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UNCERTAINTY QUANTIFICATION AND REDUCTION USING SENSITIVITY ANALYSIS AND HESSIAN DERIVATIVES

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ABSTRACT

We study the use of Hessian interaction terms to quickly identify design variables that reduce variability of system performance. To start we quantify the uncertainty and compute the variance decomposition to determine noise variables that contribute most, all at an initial design. Minimizing the uncertainty is next sought, though probabilistic optimization becomes computationally difficult, whether by including distribution parameters as an objective function or through robust design of experiments. Instead, we consider determining the more easily computed Hessian interaction matrix terms of the variance-contributing noise variables and the variables of any proposed design change. We also relate the Hessian term coefficients to subtractions in Sobol indices and reduction in response variance. Design variable changes that can reduce variability are thereby identified quickly as those with large Hessian terms against noise variables. Furthermore, the Jacobian terms of these design changes can indicate which design variables can shift the mean response, to maintain a desired nominal performance target. Using a combination of easily computed Hessian and Jacobian terms, design changes can be proposed to reduce variability while maintaining a targeted nominal. Lastly, we then recompute the uncertainty and variance decomposition at the more robust design configuration to verify the reduction in variability. This workflow therefore makes use of UQ/SA methods and computes design changes that reduce uncertainty with a minimal 4 runs per design change. An example is shown on a Stirling engine design where the top four variance-contributing tolerances are matched with two design changes identified through Hessian terms, and a new design found with 20% less variance.

Keywords: Robust Design, Simulation Based Design, Systems Engineering, Uncertainty Analysis, Uncertainty Modeling.

NOMENCLATURE

d Design variable
 H^{ij} Hessian cross term
 J^i Jacobian term

h_i Range of a noise variable used in the Hessian
 k_j Range of a design variable used in the Hessian
 n Noise variable
RDM Robust Design Method
SA Sensitivity Analysis
 S_i Main effect Sobol index
 TS_i Total effect Sobol index
UQ Uncertainty Quantification
 V_i Contribution to variance from the i^{th} noise variable
 σ_y^2 Response Variance
 y Response

1. INTRODUCTION

Parametric robust design as a method to reduce uncertainty has been well researched and developed into what has become the standard experimental *Robust Design Method* (RDM), making use of design-of-experiments to reduce the performance variability of a design due to multiple causes [1]. RDM is more than a statistical experiment, it involves a multiple step workflow including identifying possible sources of variability, quantifying their relative contribution with experiments, generating ideas for design changes that may promote variation reduction, and then quantifying the ability of design changes to reduce this variability through a further set of experiments.

Unfortunately, executing RDM remains a complex task for many industries, which has impeded adoption of RDM [2]. This is particularly evident when used in conjunction with simulation tools, which have prohibitively long manual setup times and long execution times. While automation can help reduce the burden [3-4], means are needed to more quickly identify potential design changes that can reduce variability arising from different contributing noise variables. Given that, generally at least thirty runs are needed to create a reasonable histogram of a distribution, repeating this for different design configuration alternatives is prohibitive. Computer based design of experiments, with surrogate models or otherwise, can improve upon this in a more structured exploration of the design space, but often require dozens of runs for a few design variables each with several runs over the noise variables.

We explore using rapidly computed Hessian second derivative terms to rank potential design changes. We also combine this with computed Jacobian first derivative terms to enable reshifting the mean to remain on target while reducing variation. We find that the variation reduction impact of any design change due to any causal noise variable can be estimated in 4 runs.

Next, we review related works. Then, we outline a workflow and derive the calculations to (1) identify contributing noise variables, (2) rank design changes using a hessian derived calculation, (3) construct variance and mean prediction equations, (4) compute a best set of design changes that minimize variance subject to a nominal target constraint, and (5) verify the variation reduction at a new design configuration. We demonstrate the work using an open source data project, a Stirling engine design [1].

1.1 Related Work

Robust design was introduced by Taguchi as an experimental method to study the effect of different input noise variables on performance variability, and how these can be reduced through design variable selections [5-6]. Arvidsson and Gremyr [1] provide a review of experimental RDM research. Executing RDM early in design is needed to reduce the risk of non-compliance as a design goes into production [7]. Wu and Hamada [8] highlight noise and design variable interactions and design of experimental arrays meant to highlight such terms. Montgomery [9] further derives the response variance as a Hessian interaction terms as is used here.

On the other hand, in recent years the need for RDM has increased, since systems are now increasingly design-optimized for higher performance, higher efficiency, and lower cost; see for example Arena et al [10] for a discussion on trends in defense system programs. Optimizing a system can unfortunately and unknowingly result in tighter design margins to achieve higher performance, leading to costly production problems [11]. Systems designed with tighter margins are inherently more prone to variability problems [7]. In summary, using modern design optimization methods has increased the need for clarifying and understanding how much performance variability there will be in a design, to compare the variability distribution against the targeted design margin and thereby quantify the future manufacturing quality risks.

In the past decades, another body of work has been developed to explore the use of computer-based experiments with various forms of higher discrepancy experimental sampling enabled with computer experiments over traditional design-of-experiments. Uncertainty Quantification (UQ) and Sensitivity Analysis (SA) have grown rapidly over the last several years as an interdisciplinary field [12]. Uncertainty quantification provides the means to quantify the expected variability in a new design before observing it in production. Sensitivity analysis provides the means to decompose the variation into major contributors, to identify which tolerances and noises variables are the major contributors [13]. Main effect and Total effect Sobol sensitivity indices quantify the percent contribution of

noise variables to the variance of the computed performance response uncertainty. Sobol indices typically require large samples and so surrogate models are used [14]. Pandas and Hinken studied expressing response variance as an expansion using Hessian terms [15], similar to a surrogate model of variance. We here look for design variables to reduce variance.

