{sg}(P(\eta)) \) and can show that
\[
\left\| \frac{\partial^2 \Phi_{sg}(P(\eta))}{\partial \eta \partial \eta^T} - \frac{\partial^2 W_g(P(\eta), \Sigma, \theta_0)}{\partial \eta \partial \eta^T} \right\| = o_p(1) \tag{A.38}
\]
uniformly for any \( \eta \in \overline{\Theta} \). Applying the Taylor expansion of \( \frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta_g} \) shows
\[
0 = \frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta_g} = \frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta_g^*} + \frac{\partial^2 \Phi_{sg}(P(\eta))}{\partial \eta \partial \eta^T} \bigg|_{\eta = \eta_g^*} (\hat{\eta}_{\text{MSE}g} - \eta_g^*),
\]
where \( \eta \) lies between \( \hat{\eta}_{\text{MSE}g} \) and \( \eta_g^* \). For sufficiently large \( N \), we have
\[
\hat{\eta}_{\text{MSE}g} - \eta_g^* = -\left( \frac{\partial^2 \Phi_{sg}(P(\eta))}{\partial \eta \partial \eta^T} \right)_{\eta = \eta_g^*}^{-1} \frac{\partial \Phi_{sg}(P(\eta))}{\partial \eta} \bigg|_{\eta = \eta_g^*} = O_p(1) O_p(\mu_N) = O_p(\mu_N).
\]
The proof of (76) and (77) can be done in a similar way and thus is omitted. This completes the proof.

**Appendix B**

This appendix contains the technical lemmas used in the proof in Appendix A.

**B.1 Matrix Differentials and Related Identities**

This section introduces the differentiation of a function \( f(X) \) where \( X \) is a matrix. It is assumed that \( X \) has no special structure, i.e., that the elements of \( X \) are independent. For convenience and readability, the formulas used in the paper are stated in the following lemmas.

**Lemma B1** (Petersen & Pedersen, 2012) Assume that \( b \) is a column vector, and \( A, B \) and \( X \) are matrices with compatible dimensions. Then we have
\[
\frac{\partial b^T X^T A X b}{\partial X} = (A + A^T) X b b^T \tag{B.39}
\]
\[
\frac{\partial b^T X^{-1} b}{\partial X} = -X^{-T} b b^T X^{-T} \tag{B.40}
\]
\[
\frac{\partial \log | \det(X) |}{\partial X} = X^{-T} \tag{B.41}
\]
\[
\frac{\partial (X^{-1})_{ki}}{\partial X_{ij}} = -(X^{-1})_{ki} (X^{-1})_{ij} \tag{B.42}
\]
\[
\frac{\partial \text{Tr}(A X^{-1} B)}{\partial X} = -(X^{-1} B A X^{-1})^T \tag{B.43}
\]
\[
\frac{\partial \text{Tr}(A X B X^T A^T)}{\partial X} = A^T X (B + B^T). \tag{B.44}
\]

where \((\cdot)_{ij}\) denotes the \((i, j)\)th element of a matrix.

**Lemma B2** Suppose that both \( A \) and \( B \) are positive semidefinite. If \( \text{Tr}(A B) = 0 \), then \( A B = 0 \).
Proof. Let us denote the symmetric square root factorization of $A$ by $A^\ddagger.$ Thus the trace property implies
\[
\text{Tr}(AB) = \text{Tr}(A^\ddagger A^\dagger B^\dagger B^\ddagger) \\
= \text{Tr}(A^\ddagger B^\dagger B^\ddagger A^\dagger) = \|A^\ddagger B^\ddagger\|^2 = 0.
\]
This derives that $A^\ddagger B^\ddagger = 0.$ Pre-multiplying by $A^\ddagger$ and post-multiplying by $B^\ddagger$ entails $AB = 0.$

Lemma B3 We have the following identities:
\[
\sum_{ij} (A)_{ij} J_{ij} = A, \quad (B.45)
\]
\[
Y - \Phi \tilde{\theta}^R = \sigma^2 Q^{-1} Y, \quad (B.46)
\]
\[
\tilde{\theta}^L S - \tilde{\theta}^R = \sigma^2 (\Phi^T \Phi)^{-1} \Phi^T Q^{-1} Y, \quad (B.47)
\]
\[
A(I_N + BA)^{-1} = (I_n + AB)^{-1} A, \quad (B.48)
\]
\[
\Phi^T Q^{-1} \hat{\Phi} = S^{-1}, \quad (B.49)
\]
\[
\Phi^T Q^{-T} Q^{-1} \Phi = S^{-T}(\Phi^T \Phi)^{-1} S^{-1}, \quad (B.50)
\]
\[
\Phi^T Q^{-T} Q^{-1} Y = S^{-T}(\Phi^T \Phi)^{-1} S^{-1} \tilde{\theta}^L S, \quad (B.51)
\]
\[
I_N - \sigma^2 Q^{-1} = \Phi P \Phi^T Q^{-1} = Q^{-1} \Phi P \Phi^T = \Phi R^{-1} \Phi^T, \quad (B.52)
\]
\[
\frac{\partial (Q^{-1})_{ij}}{\partial P_{st}} = - \Phi^T Q^{-T} J_{ij} Q^{-1} \Phi, \quad (B.53)
\]
\[
\frac{\partial (R^{-1})_{ij}}{\partial P_{st}} = \sigma^2 P^{-T} R^{-T} J_{ij} R^{-1} P^{-T}, \quad (B.54)
\]
where $J_{ij}$ is a matrix whose $(i, j)$-element is one and zero for all other elements.

Proof. The identities (B.45)–(B.52) can be verified by a straightforward calculation. Using (B.42) gives
\[
\frac{\partial (Q^{-1})_{ij}}{\partial P_{st}} = \sum_{a,b} \frac{\partial (Q^{-1})_{ab}}{\partial Q_{ab}} \frac{\partial Q_{ab}}{\partial P_{st}} = \sum_{a,b} (Q^{-1})_{ia} (Q^{-1})_{bj} |a|_{\Phi^T} |b|_{\Phi^T} = \sum_{a,b} (\Phi^T)^a (Q^{-T})_{ai} (Q^{-T})_{jb} \Phi_{bt} = \sum_{a,b} (\Phi^T)^a (Q^{-T})_{ai} (Q^{-T})_{jb} \Phi_{bt} = \sum_{a,b} (\Phi^T)^a (Q^{-T})_{ai} (Q^{-T})_{jb} \Phi_{bt},
\]
which implies (B.53). While (B.54) can be proved in a similar way.

B.2 Convergence Result for Extremum Estimators

Lemma B4 (Ljung, 1999, Theorem 8.2) Assume that

1) $M(\eta)$ is a deterministic function that is continuous in $\eta \in \Omega$ and minimized at the set
\[
D = \arg \min_{\eta \in \Omega} M(\eta) = \{\eta | \eta \in \Omega, M(\eta) = \min_{\eta \in \Omega} M(\eta)\}
\]
where $\Omega$ is a compact subset of $\mathbb{R}^p.$

2) A sequence of functions $\{M_N(\eta)\}$ converges to $M(\eta)$ almost surely and uniformly in $\Omega$ as $N$ goes to $\infty.$

Then $\hat{\eta}_N = \arg \min_{\eta \in \Omega} M_N(\eta)$ converges to $D$ almost surely, namely,
\[
\inf_{\tilde{\eta} \in D} \|\hat{\eta}_N - \tilde{\eta}\| \to 0, \quad \text{as} \ N \to \infty.
\]

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