The Need for Numerical Optimization

AE 6310: Optimization for the Design of Engineered Systems

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Dr. Glenn Lightsey

Lecture Notes Developed By Dr. Brian German

Georgia Institute of Technology

Daniel Guggenheim School of Aerospace Engineering

What is “optimization”?

From Merriam Webster:

Optimization (noun):

an act, process, or methodology of making something (as a design, system, or decision) as fully perfect, functional, or effective as possible; *specifically*: the mathematical procedures (as finding the maximum of a function) involved in this

Why is optimization difficult?

- If optimization is just the process of "finding a maximum of a function," didn't we learn everything we need in calculus?

To minimize (or maximize) $f(x)$…

1. Find $\frac{d}{dx}[f(x)]$ …
2. Set $\frac{d}{dx}[f(x)] = 0$ to solve for the **critical points**, x_{cr} …
3. Select the critical point(s) for which $\frac{d^2}{dx^2}[f(x_{cr})] > 0$ (<0 for maximization)

- Easy, right?
- Well, it depends. Let's look at some examples.

Example 1: Quadratic Function of One Variable

Minimize $f(x) = x^2 - x - 1$

$$\frac{df}{dx} = 2x - 1$$

$$\frac{df}{dx} = 0 \quad \Rightarrow \quad 2x - 1 = 0 \quad \Rightarrow \quad x_{cr} = \frac{1}{2}$$

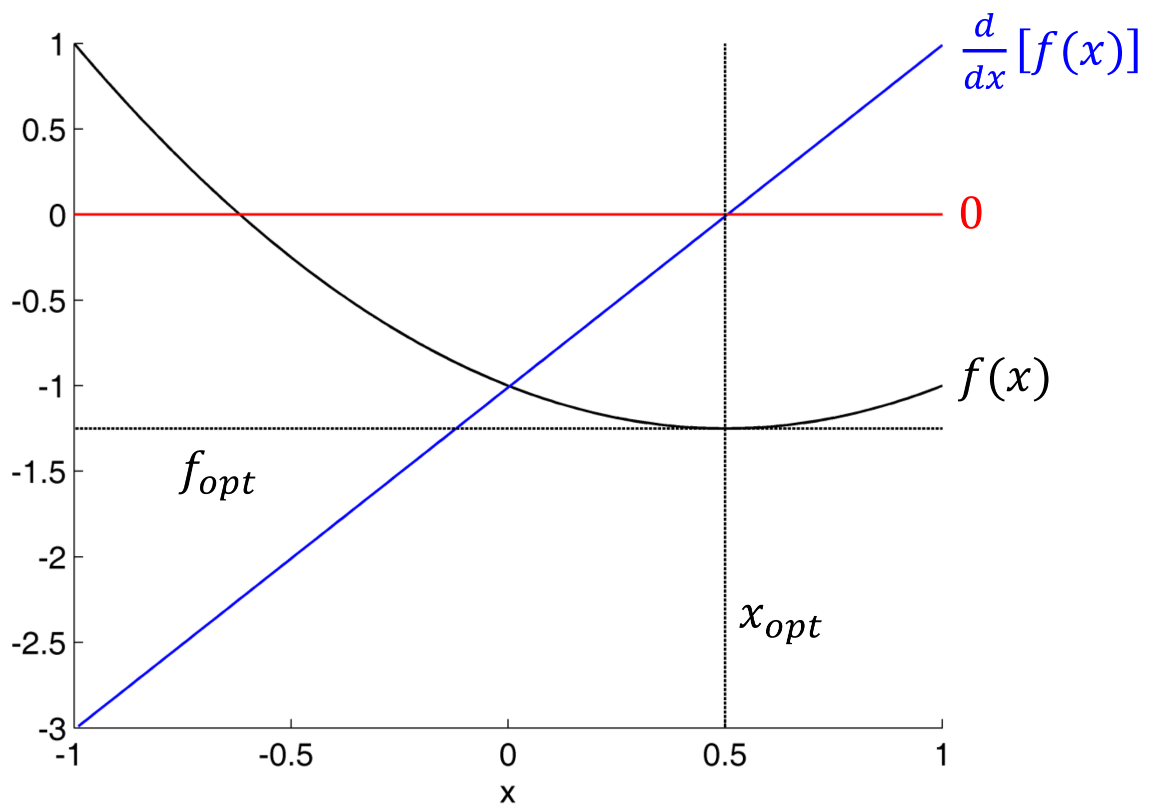
$$\frac{d^2 f}{dx^2} = \frac{d}{dx}[2x - 1] = 2 > 0 \Rightarrow x_{cr} = x_{opt}$$

$$f_{opt} = f\left(x_{opt}\right) = x_{opt}^2 - x_{opt} - 1 = \frac{1}{4} - \frac{1}{2} - 1 = -\frac{5}{4}$$

Not very difficult.

Example 1: Quadratic Function of One Variable

$$f(x) = x^2 - x - 1$$



Example 2: Cubic Function of One Variable

Minimize $f(x) = -x^3 + x^2 + \frac{1}{2}x - 1$

$$\frac{df}{dx} = -3x^2 + 2x + \frac{1}{2} = 0 \Rightarrow x_{cr} = \left\{\frac{2-\sqrt{10}}{6}, \frac{2+\sqrt{10}}{6}\right\}$$

$$\frac{d^2}{dx^2}[f(x_{cr})] = -6x_{cr} + 2 = \left\{\sqrt{10}, -\sqrt{10}\right\}$$

