

Validation by Monte Carlo Sampling of Experimental Observation Functionals

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SUMMARY

We present and analyze a validation procedure for a given state estimate u^* of the true field u^{true} based on Monte Carlo sampling of experimental observation functionals. Our method provides, given a set of N possibly noisy local experimental observation functionals over the spatial domain Ω , confidence intervals for the $L^2(\Omega)$ error in state and the error in $L^2(\Omega)$ outputs. For $L^2(\Omega)$ outputs, our approach also provides a confidence interval for the output itself, which can be used to improve the initial output estimate based on u^* . Our approach implicitly takes advantage of variance reduction, through the proximity of u^* to u^{true} , to provide tight confidence intervals even for modest values of N . We present results for a synthetic model problem to illustrate the elements of the methodology and confirm the numerical properties suggested by the theory. Finally, we consider an experimental thermal patch configuration to demonstrate the applicability of our approach to real physical systems. Copyright © 2016 John Wiley & Sons, Ltd.

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1. INTRODUCTION

According to the definition of AIAA ([7]), validation ([18]) is *the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model*. The importance of validation is twofold. First, reliable validation procedures can serve to verify that the error is less than a certain safety tolerance $\epsilon > 0$ — uncertainty quantification. Second, in the context of subsequent data assimilation ([16]), reliable error estimators can be employed to properly choose the number and location of measurements — in effect, uncertainty reduction. In this paper, we present and analyze a computational procedure to estimate the accuracy of a given state estimate based on N local experimental observations: rather than employing experimental measurements to improve our estimate of the state (data assimilation), we here wish to use experimental measurements to assess *a posteriori* the accuracy of a given deterministic state estimate of the true state (validation), and to improve the estimate of linear outputs of interest (output estimation).

From a mathematical perspective, our goal is to estimate the $L^2(\Omega)$ state-estimation error, and the signed error in $L^2(\Omega)$ output functionals. We shall denote by u^* the estimate of the (assumed) deterministic state u^{true} of a physical system over a specified spatial domain $\Omega \subset \mathbb{R}^d$. We shall further denote by $E = \|u^{\text{true}} - u^*\|_{L^2(\Omega)}$ the $L^2(\Omega)$ state-estimation error, and by $E_{\mathcal{L}} = \mathcal{L}(u^{\text{true}}) - \mathcal{L}(u^*)$ the error in the $L^2(\Omega)$ output $\mathcal{L} : L^2(\Omega) \rightarrow \mathbb{R}$. Finally, we introduce the experimental

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measurements $\{\ell_n^{\text{obs}}\}_{n=1}^N$: we assume that each experimental observation is the application of a linear functional to the physical state with no systematic noise, that is $\ell_n^{\text{obs}} = \ell(u^{\text{true}}, \nu, x_n^{\text{obs}}) + \epsilon_n$, where $x_n^{\text{obs}} \in \Omega$ is the transducer location, the constant $\nu > 0$ denotes the spatial width of the transducer, and ϵ_n is a random disturbance. The functional $\ell(\cdot, \nu, x_n^{\text{obs}})$ takes into account the averaging process performed by the experimental device. We emphasize that the state estimate u^* may reflect “training” data, but the subsequent validation is independent of the training data (i.e., based on an independent dataset).

In this work we follow a frequentist approach to derive confidence intervals for the error in state and output. For either $E_{\mathcal{L}}$ or E , we first build a Monte Carlo estimate for the error (denoted by either $\hat{E}_{\mathcal{L}}$ or $\hat{E}$). Then, we build lower and upper error bounds for the difference between the estimated error and the true error (either $E_{\mathcal{L}} - \hat{E}_{\mathcal{L}}$ or $E - \hat{E}$) based on standard large-sample methods (see, e.g., [21, Chapter 8]). In more detail, we identify three different error sources, here called finite- ν error, finite- N error, and finite-noise error: finite- ν error is related to the finite spatial width ν of the transducer (which prevents us from computing pointwise values of the error field); finite- N error is related to the finite number of measurements available; finally, finite-noise error is related to the random error in the measurements. We propose actionable lower and upper error bounds that take into account finite- N and finite-noise error in the estimate. Furthermore, we develop a mathematical theory to assess the conditions under which finite- ν error is small. We remark that the computational procedure as well as the finite- N and finite-noise analysis do not rely on any assumption on the error field $u^{\text{true}} - u^*$ — apart from a very weak regularity assumption.

Exploiting the linearity of $\mathcal{L}$, we show that we can employ our technique to provide lower and upper bounds for the quantity of interest $\mathcal{L}(u^{\text{true}})$. We demonstrate that, by applying the Monte Carlo procedure to the output error instead of to the true field, and exploiting the proximity of u^* to u^{true} , we can significantly reduce the variance of the process and thus improve the output estimate $\mathcal{L}(u^*)$ for the output $\mathcal{L}(u^{\text{true}})$. We emphasize that the improvement in the output estimate is not the consequence of the improvement of the state estimate u^* , which is not updated by our procedure.

Large-sample methods — on which we rely to address finite- N and finite-noise errors — have already been extensively used to assess the accuracy of computational models in the field of Validation and Verification (see, e.g., [25]). However, the idea of applying a Monte Carlo approach to estimate the $L^2(\Omega)$ error in state and the error in output evaluations is new: rather than comparing experimental measurements of the output with simulation predictions for the output, we exploit (quasi-)pointwise experimental measurements to deduce the error in output functionals of interest.

From the perspective of uncertainty quantification, our method complements Bayesian techniques [3, 4, 6, 19, 20] in that we make few assumptions on the error field $u^{\text{true}} - u^*$. If substantial prior information about the error field is available, we envision that our approach might be outperformed by suitable Bayesian techniques. In absence of such information our frequentist approach can still be applied and will yield good results in particular if the error $u^{\text{true}} - u^*$ is not too large.

From the perspective of uncertainty reduction, our approach may be viewed as the experimental extension of recent efforts in variance reduction techniques for Monte Carlo simulations. In more detail, the idea of using a surrogate model — in this case the state estimate u^* — to reduce the variance of a Monte Carlo process is related to the classical control variates method (see, e.g., [24, Chapter 4]) and to a number of more recent works for the estimation of statistical outputs of stochastic ODEs ([11, 12]), and stochastic PDEs ([1, 27, 17]).

Our method relies on three assumptions: (i) sensor locations are drawn randomly from a given distribution, (ii) the random disturbance is homoscedastic, and (iii) the systematic error in the measurements is small compared to the other sources of error. Measurements in arbitrary spatial points can be acquired by appealing to robotic observation platforms. We refer to [15] for an application of the former data acquisition system to acoustics. On the other hand, we observe that in distributed sensor networks ([8, 23]) locations should be selected among a set of candidate grid points; in section 2, we discuss how to extend our procedure to this scenario. The assumption of homoscedastic random noise is convenient for the analysis and is reasonably accurate in many engineering applications. Systematic error introduces a deterministic shift in our confidence

interval, which is difficult to quantify without any prior information. In section 2, we quantify under what conditions we can neglect it.

This paper is organized as follows. In section 2, we derive a confidence interval $\widehat{C}_{\mathcal{L}}$ for the error in $L^2(\Omega)$ functional outputs; we also unfold the confidence interval to develop estimates for the output $\mathcal{L}(u^{\text{true}})$. In section 3, we discuss how to extend our technique to the estimation of the $L^2(\Omega)$ error in state. Finally, in section 4, we first numerically validate our method for a synthetic example, and we then consider an experimental thermal patch configuration to demonstrate the applicability of our approach to real physical systems.

2. EXPERIMENTAL ERROR IN $L^2(\Omega)$ FUNCTIONALS

2.1. Preliminaries

By way of preliminaries, we introduce notation used throughout the paper. First, we introduce the observable domain Ω^{obs} in which we can take measurements, and the domain of interest $\Omega \subset \Omega^{\text{obs}}$. Then, we introduce the standard $L^p(\Omega^{\text{obs}})$ Banach space over Ω^{obs} endowed with the norm $\|w\|_{L^p(\Omega^{\text{obs}})} = (\int_{\Omega^{\text{obs}}} w^p dx)^{1/p}$. Here, $L^p(\Omega^{\text{obs}})$ consists of classes of equivalence of functions $\{w : \|w\|_{L^p(\Omega^{\text{obs}})} < \infty\}$. Furthermore, we introduce the space of continuous functions over Ω^{obs} , $C(\Omega^{\text{obs}})$.

Given a random variable X , we denote by $\mathbb{E}[X]$ and by $\mathbb{V}[X]$ the mean and the variance, where $\mathbb{E}$ denotes expectation. We use lower-case letters to indicate independent realizations (random variates) of X , $x_1, x_2, \dots$; on the other hand, we use upper-case letters to indicate independent copies of X , $X_1, X_2, \dots$. We refer to a function of the random variates $x_1, x_2, \dots$ as to a (statistical) estimate; while we refer to a function of the random variables $X_1, X_2, \dots$ as to a (statistical) estimator. We denote by $X \sim \mathcal{N}(m, \sigma^2)$ a Gaussian random variable with mean m and variance σ^2 . Similarly, we denote by $X \sim \text{Uniform}(\Omega)$ an uniform random variable over Ω . Furthermore, we refer to an arbitrary random variable ε such that $\mathbb{E}[\varepsilon] = 0$ and $\mathbb{V}[\varepsilon] = \sigma^2$ using the notation $\varepsilon \sim (0, \sigma^2)$. We denote by $\epsilon_1, \epsilon_2, \dots$ independent realizations of ε . Finally, we denote by $\chi_A : \mathbb{R}^d \rightarrow \{0, 1\}$ the indicator function of the set $A \subset \mathbb{R}^d$.

