A Co-kriging Multi-fidelity Surrogate Model Assisted Robust Optimization Approach

Hansi Xu, Qi Zhou, Ping Jiang, and Tingli Xie

***Abstract*—The goal of the robust optimization is to obtain the optimal solution while ensuring that the objective function value is not too sensitive to the uncertainties and the constraints are still feasible under the worst case of the variations of the uncertainty. The effectuation of engineering applications robust design optimization relies on the expensive simulation analysis, which is so time consuming that experimenters turned to mathematical models. In this work, a Co-Kriging multi-fidelity surrogate model assisted robust optimization approach is proposed to improve the efficiency of the robustness optimization. In the developed approach, the Co-Kriging multi-fidelity surrogate model is constructed to integrate the sample date from both low-fidelity (LF) and high-fidelity (HF) models. What is more, the concurrent treatment of the uncertainties from the multi-fidelity surrogate model, design variables, and noise parameters are investigated. The effectiveness and merits of the developed approach are illustrated on a benchmark numerical case.**

***Index Terms*—Co-kriging, multi-fidelity surrogate model, robust optimization, uncertainty quantification.**

I. INTRODUCTION

The concept of robustness is first proposed by Genichi Taguchi in 1940s [1] by defining it as a state where “the performance is minimally sensitive to factors causing variability”. In engineering problems, since products are expected to be robust with high quality and low cost to satisfy the consumers, robust design seems a necessity [2], [3]. To determine statistic characteristics of the product response straight, a large quantity of simulations are required in the formulations of robust design, which leads to the prohibitive computational cost brought by the increasingly complex simulations ensuring accuracy. Considering the consumption of time and the cost, surrogate model is applied in these situations. Common choices of surrogate model are polynomial functions [4], Kriging models [5], [6], radial basis function networks [7] and so on. Recent years, the multi-fidelity [8] surrogate model has become the research hotspots in the current surrogate modeling methods field for combing the high-fidelity [9], [10] analysis model with the low-fidelity analysis model of low cost and providing both the prediction and the prediction error at the non-test points.

Time-saving and cost-reducing it is, the drawback is also obvious. Simply replacing the true response surface with a surrogate model, the deviation (or “surrogate model uncertainty”) may be huge [11], which are supposed to be taken into account. In practical engineering problems, there are varied uncertainties coming from different sources, including the uncertainties of design variables and noise parameters. The former is introduced during manufacturing and measurement process, and the latter originates from physical parameters, environmental conditions [12], etc. These uncertainties could lead to great deviations in the product response of the physical system or the simulation-based engineering analysis, in which case the multiple uncertainties should be quantified appropriately.

While the existing works are either lack of a comprehensive quantification of all existing uncertainties including the design variable uncertainty, noise parameters uncertainty and the surrogate model uncertainty, nor limited to the selection of surrogate models. In this article, the whole situation has been expanded to the multi-fidelity model from the single fidelity, which made the application scope of the comprehensive uncertainty quantization method greatly expanded too. It also increased the efficiency of the robustness optimization assisted with multi-fidelity surrogate model.

This paper is organized as follows. In section 2, the background knowledge of the multi-fidelity surrogate model is briefly presented. Section 3 gives the detailed process of the proposed approach. Then, to illustrate the proposed approach, a benchmark numerical case. is provided in Section 4 to illustrate the efficiency of the proposed approach. Section 5 gives the conclusion and discussion.

II. REVIEW OF THE MULTI-FIDELITY SURROGATE MODEL

A brief review of multi-fidelity surrogate model is briefly introduced in this section. More comprehensive knowledge could be acquired in [13]-[16]. Consider two design sets consisting of two level systems of high fidelity (HF) model and low fidelity (LF) model. The low fidelity input design set and the high fidelity design set are:

$$\begin{aligned}\mathbf{X}_h &= \left[\mathbf{x}_h^{(1)},\mathbf{x}_h^{(2)},\cdots,\mathbf{x}_h^{(n)}\right]^T \\ \mathbf{X}_l &= \left[\mathbf{x}_l^{(1)},\mathbf{x}_l^{(2)},\cdots,\mathbf{x}_l^{(m)}\right]^T\end{aligned} \tag{1}$$

where n and m are the set sizes respectively.