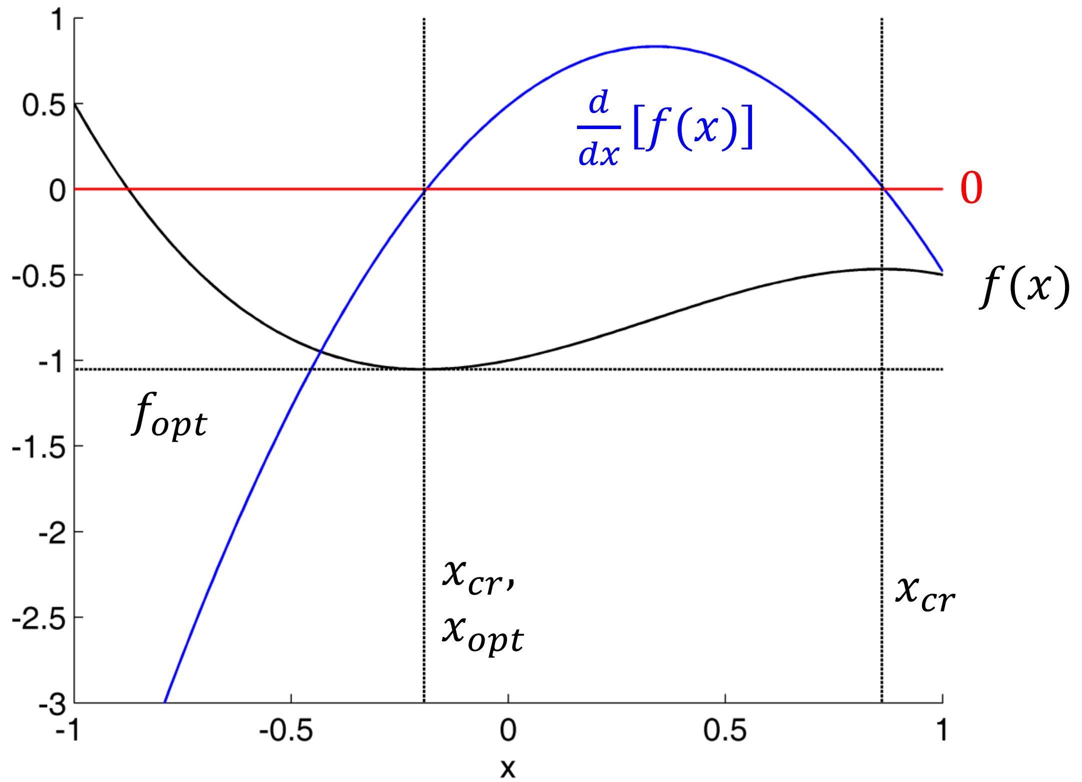
$$\Rightarrow x_{opt} = \frac{2-\sqrt{10}}{6} \approx -0.19$$

$$f_{opt} = f\left(x_{opt}\right) = -x_{opt}^3 + x_{opt}^2 + \frac{1}{2}x_{opt} - 1 \approx -1.05$$

A little harder and more tedious.

Example 2: Cubic Function of One Variable

$$f(x) = -x^3 + x^2 + \frac{1}{2}x - 1$$



Example 3: Transcendental Function of One Variable

Minimize $f(x) = \frac{1}{2}\cos\left(\frac{3\pi x}{2}\right) - 3x + 2\exp(x) - \frac{7}{2}$

$$\frac{df}{dx} = -\frac{3\pi}{4}\sin\left(\frac{3\pi x}{2}\right) - 3 + 2\exp(x) = 0$$

Finding the x_{cr} from this expression looks challenging.

What can we do?

Example 3: Transcendental Function of One Variable

This is a problem in root finding, the task of determining the x values at which a function, g, crosses zero.

We could use a technique such as Newton's Method:

$$x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)}$$

We need $\frac{d}{dx}[f(x)] = 0$, so set $g = \frac{d}{dx}[f(x)]$.

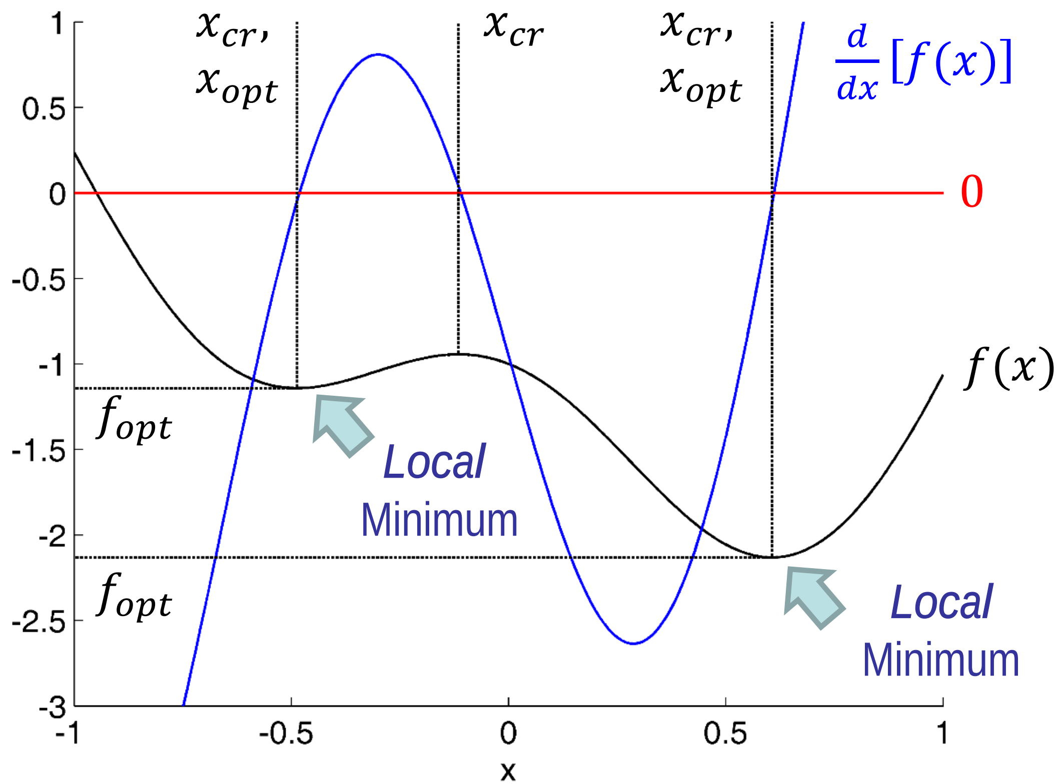
Example 3: Transcendental Function of One Variable

Before we can use Newton's Method, we need an initial guess, x_0, for the critical point.

