Basics of Optimization

Spring Progress in Mathematican and Computational Studies on Science and Engineering Problems
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NASA Glenn Research Center, Lewis Field
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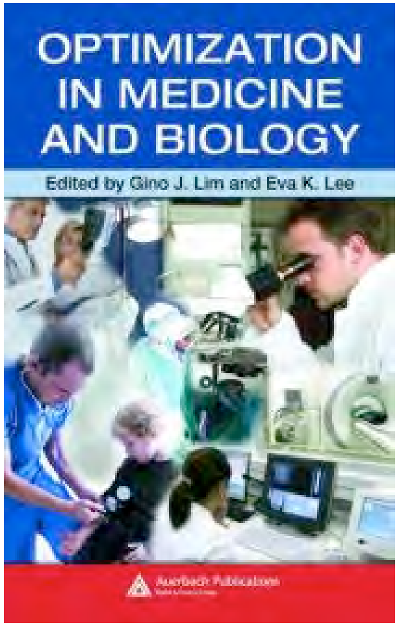
1941: Aircraft Engine Research Laboratory of the National Advisory Committee for Aeronautics (NACA)
1958: NASA Lew
begins making m
manned space fl
1999: Glenn Cen
Glenn, the first A

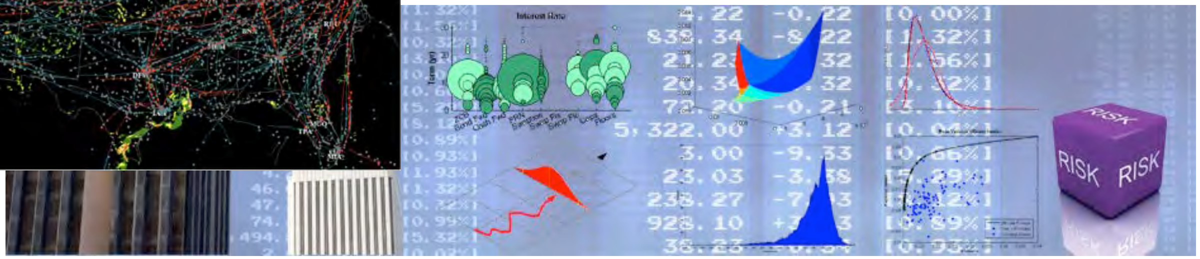
Contents

- Introduction—why do optimization
- What is optimization
- Steps in an optimization task
  - Formulation
  - Solution algorithms
- Aerospace design
- Multidisciplinary analysis and design optimization

Applications of Optimization

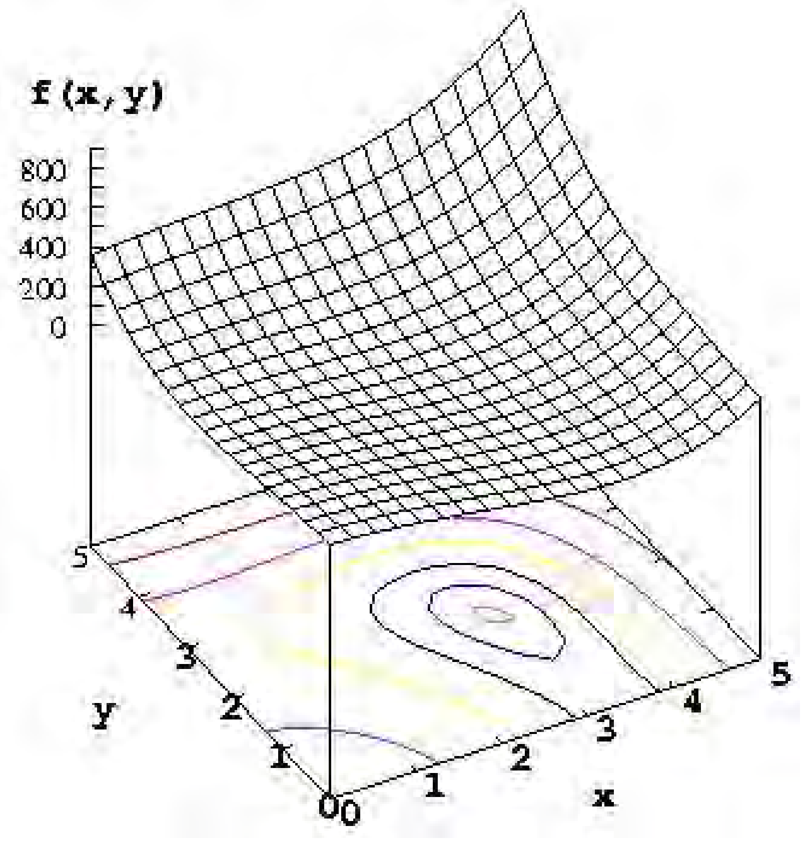
Engineering, medicine, finance, air traffic routing, war, politics, …





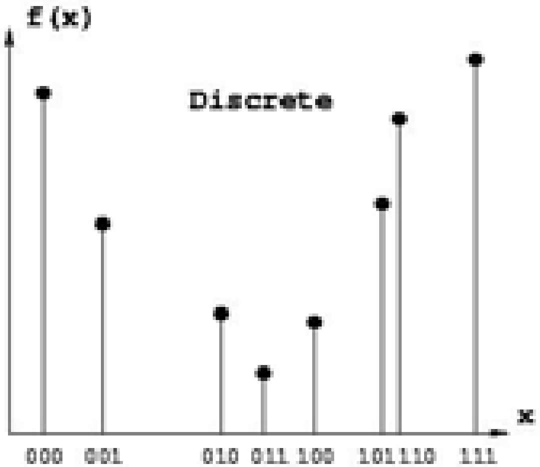
What is Optimization

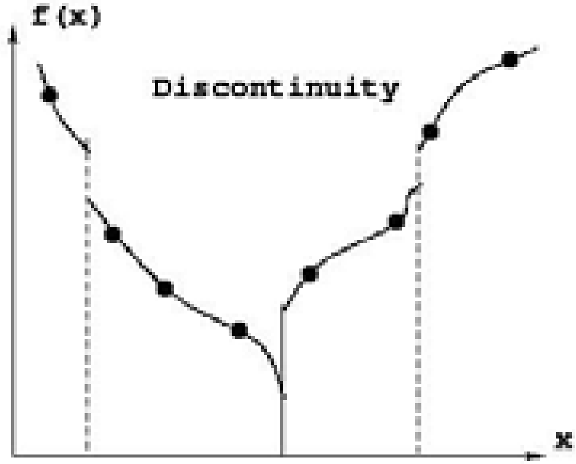
- ✧ A process of searching for a set of decision variables
  - ✓ That would minimize or maximize one or more objective functions,
  - ✓ subject to satisfying constraint

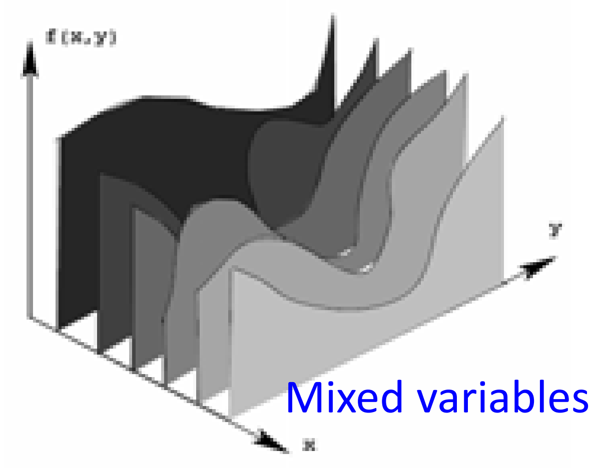


- ✧ Decision variables: (x,y)
- ✧ Objective function: f(x,y)
- ✧ Constraint functions:
  - ✓ Equality and inequality types