Using this UQ/SA approach, a design concept's variabilities can be assessed against design margins for risk of not meeting requirements. There are many examples in the literature of implementing Latin Hypercube and Quasi-Monte-Carlo methods for higher discrepancy resolution of robustness optimization against design problems [12]. These generally apply optimization search of an objective function computed based on uncertainty. Surrogate models of the mean and variance as functions of design variables can be fit. This requires samples of noise variable combinations at the design variable combinations and unfortunately can quickly lead to sampling plans with hundreds to thousands of runs.

For responses computed through computational expensive simulations, quasi Monte Carlo sequence sampling is effective, such as Sobol or Halton sequences. Unlike Latin Hypercube sampling, any initial sample can be sequentially incremented with follow-on samples of the sequence. This enables one to start with a small sample and determine how well a surrogate model can fit, and increase until a sufficient fit is achieved, thereby needing a minimal number of runs needed to compute the uncertainty and variance decomposition sensitivity analysis.

Nevertheless, these uncertainty propagation methods generally remain "black-box" simulators in nature, as they require large numbers of evaluations for quantifying uncertainty of the response. Combined with uncertainty optimization, it becomes computationally expensive for even moderate dimensional problems. There are limited attempts to interrogate the simulation model locally for improved understanding of the causes of the uncertainty or the selection of suitable design variables with which to explore optimizing (reducing) the variability. We particularly consider identifying which causes of variation (noise variables) contribute to response variation as well as whose variation effect can be mitigated by changing particular design variables.

2. ROBUSTNESS OPTIMIZATION ESTIMATION

It becomes important for computationally expensive simulations to construct sampling strategies that can capture the influence of design changes on response variability efficiently. One way to reduce sampling is to first identify the most contributing noise variables (from the initial UQ/SA), and then study how that can change with potential design changes. We then consider using Hessian second derivative values to prioritize design variables for optimization based upon their ability to reduce the contribution of selected noise variables. Next, we expand this to consider the impact on the average response, to enable constraints on any mean shift. However, first, we define terminology on the basis of uncertainty quantification and sensitivity analysis.

2.1 Uncertainty Quantification and Sensitivity Analysis

Typically, one would consider performing an analysis on minimizing variability only after first quantifying the uncertainty (UQ) as a histogram of a distribution on the response of interest. Often, one would also decompose this uncertainty into a Pareto chart of noise variables contributors as a global sensitivity analysis (GSA).

We consider here where an initial uncertainty quantification was computed. That is, for a selection of noise variables, a sample was generated and at each sample point the response evaluated, resulting in a histogram of response values. A distribution function with statistics against distribution parameters is fit, for example, a normal distribution function with mean and variance statistics. No matter the distribution, we consider variance σ_y^2 as a statistic of interest on the response y .

We also then consider the global sensitivity analysis of the total response variance σ_y^2 . Following Saltelli et al [10], we decompose the total response variance into variance contributors of the noise variables n^i , where

$$\sigma_y^2 = \sum_i V_i + \sum_{i_1 < i_2} V_{i_1 i_2} + \dots + \sum_{i_1 < i_2 < \dots < N} V_{i_1 \dots N}, \quad (1)$$

and V_i is the main effect response variance contribution of n^i and the others are higher order effects. We further consider the normalized main and total effect Sobol indices S_i and TS_i as

$$S_i = \frac{V_i}{\sigma_y^2}, \quad (2)$$

$$TS_i = S_i + (S_{1i} + S_{2i} + \dots) + (S_{12i} + S_{13i} + \dots) + \dots + \sum_{i_1 < \dots < i_{l-1} < N} S_{i_1 \dots i_{l-1} N}. \quad (3)$$

Note that S_i indicates the main effect contribution of n^i and TS_i the total effect including all interactions, and are percentage contributions of the total response variation σ_y^2 . This UQ/SA analysis forms the first step of a proposed robust design variation reduction workflow. With this, the initial design concept variability is quantified (σ_y^2) and the noise variables which contribute most are identified (those with large S_i). We now seek to find design variables that can reduce the impact of noise variables with large impact.

2.2 Hessian Interaction Terms

To study the impact of changes to different design variables, we consider the Hessian interaction matrix terms of the variance-contributing noise variables and the design variables of any proposed design changes. Hessian terms will show the influence that design variable changes have over the uncertainty contribution of noise variables. To see this, consider a Taylor Series expansion of the response at the current nominal,

$$y = f(d, n) = y_0 + \frac{\delta f}{\delta n} (n - n_0). \quad (4)$$

Typically, we compute this only for the large noise variables contributors n^i . Now consider a design variable d^j for any proposed design change. We could make the change and recompute the uncertainty quantification or similar. However, if d^j changes the UQ, it must be because d^j changed the impact of the contributing n^i . That is, the sensitivity term $\frac{\delta f}{\delta n}$ changed. Therefore, a non-zero Hessian term indicates a d^j can change the noise variable's variability influence on the response:

$$\frac{\delta}{\delta d^j} \frac{\delta}{\delta n^i} f(d, n) \neq 0. \quad (5)$$

Hence, to quickly compute how effective any design variable is at reducing response variability, one can compute the Hessian cross terms of design and noise variables denoted by

$$H^{ij} = \frac{\partial}{\partial d^j} \frac{\partial f}{\partial n^i} = \frac{\partial^2 f}{\partial d^j \partial n^i}, \quad (6)$$

and search which design variables d^j cause a significant change to the sensitivity term $\frac{\delta f}{\delta n^i}$.

Using a central finite-difference approximation, Hessian cross terms can be numerically computed as the interaction term change in response value:

$$H^{ij} = \frac{(f(d_{j+}, n_{i+}) - f(d_{j+}, n_{i-})) - (f(d_{j-}, n_{i+}) - f(d_{j-}, n_{i-}))}{4h_i h_j} \quad (7)$$

The numerator is expressed in units of the response, and can be interpreted in engineering terms as the amount of variation change possible by making the design variable shift from d_- to d_+ , due to the noise variable variation range of n_- to n_+ .