Let's make a plot.

Example 3: Transcendental Function of One Variable

$$f(x) = \frac{1}{2}\cos\left(\frac{3\pi x}{2}\right) - 3x + 2\exp(x) - \frac{7}{2}$$



We have *multiple* minima. The problem is <u>multimodal</u>.

Example 3: Transcendental Function of One Variable

But back to Newton's method…

By inspecting the plot, we can make good estimates of the locations of the critical points to serve as initial guesses.

Let's look just at the local minima and not the local maxima.

For the local minimum on the left, let's try $x_0 = -0.5$ and for the minimum on the right, let's try $x_0 = 0.5$.

Example 3: Transcendental Function of One Variable

$$x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)}$$

$$g(x) = \frac{d}{dx}[f(x)] = -\frac{3\pi}{4}\sin\left(\frac{3\pi x}{2}\right) - 3 + 2\exp(x)$$

$$g'(x) = \frac{d^2}{dx^2}[f(x)] = -\frac{9\pi^2}{8}\cos\left(\frac{3\pi x}{2}\right) + 2\exp(x)$$

$x_0 = -0.5$

step	x	dx	g(x)
0	-0.50000000	1.00000000	-0.12085758
1	-0.48666662	0.01333338	-0.00324821
2	-0.48628769	0.00037893	-0.00000273
3	-0.48628737	0.00000032	0.00000000
4	-0.48628737	0.00000000	0.00000000

$x_0 = 0.5$

step	x	dx	g(x)
0	0.50000000	1.00000000	-1.36863856
1	0.62276255	0.12276255	0.24413063
2	0.60603515	0.01672740	0.00220979
3	0.60588083	0.00015432	0.00000022
4	0.60588082	0.00000002	0.00000000

Great. We found two local minima. But how many are there?

Example 3: Transcendental Function of One Variable

It's difficult to know! Because the cosine term is periodic, there are potentially many (even an infinite number) of local minima.

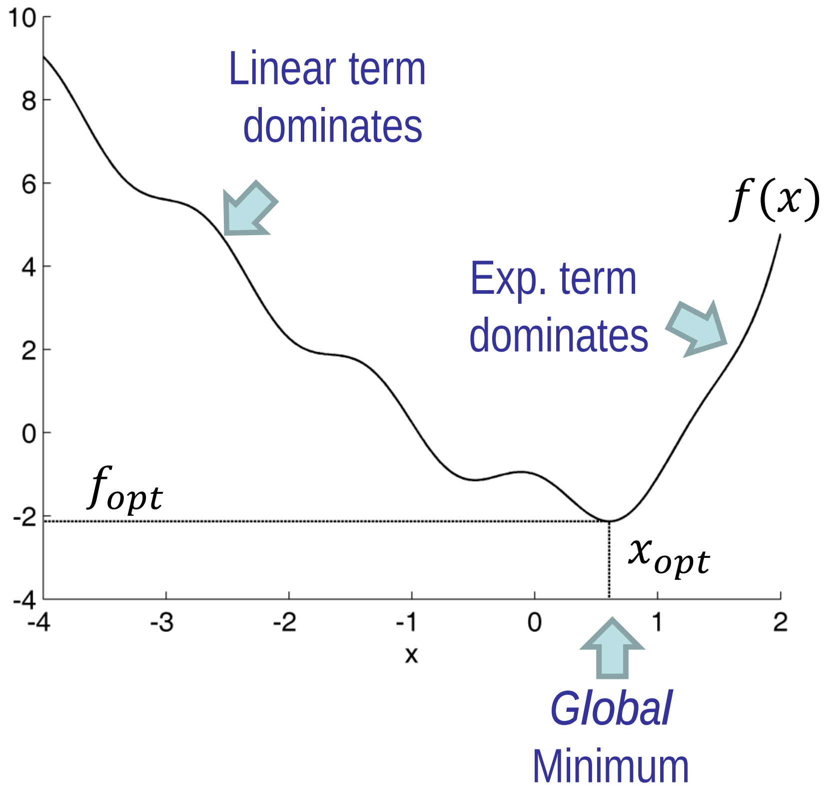
How would we ever really know if we had found all of them?