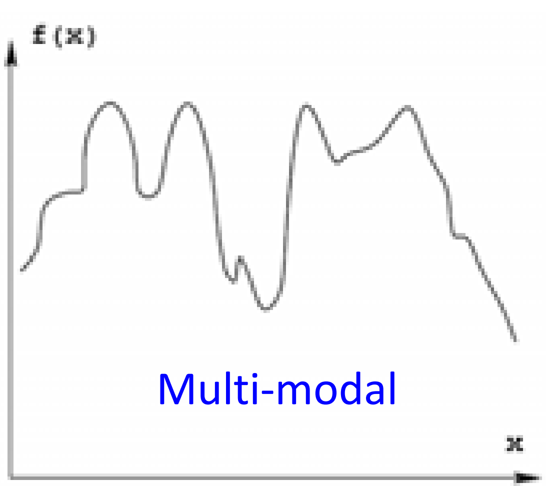
Properties of Optimization Problem



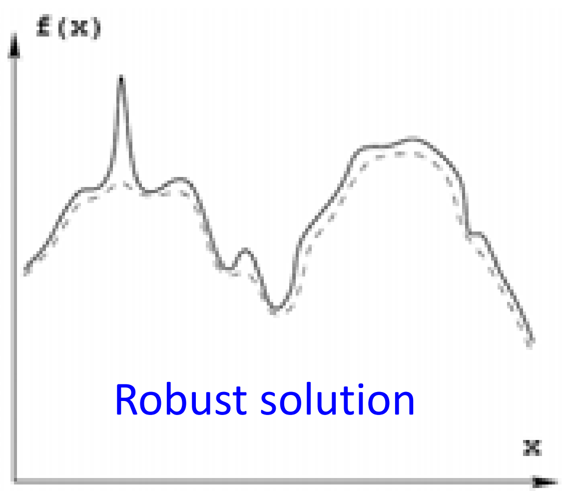




Mixed variables

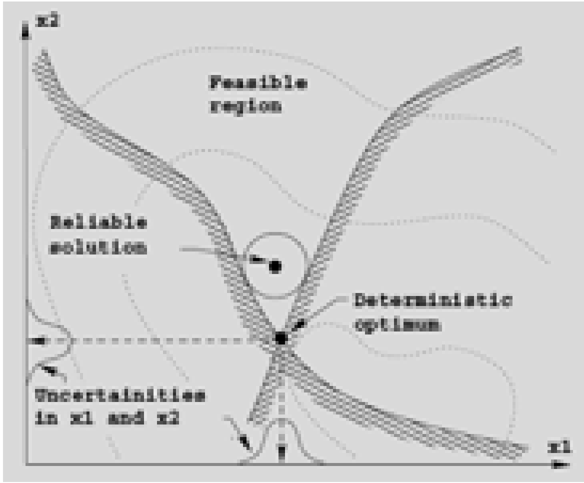


Multi-modal



Robust solution

Reliable solution



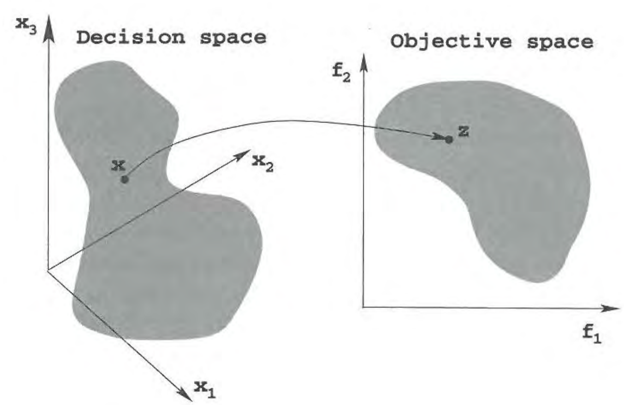
Steps in an Optimization Task

- ✧ Determine if need for optimization exists
- ✧ Formulate the Problem
  - ✓ Single objective problem
  - ✓ Multi-objective problem
- ✧ Choose an optimization algorithm
  - ✓ Criteria
- ✧ Obtain solution(s)
  - ✓ Local and global optimum
  - ✓ Constrained and unconstrained optimum
- ✧ Examine the result, reformulate and rerun if needed

Formulation of Optimization Problems

- Design variables
  - List any and every parameter related to the problem
  - Specify the type of each parameter (binary, discrete, continuous)
  - Choose a few of them as design variables
  - Use as few variables as possible, based on
    - Knowledge on the problem, experience of the user
    - Sensitivity analysis

- Constraints
  - Inequality and equality types
  - Avoid equality constraints,
    e.g. $g(x)=3$ ➔ $2 < g(x) < 3.5$
  - May be nonlinear

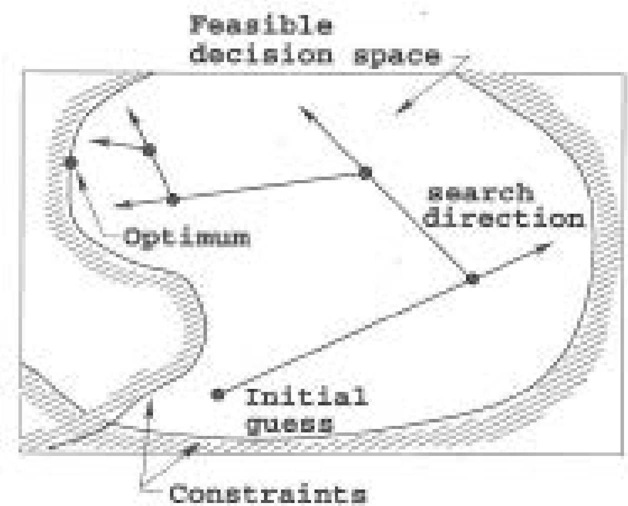


- Objective functions
  - Min or Max (convertible between them, duality)
  - Single or multiple objectives

A Typical Optimization Problem

- Decision (design) variables: $x = (x_1, x_2, \ldots, x_n)$
- Constraints for feasible solutions

$$
\begin{aligned}
&\text{Min.} \quad f(x) \\
&\text{s.t.} \quad g_j(x) \geq 0, \qquad j = 1,2,\ldots,J \\
&\qquad\quad h_k(x) = 0, \qquad k = 1,2,\ldots,K \\
&\qquad\quad x_i^L \leq x_i \leq x_i^U, \qquad i = 1,2,\ldots,n
\end{aligned}
$$



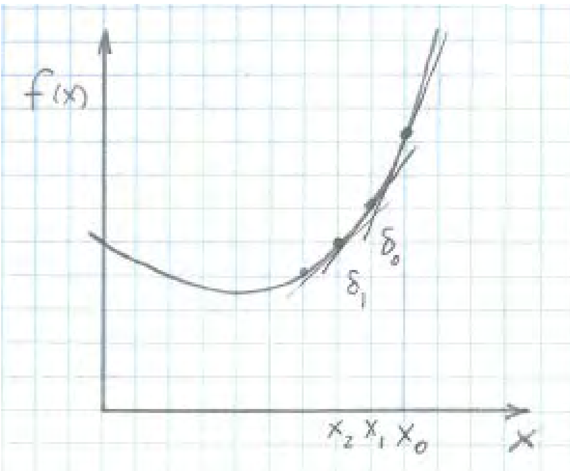
- Solutions are said to be optimal
  – Local and global optimum

Optimization Approaches

- ✧ Deterministic
  - ✓ Based on explicit gradient information
  - ✓ Converges to local optimum
  - ✓ Computationally efficient (relatively)

- ✧ Stochastic
  - ✓ Mostly, biomimetic and driven by an inherent “search” direction
  - ✓ Genetic Algorithms (GAs)
    - Based (loosely) on principles of natural evolution and survival of the fittest
  - ✓ Capable of finding global optimum
  - ✓ Suitable for problems with multiple objective functions

