Physical Parameter Calibration
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Abstract  Computer simulation models are widely used to study complex physical systems. A related fundamental topic is the inverse problem, also called calibration, which aims at learning about the values of parameters in the model based on observations. In most real applications, the parameters have specific physical meanings, and we call them physical parameters. To recognize the true underlying physical system, we need to effectively estimate such parameters. However, existing calibration methods cannot do this well due to the model identifiability problem. This paper proposes a semi-parametric model, called the discrepancy decomposition model, to describe the discrepancy between the physical system and the computer model. The proposed model possesses a clear interpretation, and more importantly, it is identifiable under mild conditions. Under this model, we present estimators of the physical parameters and the discrepancy, and then establish their asymptotic properties. Numerical examples show that the proposed method can better estimate the physical parameters than existing methods.

KEY WORDS: Computer Experiment; Identifiability; Inverse Problem; Semi-parametric Model; Reproducing Kernel Hilbert Space

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1 Introduction

With the rapid development of computational techniques and mathematical modelings, computer simulation models are adopted across almost all areas of physical science, engineering, environmental, health, and social science to understand, predict, or control complex systems (Santner et al., 2018). Compared to physical experiments, computer simulations can be much faster and less costly. Furthermore, many physical processes are difficult or impossible to conduct directly via real experiments. Therefore, computer experiments are becoming popular surrogates and auxiliary to physical experiments.

An important task in computer modeling is to solve the inverse problem using the observations of physical and simulation experiments, i.e., to identify the values of parameters within the computer model. The corresponding process is often referred to as calibration and the parameters are referred to as calibration parameters. Calibration parameters can be classified into two types, physical parameters and tuning parameters (Brynjarsdóttir and O’Hagan, 2014). Physical parameters have specific meaning within the science underlying the simulation model. Learning about their values can contribute to understanding the physical system. Tuning parameters, however, do not have physical meaning. They are often used only for construction of the computer model, and their “true” values are whatever enable the model to fit best to reality. Generally speaking, physical parameters are more important to researchers, and thus we focus on the calibration issue for them in this paper.

Physical parameters usually exist within physical systems in an implicitly nonlinear manner, and cannot be observed. In addition, computer models are built based on some assumptions and simplifications of real physical systems, and these assumptions and simplifications may not totally hold in reality. Therefore, there exists some discrepancy between a physical system and the corresponding computer model, even when we know the true values of physical parameters. These difficulties make the issue of physical parameter calibration very challenging to statisticians.

Kennedy and O’Hagan (2001) first studied the calibration issue systematically under a Bayesian framework. Their main idea is to model the discrepancy between the physical
system and the computer model as a Gaussian process. Because of the importance of calibration, Kennedy and O’Hagan’s approach has been widely used in various fields, including cylinder implosion, spot welding, hydrology, radio-logical protection, micro-cutting, and climate prediction (Goldstein and Rougier, 2004; Murphy et al., 2007). This approach has also received a great deal of attention in the statistical literature; see Higdon et al. (2008); Chang and Joseph (2014); Storlie et al. (2015); Qian and Wu (2008), among many others.

However, Kennedy and O’Hagan’s model is unidentifiable. That is, under their model, the distribution of the observed data from the physical system does not uniquely determine the corresponding calibration parameter values given the computer model. As a result, Kennedy and O’Hagan’s method can lead to unreasonable estimators of calibration parameters (Tuo and Wu, 2015, 2016). There are several Bayesian approaches to cope with this identifiability problem. For example, Bayarri et al. (2007) suggested reducing the confounding between the calibration parameters and the model discrepancy through incorporating the experts’ information into the prior distribution. Brynjarsdóttir and O’Hagan (2014) gave a concrete example in which the prior information on the model discrepancy was incorporated through a constrained Gaussian process. Plumlee (2017) proposed an improved Bayesian calibration method in which the prior distribution on the model discrepancy is orthogonal to the gradient of the computer model. However, these Bayesian approaches rely on prior information and lack theoretical guarantees.

Tuo and Wu (2015, 2016) and Wong et al. (2017) tackled the identifiability problem by defining the “true” parameter values as the ones that minimize the $L_2$ distance between the physical system and the computer model. Their $L_2$ calibration model is rigorously identifiable under a frequentist framework. Following these work, several authors proposed different methods to implement $L_2$ calibration; see e.g. the Bayesian projected calibration method (Xie and Xu, 2021) and the scaled Gaussian process method (Gu and Wang, 2017; Gu et al., 2018). Unfortunately, in most cases, the “true” parameter values in $L_2$ calibration are different from the true values of physical parameters, and thus $L_2$ calibration cannot yield accurate estimates of physical parameters. For instance, see the examples in Brynjarsdóttir and O’Hagan (2014) and Plumlee (2017).
In this paper we propose a frequentist framework for the physical parameter calibration issue. A semi-parametric model, called the discrepancy decomposition model, is introduced to describe the discrepancy between the physical system and the computer model. The discrepancy decomposition model decomposes the discrepancy into the intrinsic discrepancy and the parametric discrepancy, both of which have reasonable interpretations. Besides, our model is identifiable under mild conditions, which guarantees that the physical parameters can be identified. Under our model, we provide estimators of the physical parameters and the discrepancy, and then establish their asymptotic properties. In particular, the estimators of the physical parameters are proven to have a convergence rate of order $\sqrt{n}$. We present several examples to illustrate the proposed calibration method. The numerical results indicate that our method outperforms existing methods.

The rest of this paper is organized as follows. Section 2 reviews the calibration issue, and then introduces the discrepancy decomposition model. Its identifiability is also proven. Section 3 presents the estimation method and the corresponding asymptotics under our model. Section 4 gives numerical examples. Section 5 ends the paper with some discussion. All proofs are given in the Appendix.

2 The discrepancy decomposition model

2.1 The calibration problem

We first review the calibration problem of computer models. Suppose there is a physical system $\eta$ with a vector of control variables $\mathbf{x}$ as its input, where $\eta$ is deterministic and unknown. Denote the domain of $\mathbf{x}$ by $\Omega$, which is the closure of a bounded convex open set in $\mathbb{R}^d$. For each $\mathbf{x} \in \Omega$, the output of this physical system, $\eta(\mathbf{x}) \in \mathbb{R}$. To study the physical system, we collect the noisy responses $\{y_i\}_{i=1}^n$,

$$y_i = \eta(x_i) + \epsilon_i, \quad i = 1, ..., n, \quad (1)$$
on a set of design points \( \{x_i\}_{i=1}^n \), where \( \{\epsilon_i\}_{i=1}^n \) are independent random noises.

Suppose that we also have a deterministic computer model that is designed to approximate \( \eta \). Let \( y^s(x, \theta) \) denote the output of the computer model at inputs \( (x, \theta) \in \Omega \times \Theta \), where the superscript \( s \) stands for “simulation”, \( x \) is the same control variable as in \( \eta \), \( \theta \in \Theta = [0, 1]^q \) represents a vector of calibration variables. We focus on the case where \( \theta \) has a certain physical meaning, i.e., there is an underlying value of \( \theta \) implicitly involved in the physical system \( \eta \). Let \( \theta^p \) denote such a value, where the superscript \( p \) stands for “physical”. Generally, the calibration parameter \( \theta^p \) cannot be measured directly or cannot be controlled from the available physical experiment. The main goal of calibration is to estimate \( \theta^p \) given the physical observations \( \{y_i\}_{i=1}^n \) and the computer model \( y^s \). Let \( \delta \) denote the discrepancy between the physical system and the computer model, i.e.,

\[
\delta = \eta(x) - y^s(x, \theta).
\]  

(2)

Kennedy and O’Hagan (2001) used a Gaussian process to model \( \delta \), and developed the corresponding Bayesian calibration method. However, the true calibration parameter is unidentifiable within this framework in that the distribution of the observed data from the physical experiment cannot uniquely determine the calibration parameter given the computer model (Tuo and Wu, 2015; Xie and Xu, 2021).

Tuo and Wu (2015, 2016) avoid the identifiability problem via a natural and simple way. They redefine the “true” value of \( \theta \) as the one that minimizes the \( L_2 \) distance between \( y^s(x, \theta) \) and \( \eta(x) \), i.e.,

\[
\theta^* = \arg \min_{\theta \in \Theta} \|\eta(x) - y^s(x, \theta)\|_{L_2} = \arg \min_{\theta \in \Theta} \left( \int_{\Omega} (\eta(x) - y^s(x, \theta))^2 \, dx \right)^{1/2}.
\]

This definition is perfect when \( \theta \) is a tuning parameter. However, in the physical parameter calibration problem, \( \theta^* \) may be much different from \( \theta^p \); see Brynjarsdóttir and O’Hagan (2014), Plumlee (2017), and our numerical examples in Section 4. Therefore, we need other strategies to better identify \( \theta^p \).
2.2 Model construction

In this section, we propose a new approach to identify the physical parameters. A statistical model is constructed to approximate the relationship between the physical and computer models. Note that the discrepancy \( \delta \) in (2) is a function of \( x \) and \( \theta \). We rewrite it as

\[
\delta(x, \theta) = \eta(x) - y^s(x, \theta).
\]

Roughly speaking, the above \( \delta \) can be viewed as a total discrepancy that contains two types of discrepancies. The first type, maybe called the intrinsic discrepancy, is caused by unpractical assumptions or simplifications of the complex physical system in the construction of the computer model. The second type is caused by incorrect values of the calibration parameter used in the computer model. A possible reason of the identifiability problem is that the two types of discrepancies are entangled in conventional calibration models.

To avoid the identifiability problem, we propose an additive structure of the two types of discrepancies. Specifically, we model the total discrepancy as

\[
\delta(x, \theta) = \alpha(x) + \beta^T(x)(\theta - \theta^p), \tag{3}
\]

where \( \alpha(x) \) and \( \beta(x) = (\beta_1(x), \ldots, \beta_q(x))^T \) are unknown smooth functions, the superscript \( T \) denotes transpose, and \( \theta^p = (\theta^p_1, \ldots, \theta^p_q)^T \) is the parameter vector of interest. In model (3), \( \alpha(x) \) represents the intrinsic discrepancy due to unpractical assumptions or simplification of the physical system used in the computer model. It will not vanish even if the computer model is well calibrated with \( \theta = \theta^p \). We refer to the other term \( \beta^T(x)(\theta - \theta^p) \) as the parametric discrepancy, which is caused by incorrect identification of \( \theta \), and \( \beta(x) \) is called the discrepancy coefficient function. The parametric discrepancy will vanish when we use the correct value of \( \theta \) in the computer model. We call model (3) the discrepancy decomposition model since it decomposes the total discrepancy into the intrinsic and parametric discrepancies. The goal of this calibration modeling is to identify \( \theta^p \), and the nuisance parameters \( \alpha(x) \) and \( \beta(x) \) will be estimated at the same time.
The discrepancy decomposition model in (3) can be viewed as an approximation from the Taylor expansion. Implement the first-order Taylor expansion of \( \delta(x, \theta) \) at \( \theta^p \). After ignoring the higher-order remainder, we can see that \( \alpha(x) \) and \( \beta(x) \) correspond to \( \delta(x, \theta^p) \) and \( \frac{\partial \delta(x, \theta)}{\partial \theta} \bigg|_{\theta=\theta^p} \), respectively.

Our model uses a simple additive structure of two meaningful terms to approximate the real discrepancy. Therefore, it possesses good interpretability. In addition, we will show in the next subsection that this model is identifiable under mild conditions, which guarantees that we can next construct effective estimation for \( \theta^p \).

