



Approximation Concepts and Sensitivity Analysis



Overview

- Design space dimensionality reduction
 - active constraint sets
 - design variable linking
- Approximate analysis
 - basis reduction
 - simplified analysis
- Explicit approximations
 - Taylor series
 - response surfaces



Design Variable Linking

- Simple reduction in the number of variables by assumed relationships

$$A_1 = A_3 = X(1)$$

$$A_2 = A_4 = X(2)$$

$$A_5 = A_6 = X(3)$$

$$A_7 = A_8 = A_9 = A_{10} = X(4)$$

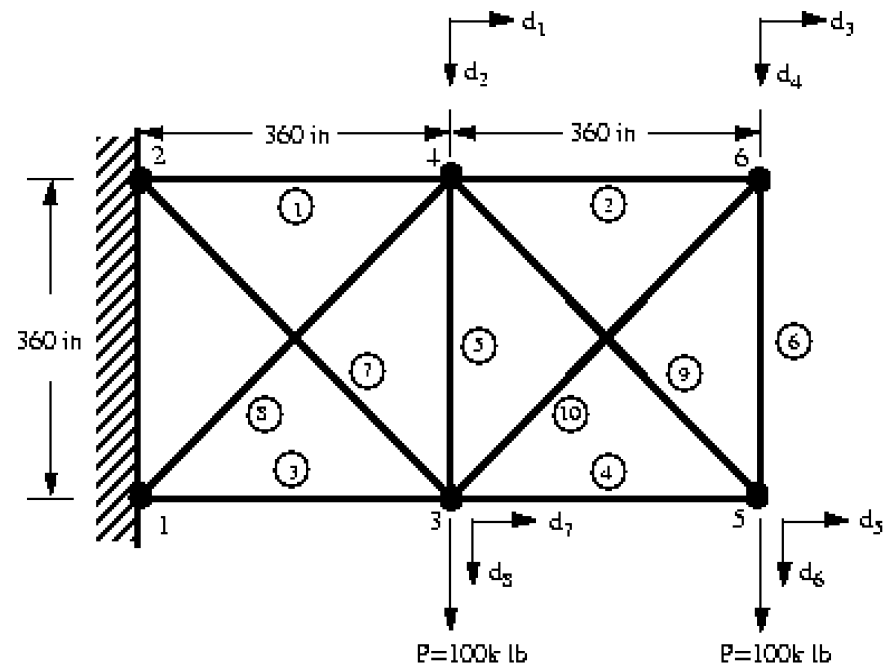
- Can also be functional relations of the type

$$A_1 = X(1) \quad A_3 = X(2)$$

$$A_2 = A_4 = 0.6X(1) + 0.4X(2)$$

$$A_5 = A_6 = X(3)$$

$$A_7 = A_8 = A_9 = A_{10} = 0.7X(3)$$





Constraint Reduction Methods

- Composite constraint representation - Kresselmeir-Stienhauser function

$$\Omega(X) = -\varepsilon + \frac{1}{\rho} \ln \sum_{j=1,m} \exp[\rho g_j(X)]$$

- function is an envelope function that represents the aggregate of the most critical constraints in the set
- choose $\rho \sim 25 - 30$ to make most critical constraint the dominant term in Ω