Gradient (Descent) Method



$$\min \quad f(x) = a(x-b)^2 + b$$

$$x_1 = x_0 - \frac{df}{dx}(x_0)\,\delta_0$$

$$x_2 = x_1 - \frac{df}{dx}(x_1)\,\delta_1$$

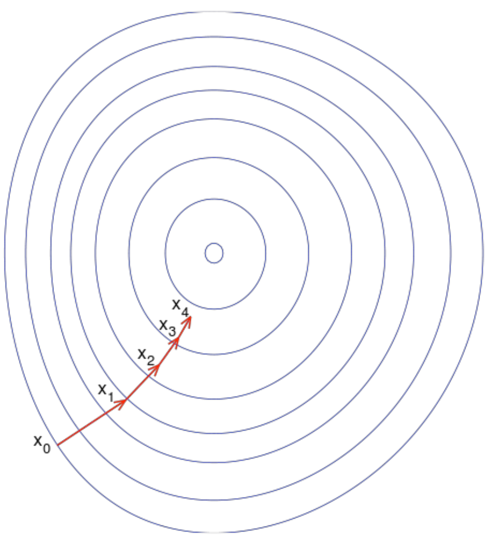
$\vdots$

Multi-Dimension space

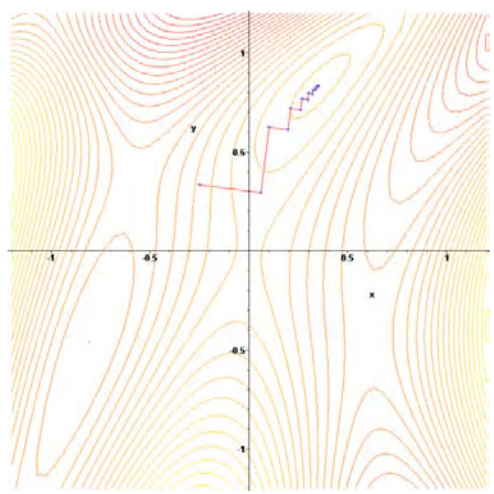
$$\min \quad f(\vec{x})$$

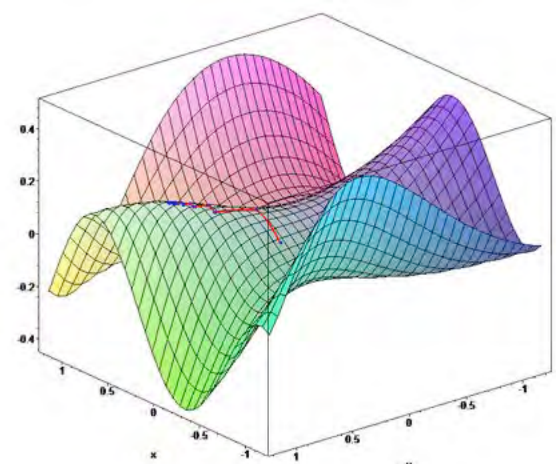
$$\vec{x}_{i+1} = \vec{x}_i - \gamma \nabla f(\vec{x}_i), \quad \gamma > 0$$

$$\text{s. t.} \quad f(\vec{x}_{i+1}) < f(\vec{x}_i)$$



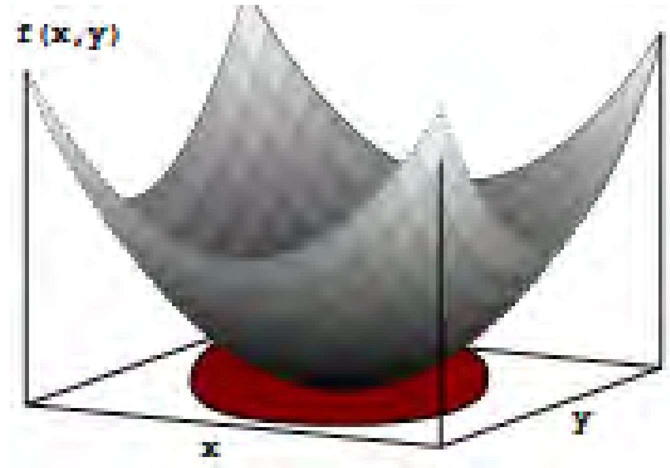
$$F(x, y) = \sin\left(\frac{1}{2}x^2 - \frac{1}{4}y^2 + 3\right)\cos(2x + 1 - e^y)$$





Constrained Optimization

- Karush-Kuhn-Tucker (KKT) conditions for optimality
  - First-order necessary conditions
  - Convex search space, convex *f*:
  - KKT point is minimum



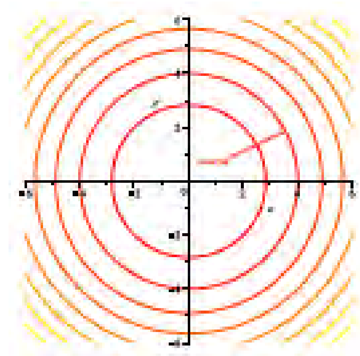
$$\nabla f(x) - \sum_{j=1}^{J} u_j \nabla g_j(x) - \sum_{k=1}^{K} v_k \nabla h_k(x) = 0$$

$$g_j(x) \geq 0, \quad j = 1, 2, \ldots, J$$

$$h_k(x) = 0, \quad k = 1, 2, \ldots, K$$

$$u_j g_j(x) = 0, \quad j = 1, 2, \ldots, J$$

$$u_j(x) \geq 0, \quad j = 1, 2, \ldots, J$$



Himmelblau Problem

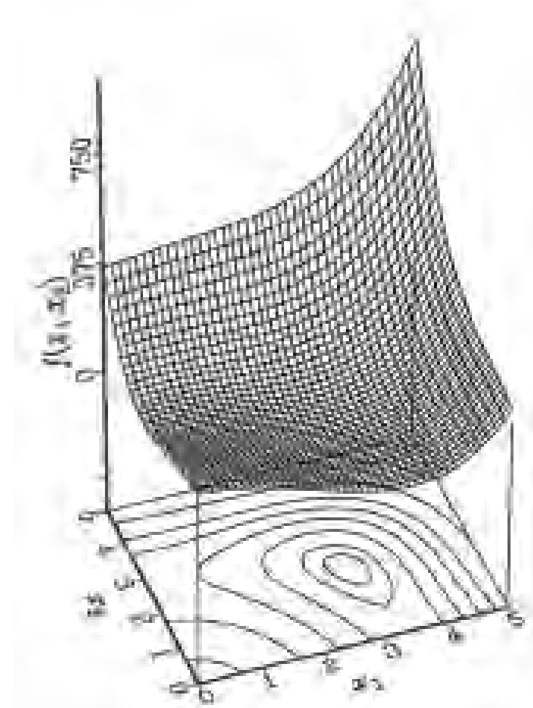
$$f(x) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2$$

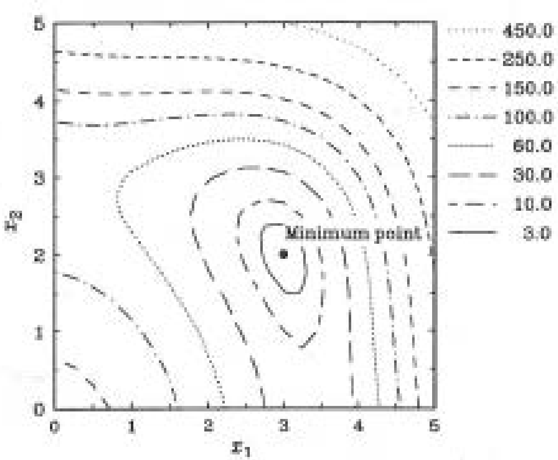
subject to

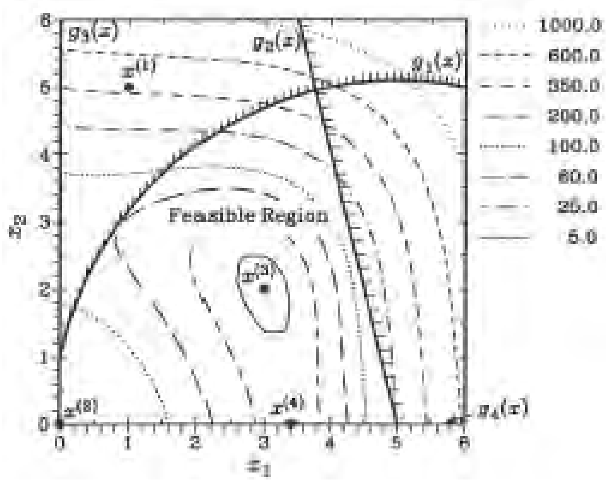
$$g_1(x) = 26 - (x_1 - 5)^2 - x_2^2 \geq 0,$$