2.3 Identifiability

We first consider the case of \( q = 1 \), i.e., \( \theta^p \) is one-dimensional. The following two assumptions can guarantee the identifiability property of the proposed model.

**Assumption 2.1.** \( \int_{\Omega} \alpha(x) dx = c \), where \( c \) is a pre-specified constant.

**Assumption 2.2.** \( \int_{\Omega} \beta(x) dx \neq 0 \).

Assumption 2.2 indicates that, if the computer model is not well calibrated (we input \( \theta \neq \theta^p \) in it), then besides the intrinsic discrepancy, there will be a non-zero gap between the physical and computer models in the average sense.

Assumption 2.1 requires that the average intrinsic discrepancy should be fixed as a known number. It should be pointed out that \( c \) cannot be assumed unknown. Otherwise, the model (3) can be written as

\[
\delta(x, \theta) = c + \alpha(x) + \beta(x)(\theta - \theta^p)
\]

with constraint \( \int_{\Omega} \alpha(x) dx = 0 \), where \( c \) is an unknown parameter. For arbitrary \( \theta_1 \neq \theta_2 \), \( \alpha_1(x) \) with \( \int_{\Omega} \alpha_1(x) dx = 0 \), and \( \beta(x) \), let \( c_1 = 0 \), \( \alpha_2(x) = \alpha_1(x) + \beta(x)(\theta_2 - \theta_1) - \int_{\Omega} \beta(x)(\theta_2 - \theta_1) dx \), and \( c_2 = \int_{\Omega} \beta(x)(\theta_2 - \theta_1) dx \). The following equality always holds for all \( x \) and \( \theta \),

\[
c_1 + \alpha_1(x) + \beta(x)(\theta - \theta_1) = c_2 + \alpha_2(x) + \beta(x)(\theta - \theta_2),
\]
which indicates that model (3) is unidentifiable. Hence we need to choose an appropriate value of $c$ in advance.

The value of $c$ describes the average difference between the physical and computer models when there is no parametric discrepancy (we input the correct $\theta^p$ in the computer model). The selection of $c$ can depend on our prior information. For instance, in the the small ball falling experiment given in Plumlee (2017) and Xie and Xu (2021), it is known that the true free fall system is usually affected by air resistance. We therefore set $c$ as a suitable positive constant in the balling falling experiment; see Section 4.2.

If there is no prior information on $c$, we can set $c = 0$ by default, which implies the ideal case where the average discrepancy is zero with $\theta = \theta^p$. For many real applications, the assumption of this ideal case is reasonable. When it does not hold, we take a subset $\Omega'$ of $\Omega$ with a positive Lebesgue measure, on which the computer model is known to be closer to the physical system by some prior. Then we can use

**Assumption 2.1'.** $\int_{\Omega'} \alpha(x) dx = 0.$

**Assumption 2.2'.** $\int_{\Omega'} \beta(x) dx \neq 0.$

to replace Assumptions 2.1 and 2.2, and this does not influence the identifiability property of our model.

We then consider the general $q \geq 1$. Take $q$ different subsets $\Omega_1, \ldots, \Omega_q$ of $\Omega$, each of which has a nonzero Lebesgue measure. The following two assumptions are generalizations of Assumptions 2.1 and 2.2, respectively.

**Assumption 2.3.** $\int_{\Omega_t} \alpha(x) dx = c_t, \quad t = 1, \ldots, q,$ where $c_1, \ldots, c_q$ are pre-specified constants.

**Assumption 2.4.** The matrix $M = (m_{st})_{s,t=1,\ldots,q}$ is nonsingular, where $m_{st} = \int_{\Omega_t} \beta_s(x) dx$ for $s, t = 1, \ldots, q$.

Similar to those in Assumption 2.1 (2.1'), $c_t$ describes the average difference between the physical and computer models over $\Omega_t$ for $t = 1, \ldots, q$ when there is no parametric discrepancy. We can select $\Omega_1, \ldots, \Omega_q$ and $c_1, \ldots, c_q$ in Assumption 2.3 by some prior information. Under
Assumption 2.4, for $\theta \neq \theta^p$, we have $(\int_{\Omega_1} \beta^T(x)(\theta - \theta^p)dx, \ldots, \int_{\Omega_q} \beta^T(x)(\theta - \theta^p)dx)^T = M(\theta - \theta^p) \neq 0$, which has a similar interpretation to Assumption 2.2 if the computer model is not well calibrated, then besides the intrinsic discrepancy, there will be a non-zero gap between the physical and computer models in some average sense. In addition, since the Lebesgue measure of the subset $\{Z = (z_{st})_{s,t=1}^q : z_{st} \in \mathbb{R}, \ Z \text{ is singular}\}$ of $\mathbb{R}^{q \times q}$ is zero, Assumption 2.4 holds almost surely.

The following theorem presents the identifiability property of the proposed model.

**Theorem 1.** Under Assumptions 2.3 and 2.4, the discrepancy decomposition model in (3) is identifiable.

**Remark 1.** From the above discussion we know that the discrepancy decomposition model (3) is unidentifiable without the constraints in Assumption 2.3. In other words, different constraints correspond to different definitions of $\theta^p$, which may not be the true values $\theta^p_0$ of the physical parameter. We define the constraints corresponding to $\theta^p_0$ as the “oracle” constraints. Generally the oracle constraints exist. Here is an example. If the computer model $y^s$ has the form of $y^s(x, \theta) = \gamma_0(x) + \gamma^T(x)\theta$, then the discrepancy decomposition model (3) holds with $\alpha(x) = \eta(x) - \gamma_0(x) + \gamma^T(x)\theta^p$ and $\beta(x) = \gamma(x)$. For any $\{\Omega\}_{t=1}^q$ in Assumption 2.3, let $c_t = \int_{\Omega_t} [\eta(x) - \gamma_0(x) + \gamma^T(x)\theta^p_0] dx$, $t = 1, \ldots, q$, which gives a group of oracle constraints.

**Assumption 2.5.** For each $j = 1, \ldots, q$, the Lebesgue measure of $\{x \in \Omega : \beta_j(x) = 0\}$ is zero.

Assumption 2.5 is not a condition for identifiability. We state it here because it has a similar interpretation to Assumption 2.4 that assumes a non-zero gap between the physical system and the computer model. This assumption will be used in the next section.

## 3 Parameter estimation and asymptotics

In this section, we provide the estimation method for the physical parameter $\theta^p$ under the discrepancy decomposition model. The corresponding asymptotic properties are established.
Analysis of the asymptotics includes three steps: (1) establishing consistency; (2) establishing convergence rates; and (3) deriving the limiting distribution.

### 3.1 Parameter estimation

Suppose we have the data \( \{(x_i, y_i)\}_{i=1}^n \) of physical experiments from \([1]\). Let \( \{\theta_i\}_{i=1}^n \subset \Theta \subset \mathbb{R}^q \). We run the computer simulator \( y^s \) on \( \{(x_i, \theta_i)\}_{i=1}^n \), and let \( \delta_i = y_i - y^s(x_i, \theta_i) \), \( i = 1, \ldots, n \). Under the discrepancy decomposition model in \([3]\), we can write

\[
\delta_i = \alpha(x_i) + \beta^T(x_i)(\theta_i - \theta^p) + \epsilon_i, \quad i = 1, \ldots, n.
\]

We need to estimate the unknown parameters, \( \alpha(x) \), \( \beta(x) \), and \( \theta^p \), based on the data \( \{(x_i, \theta_i, \delta_i)\}_{i=1}^n \).

Our study in this section employs the reproducing kernel Hilbert space (also called the native space) as a mathematical tool; see Kosorok (2008) for detailed descriptions on this space. Let \( N_k(\Omega) \) denote the reproducing kernel Hilbert space on \( \Omega \) generated by a positive definite real-valued kernel function \( k \), and let \( \| \cdot \|_{N_k} \) be the corresponding norm. By \([4]\), the estimators of \( \alpha(x) \), \( \beta(x) \), and \( \theta^p \) can be given by the following penalized least squares problem,

\[
\min_{(\theta^p, \alpha, \beta) \in \Theta \times A \times B} \frac{1}{n} \sum_{i=1}^n \left\{ \delta_i - \alpha(x_i) - \beta^T(x_i)(\theta_i - \theta^p) \right\}^2 + \lambda_n^2 \left( \| \alpha \|_{N_k}^2 + \sum_{s=1}^q \| \beta_s \|_{N_k}^2 \right),
\]

where \( A = \{ \alpha(x) \in N_k(\Omega) : \int_{\Omega_t} \alpha(x) \, dx = c_t, \ t = 1, \ldots, q \} \), \( B = N_k(\Omega) \times \cdots \times N_k(\Omega) \), and \( \lambda_n > 0 \) is a tuning parameter. Denote \( \hat{\delta} = (\delta_1, \ldots, \delta_n)^T \) and \( \hat{c} = (c_1, \ldots, c_q)^T \).

By the representer theorem (Schölkopf et al. 2001), the solutions corresponding to the nonparametric parameters \( \alpha \) and \( \beta \) to \([5]\) have the following finite-dimensional expressions,

\[
\alpha(\cdot) = \sum_{i=1}^n a_i k(x_i, \cdot), \quad \beta(\cdot) = (\beta_1(\cdot), \ldots, \beta_q(\cdot))^T = \left( \sum_{i=1}^n b_i k(x_i, \cdot), \ldots, \sum_{i=1}^n b_q k(x_i, \cdot) \right)^T.
\]

Let \( a = (a_1, \ldots, a_n)^T \), \( K = (k_1, \ldots, k_n) = (k_{ij})_{i,j=1,\ldots,n} \) with \( k_{ij} = k(x_i, x_j) \), \( b_s = (b_{s1}, \ldots, b_{sn})^T \).
for $s = 1, \ldots, q$, and $b = (b_1^T, \ldots, b_q^T)^T$. Therefore, (5) is equivalent to the following optimization problem,

$$
\min_{(\theta^p, a, b) \in \Theta \times \mathbb{R}^n \times \mathbb{R}^{nq}} \frac{1}{n} \| \delta - K a - T(\theta^p) b \|^2 + \lambda_n^2 \left\{ a^T K a + b^T (I_q \otimes K) b \right\},
$$

s.t. $Ja = c$,

where $\| \cdot \|$ denotes the Euclidean norm, $T(\theta^p) = ((\theta_1 - \theta^p) \otimes k_1, \ldots, (\theta_n - \theta^p) \otimes k_n)^T$, $\otimes$ represents the Kronecker product, $I_q$ denotes the identity matrix of order $q$, and $J = \left( \int_{\Omega_k} k(x_i, x) dx \right)_{t=1, \ldots, q, \ i=1, \ldots, n}$.