With these sample sets and the multiple models, the corresponding outputs is given as follow:

$$\begin{aligned}\mathbf{Y}_l &= f_l(\mathbf{X}_l)=\left[y_l(\mathbf{x}_l^{(1)}),y_l(\mathbf{x}_l^{(2)}),\cdots,y_l(\mathbf{x}_l^{(m)})\right]^T \\ \mathbf{Y}_h &= f_h(\mathbf{X}_h)=\left[y_h(\mathbf{x}_h^{(1)}),y_h(\mathbf{x}_h^{(2)}),\cdots,y_h(\mathbf{x}_h^{(m)})\right]^T\end{aligned} \tag{2}$$

Based on the Markov property, an autoregressive model could be constructed, which assumes that:

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$$\hat{y}_h(\mathbf{x}) = \rho \hat{y}_l(\mathbf{x}) + \delta(\mathbf{x}) \quad (3)$$

where ρ is a regression parameter playing the role of data connection between the two levels, and $\hat{y}_h(\mathbf{x})$, $\hat{y}_l(\mathbf{x})$ are the prediction response of Kriging model constructed with the initial inputs and outputs. $\delta(\mathbf{x})$ indicates a discrepancy model.

The following formula is used to describe the correlation between two design variables x and $\mathbf{x}'$:

$$\mathrm{R}(\mathbf{x},\mathbf{x}') = \exp[-d(\mathbf{x},\mathbf{x}')] = \exp\left[-\sum_{k=1}^{d}\theta_k (x_k - x'_k)^{P_k}\right] \quad (4)$$

where $\mathrm{x}=(x_1,x_2,\cdots,x_d)$, $\mathbf{x}'=(x'_1,x'_2,\cdots,x'_d)$ with d dimension. θ_k and P_k are the hyper-parameters associate with the dimension k.

The prediction response of a non-sample point $\mathbf{x}^*$ is formed as:

$$\hat{y}_h(\mathbf{x}^*) = f(\mathbf{x})^T \beta^* + c(\mathbf{x})^T C^{-1}(y - F\beta^*) \quad (5)$$

where

$$y = \begin{bmatrix} Y_l \\ Y_h \end{bmatrix}, \beta^* = (F^T C^{-1} F)^{-1} F^T \Lambda^{-1} y \quad (6)$$

$$\mathrm{c}(\mathbf{x}^*) = \begin{bmatrix} \rho\sigma_l^2 \mathrm{R}_l(\mathbf{x}_l,\mathbf{x}^*) \\ \rho^2\sigma_l^2 \mathrm{R}_l(\mathbf{x}_h,\mathbf{x}^*) + \sigma_d^2 \mathrm{R}_d(\mathbf{x}_h,\mathbf{x}^*) \end{bmatrix} \quad (7)$$

The data covariance matrix C is formed as:

$$\mathrm{C} = \begin{bmatrix} \sigma_l^2 \mathrm{R}_l(\mathrm{x}_l,\mathrm{x}_l) & \rho\sigma_l^2 \mathrm{R}_l(\mathrm{x}_l,\mathrm{x}_h) \\ \rho\sigma_l^2 \mathrm{R}_l(\mathrm{x}_l,\mathrm{x}_h) & \rho^2\sigma_l^2 \mathrm{R}_l(\mathrm{x}_h,\mathrm{x}_h) + \sigma_h^2 \mathrm{R}_h(\mathrm{x}_h,\mathrm{x}_h) \end{bmatrix} \quad (8)$$

where $f(\mathbf{x})$ and F are the regression model based on the sampled points and prediction points respectively, σ_l^2 and σ_d^2 are the process variances of the LF model and the discrepancy model respectively.

