

## Employing Sensitivity Derivatives for Robust Optimization under Uncertainty in CFD

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### Abstract

A robust optimization is demonstrated on a two-dimensional inviscid airfoil problem in subsonic flow. Given uncertainties in statistically independent, random, normally distributed flow parameters (input variables), an approximate first-order statistical moment method is employed to represent the Computational Fluid Dynamics (CFD) code outputs as expected values with variances. These output quantities are used to form the objective function and constraints. The constraints are cast in probabilistic terms; that is, the probability that a constraint is satisfied is greater than or equal to some desired target probability. Gradient-based robust optimization of this stochastic problem is accomplished through use of both first and second-order sensitivity derivatives. For each robust optimization, the effect of increasing both input standard deviations and target probability of constraint satisfaction are demonstrated. This method provides a means for incorporating uncertainty when considering small deviations from input mean values.

### Introduction

In gradient-based optimization, input data and parameters are often assumed precisely known leading to deterministic or conventional optimization. When statistical uncertainties exist in the input data or parameters, however, these uncertainties affect the design and therefore should be accounted for in the optimization. Such optimizations under uncertainty have been studied and used in structural design disciplines [1-5]; we refer to these as non-deterministic or robust design optimization procedures. In the present work robust optimization procedures are applied to a two-dimensional inviscid CFD code.

An integrated strategy for mitigating the effect of uncertainty in simulation-based design is presented in [6]; this strategy consists of uncertainty quantification, uncertainty propagation, and robust design tasks. This strategy is followed herein making use of second moment approximations and sensitivity derivatives (SD), that is, the derivatives of CFD code output with respect to code input parameters. In [7] it is shown that a statistical First Order Second Moment (FOSM) method can be used to efficiently propagate input uncertainties through finite element analyses to approximate output

uncertainty. This FOSM method is employed herein to model uncertainty propagation through the CFD code.

The SD contain information which can be used to direct the optimization search; that is, the objective and constraint gradients are functions of the CFD SD. The gradient-based robust optimization demonstrated herein for a two-dimensional airfoil problem requires both first and second-order SD from the CFD code. Reference 8 presents, discusses, and demonstrates the efficient calculation of both first and second-order SD from CFD code. Our initial verification of this present process was obtained for quasi 1-D problems using an Euler code [9]. A 3-D application of this present procedure to a flexible wing [10] obtained the required second-order SD contributions by finite differencing terms containing first-order SD.

Another earlier demonstration or application of gradient-based, robust optimization involving advanced or high-fidelity (nonlinear) CFD code was presented in [11] and [12]. Two aspects need to be pointed out in regard to the robust optimization demonstrations for CFD code modules presented herein and also in [8-12]. First, the sources of uncertainty considered were only those due to code input parameters; i.e., due to sources external to the CFD code simulation. Other computational simulation uncertainties, such as those due to physical, mathematical and numerical modeling approximations (see [13] and [14]) - essentially internal model error and uncertainty sources, were not considered. Second, the assessment of everyday operational fluctuations on performance loss, not catastrophe was addressed. Consequently, we are most concerned with aero performance behavior due to probable fluctuations, i.e., near the mean of probability density functions (pdf).

## The Integrated Statistical Approach

### *Uncertainty Quantification*

In this study, we consider the influence of uncertainty in CFD input parameterization variables. We have assumed that these input variables are statistically independent, random, and normally distributed about a mean value. This assumption not only simplifies the resulting algebra and equations, but also serves to quantify input uncertainties. Furthermore, it is not an unreasonable assumption for input flow conditions subject to random fluctuations.

### *Uncertainty Propagation*

Uncertainty propagation is accomplished by a FOSM method. The CFD system output solution of interest is approximated in Taylor series form; the approximation is an estimate of the output value for small deviations of the input. Given input random variables  $\mathbf{b}=\{b_1, \dots, b_n\}$  with mean  $\bar{\mathbf{b}} = \{\bar{b}_1, \dots, \bar{b}_n\}$  and standard deviations,  $\sigma_{\mathbf{b}} = \{\sigma_{b_1}, \dots, \sigma_{b_n}\}$ , the first order Taylor series approximation of CFD output function,  $\mathbf{F}$  is given by:

$$\mathbf{F}(\mathbf{b}) = \mathbf{F}(\bar{\mathbf{b}}) + \sum_{i=1}^n \frac{\partial \mathbf{F}}{\partial b_i} (b_i - \bar{b}_i) \quad (1)$$

where derivatives are evaluated at the mean values,  $\bar{\mathbf{b}}$ . One then obtains expected values for the mean (first moment) and variance (second moment) of the output function,  $\mathbf{F}$ , which depend on the SD and input variances,  $\sigma_{\mathbf{b}}^2$ . The mean of the output function,  $\bar{\mathbf{F}}$ , and its variance  $\sigma_{\mathbf{F}}^2$ , are approximated as