If $\theta^p$ is known, then (6) is a standard quadratic programming problem with a linear equality constraint. In most cases, the sample size $n$ is much larger than $q$, and the Lebesgue measure of the subset $\{ W = (w_{ti})_{t=1, \ldots, q, \ i=1, \ldots, n} : w_{ti} \in \mathbb{R}, \ \text{rank}(W) < q \}$ of $\mathbb{R}^{q \times n}$ is zero. Therefore, we can assume that the matrix $J$ is of full column rank. For given $\theta^p$, the solution to (6) can be given by

$$
\left( \begin{array}{c}
a(\theta^p) \\
b(\theta^p)
\end{array} \right) = D^{-1} d + D^{-1} \tilde{J} (\tilde{J}^T D^{-1} \tilde{J})^{-1} \left[ - \tilde{J}^T D^{-1} d + c \right],
$$

where $\tilde{J} = \left( \begin{array}{c} J \\ O \end{array} \right)_{2n \times q}$, $O$ is the zero matrix,

$$
D = 2 \begin{pmatrix} K^T K + \lambda_n^2 I_q & K^T T(\theta^p) \\ T^T(\theta^p) K & T^T(\theta^p) T(\theta^p) + \lambda_n^2 (I_q \otimes K) \end{pmatrix}, \text{ and } d = 2 \begin{pmatrix} K^T \delta \\ T(\theta^p) \delta \end{pmatrix}.
$$

Consequently, we can estimate $\theta^p$ by solving

$$
\min_{\theta^p \in \Theta} \frac{1}{n} \| \delta - K a(\theta^p) - T(\theta^p) b(\theta^p) \|^2 + \lambda_n^2 \left\{ a(\theta^p)^T K a(\theta^p) + b(\theta^p)^T (I_q \otimes K) b(\theta^p) \right\}.
$$

The tuning parameter $\lambda_n$ in (5) can be selected via cross-validation. Let $\hat{\theta}^p$, $\hat{\alpha}$, and $\hat{\beta} =$
$(\hat{\beta}_1, \ldots, \hat{\beta}_q)^T$ denote the solutions to (5). We estimate the discrepancy $\delta$ in (3) using

$$\hat{\delta}(x, \theta) = \hat{\alpha}(x) + \hat{\beta}^T(x)(\theta - \theta^p).$$

### 3.2 Consistency

In this subsection we present the consistency property of $\hat{\theta}_p^0$, $\hat{\alpha}$, and $\hat{\beta}$. Let $\theta^0_p$, $\alpha_0$, and $\beta_0 = (\beta_{01}, \ldots, \beta_{0q})^T$ denote the underlying true values of $\theta^p$, $\alpha$, and $\beta$ in model (3), respectively. The true discrepancy can be written as

$$\delta_0(x, \theta) = \alpha_0(x) + \beta_0^T(x)(\theta - \theta^p_0).$$

Here we assume that $\theta^p_0$ is an interior point of $\Theta$.

We need some additional notation and definitions from the theory of empirical processes (van De Geer, 2000). Let $(\mathcal{G}, \Upsilon, \| \cdot \|)$ be a function space with domain $\Upsilon$ and norm $\| \cdot \|$. For $\rho > 0$, let $J = \{ N : \text{there exists a collection } \{g_1, \ldots, g_N\} \subset \mathcal{G} \text{ such that } \sup_{g \in \mathcal{G}} \min_{1 \leq j \leq N} \| g - g_j \| \leq \rho \}$. Denote the smallest number in $J$ by $N(\rho, \mathcal{G}, \| \cdot \|)$, and take $N(\rho, \mathcal{G}, \| \cdot \|) = \infty$ if $J = \emptyset$. We call $N(\rho, \mathcal{G}, \| \cdot \|)$ the $\rho$-covering number and $H(\rho, \mathcal{G}, \| \cdot \|) = \log N(\rho, \mathcal{G}, \| \cdot \|)$ the $\rho$-entropy of $\mathcal{G}$.

Similarly, for $\rho > 0$, define $J_B = \{ N : \text{there exist pairs of functions } \{[g^L_j, g^U_j] \}_{j=1}^N \text{ with } \max_{1 \leq j \leq N} \| g^U_j - g^L_j \| \leq \rho \text{ such that for each } g \in \mathcal{G}, \ g^L_j(x) \leq g(x) \leq g^U_j(x) \text{ for all } x \in \Upsilon, \text{ for some } j = j(g) \in \{1, \ldots, N\} \}$. Let the covering number with bracketing $N_B(\rho, \mathcal{G}, d)$ represent the smallest number in $J_B$ and take $N_B(\rho, \mathcal{G}, \| \cdot \|) = \infty$ if $J_B = \emptyset$. We call $H_B(\rho, \mathcal{G}, \| \cdot \|) = \log N_B(\rho, \mathcal{G}, \| \cdot \|)$ the $\rho$-entropy with bracketing of $\mathcal{G}$.

For $g \in \mathcal{G}$, let $\| g \|_\infty = \inf \{ M > 0 : \{ x \in \Upsilon : g(x) > M \} \text{ is of Lebesgue measure zero} \}$. The following two results (van De Geer, 2000) are useful:

$$H_B(\rho, \mathcal{G}, \| \cdot \|_{L_2}) \leq H(\rho/2, \mathcal{G}, \| \cdot \|_{\infty}), \text{ for all } \rho > 0, \tag{7}$$

$$H_B(\rho, \mathcal{G}, \| \cdot \|_{L_2}) \leq H(\rho/2, \mathcal{G}, \| \cdot \|_{\infty}), \text{ for all } \rho > 0, \tag{7}$$
and for all \(v_1, \ldots, v_n \in \Upsilon\),

\[
H(\rho, \mathcal{G}, \| \cdot \|_n) \leq H(\rho, \mathcal{G}, \| \cdot \|_\infty), \text{ for all } \rho > 0, \tag{8}
\]

where \(\|g\|_n = (\sum_{i=1}^n g(v_i)^2/n)^{1/2}\) denotes the empirical norm of \(g \in \mathcal{G}\).

Define

\[
\Delta = \left\{ \delta(x, \theta) = \alpha(x) + \beta^T(x)(\theta - \theta^p) : \theta^p \in \Theta, \alpha(x) \in A \text{ and } \beta(x) \in B \right\}. \tag{9}
\]

For any \(\delta \in \Delta\), its empirical norm is

\[
\|\delta\|_n = \left\{ \frac{1}{n} \sum_{i=1}^n \delta^2(x_i, \theta_i) \right\}^{1/2}.
\]

We make the following assumptions.

**Assumption 3.1.** The sequence \(\{x_i\}_{i=1}^n\) are independently and identically distributed (i.i.d.) from the uniform distribution \(U(\Omega)\). The sequence \(\{\theta_i\}_{i=1}^n\) are i.i.d. from the uniform distribution \(U(\Theta)\). The two sequences \(\{x_i\}_{i=1}^n\) and \(\{\theta_i\}_{i=1}^n\) are independent.

**Assumption 3.2.** The error sequence \(\{\epsilon_i\}_{i=1}^n\), independent of \(\{x_i\}_{i=1}^n\) and \(\{\theta_i\}_{i=1}^n\), are uniformly sub-Gaussian, i.e.,

\[
\max_{i=1, \ldots, n} K^2(\mathbb{E} \epsilon_i^2/K^2 - 1) \leq \sigma_0^2
\]

for all \(n\), where \(K\) and \(\sigma_0\) are constants.

**Assumption 3.3.** \(\delta_0 \in \Delta\) and there exists a constant \(L\) such that \(\sup_{\delta \in \Delta} \|\delta\|_n \leq L\).

**Assumption 3.4.** For all \(\rho > 0\),

\[
H\left(\rho, \left\{ \frac{\delta - \delta_0}{\|\delta\|_{L_2} + \|\delta_0\|_{L_2}} : \delta \in \Delta \right\}, \| \cdot \|_n \right) \leq R \rho^{-\gamma},
\]

where \(R > 0\) and \(\gamma \in (0, 2)\) are constants.
Assumption 3.5. \(2H_B(\rho_n, \Delta, \| \cdot \|_{L_2}) \leq n\rho_n^2, n \geq 1, \) for some \(\{\rho_n\}\) satisfying \(\rho_n^2 \to 0\) and \(n\rho_n^2 \to \infty\).

Assumption 3.6. The tuning parameter \(\lambda_n\) in (5) satisfies \(\lambda_n^{-1} = O(n^{1/\gamma})\) and \(\lambda_n = O(n^{-1/\gamma})\), where \(\gamma\) is defined in Assumption 3.4.

Theorem 2. Under Assumptions 2.3-2.5 and 3.1-3.6, we have
\[
\| \hat{\delta} - \delta_0 \|_{L_2} = O_p(n^{-1/2+\gamma}), \quad \text{as } n \to \infty. \tag{10}
\]

In addition, for the components \(\hat{\theta}^p, \hat{\alpha}, \) and \(\hat{\beta}\) of \(\hat{\delta}\), we have
\[
\| \hat{\theta}^p - \theta_0^p \| = o_p(1), \quad \| \hat{\alpha} - \alpha_0 \|_{L_2} = o_p(1), \quad \text{and} \quad \| \hat{\beta}_j - \beta_{0j} \|_{L_2} = o_p(1), \quad j = 1, \ldots, q. \tag{11}
\]

Assumptions 3.1-3.6 in the above theorem are widely used in the literature. Assumptions 3.2 holds for many commonly-encountered distributions. For instance, if \(\epsilon_1, \ldots, \epsilon_n\) are i.i.d. from \(\mathcal{N}(0, \tau^2_0)\), then one can take \(K = 2\tau_0\) and \(\sigma_0 = \tau_0\) to satisfy it (van De Geer, 2000).

Assumption 3.3 is a common condition in the theory of empirical processes (van De Geer, 2000). Actually, given bounded \(\Omega\) and \(\Theta\), it holds for commonly-encountered function spaces on them.

Assumptions 3.4 and 3.5 can be viewed as constraints on the degrees of “compactness” or “massiveness” of the function space \(\Delta\) defined in (9). They are usually used in the theory of empirical processes (van De Geer, 2000). The following remark presents a relationship between the entropies of \(\Delta\) and \(\mathcal{N}_k\), which can be used to verify the two assumptions.

Remark 2. Let \(N = N(\rho, \mathcal{N}_k, \| \cdot \|_{\infty})\). By definition, there exists \(\mathcal{N}_e = \{f_1, \ldots, f_N\} \subset \mathcal{N}_k\) such that \(\sup_{f \in \mathcal{N}_k} \min_{1 \leq j \leq N} \| f - f_j \|_{\infty} \leq \rho\). For arbitrary fixed \(\theta^p = (\theta^p_1, \ldots, \theta^p_q)^T \in \Theta\), define \(\Delta_e = \{f_{j_0} + \sum_{s=1}^q (\theta_s - \theta^p_s) f_{j_s}: j_0, j_1, \ldots, j_q \in \{1, \ldots, N\}\}\). For any \(\delta = \alpha + \beta^T (\theta - \theta^p) \in \Delta\), it follows that \(\| \delta - \tilde{\delta} \|_{\infty} \leq \rho + 2qM\rho\) for some \(\tilde{\delta} \in \Delta_e\), where \(M = \max\{\|\theta\| : \theta \in \Theta\}\). Note that the cardinality of \(\Delta_e\) is at most \(N^{q+1}\). We actually obtain that \(N((1+2qM)\rho, \Delta, \| \cdot \|_{\infty}) \leq (N(\rho, \mathcal{N}_k, \| \cdot \|_{\infty}))^{q+1}\), which implies \(H((1+2qM)\rho, \Delta, \| \cdot \|_{\infty}) \leq (1+q)H(\rho, \mathcal{N}_k, \| \cdot \|_{\infty})\).
The following two remarks show that Assumptions 3.4 and 3.5 hold for the reproducing kernel Hilbert spaces generated by the Matérn kernel and the Gaussian kernel, which are widely used in computer experiments (Santner et al., 2018).