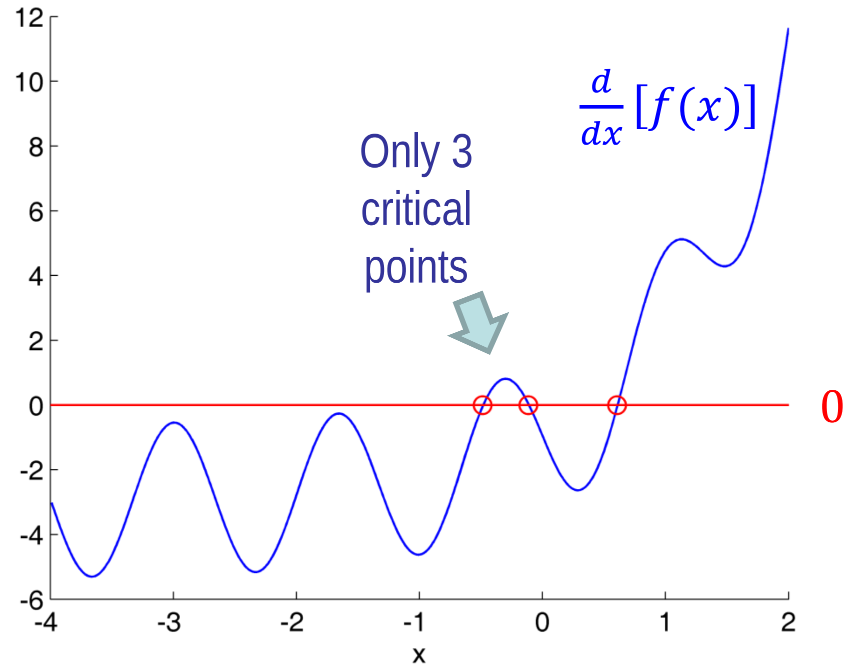
Additionally, do we care about *all* of the local minima? Maybe we want to know the <u>global minimum</u>.

Let's make a plot over a larger domain to see what we can find out.

Example 3: Transcendental Function of One Variable

$$f(x) = \frac{1}{2}\cos\left(\frac{3\pi x}{2}\right) - 3x + 2\exp(x) - \frac{7}{2}$$





It's good that we could make a plot. Often, it's not so simple. Why?

Example 4: Add a Constraint to Example 3

Minimize $$f(x) = \frac{1}{2}\cos\left(\frac{3\pi x}{2}\right) - 3x + 2\exp(x) - \frac{7}{2}$$

Subject to $$g(x) = x - \frac{1}{4} < 0$$

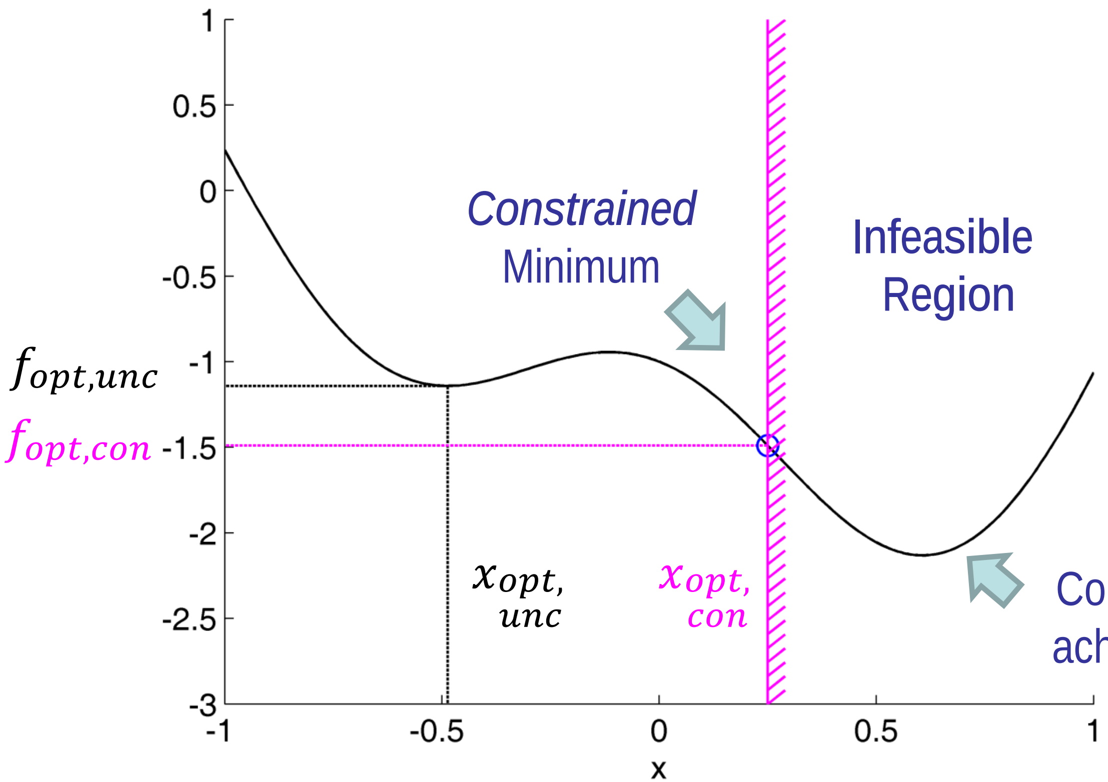
This is a problem in constrained optimization.

We have to determine whether the constraint is active.

Example 4: Add a Constraint to Example 3

Minimize $$f(x) = \frac{1}{2}\cos\left(\frac{3\pi x}{2}\right) - 3x + 2\exp(x) - \frac{7}{2}$$

Subject to $$g(x) = x - \frac{1}{4} < 0$$



Constraint prevents us from achieving the unconstrained global minimum

Example 5: Quadratic Function of Two Variables

Minimize $f(x_1, x_2) = \frac{3}{2}x_1^2 + \frac{1}{2}x_1 x_2 + 2x_2^2 - \frac{1}{2}x_1 + \frac{1}{2}x_2 - 2$

For the case of functions of multiple variables, we recall from calculus,

To minimize (or maximize) $f(\boldsymbol{x})$…

1. Find $\nabla[f(\boldsymbol{x})]$ …
2. Set $\nabla[f(\boldsymbol{x})]$ = 0 to solve for the critical points, $\boldsymbol{x}_{cr}$ …
3. Select the critical point(s) for which the **Hessian matrix**, $H[f(\boldsymbol{x}_{cr})]$ is *positive definite* (negative definite for maximization)

Sometimes step 3 does not work… We'll discuss this situation later.

