ANOTHER LOOK AT STATISTICAL CALIBRATION: A NON-ASYMPTOTIC THEORY AND PREDICTION-ORIENTED OPTIMALITY

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We provide another look at the statistical calibration problem in computer models. This viewpoint is inspired by two overarching practical considerations of computer models: (i) many computer models are inadequate for perfectly modeling physical systems, even with the best-tuned calibration parameters; (ii) only a finite number of data points are available from the physical experiment associated with a computer model. Following this new line of thinking, we provide a non-asymptotic theory and derive a prediction-oriented calibration method. Our calibration method minimizes the predictive mean squared error for a finite sample size with statistical guarantees. We introduce an algorithm to perform the proposed calibration method and connect it to existing Bayesian calibration methods. Synthetic and real examples are provided to corroborate the derived theory and illustrate some advantages of the proposed calibration method.

1. Introduction. In engineering and sciences, computer models are increasingly used for studying complex physical systems such as those in cosmology, weather forecasting, material science, and shock physics [17]. Let $Y$ denote the output from a physical system $\zeta(\cdot)$ with a set of inputs $X$. For $i = 1, \ldots, n$, assume $Y_i$ has the following form:

$$Y_i = \zeta(X_i) + \varepsilon_i,$$

(1.1)

where the random error $\varepsilon_i$ follows the independent $N(0, \sigma^2)$ distribution and the design points $X_i$ has support on $\Omega = [0, 1]^d$. Let $\eta(x, \theta)$ denote a computer model for approximating $\zeta(x)$ with inputs $x \in \Omega$ and calibration parameters $\theta \in \Theta \subset \mathbb{R}^p$. The values of $\theta$ cannot be directly measured and typically unknown in the physical data. As George Box famously stated “All models are wrong, but essentially some are useful”, even the best computer

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models are only approximations of reality. It is possible to enhance the quality of the computer model $\eta(x, \theta)$ by tuning or calibrating the calibration parameters $\theta$. But in most practical scenarios, the computer output $\eta(x, \theta)$ cannot fit the physical response $\zeta(x)$ perfectly, regardless how the calibration parameters $\theta$ are best tuned [9, 17].

Another practical fact is only a finite number, $n$, of data points are available from the physical experiment in (1.1) to tune $\theta$.

By simultaneously following these two practical considerations, we take a new look at the calibration problem. Our purpose is to optimally predict $\zeta(\cdot)$ by calibrating $\theta$ in $\eta(\cdot, \theta)$ and estimating the model discrepancy $\zeta(x) - \eta(x, \theta)$ based on a finite number of physical data. To this end, we use nonparametric approaches to modeling the physical system and the discrepancy function. We establish a non-asymptotic minimax estimation risk for nonparametric regression and achieve the optimal risk by using regularized estimators in the reproducing kernel Hilbert space (RKHS) [1, 21]. We show that our problem of prediction oriented calibration is equivalent to finding the minimizer of the model discrepancy under the RKHS norm. We further establish an exact statistical guarantee in the sense that for a finite sample of physical observations, the prediction error is minimized by using the computer model calibrated with the proposed method. Furthermore, we provide an algorithm to estimate the optimal calibration parameters and the model discrepancy.

1.1. Comparison with existing work. We discuss the differences between our frequentist calibration method and other frequentist calibration methods in the literature. [7] considers calibration using a parametric form of discrepancy. We use a nonparametric approach to better modeling the physical system and the model discrepancy. The $L_2$-calibration method in [18] minimizes the model discrepancy under the $L_2$-norm. [22] performs calibration by minimizing the model discrepancy under the empirical $l_2$-norm. Below are the main differences between [18, 22] and ours.

- Different method. Calibration in [18, 22] and our work minimizes the following different norms of the model discrepancy: the $L_2$-norm in [18], the empirical $l_2$-norm in [22] and the RKHS norm in our method.
- Different analysis. Theoretical results in [18, 22] are based on asymptotics theory assuming the number of physical observations go to infinity. Our theory is based on finite-sample properties of calibration and prediction following the fact that usually, only a finite number of physical data are available.
- Different results. The $L_2$-calibration in [18] minimizes the distance
between the physical system and the imperfect computer model, but not directly for predicting the physical system. [22] performs the least square calibration and then estimates the model discrepancy in the RKHS. However, for a finite number of physical observations, the estimation error of discrepancy can be large. To overcome this difficulty, our calibration method minimizes the predictive mean squared error for a finite sample of physical data with statistical guarantees.

Bayesian calibration was studied by [9, 14, 5, 6, 8, 15, 19], among others. Our frequentist calibration method is easier to compute and complements these Bayesian methods. Furthermore, we will discuss an interesting connection between our method and these Bayesian methods in Section 4. This link offers new justification for observed successful prediction performance of the Bayesian calibration methods in various fields.

Our non-asymptotic minimax theory is inspired by recent developments of concentration inequalities that provide valid statistical inference and estimation results for finite samples. Existing research on concentration inequalities typically addresses finite dimensional parameters for parametric models. Because our interest is computer model calibration, we develop a non-asymptotic minimax theory for nonparametric models.

The remainder of the article is organized as follows. In Section 2, we discuss the identifiability issue and formulate a prediction-oriented optimal calibration method. In Section 3, we establish a non-asymptotic minimax theory and apply it to the prediction-oriented calibration method. In Section 4, we develop an algorithm for solving our calibration problem and build a connection between our method and the Bayesian calibration method. In Section 5, we provide synthetic and real examples to corroborate the derived theory and illustrate some advantages of the proposed calibration method. We give concluding remarks in Section 6. All other proofs and algorithm are delegated to the supplementary material.

2. Prediction-oriented calibration. Since the computer model is imperfect for modeling the physical system, \( \eta(x, \theta) \neq \zeta(x) \) for any \( \theta \in \Theta \). A model discrepancy function \( \delta(x, \theta) = \zeta(x) - \eta(x, \theta) \) is commonly used [9, 13]. Equivalently, write

\[
\zeta(x) = \eta(x, \theta) + \delta(x, \theta), \quad \forall x \in \Omega, \theta \in \Theta.
\]

The goal is to accurately predict \( \zeta(\cdot) \) using the computer model, which requires calibrating \( \theta \) and estimating \( \delta(\cdot, \theta) \) simultaneously with a finite physical sample in \((1.1)\). Two main difficulties arise. The identifiability issue of \( \theta \) to be discussed in Section 2.1 and the non-negligible estimation error of
δ(·, θ) due to the finite sample of the physical data. These two issues motivate our calibration method in Section 2.2.

