

Accounting for Test Variability through Sizing Local Domains in Sequential Design Optimization with Concurrent Calibration-Based Model Validation

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ABSTRACT

We have recently proposed a new method for combined design optimization and calibration-based validation using a sequential approach with variable-size local domains of the design space and statistical bootstrap techniques. Our work was motivated by the fact that model validation in the entire design space may be neither affordable nor necessary. The method proceeds iteratively by obtaining test data at a design point, constructing around it a local domain in which the model is considered valid, and optimizing the design within this local domain. Due to test variability, it is important to know how many tests are needed to size each local domain of the sequential optimization process. Conducting an unnecessarily large number of tests may be inefficient, while a small number of tests may be insufficient to achieve the desired validity level. In this paper, we introduce a technique to determine the number of tests required to account for their variability by sizing the local domains accordingly. The goal is to achieve a desired level of model validation in each domain using the correlation between model data at the center and any other point in the local domain. The proposed technique is illustrated by means of a piston design example.

1. INTRODUCTION

A major challenge in engineering design optimization is that the computational and/or simulation models utilized for analysis to quantify objective and constraint values (and their sensitivities with respect to design variables and parameters) must remain adequately accurate in very large design spaces, both in terms of dimensionality and range. In the engineering design community, adequate accuracy of the models has been assessed by validation approaches that compare

model predictions to experimental data. Model validation for specific analysis purposes typically presents significantly less computational challenges as such models are developed with the intention to be utilized in the context of a relatively narrow scope. We believe that the approach to model validation for design optimization however, as used predominantly by the engineering design community, has several limitations:

1. Model predictions are compared to experimental data at a small number of points. Typically, this may be inadequate for large number of model inputs (dimensionality) that constitute design optimization variables and parameters, and can take values from large intervals (range).
2. Model predictions are typically compared at points for which experimental data are already available; new tests are usually not conducted. However, these points may not be relevant to the optimal design, which is determined by intersecting active constraint boundaries that may lie far away from the test points.
3. If new tests are conducted for model validation, they are all performed before the optimization process. Typically, the test points are distributed across the design space in an attempt to fill it according to the design-of-experiments paradigm. However, numerical optimization algorithms generate a sequence of design candidates (or iterates) until they converge to an optimal design according to termination criteria, desired accuracy and/or computational budget (e.g., maximum number of iterations). They rarely visit the entire design space. Thus, testing at points distributed over the entire design space may be irrelevant, and thus wasteful. We think that this is true even when using optimization algorithms that evaluate points

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in the entire design space in an attempt to find good local minima, because the test cost can outweigh these attempts.

To address the above issues, we have been presenting in a series of recent publications (Li et al., 2010; Drignei et al, 2012a and 2012b), the building blocks of a new methodology for sequential design optimization that utilizes calibration-based model validation in local (sub)domains of the design space. The above publications also provide a comprehensive literature review on model validation. Our new methodology proceeds iteratively by obtaining test data at a design point, constructing around it a local domain in which the model is considered valid, and optimizing the design within this local domain. If the optimal design associated with the local domain lies on the boundary of the latter, a new iteration is conducted with the optimal design serving as the new center point. This process either converges if the optimal design of a local domain lies in the interior of the latter or is terminated if testing resources are exhausted. In the second case, we are still left with a design that is optimal with respect to a part of the design space.

The premise of this paradigm is that testing resources are utilized more efficiently. We recognize that the new paradigm may be conflicting with the automation of the design optimization process, as it requires the temporary interruption of the design optimization process when new tests become necessary. However, we emphasize that current practice can lead to invalid and bad designs because of the three arguments we presented above, as demonstrated with an academic example in Li et al. (2010). We must decide whether we want "automated" results that may be erroneous or "semi-automated" design solutions that utilize resources efficiently and increase the likelihood of performing as predicted when built. Moreover, the proposed paradigm enables the consideration of additional model inputs as variables during the optimization process. It also enables robustness studies with respect to model inputs that are design parameters since testing resources are not exhausted a-priori but managed and allocated as the design optimization process progresses.

In section 2 we review our previous research on design optimization using local domains. In section 3 we develop the statistical models, the method for choosing the number of tests and the construction of local domains. Section 4 presents a description of the piston example, on which we apply the proposed methodology. We summarize in Section 5.

2. BRIEF METHODOLOGY REVIEW

In Li et al. (2010) we first proposed the idea of validating computational models via calibration as the design optimization process progresses using a sequential approach that resembles trust-region

methods. In this first research effort, we assumed that data can be obtained for each of the local domains that are defined during the sequential optimization process. Moreover, we held the size of the local domains (whose shapes were hyper-rectangles) fixed, and used interval-based Bayesian hypothesis testing to compute model validity at the center of each local domain. Our combined design optimization and validation method was based on calibrating model parameters (if necessary) to ensure that model validity would not fall below a threshold. Although this first method did not account for test or model uncertainty directly, and assumed fixed local domains, a contrived cantilever beam design example we used to demonstrate our idea highlighted the fact that a-priori global validation can lead to invalid and worse designs, while the proposed sequential design optimization approach using calibration-based validation in local domains converged to a valid and better design.

In Drignei et al. (2012a), we improved our methodology by varying the size of the local domains to reflect model validity. In this work, the dimensions of the hyper-rectangles around a center point design are determined such that model predictions match test data statistically for a given confidence level. Keeping the assumption that test data can be obtained for each local domain, we modeled the error between model predictions and test data as a Gaussian process and conducted calibration-based validation using a parametric bootstrap methodology involving maximum likelihood estimators of unknown model parameters. We formulated a design optimization problem based on the "thermal example" of Dowding et al. (2008) that was developed to serve as a validation benchmark problem for a validation workshop at Sandia National Laboratories. We demonstrated that i) the sequential process generates local domains of different dimensions and ii) that the active constraints (which determine the optimum) move around the design space as the models that are used to compute them are re-calibrated as necessary.

While the Gaussian process assumption is prevalent in the literature as many data sets exhibit Gaussian behavior, there are instances where this is not true. Therefore, in Drignei et al. (2012b), we used a nonparametric bootstrap statistical method that does not rely on the assumption of Gaussian (or any other) distribution. We applied the nonparametric bootstrapping technique to the same thermal example. The obtained results differed, but not substantially. Nevertheless, the ability to not have to rely on the Gaussian (or any other) distribution may be crucial for other design applications.

