# Probabilistic Modeling of Optimization Errors

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**ABSTRACT**

A structural optimization procedure for a high-speed civil transport resulted in inaccurate optimal wing structural weight due to premature convergence. The optimization error in wing structural weight appeared noisy and one sided. Probabilistic models were applied to the optimization error and the Weibull model was successfully fit to the optimization errors. Previous work showed that the probabilistic model enabled us to estimate average errors without performing very accurate optimization runs. We show that two sets of optimization results, obtained by using a different initial design point for each set, can serve to estimate the mean and standard deviation of the optimization errors.

## 1. Introduction

Optimization is an iterative procedure, which is rarely allowed to converge to high precision due to computational cost considerations. In design optimization of a complex system, sub-optimization problems are often solved within the system level optimization. Consequently, the optimization results are usually a noisy function of the parameters of the design problem. When a single optimization is flawed, it may be difficult to find the problem due to the ill-conditioning of the design space. However, when many optimization results are available such as building a response surface model based on the sub-optimization results, statistical models can be used to estimate the average error of the multiple optimization runs.

A structural optimization procedure was used to obtain accurate wing structural weight ($W_s$) for various configurations of a high-speed civil transport (HSCT). The structural optimization was solved as a sub-optimization within a configuration design optimization of the HSCT, but it resulted in noisy $W_s$ in terms of the aircraft configuration variables. The structural optimization was performed a priori on a carefully selected set of HSCT configurations to build a response surface model (*c.f.* Ref. 1) of $W_s$. An advantage of the response surface approach is that it naturally smoothes out the noise in the $W_s$ data. However, the standard assumption of the response surface fit, that the error is normal with zero mean, may not apply well to optimization errors, which tend to be one-sided[2]. In addition, a data driven model of the optimization error can be useful to consider the effects of the error in a robust design study.

Numerical optimization errors are deterministic in that computer simulation gives the same output for the same input for repeated runs. However, an optimization procedure can be very sensitive to small changes of input parameters. For example, the structural optimization of the HSCT may result in substantially different $W_s$ for slightly different HSCT configurations. Therefore, a probabilistic model can be useful to characterize the noise error of optimization problems. Moreover, other input parameters such as the convergence criteria or the initial design can affect the accuracy of the optimization procedure. The effect of the initial design point is of particular interest because one can easily change it and repeat the optimization to improve a possibly erroneous run due to convergence difficulties or local optima. We apply probabilistic models to a set of structural optimization runs of the HSCT intended for a $W_s$ response surface model, to estimate mean and standard deviation of the optimization error.

## 2. Noise Error from Structural Optimization

The application problem in this paper is a HSCT design model developed by the Multidisciplinary Analysis and Design (MAD) Center for Advanced Vehicles at Virginia Tech. A simplified version of the problem is used following Knill et al.[3] with five configuration design variables including wing root chord, wing tip chord, inboard leading edge sweep angle, airfoil thickness ratio, and fuel weight. Takeoff gross weight is minimized at the system level as a function of the five configuration variables. To improve wing weight equations based on historical data, GENESIS[4] structural optimization software based on finite element models is used. The structural optimization is a sub-optimization below the system level configuration optimization, and wing structural weight ($W_s$) is minimized in terms of 40 structural design variables, including 26 to control skin panel thickness, 12 to control spar cap areas, and two for the rib cap areas[5]. The structural optimization is performed a priori for many aircraft configurations and a response surface model is constructed. For the response surface construction, the five design variables are coded so that each ranges between –1 and +1.

The structural optimization resulted in a noisy $W_s$ in term of the HSCT configuration variables[5, 2]. Figure 1 shows $W_s$ response for 21 HSCT configurations generated by a linear interpolation between two extreme designs. Design 1 corresponds to (-1, -1, -1, -1, -1) and design 21 corresponds to (1, 1, 1, 1, 1) in a coded form of the HSCT configuration variables. Case 0 corresponds to the original results we obtained by using the default convergence criteria of GENESIS. A conservative structural design from a previous study is used as an initial design point for all of the structural optimization runs of Case 0. Designs 13, 16, and 19 of Case 0 seem to have relatively large errors. For Case 1, an initial design point perturbed from that of Case 0 was used, by multiplying each of the 40 structural design variables by factors between 0.1 – 1.9. It is seen that the results are still noisy. One interesting observation is that the noise error tends to be one-sided (greater $W_s$ than the true). That is because the noise error comes from incomplete minimization due to local optima or convergence difficulties.