2.2. General framework

We first introduce the problem we wish to address together with a number of definitions and assumptions. Given the true deterministic field $u^{\text{true}} : \Omega^{\text{obs}} \rightarrow \mathbb{R}$, an estimate for u^{true} , $u^* : \Omega^{\text{obs}} \rightarrow \mathbb{R}$, and the associated state estimation error $e := u^{\text{true}} - u^*$, we wish to exploit N local assessment observations to compute a confidence interval $\widehat{C}_{\mathcal{L}}$ for the error

$$E_{\mathcal{L}} = \mathcal{L}(e), \quad (1)$$

where $\mathcal{L} : L^2(\Omega) \rightarrow \mathbb{R}$ is of the form

$$\mathcal{L}(w) := \int_{\Omega} \zeta(x) w(x) dx, \quad (2)$$

and the kernel $\zeta : \Omega \rightarrow \mathbb{R}$ is a $L^2(\Omega)$ function such that $\mathcal{L}$ is bounded in $L^2(\Omega)$.

In order to develop the mathematical analysis, we assume that the ν -neighborhood Ω_{ν} of Ω ,

$$\Omega_{\nu} := \{x \in \Omega^{\text{obs}} : \text{dist}(x, \Omega) < \nu\}, \quad (3)$$

is compactly embedded in Ω^{obs} , $\Omega_{\nu} \subset \subset \Omega^{\text{obs}}$, for some $\nu > 0$.

We model the experimental observations at “point” x_n^{obs} as

$$\ell_n^{\text{obs}} = \ell(u^{\text{true}}, \nu, x_n^{\text{obs}}) + \epsilon_n, \quad n = 1, \dots, N. \quad (4)$$

The disturbances $\epsilon_1, \dots, \epsilon_N$ are N independent realizations of the random variable $\varepsilon \sim (0, \sigma^2)$. We emphasize that (4) corresponds to assuming that systematic experimental error is negligible. In

section 2.3.1, we quantify this assumption. The functional $\ell(\cdot, \nu, x_n^{\text{obs}}) : L^2(\Omega^{\text{obs}}) \rightarrow \mathbb{R}$ is defined as the convolution

$$\ell(w, \nu, x_n^{\text{obs}}) = \int_{\Omega^{\text{obs}}} \omega_{d,\nu}(|x - x_n^{\text{obs}}|) w(x) dx. \quad (5a)$$

The convolutional kernel $\omega_{d,\nu}$ is given by

$$\omega_{d,\nu}(r) = \frac{C(d)}{\nu^d} \omega\left(\frac{r}{\nu}\right), \quad (5b)$$

where $\nu, C(d) > 0$ are given constants, and $\omega(\cdot)$ is a positive function such that $\omega(\rho) = 0$ for $\rho \geq 1$. We emphasize that the constant $\nu > 0$ reflects the filter width of the transducer, assumed small compared to the characteristic length-scale of the true field, while $x_n^{\text{obs}} \in \Omega$ reflects the transducer position. Finally, the function ω describes the local averaging process and is analogous to the spread function employed in blurring/deblurring of images. In anticipation of the analysis, we also introduce the low-pass filter operator $\mathcal{F}_\nu : L^2(\Omega^{\text{obs}}) \rightarrow L^2(\Omega)$ such that

$$\mathcal{F}_\nu(w)(x) = \ell(w, \nu, x), \quad \forall x \in \Omega. \quad (6)$$

We can now introduce the limited observations error estimate $\widehat{E}_\mathcal{L}$ as

$$\widehat{E}_\mathcal{L}(N, \nu) := \frac{|\Omega|}{N} \sum_{n=1}^N \zeta(x_n^{\text{obs}}) \ell_n^{\text{err}}. \quad (7)$$

Here, $\ell_1^{\text{err}}, \dots, \ell_N^{\text{err}}$ are defined as

$$\ell_n^{\text{err}} = \ell_n^{\text{obs}} - \ell(u^*, \nu, x_n^{\text{obs}}). \quad (8a)$$

We observe that $\{\ell_n^{\text{obs}}\}_n$ are taken experimentally, while $\{\ell(u^*, \nu, x_n^{\text{obs}})\}_n$ are computed numerically. Recalling (6) and (4), we also observe that

$$\ell_n^{\text{err}} = \ell(u^{\text{true}}, \nu, x_n^{\text{obs}}) + \epsilon_n - \ell(u^*, \nu, x_n^{\text{obs}}) = \mathcal{F}_\nu(e)(x_n^{\text{obs}}) + \epsilon_n. \quad (8b)$$

In order to address the problem of estimating $E_\mathcal{L}$ using the pointwise estimate $\widehat{E}_\mathcal{L}$, we identify three different sources of error.

- *Finite- ν error*: since the transducers have finite spatial width, we can only measure an approximation of the pointwise values of u^{true} .
- *Finite- N error*: since the number of measurements is limited, only a finite number of error evaluations are available.
- *Finite-noise error*: since measurements are affected by homoscedastic error, we can only observe a noisy value of $\ell(u^{\text{true}}, \nu, x_n^{\text{obs}})$.

To formalize these definitions, we introduce the perfect unlimited observations error estimate

$$\widehat{E}_\mathcal{L}^\infty(\nu) = \mathcal{L}(\mathcal{F}_\nu(e)), \quad (9)$$

and then the finite- ν error

$$\Delta_\mathcal{L}^\nu(\nu) := |E_\mathcal{L} - \widehat{E}_\mathcal{L}^\infty(\nu)|, \quad (10)$$

and the combined finite- N and finite-noise error

$$\Delta_\mathcal{L}^{N,\sigma}(N, \nu) := |\widehat{E}_\mathcal{L}^\infty(\nu) - \widehat{E}_\mathcal{L}(N, \nu)|. \quad (11)$$

We emphasize that $\Delta_\mathcal{L}^\nu$ is deterministic, while $\Delta_\mathcal{L}^{N,\sigma}$ is a random variate.

We now present the outline of the remainder of this section. In section 2.3, we propose an actionable procedure to estimate a confidence interval for $\widehat{E}_\mathcal{L}^\infty(\nu)$. Then, in section 2.4, we illustrate how to exploit the confidence interval for $\widehat{E}_\mathcal{L}^\infty(\nu)$ to update the estimate of the output $\mathcal{L}(u^{\text{true}})$. In these two sections, we assume that the finite- ν error is negligible. Finally, in section 2.5, we provide conditions under which the finite- ν error is small.

2.3. Construction of the confidence interval

2.3.1. Finite-noise and finite- N error In order to derive an asymptotic bound for the finite-noise and finite- N error, it is first convenient to introduce a probabilistic interpretation of the quantities introduced in section 2.2. Towards this end, we assume that the observation points $\{x_n^{\text{obs}}\}_{n=1}^N$ are N independent realizations of the random variable $X \sim \text{Uniform}(\Omega)$, such that X and the random noise ε are independent. As a consequence, recalling (8), we have that $\{\ell_n^{\text{err}}\}_{n=1}^N$ are N independent realizations of the random variable $L^{\text{err}} = \mathcal{F}_\nu(e)(X) + \varepsilon$ and

$$\hat{E}_{\mathcal{L}}^\infty(\nu) = \mathbb{E}[|\Omega| \zeta(X) L^{\text{err}}] = \mathbb{E}[Z^{\text{obs}}], \quad (12)$$

where $Z^{\text{obs}} = |\Omega| \zeta(X) L^{\text{err}}$ is introduced to simplify the notation.

We observe that $\hat{E}_{\mathcal{L}}$ is the sample mean associated with the random variates $\{z_n^{\text{obs}} = |\Omega| \zeta(x_n^{\text{obs}}) \ell_n^{\text{err}}\}_{n=1}^N$; therefore, $\hat{E}_{\mathcal{L}} = \hat{E}_{\mathcal{L}}(x_1^{\text{obs}}, \dots, x_N^{\text{obs}})$ is an unbiased estimate for $\hat{E}_{\mathcal{L}}^\infty(\nu)$, and we can apply the Central Limit Theorem (see, e.g., [13, Theorem 21.1]) to derive an approximate confidence interval for $\hat{E}_{\mathcal{L}}^\infty$. We thus obtain:

$$\begin{aligned} \hat{C}_{\mathcal{L}}^{N,\sigma}(N, \nu, \alpha) &= \left[\hat{E}_{\mathcal{L},\text{LB}}^{N,\sigma}(N, \nu, \alpha), \hat{E}_{\mathcal{L},\text{UB}}^{N,\sigma}(N, \nu, \alpha) \right] \\ &= \left[\hat{E}_{\mathcal{L}}(N, \nu) - \frac{1}{\sqrt{N}} \hat{s}e_{\mathcal{L},N}^{\text{obs}} t_{1-\alpha/2}(N-1), \right. \\ &\quad \left. \hat{E}_{\mathcal{L}}(N, \nu) + \frac{1}{\sqrt{N}} \hat{s}e_{\mathcal{L},N}^{\text{obs}} t_{1-\alpha/2}(N-1) \right], \end{aligned} \quad (13)$$

where $t_{1-\alpha/2}(N-1)$ is the $(1-\alpha/2)$ quantile of the t-distribution with $N-1$ degrees of freedom, and $\hat{s}e_{\mathcal{L},N}^{\text{obs}} = \sqrt{\frac{1}{N-1} \sum_{n=1}^N (z_n^{\text{obs}} - \bar{z}^{\text{obs}})^2}$, $\bar{z}^{\text{obs}} = \frac{1}{N} \sum_{n=1}^N z_n^{\text{obs}}$.