In this paper, we lift the assumption that a fixed number of tests has been conducted to generate data for each local domain. In order to utilize resources as efficiently as possible, we assume that only one set of test data exists (or can be obtained) for the center point

design of each new local domain, and present a technique for conducting additional tests incrementally (one by one) if and as necessary to validate the model via calibration, so that it satisfies a user-specified accuracy threshold. We demonstrate our updated methodology for sequential design optimization and validation using a piston design example, which involves statistical surrogates for the responses of interest.

3. TEST VARIABILITY AND LOCAL DOMAIN SIZING

In this section, we first review the statistical framework to model the error between test data and model predictions. For convenience of notation, since the design example we use considers only scalar responses, we will consider the case where responses are spatially invariant and time-independent. A formulation for time-dependent, spatially variant responses is presented in Drignei et al. (2012b). We then proceed with presenting the technique for linking test variability with domain size to determine the number of required tests in order to satisfy local domain model validity requirements.

3.1 Statistical error modeling

Let $y^t(\mathbf{d}, \mathbf{p})$ and $y^m(\mathbf{d}, \mathbf{p}, \mathbf{c}(\mathbf{d}, \mathbf{p}))$ be system responses as measured in a test and predicted by a computational model, respectively, where $\mathbf{d} \in \mathcal{R}^{n_d}$ are design variables, $\mathbf{p} \in \mathcal{R}^{n_p}$ are design parameters, and $\mathbf{c} \in \mathcal{R}^{n_c}$ are model calibration parameters. We assume that several tests $y_k^t(\mathbf{x})$, $k=1, \dots, r$ are available at a point $\mathbf{x} = (\mathbf{d}, \mathbf{p}) \in \mathcal{R}^{n_d+n_p}$, with their exact number r to be determined later. We can then write

$$y_k^t(\mathbf{x}) = y^m(\mathbf{x}, \mathbf{c}) + \delta(\mathbf{x}) + \varepsilon_k(\mathbf{x}), \quad (1)$$

where $\delta(\mathbf{x})$ is the prediction bias representing the mean simulation model error, and $\varepsilon_k(\mathbf{x})$ is a zero mean random quantity representing the variability between a specific test response (fixed k) and a specific model prediction (fixed $\mathbf{c}$). Here, for simplicity reasons, we will not include the model bias explicitly. However, a bias term (random or not) can be easily included (Drignei et al., 2012b; Bayarri et al., 2007; Kennedy and O'Hagan, 2001), should there be strong evidence for it in specific applications. The above statistical model simplifies to

$$y_k^t(\mathbf{x}) = y^m(\mathbf{x}, \mathbf{c}) + \varepsilon_k(\mathbf{x}). \quad (2)$$

Since there can be several responses of interest, we denote by $\mathbf{y}^t(\mathbf{x})$ the vector of test responses, by $\mathbf{y}^m(\mathbf{x}, \mathbf{c})$ the vector of model responses and by $\boldsymbol{\varepsilon}(\mathbf{x})$ the

error vector. Due to measurement error and uncontrollable testing conditions, the test responses $\mathbf{y}^t(\mathbf{x})$ may be variable. In order to capture the error variability around the mean statistically, we model $\boldsymbol{\varepsilon}(\mathbf{x})$ as a Gaussian process with mean vector zero and covariance matrix $\boldsymbol{\Gamma}$. The latter may depend on statistical parameters $\boldsymbol{\theta}$ that also need to be estimated. If $\boldsymbol{\phi} = (\mathbf{c}, \boldsymbol{\theta})$ includes the model calibration parameters $\mathbf{c}$ and the statistical parameters $\boldsymbol{\theta}$, the Gaussian probability density function we consider is (Schervish, 1995)

$$f_{\mathbf{E}/\boldsymbol{\Phi}}(\boldsymbol{\varepsilon}(\mathbf{x})|\boldsymbol{\phi}) = \left(\frac{1}{\sqrt{2\pi}}\right)^N \frac{1}{\sqrt{\det(\boldsymbol{\Gamma})}} \exp\left(-\frac{1}{2}\boldsymbol{\varepsilon}(\mathbf{x})^T \boldsymbol{\Gamma}^{-1} \boldsymbol{\varepsilon}(\mathbf{x})\right), \quad (3)$$

where N is the length of the test data vector $\mathbf{y}^t(\mathbf{x})$. For simplification, the covariance matrix is chosen as $\boldsymbol{\Gamma} = \tau^2 \mathbf{I}$ where $\mathbf{I}$ is the identity matrix. Therefore, $\boldsymbol{\theta} = \tau^2$ in this paper.

3.2 Determining the local domain

When the point $\mathbf{x}$ is fixed, the parameter vector $\boldsymbol{\phi}$ is estimated by maximizing the likelihood function $L(\boldsymbol{\phi}|\boldsymbol{\varepsilon}(\mathbf{x})) = f_{\mathbf{E}/\boldsymbol{\Phi}}(\boldsymbol{\varepsilon}(\mathbf{x})|\boldsymbol{\phi})$ where $f_{\mathbf{E}/\boldsymbol{\Phi}}(\boldsymbol{\varepsilon}(\mathbf{x})|\boldsymbol{\phi})$ is provided by Equation (3).

Test data $\mathbf{y}^t(\mathbf{x})$ at point $\mathbf{x}$ are used to determine the size of the local domain around $\mathbf{x}$, by extending the likelihood function to include $\mathbf{x}$ as an additional statistical parameter; i.e., $L_{\text{ext}}(\mathbf{x}, \boldsymbol{\phi}|\boldsymbol{\varepsilon}(\mathbf{x}))$. We can then obtain estimated values $(\hat{\mathbf{x}}, \hat{\boldsymbol{\phi}})$ of the parameters $(\mathbf{x}, \boldsymbol{\phi})$ by maximizing the extended likelihood function L_{ext} . This is accomplished by generating error data $\bar{\varepsilon}_k(\mathbf{x})$ from the Gaussian distribution with zero mean and variance τ^2 , and re-estimating (i.e., re-calibrating) the model by maximizing the extended likelihood function L_{ext} . This process is repeated (e.g., $B=50$ times) to obtain the parametric bootstrap finite sample $\{\bar{\mathbf{x}}_b\}$, $b=1, \dots, B$ of statistical copies of $\mathbf{x}$. Then the local domain will be an ellipse including those design points $\mathbf{x}$ that satisfy

$$\sum_{i=1}^K \left(\frac{\tilde{x}_i - \bar{x}_i}{s_i} \right)^2 \leq \chi_{K, 1-\alpha}^2, \quad \text{where } x_i \text{ is the } i^{\text{th}} \text{ component of } \mathbf{x}, \tilde{x}_i \text{ is the sample mean of } x_{b,i}, s_i \text{ is the sample standard deviation of } x_{b,i} \text{ and } \chi_{K, 1-\alpha}^2 \text{ is a critical value of the chi-square distribution with } n_d+n_p \text{ degrees of freedom (the number of components of } \mathbf{x} \text{).}$$

For example, for $n_d+n_p=2$ and $\alpha=0.01$, $\chi_{K, 1-\alpha}^2=9.21$ based on the table of chi-square critical values. This is an established statistical method to obtain exact

confidence regions in multidimensional cases (Schervish, 1995). In our previous work we used rectangular shapes for the local domains to expedite the computational process. The resulting confidence level was thus only approximate.