$$\bar{\mathbf{F}} = \mathbf{F}(\bar{\mathbf{b}}) \quad \sigma_{\mathbf{F}}^2 = \sum_{i=1}^n \left( \frac{\partial \mathbf{F}}{\partial b_i} \sigma_{b_i} \right)^2 \quad (2)$$

where derivatives are evaluated at the mean values,  $\bar{\mathbf{b}}$ . Equation (2) represents a FO method for representing input parameter uncertainty propagation. The method is straightforward with the difficulty largely lying in computation of the SD.

### Robust Optimization

Conventional optimization for an objective function,  $\text{Obj}$ , that is a function of the CFD output,  $\mathbf{F}$ , state variables,  $\mathbf{Q}$ , and input (design) variables,  $\mathbf{b}$ , is routinely expressed as shown in Eq. (3). System constraints,  $\mathbf{g}$ , are represented as inequality constraints. The input variables,  $\mathbf{b}$ , are precisely known, and all functions of  $\mathbf{b}$  are therefore deterministic.

$$\min \text{Obj}, \text{ where } \text{Obj} = \text{Obj}(\mathbf{F}, \mathbf{Q}, \mathbf{b}) \quad \text{subject to} \quad \begin{aligned} \mathbf{R}(\mathbf{Q}, \mathbf{b}) &= 0 \\ \mathbf{g}(\mathbf{F}, \mathbf{Q}, \mathbf{b}) &\leq 0 \end{aligned} \quad (3)$$

For robust design, the conventional optimization, Eq. (3), must be treated in a probabilistic manner. Given uncertainty in the input variables,  $\mathbf{b}$ , all functions in Eq. (3) are no longer deterministic. The design variables are now the mean values,  $\bar{\mathbf{b}} = \{\bar{b}_1, \dots, \bar{b}_n\}$ , where all elements of  $\bar{\mathbf{b}}$  are assumed statistically independent and normally distributed with standard deviations  $\sigma_{\mathbf{b}}$ . The state equation residual equality constraint,  $\mathbf{R}$ , is deemed to be satisfied at the expected values of  $\mathbf{Q}$  and  $\mathbf{b}$ , that is the mean values  $\bar{\mathbf{Q}}$  and  $\bar{\mathbf{b}}$  for the FO approximation. The objective function is cast in terms of expected values and becomes a function of  $\bar{\mathbf{F}}$  and  $\sigma_{\mathbf{F}}$ . The other constraints are cast into a probabilistic statement: the probability that the constraints are satisfied is greater than or equal to a desired or specified probability,  $P_k$ . This probability statement is transformed (see [6]) into a constraint involving mean values and standard deviations under the assumption that variables involved are normally distributed. The robust optimization can be expressed as

$$\min \text{Obj}, \quad \text{Obj} = \text{Obj}(\bar{\mathbf{F}}, \sigma_{\mathbf{F}}, \bar{\mathbf{Q}}, \bar{\mathbf{b}}) \quad \text{subject to} \quad \begin{aligned} \mathbf{R}(\bar{\mathbf{Q}}, \bar{\mathbf{b}}) &= 0 \\ \mathbf{g}(\bar{\mathbf{F}}, \bar{\mathbf{Q}}, \bar{\mathbf{b}}) + k\sigma_{\mathbf{g}} &\leq 0, \end{aligned} \quad (4)$$

where  $k$  is the number of standard deviations,  $\sigma_{\mathbf{g}}$ , that the constraint  $\mathbf{g}$  must be displaced in order to achieve the desired or specified probability,  $P_k$ . For the FOSM approximation, standard deviations  $\sigma_{\mathbf{F}}$  and  $\sigma_{\mathbf{g}}$  are of the form given in Eq. (2) involving first-order SD. Therefore, a gradient-based optimization will then require second-order SD to compute the objective and constraint gradients. The efficient calculation of second-order SD necessary for robust optimization was demonstrated in [8]. Both conventional and robust

optimizations were performed using the Sequential Quadratic Programming (SQP) method option in the Design Optimization Tools, DOT [15].

### Application to 2-D Euler CFD

An initial verification of the present methodology was done for several quasi 1-D problems using Euler Code [9]. The methodology is demonstrated herein for a 2-D inviscid steady subsonic flow over a NACA 64A410 airfoil using an Euler code [8]. A 129 x 33 C-mesh computational grid is used with the far-field boundary approximately five chord lengths from the surface of the airfoil.