**Remark 3.** Consider the Matérn kernel function,

\[ k(s, t) = \frac{1}{\Gamma(\nu)2^{\nu-1}}\left(2\sqrt{\nu}\phi\|s - t\|\right)^\nu \Phi_\nu\left(2\sqrt{\nu}\phi\|s - t\|\right), \]

where \( \phi > 0 \) and \( \nu \geq 1 \) are constants. The reproducing kernel Hilbert space generated by this kernel function is actually the (fraction) Sobolev space \( \mathcal{H}^{\nu+d/2}(\Omega) \) (Tuo and Wu, 2015). Let \( \mathcal{H}^\mu(\Omega, R) = \{ f \in \mathcal{H}^\mu(\Omega) : \|f\|_{\mathcal{H}^\mu} \leq R \} \). Edmunds and Triebel (2010) proved that for \( \mu > d/2 \),

\[ H\left(\rho, \mathcal{H}^\mu(\Omega, R), \| \cdot \|_{\infty} \right) \leq \left( CR \right)^{d/\mu}, \]

where \( C \) is a constant independent of \( R \) and \( \rho \). Combining (7), (8), and Remark 2, we obtain that Assumptions 3.4 and 3.5 hold for \( \mathcal{H}^\mu(\Omega, R) \). Moreover, we can choose \( \lambda_n \propto n^{-\mu/2} \) to achieve the convergence rate \( \| \hat{\delta} - \delta_0 \|_{L^2} = O_p(n^{-\mu/2}) \) in Theorem 2, which is known to be optimal (Stone, 1982).

**Remark 4.** Consider the Gaussian kernel function,

\[ k(s, t) = \exp\left\{ -\frac{\|s - t\|^2}{\phi^2} \right\}, \tag{12} \]

where \( \phi > 0 \) is a constant. Let \( \mathcal{F}_k(\Omega, R) = \{ f \in \mathcal{N}_k(\Omega) : \|f\|_{\mathcal{N}_k} \leq R \} \). Zhou (2002) proved that for \( \rho < R/2 \),

\[ H\left(\rho, \mathcal{F}_k(\Omega, R), \| \cdot \|_{\infty} \right) \leq C \left( \ln \frac{R}{\rho} \right)^{d+1}, \]

where \( C \) is a constant independent of \( R \) and \( \rho \). Combining (7), (8), and Remark 2, we obtain that Assumptions 3.4 and 3.5 hold for \( \mathcal{F}_k(\Omega, R) \) with \( \gamma = 1 \).
3.3 Convergence rate

In this subsection we establish convergence rates of \( \hat{\theta}^p, \hat{\alpha}, \) and \( \hat{\beta} \). For simplicity, denote

\[
m(\theta^p, \alpha, \beta) = \left( \delta - \alpha - \beta^T (\theta - \theta^p) \right)^2,
\]

where \( \delta = \alpha_0 + \beta_0^T (\theta - \theta_0^p) + \epsilon \). Let \( \mathbb{P}_n = n^{-1} \sum_{i=1}^{n} 1(x_i, \theta_i, \epsilon_i) \) denote the empirical measure. Then (5) can be rewritten as

\[
\min_{(\theta^p, \alpha, \beta) \in \Theta \times A \times B} \mathbb{P}_n m(\theta^p, \alpha, \beta) + \lambda_n^2 \left( \|\alpha\|_{X_0}^2 + \sum_{s=1}^{q} \|\beta_s\|_{X_0}^2 \right).
\]

Define

\[
dis((\theta^p, \alpha, \beta), (\theta_0^p, \alpha_0, \beta_0)) = \|\theta^p - \theta_0^p\| + \|\alpha - \alpha_0\|_{L_2} + \sum_{s=1}^{q} \|\beta_s - \beta_{0s}\|_{L_2}.
\]

Let \( \mathbb{P} \) denote the probability measure with respect to the underlying distributions.

**Assumption 3.7.** For every \((\theta^p, \alpha, \beta)\) in a neighborhood of \((\theta_0^p, \alpha_0, \beta_0)\),

\[
-\mathbb{P}(m(\theta^p, \alpha, \beta) - m(\theta_0^p, \alpha_0, \beta_0)) \lesssim -\text{dis}^2((\theta^p, \alpha, \beta), (\theta_0^p, \alpha_0, \beta_0)),
\]

where \( \lesssim \) means “is bounded above up to a universal constant”.

**Assumption 3.8.** \( H_B(\rho, \Delta, \|\cdot\|_{L_2}) < \rho^{-\gamma} \), where \( \gamma \) is defined in Assumption 3.4 and \( \Delta = \{m(\theta^p, \alpha, \beta) - m(\theta_0^p, \alpha_0, \beta_0) : \text{dis}((\theta^p, \alpha, \beta), (\theta_0^p, \alpha_0, \beta_0)) \leq \tau \} \).

**Assumption 3.9.** There exists a constant \( \tilde{L} \) such that \( \|f\|_{\infty} \leq \tilde{L} \) for every \( f \in \Delta \).

**Theorem 3.** Under Assumptions 2.3-2.5 and 3.1-3.9 we have

\[
\|\hat{\theta}^p - \theta_0^p\| = \mathcal{O}_p(n^{-\frac{1}{2+\gamma}}), \|\hat{\alpha} - \alpha_0\|_{L_2} = \mathcal{O}_p(n^{-\frac{1}{2+\gamma}})
\]

and

\[
\|\hat{\beta}_j - \beta_{0j}\|_{L_2} = \mathcal{O}_p(n^{-\frac{1}{2+\gamma}}), \quad j = 1, \ldots, q.
\]

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By the smoothness of \( m(\cdot,\cdot,\cdot) \), Assumption 3.7 holds with reasonable boundedness assumptions. Assumption 3.8 is a common condition in the theory of empirical processes \(^{1}\) with the same \( \gamma \) as in Assumption 3.4. Combining the entropy results in Remarks 2-4 we can conclude that Assumption 3.8 holds for the Matérn kernel and the Gaussian kernel. Given bounded \( \Omega \) and \( \Theta \), Assumption 3.9 holds for commonly-encountered function spaces on them.

3.4 Asymptotic normality of \( \hat{\theta}^p \)

In this section we prove asymptotic normality of \( \hat{\theta}^p \), which implies that it possesses the \( \sqrt{n} \)-convergence rate. This rate is a parametric one, faster than that in Theorem 3. Our notation, assumptions, and proof mainly follow the paradigm developed by \(^{2}\) Ma and Kosorok (2005).

For any \( \alpha \in A \) and \( \beta \in B \), let \( \alpha(t_1) \) and \( \beta(t_2) \) be two smooth curves running through \( \alpha \) and \( \beta \) with \( \alpha(0) = \alpha \) and \( \beta(0) = \beta \), where \( A \) and \( B \) are defined in \(^{3}\). Let \( A = \{ a : a = (\partial/\partial t_1)\alpha(t_1)|_{t_1=0} \} \) and \( B = \{ b : b = (\partial/\partial t_2)\beta(t_2)|_{t_2=0} \} \) denote the tangent sets. Set

\[
m_1(\theta^p, \alpha, \beta) = \frac{\partial}{\partial \theta^p} m(\theta^p, \alpha, \beta), \quad m_2(\theta^p, \alpha, \beta)[a] = \frac{\partial}{\partial t_1}_{t_1=0} m(\theta^p, \alpha(t_1), \beta), \quad a \in A,
\]

and

\[
m_3(\theta^p, \alpha, \beta)[b] = \frac{\partial}{\partial t_2}_{t_2=0} m(\theta^p, \alpha, \beta(t_2)), \quad b \in B.
\]

Moreover, define

\[
m_{11}(\theta^p, \alpha, \beta) = \frac{\partial}{\partial \theta^p} m_1(\theta^p, \alpha, \beta), \quad m_{12}(\theta^p, \alpha, \beta)[a] = \frac{\partial}{\partial t_1}_{t_1=0} m_1(\theta^p, \alpha(t_1), \beta),
\]

and

\[
m_{21}(\theta^p, \alpha, \beta)[a] = \frac{\partial}{\partial \theta^p} m_2(\theta^p, \alpha, \beta)[a], \quad m_{22}(\theta^p, \alpha, \beta)[a_1][a_2] = \frac{\partial}{\partial t_1}_{t_1=0} m_2(\theta^p, \alpha_2(t_1), \beta)[a_1],
\]

where \( a, a_1, a_2 \in A \), and \( (\partial/\partial t_1)\alpha_2(t_1)|_{t_1=0} = a_2 \). Let \( m_2(\theta^p, \alpha, \beta)[a] = (m_2(\theta^p, \alpha, \beta)[a_1],..., \)
where \( a = (a_1, ..., a_q)^T \) and \( a_1, ..., a_q \in \mathbb{A} \). We can define \( m_{13}[b], m_{23}[a][b], m_{33}[b_1][b_2], m_{12}[a_1], \) and \( m_{22}[a_1][a_2] \) accordingly.

**Assumption 3.10.** There exist \( b^* \in \mathbb{B} \) and \( a^* = (a^*_1, ..., a^*_q)^T \in \mathbb{A}^q \) such that for any \( b \in \mathbb{B} \) and \( a = (a_1, ..., a_q)^T \in \mathbb{A}^q \),

\[
\begin{align*}
\mathbb{P}\{m_{12}(\theta^p_0, \alpha_0, \beta_0)[a] - m_{22}(\theta^p_0, \alpha_0, \beta_0)[a^*][a] - m_{32}(\theta^p_0, \alpha_0, \beta_0)[b^*][a]\} = 0, \\
\mathbb{P}\{m_{13}(\theta^p_0, \alpha_0, \beta_0)[b] - m_{23}(\theta^p_0, \alpha_0, \beta_0)[a^*][b] - m_{33}(\theta^p_0, \alpha_0, \beta_0)[b^*][b]\} = 0.
\end{align*}
\]

Let

\[
\tilde{m}(\theta^p, \alpha, \beta) = m_1(\theta^p, \alpha, \beta) - m_2(\theta^p, \alpha, \beta)[a^*] - m_3(\theta^p, \alpha, \beta)[b^*] \tag{15}
\]

and \( \tilde{\Delta} = \{ \tilde{m}(\theta^p, \alpha, \beta) - \tilde{m}(\theta^p_0, \alpha_0, \beta_0) : \text{dis}((\theta^p, \alpha, \beta), (\theta^p_0, \alpha_0, \beta_0)) \leq \tilde{M}n^{-1/(2+\gamma)} \} \), where \( \tilde{M} \) is a constant.

**Assumption 3.11.** \( H_B(\rho, \tilde{\Delta}, \| \cdot \|_{L_2}) \leq \rho^{-\gamma} \).

**Assumption 3.12.** There exists a constant \( \tilde{L} \) such that \( \| f \|_\infty \leq \tilde{L} \) for every \( f \in \tilde{\Delta} \).

**Assumption 3.13.** \( 0 < \det(I^*) < \infty \), where \( \det \) denotes the determinant of a matrix,

\[
I^* = \left\{ \mathbb{P}\{m_{11}(\theta^p_0, \alpha_0, \beta_0) - m_{21}(\theta^p_0, \alpha_0, \beta_0)[a^*] - m_{31}(\theta^p_0, \alpha_0, \beta_0)[b^*]\} \right\}^{-1}
\times \mathbb{P}\{m_{1}(\theta^p_0, \alpha_0, \beta_0) - m_2(\theta^p_0, \alpha_0, \beta_0)[a^*] - m_3(\theta^p_0, \alpha_0, \beta_0)[b^*]\}^\otimes 2
\times \left\{ \mathbb{P}\{m_{11}(\theta^p_0, \alpha_0, \beta_0) - m_{21}(\theta^p_0, \alpha_0, \beta_0)[a^*] - m_{31}(\theta^p_0, \alpha_0, \beta_0)[b^*]\} \right\}^{-1},
\]

and \( \otimes 2 \) denotes “outer product”.

**Theorem 4.** Under Assumptions 2.3, 2.5, 3.1, 3.13 we have

\[
\sqrt{n}(\hat{\theta}^p - \theta^p_0) \xrightarrow{d} \mathcal{N}(0, I^*),
\]

where \( \xrightarrow{d} \) denotes “convergence in distribution”.