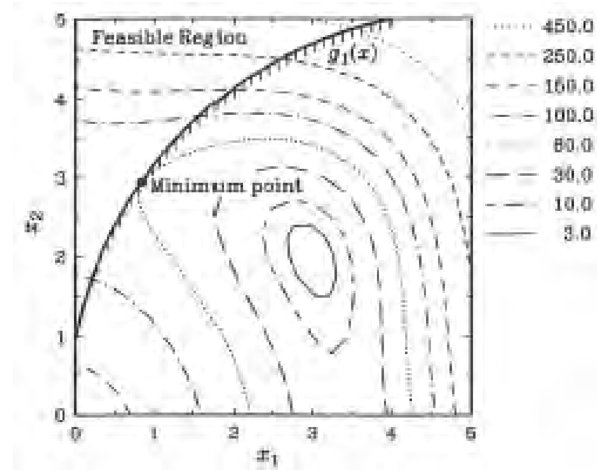
$$g_2(x) = 20 - 4x_1 - x_2 \geq 0,$$

$$x_1, x_2 \geq 0.$$









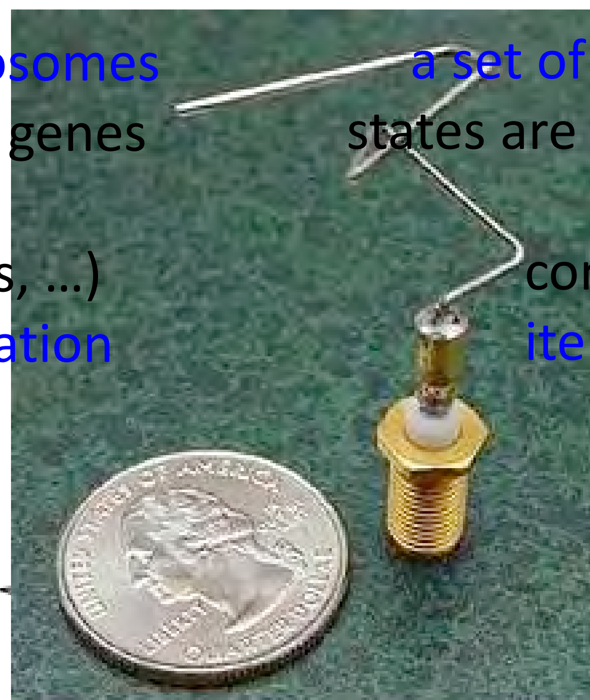
Genetic Algorithms

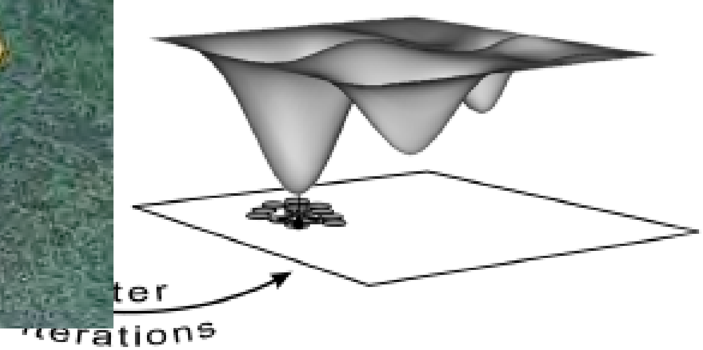
Holland (1975) "Adaptation in Natural and Artificial Systems"

- The fittest survive (Charles Darwin)
- Based on evolution of a population
- "Computer programs that evolve in ways that resemble natural selection can solve complex problems even their creators do not fully understand."

For generation *n*,

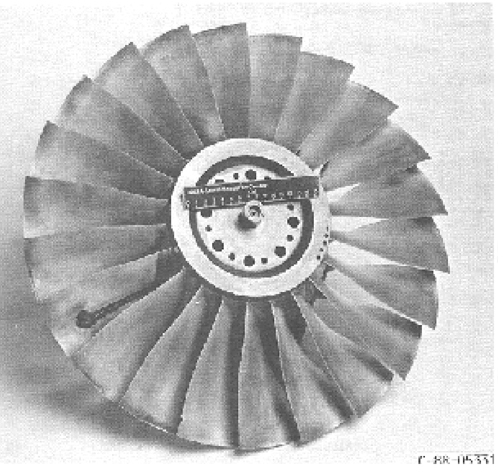
a population of chromosomes	a set of states (solutions/designs)
chromosomes consists of genes	states are functions of design variables
fitness	objective function
constraints (environments, …)	constraints (physical, …)
evolution of whole population	iteration of whole set



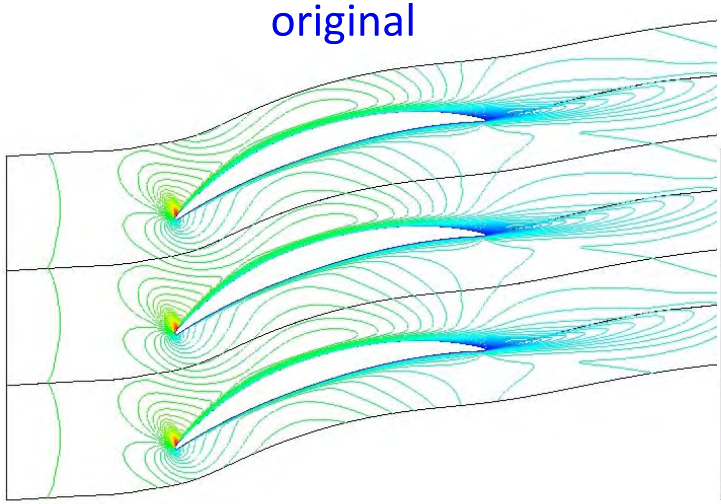


- ✧ Selection/pairing
- ✧ Crossover
- ✧ Mutation

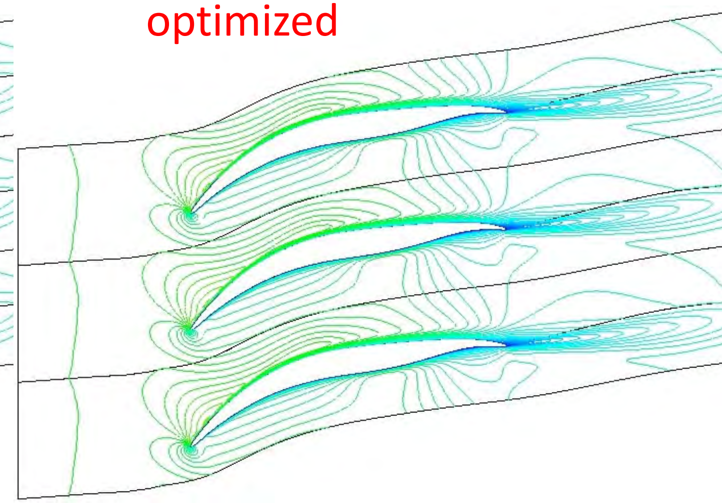
NASA Rotor 67

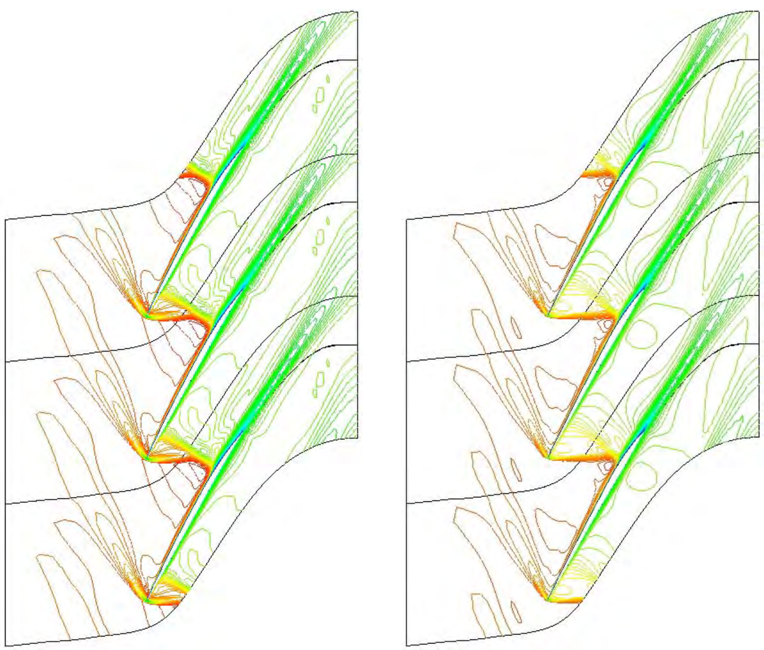


original



optimized





Oyama, A., Liou, M.-S. and S. Obayashi, *J. Propulsion & Power,* Vol. 20, 612-619, 2004.