2.1. The identifiability issue. Suppose that ζ(·) resides in a RKHS \( (H, \| \cdot \|_H) \) on \( \Omega = [0, 1]^d \). One example of \( H \) is the \( m \)th order Sobolev space \( W^m_2(\Omega) \) with \( 2m > d \):

\[
W^m_2(\Omega) = \left\{ g(\cdot) \in L^2(\Omega) \middle| \frac{\partial^{\alpha_1 + \cdots + \alpha_d} g(\cdot)}{\partial^{\alpha_1} x_1 \cdots \partial^{\alpha_d} x_d} \in L^2(\Omega), \forall \alpha_1, \ldots, \alpha_d \in \mathbb{N} \text{ with } \alpha_1 + \cdots + \alpha_d \leq m \right\}.
\]

Since \( \eta(·, \theta) \) approximates the physical system \( \zeta(·) \), we assume the following regularity condition for \( \eta(·, \theta) \).

**Assumption 2.1.** For any \( \theta \in \Theta \), the computer model \( \eta(·, \theta) \in H \).

An analogy of Assumption 2.1 was already used in [15]. But instead of assuming the function space is a RKHS, [15] considers a function space of bounded mixed derivatives. Assumption 2.1 implies that for any \( \theta \in \Theta \), \( \delta(·, \theta) = \zeta(x) - \eta(x, \theta) \) is in \( H \). This observation leads to a potential identifiability issue for \( \theta \). For example, for two different \( \theta_1 \not= \theta_2 \in \Theta \), their corresponding model discrepancies \( \delta(x, \theta_1) = \zeta(x) - \eta(x, \theta_1) \) and \( \delta(x, \theta_2) = \zeta(x) - \eta(x, \theta_2) \) are both in \( H \). This implies that both \( (\theta_1, \delta(·, \theta_1)), (\theta_2, \delta(·, \theta_2)) \in \Theta \times H \) are true for model (2.1). There are infinite truth pairs \( (\theta, \delta(·, \theta)) \in \Theta \times H \) for (2.1) by choosing arbitrary \( \theta \in \Theta \) and using \( \delta(·, \theta) = \zeta(x) - \eta(x, \theta) \). This identifiability issue was first noticed by K. Beven and P. Diggle in their discussion of [9].

If Assumption 2.1 fails, our results hold for replacing \( \delta(·, \theta) = \zeta(·) - \eta(·, \theta) \) with \( \delta(·, \theta) = P_H{\zeta(·) - \eta(·, \theta)} \), where \( P_H \) denotes the projection from \( L^2(\Omega) \) to \( H \) in the \( L^2 \)-norm. Hereinafter, we focus on the imperfect computer model under Assumption 2.1.

2.2. Definition of prediction-oriented calibration. Denote by \( \Pi \) the sampling distribution of \( X_i \) in (1.1) which is independent of \( \varepsilon_i \) and satisfies \( \Pi(\Omega) = 1 \). Assume that the density of \( \Pi \) is bounded away from zero and infinity on \( \Omega \). Let \( X^* \) be drawn from \( \Pi \) and \( Y^* = \zeta(X^*) + \varepsilon^* = \eta(X^*, \theta) + \delta(X^*, \theta) + \varepsilon^* \sim N(0, \sigma^2) \). Then for a fixed \( \theta \in \Theta \), the minimal predictive mean squared error for predicting \( Y^* \) is

\[
\inf_{\delta} \mathbb{E} \left\{ Y^* - \left[ \eta(X^*, \theta) + \delta(X^*, \theta) \right] \right\}^2 = \sigma^2 + \inf_{\delta} \| \delta(·, \theta) - \bar{\delta}(·, \theta) \|_{L^2(\Pi)}^2,
\]

(2.2)
where the infimum is over all measurable estimators.

The identifiability issue discussed in Section 2.1 indicates that there are infinite pairs of \((\theta, \delta(\cdot, \theta)) \in \Theta \times H\) satisfying model (2.1). However, for a finite sample size \(n\), the minimal estimation error \(\inf_{\tilde{\delta}} \|\delta(\cdot, \theta) - \tilde{\delta}(\cdot, \theta)\|_{L_2(\Pi)}\) does not vanish [2]. This fact motivates us to define optimal calibration \(\theta_{\text{opt-pred}}\) to minimize the minimal predictive mean squared error (2.2) over \(\theta \in \Theta\). Equivalently, we define

\[
\theta_{\text{opt-pred}} \equiv \arg \min_{\theta \in \Theta} \left\{ \inf_{\tilde{\delta}} \|\delta(\cdot, \theta) - \tilde{\delta}(\cdot, \theta)\|_{L_2(\Pi)} \right\},
\]

where the superscript “opt-pred” denotes “optimal for prediction”. By definition, \(\theta_{\text{opt-pred}}\) in (2.3) is optimal for predicting \(\zeta(\cdot)\). We will establish a non-asymptotic theory for nonparametric regression in Section 3 and introduce an algorithm in Section 4. The formulation of \(\theta_{\text{opt-pred}}\) in (2.3) is frequentist. We will discuss in Section 3.4 the differences between \(\theta_{\text{opt-pred}}\) and other frequentist calibration methods, including the \(L_2\)-calibration method [18] and the least square calibration method [22].

3. Main results. Existing theory for calibration, including [18, 22], adopts the asymptotic regime that the number of data points for the physical experiment goes to infinity. In Section 3.1, we present non-asymptotic minimax risk for nonparametric models and apply it the model calibration problem in Section 3.2. In Section 3.3, we show the improvement in prediction achieved by incorporating data from computer models. In Section 3.4, we compare our calibration method with some existing frequentist methods.

3.1. Non-asymptotic minimax theory for nonparametric regressions. We consider the nonparametric regression in (1.1), where \(\zeta(\cdot)\) resides in the RKHS \(H\). Let \(\|\cdot\|_H\) be the corresponding RKHS norm and \(K : \Omega \times \Omega \to \mathbb{R}\) be a Mercer kernel generating \((H, \|\cdot\|_H)\). By the spectral theorem, \(K\) admits the eigenvalue decomposition:

\[
K(x, x') = \sum_{\nu \geq 1} \lambda_\nu \phi_\nu(x) \phi_\nu(x'),
\]

where \(\lambda_1 \geq \lambda_2 \geq \cdots \geq 0\) are the eigenvalues and \(\{\phi_\nu : \nu \geq 1\}\) are the corresponding eigenfunctions such that \(\langle \phi_\nu, \phi_{\nu'} \rangle_{L_2(\Pi)} = \delta_{\nu\nu'}\). Here, \(\delta_{\nu\nu'}\) is the Kronecker delta. We assume the polynomial decay rate of eigenvalues in Assumption 3.1. This common assumption holds for the Sobolev space \(H = W_2^p(\Omega)\) with Lebesgue measure on \(\Omega\).
ASSUMPTION 3.1. For $2m > d$, suppose that for any $\nu \geq 1$, the eigenvalues satisfy $c_\lambda \nu^{-2m/d} \leq \lambda_\nu \leq C_\lambda \nu^{-2m/d}$ with constants $0 < c_\lambda < C_\lambda < \infty$, and the eigenfunctions are uniformly bounded: $\max_{x \in \Omega} |\phi_\nu(x)| \leq c_\phi$ with a constant $c_\phi$ for any $\nu \geq 1$.