From the engineering perspective, it is easier to interpret H^{ij} with the sign of H^{ij} only indicating the directionality of the design change. That is, we seek the sign result that if H^{ij} is positive, an increase in d would result in an increase in the response variation. To enable this, apply the absolute values over the noise variable,

Eq. (7) represents the change in response variation range of a noise variables due to the change of a design variable, with a positive value indicating variability increase with a design variable increase. More easily expressed as

$$H^{ij} = \frac{|f(d_{j+}, n_{i+}) - f(d_{j+}, n_{i-})| - |f(d_{j-}, n_{i+}) - f(d_{j-}, n_{i-})|}{4h_i h_j} \quad (8)$$

which expresses the change of variance in terms of increasing d_j .

Consider scaling H^{ij} by the range of the standard deviation of the noise factor and by a shift in design variable by δ_j . Then

$$(\Delta_{ij}\sigma_y)^2 = \sigma_i^2 |H^{ij}\delta_j| (H^{ij}\delta_j). \quad (9)$$

large negative $(\Delta_{ij}\sigma_y)^2$ indicates making a δ_j change to nominal design variable d_0^j toward d_+ will reduce noise variable n^i contribution to response variance, whereas a large positive $(\Delta_{ij}\sigma_y)^2$ indicates making a δ_j change toward d_- will reduce noise variable n^i contribution to response variance.

Dividing $(\Delta_{ij}\sigma_y)^2$ by the UQ total power variance σ_y^2 results in the expected change in a noise variable's Sobol index S_i by a design variable d^j changes. Therefore, the expected change in a noise variable's Sobol index ΔS_{ij} by making a design change from nominal is computed as

$$\Delta S_{ij} = \frac{\sigma_i^2}{\sigma_y^2} |H^{ij}\delta_j| (H^{ij}\delta_j), \quad (10)$$

A positive value of ΔS_{ij} indicates changing to d_{j+} increases S_i by ΔS_{ij} (a possibly negative amount) and that changing to d_{j-} decreases S_i by ΔS_{ij} (again a possibly negative amount). Thus, whatever the sign of ΔS_{ij} is, you would change d^j in the opposite direction to achieve a reduction in S_i .

The impact of any one ΔS_{ij} change to a Sobol index does not simply scale σ_y^2 since $\Delta S = (\sigma_{\text{new}} - \sigma_{\text{old}})^2 / \sigma_{\text{old}}^2$, but rather can be computed as

$$\frac{\Delta \sigma_y^2}{\sigma_y^2} = \left(1 + \frac{\Delta S_{ij}}{|\Delta S_{ij}|} \sqrt{|\Delta S_{ij}|} \right)^2 - 1. \quad (11)$$

Further, the overall change in response variance due to multiple design variables changed in the direction of reducing variance is the sum over the noise variable contributors and design changes

$$\sigma_{y,\text{new}}^2 = \sigma_{y,\text{old}}^2 \left(1 - \sqrt{\sum_{ij} |\Delta S_{ij}|} \right)^2. \quad (12)$$

The four Hessian values H^{ij} can also be plotted to visualize interaction impact on response variance due to design and noise variable changes. The interaction plots will show impact of design change over noise contribution if the lines are non-parallel.

2.3 Jacobian Mean Shift Term

The design changes suggested by the Hessian calculations can result not only in variance reduction, but also in mean shift. Often this is undesirable, as the nominal performance \bar{y} is targeted. In this case the Jacobian can similarly be used to compute means shifts, to shift the mean back to target while reducing the variation.

Again consider a Taylor Series expansion of the response at the current nominal n_0 ,

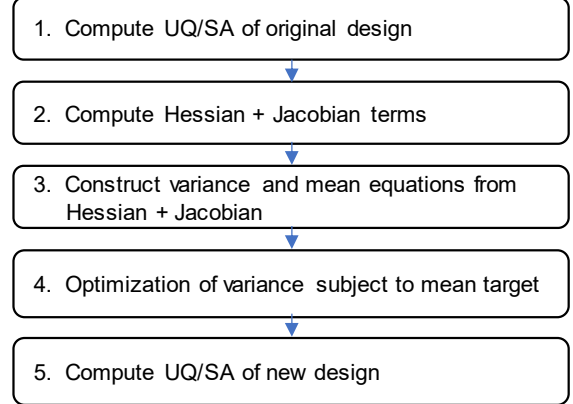


FIGURE 1: 4 STEP WORKFLOW USING HESSIANS AND JACOBIAN TERMS.

$$y = f(d, n) = y_0 + \frac{\partial f}{\partial n}(n - n_0) + \frac{\partial f}{\partial d}(d - d_0). \quad (13)$$

When changing a design variable d^j to reduce variation, the Jacobian can indicate how much the mean will shift. Further, we can use a variable d^j which has no influence on the Hessian to shift back the mean to its original value. Here,

$$J^j = \frac{1}{2} \frac{\partial f}{\partial d^j} \approx \frac{\sum_{d^j=d_+} y}{N} - \frac{\sum_{d^j=d_-} y}{N} \quad (14)$$

where N is the number of runs done in the Hessian analysis, where half are at d_+ and half are at d_- . Eq. (14) computes the half-effect of moving from the nominal center to either of the end points d_+ or d_- .

The overall change in response mean is then approximately a linear summation of the design variable changes,

$$\Delta \bar{p}(d) = \sum_j (J^j) \Delta d^j, \quad (15)$$

where again Δd^j is the amount of change to d^j in a new design configuration considered.

In combination with the variation reduction as computed by Eq. (9) and the mean shift as computed by Eq. (14), one can select design variable changes to reduce the variation while constraining the mean to a target. Design variables that reduce variation can be determined and set using Eq. (12). The associated mean shift from those changes can be computed using Eq. (15), and different design variables changed to shift the mean back to the desired target for the mean. In this way, variation can be minimized. Furthermore, the reasons for the variation reduction are made explicit. The identified design variables that can reduce the impact of identified noise variables will be clear, rather than a black box experimental optimization approach.

