Multidisciplinary System Design Optimization (MSDO)

Approximation Methods

Lecture 19

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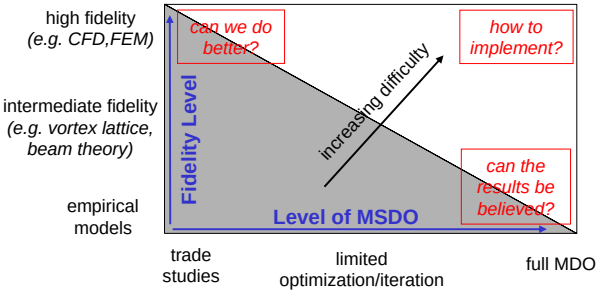
Today's Topics

- Design variable linking
- Reduced-Basis Methods
- Response Surface Approximations
- Kriging
- Variable-Fidelity Models

Why Approximation Methods?

We have seen throughout the course the constant trade-off between **computational cost** and **fidelity.**



from Giesing, 1998

Approximation methods provide a way to get high-fidelity model information throughout the optimization without the computational expense.

Approximation Methods

- Recall that the analysis or simcode must be invoked each time the optimizer selects a new design vector to try
- Typically, hundreds (thousands) of design vectors will be analyzed throughout an optimization run
- Can use **Approximation Models** (**Surrogate Models**) for objective functions and constraints
- If approximate models are inexpensive to evaluate, can analyze many more design vector options without worrying about computational resources
- Concept first introduced in structural optimization by Barthelemy and Haftka, 1993

Approximation Methods Overview

Design variable linking Reduced-basis methods	• reduce the number of design variables in the optimization code • simcode analysis full order
Response surface methods Kriging	• same number of design variables • simcode analysis simplified
Variable-fidelity methods	• combine high-fidelity and approximation models

Design Variable Linking

- Not all design variables may be independent
- For example, symmetry may exist in the problem

$$\mathbf{y} = \mathbf{T}\mathbf{x} + \mathbf{y}^C$$

optimizer uses **y**, but provides **x** to simcode for analysis

Define:

$$\underset{r\times 1}{\begin{bmatrix}\mathbf{y}\end{bmatrix}} = \underset{r\times n}{\begin{bmatrix}\mathbf{T}\end{bmatrix}} \underset{n\times 1}{\begin{bmatrix}\mathbf{x}\end{bmatrix}} + \underset{r\times 1}{\begin{bmatrix}\mathbf{y}^C\end{bmatrix}}$$

Reduced-Basis Methods

Consider r feasible design vectors: $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^r$

We could consider the desired design to be a linear combination of these basis vectors:

$$\mathbf{x}^* = \sum_{i=1}^{r} \alpha_i \mathbf{x}^i + \mathbf{x}^C$$

scalar coefficient — basis vector — added for generality

Reduced-Basis Methods

We can now optimize $J(\mathbf{x})$ by finding the optimal values for the coefficients α_i.

dimension n → dimension r

- do one full-order evaluation of resulting answer
- approach is efficient if $r << n$
- will give the true optimum only if $\mathbf{x}^*$ lies in the span of $\{\mathbf{x}^i\}$
- basis vectors could be
  - previous designs
  - solutions over a particular range (DoE)
  - derived in some other way (POD)

Reduced-Basis Example

Example using a reduced-basis approach (van der Plaats Fig 7-2): airfoil design for a unique application.

- many airfoil shapes with known performance are available
- design variables are (x,y) coordinates at chordwise locations (n~100)
- use four basis airfoil shapes (low-speed airfoils) which contain the n geometry points
- plus two basis shapes which allow trailing edge thickness to vary
- r=6 (r<<n)
- optimize for high speed, maximum lift with a constraint on drag

Reduced-Basis Example

Vanderplaats, G. N. *Numerical Optimization Techniques for Engineering Design.* Vanderplaats R&D, 1999. Figure 7-2.

Vanderplaats, G. N. *Numerical Optimization Techniques for Engineering Design.* Vanderplaats R&D, 1999. Figure 7-3.