We now present our main results. We first show a non-asymptotic minimax lower bound for the predictive mean squared error.

**Theorem 3.1.** Under the regression model (1.1) where $\zeta(\cdot) \in H$ and Assumption 3.1 holds, there exists a constant $C_1 > 0$ not depending on $n, \sigma, m, d, \|\zeta\|_H$ such that for any $n \geq 1$,

$$\inf_{\tilde{\zeta}} \sup_{\zeta \in H} \mathbb{P}\left\{ \|\tilde{\zeta} - \zeta\|_{L_2(\Pi)}^2 \geq C_1 \left[ 1 + n^{-2m/d} \left( 1 + \sigma/\|\zeta\|_H \right)^{-2d/2m+d} \right]^2 \cdot n^{-2m/d} (\|\zeta\|_H + \sigma)^2 \left( 1 + \sigma/\|\zeta\|_H \right)^{-2d/2m+d} \right\} > 0.$$ 

The proof of this theorem, given in the supplementary material, is based on Fano’s lemma [2]. Now, we show that the non-asymptotic lower bound of the theorem can be achieved by the regularized estimator in the RKHS:

$$\tilde{\zeta}_{n\lambda} = \arg \min_{g \in H} \left\{ \frac{1}{n} \sum_{i=1}^{n} (Y_i - g(X_i))^2 + \lambda \|g\|_H^2 \right\},$$

where $\lambda > 0$ is the tuning parameter. The following result shows that $\tilde{\zeta}_{n\lambda}$ is minimax optimal for a finite sample.

**Theorem 3.2.** Under the regression model (1.1) where $\zeta(\cdot) \in H$ and Assumption 3.1 holds, there exists a constant $C_2 > 0$ not depending on $n, \sigma, \|\zeta\|_H$ such that for any $n \geq 1$ and any $\alpha > 0$ with probability at least $1 - 8e^{-\alpha^2}$,

$$\|\tilde{\zeta}_{n\lambda} - \zeta\|_{L_2(\Pi)}^2 \leq C_2 \left[ 1 + \alpha^{2m/d} n^{-2m/d} \left( 1 + \sigma/\|\zeta\|_H \right)^{-2d/2m+d} \right]^2 \cdot \alpha^{2m/d} \left( \|\zeta\|_H + \sigma \right)^2 \left( 1 + \sigma/\|\zeta\|_H \right)^{-2d/2m+d},$$

where $\tilde{\zeta}_{n\lambda}$ is defined by (3.1) with $\lambda = n^{-2m/(2m+d)} \{ 4m^{1/2} (4m^2 - d^2)^{-1/2} C_\lambda^d / 4m^2 \}^{2m/(2m+d)}$. Here, $A$ is a constant not depending on $n, \sigma, \|\zeta\|_H$.

We relegate the proof of Theorem 3.2 to the supplementary material. We establish the proof by using results from empirical processes such as the
maximal inequalities and the concentration inequalities [11] and deriving some new techniques.

We make three remarks on this theorem. First, the conventional asymptotic convergence rate can be recovered from Theorem 3.2. Since $2m > d$ in Assumption 3.1,

$$\alpha^{2m-d} n^{-\frac{2m-d}{2m+d}} (1 + \sigma/\|\zeta\|_H)^{-\frac{2d}{2m+d}} = o(1), \text{ as } n \to \infty.$$ 

Thus, Theorem 3.2 yields that

$$\|\hat{\zeta}_n - \zeta\|_{L^2(\Pi)} = O_P\left\{n^{-2m/(2m+d)}\right\} \text{ as } n \to \infty.$$ 

This is a well-known rate ([3, 20, 21]).

Second, Theorems 3.1 and 3.2 together immediate imply that the non-asymptotic minimax optimal risk for estimating $\zeta \in H$ is

$$\|\tilde{\zeta} - \zeta\|_{L^2(\Pi)}^2 = C\left[1 + n^{-\frac{2m-d}{2m+d}} (1 + \sigma/\|\zeta\|_H)^{-\frac{2d}{2m+d}}\right]^2 \cdot n^{-\frac{2m}{2m+d}} (\|\zeta\|_H + \sigma)^2 (1 + \sigma/\|\zeta\|_H)^{-\frac{2d}{2m+d}},$$

for some constant $C$. This minimax risk holds for a finite sample and indicates the dependence on the signal-to-noise ratio: $\|\zeta\|_H/\sigma$ and the magnitude of signal and noise: $\|\zeta\|_H + \sigma$.

Third, Theorem 3.2 suggests a tradeoff between the approximation error and the prediction error. A smaller $\lambda$ in (3.1) corresponds to a smaller approximation error: $\frac{1}{n} \sum_{i=1}^n |Y_i - \hat{\zeta}_n(X_i)|^2$; see, e.g., [21]. In practice, we usually do not know the values of $\|\zeta\|_H$ or $\sigma$. Theorem 3.2 implies that for achieving the minimax optimal risk (3.2), the optimal $\lambda$ with a smaller value corresponds to a larger $\|\zeta\|_H$, which yields a larger risk for prediction in (3.2).

### 3.2. Optimal calibration and prediction

We apply the non-asymptotic minimax theory in Section 3.1 to derive an equivalent form for the calibration method in (2.3). The following theorem leads to an algorithm for computing $\theta_{opt-pred}$ in Section 4.

**Theorem 3.3.** Under the Assumptions in 2.1 and 3.1, for any $n \geq 1$, the calibration procedure in (2.3) is equivalent to finding the minimizer of the model discrepancy equipped with the RKHS norm:

$$\theta_{opt-pred} = \arg\min_{\theta \in \Theta} \{\|\zeta(\cdot) - \eta(\cdot, \theta)\|_H\}.$$ 

The proof of this theorem is relegated to the supplementary material. Here are some explanations. If the model discrepancy $\zeta(\cdot) - \eta(\cdot, \theta)$ has a small RKHS norm, the discrepancy is a simple function in the RKHS. Since
the sample size \( n \) is fixed and finite, a simpler function should have a more accurate estimator by using limited information from data. As discussed in Section 2, a more accurate discrepancy estimator gives a smaller prediction error for the physical system. Unlike the existing work in model calibrations, Theorem 3.3 justifies the use of RKHS norm to measure the model discrepancy, which is different from the \( L_2 \)-norm [18] and the empirical \( l_2 \)-norm [22].