2.4 Workflow

The previous sections derived the necessary mathematics for using Hessian and Jacobian terms to reduce variation. We now present a five-step workflow to execute this practically. First, we

quantify response uncertainty and identify input noise variables with large sensitivity contribution. Then an interaction term Hessian matrix calculation is performed to quickly screen design variables for their variation reduction capability against these contributing sources of variation. Each proposed design variable needs only 4 runs to determine if it can reduce the variation contribution of a noise variable, per Eq. (12), and the impact on the mean shift determined per Eq. (15). Having identified design variables to change and by how much, a new design is computed as a constrained optimization, using the summation of variation reductions predicted by the Hessian analysis and keeping the nominal constrained on target through the summation of Jacobian terms. Lastly, an uncertainty quantification at the new design computes the variation reduction. This is outlined in Figure 1.

The first step in the workflow is to compute uncertainty quantification and sensitivity analysis. We apply the open source toolchain developed by Sanchez et al. [3]. The Python based toolchain is developed to screen causal variables, and then apply quasi-Monte-Carlo uncertainty quantification sampling and global sensitivity analysis to quantify engine power variability and identify input noise variables with the largest sensitivity contribution. There are several computational tasks scripted to first construct UQ samples: run a standalone simulation code to compute response values at each UQ sample point, best-fit a surrogate model to the UQ sample points, and finally perform a GSA with the surrogate model by generating a large number of Saltelli sample points to compute Sobol indices. The results are the sensitivity contribution of each input noise variable. The GSA indicated which input parameters are the largest contributors to the response variance.

Next in Step 2 we compute Hessian and Jacobian terms to reduce the sensitivity of the high contributing noise variables n^i by considering design changes d^j . For each high contributing noise variables n^i , each design change d^j is considered by computing the Hessian term Eq. (8) and Jacobian term Eq. (14). This is only 4 runs for every noise and design variable combination.

Next in Step 3 we assemble an overall variation reduction equation as the sum of terms Eq. (12). We also assemble an overall mean shift equation as the sum of terms Eq. (15). Then in Step 4 we can use these two equations to find the changes to the design variables that minimize the variation subject to the mean fixed to a target.

Lastly in Step 5, we recompute the UQ/SA at the new values of the design variables. This confirms the variation reduction and the targeting of the mean response.

3. EXAMPLE STIRLING ENGINE

In previous work, [3-4] workflows were developed applying uncertainty quantification and sensitivity analysis methods to identify root causes of manufacturing quality problems and in [16] a workflow was developed using design of experiments to achieve robustness improvement. Here we build on these previous works to now consider the greater insight and fewer runs offered by the Hessian approach.

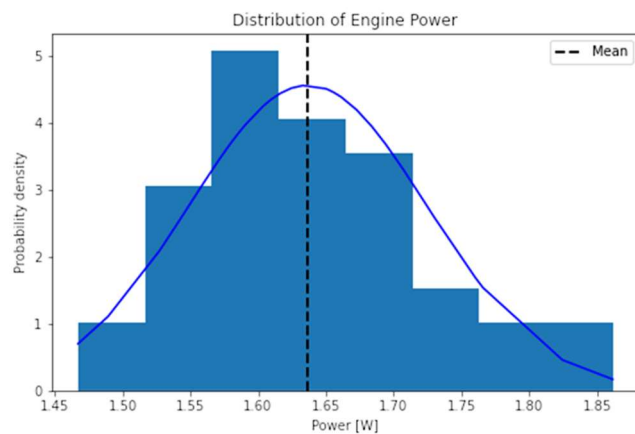


FIGURE 2: UNCERTAINTY OF ENGINE POWER AT NOMINAL DESIGN.

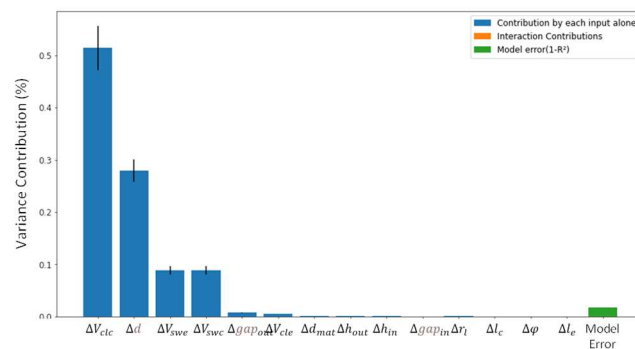


FIGURE 3: SOBEL SENSITIVITY ANALYSIS OF THE MODEL COMPUTED POWER VARIABILITY AT NOMINAL DESIGN.

In these previous works, we introduced the example of a miniature Stirling engine case study. At Aalto University students fabricated, assembled, and tested Stirling engines as part of the senior level machine design course. Students measured the speed at which the crank shaft rotates when there is no torque load applied, the no-load speed. The no-load speed tests demonstrated 25% variation in speed across the fabricated engines, due to variations in fabrication. This outcome exposed the high sensitivity of the Stirling engine to manufacturing and assembly variations. Here we follow the 5 step approach of Figure 1 to explore if the variability of the design could be reduced through parametric design changes. We compare the insight and speed of the approach with earlier RDM results which made use of design of experiments, and show this approach offers more insight to causes and mitigations with less computation.

3.1 Step 1 UQ/SA

Following Figure 1, the first step of the workflow is to quantify the uncertainty at the original design and determine noise variable contributors through a sensitivity analysis. We used the toolchain developed in [3], which creates UQ samples using

Latin Hypercube sampling and runs an external Matlab code to compute the engine power at each point. Figure 2 shows the histogram of the thermodynamic power response. The average power is 1.64 W with a standard deviation of ± 0.09 W.