In the semiparametric theory, \( \tilde{m} \) in Assumption 3.10 is called “efficient score function”; see Ma and Kosorok (2005); van Der Vaart (1998) for detailed discussion on construction.
of $\tilde{m}$ and the tangent sets. Assumptions 3.11 and 3.12 are similar to Assumptions 3.8 and 3.9, respectively, and thus they can be verified by the same arguments. Assumption 3.13 corresponds to the nonsingular information condition for general maximum likelihood estimation.

Remark 5. Our theoretical results require that the design $\{(x_i, \theta_i)\}_{i=1}^n$ are i.i.d. from the uniform distribution $U(\Omega \times \Theta)$; see Assumption 3.1. In practice, space-filling designs are commonly used to achieve better uniformity than random sampling (Santner et al., 2018). Let $\{x_i\}_{i=1}^n$ and $\{\theta_i\}_{i=1}^m$ be space-filling designs on $\Omega$ and $\Theta$, respectively. A simple design strategy is to conduct the physical experiment on $\{x_i\}_{i=1}^n$ and to conduct the computer experiment on $\{(x_i, \theta_j)\}_{i=1,...,n,j=1,...,m}$. Consequently we implement our estimation method in Section 3.1 based on the dataset $\{(x_i, \theta_j, \delta_{ij})\}_{i=1,...,n,j=1,...,m}$ of size $m \times n$, where $\delta_{ij} = y_i - y^s(x_i, \theta_j)$, $i = 1, \ldots, n$, $j = 1, \ldots, m$.

4 Numerical examples

This section provides four numerical examples to illustrate our estimates of physical parameters under the discrepancy decomposition model. In our method the Gaussian kernel function in (12) is used with the parameter $\phi$ chosen by the cross-validation method.

4.1 A toy example

Let the physical system and the corresponding computer model be

$$
\begin{align*}
\eta(x) &= \theta^p x + \sin(2\pi x), \\
y^s(x, \theta) &= \theta x,
\end{align*}
$$

where the true value of $\theta^p$ is 3. We have

$$
\delta(x, \theta) = \sin(2\pi x) - x(\theta - \theta^p),
$$
Table 1: Numerical results in the toy example

| True value: 3 | $\sigma^2 = 0.01$ | Mean | MSE    | $\sigma^2 = 0.1$ | Mean | MSE    |
|---------------|------------------|------|--------|------------------|------|--------|
| n = 31        | 2.997            | 1.50×10^{-5} | 3.023 | 7.67×10^{-4}    |
| n = 61        | 2.998            | 9.64×10^{-6}  | 3.015 | 2.81×10^{-4}    |

which is a special case of the discrepancy decomposition model (3) with intrinsic discrepancy $\alpha(x) = \sin(2\pi x)$ and discrepancy coefficient function $\beta(x) = -x$. Moreover, some algebra yields $\int_0^1 \sin(2\pi x)dx = 0$ and $\int_0^1 (-x)dx \neq 0$, which satisfy Assumptions 2.1 ($c = 0$) and 2.2 respectively.

We first try the $L_2$ calibration method (Tuo and Wu, 2015, 2016). The true value $\theta^*_0$ under the $L_2$ calibration framework is defined as the minimizer of $\|\eta(\cdot) - y^*(\cdot, \theta)\|_{L_2(0,1)}^2$. It is not hard to obtain $\theta^*_0 = 2.522$ in this example. Clearly, the $L_2$ calibration method cannot give an accurate estimate for $\theta^p$.

We next conduct our calibration method based on observations $\{(x_i, \theta_j, \delta_{ij})\}_{i=1,...,n,j=1,...,m}$ from the design in Remark 5, where $x_i = (i-1)/(n-1)$, $i = 1, \ldots, n$, $\theta_j = 2 + 2(j-1)/(m-1)$, $j = 1, \ldots, m$, and the random error in the physical data is generated from $N(0, \sigma^2)$. We fix $m = 101$, and consider two values of $n$ (with $n = 31$ and $n = 61$) and two levels of $\sigma^2$ (with $\sigma^2 = 0.01$ and $\sigma^2 = 0.1$). The means and mean squared errors (MSEs) of our estimator $\hat{\theta}^p$ given by (5) over 50 replicates are reported in Table 1. We can see that our calibration method can accurately estimate the physical parameter.

4.2 The ball falling experiment

The second example is the free fall experiment introduced by Plumlee (2017), which has a real physical background. The experiment is conducted to estimate the gravitational acceleration $\theta^p$; see Plumlee (2017) for details. Let a ball be released at vertical height eight meters with initial velocity $-1$ m/s. The physical system, which describes the ball’s vertical position $\eta$
at time $x$, and its computer model are given by

\[
\begin{align*}
\eta(x) &= 5 \log \left\{ \frac{50}{49} - 50 \tanh^2 \left[ \sqrt{2}x + \tanh^{-1}(0.02) \right] / 49 \right\} / 2 + 8, \\
y^*(x, \theta) &= 8 - x - \theta x^2 / 2, \\
\end{align*}
\]

where the true value of $\theta^p$ is 10. We have

\[
\delta(x, \theta) = \frac{5}{2} \log \left\{ \frac{50}{49} - \frac{50}{49} \tanh^2 \left[ \sqrt{2}x + \tanh^{-1}(0.02) \right] / 2 \right\} + x + \frac{1}{2} \theta^p x^2 + \frac{1}{2} x^2 (\theta - \theta^p),
\]

which is a special case of the discrepancy decomposition model (3) with intrinsic discrepancy

\[
\alpha(x) = 5 \log \left\{ \frac{50}{49} - 50 \tanh^2 \left[ \sqrt{2}x + \tanh^{-1}(0.02) \right] / 49 \right\} / 2 + x + \theta^p x^2 / 2 \quad (16)
\]

and discrepancy coefficient function $\beta(x) = x^2 / 2$.

In this example we can compute the true value in $L_2$ calibration, $\theta^*_0 = 7.41$, which is different from the true value 10. For our method, different constraints on $\alpha(x)$ in (16) yield different values of $\theta^p$. First consider the default constraint with $c = 0$ in Assumption 2.1 which gives $\theta^p = 7.755$, closer to the true value 10 than $\theta^*_0$. Note that the computer
Table 2: Numerical results in the ball falling experiment

| True value:10 | $\int_0^1 \alpha(x)dx = 0$ | $\int_0^{0.5} \alpha(x)dx = 0$ | $\int_0^1 \alpha(x)dx = 0.374$ |
|---------------|-------------------------------|-------------------------------|-------------------------------|
|               | Mean    | MSE   | Mean    | MSE   | Mean    | MSE   |
| n = 31        | 7.61    | $2.09 \times 10^{-2}$ | 8.67    | $7.67 \times 10^{-2}$ | 9.81    | $3.72 \times 10^{-2}$ |
| n = 61        | 7.64    | $1.40 \times 10^{-2}$ | 8.86    | $8.32 \times 10^{-3}$ | 9.88    | $1.48 \times 10^{-2}$ |

model $y^a$ does not take the air resistance into account. It can be expected that the intrinsic discrepancy $\alpha(x)$ is increasing with time $x$, which indicates that $y^a$ becomes closer to the real physical system $\eta(x)$ for small $x$. Therefore, we can adopt the constraint $\int_0^\tau \alpha(x)dx = 0$ with small $\tau$ to improve our estimator. For instance, $\tau = 0.5$ gives $\theta^p = 8.941$, which is much better. We can also use a positive $c$ in Assumption 2.1 to improve our estimator since we known $\alpha(x) > 0$. Figure 1 shows the values of $\theta^p$ in our model with varying $\tau$ or $c$. It can be seen that our method always outperforms $L_2$ calibration. In particular, there exists an oracle value $c = 0.374$ such that $\theta^p$ achieves the true physical value 10.

Next, we use simulations to evaluate our calibration method based on observations $\{(x_i, \theta_j, \delta_{ij})\}_{i=1,...,n, j=1,...,m}$ from the design in Remark 5, where $x_i = (i - 1)/(n - 1)$, $i = 1, \ldots, n$, $\theta_j = 7 + 5(j - 1)/(m - 1)$, $j = 1, \ldots, m$, and the random error in the physical data is generated from $\mathcal{N}(0, 0.01^2)$. We fix $m = 201$, and consider two values of $n$ (with $n = 31$ and $n = 61$). Under the three constraints, $\int_0^1 \alpha(x)dx = 0$, $\int_0^{0.5} \alpha(x)dx = 0$, and $\int_0^1 \alpha(x)dx = 0.374$, the means and MSEs of our estimator $\hat{\theta}^p$ over 50 replicates are reported in Table 2. We can see that $\hat{\theta}^p$ can accurately estimate the value of $\theta^p$ with the corresponding constraint.
4.3 The simple machine model

The third example is the simple machine model in Brynjarsdóttir and O’Hagan (2014). The physical system and the computer model are given by

\[
\begin{align*}
\eta(x) &= \theta p x / (1 + 0.05 x), \\
y^*(x, \theta) &= \theta x,
\end{align*}
\]

where the true value of \( \theta p \) is 0.65. We have

\[
\delta(x, \theta) = \left( \frac{0.65 x}{1 + 0.05 x} - \theta p x \right) - x(\theta - \theta p),
\]

which is a special case of the discrepancy decomposition model (3) with intrinsic discrepancy \( \alpha(x) = 0.65 x / (1 + 0.05 x) - \theta p x \) and discrepancy coefficient function \( \beta(x) = -x \).

We first compute the true value in \( L_2 \) calibration, \( \theta_0^* = 0.5658 \), which is different from the true value 0.65. We then try the proposed method. Without prior information, we can adopt the default constraint \( \int_{0.2}^{4} \alpha(x) dx = \int_{0.2}^{4} \left( 0.65 x / (1 + 0.05 x) - \theta p x \right) dx = 0 \), which gives
θ^p = 0.5744. This is slightly closer to the true value 0.65 than θ^*_0.

If some physical data are available, we can obtain better constraints that yield better estimators of θ^p. Figure 2 shows the curve of the computer model and 31 observations from the true physical process. It can be seen that the computer model is close to the physical system for small x. We hence take the constraint ∫_τ^4 α(x)dx = 0 with τ < 4 to improve our estimator. For instance, taking τ = 1 gives θ^p = 0.628, which is much better.

Similar to Figure 1, Figure 3 shows the values of θ^p in our model with varying c and τ in constraints ∫_τ^4 α(x)dx = 0 and ∫_τ^4 α(x)dx = −c, respectively. We can see that θ^p from smaller τ or larger c in our model is closer to the true value, and our estimates are uniformly better than L_2 calibration. In particular, taking c = 0.6035 gives the exact true value θ^p = 0.65.