Example 5: Quadratic Function of Two Variables

Minimize $f(x_1, x_2) = \frac{3}{2}x_1^2 + \frac{1}{2}x_1x_2 + 2x_2^2 - \frac{1}{2}x_1 + \frac{1}{2}x_2 - 2$

Let's try it:

$$\nabla[f(\boldsymbol{x})] = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \mathbf{0} \Rightarrow \begin{matrix} \frac{\partial f}{\partial x_1} = 3\mathrm{x}_1 + \frac{1}{2}x_2 - \frac{1}{2} = 0 \\ \frac{\partial f}{\partial x_2} = \frac{1}{2}x_1 + 4x_2 + \frac{1}{2} = 0 \end{matrix}$$

$$\Downarrow$$

$$\begin{bmatrix} 3 & 1/2 \\ 1/2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1/2 \\ -1/2 \end{bmatrix} \Rightarrow \begin{bmatrix} x_{1,cr} \\ x_{2,cr} \end{bmatrix} \approx \begin{bmatrix} 0.19 \\ -0.15 \end{bmatrix}$$

Okay, we have one critical point.

(How would we know if a critical point did not exist?)

Example 5: Quadratic Function of Two Variables

Let’s now determine whether the critical point is a minimum.

To do so, first calculate the Hessian matrix:

$$H(\boldsymbol{x}) = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1 \partial x_2} \\ \dfrac{\partial^2 f}{\partial x_2 \partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 3 & 1/2 \\ 1/2 & 4 \end{bmatrix}$$

Next, calculate its characteristic polynomial:

$$\det(\lambda I - H) = 0 \Rightarrow \det \begin{bmatrix} \lambda - 3 & -1/2 \\ -1/2 & \lambda - 4 \end{bmatrix} = 0$$

Example 5: Quadratic Function of Two Variables

$$\det\begin{bmatrix}\lambda-3 & -1/2\\ -1/2 & \lambda-4\end{bmatrix}=0 \qquad \Rightarrow \qquad \lambda^2-7\lambda+\frac{47}{4}=0$$

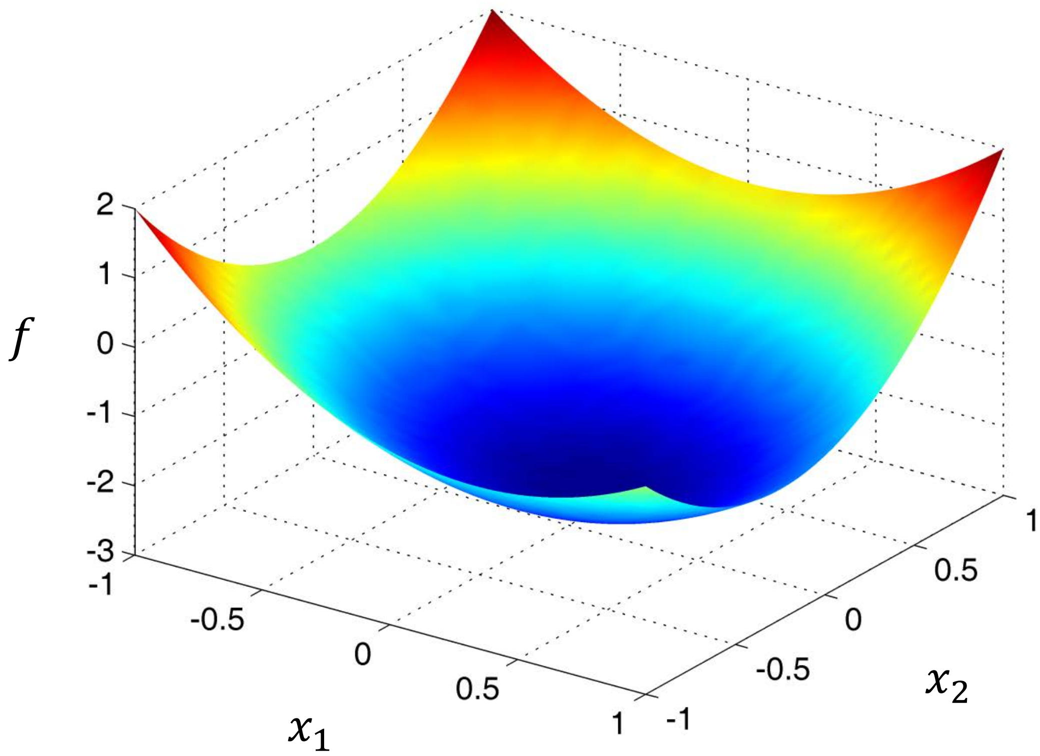
$$\Rightarrow \qquad \lambda\approx\begin{bmatrix}4.21\\ 2.79\end{bmatrix}$$

Since both eigenvalues are positive, $H(\boldsymbol{x})$ is positive definite.

The critical point is therefore a (local) minimum.