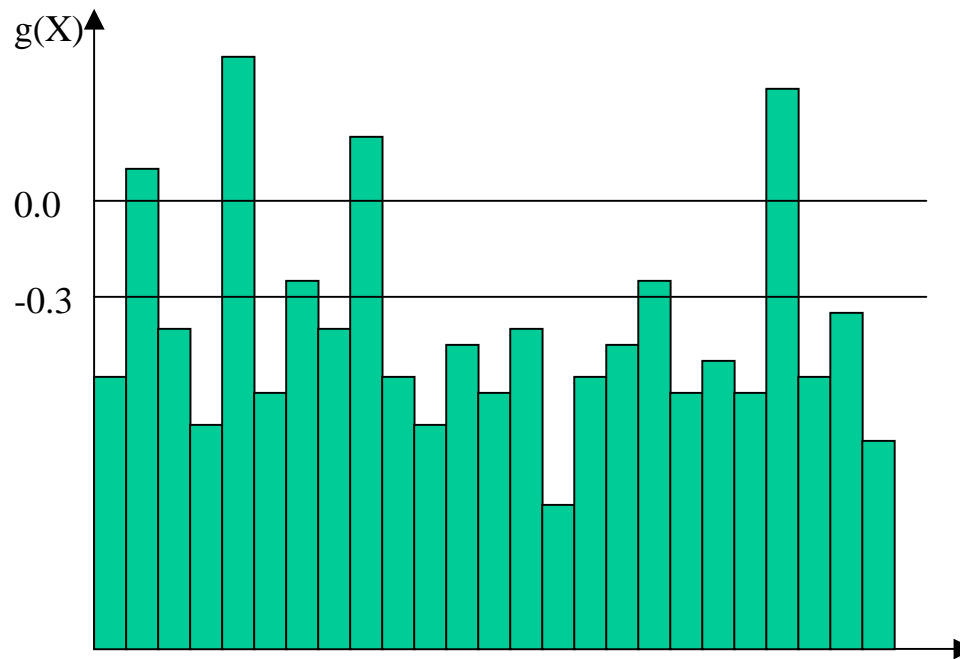


Constraint Deletion Strategy

- Many constraints are satisfied with a large margin - far from critical, and can be temporarily ignored from the optimization process
- Gradient calculations are significant source of computational expense
 - fewer constraints imply fewer gradient calculations
- Constraint deletion can be based on
 - deleting currently non-critical constraints
 - regionalization - applicable in structural design, for example



Constraint Deletion



- Retain all constraints with $g > -0.3$ only



Approximate Analysis

- Basis reduction method
 - let a vector Y define the actual design
 - for example, Y could consist of 25 cross-sectional areas of truss elements
 - develop a number of design alternatives $Y^i, i = 1, N$
- The vector Y to be used in analysis is then computed as

$$Y = \sum_{i=1}^N X_i Y^i$$

- where X_i are the independent design variables



Basis Reduction

- Reduction in the number of independent design variables
 - will help establish an upper bound on the optimal objective function value
- Improves the conditioning of the optimization problem
- Careful selection of basis vectors greatly helps in getting to the true optimum
 - use prior designs/experience base to select basis vectors



Simplified Analysis

- Basis approach
 - create a detailed analysis model
 - create a simplified analysis model
 - compare results for the initial design using the two models and modify simplified model so that results correlate with those of exact model
 - optimize using simplified model and perform a detailed analysis of the optimal design
 - if agreement is good, stop, else modify simplified model and repeat
- Approach can be very efficient in those problems where detailed model is very expensive



Response Surface Approximations

- Particularly useful when only function information is available to create the approximations
 - if we have a number of designs X_i distributed over the design domain, we can fit a polynomial (assumed order) to these data points
 - full second order polynomial will require $1+N+N(N+1)/2$ data points
 - works well for expensive analysis cases when number of variables is small
 - is also useful in those cases where function values are determined experimentally



Taylor Series Approximations

- As described earlier, one can create first or higher-order function approximations
 - first-order approximations are the basis of sequential linear programming
 - first-order approximation is preferred as second or higher order gradients are both expensive, and generally less accurate
- Assist in improving the quality of approximations by choosing variables appropriately
 - choose variables so that linear or quadratic models adequately model the response behavior



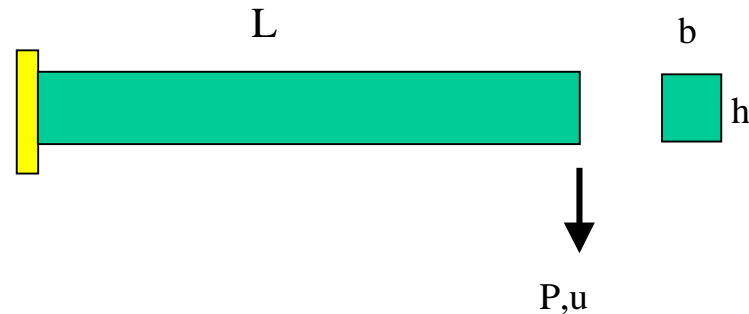
Use of Intermediate Variables

- If design variable is h , one can construct a linear approximation for u as follows (not exact)

$$\bar{u} = u_0 + \frac{\partial u}{\partial h}(h - h_0) = u_0 - \frac{12PL^3}{EBh^4}$$

- If design variable is chosen as the reciprocal moment of inertia, the approximation is exact

$$\bar{u} = u_0 + \frac{\partial u}{\partial I} \left(\frac{1}{I} - \frac{1}{I_0} \right) (-I_0^2) = \frac{PL^3}{3EI}$$



$$u_0 = \frac{PL^3}{3EI} = \frac{4PL^3}{Ebh^3}$$



Use of Intermediate Response

- Consider approximation for stresses in rod elements
 - stress $\sigma = F / A$ and if A is design variable, then stress is nonlinearly varying with A
 - intermediate variable choice would be to designate $1/A$ as the design variable
 - alternative, approximate the internal force F as a linear function of A

$$\bar{F} = F^0 + \nabla F^T \Delta A$$

- stresses are then computed explicitly from (nonlinear)

$$\bar{\sigma} = \frac{F^0 + \nabla F^T \Delta A}{A}$$



Conservative Approximations

- We would like to have approximate value of constraints to be more positive
 - such a conservative approximation ensures that the true constraint (when evaluated) is less likely to be violated
- This approximation is conservative with respect to a linear approximation (no guarantee with respect to actual constraint)