The confidence interval $\hat{C}_{\mathcal{L}}^{N,\sigma}$ is asymptotically correct for $\hat{E}_{\mathcal{L}}^\infty$, its size vanishes as N goes to infinity, and it can be computed in real time ($O(N)$ -computational complexity). In addition, the quantity $\frac{1}{\sqrt{N}} \hat{s}e_{\mathcal{L},N}^{\text{obs}} t_{1-\alpha/2}(N-1)$ asymptotically bounds the finite- N and finite-noise error $\Delta_{\mathcal{L}}^{N,\sigma}$ in (11) with confidence $1-\alpha$. We remark that this procedure can be extended to the case of multiple outputs. We refer to [5] for a thorough analysis of multivariate normal confidence regions. We further observe that other non-parametric strategies for the construction of confidence regions can be applied in lieu of the normal confidence intervals employed in this work. In this respect, we mention bootstrap confidence intervals (see [10, 9] and [28, Chapter 3]).

Our construction relies on the assumptions that we can take measurements in arbitrary spatial points and that systematic noise is negligible. Remark 1 shows how to extend our approach to the case in which sensor locations should be selected among a set of candidate grid points. On the other hand, Remark 2 provides a condition under which systematic noise is negligible.

Remark 1

We shall now discuss the case in which sensor locations should be selected among a set of candidate grid points $\{x_j^{\text{grid}}\}_{j=1}^{\mathcal{N}}$. With this in mind, we shall define the functional $\mathcal{L}^{\text{grid}} : C(\Omega) \rightarrow \mathbb{R}$ as

$$\mathcal{L}^{\text{grid}}(u) = |\Omega| \sum_{j=1}^{\mathcal{N}} u(x_j^{\text{grid}}) \zeta(x_j^{\text{grid}}) w_j, \quad (14)$$

where $\{w_j\}_{j=1}^{\mathcal{N}}$ is a set of suitable positive weights such that $\sum_{j=1}^{\mathcal{N}} w_j = 1$. We shall further define the probability distribution P^{grid} such that $P^{\text{grid}}(x_j^{\text{grid}}) = w_j$, $j = 1, \dots, \mathcal{N}$.

Exploiting the definitions above, it is straightforward to verify that if $X_1, \dots, X_N$ are N independent copies of the random variable $X \sim P^{\text{grid}}$ then

$$\mathbb{E}[|\Omega| \zeta(X) L^{\text{err}}] = \mathcal{L}^{\text{grid}}(\mathcal{F}_\nu(e)), \quad n = 1, \dots, N.$$

Therefore, $\hat{E}_{\mathcal{L}}$ is an unbiased estimate for $\mathcal{L}^{\text{grid}}(\mathcal{F}_\nu(e))$: provided that $|\mathcal{L}^{\text{grid}}(\mathcal{F}_\nu(e)) - \mathcal{L}(\mathcal{F}_\nu(e))|$ is small, we can rely on $\hat{C}_{\mathcal{L}}^{N,\sigma}$ to estimate $\hat{E}_{\mathcal{L}}^\infty(\nu)$. This observation suggests (for smooth problems) a grid informed by high-order quadrature schemes.

Remark 2

Let us assume that $\epsilon_1, \dots, \epsilon_N$ are independent realizations of the random variable $\varepsilon \sim (\delta, \sigma^2)$ with $\delta \neq 0$. Then, $\widehat{C}_{\mathcal{L}}^{N, \sigma}$ is an asymptotically-correct $(1 - \alpha)$ confidence interval for $E_{\mathcal{L}}^{\infty}(\nu) + |\Omega| \delta \mathbb{E}[\zeta(X)]$. Therefore, we can neglect the effect of systematic noise if and only if

$$|\Omega| \delta \mathbb{E}[\zeta(X)] \ll \frac{1}{\sqrt{N}} \widehat{se}_{\mathcal{L}, N}(\delta) t_{1-\alpha/2}(N-1), \quad (15)$$

where the argument δ at the right-hand side stresses the fact that the sample standard deviation depends on δ .

2.3.2. Computational procedure Algorithm 1 outlines the computational procedure to generate the confidence interval $\widehat{C}_{\mathcal{L}}^{N, \sigma}$ for $\widehat{E}_{\mathcal{L}}^{\infty}(\nu)$. Provided that $\Delta_{\mathcal{L}}^{\nu}(\nu)$ is negligible, we can rely on the same procedure to estimate $E_{\mathcal{L}}$.

Algorithm 1 Confidence region for $\widehat{E}_{\mathcal{L}}^{\infty}(\nu)$

Input N number of measurements
 $u^* : \Omega^{\text{obs}} \rightarrow \mathbb{R}$ approximated field
Output $\widehat{C}_{\mathcal{L}}^{N, \sigma}$ confidence interval for $\widehat{E}_{\mathcal{L}}^{\infty}(\nu)$

- 1: Draw N independent realizations $\{x_n^{\text{obs}}\}_n$ from $X \sim \text{Uniform}(\Omega)$, and collect the experimental results $\{\ell_n^{\text{obs}}\}_n$.
 - 2: Compute $\ell_n^{\text{err}} = \ell_n^{\text{obs}} - \ell(u^*, \nu, x_n^{\text{obs}})$ for $n = 1, \dots, N$.
 - 3: $\widehat{E}_{\mathcal{L}}(N, \nu) := \frac{|\Omega|}{N} \sum_{n=1}^N \ell_n^{\text{err}} \zeta(x_n^{\text{obs}})$.
 - 4: Compute the confidence region $\widehat{C}_{\mathcal{L}}^{N, \sigma}$ of (13).
-

The computational cost associated with the procedure is very limited. If the approximated field u^* is discretized through the Finite Element method ([2]), calculation of $\ell(u^*, \nu, x_n^{\text{obs}})$ requires a search to find the element of the FE triangulation to which x_n^{obs} belongs. For structured grids, this operation is independent of the mesh size, while for unstructured grids it scales in general with the size of the mesh. In both cases, the cost is negligible if compared to the cost of acquiring experimental data.

If sensor locations should be selected among a set of grid points $\{x_j^{\text{grid}}\}_{j=1}^N$ (cf. Remark 1), we first introduce the functional $\mathcal{L}^{\text{grid}}$ (14) by selecting the weights $\{w_j\}_{j=1}^N$; then we draw $\{x_n^{\text{obs}}\}_n$ from $X \sim P^{\text{grid}}$, and we collect the corresponding experimental results $\{\ell_n^{\text{obs}}\}_n$. The remainder of the Algorithm (steps 2-4) remains unchanged.

2.4. Variance analysis and output updates

Proposition 2.1 provides a formula for the asymptotic behavior of the square of $\widehat{se}_{\mathcal{L}, N}^{\text{obs}}$ defined in (13).

Proposition 2.1

Let $\{X_n\}_n$ and $\{\varepsilon_n\}_n$ be N independent copies of the two independent random variables $X \sim \text{Uniform}(\Omega)$ and $\varepsilon \sim (0, \sigma^2)$. Then, the following limit holds in the almost sure sense:

$$\lim_{N \rightarrow \infty} \left(\widehat{se}_{\mathcal{L}, N}^{\text{obs}} \right)^2 = |\Omega|^2 \left(\mathbb{V}[\zeta(X) \mathcal{F}_{\nu}(e)(X)] + \mathbb{E}[\zeta(X)^2] \sigma^2 \right). \quad (16)$$