3.3 Determining the number of required tests for each local domain

In our previous work, we assumed that the model is validated through calibration in a local domain D *uniformly*, i.e., that the model is valid at each point inside the local domain. However, model validity may vary at different points of the local domain, with points farther away from its center (where test data are available) possibly having lower validity. This behavior stems from the Gaussian asymptotic distribution of the maximum likelihood estimators and the generalized least squares estimators that were used in our parametric and non-parametric bootstrap approaches, respectively. Moreover, we need to account for test variability while sizing the local domains (in our previous work we assumed that data are available from a fixed number of tests).

We propose therefore, an enhanced calibration-based validation procedure that is based on the distance between the point at which we have test data (the center of the local domain) and the point at which we want to utilize the model. This enhanced technique is based on the assumption that test and model data are statistically similar at the center of the local domain, while this statistical similarity decreases as the distance from the center point increases.

We define a pointwise validation measure at $\mathbf{x}$ as the correlation between model data at the center $\mathbf{x}_c$ of the domain and model data at point $\mathbf{x}$. This could be an empirical correlation, or a more sophisticated model correlation. In this paper, we use the surrogate model correlation

$$V(\mathbf{x}) = C(\mathbf{x}, \mathbf{x}_c), \quad (4)$$

which is described in detail in the next section. This correlation inherently depends on the distance between the two points $\mathbf{x}$ and $\mathbf{x}_c$. Furthermore, we define the *validation level* of the local domain D as

$$V_L = \min_{\mathbf{x} \in D} V(\mathbf{x}). \quad (5)$$

It expresses a minimally acceptable model correlation between data at the center and data within the local domain. This new validation measure is a generalization and a refinement of our previous dichotomous validation measure, where the model at a validating design point was either validated or not, depending on whether it was included in the local domain or not.

Using statistical arguments, one can demonstrate that if the number of tests at the center design point increases from 1 to r , the local domain shrinks, and its size is expected to decrease by a factor of order r . This

follows from the asymptotic distribution of maximum likelihood. Therefore, by increasing the number of tests, we obtain a local domain that is more strongly validated according to the proposed validation level of Equation (5) because all its points are closer to the center design point where the test data are available. However, increasing the number of tests also increases the cost. Thus, there is a trade-off between the cost and the degree of model validation of the local domain. We propose the following algorithm for choosing the number of tests r in each local domain:

1. Start with a minimum number of tests r_0 and obtain the local domain using high confidence level, for example 99%. In this local domain, compute the validation level of Equation (5).
2. If the validation level is above a high pre-established threshold (e.g. 0.99), stop the algorithm and choose $r=r_0$.
3. If the validation level is below the threshold, increase the number of tests r by one and repeat steps 1 and 2 above.

In general, the confidence level used to construct the local domains does not need to be equal to the validation level threshold.

3.4 Design optimization

Ultimately, we are interested in optimizing a design objective subject to constraints where the objective and constraints are evaluated using model predictions for the responses of interest. A piston design optimization example is presented in the next section. The following steps summarize the proposed sequential design optimization approach with concurrent calibration-based model validation using elliptic local domains whose size is determined by accounting for test variability using a parametric bootstrap.

1. Choose an initial point $\mathbf{x}^{(0)}$, where both test data and model predictions are generated.
2. Calibrate the computer (prediction) model at the current point using maximum likelihood estimation, parametric bootstrap and an initial number r_0 of test data.
3. Obtain the elliptic local domain surrounding this point.
4. Compute the validation level of the current local domain. If it is below a specified threshold, conduct an additional test, go back to Step 3 and compute a new elliptic local domain using the additional test data. If it satisfies the validation level threshold go to Step 5.
5. Solve the design optimization problem in the local domain defined at Step 3.

6. If the optimal design obtained at Step 5 is on the boundary of the local domain, go to Step 2. Otherwise, stop.

4. EXAMPLE: PISTON DESIGN

Automotive piston design is a challenging problem involving complex physics and requiring satisfaction of multiple performance objectives. Efforts to reduce engine vibration and radiated noise while improving durability, fuel economy and reliability are critical. Important piston design requirements include high scuff resistance, low friction and wear, and low noise. It is common practice to determine the optimal piston skirt profile so that the maximum contact pressure at the piston-bore interface is kept low in order to avoid scuffing. Reduced friction and low piston slap noise are used as additional design requirements.

Despite the small clearance between the piston and the cylinder bore, the piston undergoes a secondary motion within the bore, which can generate unwanted sound and vibration. The secondary motion is caused by the piston side thrust, which changes direction due to the connecting rod angularity. As a result, the piston moves laterally from one side of the bore to the other and also tilts within the bore clearance. It eventually collides against the cylinder wall. This impact is commonly known as piston slap.

To improve the friction, noise and scuffing performance, the piston is designed with barrel and ovality shapes. Because of the barrel shape, the side

load on the piston skirt gets distributed more evenly resulting in a much wider contact pattern and lower skirt pressure improving the piston's scuffing propensity. The piston ovality also improves the piston's scuffing propensity and also provides additional clearance to parts of the skirt to compensate for the piston's thermal expansion. The piston slap cannot be eliminated completely although it can be significantly reduced with a good piston skirt profile. The combination of a deformed cylinder with a deformed, profiled piston (oval and barrel shapes) defines the clearance at running conditions affecting therefore, the performance of the piston.