– linear

$$g_L = g(X^0) + \sum_{i=1}^N \left. \frac{\partial g}{\partial X_i} \right|_{X^0} (X_i - X_i^0)$$

– reciprocal

$$g_R = g(X^0) - \sum_{i=1}^N \left. \frac{\partial g}{\partial X_i} \right|_{X^0} \left(\frac{1}{X_i} - \frac{1}{X_i^0} \right) (X_i^0)^2$$



Conservative Approximations

- If the approximation to $g(X)$ is to be conservative

- use linear approximation if $(X_i^0) \frac{\partial g}{\partial X_i} \Big|_{X^0} \geq 0$

- use reciprocal approximation if $(X_i^0) \frac{\partial g}{\partial X_i} \Big|_{X^0} < 0$

- If X_i is close to zero or in the process of crossing zero, use linear approximation



Sensitivity Analysis - Overview

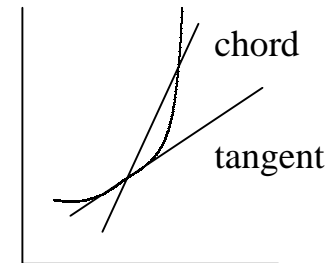
- Finite difference method
- Quasi-analytical method
- Analytical method
- Coupled system sensitivity
- Problem parameter sensitivity



Finite Difference Approach

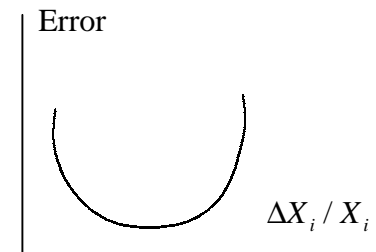
- Forward difference

$$\frac{df}{dX} = \frac{f(X + \Delta X) - f(X)}{\Delta X}$$



- Central difference

$$\frac{df}{dX} = \frac{f(X + \Delta X) - f(X - \Delta X)}{2\Delta X}$$



- Optimal step size must be chosen - optimal step size cannot simply be the smallest due to round-off errors



Quasi-Analytical Approach

- Apart from accuracy concerns, finite difference is very expensive if analysis is computationally cumbersome
 - for a N variable problem, each finite difference calculation requires N+1 function analyses
- Quasi-analytical method is based on carrying out an analytical differentiation, and alleviating computational costs and complexity by computing key derivatives by the finite difference approach
 - consider a set of equations as follows

$$F[X, u(X)] = 0$$



Quasi-Analytical Approach

- Analytically differentiating this equation with respect to the design variables X

$$\frac{\partial F}{\partial X} + \frac{\partial F}{\partial u} \frac{\partial u}{\partial X} = 0$$

- The terms $\frac{\partial F}{\partial X}$ and $\frac{\partial F}{\partial u}$ can be computed by finite difference
- As an example consider the finite element equation for static analysis $[K]\{u\}=\{P\}$



Quasi-Analytical Approach

- Analytical differentiation with respect to X yields

$$\frac{\partial K}{\partial X} u + K \frac{\partial u}{\partial X} = \frac{\partial P}{\partial X}$$

– or
$$\frac{\partial u}{\partial X} = (K)^{-1} \left(\frac{\partial P}{\partial X} - \frac{\partial K}{\partial X} u \right)$$

- Recall that true finite difference would require new $[K]$ matrix for each design perturbation, and factorization of this matrix to solve for corresponding displacement response



Analytical Sensitivity- Unit Load Method

Applications in Structural Design

- If we need to selectively compute the sensitivity of a displacement component with respect to design variables, we could use the unit-load method
- First define [H] as

$$[H] = \left[\left[\frac{\partial P}{\partial X_1} \right], \dots, \left[\frac{\partial P}{\partial X_N} \right] \right] - \left[\left[\frac{\partial K}{\partial X_1} \right] \{u\}, \dots, \left[\frac{\partial K}{\partial X_N} \right] \{u\} \right]$$

- Also, a desired displacement u_j is expressed as $u_j = \{Q_j\}^T \{u\}$ where $\{Q_j\}$ is a virtual load vector with unity at j-th location and zero elsewhere



Analytical Sensitivity- Unit Load Method Applications in Structural Design

- The differentiation of u_j with respect to X gives

$$\left\{ \frac{\partial u_j}{\partial X} \right\}^T = \{Q_j\}^T \left[\frac{\partial u}{\partial X} \right]$$

- And since the virtual displacement corresponding to the virtual load is obtained as $[K]\{u_j^Q\} = \{Q_j\}$ the above equation becomes

$$\left\{ \frac{\partial u_j}{\partial X} \right\}^T = \{u_j^Q\}^T [K] \left[\frac{\partial u}{\partial X} \right] = \{u_j^Q\}^T [H]$$