Next, we use simulations to evaluate our calibration method based on observations \{(x_i, θ_j, δ_{ij})\}_{i=1,...,n,j=1,...,m} from the design in Remark 5, where x_i = 0.2 + 3.8(i − 1)/(n − 1), i = 1, ..., n, θ_j = 0.55 + 0.2(j − 1)/(m − 1), j = 1, ..., m, and the random error in the physical data is generated from \mathcal{N}(0, 0.01^2). We fix m = 101, and consider two values of n (with n = 31 and n = 61). The means over 50 replicates of our estimators under three constraints are reported in Table 3. We also show the results from the KO (Kennedy and O’Hagan).
Table 3: Numerical comparison in the simple machine model

| True value: 0.65 | DD model with $\int_0^4 \alpha(x)dx = 0$ | DD model with $\int_0^1 \alpha(x)dx = 0$ | DD model with $\int_0^4 \alpha(x)dx = -0.6035$ | KO model | KO model with informative prior |
|-----------------|---------------------------------|---------------------------------|---------------------------------|--------|-------------------------------|
| $n = 31$        | Mean 0.574 Mean 0.629 Mean 0.650 Mean 0.535 Mean 0.641 | $n = 61$ Mean 0.574 Mean 0.629 Mean 0.650 Mean 0.533 Mean 0.638 |

(DD stands for “discrepancy decomposition”)

From Table 3 we can find that the KO model with informative prior performs well. However, such prior includes strong quantitative conditions on the derivatives of the discrepancy, which are not easy to obtain (Brynjarsdóttir and O’Hagan, 2014). In the proposed method we do not need so informative prior. Some roughly qualitative information can help our model to yield good estimates of $\theta^p$. Even without informative prior, our method is better than the original KO and $L_2$ calibration methods.

### 4.4 The spring vibration model

The last example is the spring vibration model, which also has a real physical background. Stretch one side of a spring and then release it. We want to estimate its elasticity coefficient $\theta$ by recording the displacement $y$ of the spring at time $x$. By Hooke’s law, the force on the spring is equal to $-\theta y$; by Newton’s law, the acceleration $a = \frac{d^2 y}{dx^2} = -\theta y/m_s$, where $m_s$ is the mass of the spring. Combining these, we have the following differential equation,

$$\frac{d^2 y}{dx^2} + \frac{\theta}{m_s} y = 0.$$  \hfill (17)

The above equation does not take the spring’s resilience into account. Note that the spring is subjected to resistance proportional to the speed. The spring vibration can be better described by the following differential equation,

$$\frac{d^2 y}{dx^2} + \frac{k}{m_s} \frac{dy}{dx} + \frac{\theta}{m_s} y = 0,$$  \hfill (18)
where \( k \) is the resistance coefficient. We treat the solutions to (18) and (17) as the real physical system and its computer model, respectively. Let \( m_s = 1 \), \( k = 0.5 \), and the initial displacement be 1. The physical system and its computer model are given by

\[
\eta(x) = \exp(-0.5x) \cos(\sqrt{\theta^p}x), \quad x \in [0, 6.5], \quad \theta \in [1, 2.5],
\]

where the true value of \( \theta^p \) is 2. Then we have

\[
\delta(x, \theta) = \exp(-0.5x) \cos(\sqrt{\theta^p}x) - \cos(\sqrt{\theta}x).
\]

Note that here \( \delta(x, \theta) \) does not satisfy our discrepancy decomposition model (3).

First, we can compute the true value in \( L_2 \) calibration, \( \theta^*_0 = 1.76 \). Next, we use simulations to evaluate our calibration method based on observations \( \{(x_i, \theta_j, \delta_{ij})\}_{i=1}^{n} \) \( \{j=1}^{m} \) from the design in Remark 5, where \( x_i = 6.5(i - 1)/(n - 1), \quad i = 1, \ldots, n, \quad \theta_j = 1 + 1.5(j - 1)/(m - 1), \quad j = 1, \ldots, m, \) and the random error in the physical data is generated from \( \mathcal{N}(0, 0.01^2) \). We fix \( m = 101 \), and consider two values of \( n \) (with \( n = 31 \) and \( n = 61 \)). Without any prior information, we use the default constraint \( \int_0^{6.5} \alpha(x)dx = 0 \). The means and MSEs of our estimator \( \hat{\theta}^p \) over 50 replicates are reported in Table 4. We can see that our calibration method based on the discrepancy decomposition model is still better than \( L_2 \) calibration.
Table 5: Comparison of existing methods with our method in two aspects

|                        | Study true value of $\theta^p$ | Identifiability |
|------------------------|--------------------------------|-----------------|
| KO model               | ×                              | ×               |
| KO model with informative prior | ✓                              | ×               |
| L_2 calibration        | ⊚                              | ✓               |
| DD model               | ⊚                              | ✓               |
| DD model with informative prior | ✓                              | ✓               |

(DD stands for “discrepancy decomposition”)

5 Conclusion and discussion

In this article we develop a new frequentist framework for physical parameter calibration. This framework builds the discrepancy decomposition model for the discrepancy function $\delta$, which decomposes $\delta$ into two parts: the intrinsic discrepancy and parametric discrepancy. Under the framework, $\theta^p$ and $\delta$ are both well and meaningfully defined. Using the kernel method, our framework yields their estimators with good performance. On the theoretical aspect, the estimators enjoy the optimal convergence rates under reasonable conditions. On the numerical aspect, several examples indicate that our estimator is closer to the true value of $\theta^p$ than existing methods.

Brynjarsdóttir and O’Hagan (2014) stated the following three objectives of calibration: to study the true values of the physical parameters, to predict the physical system’s behaviour within the scope of the observations (interpolation), and outside the scope of the observations (extrapolation); see also Wong et al. (2017). Note that all existing popular methods possess the interpolation property, but cannot perform well in extrapolation. Here we focus on the first objective, and compare the identifiability property and estimation accuracy of the popular KO model, $L_2$ calibration, and our discrepancy decomposition model in Table 5. The notation ⊚ in the table means that the method works well only under certain conditions. From the table, the KO model lacks identifiability, and $L_2$ calibration can find the true value of $\theta^p$ only when the model discrepancy is negligible (Wong et al., 2017). Compared with them, the proposed method possesses both identifiability and accuracy. Even with the default constraint, it yields better estimates than existing methods. With informative prior,
we can modify the constraint to produce exact estimates of the true physical parameters.

“All models are wrong, but some are useful.” When our discrepancy decomposition model does not hold, the true value of \( \theta^p \) under our framework is actually defined as the solution to

\[
\min_{(\theta^p, \alpha, \beta) \in \Theta \times A \times B} \left\| \eta(x) - y^s(x, \theta) - \alpha(x) - \beta^T(x)(\theta - \theta^p) \right\|_{L_2(\Omega \times \Theta)}.
\]

Therefore, our method can be viewed as a high-order version of \( L_2 \) calibration in approximating the discrepancy. This may be the reason why our method is better than \( L_2 \) calibration even when the proposed model does not hold; see the example in Section 4.4. In addition, the discrepancy decomposition model provides another angle to look into the calibration problem, and some future researches can be developed along this direction.

**Appendix A: Proof of Theorem 1**

*Proof.* Suppose

\[
\tilde{\alpha}(x) + \tilde{\beta}^T(x)(\theta - \theta^p) = \bar{\alpha}(x) + \tilde{\beta}^T(x)(\theta - \theta^p),
\]

which can be rewritten as

\[
(\tilde{\beta}(x) - \bar{\beta}(x))^T(\theta - \theta^p) = \tilde{\beta}^T(x)(\theta^p - \bar{\theta}^p) + \tilde{\alpha}(x) - \bar{\alpha}(x).
\]

Note that the left side of (20) relies on \( \theta \), while the right side is independent of \( \theta \). Since \( \theta \) is valued in an infinite set, the equation holds if and only if

\[
\tilde{\beta}(x) = \bar{\beta}(x).
\]

Write \( \beta(x) = \tilde{\beta}(x) = \bar{\beta}(x) \), and plug this into (19). We have

\[
\beta^T(x)(\bar{\theta}^p - \bar{\theta}^p) = \tilde{\alpha}(x) - \bar{\alpha}(x).
\]
By Assumption 2.3, integrating $x$ over $\Omega$ on both sides yields
\[
\int_{\Omega_t} \beta^T(x)(\tilde{\theta}^p - \bar{\theta}^p)dx = 0, \quad t = 1, \ldots, q.
\]
By Assumption 2.4, the above equation implies $\tilde{\theta}^p = \bar{\theta}^p$, and then $\tilde{\alpha}(x) = \bar{\alpha}(x)$ by (21). 

Appendix B: Proofs in Section 3

B.1 Some notation and lemmas

In this subsection, we present some notation and lemmas that are useful to prove Theorem 2. Let
\[
(\epsilon, \delta)_n = \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \delta(x_i, \theta_i), \quad \|\epsilon\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} \epsilon_i^2,
\]
\[
\|\delta - \delta_0\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} (\delta_i - \delta_0(x_i, \theta_i))^2,
\]
\[
\|\delta - \hat{\delta}\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} (\delta_i - \hat{\delta}(x_i, \theta_i))^2.
\]

The following lemma will play a key role in the proof of Theorem 2. It can be found in Lemma 8.4 of van De Geer (2000).

**Lemma 1.** Suppose $\epsilon_1, \ldots, \epsilon_n$ is uniformly sub-Gaussian, $H(\rho, \Delta, \|\cdot\|_n) \leq R\rho^{-\gamma}$ for all $\rho > 0$, and $\sup_{\delta \in \Delta} \|\delta\|_n \leq L$, where $R > 0$, $\gamma \in (0, 2)$, and $L > 0$ are constants. Then for some constant $c$ depending on $R, \gamma, L, K$, and $\sigma_0$, we have
\[
P \left( \sup_{\delta \in \Delta} \frac{\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \epsilon_i \delta(x_i, \theta_i)}{\|\delta\|_n^{1-\frac{\gamma}{2}}} \geq T \right) \leq c \exp \left( -\frac{T^2}{c^2} \right) \quad \text{for all } T \geq c.
\]

**Lemma 2.** Under Assumptions 2.3, 2.4 and 3.1, 3.6, we have
\[ \| \hat{\delta} - \delta_0 \|_n = \mathcal{O}_p(\lambda_n). \] (22)

**Proof.** Under Assumption 3.2 and 3.4, by Lemma 1, we get
\[
\sup_{\delta \in \Delta} \frac{|(\epsilon, \delta - \delta_0)_n|}{\| \delta - \delta_0 \|_{1/n}^{1 - \gamma/2}} = \mathcal{O}_p(n^{-\frac{1}{2}}). \tag{23}
\]

By the definition of \( \hat{\delta} \), we have
\[
\| \delta - \hat{\delta} \|_n^2 + \lambda_n^2 \left( \| \hat{\alpha} \|_{\mathcal{N}_k}^2 + \sum_{j=1}^q \| \hat{\beta}_j \|_{\mathcal{N}_k}^2 \right) \leq \| \delta - \delta_0 \|_n^2 + \lambda_n^2 \left( \| \alpha_0 \|_{\mathcal{N}_k}^2 + \sum_{j=1}^q \| \beta_{0j} \|_{\mathcal{N}_k}^2 \right). \tag{24}
\]

Since \( \Omega \) is compact and kernel function \( k \) is symmetric positive, \( \mathcal{N}_k(\Omega) \) has a continuous linear embedding into \( L_2(\Omega) \) (Tuo, 2019). Specifically, for any \( f \in \mathcal{N}_k(\Omega) \), we have
\[
\| f \|_{\mathcal{N}_k(\Omega)} \leq \left( \int_{\Omega} k(x, x) \, dx \right) \| f \|_{L_2}. 
\]

Note that \( \int_{\Omega} k(x, x) \, dx \) is a constant. Hence, for each \( \alpha \in A, \beta \in B, \) and \( v \in \mathbb{R}^q, \) \( \| \alpha \|_{L_2}, \| \alpha \|_{\mathcal{N}_k}, \| \beta^T v \|_{L_2} \) and \( \| \beta^T v \|_{\mathcal{N}_k} \) are all finite. Then, rewrite (24) as
\[
\| \delta - \hat{\delta} \|_n^2 + \lambda_n^2 \left( \| \hat{\alpha} \|_{\mathcal{N}_k}^2 + \sum_{j=1}^q \| \hat{\beta}_j \|_{\mathcal{N}_k}^2 \right) \leq 2(\epsilon, \delta - \delta_0)_n + \lambda_n^2 \left( \| \alpha_0 \|_{\mathcal{N}_k}^2 + \sum_{j=1}^q \| \beta_{0j} \|_{\mathcal{N}_k}^2 \right). \tag{25}
\]