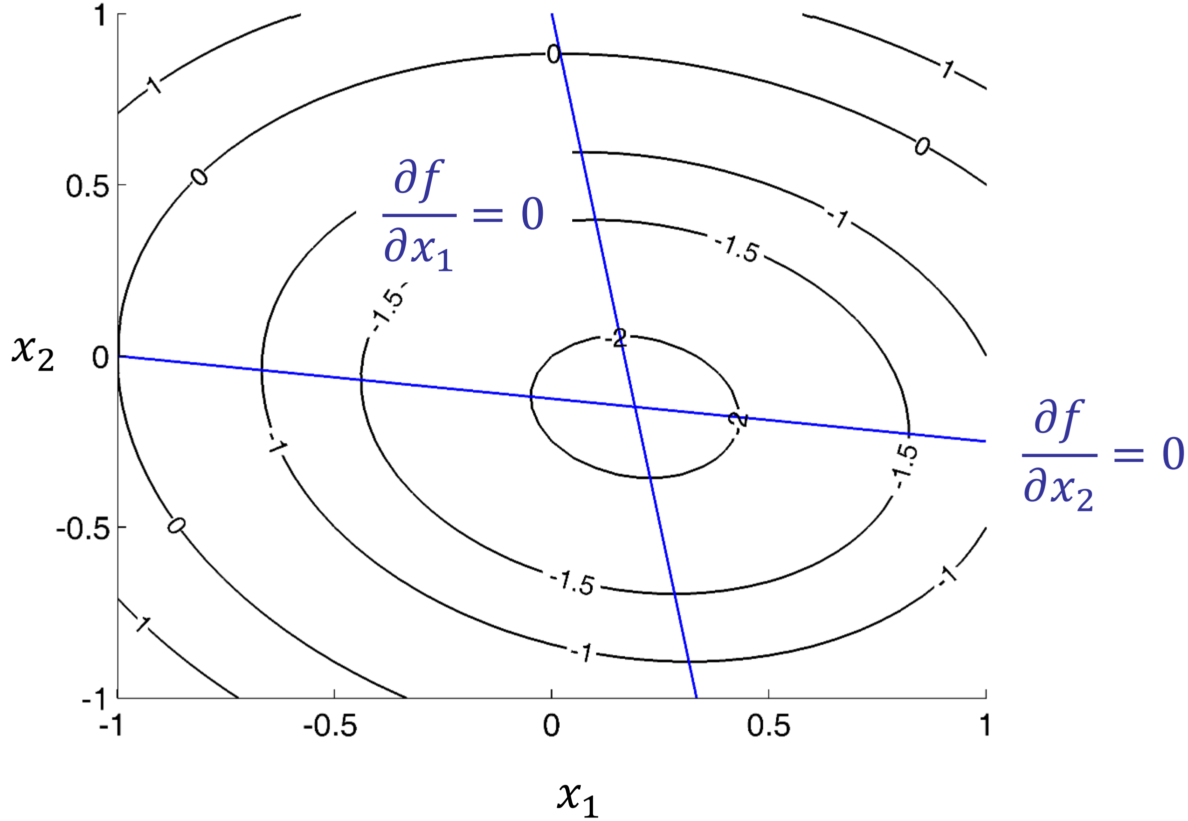
Example 5: Quadratic Function of Two Variables

Minimize $f(x_1, x_2) = \frac{3}{2}x_1^2 + \frac{1}{2}x_1x_2 + 2x_2^2 - \frac{1}{2}x_1 + \frac{1}{2}x_2 - 2$



Example 5: Quadratic Function of Two Variables

Minimize $f(x_1, x_2) = \frac{3}{2}x_1^2 + \frac{1}{2}x_1 x_2 + 2x_2^2 - \frac{1}{2}x_1 + \frac{1}{2}x_2 - 2$



Example 5: Quadratic Function of Two Variables

You can imagine how much more difficult this would have been with:

- A higher order polynomial or transcendental function
- Constraints
- More variables, $(x_1, \dots, x_n)$

Example 6: Expensive "Black Box" Functions

Minimize	$f(\boldsymbol{x})$
Subject to	$\mathbf{h}(\boldsymbol{x}) = \mathbf{0}$,
	$\boldsymbol{g}(\boldsymbol{x}) < \mathbf{0}$

- The functions $f(\boldsymbol{x})$, $\mathbf{h}(\boldsymbol{x})$, and $\boldsymbol{g}(\boldsymbol{x})$ are of unknown form, i.e. we cannot write them out in terms of known functions (polynomials, trig functions, exponentials, etc.).
- The functions may be engineering analysis tools, e.g. CFD or FEA solvers.
- The tools may be expensive to run, i.e. they may require considerable "wall time" and computing resources

Example 6: Expensive "Black Box" Functions

There are a lot of difficulties with these problems:

- Difficult to do "textbook" calculus analyses associated with known functional forms
- We have to "query" or "sample" the function every time we want to obtain 1 point, and this is problematic for expensive functions
- We cannot even make good plots, i.e. a plot takes MANY points!
- Besides, there are probably too many variables, $(x_1, \ldots, x_n)$ to be able to visualize adequately
- Functions are often strongly nonlinear and may even have discontinuities

Engineering Analysis

Given a system, how do we expect it to perform?

$$\boldsymbol{x} \longrightarrow \boxed{\mathrm{A}} \longrightarrow \boldsymbol{f}(\boldsymbol{x}), \boldsymbol{h}(\boldsymbol{x}), \boldsymbol{g}(\boldsymbol{x})$$