Next, a surrogate model is fit through the UQ sample points for use in the sensitivity analysis. A vast selection of machine learning methods are available in the Python code library scikit-learn [17] and used in our toolchain. Here we applied Kernel Ridge Regression with a cross-validated grid search routine implemented for hyperparameter tuning. The resulting surrogate model matched the simulation with $r^2 = 0.98$ on the test data. With this surrogate model, Saltelli samples were generated and Sobol indices computed. Figure 3 shows the resulting variance contribution to the power variability by each noise variable alone and by higher order interactions.

The sensitivity analysis indicates variation of the clearance volume and swept volume of compression chamber, the power piston diameter and variation of the swept volume of the expansion piston as the largest contributors to power variability.

3.2 Unconstrained Minimization

The second step in the workflow is to construct interaction in Hessian terms to quickly compute the effect of any design change has on reducing contributions to response variability. First, design variables are selected. We make use of input volumetric variables compounded from dimensional geometry of the engine. Clearance and swept volumes from compression and expansion sides (V_{clc} , V_{swc} , V_{cle} , V_{swe}) were selected as design variable d^j . From the GSA the largest contributors to engine power variability were (ΔV_{clc} , ΔV_{swc} , ΔV_{swe} , Δd) and so used as noise variables n^i . We defined $\pm 4\sigma$ ranges for the noise variables and a reasonable $\pm 20\%$ range of optimization for the design variables.

The Hessian cross terms are constructed in terms of the 4 noise variables and 4 design variables, 16 combinations requiring a total of 64 runs. Table 1 shows how changing a design variable from -20% to +20% results in the tabulated 8 σ thermodynamic power range (W), using Eq. (8). It shows, for example, that when changing the design variable $V_{clc} + 20\%$, the variability in thermodynamic power due to the manufacturing variation ΔV_{clc} will go down by ± 0.01 W, a significant reduction of the ± 0.09 W standard deviation. Table 1 also shows that the contribution to thermodynamic power variation due to ΔV_{swc} and ΔV_{swe} are not significantly affected by any of the proposed design changes, since rows 2 and 3 all have small terms.

Improved understanding is provided by normalizing the results of Table 1 into percentages as Sobol indices, using Eq. (2). Table 2 shows the impact on a noise variable's Sobol index S_i by changing a design variable by 20%. These are the additive changes to each main effect Sobol index. Note these are not multipliers on the total variance and do not show how much the total variance is percentage reduced. Rather, Eq.s (11) and (12) are needed, with results shown in Table 3.

The interaction impact on response variance indicates making an increase of 20% to the nominal V_{clc} will reduce the

$\Delta_{ij}\sigma_y$ (W)		Design			
		V_{clc}	V_{swc}	V_{cle}	V_{swe}
Noise	ΔV_{clc}	-0.010	0.005	-0.002	0.009
	ΔV_{swc}	-0.001	-0.002	0.000	0.004
	ΔV_{swe}	-0.002	0.003	0.000	0.000
	Δd	-0.008	0.005	-0.001	0.008

TABLE 1: HESSIAN INTERACTION.

ΔS_{ij} (%)		Design				
		V_{clc}	V_{swc}	V_{cle}	V_{swe}	$(V_{clc}, -V_{swe})$
Noise	ΔV_{clc}	-1.21	0.35	-0.03	1.13	-4.68
	ΔV_{swc}	-0.03	-0.06	0.00	0.26	-0.47
	ΔV_{swe}	-0.04	0.13	0.00	0.00	-0.04
	Δd	-0.93	0.28	-0.03	0.88	-3.63
	All	-1.49	0.53	-0.04	1.58	-6.08

TABLE 2: INTERACTION IMPACT ON SOBOL INDICES.

$\Delta_{ij}\sigma_y^2$ (%)		Design				
		V_{clc}	V_{swc}	V_{cle}	V_{swe}	$(V_{clc}, -V_{swe})$
Noise	ΔV_{clc}	-20.8	12.2	-3.7	22.4	-38.6
	ΔV_{swc}	-3.4	-5.0	-0.6	10.5	-13.2
	ΔV_{swe}	-4.1	7.2	-0.7	-0.6	-4.1
	Δd	-18.4	10.8	-3.2	19.7	-34.5
	All	-27.9	14.0	-4.1	23.6	-43.2

TABLE 3: INTERACTION IMPACT ON VARIANCE.

contribution of ΔV_{clc} variance by 21% whereas making an decrease of 20% to the nominal V_{swe} will reduce the contribution of ΔV_{clc} variance by 22%. Overall, Eq. (12) indicates that in combination making the two design changes together will show a 39% power variance reduction, all due to the input noise variation on ΔV_{clc} alone, and a 43% reduction due to all four input noise variations. Note that no design changes had any impact on the thermodynamic power variation caused by ΔV_{swc} or ΔV_{swe} input noise variations, rows 2 and 3 are near zero. This Hessian approach provides insight into how and why design changes reduce response variation.

Figure 4 shows the Hessian calculation results graphically as a matrix plot. Each matrix column is a design variable and each matrix row is a noise variable. Each plot therefore has a design variable x-axis with thermodynamic power as the y-axis, and two lines of the response with the noise variable high and low. Therefore, parallel lines indicate no impact of a design change over a noise contribution, and highly non-parallel lines show a strong ability of the design variable to reduce the impact of the noise variable. Design variable values are sought which bring the two lines together. The upper left plot indicates a large change to design variable V_{clc} will reduce ΔV_{clc} variability