Proof

Recalling the law of large numbers, it is sufficient to show that

$$\mathbb{V}[Z^{\text{obs}}] = |\Omega|^2 \left(\mathbb{V}[\zeta(X) \mathcal{F}_{\nu}(e)(X)] + \mathbb{E}[\zeta(X)^2] \sigma^2 \right),$$

where $Z^{\text{obs}} = |\Omega| \zeta(X) (\mathcal{F}_\nu(e)(X) + \varepsilon)$. Since X and ε are independent, $\mathbb{E}[f(X)g(\varepsilon)] = \mathbb{E}[f(X)]\mathbb{E}[g(\varepsilon)]$ for any pair (f, g) of measurable functions (see, e.g., [13, Theorem 10.1]). Therefore, we obtain

$$\begin{aligned} \mathbb{E}[Z^{\text{obs}}] &= \mathbb{E}[|\Omega| \zeta(X) (\mathcal{F}_\nu(e)(X) + \varepsilon)] \\ &= |\Omega| \left(\mathbb{E}[\zeta(X) \mathcal{F}_\nu(e)(X)] + \mathbb{E}[\zeta(X)] \underbrace{\mathbb{E}[\varepsilon]}_{=0} \right) = |\Omega| \mathbb{E}[\zeta(X) \mathcal{F}_\nu(e)(X)], \end{aligned}$$

and

$$\begin{aligned} \mathbb{E}[(Z^{\text{obs}})^2] &= |\Omega|^2 \left(\mathbb{E}[(\zeta(X) \mathcal{F}_\nu(e)(X))^2] + \mathbb{E}[\zeta(X)^2] \underbrace{\mathbb{E}[\varepsilon^2]}_{=\sigma^2} + 2\mathbb{E}[\zeta(X)^2 \mathcal{F}_\nu(e)(X)] \underbrace{\mathbb{E}[\varepsilon]}_{=0} \right). \\ &= |\Omega|^2 \left(\mathbb{E}[(\zeta(X) \mathcal{F}_\nu(e)(X))^2] + \mathbb{E}[\zeta(X)^2] \sigma^2 \right). \end{aligned}$$

This follows recalling that $\mathbb{V}[W] = \mathbb{E}[W^2] - (\mathbb{E}[W])^2$ for any random variable W . $\square$

The limit (16) and the confidence interval (13) show that the variance of the Monte Carlo process is the sum of two contributions: the first one is related to the accuracy of the state estimate u^* , the second one is related to the magnitude of the noise. The first term vanishes when $u^{\text{true}} = u^*$ (perfect approximation), while the second term vanishes when the measurements are noise-free. Provided that the noise is small, if the error $e = u^{\text{true}} - u^*$ is also small, we can accurately estimate the error for modest values of N .

Due to the linearity of $\mathcal{L}$, and provided that the finite- ν error is negligible, we can also use our error estimator $\hat{E}_\mathcal{L}$ to improve the estimate for the output. We have indeed that

$$\lim_{N \rightarrow \infty} \mathcal{L}(u^*) + \hat{E}_\mathcal{L}(N, \nu) = \mathcal{L}(u^* - \mathcal{F}_\nu(u^*)) + \mathcal{L}(\mathcal{F}_\nu(u^{\text{true}})) \simeq \mathcal{L}(u^{\text{true}}). \quad (17)$$

Clearly, the variance associated with the process $\mathcal{L}(u^*) + \hat{E}_\mathcal{L}(N, \nu)$ satisfies (16). On the other hand, if we apply the Monte Carlo procedure to the true field, we obtain

$$\lim_{N \rightarrow \infty} \left(\hat{s}_{\mathcal{L}, N}^{\text{obs}} \right)^2 = |\Omega|^2 \left(\mathbb{V}[\zeta(X) \mathcal{F}_\nu(u^{\text{true}})(X)] + \mathbb{E}[\zeta(X)^2] \sigma^2 \right).$$

Thus, by applying the Monte Carlo procedure to the output error instead of to the true field, we can significantly reduce the variance associated to the process and thus improve the output estimate even for modest values of N . As stated in the introduction, this idea is related to control variates method for variance reduction ([24]), and also to multi-level Monte Carlo approaches ([11, 12, 1, 27, 17]). In section 4, we assess numerically the practical relevance of (17).

2.5. Analysis of the finite- ν error

In section 2.3, we have proposed an actionable procedure to compute a confidence region $\hat{\mathcal{C}}_\mathcal{L}^{N, \sigma}$ for $\hat{E}_\mathcal{L}^\infty(\nu)$. In this section, we investigate under what assumptions we can neglect the finite- ν error $\Delta_\mathcal{L}^\nu(\nu) = |E_\mathcal{L} - \hat{E}_\mathcal{L}^\infty(\nu)|$ and then interpret $\hat{\mathcal{C}}_\mathcal{L}^{N, \sigma}$ as an appropriate confidence interval for $E_\mathcal{L}$. We refer to [26, Appendix A] for further details.

We present the error bound for $\Delta_\mathcal{L}^\nu(\nu)$. We assume that the filter width ν is such that $\Omega_\nu \subset \subset \Omega$; we further assume that $\omega(r) \leq M$ for all $r \geq 0$ and for some $M > 0$. Then, if $\nabla e \in L^q(\Omega_\nu)$ for some $q > d$, we have

$$|E_\mathcal{L} - \hat{E}_\mathcal{L}^\infty| \leq C_\omega \nu^{1-d/q} |\Omega|^{1/2} \|\zeta\|_{L^2(\Omega)} \|\nabla e\|_{L^q(\Omega_\nu)}, \quad (18)$$

where C_ω depends on the exponent q , on the dimension d , and on the filter shape ω . We observe that bound (18) is not actionable since $\|\nabla e\|_{L^q(\Omega_\nu)}$ is unknown; in section 4.1, we investigate numerically the actual magnitude of $\Delta_\mathcal{L}^\nu(\nu)$ for the problems considered.

Unlike finite- N and finite-noise error, finite- ν error admits a physical interpretation: it is a balance between the filter width ν and the characteristic spatial length scale of the error field. Furthermore, finite- ν error is related to the so-called *minimum detectable signal* in radar systems [22] since it represents a way of assessing the maximum accuracy of our estimate. However, in radar systems this concept has a different physical interpretation: it is the ratio between signal and noise.

3. EXPERIMENTAL $L^2(\Omega)$ A POSTERIORI ERROR ESTIMATOR

3.1. General framework

We now tailor the analysis of section 2 to the *a posteriori* error estimation of the $L^2(\Omega)$ -error $E = \|u^{\text{true}} - u^*\|_{L^2(\Omega)}$. Due to the nonlinearity of E , the procedure is more involved; however, the same ideas apply also to this case.

Given $\{\ell_n^{\text{err}}\}_{n=1}^N$ introduced in (8), we define the limited observations error estimate

$$\hat{E}(N, \nu) := \sqrt{\frac{|\Omega|}{N} \sum_{n=1}^N (\ell_n^{\text{err}})^2}. \quad (19)$$

Then, we define the perfect unlimited observations error estimate

$$\hat{E}^\infty(\nu) := \|\mathcal{F}_\nu(e)\|_{L^2(\Omega)}. \quad (20)$$

Finally, we define the finite- ν error

$$\Delta^\nu(\nu) := |E - \hat{E}^\infty(\nu)|, \quad (21)$$

and the combined finite- N and finite-noise error

$$\Delta^{N, \sigma}(N, \nu) := |\hat{E}^\infty(\nu) - \hat{E}(N, \nu)|. \quad (22)$$

In the remainder of this section, we first propose a confidence interval for $\hat{E}^\infty(\nu)$, and we present an error bound for $\Delta^\nu(\nu)$.

3.2. Construction of the confidence interval

3.2.1. Finite-noise and finite- N error We first consider the case in which the variance σ^2 associated with the random noise is known *a priori*. Given $X \sim \text{Uniform}(\Omega)$, we define the random variable $Y^{\text{obs}} = |\Omega|((L^{\text{err}})^2 - \sigma^2)$, where $L^{\text{err}} = \mathcal{F}_\nu(e)(X) + \varepsilon$, and X and ε are assumed to be independent. We observe that

$$\mathbb{E}[Y^{\text{obs}}] = (\hat{E}^\infty(\nu))^2. \quad (23)$$

Therefore, assuming that σ^2 is known, and exploiting the positivity of $\hat{E}^\infty(\nu)$, we can apply the Central Limit Theorem to derive an approximate confidence interval for $\hat{E}^\infty(\nu)$:

$$\begin{aligned} \hat{C}^{N, \sigma}(N, \nu, \alpha, \sigma) &= [\hat{E}_{\text{LB}}^{N, \sigma}(N, \nu, \alpha, \sigma), \hat{E}_{\text{UB}}^{N, \sigma}(N, \nu, \alpha, \sigma)] \\ &= \left[\sqrt{\left(\left(\hat{E}_{\text{mod}}(N, \nu, \sigma) \right)^2 - \frac{1}{\sqrt{N}} t_{1-\alpha/2}(N-1) \hat{s}e_{Y^{\text{obs}}, N} \right)_+}, \right. \\ &\quad \left. \sqrt{\left(\left(\hat{E}_{\text{mod}}(N, \nu, \sigma) \right)^2 + \frac{1}{\sqrt{N}} t_{1-\alpha/2}(N-1) \hat{s}e_{Y^{\text{obs}}, N} \right)_+} \right]. \end{aligned} \quad (24a)$$