Efforts have been made to reduce the error of the HSCT structural optimization. Papila and Haftka[6] repaired erroneous optimizations by changing optimization algorithms or trying different initial designs. After extensive experiments with convergence criteria, it was found that the most effective way to improve the optimization was to tighten one of the convergence criteria[7]. However, it was not trivial to choose the right convergence tolerances, and the tightened convergence tolerances more than doubled the cost of the optimization.

The authors[7] applied probabilistic models to the optimization error. The Weibull distribution successfully modeled the error for several cases of different GENESIS convergence criteria. In addition, an indirect approach was devised, using two sets of optimization results for different convergence criteria. The indirect approach gave reasonable estimates of the average error without requiring high-fidelity optimization runs. In this paper, we will show that the Weibull model is useful for optimization runs with different initial design points and that the indirect approach can be applied to optimization runs with two different initial designs. Changing the initial design of the optimization is straightforward and may have a computational advantage over tightening the convergence criteria.

To study the error in $W_s$ from the structural optimization, we used a mixed experimental design of 126 HSCT configurations[6], intended to permit fitting a quadratic or cubic polynomial of the five-variable HSCT design problem to create a $W_s$ response surface approximation. Optimization error, $e$, is defined as

$$e = W_s - W_s^t, \qquad (1)$$

where $W_s$ is the calculated optimum and $W_s^t$ is the true optimum, which is unknown for many practical engineering optimization problems. To estimate $W_s^t$, we need to perform high-fidelity optimization runs that can be expensive. We estimated $W_s^t$ by taking the best of repeated GENESIS runs: Case 0 and Case1 with different initial designs as described above and additional six cases with different sets of convergence criteria[7]. The optimization error, $e$, was calculated for each of the 126 HSCT configurations. Then, the mean and standard deviation of $e$ were estimated for each case of different GENESIS parameters,

$$\hat{m}_{data} = \frac{\sum_{i=1}^{n} e_i}{n} = \bar{e}, \quad \hat{s}_{data} = \sqrt{\frac{\sum_{i=1}^{n} (e_i - \bar{e})^2}{n-1}}, \qquad (2)$$

where $n$ (= 126) is the sample size. Table 1 shows that the average errors were not much different between Case 0 and Case 1, 5.51% and 5.34%, respectively. In terms of computational cost, Cases 0 and 1 took almost the same CPU time per GENESIS run since the only difference is the initial design point.

## 3. Probabilistic Modeling of Optimization Error

With multiple structural optimization runs available, we can obtain a data driven model of the optimization error by fitting a probability distribution. We use the maximum likelihood estimation (MLE) method for the distribution fit[8]. In MLE, we find a vector of distribution parameters, b, to maximize the likelihood function, $l(\mathrm{b})$, which is a product of the probability density function, $f$, over the sample data $x_i$ ($i$ = 1, …, $n$),

$$l(\mathrm{b}) = \prod_{i=1}^{n} f(x_i;\mathrm{b}). \tag{3}$$

The quality of fit is checked via the $c^2$ goodness-of-fit test[8], which is essentially a comparison of histograms between the data and the fit. The test results will be given in terms of the $p$-value. A $p$-value near one implies a good fit and a small chance that the data is inconsistent with the distribution. Conversely, a small $p$-value implies a poor fit and a high chance that the data is inconsistent with the distribution.

Considering the one-sidedness of the optimization error, we selected the Weibull distribution[8, 9], which is defined by a shape parameter, $a$, and a scale parameter $b$. The probability density function (PDF) of the Weibull distribution is

$$f(x) = \begin{cases} a b^{-a} x^{a-1} \exp\left(-\left(\frac{x}{b}\right)^{a}\right) & if\ x \ge 0 \\ 0 & if\ x < 0 \end{cases}. \tag{4}$$

Once we obtain the fit parameters, $a$ and $b$, estimates of mean and standard deviation of $e$ can be calculated from

$$\hat{m}_{fit} = \frac{b}{a}\Gamma\left(\frac{1}{a}\right), \quad \hat{s}_{fit} = \frac{b^2}{a}\left\{2\Gamma\left(\frac{2}{a}\right) - \frac{1}{a}\left[\Gamma\left(\frac{1}{a}\right)\right]^2\right\}, \tag{5}$$

where $\Gamma$ is the gamma function.