We now discuss the non-asymptotic minimax risk for predicting \( \zeta(\cdot) \) based on the calibration parameters \( \theta^{\text{opt-pred}} \). As a corollary of Theorem 3.1, the following result gives a lower bound of the predictive mean squared error when using the computer model calibrated by \( \theta^{\text{opt-pred}} \) and an estimator of the model discrepancy.

**Corollary 3.4.** Under the regression model (1.1) where \( \zeta(\cdot) \in \mathcal{H} \) and Assumption 2.1 and 3.1 hold, then for any \( n \geq 1 \),

\[
\inf_{\delta} \sup_{\zeta \in \mathcal{H}} \mathbb{P} \{ \| \eta(\cdot, \theta^{\text{opt-pred}}) + \tilde{\delta}(\cdot) - \zeta(\cdot) \|^2_{L_2(\Pi)} \geq C_1 \left[ 1 + n^{-\frac{2m-d}{4m+2d}} \left( 1 + \sigma/\| \zeta - \eta(\cdot, \theta^{\text{opt-pred}}) \|_{\mathcal{H}} \right)^{-\frac{2d}{2m+d}} \right] \left( \| \zeta - \eta(\cdot, \theta^{\text{opt-pred}}) \|_{\mathcal{H}} + \sigma \right)^2 \left( 1 + \sigma/\| \zeta - \eta(\cdot, \theta^{\text{opt-pred}}) \|_{\mathcal{H}} \right)^{-\frac{2d}{2m+d}} > 0.
\]

Here, the constant \( C_1 \) is the same as in Theorem 3.1 that does not depend on \( n, \sigma, m, d, \| \zeta - \eta(\cdot, \theta^{\text{opt-pred}}) \|_{\mathcal{H}} \).

As a corollary of Theorem 3.2, we show that the non-asymptotic lower bound in Corollary 3.4 can be achieved by the regularized estimator for the model discrepancy in the RKHS \( \mathcal{H} \):

\[
(3.3) \quad \hat{\delta}_{n,\lambda}(\cdot, \theta) = \arg \min_{h \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} [ Y_i - \eta(X_i, \theta) - h(X_i)]^2 + \lambda \| h \|^2_{\mathcal{H}} \right\},
\]

where \( \lambda > 0 \) is the tuning parameter.

**Corollary 3.5.** Under the regression model (1.1) where \( \zeta(\cdot) \in \mathcal{H} \) and Assumption 2.1 and 3.1, for any \( n \geq 1 \) and any \( \alpha > 0 \) with probability at
least 1 \(- 8e^{-\alpha^2}\),
$$\|\eta(\cdot, \theta_{\text{opt-pred}}) + \tilde{\delta}_{n\lambda}(\cdot, \theta_{\text{opt-pred}})\|_{L_2(\Pi)}^2$$
$$\leq C_2 \left[ 1 + \alpha_2 \frac{2m - d}{2m + d} n^{-\frac{2m - d}{2m + d}} \left( 1 + \sigma / \|\zeta(\cdot) - \eta(\cdot, \theta_{\text{opt-pred}})\|_H \right) \right]^{\frac{2d}{2m + d}} \cdot n^{-\frac{2m - d}{2m + d}} \left( \|\zeta(\cdot) - \eta(\cdot, \theta_{\text{opt-pred}})\|_H + \sigma \right)^2 \left( 1 + \sigma / \|\zeta(\cdot) - \eta(\cdot, \theta_{\text{opt-pred}})\|_H \right)^{-\frac{2d}{2m + d}},$$
where $\tilde{\delta}_{n\lambda}$ is defined by (3.3) with
$$\lambda = n^{2m/(2m+d)} (4m^{1/2}(4m-d)^{-1/2} \cdot C_{\lambda}^{d/4m} (\alpha A + \sigma c_{\phi} (1+\sqrt{2} \alpha) / \|\zeta(\cdot) - \eta(\cdot, \theta_{\text{opt-pred}})\|_H) )^{1/(2m+d)}.$$ Here, $C_2$ and $A$ are the same as in Theorem 3.2 that do not depend on $n, \sigma, \|\zeta - \eta(\cdot, \theta_{\text{opt-pred}})\|_H$.

Corollary 3.4 and 3.5 together imply that the non-asymptotic minimax optimal risk for predicting $\zeta \in H$ by the computer model with $\theta_{\text{opt-pred}}$ is
$$\|\eta(\cdot, \theta_{\text{opt-pred}}) + \tilde{\delta}(\cdot)\|_{L_2(\Pi)} \geq C \left[ 1 + n^{-\frac{2m - d}{2m + d}} \left( 1 + \frac{\sigma}{\min_{\theta \in \Theta} \|\zeta - \eta(\cdot, \theta)\|_H} \right)^{-\frac{2d}{2m + d}} \right]^2 \cdot n^{-\frac{2m - d}{2m + d}} \left( \min_{\theta \in \Theta} \|\zeta - \eta(\cdot, \theta)\|_H + \sigma \right)^2 \left( 1 + \frac{\sigma}{\min_{\theta \in \Theta} \|\zeta - \eta(\cdot, \theta)\|_H} \right)^{-\frac{2d}{2m + d}}.$$
Moreover, this minimax optimal risk can be obtained by
$$\zeta_{n\lambda}^{\text{opt-pred}}(\cdot) \equiv \eta(\cdot, \theta_{\text{opt-pred}}) + \tilde{\delta}_{n\lambda}(\cdot, \theta_{\text{opt-pred}}),$$
where $\tilde{\delta}_{n\lambda}$ is defined by (3.3).

3.3. Improved prediction using the computer model. The minimax optimal predictor (3.4) combines the merits of parametrics (for computer model) and nonparametrics (for the discrepancy estimator). We compare (3.4) with its counterpart of the minimax optimal predictor (3.1) without using the computer model.

**Theorem 3.6.** Under the regression model (1.1) where $\zeta(\cdot) \in H$ and Assumption 2.1 and 3.1, if
$$\min_{\theta \in \Theta} \|\zeta(\cdot) - \eta(\cdot, \theta)\|_H < \|\zeta\|_H,$$
then $\zeta_{n\lambda}^{\text{opt-pred}}(\cdot)$ defined by (3.4) with the aid of the computer model achieves a smaller upper bound of the predictive mean squared error than $\tilde{\zeta}_{n\lambda}(\cdot)$ defined by (3.1) without using the information of the computer model.
The proof of this theorem is given in the supplementary material. Here is a remark on the condition (3.5). The computer model $\eta(\cdot, \theta)$ is built based on some physics for the system $\zeta(\cdot)$ and Theorem 3.3 shows that $\eta(\cdot, \theta_{\text{opt-pred}})$ is the best approximation to $\zeta(\cdot)$ within the family $\{\eta(\cdot, \theta), \theta \in \Theta\}$. Although the computer model is imperfect for modeling the physical system, $\eta(\cdot, \theta_{\text{opt-pred}})$ can still capture some major shape of $\zeta(\cdot)$ and consequently $\zeta(\cdot) - \eta(\cdot, \theta_{\text{opt-pred}})$ has less variation or smoother in $\mathcal{H}$ than the original $\zeta(\cdot)$ does. Hence, we assume that $\|\zeta(\cdot) - \eta(\cdot, \theta_{\text{opt-pred}})\|_{\mathcal{H}} < \|\zeta\|_{\mathcal{H}}$, which is exactly the condition (3.5).