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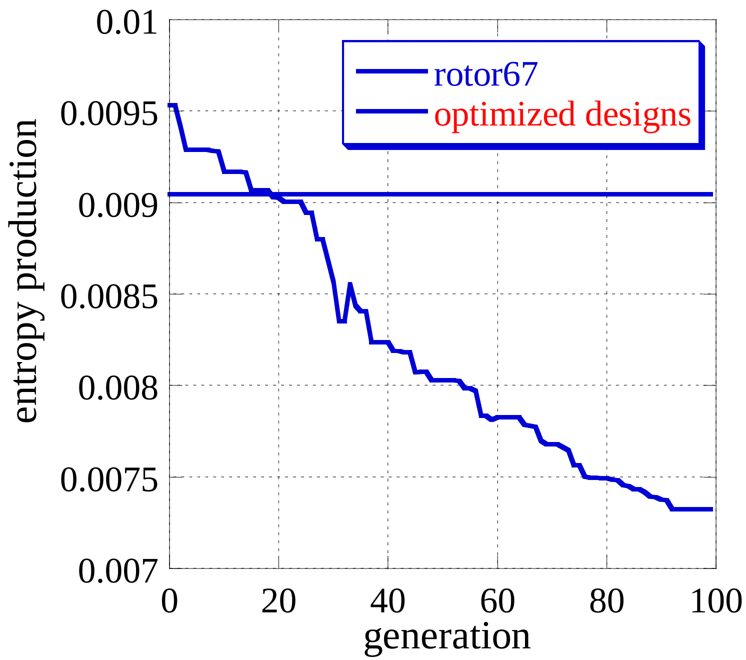
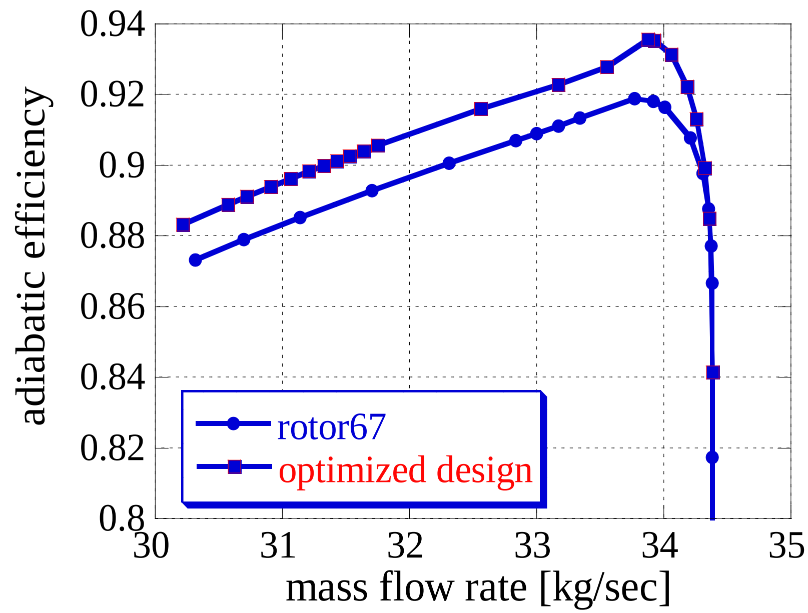
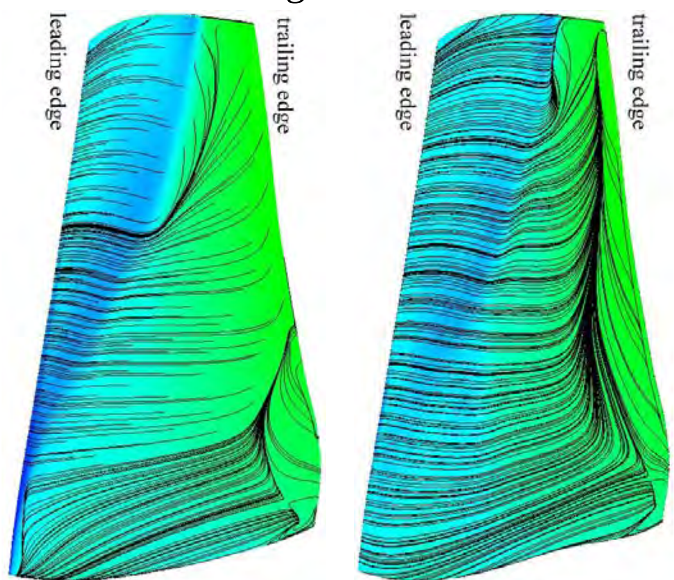




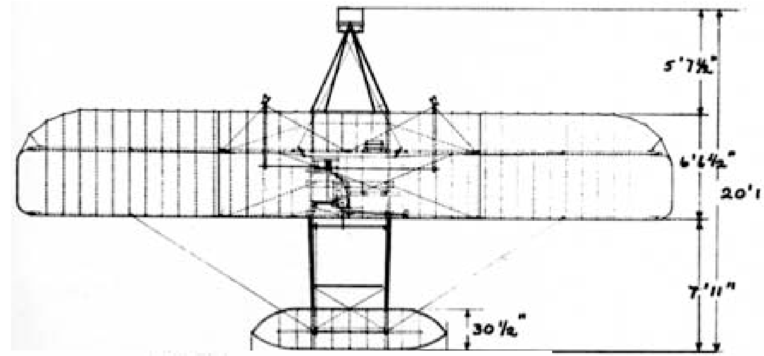


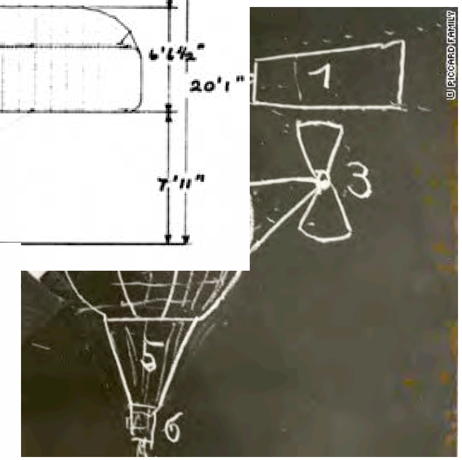
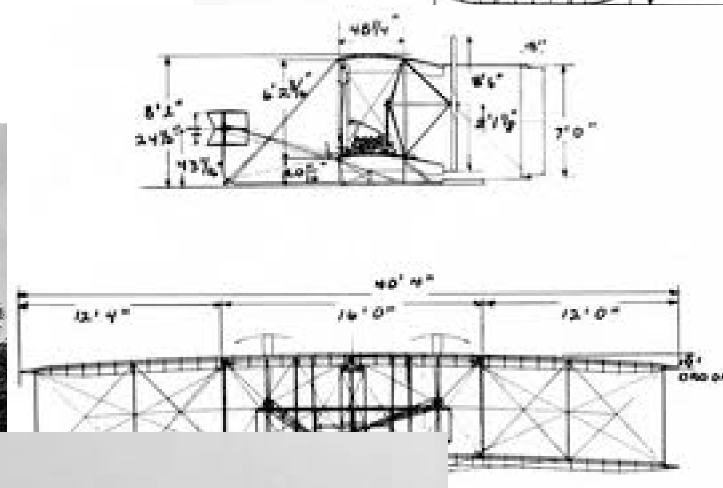
A 2% increase in efficiency!

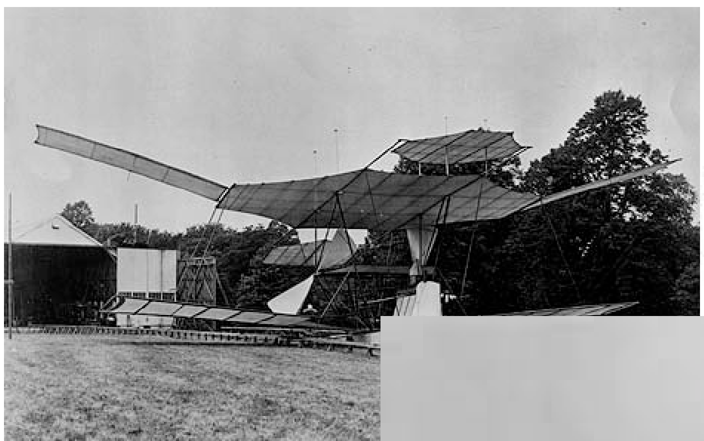
Yielded milder flow separation, less losses