Here, $(a)_+ = \max\{a, 0\}$, the modified estimate $\hat{E}_{\text{mod}}$ is defined as

$$\hat{E}_{\text{mod}}(N, \nu, \sigma) = \sqrt{\left(\left(\hat{E}(N, \nu) \right)^2 - |\Omega|\sigma^2 \right)_+}, \quad (24b)$$

while $t_{1-\alpha/2}(N-1)$ is the $(1-\alpha/2)$ quantile of the t-distribution with $N-1$ degrees of freedom, and $\widehat{se}_{Y^{\text{obs}},N}$ is the sample standard deviation associated with the N independent realizations of Y^{obs} :

$$\widehat{se}_{Y^{\text{obs}},N} := \sqrt{\frac{1}{N-1} \sum_{n=1}^N \left(|\Omega| (\ell_n^{\text{err}})^2 - \left(\widehat{E}(N, \nu) \right)^2 \right)^2}. \quad (24c)$$

We now consider the case in which $\sigma \in [\sigma_{\text{LB}}, \sigma_{\text{UB}}]$ for some known constants $\sigma_{\text{LB}}, \sigma_{\text{UB}} > 0$. Since $\widehat{se}_{Y^{\text{obs}},N}$ is independent of σ^2 , the noise variance σ^2 only shifts the confidence region $\widehat{C}^{N,\sigma}$ along the real axis. Therefore, finite- N and finite-noise errors can be asymptotically decoupled in the limit of $N \rightarrow \infty$. The latter observation helps us manage uncertainty through the value of σ^2 : if we are confident that $\sigma \in [\sigma_{\text{LB}}, \sigma_{\text{UB}}]$, we can modify (24) as follows:

$$\begin{aligned} \widehat{C}^{N,\sigma}(N, \nu, \alpha, \sigma) &= \left[\widehat{E}_{\text{LB}}^{N,\sigma}(N, \nu, \alpha, \sigma), \widehat{E}_{\text{UB}}^{N,\sigma}(N, \nu, \alpha, \sigma) \right] \\ &= \left[\sqrt{\left(\left(\widehat{E}_{\text{mod,LB}}(N, \nu, \sigma) \right)^2 - \frac{1}{\sqrt{N}} t_{1-\alpha/2}(N-1) \widehat{se}_{Y^{\text{obs}},N} \right)}_+, \right. \\ &\quad \left. \sqrt{\left(\left(\widehat{E}_{\text{mod,UB}}(N, \nu, \sigma) \right)^2 + \frac{1}{\sqrt{N}} t_{1-\alpha/2}(N-1) \widehat{se}_{Y^{\text{obs}},N} \right)}_+ \right], \end{aligned} \quad (25a)$$

where $\widehat{E}_{\text{mod,LB}}(N, \nu, \sigma)$, and $\widehat{E}_{\text{mod,UB}}(N, \nu, \sigma)$ are defined as

$$\begin{aligned} \widehat{E}_{\text{mod,LB}}(N, \nu, \sigma) &= \sqrt{\left(\left(\widehat{E}(N, \nu) \right)^2 - |\Omega| \sigma_{\text{UB}}^2 \right)}_+, \\ \widehat{E}_{\text{mod,UB}}(N, \nu, \sigma) &= \sqrt{\left(\left(\widehat{E}(N, \nu) \right)^2 - |\Omega| \sigma_{\text{LB}}^2 \right)}_+. \end{aligned} \quad (25b)$$

3.2.2. Computational procedure Algorithm 2 summarizes the computational procedure. Unlike the case of $L^2(\Omega)$ outputs, we must provide an estimate for σ^2 . As for $L^2(\Omega)$ functionals, if the finite- ν error is modest, we can employ the same procedure to estimate E .

Algorithm 2 Confidence region for $\widehat{E}^\infty(\nu)$

Input	N	number of measurements
	$\sigma_{\text{LB}}, \sigma_{\text{UB}}$	lower and upper bound for the noise standard deviation σ
	$u^* : \Omega^{\text{obs}} \rightarrow \mathbb{R}$	approximated field
Output	$\widehat{C}^{N,\sigma}$	confidence interval for $\widehat{E}^\infty(\nu)$

- 1: Draw N independent realizations $\{x_n^{\text{obs}}\}_n$ from $X \sim \text{Uniform}(\Omega)$, and collect the experimental results $\{\ell_n^{\text{obs}}\}_n$.
 - 2: Compute $\ell_n^{\text{err}} = \ell_n^{\text{obs}} - \ell(u^*, \nu, x_n^{\text{obs}})$ for $n = 1, \dots, N$.
 - 3: $\widehat{E}(N, \nu) := \sqrt{\frac{|\Omega|}{N} \sum_{n=1}^N (\ell_n^{\text{err}})^2}$.
 - 4: Compute the confidence region $\widehat{C}^{N,\sigma}$ of (25).
-

3.3. Analysis of the finite- ν error

We briefly comment on the finite- ν error $\Delta^\nu(\nu)$. With this in mind, we assume that (i) $\Omega_\nu \subset \subset \Omega$, (ii) $\omega(r) \leq M$ for all $r \geq 0$ and for some $M > 0$, and (iii) $\nabla e \in L^q(\Omega_\nu)$ for some $q > d$. Then, it is

possible to prove the following estimate

$$\Delta^\nu(\nu) \leq C_\omega \sqrt{|\Omega|} \nu^{1-d/q} \|\nabla e\|_{L^q(\Omega_\nu)}, \quad (26)$$

where $C_\omega > 0$. As for $L^2(\Omega)$ functionals, finite- ν error $\Delta^\nu(\nu)$ depends on the balance between filter width ν and characteristic spatial length scale of the error field. We refer to [26, Appendix A] for the proof of (26), and to the numerical results for a rigorous assessment of the practical effect of this contribution for a controlled synthetic example.

4. NUMERICAL RESULTS

4.1. A synthetic problem

We first assess our computational procedures through a synthetic problem. Towards this end, we consider the parametric problem:

$$\begin{cases} -\nabla \cdot (\kappa(\mu) \nabla u(\mu)) = 0 & \text{in } \Omega^{\text{obs}} \\ \kappa(\mu) \frac{\partial u}{\partial n} = g & \text{on } \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \\ u(\mu) = 0 & \text{on } \Gamma_4 \end{cases} \quad (27a)$$

where $\Omega^{\text{obs}} = \bigcup_{i=1}^9 \Omega_i$, and

$$\kappa(x, \mu) = \begin{cases} 1 & \text{in } \Omega_1, \\ \mu_i & \text{in } \Omega_{i+1}, \quad i = 1, \dots, 8; \end{cases} \quad g(x) = \begin{cases} 1 & \text{on } \Gamma_1, \\ 0 & \text{on } \Gamma_2, \\ 1 - 2x_1 & \text{on } \Gamma_3. \end{cases} \quad (27b)$$

Figure 1 shows the computational domain. We consider the domain of interest $\Omega = \Omega_5$. In order to assess our method, we generate the true field u^{true} and the approximate field u^* by considering the solution to (27) obtained using a Finite Element (FE) solver for different choices of the parameter μ :

$$u^{\text{true}} = u(\mu^{\text{true}} = [1, 1, 1, 1, 1, 1, 1, 1]), \quad u^* = u(\mu^* = [1, 1.2, 1.5, 0.6, 1.6, 1.3, 1.1, 1]).$$

We resort to a $\mathbb{P}^3$ Finite Element discretization with $\mathcal{N} = 37249$ degrees of freedom. Figure 2 shows the true field and the error field over Ω^{obs} and highlights the domain of interest Ω .

Local experimental observations are assumed to be truncated Gaussians with $\nu = 2r_{\text{Gauss}}$, and standard deviation equal to r_{Gauss} :

$$\omega_{d,\nu}(r) = C(r_{\text{Gauss}}, d) \exp\left(-\frac{r^2}{2r_{\text{Gauss}}^2}\right) \chi_{\{r < 2r_{\text{Gauss}}\}}(r). \quad (28)$$

In all the simulations, we consider observations of the form

$$\ell_n^{\text{obs}} = \ell(u^{\text{true}}, \nu, x_n^{\text{obs}}) + \epsilon_n,$$

where $\epsilon_1, \dots, \epsilon_N$ are N independent random variates of the Gaussian random variable $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

4.1.1. Error in $L^2(\Omega)$ outputs We first consider the case of $L^2(\Omega)$ outputs. We wish to estimate the error associated with the output

$$\mathcal{L}(u^{\text{true}}) = \frac{1}{|\Omega|} \int_{\Omega} u^{\text{true}} dx,$$

corresponding to $\zeta = 1/|\Omega|$. For this choice of $\mathcal{L}$, we have

$$\mathcal{L}(u^{\text{true}}) = -1.9588, \quad \mathcal{L}(u^*) = -1.8464.$$

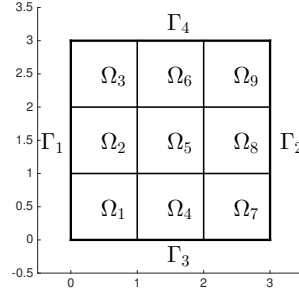


Figure 1. Thermal block synthetic problem: computational domain.