The predictor (3.4) is a parametrically-guided nonparametric predictor, where $\eta(\cdot, \theta)$ can have a parametric form.

3.4. Comparison with existing frequentist calibration methods. We compare the calibration procedure in $\theta_{\text{opt-pred}}$ defined by (2.3) with two other frequentist calibration methods: the $L_2$-calibration and the least square calibration. The $L_2$-calibration method in [18] is defined as follows:

$$\hat{\theta}_{n}^{L_2} = \arg \min_{\theta \in \Theta} \left\{ \| \hat{\zeta}_{n\lambda}(\cdot) - \eta(\cdot, \theta) \|_{L_2(\Pi)} \right\},$$

where $\hat{\zeta}_{n\lambda}(\cdot)$ is defined by (3.1). The least square calibration method in [22] minimizes the model discrepancy equipped with the empirical $l_2$-norm:

$$\hat{\theta}_{n}^{l_2} = \arg \min_{\theta \in \Theta} \left\{ \frac{1}{n} \sum_{i=1}^{n} [Y_i - \eta(X_i, \theta)]^2 \right\}.$$  

In particular, [22] estimates the model discrepancy after calibrating $\theta = \hat{\theta}_{n}^{l_2}$:

$$\hat{\zeta}_{n\lambda}(\cdot, \hat{\theta}_{n}^{l_2}) = \arg \min_{\delta(\cdot) \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} [Y_i - \eta(X_i, \hat{\theta}_{n}^{l_2}) - \delta(X_i)] + \lambda \| \delta \|_{\mathcal{H}}^2 \right\},$$

and a predictor for $\zeta(\cdot)$ is given by $\eta(\cdot, \hat{\theta}_{n}^{l_2}) + \hat{\zeta}_{n\lambda}(\cdot, \hat{\theta}_{n}^{l_2})$.

Remark 3.1. The differences between $\theta_{\text{opt-pred}}$, $\hat{\theta}_{n}^{L_2}$, and $\hat{\theta}_{n}^{l_2}$ are as follows.

- Calibration results. We have that $\theta_{\text{opt-pred}} = \arg \min_{\theta \in \Theta} \{ \| \zeta(\cdot) - \eta(\cdot, \theta) \|_{\mathcal{H}} \}$ and

$$\mathbb{P} \left\{ \hat{\theta}_{n}^{L_2}, \hat{\theta}_{n}^{l_2} \to \theta^{L_2} \right\} \equiv \arg \min_{\theta \in \Theta} \{ \| \zeta(\cdot) - \eta(\cdot, \theta) \|_{L_2(\Pi)} \} \text{ as } n \to \infty \} > 0.$$  

Since $\hat{\theta}_{n}^{L_2}$ and $\hat{\theta}_{n}^{l_2}$ converge to a different minimizer than $\theta_{\text{opt-pred}}$, the calibration result in $\theta_{\text{opt-pred}}$ is different from $\hat{\theta}_{n}^{L_2}$ and $\hat{\theta}_{n}^{l_2}$. 
• Prediction. For a finite sample size $n$, the predictor with $\theta_{\text{opt-pred}}$ achieves a smaller upper bound of the predictive mean squared error comparing with the predictor with $\widehat{\theta}_{\text{L2}}^n$ in [18] and the predictor with $\widehat{\theta}_{\text{L2}}^n$ in [22].

We provide a proof of Remark 3.1 in the supplementary material.

4. An algorithm. We propose an algorithm to compute the optimal calibration $\theta_{\text{opt-pred}}$ in (2.3). From Theorem 3.3,

\begin{equation}
\theta_{\text{opt-pred}} = \arg\min_{\theta \in \Theta} \{ \| \delta(\cdot, \theta) \|_H^2 \},
\end{equation}

where the discrepancy $\delta(\cdot, \theta)$ is subject to the constraint (2.1). By evaluating (2.1) at the training data, we have

\begin{equation}
Y_i = \zeta(X_i) + \varepsilon_i = \eta(X_i, \theta) + \delta(X_i, \theta) + \varepsilon_i, \quad \forall \theta \in \Theta, i = 1, \ldots, n.
\end{equation}

By using the Lagrange multiplier method for (4.1) with the constraint (4.2), we need to find $\theta \in \Theta$ and $\delta(\cdot) \in H$ for minimizing

\begin{equation}
\frac{1}{n} \sum_{i=1}^n [Y_i - \eta(X_i, \theta) - \delta(X_i)]^2 + \lambda \| \delta \|_H^2,
\end{equation}

where $\lambda > 0$ is a tuning parameter.

The optimization problem in (4.3) can be solved iteratively as follows. We introduce some notation. Recall that $K$ is the reproducing kernel of $(H, \| \cdot \|_H)$. Let $\Sigma$ be the $n \times n$ kernel matrix with $ij$th entry $K(X_i, X_j)$. Denote by $\vec{Y} = (Y_1, \ldots, Y_n)^\top$, $\eta(\vec{X}, \theta) = (\eta(X_1, \theta), \ldots, \eta(X_n, \theta))^\top$, $\delta(\vec{X}, \theta) = (\delta(X_1, \theta), \ldots, \delta(X_n, \theta))^\top$, and $\zeta(\vec{X}) = (\zeta(X_1), \ldots, \zeta(X_n))^\top$.

For any fixed $\theta \in \Theta$, the minimizer $\hat{\delta}(\cdot)$ of (4.3) is the same as the regularized estimator $\hat{\delta}_{n\lambda}(\cdot, \theta)$ in (3.3). By the representer lemma [10],

\begin{equation}
\hat{\delta}_{n\lambda}(\cdot, \theta) = \sum_{i=1}^n c_i K(X_i, \cdot),
\end{equation}

where the coefficient $c = (c_1, \ldots, c_n)^\top \in \mathbb{R}^n$ is given by

\begin{equation}
c = c(\theta) = (\Sigma + n \lambda I)^{-1} [\vec{Y} - \eta(\vec{X}, \theta)].
\end{equation}

The tuning parameter $\lambda$ can be selected by the generalized cross-validation (GCV) in [4]. Let $A(\lambda)$ be the influence matrix satisfying $\hat{\delta}_{n\lambda}(\vec{X}, \theta) = A(\lambda)[\vec{Y} - \eta(\vec{X}, \theta)]$. The GCV estimate of $\lambda$ is the minimizer of

\begin{equation}
\text{GCV}(\lambda) = \frac{n^{-1} \| \vec{Y} - \eta(\vec{X}, \theta) - \hat{\delta}_{n\lambda}(\vec{X}, \theta) \|^2}{[n^{-1} \text{tr}(I - A(\lambda))]^2}.
\end{equation}
GCV gives a consistent estimate of the optimal \( \lambda \) in Corollary 3.5 [12, 21]. Another popular technique for selecting the tuning parameter is fivefold or tenfold cross-validation. Since the computational load of GCV is smaller, it will be used for simulations in Section 5.