The mean square error (MSE) of prediction is:

$$s^2(\mathbf{x}) = c' + u^T (F^T C^{-1} F)^{-1} u - c^T C^{-1} c \quad (9)$$

where $u = F^T C^{-1} c - f$ and $c' = \rho^2\sigma_l^2 + \sigma_d^2$. It should be noted that since the Co-kriging model is also a kind of interpolation method based on high fidelity data, it is obvious that the mean square error at the high fidelity points is 0.

III. Quantifying the Compound Effect of Multiple Uncertainties

Define a design variable as $\mathbf{x} = [x_1, x_2, \ldots, x_d]$, to represent the uncertainty of it, the design variables could be formed as:

$$\begin{aligned} &\mathrm{x} = \bar{\mathrm{x}} + \mathrm{d} \\ &\mathrm{d} \sim N(0, \sigma_{\mathrm{x}}^2) \end{aligned} \quad (10)$$

where the vector $\mathrm{d} = [d_1, d_2, \cdots, d_d]$ obeys a multivariate normal distribution with mean of 0 and a covariance matrix σ_{x}, which means the vector $\mathbf{x}$ follows a multivariate normal distribution $\mathrm{x} \sim N(\bar{\mathrm{x}}, \sigma_{\mathrm{x}}^2)$. It should be noted that the deterministic part $\bar{\mathrm{x}} = [\bar{\mathrm{x}}_1, \bar{\mathrm{x}}_2, \cdots, \bar{\mathrm{x}}_d]$ is the design input value designers set. For the noise parameter, $\mathbf{W} = [w_1, w_2, \ldots, w_n]$ obeying the multivariate normal distribution $\mathbf{W} \sim N(\bar{\mathbf{W}}, \sigma_{\mathbf{W}}^2)$ is defined. Notice that the difference between $\bar{\mathrm{x}}$ and $\bar{\mathbf{W}}$ is that the latter one is not designable but uncontrollable instead. Let $y(\mathrm{x},\mathbf{W})$ denote the true response of a computationally expensive simulator as a function of x and $\mathbf{W}$.

The robust design objective [17] in this section is to find the optimal solution $\mathrm{x}^* = \arg\max_{\mathrm{x}} f(\mathrm{x})$ or $\mathrm{x}^* = \arg\min_{\mathrm{x}} f(\mathrm{x})$. The robust design objective function is formed as:

$$f(\mathrm{x}) = \mu(\mathbf{x}) \pm \mathrm{c}\sigma(\mathbf{x}) \quad (11)$$

where $\mu(\mathbf{x})$ and $\sigma(\mathbf{x})$ are the mean and standard deviation of the response value $y(\mathrm{x},\mathbf{W})$. A specific constant value c reflects the risk attitude. What is more, if the response $f(\mathrm{x})$ follows a normal distribution, the value of c (usually selected as 1, 2, 3, etc.) could represent the different confidence levels of prediction intervals. The choice of "$\pm$" is associated with the robust design objective. For example, to maximize the objective function, "$-$" is selected for robust consideration.

If the true response value could be got easily, only two kinds of uncertainties are considered in this scenario, that is the design variable uncertainty and the noise parameter uncertainty. Then, the close form solutions of the response mean and variance are shown below.

$$\begin{aligned} \mu_{\mathrm{W}}(\mathbf{x}) &= E\left[y(\mathrm{x},\mathbf{W})\right] \\ &= \int_{\mathbf{W}}\int_{\mathrm{d}} y(\bar{\mathrm{x}}+\mathrm{d},\mathbf{W})\, p(\mathrm{d})\, p(\mathrm{W})\, d\mathbf{d}d\mathbf{W} \end{aligned} \quad (12)$$