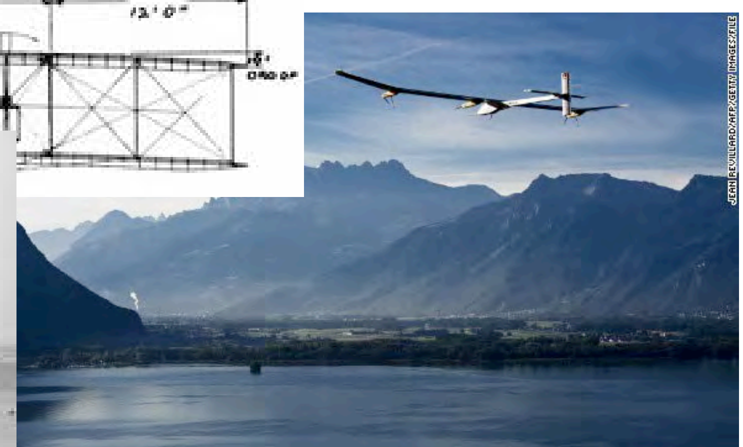
Real-world Engineering Project

- Motivation, ideas
- Sketches (“back of envelope”)
- Prototype
- Analysis
- Building
- Testing

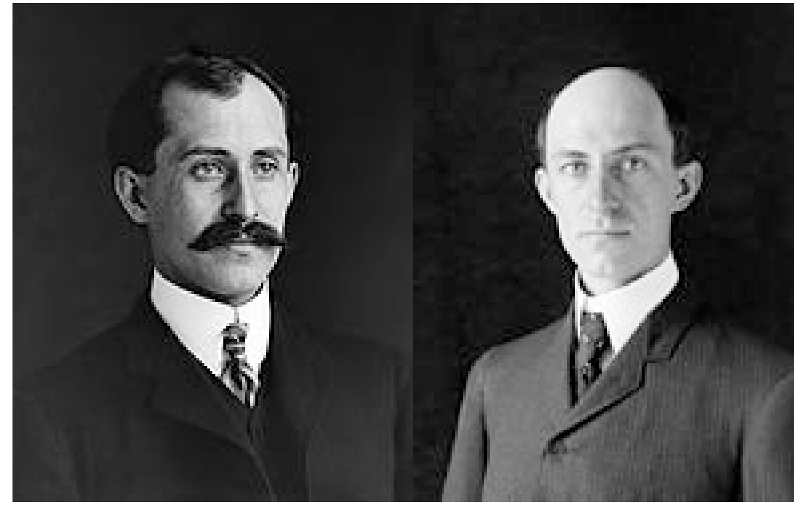


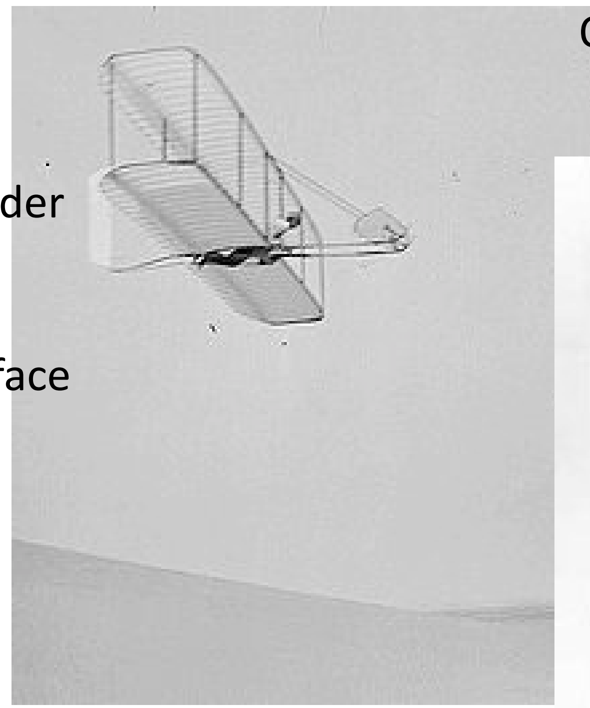


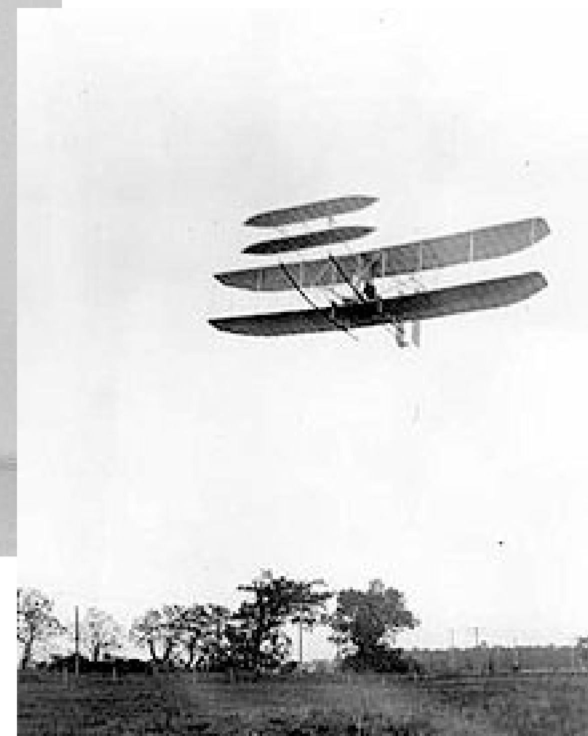


Wright Brothers' Flight



Orville Wilbur





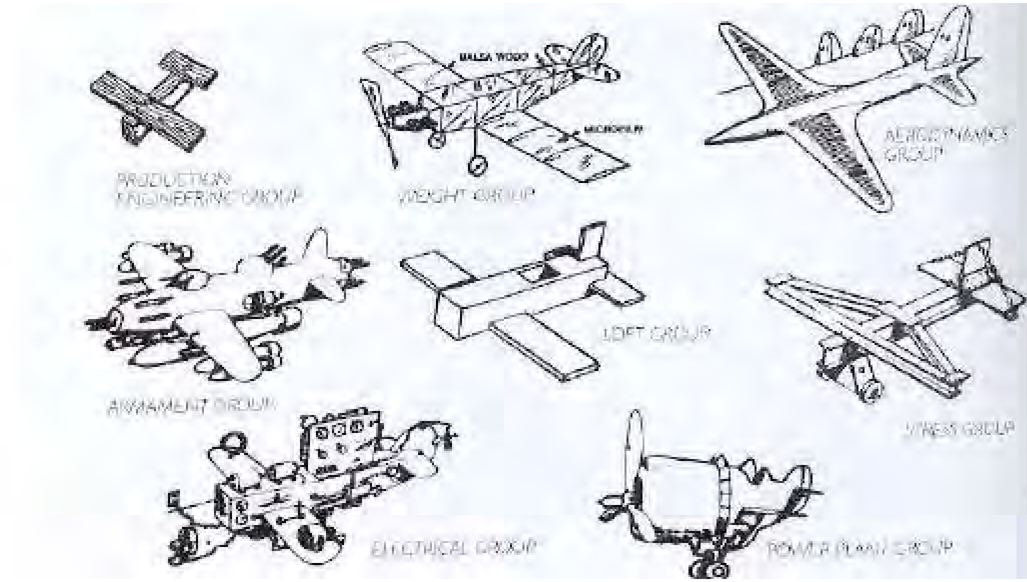
First powered aircraft flown under pilot's control, Dec. 17, 1903

40 ft span, 505 sq. ft airfoil surface
750 pounds with pilot
12 hp motor

Four flights
850 ft max distance
59 sec max duration

Design of a Complex Engineering System

- ✧ Engineering system is typica
  - ✓ Multidisciplinary
  - ✓ Complex and nonlinear
  - ✓ Unknown/uncertainty
  - ✓ Hard to analyze
  - ✓ Hard to build



- ✧ Achieving a desirable performance requires Design and Optimization
  - ✓ Multiple objectives, constraints, uncertainties,
  - ✓ Multilevel optimization
  - ✓ Multidisciplinary
  - ✓ Decision making/formulation
  - ✓ Expensive to compute

Modern Aerospace Design

- Computation-based design
- Integration of high-fidelity modeling in multiple disciplines
- Challenges
  - Fidelity and applicability of modeling
  - Integration: efficiency, adaptability (models, computer systems, …), easiness to use
  - Verification and validation
- A new paradigm–Multidisciplinary Design Analysis and Optimization (MDAO), in which the synergistic effects of various interacting disciplines/phenomena are explored and exploited at every stage of the design process
- Challenges
  - Issues with optimization, such as choice of approaches, problem formulation, …
  - Configuration and its definition
  - Integration with CAD, mesh generation
  - Integration of different fidelity levels
  - Analysis of resulting designs
  - …
- Optimization