For any fixed \( \delta(\cdot) = \delta_{n\lambda}(\cdot, \theta) \) from (4.4), the minimizer \( \theta \) of (4.3) is the same as

\[
(4.7) \quad \arg \min_{\theta \in \Theta} \left\{ (\bar{Y} - \eta(\bar{X}, \theta))^\top (\Sigma + n\lambda)^{-1} (\bar{Y} - \eta(\bar{X}, \theta)) \right\}.
\]

Since the objective function in (4.7) is a weighted version of the empirical \( l_2 \)-norm \( \| \bar{Y} - \eta(\bar{X}, \theta) \|^2 / n \), (4.7) gives a different calibration result than the least square calibration method (3.6).

Putting the above building blocks together, our algorithm for optimizing (4.3) iterates between (4.4) and (4.7). In each iteration, (4.3) is decreased. The algorithm can start with the calibration parameters from the least square calibration method. Applying later iterations of the algorithm continuously improves the initial values for prediction. Our experience indicates that a small number of iterations is sufficient to obtain good performance of the algorithm. In our simulation studies, we find that the objective function (4.3) decreases fast in the first iteration and becomes close to the objective function at convergence. This motivates a one-step update procedure:

1. Initialization: Solve the least square calibration problem in (3.6) to obtain \( \theta = \theta_1^2 \).
2. Solve for \( \hat{\delta}_{n\lambda}(\cdot, \theta) \) in (4.4), and tune \( \lambda \) according to GCV. Fix \( \lambda \) at the chosen value in later steps.
3. For \( \hat{\delta}_{n\lambda}(\cdot, \theta) \) obtained in step 2, solve for \( \theta \) in (4.7).
4. With the new \( \theta \), solve for \( \hat{\delta}_{n\lambda}(\cdot, \theta) \) in (4.4).

4.1. Connection with Bayesian calibration. We now link our frequentist calibration method to the Bayesian calibration method in [9]. [9] uses Gaussian processes [16] as priors for the computer model \( \eta(\cdot, \theta) \) and the discrepancy \( \delta(\cdot, \theta) \). Recall that \( K \) is the reproducing kernel of the RKHS \( (\mathcal{H}, \| \cdot \|_{\mathcal{H}}) \).

We consider the following priors

\[
(4.8) \quad \zeta(x) = \eta(x, \theta) + \delta(x),
\]

where \( \eta(x, \theta) = \sum_{j=1}^{p} \theta_j h_j(x), \theta \sim N(0, \alpha I), \delta(x) \sim N(0, \beta K(\cdot, \cdot)) \).

Here, \( h_j(x) \) are deterministic functions and \( \alpha, \beta \) are positive hyperparameters. The following proposition builds a connection between the Bayesian
calibration method and the optimization step in (4.3) for our calibration method.

**Proposition 4.1.** Suppose that the prior for $\zeta(\cdot)$ is given by (4.8) and denote the posterior mean $\hat{\zeta}_\alpha(x) = E[\zeta(x)|Y_1, \ldots, Y_n]$. Let the predictor corresponding to the optimal calibration be $\hat{\zeta}_{n\lambda}^{\text{opt-pred}}(\cdot) = \eta(\cdot, \hat{\theta}_{\text{opt-pred}}, \hat{\delta}_{n\lambda})$, which is an estimator of (3.4) and

$$(\hat{\theta}_{\text{opt-pred}}^{\text{opt-pred}}, \hat{\delta}_{n\lambda}) = \arg\min_{\theta \in \Theta, \delta \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^{n} [Y_i - \eta(X_i, \theta) - \delta(X_i)]^2 + \lambda \|\delta\|_2^2 \right\}$$

with $\lambda = \sigma^2/n\beta$. Here, $\alpha$ and $\beta$ are defined in (4.8). Then, $\lim_{\alpha \to \infty} \hat{\zeta}_\alpha(x) = \hat{\zeta}_{n\lambda}^{\text{opt-pred}}(x)$ for any $x \in \Omega$.

The proof of this proposition is given in the supplementary material. The proposition sheds new lights on why the prediction of the Bayesian calibration method works well in practice.

The Bayesian calibration method is more time consuming to compute than frequentist calibration methods such as ours.

5. **Simulation and real examples.** We illustrate of the prediction accuracy of the proposed calibration method using several examples. Our simulation study consists of Example 5.1, 5.2, 5.3, where the tuning parameters for regularized estimators are selected by the GCV. The prediction accuracy is measured by the predictive mean squared error estimated by a Monte Carlo sample of 1000,000 test points from the same distribution as the training points. A real data example is given in Example 5.4.

**Example 5.1.** Consider a physical system $\zeta(x) = \exp(\pi x/5) \sin 2\pi x, x \in [0, 1]$. The physical data are generated by (1.1) with $X_i \sim \text{Unif}([0, 1]), \varepsilon_i \sim N(0, \sigma^2)$ for $i = 1, \ldots, 50$. Four different noise variances are investigated: $\sigma^2 = 0.1, 0.25, 0.5, 1$. Suppose that the computer model is

$$\eta(x, \theta) = \zeta(x) - \sqrt{\theta^2 - \theta} + 1(\sin 2\pi \theta x + \cos 2\pi \theta x) \text{ for } \theta \in [-1, 1].$$

Since $\theta^2 - \theta + 1 \geq 3/4$ for any $-1 \leq \theta \leq 1$, the model discrepancy between $\eta(\cdot, \theta)$ and $\zeta(\cdot)$ always exists no matter how $\theta$ is chosen. We use the Matérn kernel $K(x_1, x_2) = (1 + |x_1 - x_2|/\psi)\exp\{-|x_1 - x_2|/\psi\}$, where the scale parameter $\psi$ is chosen by the five-fold cross-validation. Figure 1 plots the squared model discrepancy with different norms: $\|\zeta(\cdot) - \eta(\cdot, \theta)\|_{L_2(\Pi)}^2$ and $\|\zeta(\cdot) - \eta(\cdot, \theta)\|_{\mathcal{H}}^2$. The corresponding minimizers are different given as $\theta_{L_2} \approx \ldots$
\(-0.1780\) and \(\theta_{\text{opt-pred}} \approx 0.3740\) (a local minimizer of \(\|\zeta(\cdot) - \eta(\cdot, \theta)\|^2_H\) in \([-0.4, 0]\) is \(\theta_{\text{opt-pred}} \approx -0.1230\)), which illustrates the first part of Theorem 3.1.