An analytical model was developed by Patel et al. (2010) and Paras et al. (2007) to simulate the piston secondary dynamics and piston-bore contact for an asymmetric half piston model. The model includes several important physical attributes such as bore distortion due to mechanical and thermal deformation, inertia loading, piston barrelity and ovality, piston flexibility and skirt-to-bore clearance. The model accounts for piston kinematics, rigid-body dynamics and skirt flexibility.

Based on a sensitivity study (Patel, 2009) seven key design variables were identified as the biggest contributors on piston friction, noise and scuffing. Table 1 provides the lower and upper bound for each design variable. All variables are assumed normally distributed. Table 1 also provides their standard deviation.

Table 1. Piston design variables

	Design variables	Units	Lower bound	Upper bound	Standard deviation
1	Pin offset	mm	-1	1	0.1
2	Cold clearance	μm	0	0.025	0.005
3	Clearance at section A_2	μm	0.1	0.2	0.05
4	Ovality at section A_2	-	0.4	0.9	0.1
5	Barrelity at section A_2	-	1.5	4.0	0.2
6	Cylinder bore distortion	deg	60	120	10
7	Coefficient of friction	-	0.05	0.2	0.05

Figure 2 shows some piston design details. From the front view, the piston has a barrel shape which allows different level of clearance at different sections. The piston skirt is divided into three main sections; top section A_2 , middle section A_1 , and bottom section A . The clearance between the skirt and the liner in the middle section represents the cold-clearance. The oval shape is defined at three sections along the piston skirt similarly to the piston barrelity. Because of its criticality, the piston

ovality at the top-section is used as a design variable. Finally, the piston pin offset and the cold clearance are also design variables. The pin offset is the distance between the piston centerline to the piston pin-hole centerline.

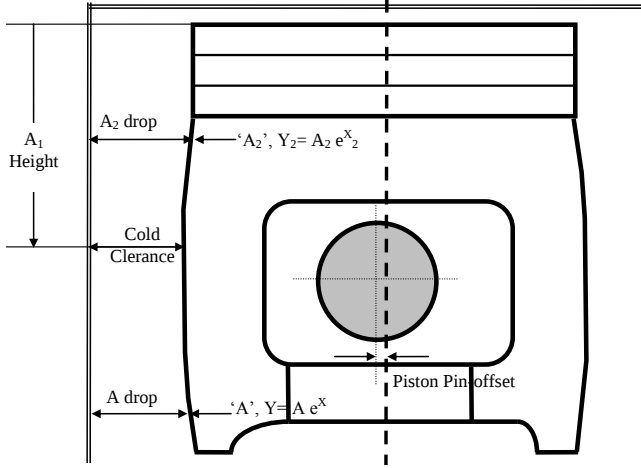


Figure 2. Piston geometric dimensions

Here, the design vector $\mathbf{x}$ consists of two design variables (pin offset and cold clearance), whereas the calibration vector $\mathbf{c}$ includes the remaining five variables in Table 1. Denoting by $f_1(\mathbf{x}, \mathbf{c})$ the skirt pressure, by $g_1(\mathbf{x}, \mathbf{c})$ the total friction power loss and by $g_2(\mathbf{x}, \mathbf{c})$ the kinetic energy loss, the design optimization problem is formulated as

$$\begin{aligned} \min_{\mathbf{x}} \quad & f_1(\mathbf{x}, \mathbf{c}) \\ \text{subject to} \quad & g_1(\mathbf{x}, \mathbf{c}) \leq 2 \\ & g_2(\mathbf{x}, \mathbf{c}) \leq 7850. \end{aligned} \quad (6)$$

The model response vector in this example is thus given by $\mathbf{y}^m(\mathbf{x}, \mathbf{c}) = [f_1(\mathbf{x}, \mathbf{c}), g_1(\mathbf{x}, \mathbf{c}), g_2(\mathbf{x}, \mathbf{c})]^T$.

4.1 Model surrogates

The models developed by Patel et al. (2010) and Paras et al. (2007) for simulating the piston motion and computing the responses f_1 , g_1 and g_2 are computationally expensive and thus prohibitive for optimization. Therefore, following established methodology on design and analysis of computer experiments (Santner et al., 2003; Fang et al., 2006), we constructed separate scalar surrogates for each response using data at 100 points of the 7-dimensional input space chosen according to a maximin design criterion (Morris et al., 1993). We assumed a Gaussian distribution for each surrogate y , with

constant mean μ and Gaussian correlation (Currin et al., 1991)

$$C(x_i, x_j) = \sigma^2 \exp\left[-\sum_{k=1}^7 \theta_k (x_{k,i} - x_{k,j})^2\right],$$

for $i, j = 1, \dots, 100$, where $x_{k,i}$ are input coordinates scaled to the interval $[0, 1]$, and $k = 1, \dots, 7$. The unknown parameters θ_k, μ, σ^2 are estimated by maximum likelihood estimation. Denote by $\mathbf{C}$ the matrix with elements $C(x_i, x_j)$ and by $\mathbf{Y}$ the vector of model data.

The surrogate at a new input of coordinates $x_{k,0}$ is chosen to be the conditional mean

$$\hat{\mathbf{y}} = \mu + \mathbf{C}_0^T \mathbf{C}^{-1} (\mathbf{Y} - \mu \mathbf{1}), \quad (7)$$

with the conditional variance $\sigma^2(1 - \mathbf{C}_0^T \mathbf{C}^{-1} \mathbf{C}_0)$ for the surrogate error. In Equation (7), the vector $\mathbf{C}_0$ has components

$$C_0(i) = \sigma^2 \exp\left[-\sum_{k=1}^7 \theta_k (x_{k,i} - x_{k,0})^2\right], \quad \text{for } i = 1, \dots, 100 \quad \text{and}$$

$\mathbf{1}$ represents a unit vector.

In the rest of the paper we replace the model data $\mathbf{y}^m(\mathbf{x}, \mathbf{c})$ with surrogates $\hat{\mathbf{y}}^m(\mathbf{x}, \mathbf{c})$ throughout the input space.

The surrogate surfaces may be characterized by artificial, local optima. As the results below will show, this may be a potential drawback in using surrogates in optimization processes. One can decrease the potential of such artificial local optima by increasing the sample of design points, at the expense of a more computationally intensive and/or numerically unstable procedure. Alternatively, starting the optimization process from different initial conditions may lead to the global optimum.

Table 2 presents the maximum likelihood estimated statistical parameters for the three surrogates. Figure 1 shows the cross-validation plots, indicating that the surrogates are acceptably accurate. The “leave-one-out” cross-validation method has been used. The plots in Figure 1 show the actual model response data versus the cross-validation surrogate model response data at all 100 points. In such plots, the closer the scatter-plot is to the main diagonal, the better the statistical surrogate is.