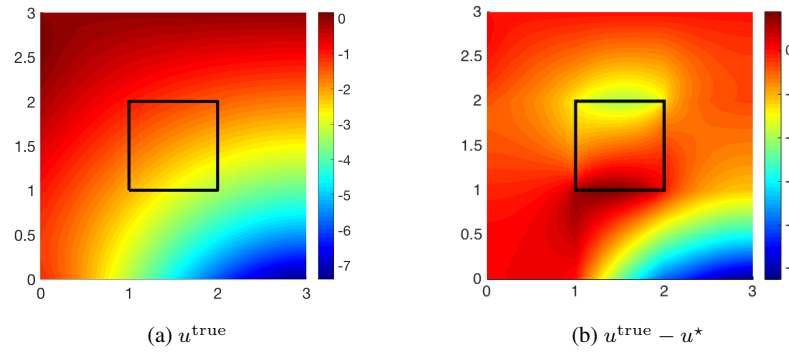

 Figure 2. Thermal block synthetic problem: visualization of the true field and of the error field. The domain Ω is the rectangular region inside the black boundary.

Figure 3 shows the behavior of the error estimator $\hat{E}_{\mathcal{L}}$ and of the lower and upper bounds $\hat{E}_{\mathcal{L},\text{LB}}^{N,\sigma}$ and $\hat{E}_{\mathcal{L},\text{UB}}^{N,\sigma}$ with respect to N for two values of σ . In this test, we consider $\alpha = 0.1$, $r_{\text{Gauss}} = 0.1$. We observe that in the noise-free case ($\sigma = 0$), $\hat{E}_{\mathcal{L}}$ is an accurate approximation of $E_{\mathcal{L}}$ for $N \gtrsim 5$, and that $\hat{E}_{\mathcal{L}}^{N,\sigma}$ is a meaningful confidence interval for $E_{\mathcal{L}}$ for $N \gtrsim 10$. By comparing Figure 3(a), and Figure 3(b), we observe that the convergence with N depends on the magnitude of noise as expected from the theory (see equation (16)).

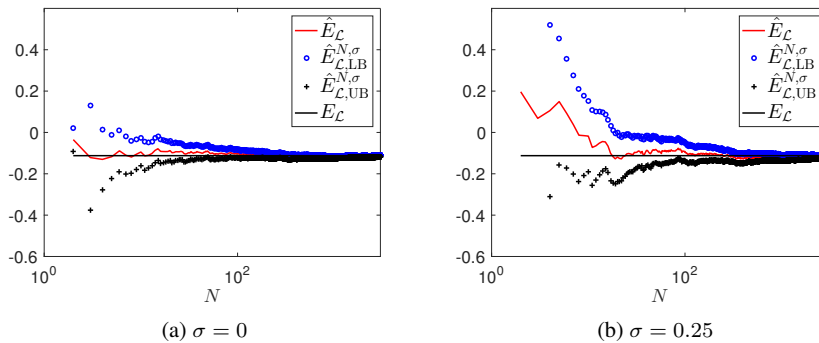

 Figure 3. Thermal block synthetic problem: $(1 - \alpha)$ - confidence interval for the output error ($\alpha = 0.1$, $r_{\text{Gauss}} = 0.1$, $\mathcal{L}(u^{\text{true}} - u^*) = -0.1124$).

Figure 4 shows that we can use our procedure to build a confidence interval for $\mathcal{L}(u^{\text{true}})$. This observation confirms the result in (17). We observe that we can use our strategy to update the estimate for $\mathcal{L}(u^{\text{true}})$ for $N \gtrsim 10$ in the noise-free case, and for $N \gtrsim 20$ in the noisy case.

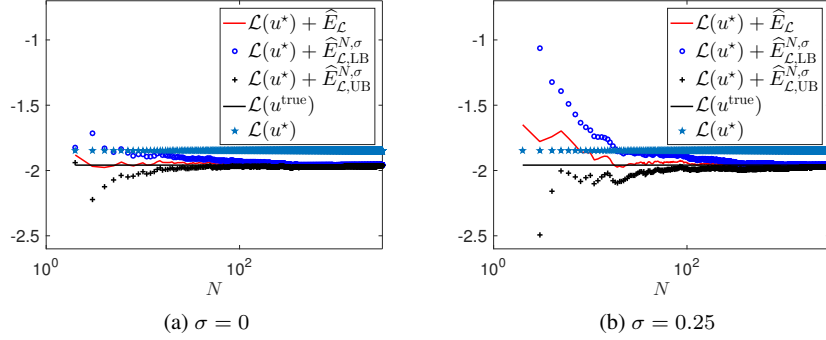


Figure 4. Thermal block synthetic problem: $(1 - \alpha)$ -confidence interval for the output ($\alpha = 0.1$, $r_{\text{Gauss}} = 0.1$, $\mathcal{L}(u^{\text{true}}) = -1.9288$).

Figure 5 shows the behavior of the size of the confidence interval, $|\hat{\mathcal{C}}_{\mathcal{L}}^{N,\sigma}|$, for two different choices of σ , and for $u^* = 0$ and $u^* = u(\mu^*)$. We denote by $\hat{\mathcal{C}}_{\mathcal{L},1}^{N,\sigma}$ the region associated with $u^* = u(\mu^*)$, and by $\hat{\mathcal{C}}_{\mathcal{L},2}^{N,\sigma}$ the region associated with $u^* = 0$. As in the previous test, we set $\alpha = 0.1$, $r_{\text{Gauss}} = 0.1$. We observe that $|\hat{\mathcal{C}}_{\mathcal{L},1}^{N,\sigma}(N = 10)| \approx |\hat{\mathcal{C}}_{\mathcal{L},2}^{N,\sigma}(N = 150)|$ in the noise-free case, and $|\hat{\mathcal{C}}_{\mathcal{L},1}^{N,\sigma}(N = 10)| \approx |\hat{\mathcal{C}}_{\mathcal{L},2}^{N,\sigma}(N = 40)|$ in the noisy case. The results show that our procedure takes advantage of the proximity of u^* to u^{true} to reduce the variance of the process. We observe that the variance reduction strategy is less effective in the presence of experimental noise: this is in good agreement with estimate (16).

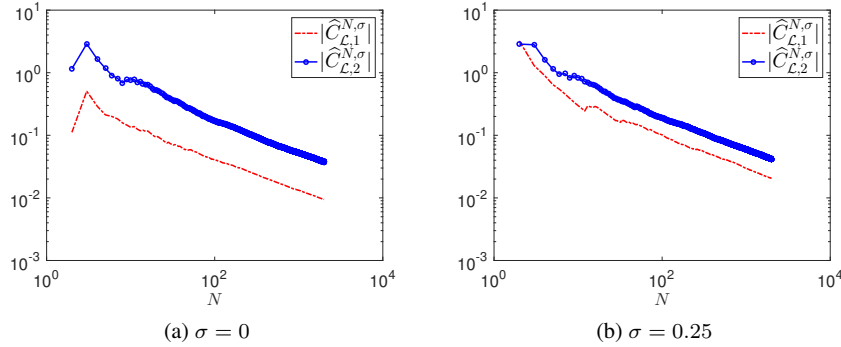


Figure 5. Thermal block synthetic problem: size of the confidence interval $|\hat{\mathcal{C}}_{\mathcal{L}}^{N,\sigma}|$ for two different choices of σ , and for $u^* = 0$ and $u^* = u(\mu^*)$ ($\alpha = 0.1$, $r_{\text{Gauss}} = 0.1$).

4.1.2. $L^2(\Omega)$ error We now consider the problem of estimating the $L^2(\Omega)$ error. Figure 6 shows the behavior of $\hat{E}$, $\hat{E}_{\text{mod}}$, and the lower and upper bounds $\hat{E}_{\text{LB}}^{N,\sigma}$ and $\hat{E}_{\text{UB}}^{N,\sigma}$ with respect to N and for two values of σ . In this test, we consider $\alpha = 0.1$, $r_{\text{Gauss}} = 0.05$, and we assume that we know the value of σ . We observe that our procedure provides a meaningful upper bound for the error for $N \gtrsim 5$ in the noise-free case, and for $N \gtrsim 20$ in the noisy case.

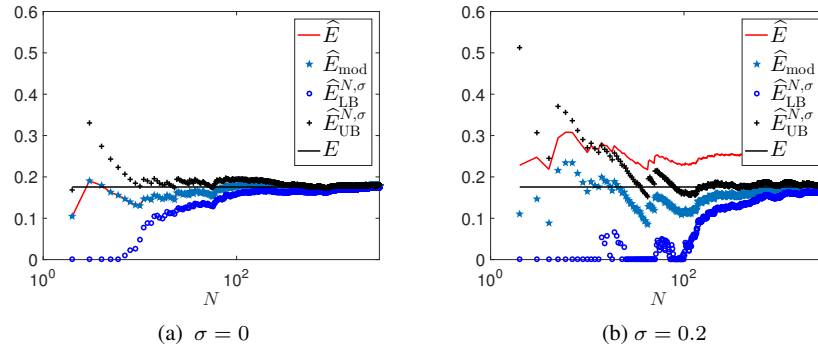


Figure 6. Thermal block synthetic problem: confidence intervals for the $L^2(\Omega)$ error for two different choices of σ ($\alpha = 0.1$, $r_{\text{Gauss}} = 0.05$, $\|u^{\text{true}} - u^*\|_{L^2(\Omega)} = 0.1756$).