For the current study, the airfoil angle of attack,  $\alpha$  and the free-stream Mach number,  $M_{inf}$ , will be taken as statistically independent random variables. The CFD output is both the lift coefficient,  $C_l$  and the pitching moment coefficient,  $C_m$ . Applying the approach previously outlined yields

Input random variables:  $\mathbf{b}=\{\alpha, M_{inf}\}$  CFD output function:  $\mathbf{F}=\{C_l, C_m\}$ .

$$\begin{aligned} \bar{C}_l &= C_l(\bar{\alpha}, \bar{M}_{inf}) & \bar{C}_m &= C_m(\bar{M}_{inf}, \bar{\alpha}) \\ \sigma_{C_l}^2 &= \left( \frac{\partial C_l}{\partial \alpha} \sigma_{\alpha} \right)^2 + \left( \frac{\partial C_l}{\partial M_{inf}} \sigma_{M_{inf}} \right)^2 & \sigma_{C_m}^2 &= \left( \frac{\partial C_m}{\partial \alpha} \sigma_{\alpha} \right)^2 + \left( \frac{\partial C_m}{\partial M_{inf}} \sigma_{M_{inf}} \right)^2 \end{aligned} \quad (5)$$

To demonstrate the optimizations, a simple target-matching problem is selected; a unique answer is obtained when an equality constraint is enforced. The CFD code is run for given  $\alpha$  and  $M_{inf}$ ; the resulting  $C_l(\alpha, M_{inf})$  and corresponding  $C_m(\alpha, M_{inf})$  are taken as the target values  $C_{lt}$  and  $C_{mt}$ , respectively. For this conventional optimization, the objective function and constraint are cast as

$$\begin{aligned} \min \text{Obj}, \quad \text{Obj} &= \text{Obj}(C_l, \alpha, M_{inf}) = [C_l(\alpha, M_{inf}) - C_{lt}]^2 \\ \text{subject to} \quad \mathbf{R}(\alpha, M_{inf}) &= 0 & (6) \\ C_m(\alpha, M_{inf}) - C_{mt} &= 0 \end{aligned}$$

The robust optimization is expressed as

$$\begin{aligned} \min \text{Obj}, \quad \text{Obj} &= \text{Obj}(\bar{C}_l, \sigma_{C_l}, \bar{\alpha}, \bar{M}_{inf}) = [\bar{C}_l(\bar{\alpha}, \bar{M}_{inf}) - C_{lt}]^2 + \sigma_{C_l}^2 \\ \text{subject to} \quad \mathbf{R}(\bar{\alpha}, \bar{M}_{inf}) &= 0 & (7) \\ C_m(\bar{\alpha}, \bar{M}_{inf}) - C_{mt} + k\sigma_{C_m} &= 0 \end{aligned}$$

Note that for  $\sigma_{\alpha} = \sigma_{M_{inf}} = 0$  in Eq. (7), the conventional optimization is obtained.

## Sample Results & Discussion

Optimization results were generated using the 2-D CFD code and the procedure given by Eq. (3) and (4). Two cases are presented. For case 1,  $P_k$  is fixed at  $k=1$ , i.e.,  $P_1=84.13\%$ , and the effect of increasing the input variable standard deviations is addressed. For case 2, the standard deviations of the input variables are fixed at 0.01 and  $P_k$  increases.

In Table 1, results for case 1 of the robust optimization are displayed. For  $\sigma_\alpha = \sigma_{\text{Minf}} = \sigma$  ranging from 0 to 0.08, optimal values for the input variables  $(\bar{\alpha}, \bar{\text{Minf}})$  are listed. As  $\sigma$  increases, so does  $\sigma_{\text{Cm}}$ . Accordingly, the mean values,  $(\bar{\alpha}, \bar{\text{Minf}})$  which minimize the objective function and satisfy the probabilistic constraint, become increasingly displaced from the target moment coefficient,  $\text{Cmt}$ . This is shown in Fig. 1. The robust design points track the dashed curve for  $\bar{\text{Cl}} = \text{Clt}$  with some displacement due to the  $\sigma_{\text{Cl}}^2$  term of the objective, Eq. (7). Note that  $\text{Cm}(\bar{\alpha}, \bar{\text{Minf}})$  is displaced from the solid curve  $\text{Cm} = \text{Cmt}$  by  $k\sigma_{\text{Cm}}$ , as required by the probabilistic constraint. This displacement can be viewed as the probabilistic solution dependent or "effective" safety margin.