Coupled System Sensitivity

- What happens when finite difference approach is applied to a coupled complex system?
 - perturb one variable at a time, iterate the coupled analyses to convergence - everyone must act in concert (also very expensive)
 - small perturbations required to ensure accuracy may generate nothing more than numerical noise in a coupled system analysis - perturb isolated stringer and hope to see meaningful change in aircraft range???
 - large differences are employed but at the risk of severe loss in accuracy



Coupled System Sensitivity - GSE1

- Consider a multidisciplinary system with two subsystems A and B

- system equations can be written in symbolic form as

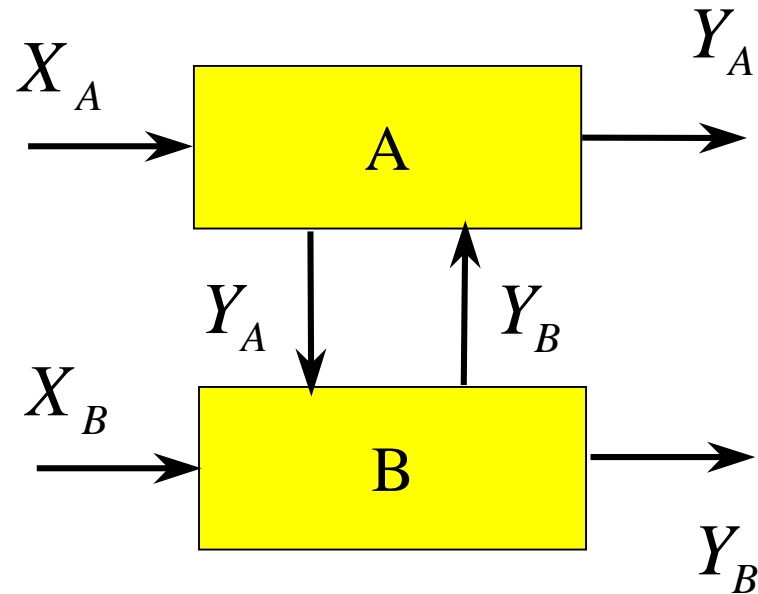
$$A[(X_A, Y_B), Y_A] = 0$$

$$B[(X_B, Y_A), Y_B] = 0$$

- rewrite these as follows

$$Y_A = Y_A(X_A, Y_B)$$

$$Y_B = Y_B(X_B, Y_A)$$





Coupled System Sensitivity - GSE1

- First-order Taylor series representation

$$\frac{dY_A}{dX_A} = \frac{\partial Y_A}{\partial X_A} + \frac{\partial Y_A}{\partial Y_B} \frac{dY_B}{dX_A}$$
$$\frac{dY_B}{dX_B} = \frac{\partial Y_B}{\partial X_B} + \frac{\partial Y_B}{\partial Y_A} \frac{dY_A}{dX_B}$$

- And using a chain rule of derivatives

$$\frac{dY_A}{dX_B} = \frac{\partial Y_A}{\partial Y_B} \frac{\partial Y_B}{\partial X_A}$$
$$\frac{dY_B}{dX_A} = \frac{\partial Y_B}{\partial Y_A} \frac{\partial Y_A}{\partial X_A}$$



Coupled System Sensitivity - GSE1

- These equations can be represented in matrix notation as

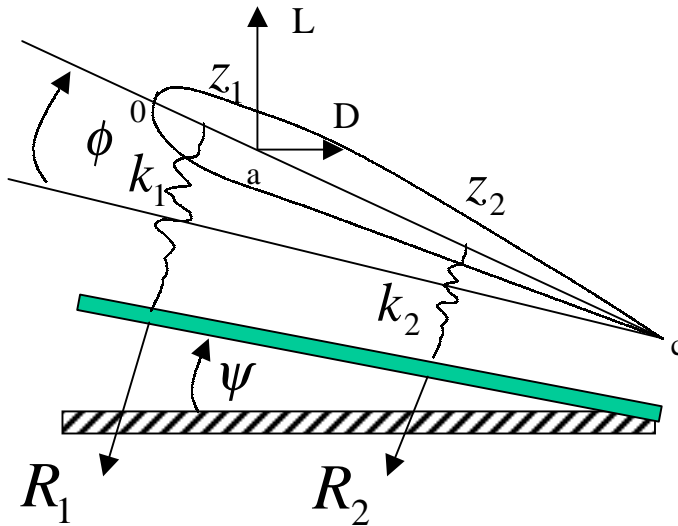
$$\begin{bmatrix} I & -\frac{\partial Y_A}{\partial Y_B} \\ -\frac{\partial Y_B}{\partial Y_A} & I \end{bmatrix} \begin{bmatrix} \frac{dY_A}{dX_A} \\ \frac{dY_B}{dX_A} \end{bmatrix} = \begin{bmatrix} \frac{\partial Y_A}{\partial X_A} \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} I & -\frac{\partial Y_A}{\partial Y_B} \\ -\frac{\partial Y_B}{\partial Y_A} & I \end{bmatrix} \begin{bmatrix} \frac{dY_A}{dX_B} \\ \frac{dY_B}{dX_B} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{\partial Y_B}{\partial X_B} \end{bmatrix}$$