## 4. Direct Fit of Probabilistic Model to Optimization Error

A straightforward approach to finding a probabilistic model of the optimization error is to fit a model distribution to $e$, calculated from Eq. 1. This approach is denoted a *direct fit*. The Weibull model was fitted to Case 0 and Case 1, and the results are summarized in Table 2. $p$-values of the $c^2$ test indicated a poor fit for Case 0, while the fit was acceptable for Case 1 with a 5% confidence level. Figure 2 compares histograms of the optimization error, $e$, with the predicted frequencies from the fitted Weibull models. It is seen that the error distribution has a mode near zero and decreases rapidly for large error. The Weibull fits give reasonable descriptions of the error distribution for both Case 0 and Case 1, although the $c^2$ test implied an unsatisfactory fit for Case 0.

The average errors estimated from the fit, $\hat{m}_{fit}$, were in reasonable agreements with $\hat{m}_{data}$: -5.63% and –8.54% discrepancies for Case 0 and Case 1, respectively. The estimates of standard deviation from the fits, $\hat{s}_{fit}$, were less accurate particularly for Case 1, with a discrepancy of –14.6% and –23.4%, for Case 0 and Case 1, respectively. Figure 3, comparing cumulative frequencies of $e$ between the data (bars) and the direct fit (solid line), indicates that the Weibull model is suited for the optimization errors for both Case 0 and Case 1. As a result, we obtained data driven probabilistic models for the optimization error.

## 5. Indirect Fit of Probabilistic Model to Optimization Error

The direct fit approach is expensive because $W_s^t$ needs to be estimated from higher-fidelity optimizations with tightened convergence criteria. Moreover, high-fidelity optimizations are not always available. Alternatively, Kim et al.[7] used an indirect fit approach of finding a distribution of differences of optimal values from two different convergence settings. For the indirect fit, however, it is not necessary to use different convergence parameters. The approach can be extended to using different initial points (*e.g.*, Cases 0 and 1). The basic idea of the indirect fit is to generate two sets of optimization results with different *optimization parameters* such as convergence criteria or initial design, which can affect results of the optimization. Changing convergence settings may require expert level knowledge depending on the optimization software, whereas it is simpler to change initial designs to generate other sets of optimization results for many optimization problems.

For two optimization results, $W_s^1$ with optimization parameter setting #1 and $W_s^2$ with optimization parameters setting #2, model the optimization errors as random variables $s$ and $t$,

$$s = W_s^1 - W_s^t \qquad (6)$$
$$t = W_s^2 - W_s^t.$$

To remove $W_s^t$ from the equation, the difference of $s$ and $t$ is defined as the *optimization difference* $x$,

$$x = s - t = (W_s^1 - W_s^t) - (W_s^2 - W_s^t) = W_s^1 - W_s^2. \qquad (7)$$

If $s$ and $t$ are independent, the probability density function (PDF) of $x$ can be obtained by a convolution of the PDF functions $g(s; b_1)$ and $h(t; b_2)$,

$$f(x; b_1, b_2) = \int_{-\infty}^{\infty} g(s; b_1) h(s - x; b_2) ds. \qquad (8)$$

Note that the optimization difference $x$ is easily calculated from $W_s^1$ and $W_s^2$ that are readily available. Then, we can fit Eq. 8 to the optimization differences via MLE.

The indirect fit was performed using the Weibull distribution on the pair of Cases 0 and 1. Recall that relatively large perturbations (multiplication factors between 0.1 – 1.9) were applied to the initial design point. The large perturbation was intended to reduce dependence (correlation) of $W_s$ between Case 0 and Case 1. The $c^2$ test on the optimization difference indicated a reasonable fit with a $p$-value of 0.5494. From the indirect fit, we estimate the mean and standard deviation of the optimization error of each of the two cases involved. Table 3 shows that the estimates of mean error by the indirect fit, $\hat{m}_{fit}$, have reasonable agreements with $\hat{m}_{data}$: -14.7% and –19.4% discrepancies for Case 0 and Case 1, respectively. The estimates of standard deviation, $\hat{s}_{fit}$, are also in a reasonable match with $\hat{s}_{data}$: 12.0% and 0.704% discrepancies for Case 0 and Case 1, respectively.