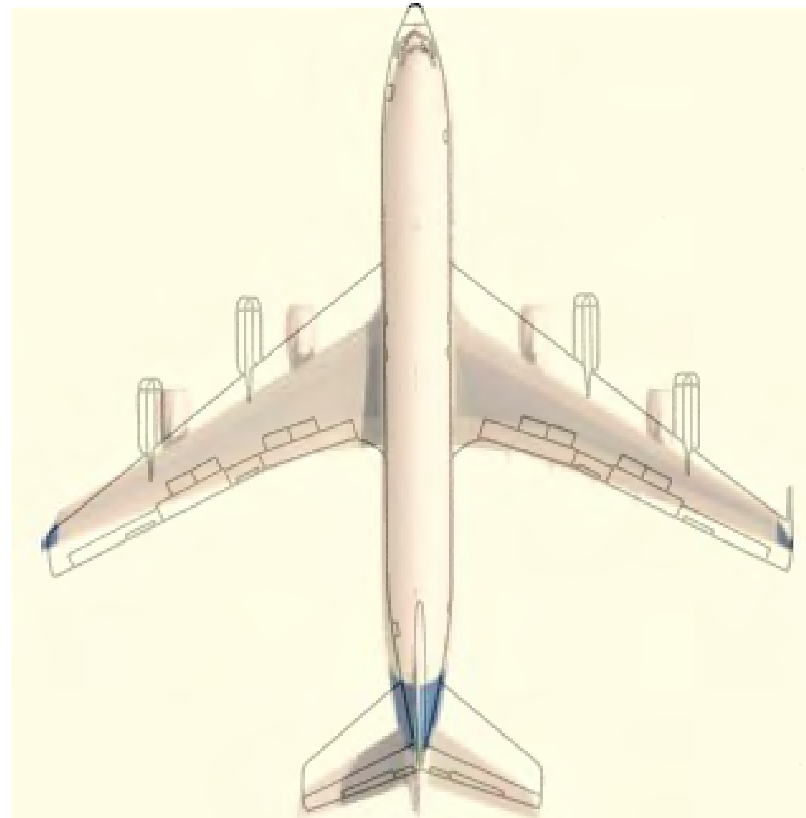
Complex System Development is Evolutionary

- **Design is often determined more by the problem formulation (parameterization, constraints) than by the optimization process.**

- **Design as parametric optimization can be problematic.**

- **To achieve more than evolutionary improvements requires advances in modeling, simulation, and multidisciplinary design.**

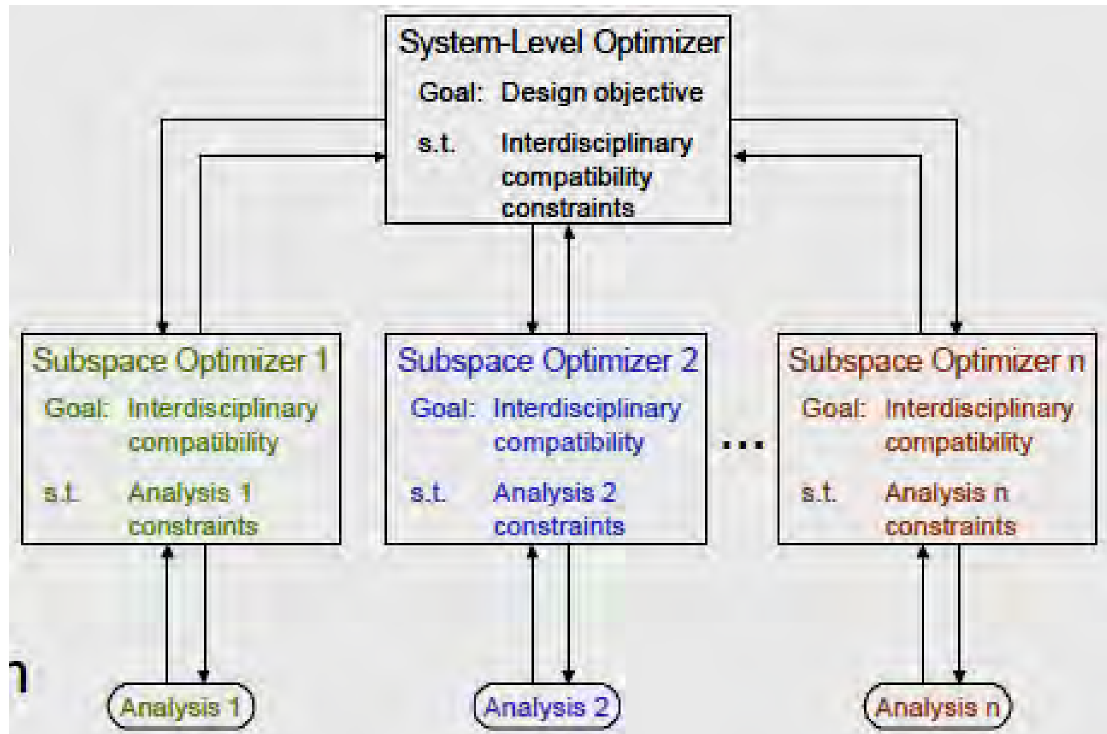
- **MDAO is a broadly applicable field, but has been pioneered in aerospace because of the maturity of modeling and**



Boeing 707: 1958, M 0.82
Airbus 340: 1993, M 0.86

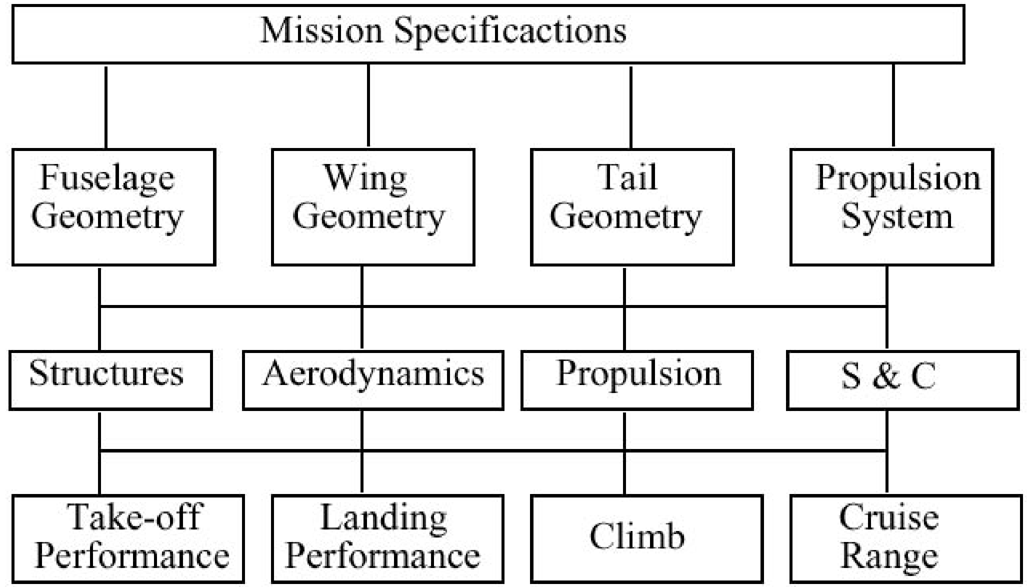
A typical MDAO problem

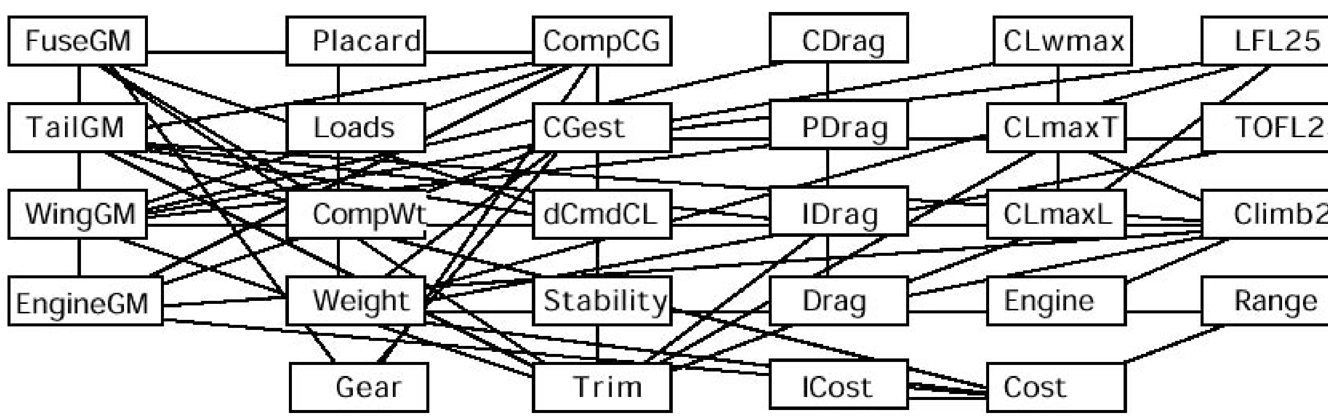
- ✧ Bilevel Multi-obj. Opt.
  - Uncertainty
  - Coupling process
  - Computational cost
  - Other practicalities
- ✧ Choose an MDO algorithm
- ✧ Solve for optimal solutions