The results for case 2 of the robust optimization, where  $\sigma_\alpha = \sigma_{\text{Minf}}$  is fixed at 0.01, and  $P_k$  increases from 50 percent to 99.99 percent ( $k=0$  to 4) are given in Table 2. With an increase in  $P_k$ ,  $\text{Cm}(\bar{\alpha}, \bar{\text{Minf}})$  is displaced from the solid curve  $\text{Cm} = \text{Cmt}$  by  $k\sigma_{\text{Cm}}$ , as required by the probabilistic constraint. Accordingly, the mean values,  $(\bar{\alpha}, \bar{\text{Minf}})$ , which minimize the objective function and satisfy the constraint, again become increasingly displaced from those at the target value,  $\text{Cmt}$ . Note the significant displacement of the solution from the target when  $P_k$  is large, i.e., when one is attempting to incorporate the tails of the pdf. In order to increase the probability of constraint satisfaction from 97.77 percent to 99.99 percent, one sees a significant change in  $(\bar{\alpha}, \bar{\text{Minf}})$  for a mere gain of 2 percent in constraint satisfaction.

## Concluding Remarks and Challenges

The present results represent an implementation of the approximate statistical moment method for robust optimization in a 2-D inviscid subsonic CFD code. Assuming statistically independent, random, normally distributed input variables, the uncertainties in the input variables were incorporated into a robust optimization procedure where statistical moments involving first-order sensitivity derivatives appeared in the objective function and system constraints. Second-order sensitivity derivatives were used in a gradient-based robust optimization. The approximate methods used throughout the analyses are valid when considering robustness about input parameter mean values.

Collectively, these results demonstrate the possibility for an approach to treat input parameter uncertainty and its propagation in gradient-based design optimization that is governed by complex CFD analysis solutions. It has been demonstrated on a relatively simple CFD code and problem; there are computational resource issues to be addressed in application to 3-D CFD codes and problems if analytical second-order SD are used.

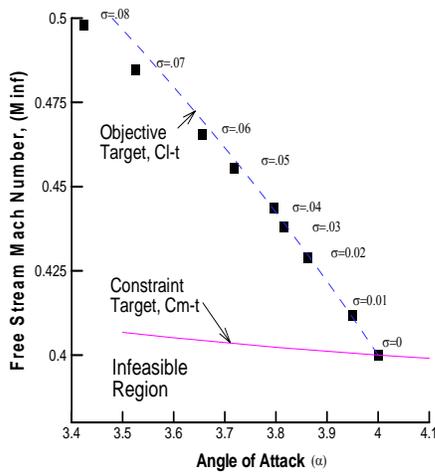


Figure 1. Optimization results in design space ( $\alpha$ ,  $\overline{M}_{inf}$ ),  $P_k$  fixed at  $P_1$ .

$\sigma$	$\overline{\alpha}$	$\overline{M}_{inf}$	Obj	$\sigma_{Cl}$	$\sigma_{Cm}$
0	4.00	0.4	0.0000	0.000	0.0000
0.01	3.95	0.411	0.0000	0.006	0.0005
0.02	3.86	0.428	0.0001	0.012	0.0010
0.03	3.81	0.437	0.0004	0.019	0.0016
0.04	3.79	0.443	0.0007	0.026	0.0022
0.05	3.72	.455	0.0011	0.034	0.0029
0.06	3.66	.465	0.0018	0.042	0.0037
0.07	3.52	.484	0.0029	0.053	0.0047
0.08	3.42	.498	0.0042	0.064	0.0058

Table 1. Figure 1 data,  $\sigma_{minf}=\sigma_{\alpha}=\sigma$ ,  $P_k = P_1$

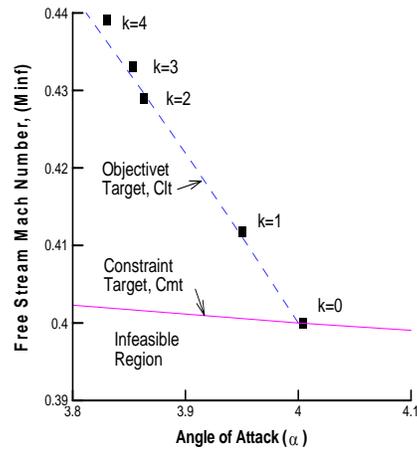


Figure 2. Optimization results in design space ( $\alpha$ ,  $\overline{M}_{inf}$ ),  $\sigma$  fixed at 0.01.

K	$P_k$	$\overline{\alpha}$	$\overline{M}_{inf}$	Obj	$\sigma_{Cl}$	$\sigma_{Cm}$
0	0.500	4.00	0.400	0.000000	0.000	0.0000
1	0.841	3.95	0.411	0.000033	0.0057	0.00047
2	0.977	3.86	0.428	0.000037	0.0061	0.00051
3	0.998	3.85	0.433	0.000039	0.0063	0.00052
4	0.999	3.83	0.439	0.000043	0.0064	0.00054

Table 2. Figure 2 data,  $\sigma$  fixed at 0.01

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