Proper Orthogonal Decomposition

Also known as principal components analysis, Kahunen-Loève decomposition, singular value decomposition

$$\mathbf{x}^* = \sum_{i=1}^{r} \alpha_i \varphi^i$$

- The r basis vectors φ_i are orthogonal
- They are computed from M empirical solutions $\{\mathbf{x}^1, \mathbf{x}^2, \ldots \mathbf{x}^M\}$
- They are optimal in the sense that they minimize the error between the original and the projected data

$$\max_{\varphi} \frac{\left\langle \left| (\mathbf{x}, \varphi) \right|^2 \right\rangle}{\left\| \varphi \right\|^2}$$

Proper Orthogonal Decomposition

These optimal basis functions can be calculated by:

1. Evaluating the correlation matrix:

$$R_{ij} = \mathbf{x}^{i\mathrm{T}} \mathbf{x}^j$$

2. Solving the $M \times M$ eigenvalue problem:

$$R\mathbf{v}_i = \lambda_i \mathbf{v}_i$$

3. Constructing the basis vectors:

$$\varphi_j = \sum_{i=1}^{M} v_j^i \mathbf{x}^i$$

Use components of the jth eigenvector to calculate the jth POD basis vector. The jth eigenvalue tells us how important is the jth basis vector.

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Response surface methods Kriging	• same number of design variables • simcode analysis simplified
Variable-fidelity methods	• combine high-fidelity and approximation models

Response Surface Methodology

- Keep the same number of design variables, but simplify the simcode analysis
- Create approximating functions to objective and constraints
- Optimize using the approximations
- Update approximations using current optimal solution guess and repeat
- Response surfaces are smooth even if design space is noisy
- Polynomial-based modeling technique
- Provide compact, explicit functional relationship between response and design variables
- Least squares is computationally inexpensive and easy to implement

Local Approximations

Most common are Taylor series expansions:

$$J(\mathbf{x}) = J(\mathbf{x}^0) + \left[\nabla J(\mathbf{x}^0)\right]^T \delta\mathbf{x} + \frac{1}{2}\delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^0)\delta\mathbf{x} + \cdots$$

$$\delta\mathbf{x} = \mathbf{x} - \mathbf{x}^0$$

- Could use the first two terms $\Rightarrow$ linear approximation
- Solve, reanalyze and repeat = sequential linear programming
- Could also include quadratic term:

$$J(\mathbf{x}) = J(\mathbf{x}^0) + \left[\nabla J(\mathbf{x}^0)\right]^T \delta\mathbf{x} + \frac{1}{2}\delta\mathbf{x}^T \mathbf{H}(\mathbf{x}^0)\delta\mathbf{x} + \cdots$$

update requires: 1 function evaluation; n function evaluations; $n(n+1)/2$ function evaluations

Local Approximations

- It is expensive to update the gradient vector and Hessian matrix
- One approach:
  - perform several approximation cycles updating only the constant term
  - then update the linear term and repeat
  - finally, update the Hessian only when no other progress can be made
- If the design space is highly nonlinear, there is no guarantee that this approach will work

Response Surface Methodology

- Another approach: use what information is available to create the approximation
- Use this approximation to make a small move in the design variables
- Analyze the result precisely $\Rightarrow$ new function evaluation
- Use the new function evaluation to improve the approximation to the design space

$\Rightarrow$ **Fit a response surface**

- Can use a quadratic or higher order surface
- Might choose to use only some of the function evaluations (*e.g.* those in a local neighborhood)

RSM

e.g. define $\Delta J = J(\mathbf{x}) - J(\mathbf{x}^0)$

quadratic approximation:

$$\begin{aligned}\Delta J &= \nabla J^{\mathrm{T}}\delta\mathbf{x} + \delta\mathbf{x}^{\mathrm{T}}\mathbf{H}\delta\mathbf{x} \\ &= \frac{\partial J}{\partial x_1}\delta x_1 + \frac{\partial J}{\partial x_2}\delta x_2 + \ldots + \frac{\partial J}{\partial x_n}\delta x_n \\ &+ \frac{1}{2}\left(H_{11}\delta x_1^2 + H_{22}\delta x_2^2 + \ldots + H_{nn}\delta x_n^2\right) \\ &+ H_{12}\delta x_1\delta x_2 + H_{13}\delta x_1\delta x_3 + \ldots + H_{1n}\delta x_1\delta x_n \\ &+ H_{23}\delta x_2\delta x_3 + \ldots + H_{n-1,n}\delta x_{n-1}\delta x_n\end{aligned} \qquad (*)$$