Table 2. Surrogate maximum likelihood estimates

Surrogate response	μ	θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7	σ
Skirt pressure	37.1286	18.2107	0.1692	0.6668	39.6980	0.2646	0.2141	0.0368	12.6683
Friction power loss	2.0366	0.0043	0.6496	0.1698	0.4760	1.7270	3.0177	4.6468	1.3090
Kinetic energy loss	8519	0.1070	0.0000	0.2302	0.0000	15.9649	57.2604	0.2637	1362

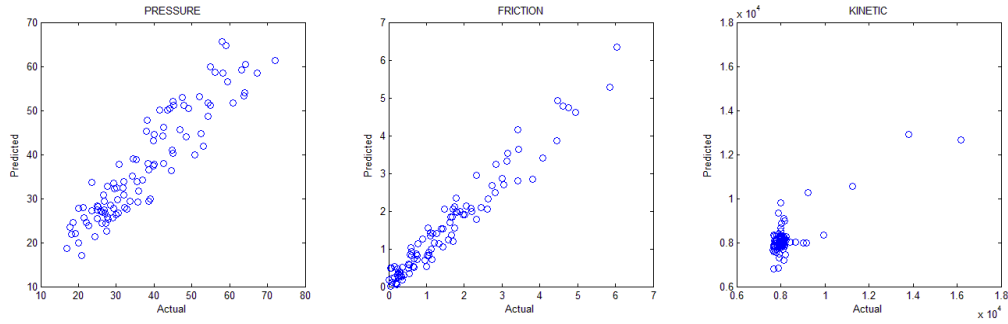


Figure1. Surrogate cross-validation results

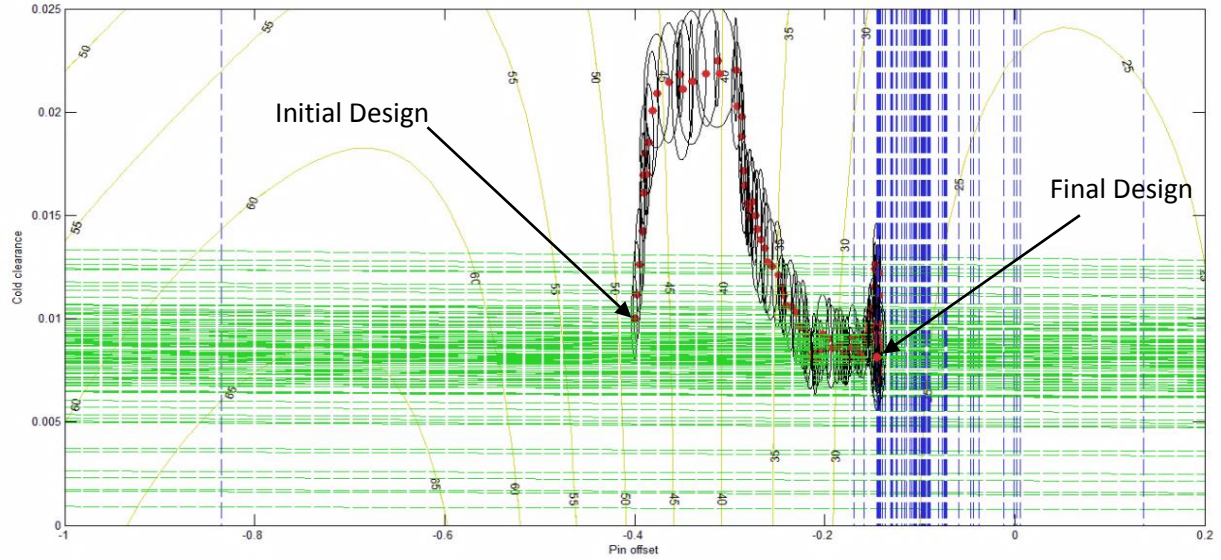


Figure 2a. Optimization results with variable number of tests for initial guess: pin offset = -0.4, cold clearance = 0.01; objective iso-contours in yellow, friction power loss constraint boundaries in green and kinetic energy loss constraint boundaries in blue

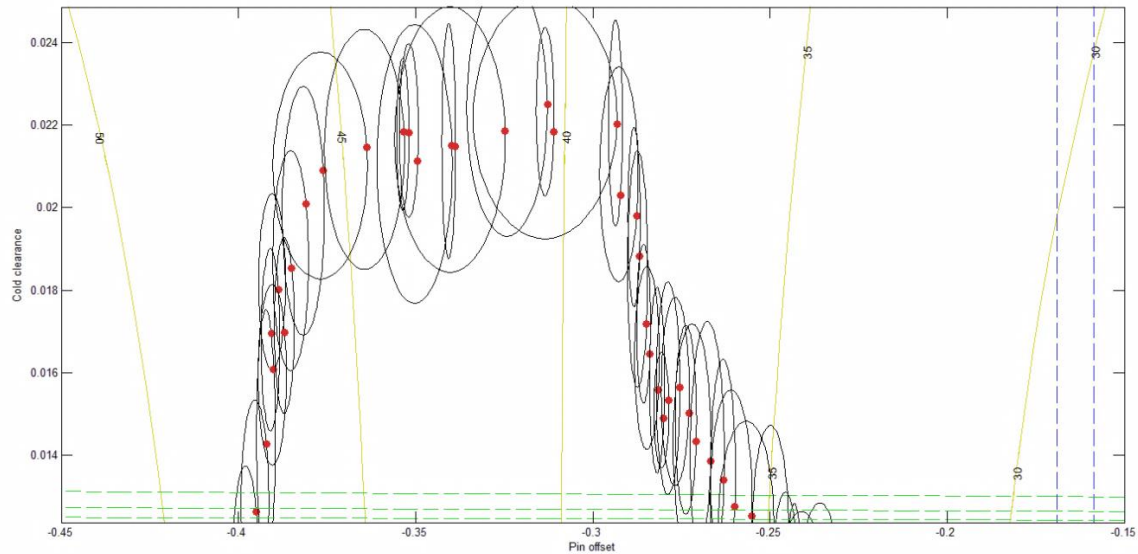


Figure2b. A zoom-in of Figure 2a, illustrating the upper part of the optimization process; objective iso-contours in yellow, friction power loss constraint boundaries in green and kinetic energy loss constraint boundaries in blue