- Total derivatives can be computed if partial sensitivities computed in each subsystem are known - the latter can be computed locally within the subsystems



Example - Wing on Elastic Support



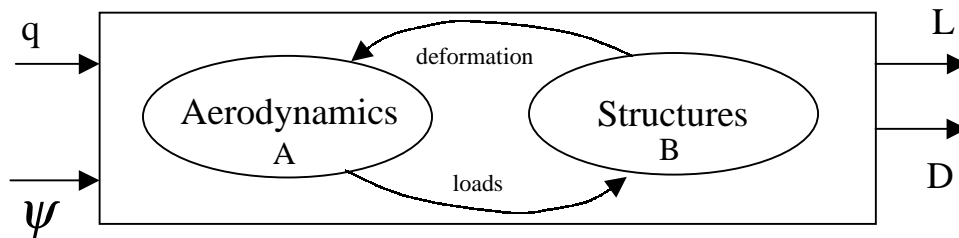
b – span

c – chord

$$\bar{z}_1 = z_1 / c; \bar{z}_2 = z_2 / c; \bar{a} = a / c$$

$$\bar{h}_1 = \bar{a} - \bar{z}_1; \bar{h}_2 = -\bar{a} + \bar{z}_2$$

$$p = \bar{h}_1 / \bar{h}_2 \quad S = b \cdot c$$



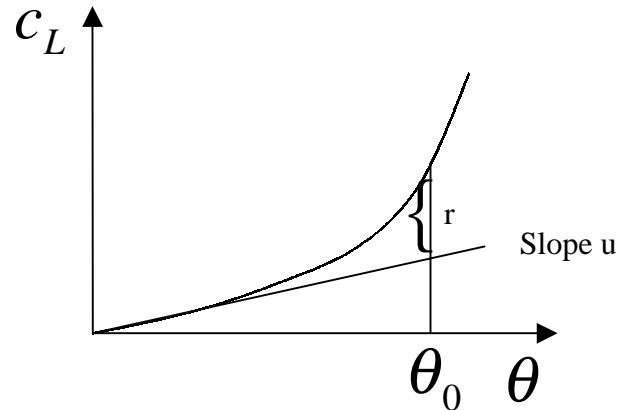
$$B = 100cm, c = 10cm, \bar{z}_1 = 0.2,$$

$$\bar{z}_2 = 0.7, \bar{a} = 0.25, q = 1N / cm^2$$

$$k_1 = 4000N / cm, k_2 = 2000N / cm$$



Example - Wing on Elastic Support



$$u = 5 / \text{rad}; r = 2$$

$$\theta_0 = 0.26 \text{ rad}; \psi = 0.05 \text{ rad}$$

$$c_L = u\theta + r(1 - \cos((\pi / 2)(\theta / \theta_0)))$$

$$q = \frac{1}{2} \rho V^2 \quad d_i = R_i / k_i \quad \phi = \frac{d_1 - d_2}{z_2 - z_1}$$