(all derivatives and entries of **H** are evaluated at $\mathbf{x}^0$)

RSM

Assume we have evaluated the baseline plus q designs:

$$\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^q \rightarrow J^0, J^1, \ldots J^q$$

We could write q equations of the form $(*)$ using

$$\left(\mathbf{x}^1 - \mathbf{x}^0, J^1 - J^0\right), \left(\mathbf{x}^2 - \mathbf{x}^0, J^2 - J^0\right), \cdots, \left(\mathbf{x}^q - \mathbf{x}^0, J^q - J^0\right)$$

There is a total of $N=n+n(n+1)/2$ unknowns:

$$\frac{\partial J}{\partial x_1}, \frac{\partial J}{\partial x_2}, \ldots, \frac{\partial J}{\partial x_n}, H_{11}, H_{12}, \ldots, H_{nn}$$

RSM

- q equations, N unknowns
- If $q<N$, only some coefficients can be calculated
- If $q>N$, use weighted least squares
- Weight designs closer to current $\mathbf{x}^q$ more heavily
- In general, use $q \geq n+1$ initial designs so an initial linear approximation can be provided
- If have baseline plus n designs, can fit a linear approximation in each direction (*i.e.* a hyperplane)
- If have more solutions, can fit a quadratic or higher order surface

RSM

- In other words, fit objective function with a polynomial
- *e.g.* quadratic approximation:

$$J(\mathbf{x}) = \mathbf{a_0} + \sum_i b_i x_i + \sum_i c_{ii} x_i^2 + \sum_{i,j<i} c_{ij} x_i x_j$$

- Update model by including a new function evaluation then doing least squares fit to compute the new coefficients

RSM

Estimation problem: $\mathbf{J} \approx \mathbf{X}\,\mathbf{c}$

$$\mathbf{J} = \begin{bmatrix} J^1 & J^2 & \cdots & J^M \end{bmatrix}^{\mathrm{T}}$$

J=vector containing *M* responses

$$\mathbf{x} = \begin{bmatrix} 1 & x_1^1 & x_2^1 & \cdots & x_1^1 x_1^1 & \cdots \\ 1 & x_1^2 & & & & \\ \vdots & \vdots & & & & \\ & & & & & \\ 1 & x_1^M & x_2^M & & x_1^M x_1^M & \end{bmatrix}$$

$$\mathbf{c} = \begin{bmatrix} c_0 \\ c_1 \\ \\ c_{p-1} \end{bmatrix}$$

c=vector containing *p* coefficients

x=*M*×*p* matrix containing *M* design vector inputs as rows. Columns depend on approximation.

Least squares solution: $\mathbf{c} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{J}$

Kriging

- RSM tends to create a global model of the design space (especially if all points weighted equally in the LS)
- May be of limited accuracy when multiple extrema exist (especially quadratic polynomial models)
- Kriging : combine global model of design space with a model for local deviations which interpolates sample points
- Developed in fields of spatial statistics and geostatistics
- Original statistical techniques developed by mining engineer D.G. Krige
- Interpolation-based modeling technique
- Computationally more expensive and not as simple to implement as RSM

Kriging

Unknown function to be modeled expressed as:

$$J(\mathbf{x}) = f(\mathbf{x}) + Z(\mathbf{x})$$

- known function
- "global" model for design space
- *e.g.* use RSM to fit $f(\mathbf{x})$ using *M* observations

- Gaussian random function
- zero mean
- variance σ^2
- "localized" deviation from global model

$$\mathrm{cov}\left[Z(\mathbf{x}^i), Z(\mathbf{x}^j)\right] = \sigma^2 \mathbf{R}\left[R(\mathbf{x}^i, \mathbf{x}^j)\right]$$

covariance matrix of $Z(\mathbf{x})$ — correlation matrix — correlation function

Approximation Methods Overview

Design variable linking
Reduced-basis methods

- reduce the number of design variables in the optimization code
- simcode analysis full order