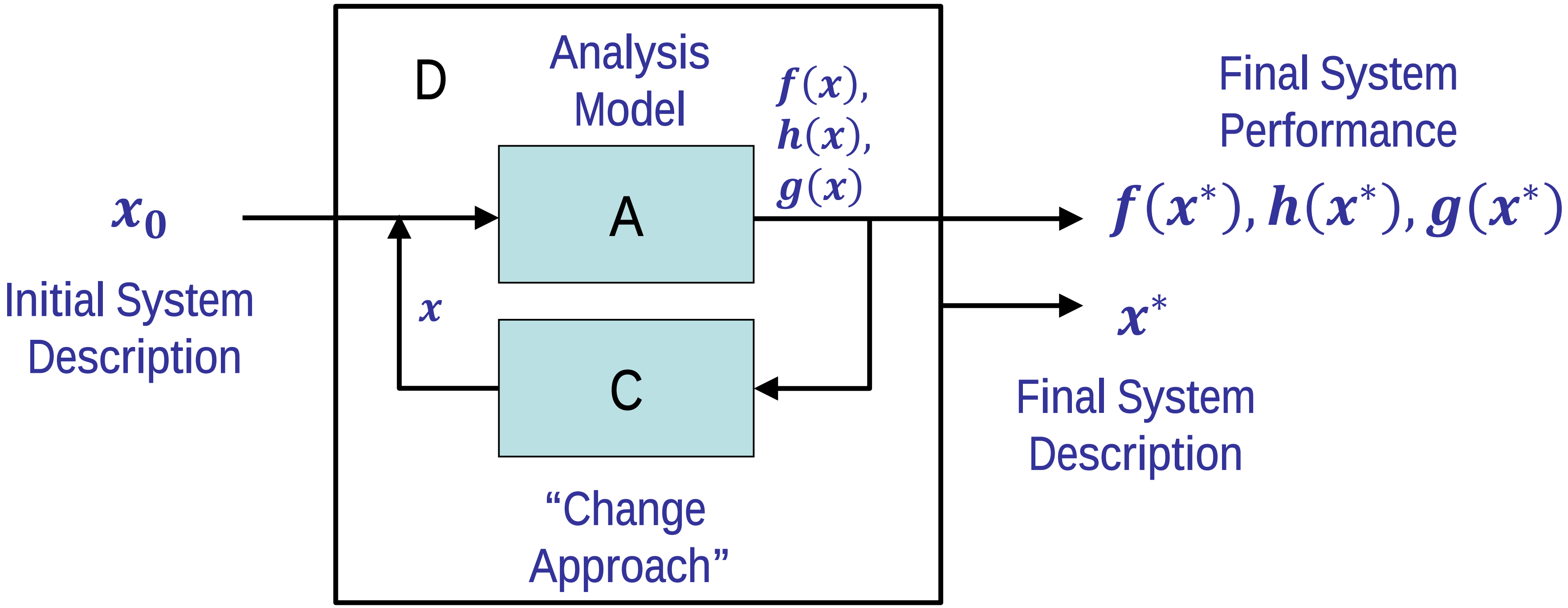
System Description
(*Design Variables*)

Analysis
Model

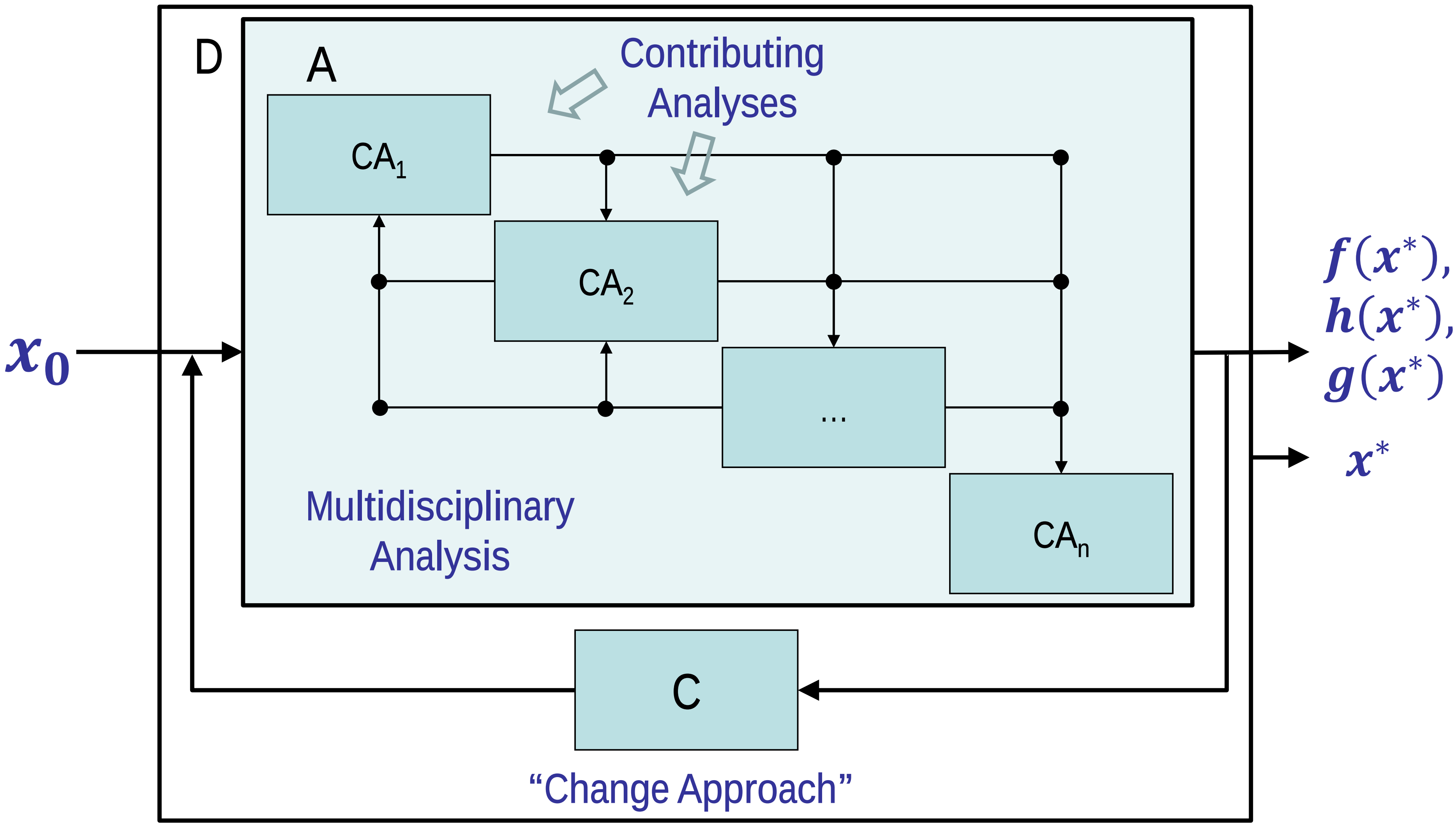
Predicted System
Performance
*(Design Attributes,
Responses)*

Engineering Design

Given a desired performance or a measure for ranking systems based on their performance, what system do we want?