Table 3. Summary of optimization results with variable number of tests for initial guess: pin offset = -0.4, cold clearance = 0.01

Step #	Ellipse semiaxis length		r	Validation level	Clearance at A ₂ section	Ovality at A ₂ section	Barrelity at A ₂ section	Cylinder Bore Distortion	Coeff. of Friction	Pin Offset optimum	Cold clearance optimum
	a	b									
0	0.0030	0.0021	2	0.9960	0.1585	0.6301	2.7647	87.6363	0.1057	-0.3977	0.0112
1	0.0036	0.0024	2	0.9944	0.1524	0.6290	2.7705	88.5236	0.1014	-0.3949	0.0126
2	0.0039	0.0024	2	0.9936	0.1491	0.6347	2.7769	88.8969	0.0946	-0.3921	0.0143
3	0.0027	0.0030	2	0.9905	0.1503	0.6346	2.7722	88.6851	0.0968	-0.3907	0.0169
4	0.0027	0.0021	3	0.9948	0.1531	0.6209	2.7538	88.0373	0.1150	-0.3888	0.0180
5	0.0036	0.0021	5	0.9954	0.0498	0.5966	2.9990	91.8587	0.0602	-0.3902	0.0161
6	0.0039	0.0021	5	0.9954	0.1330	0.6359	2.7923	89.9825	0.0740	-0.3869	0.0170
7	0.0027	0.0021	5	0.9955	0.1409	0.6420	2.8061	89.8938	0.0793	-0.3849	0.0185
8	0.0052	0.0027	12	0.9944	0.1441	0.6385	2.7775	89.1672	0.0863	-0.3809	0.0201
9	0.0061	0.0030	5	0.9912	0.1209	0.6286	2.7690	90.1270	0.0723	-0.3760	0.0209
10	0.0134	0.0027	14	0.9933	0.1482	0.6326	2.7592	88.6176	0.1089	-0.3637	0.0215
11	0.0112	0.0030	20	0.9928	0.1496	0.6302	2.7541	88.2910	0.1097	-0.3533	0.0218
12	0.0018	0.0018	8	0.9966	0.1282	0.6202	2.7471	89.8001	0.1343	-0.3519	0.0218
...	...	...	...	...	...	...	...	...	...	...	...
96	0.0018	0.0015	2	0.9978	0.1508	0.6428	2.7446	86.5974	0.1124	-0.1453	0.0082
97	0.0036	0.0012	2	0.9982	0.1456	0.6442	2.7623	85.3336	0.1023	-0.1450	0.0081

Table 4. Summary of optimization results with fixed number of tests for initial guess: pin offset = -0.4, cold clearance = 0.01

Step #	Ellipse semiaxis length		r	Validation level	Clearance at A ₂ section	Ovality at A ₂ section	Barrelity at A ₂ section	Cylinder Bore Distortion	Coeff. of Friction	Pin Offset optimum	Cold clearance optimum
	a	b									
0	0.0030	0.0021	2	0.9960	0.1585	0.6301	2.7647	87.6363	0.1057	-0.3977	0.0112
1	0.0036	0.0024	2	0.9944	0.1524	0.6290	2.7705	88.5236	0.1014	-0.3949	0.0126
2	0.0039	0.0024	2	0.9936	0.1491	0.6347	2.7769	88.8969	0.0946	-0.3921	0.0143
3	0.0027	0.0030	2	0.9905	0.1503	0.6346	2.7722	88.6851	0.0968	-0.3907	0.0169
4	0.0046	0.0052	2	0.9767	0.1490	0.6358	2.7780	88.9326	0.0940	-0.3882	0.0215
5	0.0452	0.0061	2	0.9621	0.1665	0.6532	2.9547	90.2804	0.1133	-0.3448	0.0217
6	0.1505	0.0058	2	0.9122	0.1783	0.6597	2.9875	89.8286	0.1098	-0.2151	0.0224
7	0.0455	0.0067	2	0.9586	0.1473	0.6335	2.8164	89.8114	0.0943	-0.1677	0.0208
8	0.0294	0.0067	2	0.9656	0.1555	0.6332	2.7942	88.1026	0.0928	-0.1456	0.0175
9	0.0167	0.0070	2	0.9530	0.1510	0.6327	2.7808	87.5601	0.0924	-0.1352	0.0138
10	0.0030	0.0027	2	0.9925	0.1519	0.6335	2.7838	87.1252	0.0929	-0.1342	0.0114
11	0.0039	0.0024	2	0.9948	0.1512	0.6336	2.7844	87.7648	0.0880	-0.1326	0.0098
12	0.0024	0.0018	2	0.9965	0.1490	0.6322	2.7757	87.5562	0.0931	-0.1318	0.0084
...	...	...	...	...	...	...	...	...	...	...	...
48	0.0003	0.0012	2	0.9986	0.1647	0.6465	2.8418	87.1074	0.0786	0.0000	0.0019
49	0.0003	0.0009	2	0.9989	0.1535	0.6353	2.8059	89.0702	0.0780	0.0000	0.0019

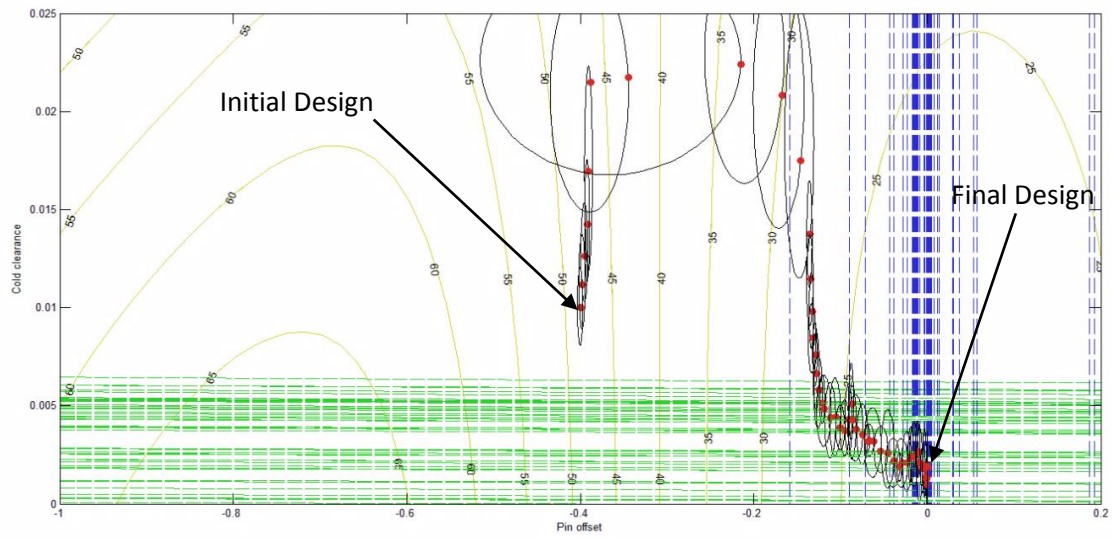


Figure 3. Optimization results with fixed number of tests for initial guess: pin offset = -0.4, cold clearance = 0.01; objective iso-contours in yellow, friction power loss constraint boundaries in green and kinetic energy loss constraint boundaries in blue