Response surface methods
Kriging

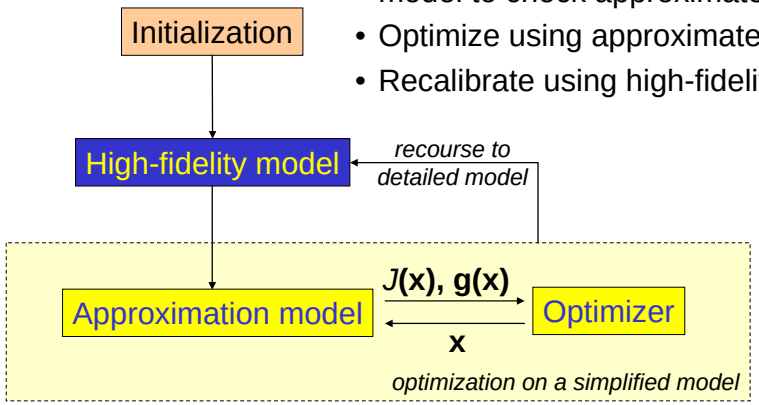
- same number of design variables
- simcode analysis simplified

Variable-fidelity methods

- combine high-fidelity and approximation models

Variable Fidelity Models

- Use information from high-fidelity model to check approximate designs
- Optimize using approximate model
- Recalibrate using high-fidelity model



From: Fig. 1, Alexandrov et al.

Variable Fidelity Models

Questions:

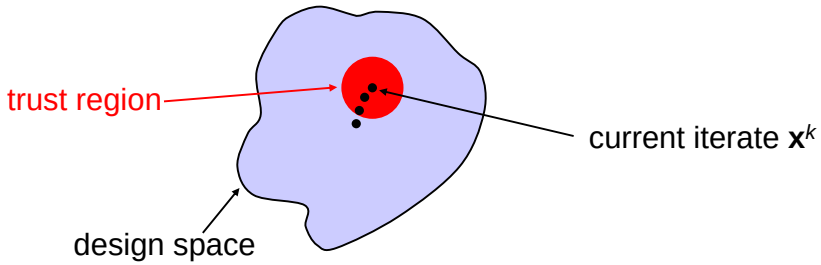
- What do we do when the design derived from the low-fidelity optimization does not provide an improvement in the true objective?
- How can we use information about the predictive capability of the approximation model to decide when to go back to the high-fidelity model?
- How do we decide when to update the approximate model?

Variable Fidelity Models

When optimization with approximation model is unsuccessful, there are two possible approaches:

1. Improve the fidelity of the approximate model
2. Do “less” optimization

One option: use a **trust region** approach



Trust Region Approach

Classic approach:

- Regulate the length of the steps taken by the iterative optimization algorithm
- Regulate based on quality of current approximation model

e.g. Quadratic Taylor series model:

$$J(\mathbf{x}^k + \mathbf{s}) \approx q^k(\mathbf{x}^k + \mathbf{s}) = J(\mathbf{x}^k) + \left[\nabla J(\mathbf{x}^k)\right]^T \mathbf{s} + \frac{1}{2}\mathbf{s}^T \mathbf{B}^k \mathbf{s}$$

where $\mathbf{s}$ is the prospective step in the design variables, $\Delta\mathbf{x}$, and $\mathbf{B}^k$ is a model of the Hessian matrix at $\mathbf{x}^k$.

Trust Region Approach

- Restrict the step size to a region in which we trust the quadratic model to approximate J well
- Done by adding a constraint on the step

$\Rightarrow$ trust region subproblem

$$\begin{aligned} &\min q^k(\mathbf{x}^k + \mathbf{s}) \\ &\text{s.t.} \quad \|\mathbf{s}\| \le \delta^k \end{aligned}$$

- In practice, variables are scaled to improve performance (step size can vary in different directions)
- Then decide whether to accept the step:

$$\mathbf{x}^{k+1} = \begin{cases} \mathbf{x}^k + \mathbf{s} & \text{if } J(\mathbf{x}^k + \mathbf{s}) < J(\mathbf{x}^k) \\ \mathbf{x}^k & \text{otherwise} \end{cases}$$

Trust Region Update

- Trust radius, δ^k, is updated adaptively
- Update depends on predictive quality of quadratic model:
  - ➢ if model did a good job of predicting J, or if there was more improvement than predicted, then increase δ^k
  - ➢ if model did a bad job of predicting J (J increased or decrease was much lower than predicted), then decrease δ^k
  - ➢ if model did an acceptable job of predicting J, then do not change δ^k