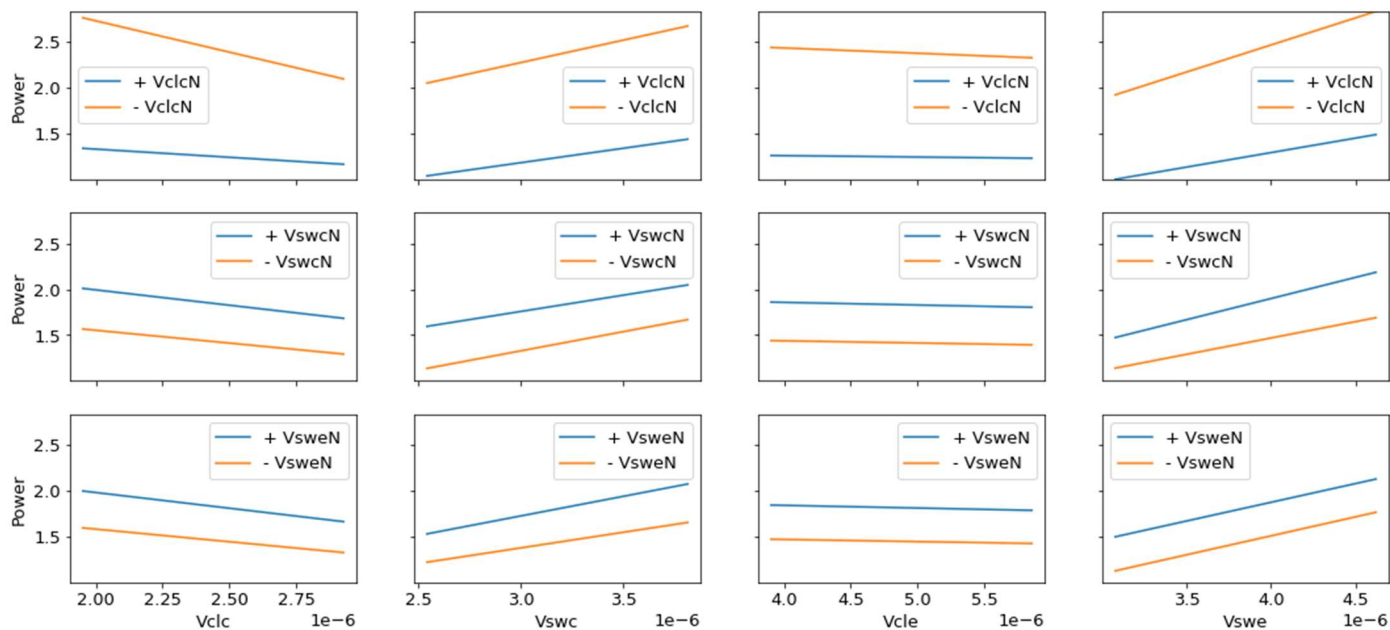


FIGURE 4: INTERACTION HESSIAN GRAPHS.

contribution to Power. The upper right plot indicates a large change to design variable Vswc will have no impact on Vclc Variability contribution to Power.

Having identified new design values for Vclc and Vswc, we proceed to compute UQ/SA at the new design. Figure 5 shows the uncertainty of engine power at new design configuration. The standard deviation went down from $\pm 0.09W$ to $\pm 0.06W$, indicating a (squared) variance reduction by 49%, similar as the Hessian reduction predicted 43% given by Eq. (12).

Next, we continue with Step 4 of the workflow and recompute a sensitivity analysis to confirm total response variance contributions. Figure 6 shows how the power variance was reduced, and that it was due to the Vclc noise variable contribution being reduced. This is as expected from the Hessian analysis which showed the design changes only mitigate the impact of the Vclc noise contribution.

3.3 Constrained Variation Reduction

Although a 49% reduction on variance was achieved at the new design, the mean power was shifted down to 1.21W from 1.64W. To constrain the mean power from shifting, the Jacobian terms can be used to shift back the mean closer to the mean at nominal design. We therefore revert back to Step 2 of the workflow and following Eq. (14) we computed the change in power J^i due to changes in design variable d^j . This is shown in Table 4. As can be seen, we would expect the average power to shift down by 0.45W with the 20% design changes to Vclc and Vswe.

Similar to Figure 4, one can create variable plots of the power response values versus each design variable. Figure 7 shows how average power changes when each design variable changes by $\pm 20\%$. The Hessian calculation showed that design variables Vclc and Vswe influence on variance response, whereas design variable Vswc and Vcle do not. Changing design

variables Vclc by -20% and Vswe by +20%, as suggested by the Hessian calculations, will cause not only a reduction in response variance but also a shift in response mean. Hence, Vswc and Vcle can be changed to compensate and shift back average power.

3.4 Optimization

The fourth step in the workflow is to solve an optimization to calculate the amount of change required for each design variable to produce the same response as the nominal design variables but with a reduced standard deviation. The objective function was set to minimize variation and constraints were added to maintain an average power change of zero and a design space from -20% to 20%.

Eq. (12) for the power variance and the Jacobian derived Eq. (15) can be simultaneously solved in a constrained optimization

$$\begin{aligned} \text{Find } d_* = \arg \min_d \sigma_p^2 \\ \text{Subjected to } \Delta \bar{p} \geq 0 \\ -0.2 \leq \Delta d \leq 0.2 \end{aligned} \quad (16)$$

The result is a new design configuration shown in Table 4. The solution showed an expected 13% reduction in variance with no change in mean. Notice the solution drove Vclc large and Vswe small, as before. However, the solution did not drive Vswe by +20%, but rather by -7%. This is because of the associated mean shift. The term Vswc can shift the mean but does not change the variation, and it was changed to +20%, accounting for approximately +0.25W increase in mean. This restricts the extent of the Vswe shift.

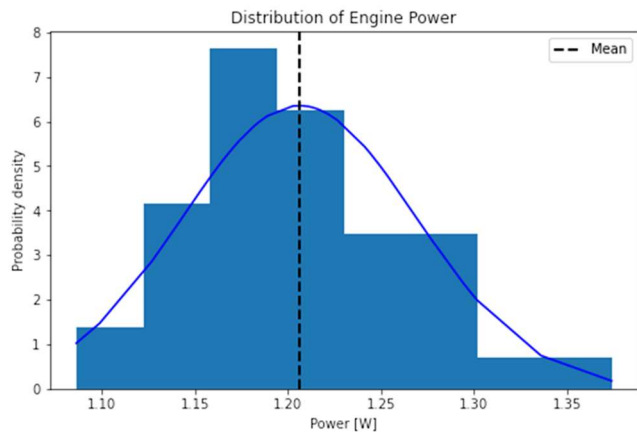


FIGURE 5: UNCERTAINTY OF ENGINE POWER AT NEW DESIGN CONFIGURATION.