Fig 1: Normalized model discrepancy equipped with \(L_2(\Pi)\)-norm and RKHS-norm in Example 5.1.

We compare the prediction accuracy of four frequentist calibration methods:

1) The computer model with \(L_2\)-calibration (abbreviated as “No Bias Corr.”), which is the \(\eta(\cdot, \hat{\theta}_n^{L_2})\) in Section 3.4 without the model discrepancy correction;

2) The nonparametric predictor (abbreviated as “N.P.”), which is the \(\hat{\zeta}_{n\lambda}(\cdot)\) obtained by (3.1) in Section 3.1;

3) The predictor in [22] (abbreviated as “LS. Cal.”), which is the \(\eta(\cdot, \hat{\theta}_n^{L_2}) + \hat{\delta}_{n\lambda}(\cdot, \hat{\theta}_n^{L_2})\) in Section 3.4 based on the least square calibration;

4) Our predictor (abbreviated as “Opt. Cal.”), which is the \(\zeta_{n\lambda}^{\text{opt-pred}}\) in Section 3.2 based on the proposed calibration and computed by the algorithm in Section 4.

For each chosen noise variance, we replicate the data generation, calibration and prediction procedures 1,000 times and average the results for each method across the replicates. The resulting average predictive mean squared errors and its associated standard errors are given in Table 1. The computer model with \(L_2\)-calibration (i.e., “No Bias Corr.”) gives the largest predictive
mean squared error, which shows that an estimator for the model discrepancy is necessary. “No Bias Corr.” has the smallest standard error which is not surprising because the parametric estimation of \( \theta \) here has a faster rate of convergences than nonparametric estimations required for other three methods. Table 1 indicates that our method “Opt. Cal.” and the predictor in [22] “LS. Cal.” outperform the nonparametric predictor “N.P.”. This advantage illustrates the improved predictions by computer models as indicated in Theorem 3.6. Furthermore, “Opt. Cal.” gives smaller prediction errors than “LS. Cal.”, which agrees with the second part of Theorem 3.1. Overall, for a finite sample size \( n = 50 \), the proposed method “Opt. Cal.” outperforms the other frequentist predictors in the settings studied.

### Table 1
Comparison of predictive mean squared errors for Example 5.1. PMSE = predictive mean squared error, SE = standard error

| \( \sigma^2 = 0.1 \) | Average of PMSE | SE of PMSE | \( \sigma^2 = 0.25 \) | Average of PMSE | SE of PMSE |
|-------------------|----------------|------------|-----------------------|----------------|------------|
| No Bias Corr.     | 0.3492         | 0.0174     | 0.3601                | 0.0270         |
| N.P.              | 0.1701         | 0.0594     | 0.2327                | 0.0680         |
| LS. Cal.          | 0.1152         | 0.0604     | 0.1693                | 0.0580         |
| Opt. Cal.         | **0.0922**     | 0.0515     | **0.1434**            | 0.0552         |

| \( \sigma^2 = 0.5 \) | Average of PMSE | SE of PMSE | \( \sigma^2 = 1 \) | Average of PMSE | SE of PMSE |
|-------------------|----------------|------------|-----------------------|----------------|------------|
| No Bias Corr.     | 0.3744         | 0.0407     | 0.3985                | 0.0666         |
| N.P.              | 0.2810         | 0.0930     | 0.3417                | 0.1367         |
| LS. Cal.          | 0.1924         | 0.0683     | 0.2074                | 0.0853         |
| Opt. Cal.         | **0.1684**     | 0.0656     | **0.1838**            | 0.0788         |

EXAMPLE 5.2. Consider a two-dimensional physical system

\[
\zeta(x_1, x_2) = \frac{2}{3} \exp(x_1 + 0.2) - x_2 \sin 0.4 + 0.4 \\
+ \exp(-x_1) \left( x_1 + \frac{1}{2} \right) \left( x_2^2 + x_2 + 1 \right), \quad (x_1, x_2) \in [0, 1]^2.
\]

Suppose that the computer model is

\[
\eta(x_1, x_2; \theta_1, \theta_2) = \frac{2}{3} \exp(x_1 + \theta_1) - x_2 \sin \theta_2 + \theta_2, \quad (\theta_1, \theta_2) \in [0, 1]^2.
\]
The model discrepancy exists between $\eta(\cdot; \theta_1, \theta_2)$ and $\zeta(\cdot)$. Assume the physical data are generated by (1.1) with a uniform design on $[0, 1]^2$ and $n = 50$. We consider four levels of $\sigma^2 = 0.03, 0.05, 0.07, 0.1$, and use the Matérn kernel $K(x_1, x_2) = (1 + \|x_1 - x_2\|/\psi) \exp\{-\|x_1 - x_2\|/\psi\}$ with $\psi$ chosen by the five-fold cross-validation. For each level of $\sigma^2$, we replicate the data generation, calibration and prediction procedures 1,000 times for all the methods and average the results for each method across the replicates. Table 2 summarizes the results, where the abbreviations of the methods are the same as those in Example 5.1. Once again, the proposed method “Opt. Cal.” outperforms the other three frequentist calibration methods in terms of the predictive mean squared error.

### Table 2

Comparison of predictive mean squared errors for Example 5.2. PMSE = predictive mean squared error, SE = standard error

| $\sigma^2$ | Average of PMSE | SE of PMSE | $\sigma^2$ | Average of PMSE | SE of PMSE |
|------------|-----------------|------------|------------|-----------------|------------|
| 0.03       |                 |            | 0.05       |                 |            |
| No Bias Corr. | 0.1690          | 0.0027     | 0.1691     | 0.0027          |            |
| N.P.       | 0.1155          | 0.0512     | 0.1823     | 0.0850          |            |
| LS. Cal.   | 0.0611          | 0.0198     | 0.0743     | 0.0212          |            |
| Opt. Cal.  | **0.0564**      | 0.0187     | **0.0691** | 0.0205          |            |

| $\sigma^2$ | Average of PMSE | SE of PMSE | $\sigma^2$ | Average of PMSE | SE of PMSE |
|------------|-----------------|------------|------------|-----------------|------------|
| 0.07       |                 |            | 0.1        |                 |            |
| No Bias Corr. | 0.1692          | 0.0028     | 0.1694     | 0.0028          |            |
| N.P.       | 0.2425          | 0.1159     | 0.3327     | 0.1453          |            |
| LS. Cal.   | 0.0825          | 0.0224     | 0.0906     | 0.0235          |            |
| Opt. Cal.  | **0.0776**      | 0.0220     | **0.0863** | 0.0234          |            |