Multidisciplinary Design



Some “Change Approaches”

- Intuition and experience
- Trial and error
- Single variable trade studies (line plots)
- Multi-variable trade studies (carpet and contour plots)
- Optimization

The State-of-the-Art in Engineering Optimization

- Optimization is rather “new” to engineering design practice

- Why?
  - For new types of systems, the main issue is **feasibility**, not optimality, i.e. make *something that works* before you make something that works *better.*
  - Historically, engineers have been educated in the tradition of hands-on problem solving and invention, not mathematical methods for optimization.
  - Computing has been inadequate to support the required analysis and optimization algorithms.

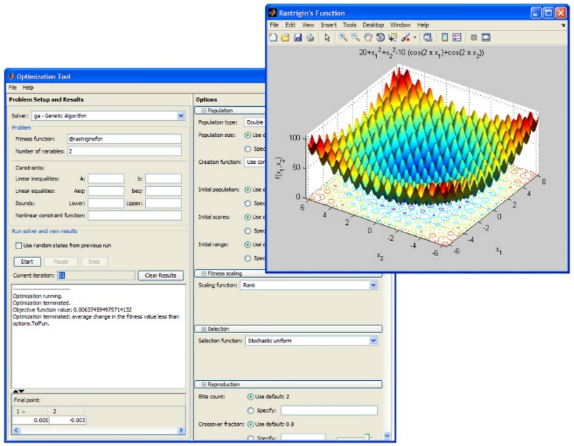
The State-of-the-Art in Engineering Optimization

Things have been changing

- Much of design is now incremental. Feasible concepts have been achieved, e.g. cars and airplanes, and we are now seeking to improve the designs.
- Engineering education now has more content in mathematics and computing.
- Computers are now much more capable.

Commercial Optimization Software

Matlab Optimization Toolboxes



Optimization Toolbox: Unconstrained, constrained, SQP, LP, MILP, root finding.

Global Optimization Toolbox: GA, Particle Swarm, Simulated Annealing, Multi-objective GA

SNOPT

"…for solving large-scale optimization problems (linear and nonlinear programs). It is especially effective for nonlinear problems whose functions and gradients are expensive to evaluate."

TOMLAB (for Matlab)

"Over 100 different algorithms for linear, discrete, global and nonlinear optimization."

http://tomopt.com/tomlab/

KNITRO

"**KNITRO** is designed for large problems with dimensions running into the hundred thousands. It is effective for solving **linear, quadratic, and nonlinear** smooth optimization problems, both **convex and nonconvex**."

http://www.ziena.com/knitro.html

Commercial Optimization Software

GAMS

"The General Algebraic Modeling System (GAMS) is a high-level modeling system for mathematical programming and optimization. It consists of a language compiler and a stable of integrated high-performance solvers. GAMS is tailored for complex, large scale modeling applications, and allows you to build large maintainable models that can be adapted quickly to new situations."

http://www.gams.com/

AMPL

"AMPL integrates a modeling language for describing optimization data, variables, objectives, and constraints; a command language for browsing models and analyzing results; and a scripting language for gathering and manipulating data and for implementing iterative optimization schemes"

http://ampl.com/

Gurobi

"State-of-the-art solver for linear programming (LP), quadratic and quadratically constrained programming (QP and QCP), and mixed-integer programming (MILP, MIQP, and MIQCP)"

http://www.gurobi.com/

CPLEX

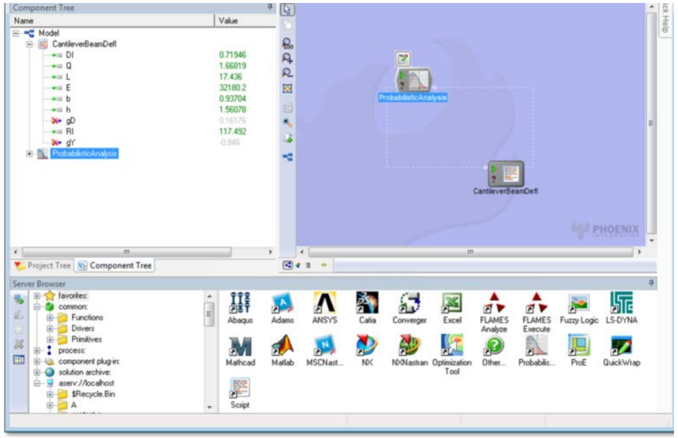
"High-performance mathematical programming solver for linear programming, mixed integer programming, and quadratic programming"

http://www-01.ibm.com/software/commerce/optimization/cplex-optimizer/

Multi-Disciplinary Optimization Software

www.esteco.com

PHX ModelCenter



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Isight

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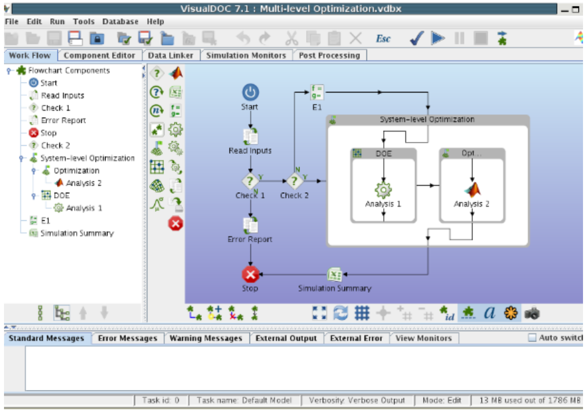
VisualDOC



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