$$\begin{aligned} \sigma_{\mathrm{W}}^2(\mathbf{x}) &= \mathbf{Var}[\mathrm{y}(\mathbf{x},\mathbf{W})] \\ &= E[\mathrm{y}^2(\mathbf{x},\mathbf{W})] - E[\mathrm{y}(\mathbf{x},\mathbf{W})]^2 \\ &= \int_{\mathbf{W}}\int_{\mathrm{d}} y^2(\bar{\mathrm{x}}+\mathrm{d},\mathbf{W}) p(\mathbf{d}) p(\mathbf{W})\, d\mathbf{d}d\mathbf{W} \\ &\quad - \left[\int_{\mathbf{W}}\int_{\mathrm{d}} y(\bar{\mathrm{x}}+\mathrm{d},\mathbf{W}) p(\mathbf{d}) p(\mathbf{W})\, d\mathbf{d}d\mathbf{W}\right]^2 \end{aligned} \quad (13)$$

where $p(\mathrm{d})$ and $p(\mathrm{W})$ are the probability density distribution function of $\mathrm{d} = [d_1, d_2, \cdots, d_d]$, $\mathbf{W} = [w_1, w_2, \ldots, w_n]$.

It is typical that the calculating of (12) and (13) seems too computationally expensive for needing many evaluations of $y(\mathrm{x},\mathbf{W})$. In order to simplify the calculation, a multi-fidelity surrogate model is applied. Based on multi-fidelity simulation, the sample sets with different fidelity levels are acquired to construct a CK model, which greatly reduces the time cost and other expense. Another benefit is that the CK model provides a prediction and the mean squared error (MSE) at every un-sampled points. The CK model prediction response is written as $\hat{y}(\mathbf{x},\mathbf{W})$ to distinguish it from the true response value, and $\sigma_{CK}^2(\mathrm{x},\mathbf{W})$ is the MSE of the CK model. The error function is formed as follow:

$$\sigma_y(\mathrm{x},\mathbf{W}) = \hat{y}(\mathrm{x},\mathbf{W}) - y(\mathrm{x},\mathbf{W}) \quad (14)$$

where

$$\sigma_y(\mathrm{x},\mathbf{W}) \sim N\left(0, \sigma_{CK}^2(\mathrm{x},\mathbf{W})\right) \quad (15)$$

If ignoring the surrogate model uncertainty, $\mathrm{y}(\mathbf{x},\mathbf{W})$ would be simply replaced by $\hat{\mathrm{y}}(\mathbf{x},\mathbf{W})$ in (13) and (14), but it is obviously not proper. In this case, the robust design objective function should be recalculated, as the surrogate model brought the interpolation uncertainty into consideration. The mean and the variance of the prediction response value with the affection of multiple uncertainties are formed as follow:

$$\begin{aligned}\mu_{\mathbf{W+CK}}(\mathbf{x}) &= E\lfloor y(\mathrm{x},\mathbf{W})\rfloor \\ &= E\left[\hat{y}(\mathrm{x},\mathbf{W})\right]+\mathrm{E}\left[\sigma_y(\mathrm{x},\mathbf{W})\right] \\ &= \int_{\mathrm{W}}\int_{\mathrm{d}}\hat{y}(\bar{\mathrm{x}}+\mathrm{d},\mathbf{W})\,p(\mathrm{d})\,p(\mathrm{W})\,d\mathbf{d}\mathbf{W}\end{aligned} \tag{16}$$