$$\theta = \psi + \phi$$

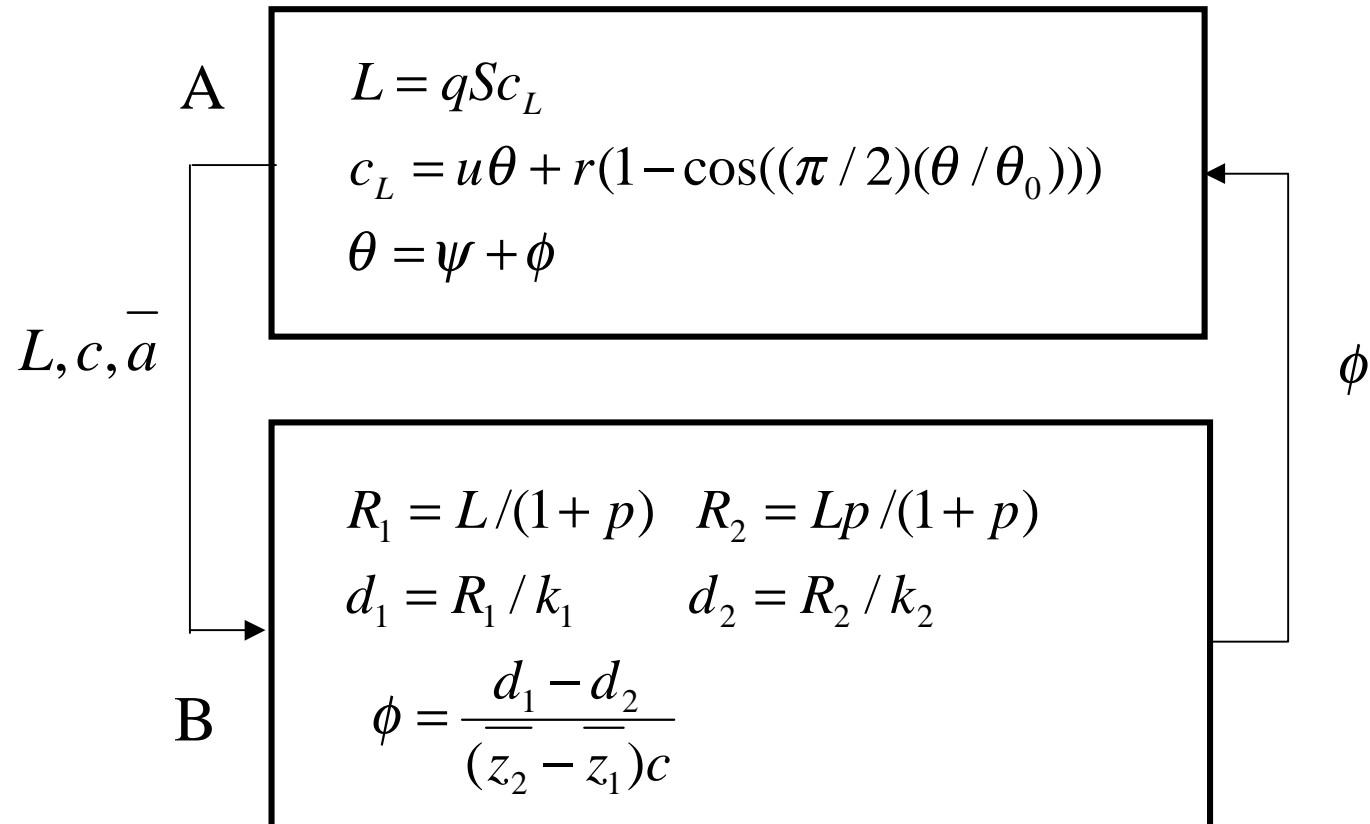
$$X = \{S, u, r, \theta_0, c, \bar{a}, \bar{\psi}, \bar{z}_1, \bar{z}_2, k_1, k_2\}$$

$$Y_A = \{L, c, \bar{a}\}$$

$$Y_B = \{\phi\}$$



Wing on Elastic Support - Simplified





Wing on Elastic Support - Results

- Solution point is for $L=502.3$, $\phi = 0.0176$, $\psi = 0.05$ and we are interested in $dL/d\psi$ and $d\phi/d\psi$
- By finite differences (step size 0.0025) these are 14925.16 N/rad and 0.5221287 rad/rad
- The GSE equation becomes

$$\begin{bmatrix} I & -\frac{\partial L}{\partial \phi} \\ -\frac{\partial \phi}{\partial L} & I \end{bmatrix} \begin{Bmatrix} \frac{dL}{d\psi} \\ \frac{d\phi}{d\psi} \end{Bmatrix} = \begin{Bmatrix} \frac{\partial L}{\partial \psi} \\ 0 \end{Bmatrix}$$



Wing on Elastic Support - Results

- From aerodynamics (locally)

$$\frac{\partial L}{\partial \psi} = 9805.105 = \frac{\partial L}{\partial \phi}$$

- From structures (locally)

$$\frac{\partial \phi}{\partial L} = 0.000035 \text{ rad} / N$$

- Substituting in GGE equations and solving

$$\frac{dL}{d\psi} = 14928.12 \frac{N}{\text{rad}}, \quad \frac{d\phi}{d\psi} = 0.5224841 \frac{\text{rad}}{\text{rad}}$$



Automatic Differentiation

- Contains a generic differentiation program
 - takes analysis code in C or in Fortran
 - takes user defined input on dependent and independent variables
 - introduces statements that generate sensitivity information
 - uses the chain rule to achieve this objective
 - modified program is the original + new statements that compute the required sensitivity
 - new statements are embedded calls to specific subroutines



Automatic Differentiation

- Program source increases in size
- Differentiation rules are similar to those in MACSYMA
 - while MACSYMA would have produced long symbolic expressions, this approach computes and saves only the numerical value of the differentiated expression
- Process is subject to only truncation errors - otherwise numerically exact
- Some extra storage is required to store derivative values - kept only as long as needed
- Process is neither finite differencing, symbolic, or quasi-analytical