4.1.3. Finite- ν error In Figure 7, we investigate the effect of the finite width ν in output error and $L^2(\Omega)$ error estimation[†]. Figure 7(a) shows the behavior of $\hat{E}_{\mathcal{L}}$, $\hat{E}_{\mathcal{L},\text{LB}}^{N,\sigma}$ and $\hat{E}_{\mathcal{L},\text{UB}}^{N,\sigma}$ with respect to r_{Gauss} for $N = 2000$. Similarly, Figure 7(b) shows the behavior of $\hat{E}$, $\hat{E}_{\text{LB}}^{N,\sigma}$ and $\hat{E}_{\text{UB}}^{N,\sigma}$ with r_{Gauss} for the same value of N . We observe that $\hat{E} - E \sim Cr_{\text{Gauss}}$ as $r_{\text{Gauss}} \rightarrow 0^+$: since for our choice of u^{true} and u^* we have that ∇e is bounded, and recalling that $\nu = 2r_{\text{Gauss}}$, this empirically confirms the error bound (26).

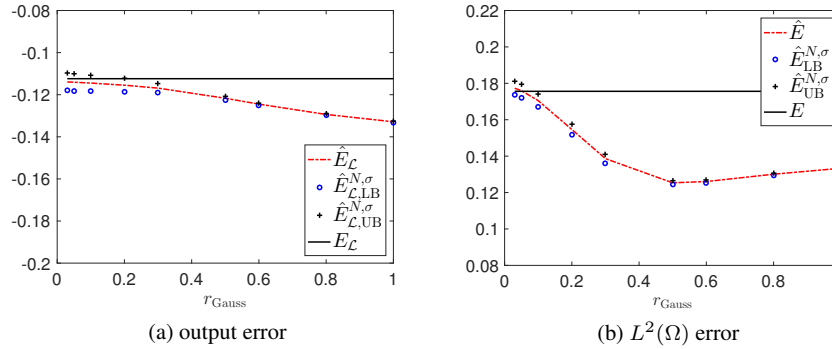


Figure 7. Thermal block synthetic problem: confidence intervals for output error and $L^2(\Omega)$ error for different values of r_{Gauss} ($\sigma = 0$, $\alpha = 0.1$, $N = 2000$).

4.1.4. Analysis of the finite-grid case We now consider the case in which sensor locations should be selected among a set of grid points $\{x_j^{\text{grid}}\}_{j=1}^N$. Towards this end, we consider two different cases: (i) a 10 by 10 grid of equispaced sensors in Ω , and (ii) a 10 by 10 grid associated with the Gaussian quadrature points in Ω . Figure 8 shows the grids. For the first grid we define $\mathcal{L}^{\text{grid}}$ (14) using uniform weights $w_j = \frac{1}{100}$, while for the second grid we consider the weights associated with Gaussian quadrature.

Figure 9 shows the behavior of the confidence intervals for $E_{\mathcal{L}}$ and for $\mathcal{L}(u^{\text{true}})$. We here set $r_{\text{Gauss}} = 0.1$. We observe that for the Gaussian case results are comparable with the results shown in Figures 3 and 4; on the other hand, for the uniform case we observe that $\mathcal{L}^{\text{grid}}(\mathcal{F}_{\nu}(e)) - \mathcal{L}(\mathcal{F}_{\nu}(e))$ is not negligible.

[†]For $r_{\text{Gauss}} \geq 0.5$, condition $\Omega_{\nu} \subset \subset \Omega^{\text{obs}}$ does not hold; in this case, we simply adjust the constant $C = C(r_{\text{Gauss}}, d, x)$ in (28) by imposing that $\ell(1, \nu, x) = 1$ for any $x \in \Omega$.

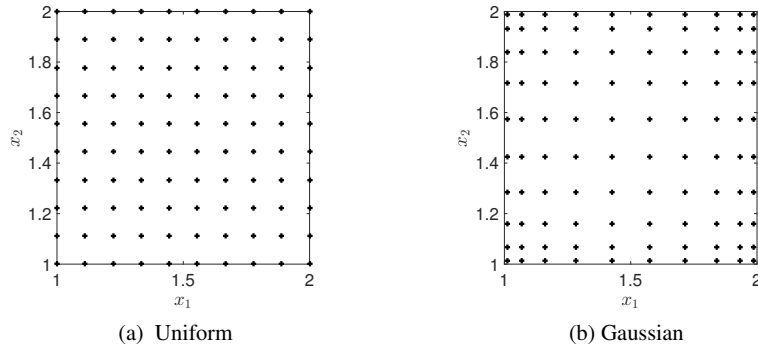
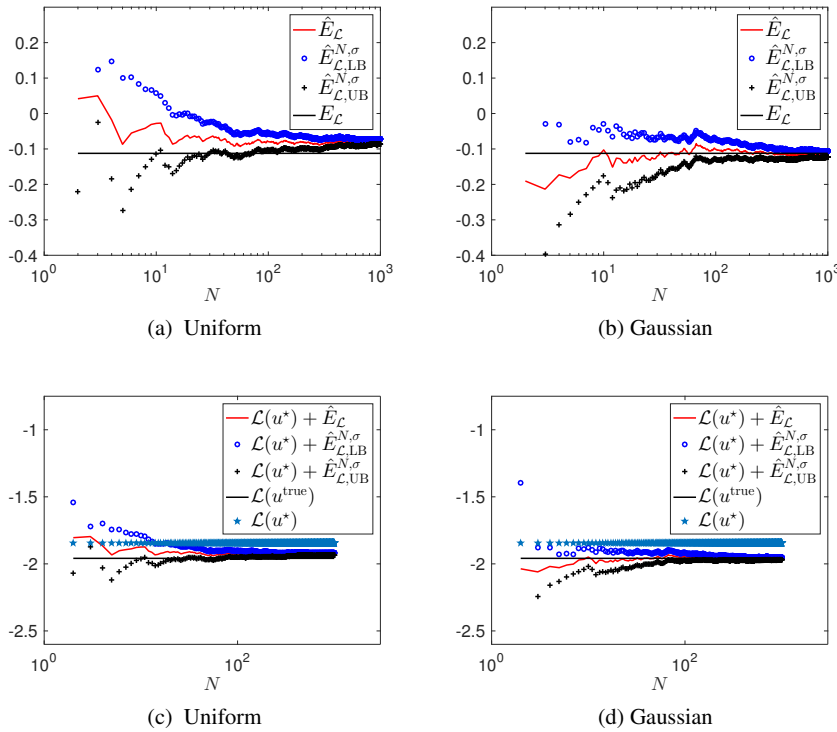


Figure 8. Thermal block synthetic problem: sensor grids.

Figure 9. Thermal block synthetic problem: confidence intervals for the output error and for the output ($\sigma = 0$, $r_{\text{Gauss}} = 0.1$, $\alpha = 0.1$).

4.2. A physical problem

4.2.1. Physical system As our second example, we consider a physical (experimental) system: a thermal patch problem in which a 1.5mm thick acrylic sheet is heated from behind by a resistive patch[‡]. The goal of a data assimilation procedure is to estimate the temperature field over a portion Ω^{obs} of the external surface of the plate heated by the patch in the steady-state limit. We can then assess the accuracy of the state estimate with the Monte Carlo procedure developed in this paper.

[‡]Heat is generated through an electrical resistance. Input power is 0.667W.

We use an IR camera (Fluke Ti 9) to take measurements in the rectangular region $\Omega^{\text{obs}} = [-23.85, 23.85] \times [-17.85, 17.85]$ mm centered on the patch. After the patch power is turned on, we take measurements using a sampling time of 4 seconds until steady state is reached; the total duration of the experiment is roughly 5 minutes. The external temperature is about 20°C , roughly constant throughout the experiment. Each surface measurement taken from the IR camera corresponds to 160×120 pixel-wise measurements; the pixel size is roughly $\Delta h^{\text{device}} = 0.3\text{mm}$, which is much smaller than the spatial length scale of the phenomenon of interest. Figure 10 shows the experimental apparatus: Figure 10(a) shows the IR camera employed to take measurements; Figure 10(b) shows a section of the experimental apparatus; Figure 10(c) shows the geometry of the patch, ($\hat{L} = 22.606\text{mm}$, $\hat{H} = 9.271\text{mm}$).

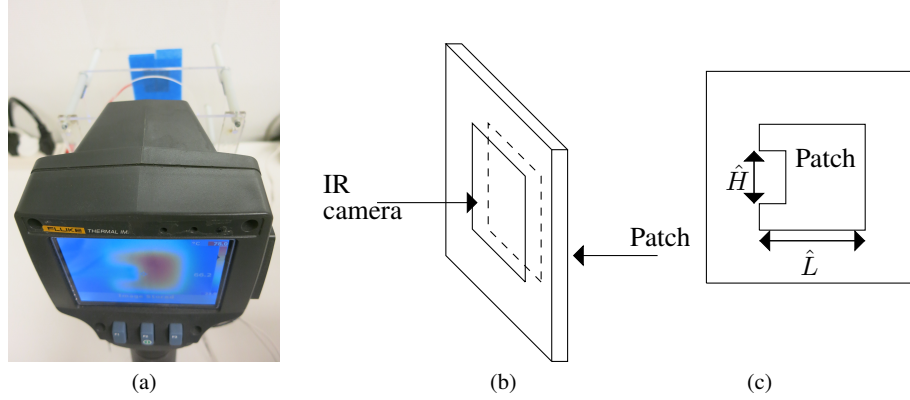


Figure 10. Thermal patch problem. Figure (a): IR camera. Figures (b) and (c): mathematical description of the acrylic sheet. $\hat{L} = 22.606\text{mm}$, $\hat{H} = 9.271\text{mm}$.