$$\begin{aligned}\sigma^2_{\mathbf{W+CK}}(\mathbf{x}) &= \mathbf{Var}[\mathrm{y}(\mathrm{x},\mathbf{W})] \\ &= E[\mathrm{y}^2(\mathrm{x},\mathbf{W})]-E[\mathrm{y}(\mathrm{x},\mathbf{W})]^2 \\ &= \int_{\mathrm{W}}\int_{\mathrm{d}} y^2(\mathrm{x},\mathbf{W})p(\mathbf{d})p(\mathbf{W})d\mathbf{d}\mathbf{W} \\ &\quad -\left[\int_{\mathrm{W}}\int_{\mathrm{d}} y(\mathrm{x},\mathbf{W})p(\mathbf{d})p(\mathbf{W})d\mathbf{d}\mathbf{W}\right]^2 \\ &= \int_{\mathrm{W}}\int_{\mathrm{d}}\left(\hat{y}(\mathrm{x},\mathbf{W})+\sigma_y(\mathbf{x},\mathbf{W})\right)^2 p(\mathbf{d})p(\mathbf{W})d\mathbf{d}\mathbf{W} \\ &\quad -\left[\int_{\mathrm{W}}\left(\hat{y}(\mathbf{x},\mathbf{W})+\sigma_y(\mathbf{x},\mathbf{W})\right)p(\mathbf{d})p(\mathbf{W})d\mathbf{d}\mathbf{W}\right]^2 \\ &= \int_{\mathrm{W}}\int_{\mathrm{d}}\left(\hat{y}^2(\mathbf{x},\mathbf{W})+\sigma_y^2(\mathbf{x},\mathbf{W})\right)p(\mathbf{d})\,p(\mathbf{W})\,d\mathbf{d}\mathbf{W} \\ &\quad +2\int_{\mathrm{W}}\int_{\mathrm{d}}\hat{y}(\mathbf{x},\mathbf{W})\sigma_y(\mathbf{x},\mathbf{W})p(\mathbf{d})\,p(\mathbf{W})\,d\mathbf{d}\mathbf{W} \\ &\quad -\left[\int_{\mathrm{W}}\int_{\mathrm{d}}\hat{y}(\mathbf{x},\mathbf{W})p(\mathbf{d})p(\mathbf{W})d\mathbf{d}\mathbf{W}\right]^2 \\ &= \int_{\mathrm{W}}\int_{\mathrm{d}}\hat{y}^2(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})p(\mathbf{d})\,p(\mathbf{W})\,d\mathbf{d}\mathbf{W} \\ &\quad -\left[\int_{\mathrm{W}}\int_{\mathrm{d}}\hat{y}(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})p(\mathbf{d})p(\mathbf{W})d\mathbf{d}\mathbf{W}\right]^2 \\ &\quad +\int_{\mathrm{W}}\int_{\mathrm{d}}\sigma_y^2(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})p(\mathbf{d})\,p(\mathbf{W})\,d\mathbf{d}\mathbf{W} \\ &= \mathrm{Var}\left[\hat{y}(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})\right]+E\left[\sigma^2_{CK}(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})\right]\end{aligned} \tag{17}$$

Both (16) and (17) are close form solutions, and CK model could give the values of $\sigma^2_{CK}(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})$ and $\hat{y}(\bar{\mathbf{x}}+\mathbf{d},\mathbf{W})$ directly. Adaptive Simpson method or Monto Carlo method could help the calculation.

IV. An Illustrative Benchmark Numerical Case

To validate the benefits of our method considering the uncertainties of surrogate model, design variables and noise parameters, the one-dimensional mathematical example is illustrated. In this case, we consider two mathematical functions as the high fidelity system and the low fidelity system respectively, and the high fidelity function derives from the beak function.

$$\begin{aligned} HF:\ \mathrm{y}_h = g(x,w) &= 3(1-w^2)\exp\left[-(x+1)^2-w^2\right] \\ &\quad -10(-x^5-w^3+\frac{w}{5})\exp\left(-x^2-w^2\right) \\ &\quad -\frac{1}{3}\exp\left[-x^2-(w+1)^2\right] \\ LF:\ \mathrm{y}_l = g(0.9x,0.8w) & \end{aligned} \tag{18}$$

The feasible design interval is $x\in[-2,2]$. As a matter of fact, the design variable x is formed as $x=\bar{x}+\mathbf{d}$, in which $\bar{x}$ is the variable, and $\mathrm{d}\sim N(0,0.009^2)$ is used to show the uncertainty. We consider the uncertainty of noise parameter w the same way as $w=-1+\sigma_w, \sigma_w\sim N(0,0.5^2)$, so the feasible interval of w is:

$$w\in\left[-1-3\times\sigma_w,-1+3\times\sigma_w\right]=\left[-2.5,0.5\right] \tag{19}$$

The response value surface of the beak function is presented in Fig. 1.