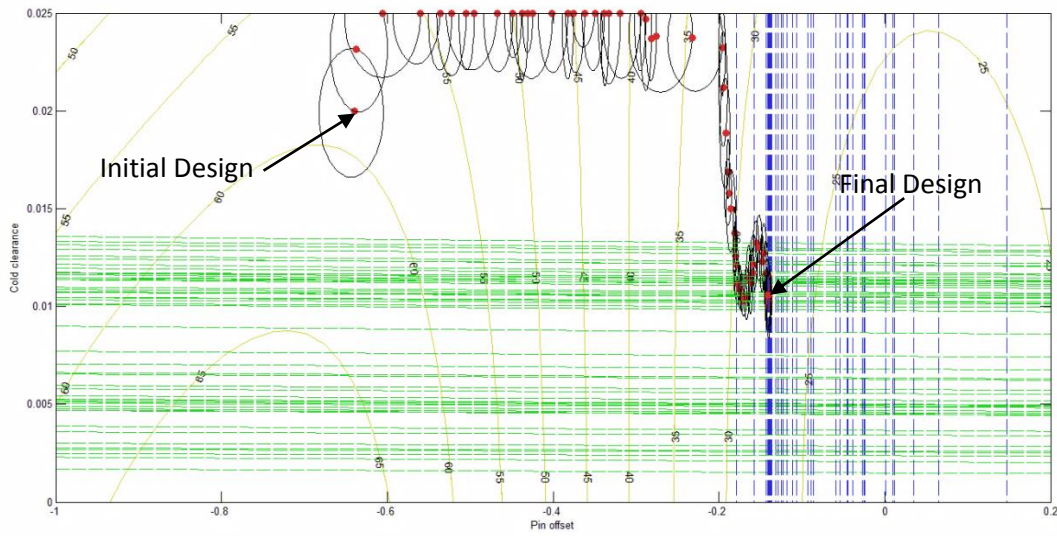


Figure 4. Optimization results with variable number of tests for initial guess: pin offset = -0.64, cold clearance = 0.02; objective iso-contours in yellow, friction power loss constraint boundaries in green and kinetic energy loss constraint boundaries in blue

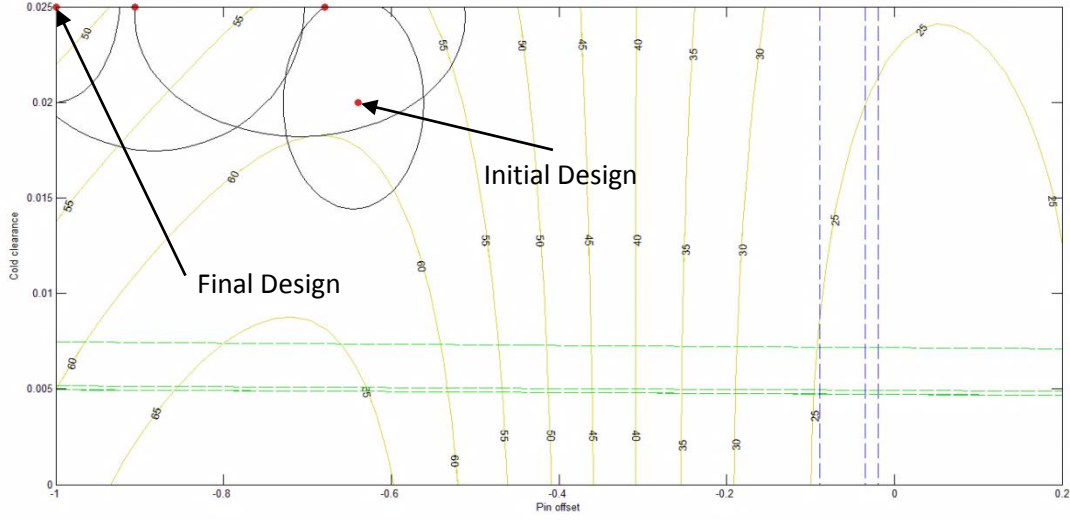


Figure 5. Optimization results with fixed number of tests for initial guess: pin offset = -0.64, cold clearance = 0.02; objective iso-contours in yellow, friction power loss constraint boundaries in green and kinetic energy loss constraint boundaries in blue

Table 5. Summary of results as a function of number of tests necessary to obtain the first local domain when algorithm starts at pin offset = -0.35 and cold clearance = 0.022.

r	Ellipse semiaxis length		Validation level	Clearance at A_2 section	Ovality at A_2 section	Barrelity at A_2 section	Cylinder Bore Distortion	Coeff. of Friction
	a	b						
2	0.0256	0.0024	0.9473	0.1362	0.6258	2.7579	89.0112	0.0798
3	0.0153	0.0024	0.9475	0.1438	0.6284	2.7790	89.2401	0.0860
4	0.0116	0.0022	0.9553	0.1408	0.6278	2.7728	89.1668	0.0802
5	0.0053	0.0021	0.9613	0.1398	0.6275	2.7669	88.9502	0.0763
6	0.0078	0.0021	0.9591	0.1354	0.6274	2.7658	89.1418	0.0711
7	0.0073	0.0023	0.9534	0.1474	0.6319	2.7846	88.8173	0.0713
8	0.0068	0.0017	0.9744	0.1591	0.6361	2.7999	88.1488	0.0706
9	0.0074	0.0018	0.9710	0.1589	0.6368	2.8016	87.8803	0.0633
10	0.0118	0.0018	0.9725	0.1417	0.6304	2.7789	88.9059	0.0643
11	0.0069	0.0011	0.9882	0.1541	0.6364	2.8116	88.9887	0.0631
12	0.0042	0.0015	0.9794	0.1558	0.6370	2.8125	88.8671	0.0630
13	0.0035	0.0014	0.9836	0.1421	0.6309	2.7857	89.0676	0.0618
14	0.0061	0.0019	0.9714	0.1435	0.6300	2.7742	88.1697	0.0589
15	0.0050	0.0016	0.9764	0.0933	0.6206	2.7298	90.5046	0.0585
16	0.0062	0.0017	0.9734	0.1264	0.6270	2.7848	90.0593	0.0628
17	0.0021	0.0013	0.9862	0.1442	0.6331	2.8202	89.8644	0.0647
18	0.0025	0.0011	0.9907	0.1333	0.6273	2.7825	89.6645	0.0650