Automatic Differentiation Example

Solve $y = x \cos(uxy)$

y – dependent

x, u – independent

Given u & x

```
Y = YIN
DO 100 I = 1, N1
  YNXT = X * COS(U * X * Y)
  IF((YNXT - Y)/YNXT.LE.TOL)GOTO 101
  Y = YNXT
100 CONTINUE
101 CONTINUE
  Y = YNXT
  PRINT, Y
END
```

Solve $y = x \cos(uxy)$

y – dependent

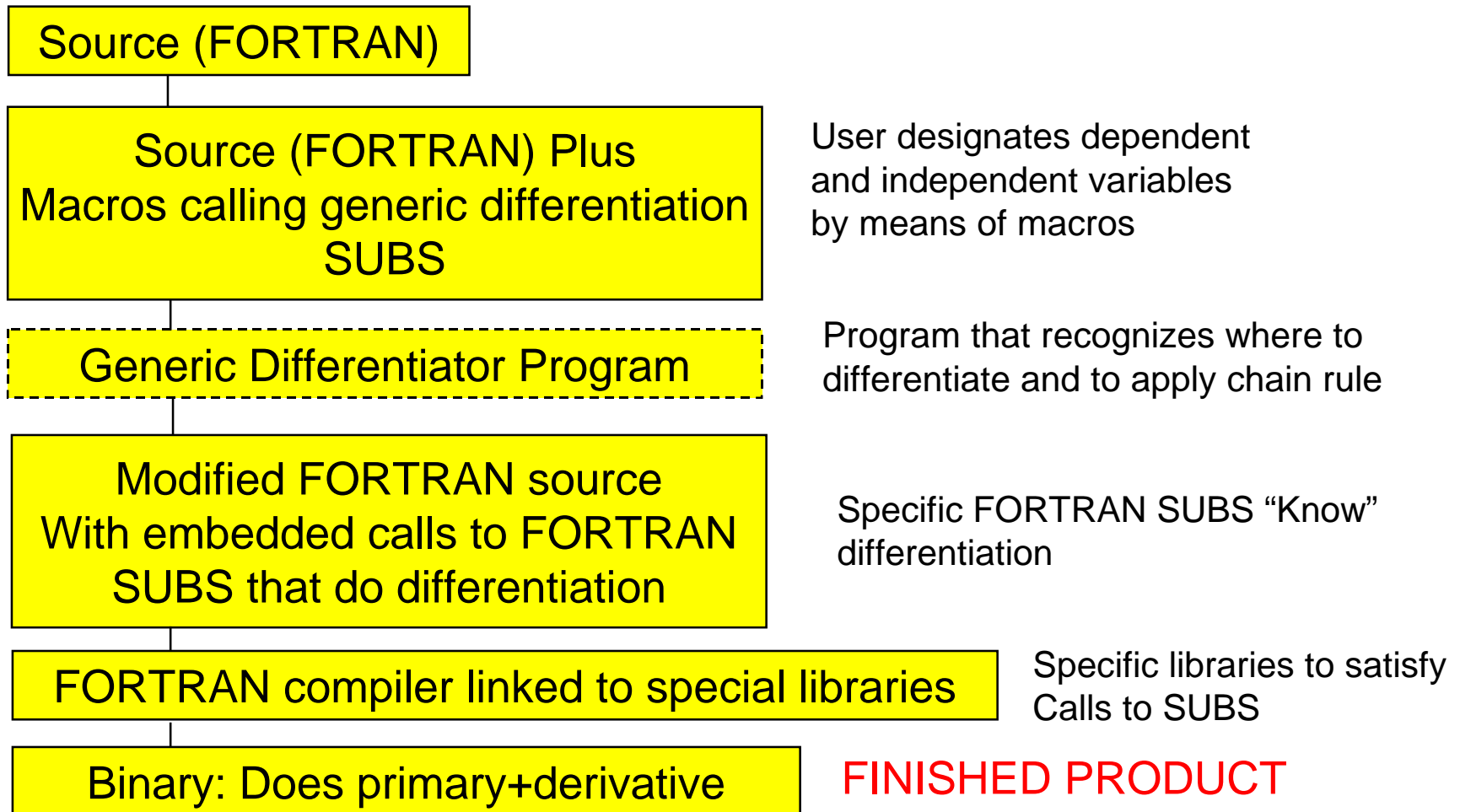
x, u – independent

Given u & x

```
Y = YIN          DY = DYIN
DO 100 I = 1, N1
  YNXT = X * COS(U * X * Y)
  DYNXT=COS(U*X*Y) - X*U*Y*SIN(U*X*Y)
             + (-X * U * X * SIN(U * X * Y) * DY
IF((YNXT - Y)/YNXT.LE.TOL)GOTO 101
  Y = YNXT          DY = DYNXT
100 CONTINUE
101 CONTINUE
  Y = YNXT          DY = DYNXT
  PRINT, Y
END
```