Trust Region Update

- Numerically, compare actual and predicted decrease:

$$r = \frac{J(\mathbf{x}^k) - J(\mathbf{x}^k + \mathbf{s})}{J(\mathbf{x}^k) - q(\mathbf{x}^k + \mathbf{s})}$$

- Define constants r_1, r_2 ($r_1 < r_2$) and apply the rules:
  - if $r < r_1$, decrease the trust radius
  - if $r > r_2$, increase the trust radius
- Typical values are $r_1 = 0.1$, $r_2 = 0.75$
- Note that prediction of ascent/descent is more important than prediction of actual value

Classic Trust Region Algorithm

Choose $\mathbf{x}^0 \in \mathbb{R}^n$ and $\delta^0 > 0$

For k=0,1,... until convergence do {

Find an approximate solution $\mathbf{s}_k$ to the subproblem:

$$\min q^k(\mathbf{x}^k + \mathbf{s})$$
$$\text{s.t.} \quad \|\mathbf{s}\| \le \delta^k$$

Compare the actual and predicted decrease:

$$r = \frac{J(\mathbf{x}^k) - J(\mathbf{x}^k + \mathbf{s})}{J(\mathbf{x}^k) - q(\mathbf{x}^k + \mathbf{s})}$$

Update $\mathbf{x}^k$ and δ^k

}

From Fig. 2, Alexandrov et al.

β-Correlation Method

- Basic idea is to take low-fidelity approximate model, J_a, and correct it by scaling
- Define the scale factor:

$$\beta = \frac{J(\mathbf{x})}{J_a(\mathbf{x})}$$

Given the current design $\mathbf{x}^k$, build a first order model of β about $\mathbf{x}^k$:

$$\beta^k(\mathbf{x}) = \beta(\mathbf{x}^k) + \nabla\beta(\mathbf{x}^k)(\mathbf{x} - \mathbf{x}^k)$$

Optimize with approximate model and use local model of β to scale result :

$$J(\mathbf{x}) \approx \beta^k J_a(\mathbf{x})$$

Variable Complexity Model

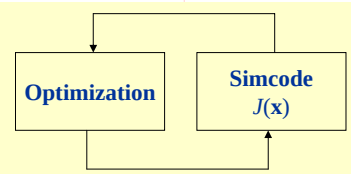
- iSight uses a Variable Complexity Model (VCM)
- Use two simcodes for the same physical process:
  (1) more accurate, longer running (exact) $J(\mathbf{x})$
  (2) less accurate, shorter running (approx.) $J_a(\mathbf{x})$
- Compute a multiplicative or additive correction factor, σ:

$$\sigma = \frac{J(\mathbf{x}^0)}{J_a(\mathbf{x}^0)}$$
$$J(\mathbf{x}) = \sigma J_a(\mathbf{x})$$

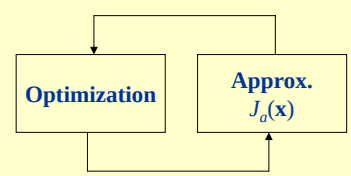
or

$$\sigma = J(\mathbf{x}^0) - J_a(\mathbf{x}^0)$$
$$J(\mathbf{x}) = \sigma + J_a(\mathbf{x})$$

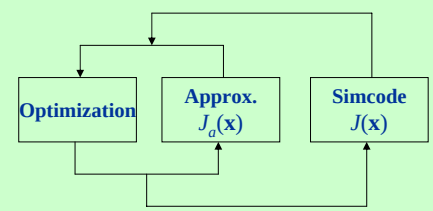
VCM



Conventional optimization with simcode



Conventional optimization with approximate model



Optimize with approximate model, update with simcode:

1. Run both models, calculate σ^0
2. Optimize using approximate model and σ^0
3. Update correction factor using simcode and repeat

Lecture Summary

- Approximation methods are one way to capture high-fidelity responses without the computational cost
- Design variable linking if physical problem allows
- Reduced-basis methods use low-order representation of the design vector
  - use previous designs, DoE or POD
- Response surface methodology
  - use polynomial models
  - weighted least squares
- Kriging
  - interpolation models
  - global + local behavior
- Variable-fidelity models
  - Trust region approach
  - β-correlation

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