4.2 Design optimization results

Figure 2 and Table 3 summarize the results of the optimization process, implementing the technique presented in Section 3. Test data $y^t(\mathbf{x})$ were simulated from the Gaussian distribution with mean $\hat{y}^m(\mathbf{x}, \mathbf{c})$ and standard deviation $\tau = 0.1$. The initial guess used for optimization was pin offset = -0.4 and cold clearance = 0.01. The optimization within each local domain started at

the center of the ellipse. Objective function iso-contours are shown in yellow only for the last step of the optimization process. Constraint boundaries are shown in green and blue for the friction power and kinetic energy losses, respectively. The constraint boundaries "move" about the design space as the sequential optimization process progresses due to the re-calibration of the models as necessary.

Due to the many steps of the sequential optimization process, Table 3 includes only the first 13 and the last 2 steps. The initial number of tests for each local domain is $r_0=2$. One can see that after the first 4 steps the number of tests per local domain increases to achieve the required high validation level. Towards the end of the sequential optimization process the validation level is high enough that no additional tests are required, so the last local domains are based on $r_0=2$ tests. Figure 3 and Table 4 show results for fixed number of tests ($r_0=2$) at each local domain of the sequential optimization process. One can see that the local domains in the middle stage of the sequential optimization process are larger. Therefore, the points located near the boundaries of the local domains are assumed to be not as valid as the points closer to the center of the ellipse, where test data are available. These ellipses are, in fact, much larger than those towards the middle stage of the optimization process in Figure 2a. This was to be expected, since additional tests will decrease the area of the local domains. The validation levels reported in Tables 3 and 4 were computed using 1000 sample points within each local domain.

Not using the new method that controls the size of the local domain may result in obtaining different optimal designs. Indeed, the optimal design in Table 3 is pin offset=-0.1450 and cold clearance = 0.0081, whereas the optimal design in Table 4 is pin offset=0.0000 and cold clearance = 0.0019. A pin offset value very close to 0 is not meaningful from an engineering point of view.

We have replicated the optimization process several times using the same initial guess. The results differ slightly due to the different sets of random numbers. While there are differences among statistically replicated optimization paths, the ones using the new method tend to converge to an optimal design farther away from the origin than those not using it. The possible cause of this behavior is the qualitative change in the optimization surface around the objective function iso-contour of 40 MPa. Specifically, this line appears to separate the area including the local maximum associated with the contour line 65 MPa from the local minimum associated with the contour line 25 MPa. In general, one would like to have a more conservative optimization method that uses small steps in such areas of qualitative changes. The optimization based on the presented method seems to naturally reduce the size of local domains in this area, whereas the method used in our previous work did not.

Figures 4 and 5 depict what happens when considering a different initial guess for the sequential design optimization process, namely pin offset = -0.64, cold clearance = 0.02 where the optimization within each local domain started at the extreme left end of each ellipse. Using the enhanced technique that accounts for test variability when sizing the local domain (new validation measure), the final optimal values are similar to those obtained using the previous initial guess (Figure 4). This is not the case when the number of tests is held fixed

for each local domain. In this case, the optimization process converges to an inferior local optimum (Figure 5). Even though this may have been caused by the surrogates, the enhanced technique did not get trapped in this local optimum. We conclude that varying the local domain size according to test variability may have advantages regarding the quality of the obtained optimal designs, even though this may come at the expense of additional tests.

To provide insight on how the validation level changes with the number of tests, we started the optimization algorithm at a new initial design with pin offset = -0.35 and cold clearance = 0.022 and stopped the algorithm after the first local domain was identified. A number of $r = 18$ tests were necessary to achieve the prescribed validation level of 0.99. Figure 6 shows the validation level as the number of tests varies from 2 to 18. As expected, adding more tests increases the validation level although the increase is not monotonic. Table 5 provides more details for the 18 tests showing that in general the size of the ellipses decreases with the number of tests. It should be noted that each row in Tables 3 and 4 show only the last row of Table 5 for each identified local domain.

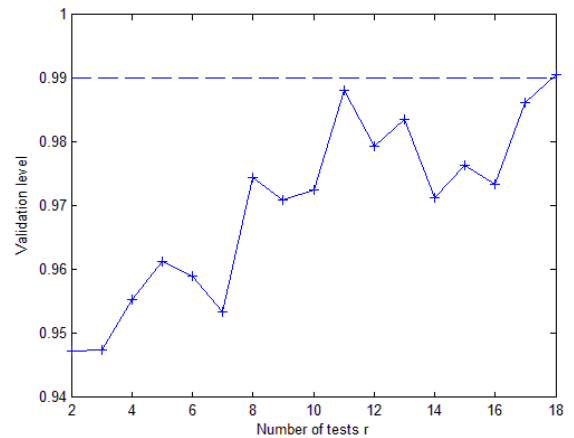


Figure 6. Validation level versus number of tests to obtain the first local domain for an initial pin offset = -0.35 and cold clearance = 0.022.

5. SUMMARY

In our recently developed methodology for sequential design optimization with concurrent, calibration-based model validation, the number of tests to obtain data was assumed constant for each local domain. Recognizing that test variability can play a significant role in the statistical error models we employ, we developed a new method that accounts for it when determining the size of local domains within which we can assume that the models used to obtain objective and constraint function values are sufficiently valid.

Using an automotive piston design example, we have demonstrated again that local model calibration is

necessary to ensure that the sequence of design optimization candidates is validated. Moreover, we have shown that test variability can be accounted for as necessary by varying the size of the local domains to ensure that validity thresholds are satisfied. Finally, for the particular example considered in this paper, we observe that optimal designs obtained using the proposed method are superior to these obtained without using it.

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