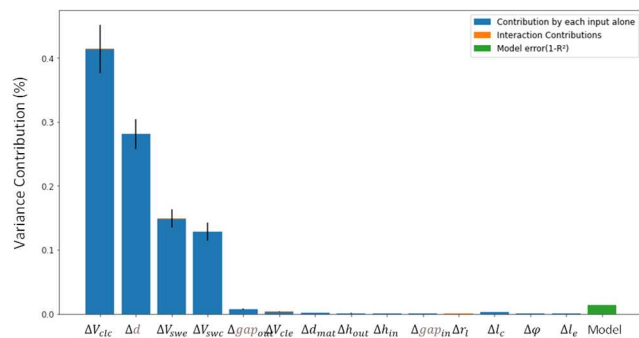


FIGURE 6: SOBOLE SENSITIVITY ANALYSIS OF THE MODEL COMPUTED POWER VARIABILITY AT NEW DESIGN.

3.5 UQ at New Design

To confirm a variation reduction and a mean power similar to the nominal design, we proceed with Step 5 to quantify uncertainty at the new design. Figure 8 shows the standard deviation and mean power of the new design. The new design configuration shows a standard deviation of $\pm 0.078W$ and an average power of $1.63W$. This result shows a (squared) reduction of 20% in variance and no change in average power in relation to nominal design. This actual is in agreement with the variation reduction predicted with the Hessian terms of 13%.

4. DISCUSSION: VALIDATION WITH UNCERTAINTY OPTIMIZATION

The approach successfully computed a new design with less variability, and successfully found a new design with less variability constrained to target the nominal average power. Further, the approach made use of only 48 runs to quantify the impact potential of 4 design variable changes on the contributions of 3 significantly contributing noise variables. Insight was provided that only one of the three most contributing noise variables can be impacted by the proposed design changes.

The results can be compared against a more comprehensive exploration of the design and noise space using robust

ΔP (W)	Vclc	Vswc	Vcle	Vswe
	-0.31	0.49	-0.05	0.60

TABLE 4: JACOBIAN MEAN SHIFTS FROM NOMINAL.

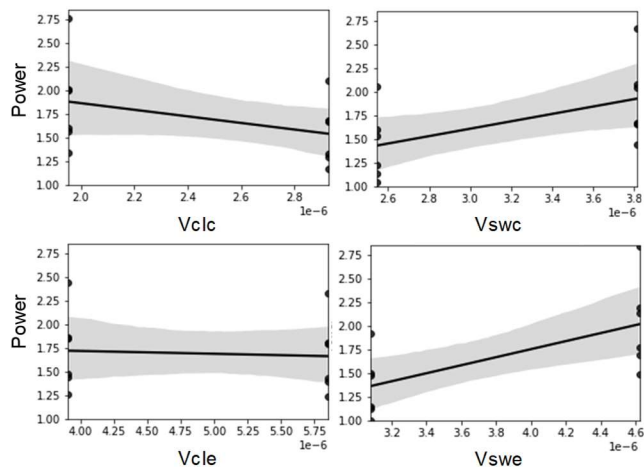


FIGURE 7: MAIN EFFECT JACOBIAN GRAPHS.

optimization. In earlier work [13] a full RDM design of experiments was undertaken, using 100 sample points over the design space with 40 sample points used in a UQ to cover the noise space. This resulted in 4000 runs total. At each design space point, the 40 points UQ was executed and the mean and variance of the power computed. To these, two statistics computed at each point in the design space, and surrogate models were fit. Then a Pareto optimization was solved to show the best combinations of mean and variance of power over the $\pm 20\%$ domain of the design variables. This is shown in Figure 9.

As can be seen, the Hessian approach solved the problem well despite using much less runs than a traditional RDM design of experiments approach. The unconstrained Hessian solution when varying only two design variables by 20% is shown, which approaches the unconstrained solution over all four variables. The constrained solution found by the Hessian approach generated the same design variable combination solution as the full RDM approach, though the predicted variance was not as precise.

Overall, we find the Hessian approach to variation reduction exploration intuitive and insightful. It allows one to quickly screen design variables for their ability to reduce response variance, and with a clear indicator of how the design variable is doing this, in terms of interaction contributions of significant noise variables.

5. CONCLUSION

The traditional and well researched robust design methodology (RDM) makes use of design of experiments to identify design changes that can reduce performance variability. Such optimization of uncertainty becomes computationally difficult,

Design	Nominal	New	Change%
Vclc	2.44E-06	2.93E-06	120
Vswc	3.18E-06	3.82E-06	120
Vcle	4.88E-06	3.91E-06	80
Vswe	3.85E-06	3.59E-06	93

TABLE 5: NEW DESIGN CONFIGURATION.

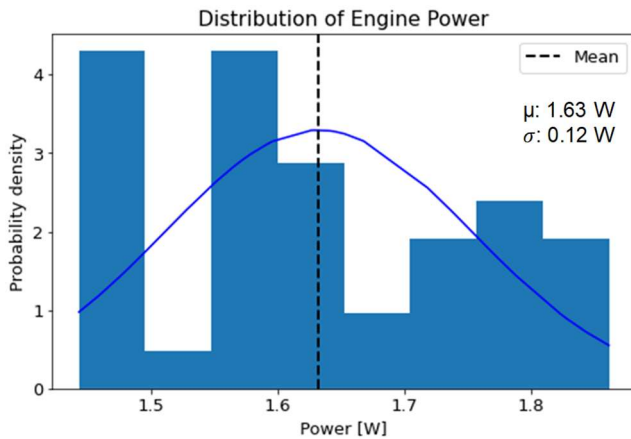


FIGURE 8: UNCERTAINTY OF ENGINE POWER AT NEW DESIGN CONFIGURATION.

whether through direct optimization of quantified uncertainty as an objective function or through Taguchi robust design of experiments.