We define the observed thermal field u^{obs} as the spatial field obtained from the IR camera at steady state and we consider the state estimate u^* corresponding to the Finite Element solution to a properly-tuned steady-heat transfer PDE model (see [26, Chapter 4.5.2]). We also introduce the domain of interest $\Omega = (-0.5\hat{L}, 0.5\hat{L}) \times (-0.5\hat{L}, 0)$. Figure 11 shows the observed field u^{obs} , the error field $e^{\text{obs}} = u^{\text{obs}} - u^*$, and the domain Ω .

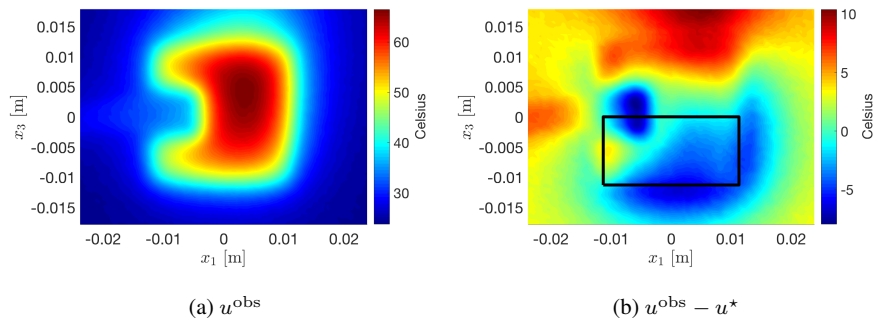


Figure 11. Thermal patch problem: visualization of the observed field and of the error field. The domain Ω is the rectangular region inside the black boundary.

The IR camera is a luxury since full-field information is typically not available. In actual practice, we envision a system with a local sensor or a small sensor array. For this reason, we synthesize local measurements – the experimental input to our method – from the IR camera data to obtain $\ell_n^{\text{obs}} = \ell(u^{\text{obs}}, \nu, x_n^{\text{obs}})$, where $\ell(\cdot, \nu, \cdot)$ is a truncated-Gaussian functional with support in the ball of radius $\nu = 6\Delta h^{\text{device}} = 1.8\text{mm}$ and standard deviation $\nu/2$. This corresponds to a weighted

average over roughly 144 pixel-wise measurements. Observation points are chosen as independent realizations of a discrete uniform distribution over the pixels' centers. We observe that the IR camera permits us to conduct convergence studies that would typically not be feasible in actual field deployment.

We now briefly comment on the noise in the dataset and we define the true field. In Figure 12, we show two spatial slices of the field $u^{\text{obs}} - u^{\text{filt}}$. The field u^{obs} is obtained directly from the IR camera, while u^{filt} is obtained applying a Wiener filter (see, e.g., [14]) based on a 3 by 3 pixel averaging to the field u^{obs} . Comparing u^{filt} and u^{obs} , we can deduce that the magnitude of noise in the measurements is approximately $\pm 0.5^\circ\text{C}$, roughly independent of the spatial position. In what follows, we set $u^{\text{true}} = u^{\text{filt}}$. We emphasize that measurements are computed based on u^{obs} .

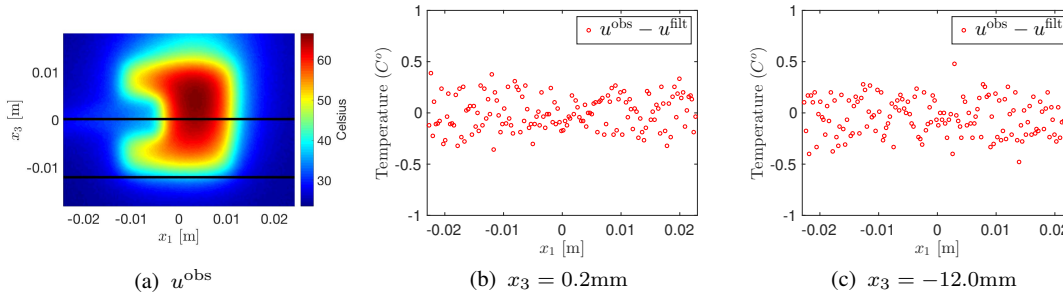


Figure 12. Thermal patch problem: comparison between filtered and unfiltered fields. Figure (a): observed thermal field u^{obs} . Figures (b) and (c): spatial slices of the difference $u^{\text{obs}} - u^{\text{filt}}$.

4.2.2. *Numerical results* We wish to estimate the error associated with the output

$$\mathcal{L}(u^{\text{true}}) = \frac{1}{|\Omega|} \int_{\Omega} u^{\text{true}} dx,$$

and the $L^2(\Omega)$ error over Ω , $\|u^{\text{true}} - u^{\star}\|_{L^2(\Omega)}$. We observe that

$$\mathcal{L}(u^{\text{true}}) = 50.0640^\circ\text{C}, \quad \mathcal{L}(u^{\star}) = 52.5965^\circ\text{C},$$

and[§]

$$\|u^{\text{true}} - u^{\star}\|_{L^2(\Omega)} = 0.0529[^\circ\text{C} \times \text{m}].$$

Figure 13 shows the results. We observe that for $N \simeq 10$ the 90% confidence interval for the output error contains the true value, and has a half-amplitude equal to 1°C (Figure 13(a)); therefore, we can use $\hat{E}_{\mathcal{L}}$ to update the estimate of the output (Figure 13(b)). Similarly, we are able to construct meaningful confidence intervals for the $L^2(\Omega)$ error for $N \gtrsim 10$ (Figure 13(c)). This shows that, also in this case, our procedure is able to provide accurate confidence intervals for modest values of N .

5. CONCLUSIONS AND PERSPECTIVES

We propose a Monte Carlo experimental procedure that provides confidence intervals for the $L^2(\Omega)$ error in state and the signed error in $L^2(\Omega)$ outputs. The procedure relies on a state estimate $u^{\star}$ for the true field u^{true} and on N possibly noisy local experimental functionals, and is based on the identification of three different sources of error: the finite- ν , the finite- N error, and the finite-noise error. Finite- N and finite-noise errors can be bound through an asymptotically rigorous statistical

[§]To provide a benchmark value, we observe that $\|u^{\text{true}} - \mathcal{L}(u^{\text{true}})\|_{L^2(\Omega)} = 0.1275[^\circ\text{C} \times \text{m}]$.

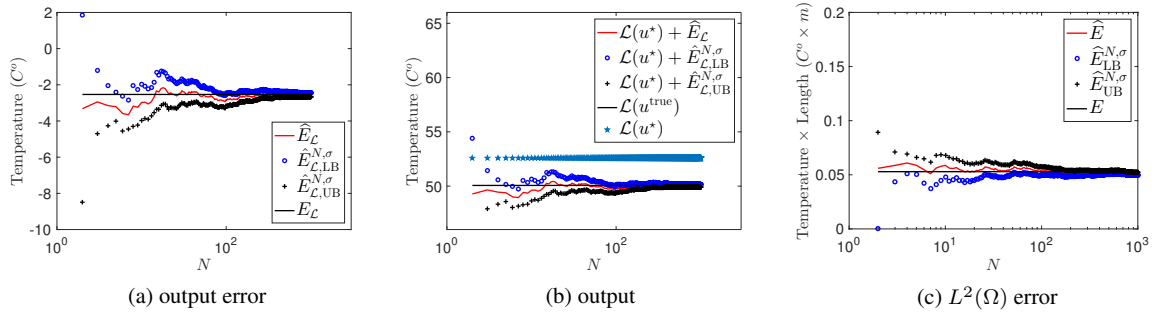


Figure 13. Thermal patch: confidence intervals for the output error, the output, and the $L^2(\Omega)$ error ($\alpha = 0.1$, $r_{\text{Gauss}} = 0.09\text{mm}$, $\mathcal{L}(u^{\text{true}} - u^*) = -2.5325^{\circ}\text{C}$, $\|u^{\text{true}} - u^*\|_{L^2(\Omega)} = 0.0529[^{\circ}\text{C} \times \text{m}]$).

procedure. On the other hand, the effect of ν depends on the spatial scale of the field and on the transducer resolution, and can only be assessed on a case-by-case basis.

We now identify a number of open problems that are the subject of ongoing research. First, we wish to extend our approach to heteroscedastic noise and to more general sampling strategies. Second, we wish to consider time-dependent problems. In this respect, for sequential estimates, we distinguish between the case of fixed sensors and the case of movable sensors. For the former, our approach seems to be readily extendable; for the latter, we envision that the error estimation procedure should be coupled with adaptive strategies for the choice of the transducer paths.

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