**Example 5.3.** We now compare the proposed calibration method with some Bayesian calibration method. Consider a falling ball example in [15] where the physical system is

$$
\zeta(x) = 8 + \frac{5}{2} \log \left( \frac{50}{49} - \frac{50}{49} \tanh \left( \tanh^{-1}(\sqrt{0.02}) + \sqrt{2}x \right)^2 \right), \quad x \in [0, 1]
$$

and the computer model derived from Newton’s second law is $\eta(x; v_0, g) = 8 + v_0 x - gx^2/2$. Here, calibration parameters $(v_0, g)$ are the vertical velocity and the acceleration rate, respectively. The model discrepancy exists between $\zeta(\cdot)$ and $\eta(\cdot; v_0, g)$. Suppose that the physical data are generated
by (1.1) with a uniform design on [0, 1] and \( n = 30 \). We compare the proposed method “Opt. Cal.” with two Bayesian methods in terms of prediction accuracy:

1) The Bayesian method in Kennedy and O’Hagan [9] (abbreviated as “KO”);
2) The Bayesian predictor using an orthogonal Gaussian process in \( L_2 \)-norm as the prior (abbreviated as “OGP”) proposed by [15].

The Matérn kernel \( K(x_1, x_2) = (1 + |x_1 - x_2|/\psi) \exp\{-|x_1 - x_2|/\psi\} \) with parameter \( \psi = 1 \) is used as the reproducing kernel for “Opt. Cal.” and the prior covariance function for both “KO” and “OGP”. Four levels of \( \sigma^2 = 0.0025, 0.01, 0.0625, 0.25 \) are considered. For each level of \( \sigma^2 \), we replicate the data generation, calibration and prediction procedures 1,000 times. Table 3 summarizes the prediction results. Here “KO” has large prediction errors and large posterior variances compared with “OGP” and “Opt. Cal.”. “OGP” provides stable and accurate predictions and our method “Opt. Cal.” gives even smaller prediction errors for some \( \sigma^2 \) levels.

### Table 3
Comparison of predictive mean squared errors for Example 5.3. PMSE = predictive mean squared error, SE = standard error

| \( \sigma^2 \) | Average of PMSE | SE of PMSE | Average of PMSE | SE of PMSE |
|---|---|---|---|---|
| 0.1 | 0.5413 | 2.3944 | 5.8596 | 29.0264 |
| 0.2 | 0.0147 | 0.0132 | 0.0230 | 0.0249 |
| 0.0091 | 0.0084 | **0.0166** | 0.0168 |

| \( \sigma^2 \) | Average of PMSE | SE of PMSE | Average of PMSE | SE of PMSE |
|---|---|---|---|---|
| 0.4 | 1.4644 | 4.3802 | 18.5433 | 97.3962 |
| 0.8 | 0.0500 | 0.0478 | 0.0952 | 0.0995 |
| **0.0318** | 0.0338 | **0.0620** | 0.0677 |

**Example 5.4 (Real data example).** We analyze a real dataset from a single voltage clamp experiment on sodium ion channels of cardiac cell membranes. This dataset consists of 19 outputs and is from [15]. The response variable is the normalized current for maintaining a fixed membrane potential of \(-35\)mV and the input variable is the logarithm of time. Suppose the computer model for this experiment is the Markov model for sodium ion channels given by \( \eta(x, \theta) = e_1^T \exp(\exp(x)A(\theta))e_4 \), where \( \theta = (\theta_1, \theta_2, \theta_3)^T \in \)
For this example, we compare the frequentist methods in Example 5.1 and 5.2, and Bayesian methods in Example 5.3. The Matérn kernel $K(x_1, x_2) = (1 + |x_1 - x_2|/\psi) \exp\{-|x_1 - x_2|/\psi\}$ with $\psi = 1$ is used for all methods and the Metropolis-Hastings algorithm is applied to sample from the posterior of $\theta$ for Bayesian methods. In each experiment, we perform five-fold cross-validation where the data is randomly partitioned into five roughly equal-sized parts: four parts are for training and the rest part is for testing. The cross-validation process is repeated five times, with each of the five parts is used once for testing. Then, the five predictive mean squared errors are averaged to give a single predictive mean squared error. We replicate the data generation, calibration and prediction procedure 100 times and average the results.

Table 4 summarizes the prediction results, with the abbreviations of the methods given in Examples 5.1 and 5.3. “No Bias Corr.” gives the largest predictive mean squared error among the four frequentist methods, indicating the existence of model discrepancy. Here all the frequentist methods outperform the two Bayesian methods. “No Bias Corr.” outperforms “LS. Cal.”. This indicates that if the calibration parameter is not chosen well, the use of computer model does not improve prediction. Overall, the proposed method “Opt. Cal.” gives the smallest prediction error among all the methods applied to this example.

| Method          | Average of PMSE | SE of PMSE |
|-----------------|-----------------|------------|
| KO              | 0.0045          | 0.0131     |
| OGP             | 9.4387 × 10^{-4}| 0.0022     |
| No Bias Corr.   | 4.2823 × 10^{-4}| 6.2333 × 10^{-4} |
| N.P.            | 2.5916 × 10^{-4}| 2.2522 × 10^{-4} |
| LS. Cal.        | 3.0521 × 10^{-4}| 6.3797 × 10^{-4} |
| Opt. Cal.       | **1.6323 × 10^{-4}** | 2.1335 × 10^{-4} |
6. Concluding remarks and discussions. We have proposed a new look at the model calibration issue in computer models. This viewpoint simultaneously considers two facts regarding how computer models are used in practice: computer models are inadequate for physical systems, regardless how the calibration parameters are tuned; and only a finite number of data points are available from the physical experiment associated with a computer model. We establish a non-asymptotic minimax theory and derive an optimal prediction-oriented calibration method. Through several examples, the proposed calibration method has some advantages in prediction when compared with some existing calibration methods. We have developed an algorithm to carry out the proposed calibration method and built a link between our method and the Bayesian calibration method. Beyond calibration of computer models, our method can be applied to calibrate unknown parameters for general misspecified models in statistics and engineering. In many applications, bounded linear functional information such as derivative data are observed or can be easily calculated together with the function observations. It would be interesting to include all these data in our proposed calibration method.

SUPPLEMENTARY MATERIAL

Supplement to “Another look at Statistical Calibration: Non-Asymptotic Theory and Prediction-Oriented Optimality”. (; .pdf). The supplementary materials contain proofs of technical results in this paper.

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