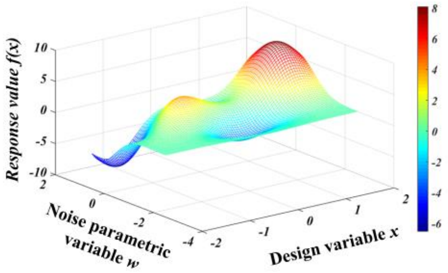

Fig. 1. The HF model.

Based on 6 high fidelity samples and 8 low fidelity samples acquired by Optimal Latin Hypercube technique, the CK (Co-Kriging) model is constructed, the prediction response surface of which is presented in Fig. 2. The robust design objective is to find the maximization of $f(\mathbf{x})$, so the robust design objective function is:

$$f(\mathrm{x})=\mu(\mathbf{x})-\mathrm{c}\sigma(\mathbf{x}) \tag{20}$$

where $c=3$, represent the probability of 0.9987.

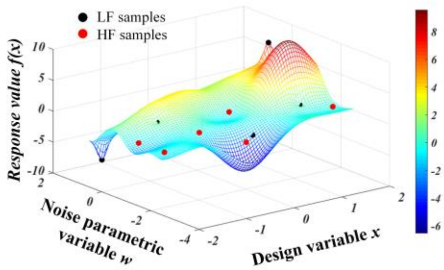

Fig. 2. The CK model based on 6 LF samples and 8 HF samples.

Fig. 3 gives a comparison of two different kinds of the objective response PIs. The mean μ_Δ and the standard deviation σ_Δ in Fig. 3(a) is calculated using (12), (13). $\mu_{\Delta+MF}$ and $\sigma_{\Delta+MF}$ is given by (16), (17). From the comparison results, it is obvious that under the same confidence level, the PI of the proposed method (b) is much wider than that of the conventional method (a).

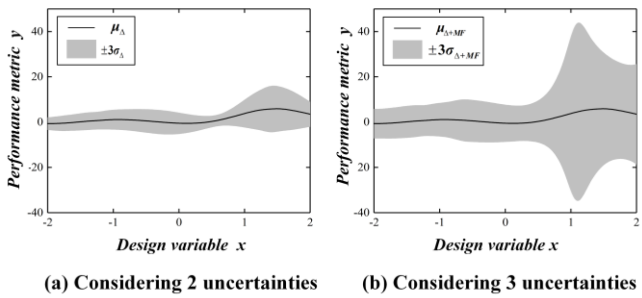

Fig. 3. The 99.87% prediction interval.

For the robust design objective is to find the maximum of the function, the lower boundary of the PI is used for the point searching. The result is presented in Fig. 4. The robust design objected function constructed with the conventional method only considered the design variable uncertainty and the noise parameter uncertainty, and the optimal solution is presented at point B ($x^* = 0.7184$), point A ($x^* = -1.1787$) is the optimal solution of the robust design objected function constructed with the proposed method considering the uncertainties of surrogate model, design variables and noise parameters. It can be seen clearly that these two optimal solutions under different scenarios are very much different.

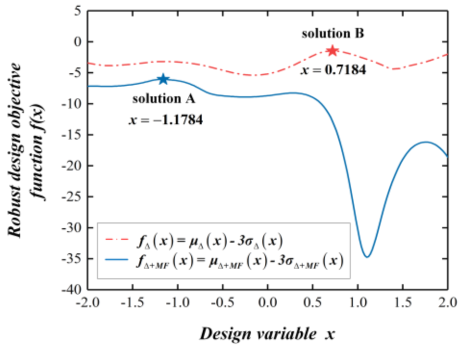

Fig. 4. Robust objective functions considering different kinds of uncertainties.

It is obvious that the two points are much different. The robust objective function of true mathematical function HF is tested in Fig. 5 for better validating the benefits of our method.