Here we made use of the more easily computed Hessian interaction matrix elements of the variance-contributing noise variables and the variables of any proposed design changes. Design variable changes with large Hessian terms against noise variables are design changes that can reduce variability. Further, the Jacobian terms of these design changes can indicate which design variables can shift the mean response, to maintain a desired performance target. Using a combination of the more easily computed Hessian and Jacobian terms, design changes can be proposed to reduce variability while maintaining a targeted nominal.

We relate here the Hessian predicted reductions to the associated reductions in Sobol indices that indicate the percentage contribution of noise variables. We also relate these to the percentage reduction expected in the response variance. This allows for rapid interpretation of the impact of different design variable changes in a UQ/SA optimization workflow.

The most basic industrial RDM workflow is to estimate the variance of a design concept, then propose design changes and then estimate the reduced variance after making the design changes. We applied this workflow to computational practice through uncertainty quantification and sensitivity analysis as a first and last step. An example was shown on a Stirling engine design where the impact of the top three variance-contributing tolerances were studied for variation reduction. The approach

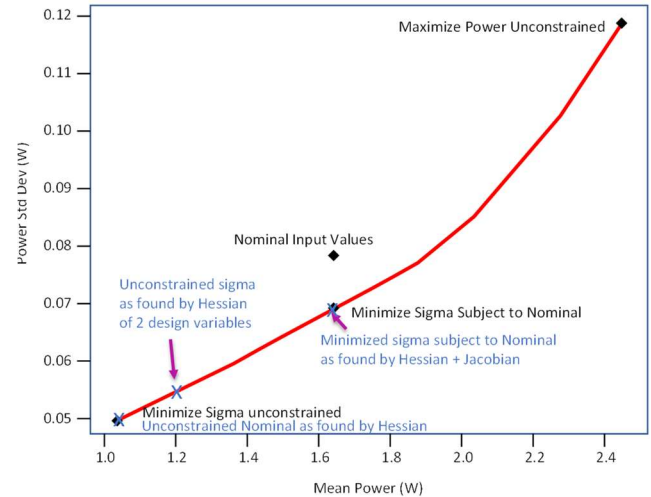


FIGURE 9: PARETO OPTIMAL SOLUTIONS AND HESSIAN RESULTS.

quickly identified two significant design variables, and found a new design with 20% less variance and no change in nominal average power. Overall we find this Hessian based RDM approach useful for classes of problems with high computational burdens.

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REFERENCES

- [1] Arvidsson, M. and Gremyr, I. "Principles of robust design methodology." *Quality and Reliability Engineering International* Vol. 24 No. 1 (2008): pp.23-35. DOI. doi.org/10.1002/qre.864
- [2] Arvidsson, M. and Gremyr, I. and Johansson, P. "Use and knowledge of robust design methodology: A survey of Swedish industry." *J. Eng. Des.* Vol. 14 No. 2 (2003): pp.129-143. DOI. 10.1080/0954482031000138192
- [3] Otto, K. and Sanchez, J. "Model Based Root Cause Analysis of Manufacturing Quality Problems Using Uncertainty Quantification and Sensitivity Analysis." *ASME International Design Engineering Technical Conferences* Vol. 1 (2019) DOI. 10.1115/DETC2019-97766
- [4] Otto, K., Wang, J. and Uyan, T. "Using Open Source Code Libraries for Robust Design Analysis." *Proceedings of the International Conference on Engineering Design ICED* Vol. 2019-August (2019): pp.1733-1741. DOI. 10.1017/dsi.2019.179
- [5] Taguchi, G. *Introduction to Quality Engineering: Designing Quality into Products and Processes*. Asian Productivity Organization (1986).
- [6] Taguchi, G. C. S. and Taguchi S. *Robust Engineering*. New York: McGraw Hill (2000).
- [7] Thornton, A. C. *Variation Risk Management: Focusing Quality Improvements in Product Development and Production*. John Wiley & Sons (2003).

- [8] Wu, J., and Hamada, M., *Experiments: planning, analysis, and optimization*. John Wiley & Sons (2011).
- [9] Montgomery, D. *Design and analysis of experiments*. John Wiley & Sons (2017).
- [10] Arena, M., Leonard, R., Murray, S. and Younossi, O. “Historical Cost Growth of Completed Weapon System Programs.” Santa Monica, CA. 2006.
- [11] Tan, J., Otto, K. and Wood, K. “Relative impact of early versus late design decisions in systems development.” *Design Science* Vol.3 (2017): pp.#. DOI. 10.1017/dsj.2017.13
- [12] Iooss, B. and Lemaître P. “A review on global sensitivity analysis methods.” *Oper. Res. Comput. Sci. Interfaces Ser.* Vol. 59 No. 30 (2015): pp.101-122. DOI.1007/978-1-4899-7547-8_5.
- [13] Saltelli, A. et al. *Global Sensitivity Analysis. The Primer*. John Wiley & Sons (2008).
- [14] Jin, R., Chen, W., and Simpson, T. “Comparative studies of metamodeling techniques under multiple modelling criteria.” *Structural and Multidisciplinary Optimization* DOI.10.1007/s00158-001-0160-4.
- [15] Panda, K. and. Hicken, J. “Hessian-based Dimension Reduction for Optimization Under Uncertainty” *Multidisciplinary Analysis and Optimization Conference AIAA* (2018). DOI. 10.2514/6.2018-3102.
- [16] Sanchez, J., Björkman, Z. and Otto, K., “Robustness improvement using open source code libraries.” *Proc. Des. Soc. Des. Conf.1* (2020): pp.365-374. DOI.10.1017/dsd.2020.82.
- [17] Pedregosa, F. et al., “Scikit-learn: Machine Learning in Python.” *J. Mach. Learn. Res.* Vol. 12 No. 1 (2011): pp.2825-2830. URL <http://jmlr.org/papers/v12/pedregosa11a.html>.