If \( \| \hat{\alpha} \|_{\mathcal{N}_k}^2 + \sum_{j=1}^q \| \hat{\beta}_j \|_{\mathcal{N}_k}^2 \geq \| \alpha_0 \|_{\mathcal{N}_k}^2 + \sum_{j=1}^q \| \beta_{0j} \|_{\mathcal{N}_k}^2 \), combining (23) and (25) yields
\[
\| \delta - \delta_0 \|_n^2 \leq \mathcal{O}_p(n^{-\frac{1}{2}}) \| \delta - \delta_0 \|_{1/n}^{1 - \gamma/2},
\]
which implies (22) straightforwardly.
If \( \| \hat{\delta} \|_{X_k}^2 + \sum_{j=1}^q \| \hat{\beta}_j \|_{X_k}^2 < \| \alpha_0 \|_{X_k}^2 + \sum_{j=1}^q \| \beta_{0j} \|_{X_k}^2 \), combining (23) and (25) yields
\[
\| \hat{\delta} - \delta_0 \|_n \leq O_p(n^{-\frac{1}{2}}) \| \hat{\delta} - \delta_0 \|_n^{1-\frac{1}{2}} + \lambda_n^2 \left( \| \alpha_0 \|_{X_k}^2 + \sum_{j=1}^q \| \beta_{0j} \|_{X_k}^2 \right).
\]

Therefore, either
\[
\| \hat{\delta} - \delta_0 \|_n \leq O_p(n^{-\frac{1}{2}}) \| \hat{\delta} - \delta_0 \|_n^{1-\frac{1}{2}} \tag{26}
\]
or
\[
\| \hat{\delta} - \delta_0 \|_n \leq \lambda_n^2 \left( \| \alpha_0 \|_{X_k}^2 + \sum_{j=1}^q \| \beta_{0j} \|_{X_k}^2 \right). \tag{27}
\]

Clearly, (27) implies (22), and (26) gives \( \| \hat{\delta} - \delta_0 \|_n = O_p(n^{-\frac{1}{2}}) = O_p(\lambda_n) \). This completes the proof.

The proof of Theorem 3 will use the following two lemmas, which can be found in Theorem 3.2.5 and Lemma 3.4.2 of van Der Vaart and Wellner (2000).

**Assumption 5.1.** For sufficiently small \( \tau \), the centered process \( (\mathbb{P}_n - \mathbb{P})(m(\theta^p, \alpha, \beta) - m(\theta^p_0, \alpha_0, \beta_0)) \) satisfies
\[
\mathbb{E} \sup_{\text{dis} ((\theta^p, \alpha, \beta), (\theta^p_0, \alpha_0, \beta_0)) \leq \tau} | \sqrt{n}(\mathbb{P}_n - \mathbb{P})(m(\theta^p, \alpha, \beta) - m(\theta^p_0, \alpha_0, \beta_0)) | \lesssim \phi_n(\tau),
\]
for function \( \phi_n \) such that \( \tau \mapsto \phi_n(\tau)/\tau^\nu \) is decreasing for some \( \nu < 2 \) (not depending on \( n \)), where \( m(\cdot, \cdot, \cdot) \) and \( \text{dis} \) are defined in (13) and (14), respectively.

**Lemma 3.** Under Assumptions [3.7 and 5.1], suppose there exists a sequence \( \{r_n\} \) satisfying
\[
r_n^2 \phi_n \left( \frac{1}{r_n} \right) \leq \sqrt{n},
\]
where \( \phi_n \) is defined in Assumption [5.1]. If \( \mathbb{P}_n(m(\theta^p, \hat{\alpha}, \hat{\beta}) - m(\theta^p_0, \alpha_0, \beta_0)) = O_p(r_n^{-2}) \) and
\((\hat{\theta}^p, \hat{\alpha}, \hat{\beta})\) converges to \((\theta^p_0, \alpha_0, \beta_0)\) in probability, then

\[
r_n \text{dis}((\hat{\theta}^p, \hat{\alpha}, \hat{\beta}), (\theta^p_0, \alpha_0, \beta_0)) = O_p(1).
\]

**Lemma 4.** Let \(\mathcal{F}\) be a class of measurable functions such that \(\mathbb{P}f^2 < \tau^2\) and \(\|f\|_\infty \leq M\) (\(M\) is a constant) for every \(f \in \mathcal{F}\). Then

\[
\mathbb{E} \sup_{f \in \mathcal{F}} |\sqrt{n}(\mathbb{P}_n - \mathbb{P})f| \lesssim J_B(\tau, \mathcal{F}, \|\cdot\|_{L_2}) \left(1 + M \frac{J_B(\tau, \mathcal{F}, \|\cdot\|_{L_2})}{\tau^2 \sqrt{n}}\right),
\]

where \(J_B(\tau, \mathcal{F}, \|\cdot\|_{L_2}) = \int_0^\tau \sqrt{1 + H_B(\rho, \mathcal{F}, \|\cdot\|_{L_2})} d\rho\).

**B.2 Proof of Theorem 2**

**Proof.** Under Assumption 3.5, applying Lemma 5.16 of van De Geer (2000) gives

\[
\limsup_{n \to \infty} \mathbb{P} \left( \sup_{\delta \in \Delta, \|\delta\|_{L_2} > 2^{\rho_n}/\kappa} \left| \frac{\|\delta\|_n}{\|\delta\|_{L_2}} - 1 \right| \geq \xi \right) = 0 \tag{28}
\]

for each \(0 < \xi < 1\). Then, combining (28) and Lemma 2 gives (10).

Next, we prove (11). We only consider the case of \(q = 2\), and the proof for other \(q\) is similar. Let \(\mathbb{P}_\epsilon\) and \(\mathbb{P}_u\) denote the probability measures induced by the random error \(\epsilon\) and the uniform distribution on \(\Omega \times \Theta\), respectively.

Note that (10) implies \(\|\hat{\delta} - \delta_0\|_{L_2} \xrightarrow{\mathbb{P}_\epsilon} 0\), where \(\xrightarrow{\mathbb{P}_\epsilon}\) denotes “convergence in probability measure \(\mathbb{P}_\epsilon\)”. Let \(\hat{\alpha}'\) be any subsequence of \(\hat{\alpha}\), and \(\hat{\beta}_j'\) and \(\hat{\theta}_j'\) be the corresponding subsequence of \(\hat{\beta}_j\) and \(\hat{\theta}_j^p\) \((j = 1, 2)\). Consequently, \(\hat{\delta}' = \hat{\alpha}' + \sum_{j=1}^2 (\theta_j - \hat{\theta}_j')\hat{\beta}_j'\) is a subsequence of \(\hat{\delta}\). By the relationship between “convergence in probability” and “convergence almost surely”, \(\hat{\delta}'\) has a subsequence \(\hat{\delta}'' = \hat{\alpha}'' + \sum_{j=1}^2 (\theta_j - \hat{\theta}_j'')\hat{\beta}_j''\) such that \(\|\hat{\delta}'' - \delta_0\|_{L_2} \xrightarrow{\text{a.s.}\epsilon} 0\), where a.s.\(\epsilon\) stands for “almost surely in the sample space \(\Xi\) of \(\epsilon\)”. Then there exists a subset \(\Xi_1 \subset \Xi\) of probability one such that for every \(\omega \in \Xi_1\), \(\|\hat{\delta}''[\omega] - \delta_0\|_{L_2} \to 0\).

For fixed \(\omega \in \Xi_1\), we have \(\hat{\delta}''[\omega] \xrightarrow{\mathbb{P}_u} \delta_0\), where \(\xrightarrow{\mathbb{P}_u}\) denotes “convergence in probability measure \(\mathbb{P}_u\)”. By the relationship between “convergence in probability” and “convergence
almost surely” again, any subsequence of \( \hat{\delta}''[\omega] \) has a subsequence that converges to \( \delta_0 \) almost surely in \( \Omega \times \Theta \), and such a sequence is still a subsequence of \( \hat{\delta}'[\omega] \). Without loss of generality, we write \( \hat{\delta}''[\omega] \xrightarrow{a.s.u} \delta_0 \), where \( a.s.u \) stands for “almost surely in \( \Omega \times \Theta \).

Let \( \tilde{\theta} = (\tilde{\theta}_1, \tilde{\theta}_2)^T \), \( \hat{\theta} = (\hat{\theta}_1, \hat{\theta}_2)^T \in \Theta \) with \( \tilde{\theta}_1 \neq \hat{\theta}_1 \) and \( \tilde{\theta}_2 \neq \hat{\theta}_2 \). We have

\[
\hat{\delta}''(x, (\tilde{\theta}_1, \tilde{\theta}_2)^T)[\omega] = \left( \hat{\alpha}''(x) + (\tilde{\theta}_1 - \hat{\theta}_1)\hat{\beta}'_1(x) + (\tilde{\theta}_2 - \hat{\theta}_2)\hat{\beta}'_2(x) \right)[\omega],
\]

(29)

\[
\hat{\delta}''(x, (\tilde{\theta}_1, \hat{\theta}_2)^T)[\omega] = \left( \hat{\alpha}''(x) + (\tilde{\theta}_1 - \hat{\theta}_1)\hat{\beta}'_1(x) + (\hat{\theta}_2 - \hat{\theta}_2)\hat{\beta}'_2(x) \right)[\omega],
\]

(30)

and

\[
\hat{\delta}''(x, (\hat{\theta}_1, \tilde{\theta}_2)^T)[\omega] = \left( \hat{\alpha}''(x) + (\hat{\theta}_1 - \hat{\theta}_1)\hat{\beta}'_1(x) + (\tilde{\theta}_2 - \hat{\theta}_2)\hat{\beta}'_2(x) \right)[\omega],
\]

(31)

converge to \( \delta_0(x, (\tilde{\theta}_1, \tilde{\theta}_2)^T) \), \( \delta_0(x, (\hat{\theta}_1, \tilde{\theta}_2)^T) \), and \( \delta_0(x, (\tilde{\theta}_1, \hat{\theta}_2)^T) \), respectively. Let (29) - (30) and (29) - (31), and this yields

\[
\hat{\beta}'_1[\omega] \xrightarrow{a.s.u} \beta_{01} \quad \text{and} \quad \hat{\beta}'_2[\omega] \xrightarrow{a.s.u} \beta_{02}.
\]

(32)

By noting that \( \Theta \) is bounded and that \( \hat{\alpha}'' = \hat{\delta}'' - (\hat{\theta}_1 - \hat{\theta}_1')\hat{\beta}'_1 - (\hat{\theta}_2 - \hat{\theta}_2')\hat{\beta}'_2 \), (32) implies \( \hat{\alpha}''[\omega] \xrightarrow{a.s.u} \alpha_0 \). Furthermore, by Assumption 2.5 we have \( \hat{\theta}'_j[\omega] \longrightarrow \theta^p_{0j}, \quad j = 1, 2 \).