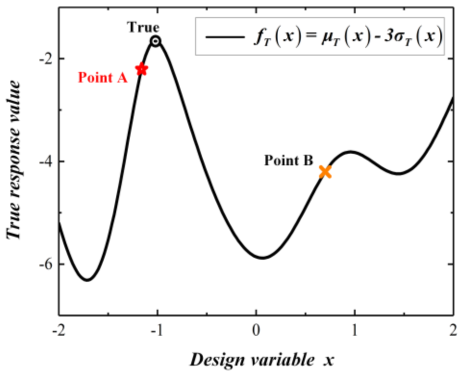

Fig. 5. The true robust objective function.

The true robust objective function is constructed with the true mathematical function, here the high fidelity system function (HF) is chosen. Since we used the true response value instead of the surrogate model value, there is no need to consider the surrogate model uncertainty. The function in Fig. 4 considers only the design variable uncertainty and the noise parameter uncertainty. It is obvious that point C ($x^* = -1.0213$) is the true optimal solution and the point A ($x^* = -1.1787$) of the proposed method is much closer to the true point than the point B ($x^* = 0.7184$). More detailed information is presented in Table I.

TABLE I: THE ARRANGEMENT OF CHANNELS

	x^*	$\mu_w(x^*)$	$\sigma_w(x^*)$	$\mu_w(x^*)-3\sigma_w(x^*)$
Point A	-1.1787	0.6229	0.9928	-2.3554
Point B	0.7184	-0.7319	1.1390	-4.1489
Point C	-1.0213	1.2304	0.9634	-1.6598

For a better explanation of why point B deviates from the true optimal solution so much, a close look at the difference between the two STD functions is shown in Fig. 6(a).

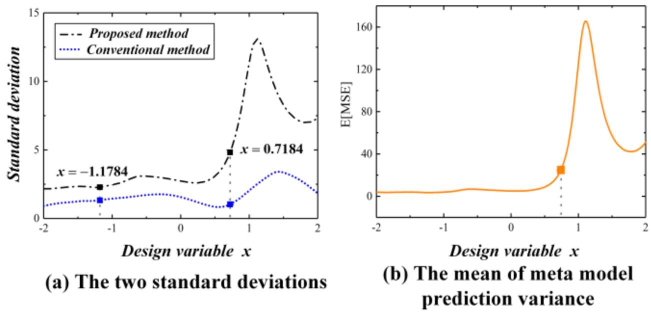

Fig. 6. STDs of (a) the response under different uncertainty situations (b) Mean of the prediction variance.

Our proposed method quantifies the STD larger than that using the conventional way at the same point $x^* = 0.7184$, in other words, the conventional way tended to estimate the STD. It would be clearer with the help of a comparison to the mean of the prediction error $E[MSE]$ presented in Fig. 6(b), and the mean of the prediction error could be treated as the surrogate model uncertainty assisted with the design variable uncertainty and the noise parameter uncertainty. It is interesting to note that the STD constructed with the proposed method rises sharply, in line with the mean of the prediction variance, which means the surrogate uncertainty has a great influence on the optimal solution finding procedure. The effectiveness of our proposed method can be confirmed.

V. CONCLUSION AND DISCUSSION

In this paper, a new robust optimization approach assisted with Co-Kriging multi-fidelity surrogate model is developed. To improve the efficiency of the robustness optimization, the multi-fidelity surrogate model is constructed to integrate the sample date from both low-fidelity (LF) and high-fidelity (HF) models. Besides, the quantification of the all three kinds of uncertainties (the surrogate model uncertainty, design variables uncertainty, and noise parameters uncertainty), which greatly complicated the existing formulations of robust design model. A numerical case has validated the effectiveness of the proposed method. The comparison results showed that the proposed Co-Kriging multi-fidelity surrogate model assisted robust optimization approach considers the compound affection of different kinds of uncertainties is more accurate and effective to find the robust optimal solution than the conventional methods.

As the future work, how to improve the "one shot" model constructing process will be investigated.

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