Representative Analysis Architecture

- Flow structure and connectivity seems straightforward and logical
- But incredibly unwieldy—inefficient, prone to mistakes and hard to maintain

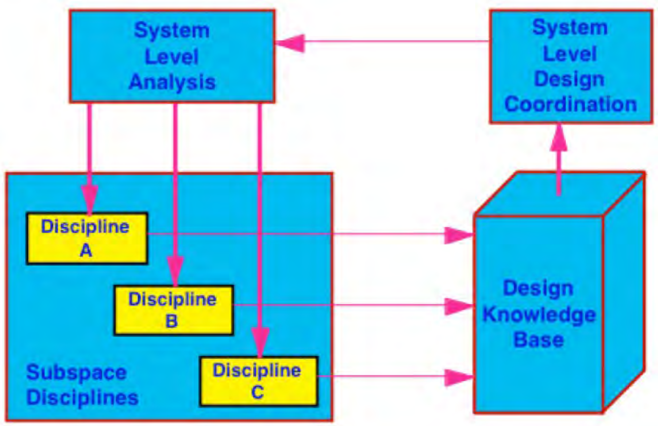




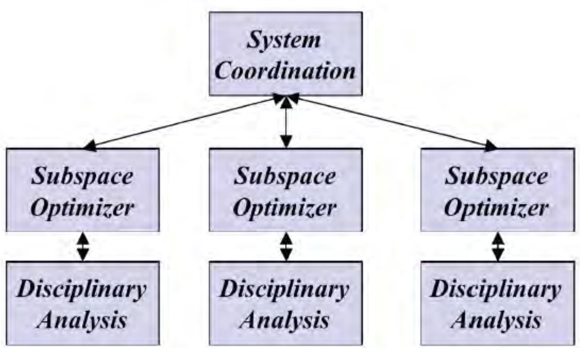
Tables taken from I. Kroo's presentation given for NASA

Distributed Design

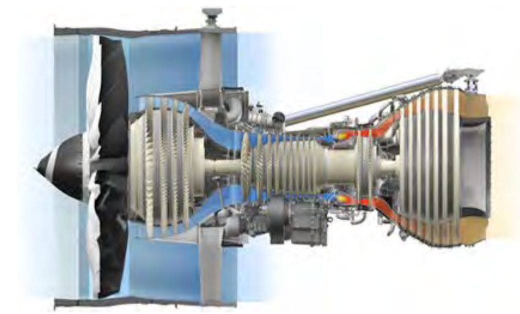
- Decomposition of the design problem
  - Design variables, constraints, disciplines, components, …

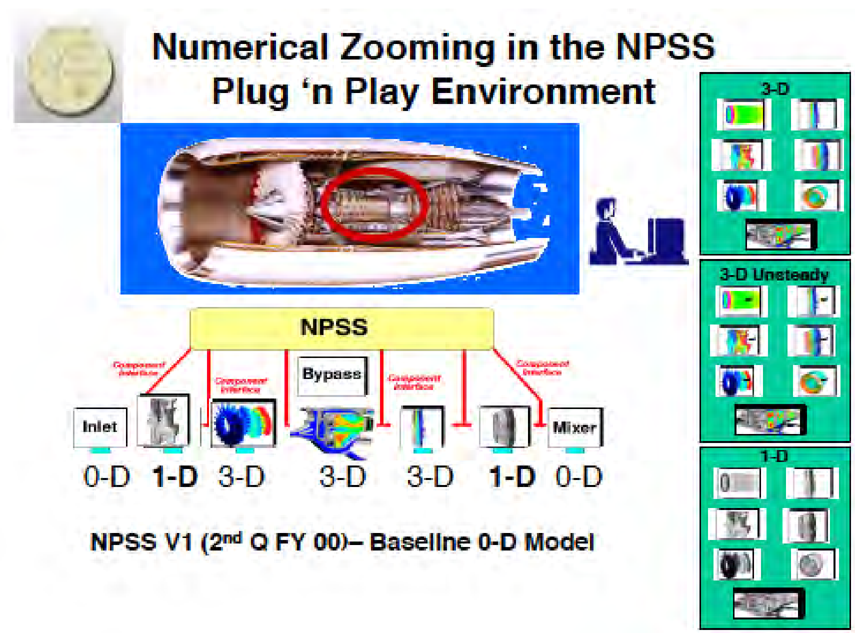


Concurrent subspace optimization



Collaborative optimization





Numerical Propulsion System Simulation

Taken from G. Follen

Taken from I. Kroo, VKI lecture, 2004

Adjoint Optimization Method

Objective function

$$f = f(Q, D), \quad Q = \text{flow variables}, \; D = \text{design variables}$$

$$\frac{df}{dD} = \left[\frac{\partial f}{\partial Q} \frac{\partial Q}{\partial D} + \frac{\partial f}{\partial D} \right]$$

These variations are subject to satisfying the flow (Navier-Stokes) equations

$$R = R(Q, D) = 0$$

Form an adjoint system via the Lagrangian multiplier

$$\hat{f} = f - \Lambda^T R$$

$$\frac{d\hat{f}}{dD} = \left[\frac{\partial f}{\partial Q} - \Lambda^T \frac{\partial R}{\partial Q} \right] \frac{\partial Q}{\partial D} + \left[\frac{\partial f}{\partial D} - \Lambda^T \frac{\partial R}{\partial D} \right]$$

=0

Determine Λ (adjoint variables) from the adjoint equations

$$\left[\frac{\partial R}{\partial Q} \right]^T \Lambda = \left[\frac{\partial f}{\partial Q} \right]$$

Adjoint Optimization Method

Then the search gradient is obtained

$$\frac{df}{dD} = \left[\frac{\partial f}{\partial D} - \Lambda^T \frac{\partial R}{\partial D} \right]$$

And the step size for the design variables:
Linear method

$$\delta D = -\varepsilon \frac{df}{dD}$$

Nonlinear method is expensive as it requires Hessian

$$\frac{d^2 f}{dD_i dD_j}$$

Concluding Remarks

- Optimization is common in practice, it is an essential step in engineering development, resulting in
  - Better design
  - Innovative solutions
  - Better understanding of the system
- Often theory is sound, but not easy to use in practice
  - Optimization algorithm is only a means to an end
- Choose an optimization algorithm better suited for the problem
- Ideas and formulation are the key to optimization

Any Questions?

Thank you for your attention!

No Free Lunch (NFL) Theorem

In the context of optimization

Wolpert and McCardy (IEEE TEC, 1997)

Algorithms A1 and A2

For All possible problems F

Performances P1 and P2 using A1 and A2 for a fixed number of evaluations

P1 = P2

- NFL breaks down for a class of problems or algorithms
- Find the best algorithm for a class of problems
- Unimodal, multi-modal, quadratic etc.

Optimality Conditions for Unconstrained Minimum Points

- Single variable: df/dx = 0, $d^2f/dx^2>0$
- General rule: Identify first non-zero derivative at point x, say its order is n. If n is even, the sign of that derivative, + or –, determines minimum or maximum, respectively.
- Multiple variables: $\nabla f = 0$, Hessian matrix H(f) is positive definite for minimum
  - A matrix is + definite, if all eigenvalues are positive