Figure 3 shows that the cumulative frequencies predicted by the indirect fit are in reasonable agreement with the data, and the indirect fits are comparable to the direct fits. The indirect approach is computationally more efficient than the direct fit because it does not require expensive higher-fidelity optimization runs. We extended the indirect approach by utilizing a simpler procedure of using different initial design points, and the Weibull model allowed us to estimate well the mean and standard deviation of the error from two sets of low-fidelity optimizations. The results demonstrate a usefulness of the probabilistic model of the optimization error.

## 6. Concluding Remarks

The structural optimization procedure for our HSCT design studies produced inaccurate optimal wing structural weight ($W_s$) because of convergence difficulties. Probabilistic models were applied to the noise error in $W_s$, by utilizing multiple optimization runs originally used for a response surface model. The Weibull model was successfully fit to the optimization errors and gave reasonable estimates of average errors. As a result, we obtained a data-driven probabilistic model of the optimization error.

An indirect fit approach using differences between two optimization results enabled us to estimate the average errors of low fidelity optimizations without performing expensive high-fidelity optimizations. We extended the indirect fit approach by using different initial design points instead of different convergence settings. Since initial design points are optimization parameters that are simple and straightforward to change, one may apply the indirect approach to estimate errors of various optimization problems.

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Table 1: Average error of the HSCT structural optimization runs on 126 HSCT configurations for two cases with different initial design points.

| | Case 0 | Case 1 |
|---|---|---|
| Description | Using the original initial point | Using a perturbed initial point from the original |
| Mean $W_s$ | 85340 *lb.* | 85202 *lb.* |
| Mean error (Percentage error to the true $W_s$) | 4458 *lb.* (5.51%) | 4321 *lb.* (5.34%) |
| Average CPU time on a SGI Origin | 75.5 sec. | 76.5 sec. |

Table 2: Results of direct fit of the Weibull model.

| | Case 0 | Case 1 |
|---|---|---|
| $\hat{m}_{data}$ | 4458 | 4321 |
| $\hat{m}_{fit}$ (discrepancy w.r.t. $\hat{m}_{data}$) | 4207 (-5.63%) | 3952 (-8.54%) |
| $\hat{s}_{data}$ | 8383 | 9799 |
| $\hat{s}_{fit}$ (discrepancy w.r.t. $\hat{s}_{data}$) | 7157 (-14.6%) | 7505 (-23.4%) |
| $a$ | 0.6161 | 0.5646 |
| $b$ | 2891 | 2415 |
| $p$-value of $c^2$ test | 0.0005 | 0.0925 |

Table 3: Results of indirect fit of the Weibull model.

| | Case 0 | Case 1 |
|---|---|---|
| $\hat{m}_{data}$ | 4458 | 4321 |
| $\hat{m}_{fit}$ (discrepancy w.r.t. $\hat{m}_{data}$) | 3804 (-14.7%) | 3481 (-19.4%) |
| $\hat{s}_{data}$ | 8383 | 9799 |
| $\hat{s}_{fit}$ (discrepancy w.r.t. $\hat{s}_{data}$) | 9393 (12.0%) | 9868 (0.704%) |
| $a$ | 0.4666 | 0.4262 |
| $b$ | 1659 | 1236 |
| $p$-value of $c^2$ test | 0.5494 | |