Automatic Differentiation Sequence of Operations





Sensitivity Based on Complex Variables

- Designating X as a vector of complex numbers $X_i = X_i^r + ih$

- Carry out a Taylor series expansion with a complex step size

$$f(x+i\Delta x) = f(x) + i(\Delta x)f'(x) - (\Delta x)^2 f''(x)/2! - i(\Delta x)^3 f'''(x)/3! + \dots$$

- Using the imaginary part of the function yields

$$f'(x) \sim \text{Im}[f(x+i\Delta x)] / \Delta x$$

- Has truncation errors of $O(\Delta x^2)$



Sensitivity Based on Complex Variables

- Given an analysis code with inputs x_1 , x_2 , x_3 and output y
- Simply declare x and y to be both complex numbers
- For step length Δx initialize $\text{Re}x_1 + \Delta x$, $\text{Re}x_2+i0$, and $\text{Re}x_3+i0$, and compute the complex output y
- Compute derivative $dy/dx_1 = \text{Im}(y) / \Delta x$
- Reset with step size on variable x_2 , and repeat.

- Note that this approach can be used with selected x_i components only.



Sensitivity Based on Complex Variables

- Advantages
 - No need to code anything except $dy/dx = \text{Im}(y) / \Delta x$
 - Insensitive to h
- Disadvantage
 - Cost about the same as in ordinary finite differencing with added overhead for handling complex numbers



Sensitivity Based on Complex Variables

- Carry out a Taylor series expansion with a complex step size

$$f(x+i\Delta x) = f(x) + i(\Delta x)f'(x) - (\Delta x)^2 f''(x)/2! - i(\Delta x)^3 f'''(x)/3! + \dots$$

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- Note that this approach can be used with selected x_i components only.



Sensitivity of Optimum WRT Preassigned Problem Parameters

- Useful in obtaining estimates of new optimal design due to a perturbation in one or more problem parameters
- This sensitivity is of practical value in hierarchical decomposition strategies

$$\text{Minimize } f(X, p)$$

$$\text{Subject to } g_j(X, p) \leq 0 \quad j = 1, m$$

- Optimal solution $f^*(X^*, p)$ and $X^*(p)$, $g_k(X^*, p) = 0$ are active constraints at the optimum
- Sensitivities df^*/dp and dX^*/dp can be obtained by differentiation of the Kuhn-Tucker conditions of optimality
 - requires active constraints remain active after perturbation
 - requires second-order sensitivity information



Sensitivity of Optimum WRT Preassigned Problem Parameters

- Assume that an optimal solution X^* has been obtained - the K-T conditions for optimality

$$\nabla f(X^*) + \sum_{j \in J} \lambda_j \nabla g_j(X^*) = 0$$

$$g_j(X^*) = 0, \lambda_j > 0, j \in J$$

- For some small change in problem parameter, we require that K-T conditions remain valid - differentiating these conditions wrt p one obtains

$$\begin{bmatrix} A_{n \times n} & B_{n \times J} \\ B^T_{J \times n} & O_{J \times J} \end{bmatrix} \begin{Bmatrix} \delta X \\ \delta \lambda \end{Bmatrix} + \begin{Bmatrix} c_{n \times 1} \\ d_{J \times 1} \end{Bmatrix} = 0$$



Sensitivity of Optimum WRT Preassigned Problem Parameters

- Where the submatrices and sub-vectors are defined as follows

$$A_{ik} = \frac{\partial^2 f}{\partial X_i \partial X_k} + \sum_{j \in J} \lambda_j \frac{\partial^2 g_j}{\partial X_i \partial X_k} \quad B_{ij} = \frac{\partial g_j}{\partial X_i}, j \in J$$

$$c_i = \frac{\partial^2 f}{\partial X_i \partial p} + \sum_{j \in J} \lambda_j \frac{\partial^2 g_j}{\partial X_i \partial p} \quad d_j = \frac{\partial g_j}{\partial p}, j \in J$$

$$\delta X = \left\{ \begin{array}{c} \frac{\partial X_1}{\partial p} \\ \frac{\partial p}{\partial p} \\ \bullet \\ \bullet \\ \frac{\partial X_n}{\partial p} \\ \frac{\partial p}{\partial p} \end{array} \right\} \quad \delta \lambda = \left\{ \begin{array}{c} \frac{\partial \lambda_1}{\partial p} \\ \frac{\partial p}{\partial p} \\ \bullet \\ \bullet \\ \frac{\partial \lambda_n}{\partial p} \\ \frac{\partial p}{\partial p} \end{array} \right\}$$