By the relationship between “convergence in probability” and “convergence almost surely” and the dominated convergence theorem, we have

\[
\|\hat{\theta}' - \theta'^p_0\| \xrightarrow{P} 0, \quad \|\hat{\alpha} - \alpha_0\|_{L_2} \xrightarrow{P} 0 \quad \text{and} \quad \|\hat{\beta}'_j - \beta_{0j}\|_{L_2} \xrightarrow{P} 0, \quad j = 1, 2.
\]

This completes the proof of (11).
B.3 Proof of Theorem 3

Proof. We apply Lemma 3 to prove Theorem 3 and need to check the conditions of Lemma 3. For each $m(\theta^p, \alpha, \beta) - m(\theta^p_0, \alpha_0, \beta_0) \in \Delta_T$, we have

$$\mathbb{P}[m(\theta^p, \alpha, \beta) - m(\theta^p_0, \alpha_0, \beta_0)]^2$$

$$= \mathbb{P}[2\delta_e - \alpha - \beta^T(\theta - \theta^p) - \alpha_0 - \beta_0^T(\theta - \theta^p_0)]^2 \left[\alpha_0 - \alpha + \beta_0^T(\theta - \theta^p) - \beta^T(\theta - \theta^p)\right]^2$$

$$\lesssim \mathbb{P}[\alpha_0 - \alpha + \beta_0^T(\theta - \theta^p_0) - \beta_0^T(\theta - \theta^p) - \beta^T(\theta - \theta^p)]^2$$

$$= \mathbb{P}[\alpha_0 - \alpha + \beta_0^T(\theta^p - \theta^p_0) + (\beta_0 - \beta)^T(\theta - \theta^p)]^2$$

$$= \mathbb{P}[(\alpha_0 - \alpha)^2 + (\beta_0^T(\theta^p - \theta^p_0))^2 + ((\beta_0 - \beta)^T(\theta - \theta^p))^2$$

$$+ 2(\alpha_0 - \alpha)(\beta_0^T(\theta^p - \theta^p_0)) + 2(\alpha_0 - \alpha)(\beta_0 - \beta)^T(\theta - \theta^p)$$

$$+ 2(\beta_0^T(\theta^p - \theta^p_0))(\beta_0 - \beta)^T(\theta - \theta^p)] \quad (33)$$

Note that

$$\mathbb{P}(\alpha_0 - \alpha)^2 \leq \tau^2, \quad \mathbb{P}(\beta_0^T(\theta^p - \theta^p_0))^2 \leq M_1^2 \tau^2, \quad \text{and} \quad \mathbb{P}((\beta_0 - \beta)^T(\theta - \theta^p))^2 \leq qM_2^2 \tau^2,$$

where $M_1 = \max_{j, x} |\beta_{0j}(x)|$ and $M_2 = \max_{j, \theta} |\theta_j|$, which yield

$$2\mathbb{P}(\alpha_0 - \alpha)(\beta_0^T(\theta^p - \theta^p_0)) \leq M_1 \left(\mathbb{P}(\alpha_0 - \alpha)^2 + \mathbb{P}(\theta^p - \theta^p_0)^2\right) \leq 2M_1 \tau^2,$$

$$2\mathbb{P}(\alpha_0 - \alpha)(\beta_0 - \beta)^T(\theta - \theta^p) \leq \mathbb{P}(\alpha_0 - \alpha)^2 + \mathbb{P}((\beta_0 - \beta)^T(\theta - \theta^p))^2 \leq (1 + qM_2^2) \tau^2,$$

and

$$2\mathbb{P}((\beta_0^T(\theta^p - \theta^p_0))(\beta_0 - \beta)^T(\theta - \theta^p)) \leq \mathbb{P}(\beta_0^T(\theta^p - \theta^p_0))^2 + \mathbb{P}((\beta_0 - \beta)^T(\theta - \theta^p))^2 \leq (M_1^2 + qM_2^2) \tau^2.$$

Combining them with (33), we get

$$\mathbb{P}(m(\theta^p, \alpha, \beta) - m(\theta^p_0, \alpha_0, \beta_0))^2 \lesssim \tau^2.$$
By Lemma 4 and Assumption 3.8, we have

\[
\begin{align*}
\mathbb{E} \sup_{\text{dis}((\theta^p, \alpha, \beta), (\theta^0, \alpha_0, \beta_0)) \leq \tau} & |\sqrt{n}(\mathbb{P}_n - \mathbb{P})(m(\theta^p, \alpha, \beta) - m(\theta^0, \alpha_0, \beta_0))| \\
\lesssim & \ J_B(\tau, \Delta, \|\cdot\|_{L_2}) \left(1 + \tilde{L} J_B(\tau, \Delta, \|\cdot\|_{L_2}) \frac{\tau^2}{\tau \sqrt{n}}\right) \\
\lesssim & \ \tau^{1-\gamma/2} + \tilde{L} n^{-\frac{1}{2}} \tau^{-\gamma}. \quad (34)
\end{align*}
\]

Hence we can take \( \phi_n(\tau) = \tau^{1-\gamma/2} + \tilde{L} n^{-\frac{1}{2}} \tau^{-\gamma} \) in Assumption 5.1, and verify \( n^{2/(2+\gamma)} \phi_n(n^{-1/(2+\gamma)}) \leq \sqrt{n} \). By \( \lambda_n = O(n^{-1/(2+\gamma)}) \), we have

\[
\mathbb{P}_n(m(\hat{\theta}^p, \hat{\alpha}, \hat{\beta}) - m(\theta^0, \alpha_0, \beta_0)) = O_p(n^{-\frac{2}{2+\gamma}}). \quad (35)
\]

Note that we have proven that \((\hat{\theta}^p, \hat{\alpha}, \hat{\beta})\) converges to \((\theta^0, \alpha_0, \beta_0)\) in Theorem 2. Combining this with (35), by Lemma 3 we obtain

\[
\text{dis}((\theta^p, \alpha, \beta), (\theta^0, \alpha_0, \beta_0)) = O_p(n^{-\frac{1}{2+\gamma}}).
\]

By the definition of \text{dis} in (14), the above equation implies Theorem 3. \( \square \)

**B.4 Proof of Theorem 4**

*Proof.* Under Assumptions 3.11 and 3.12, similar to the proof of (34), we get

\[
\sup_{\text{dis}((\theta^p, \alpha, \beta), (\theta^0, \alpha_0, \beta_0)) \leq \tilde{M} n^{-1/(2+\gamma)}} |\sqrt{n}(\mathbb{P}_n - \mathbb{P})(\bar{m}(\theta^p, \alpha, \beta) - \bar{m}(\theta^0, \alpha_0, \beta_0))| = o_p(1), \quad (36)
\]

where \( \bar{m}(\cdot, \cdot, \cdot) \) is defined in (15). Note that we have shown that \( \text{dis}((\hat{\theta}^p, \hat{\alpha}, \hat{\beta}), (\theta^0, \alpha_0, \beta_0)) = O_p(n^{-\frac{1}{2+\gamma}}) \) in Theorem 3. Combining this with (36) gives

\[
\sqrt{n}(\mathbb{P}_n - \mathbb{P})\bar{m}(\hat{\theta}^p, \hat{\alpha}, \hat{\beta}) = \sqrt{n}(\mathbb{P}_n - \mathbb{P})\bar{m}(\theta^0, \alpha_0, \beta_0) + o_p(1). \quad (37)
\]
On the other hand, note that

$$\frac{\partial}{\partial \theta^p} \left( \mathbb{P}_n m(\theta^p, \hat{\alpha}, \hat{\beta}) + \lambda_n^2 (\|\hat{\alpha}\|^2_{\mathcal{N}_0} + \sum_{s=1}^q \|\hat{\beta}_s\|^2_{\mathcal{N}_0}) \right) \bigg|_{\theta^p = \theta^*} = 0.$$ 

Since $\lambda_n = O(n^{-1/(2+\epsilon)})$, we have

$$\mathbb{P}_n m_1(\hat{\theta}^p, \hat{\alpha}, \hat{\beta}) = O(n^{-\frac{2}{2+\epsilon}}).$$

In the same way, we get

$$\mathbb{P}_n m_2(\hat{\theta}^p, \hat{\alpha}, \hat{\beta})[a^*] = O(n^{-\frac{2}{2+\epsilon}}) \quad \text{and} \quad \mathbb{P}_n m_3(\hat{\theta}^p, \hat{\alpha}, \hat{\beta})[b^*] = O(n^{-\frac{2}{2+\epsilon}}).$$

It follows that

$$\mathbb{P}_n \tilde{m}(\hat{\theta}^p, \hat{\alpha}, \hat{\beta}) = o_p(n^{-\frac{1}{2}}). \quad (38)$$

Combining (37) and (38) yields

$$\sqrt{n} \mathbb{P} \left( \tilde{m}(\hat{\theta}^p, \hat{\alpha}, \hat{\beta}) - \tilde{m}(\theta_{0,p}^p, \alpha_0, \beta_0) \right) = -\sqrt{n} \mathbb{P}_n \tilde{m}(\theta_{0,p}^p, \alpha_0, \beta_0) + o_p(1). \quad (39)$$

The left side of (39) can be written as

$$\mathbb{P} \left( m_{11}(\theta_{0,p}^p, \alpha_0, \beta_0) - m_{21}(\theta_{0,p}^p, \alpha_0, \beta_0)[a^*] - m_{31}(\theta_{0,p}^p, \alpha_0, \beta_0)[b^*] \right) \times (\hat{\theta}^p - \theta_{0,p}^p) +$$

$$\mathbb{P} \left( m_{12}(\theta_{0,p}^p, \alpha_0, \beta_0)[a] - m_{22}(\theta_{0,p}^p, \alpha_0, \beta_0)[a^*] \left[ \frac{\alpha - \alpha_0}{\|\alpha - \alpha_0\|_{L_2}} \right] - m_{32}(\theta_{0,p}^p, \alpha_0, \beta_0)[b^*] \right) \times \|\hat{\alpha} - \alpha_0\|_{L_2} +$$

$$\mathbb{P} \left( m_{13}(\theta_{0,p}^p, \alpha_0, \beta_0)[b] - m_{23}(\theta_{0,p}^p, \alpha_0, \beta_0)[a^*] \left[ \frac{\beta - \beta_0}{\|\beta - \beta_0\|_{L_2}} \right] - m_{33}(\theta_{0,p}^p, \alpha_0, \beta_0)[b^*] \right) \times \sum_{s=1}^q \|\hat{\beta}_s - \beta_{0,s}\|_{L_2}$$

$$= O(\|\hat{\theta}^p - \theta_{0,p}^p\|^2) + O(\|\hat{\alpha} - \alpha_0\|^2_{L_2}) + O((\sum_{s=1}^q \|\hat{\beta}_s - \beta_{0,s}\|_{L_2})^2) - \mathbb{P}_n \tilde{m}(\theta_{0,p}^p, \alpha_0, \beta_0) + o_p(n^{-\frac{1}{2}}).$$

36
By Theorem 3 and Assumption 3.10, we combine the above equation with (39), and get

\[ P_m(\theta_0^p, \alpha_0, \beta_0) - m_2(\theta_0^p, \alpha_0, \beta_0)[a^*] - m_3(\theta_0^p, \alpha_0, \beta_0)[b^*]) \times (\hat{\theta}^p - \theta_0^p) \]
\[ = -P_n\tilde{m}(\theta_0^p, \alpha_0, \beta_0) + o_p(n^{-\frac{1}{2}}), \]

which implies

\[ \sqrt{n}(\hat{\theta}^p - \theta_0^p) = -\sqrt{n}\left\{ P_m(\theta_0^p, \alpha_0, \beta_0) - m_2(\theta_0^p, \alpha_0, \beta_0)[a^*] - m_3(\theta_0^p, \alpha_0, \beta_0)[b^*]) \right\}^{-1} \]
\[ \times P_n\tilde{m}(\theta_0^p, \alpha_0, \beta_0) + o_p(1). \]

This completes the proof of Theorem 4. □

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