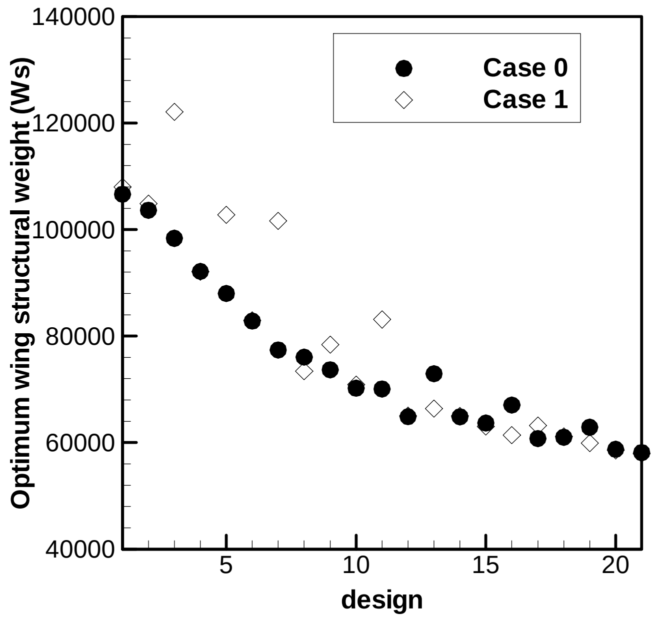
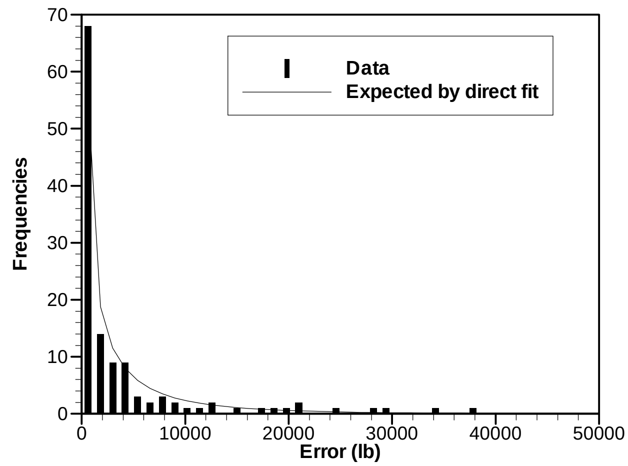
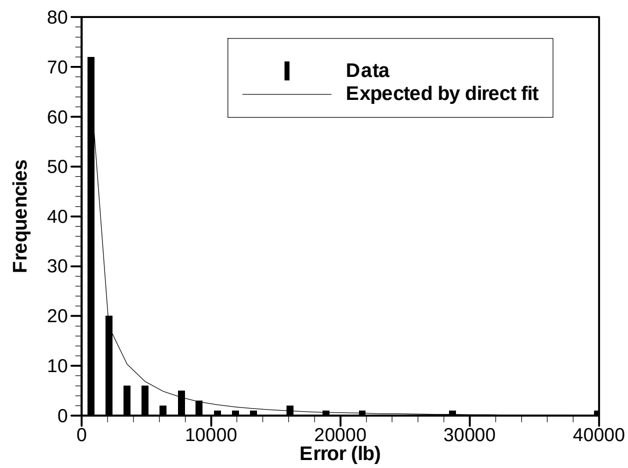



Figure 1: Noisy $W_s$ response from structural optimization. Case 0 and Case 1 used different initial design points.

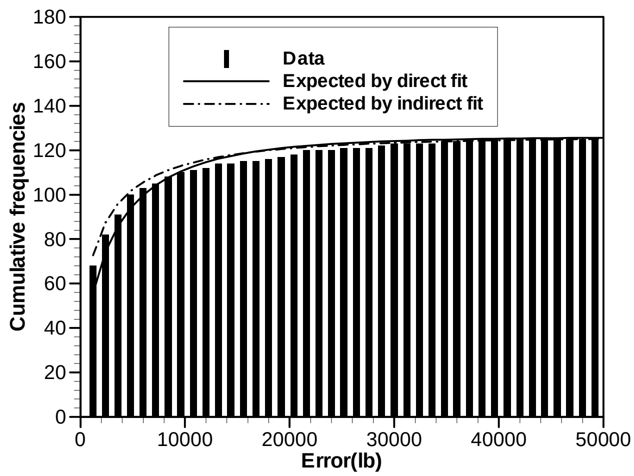



(a) For Case 0

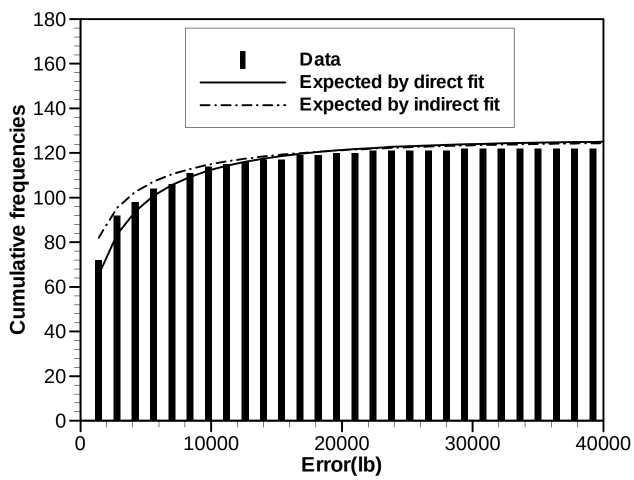



(b) For Case 1

Figure 2: Comparison of histograms of error and direct fits of the Weibull model.



(a) For Case 0



(b) For Case 1

Figure 3: Comparison of cumulative frequencies between direct and indirect fit of the Weibull model.