ME128 Computer-Aided Mechanical Design
Course Notes
Introduction to Design Optimization

2. OPTIMIZATION

Design optimization is rooted as a basic problem for design engineers. It is, of course, a rare situation in which it is possible to represent fully all the complexities of a design, appropriate objectives, if functionally quantifiable, or constraints. Thus, as with many design optimization problems, a particular optimization formulation should be regarded only as an approximation and the appropriate assumptions and limitations clearly spelled out. Optimization in design, then, should be regarded as a tool of conceptualization and analysis rather than as a principle yielding the philosophically correct solution. As you will find in engineering practice, the results of your design optimization analysis may only provide direction for the design rather than produce definitive design parameters.

We will look at two classes of optimization problems, linear and non-linear optimization, for the unconstrained and constrained case. We will also look at some numerical optimization algorithms, though if you're interested in this topic, a more detailed study of optimization can be found in IEOR262B.

2.1. Linear Programming

A linear programming problem is characterized by linear functions of the unknowns. The objective is linear in the unknowns and the constraints are linear equalities or inequalities. In engineering, one often reduces highly complex (and possibly intractable) non-linear problems into linear problems (e.g., polynomial approximation, Taylor series expansion, and linearization about a stability point) which can be solved by a variety of well-known and efficient linear optimization algorithms and tools.

Any linear program can be transformed into the following standard form:

Minimize $c_1x_1 + c_2x_2 + \ldots + c_nx_n$

Subject to

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2 \\
&\vdots \\
a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n &= b_m
\end{aligned}
$$

and

$$x_1 \geq 0 \ ; \ x_2 \geq 0 \ ; \ \ldots \ ; \ x_n \geq 0$$

where the b_i's, c_i's and a_{ij}'s are fixed real constants, and the x_i's are real numbers to be determined.

In matrix notation, (variables in bold face denote a matrix or a vector), the standard problem becomes:

Minimize	$\mathbf{c}^T\mathbf{x}$
Subject to	$\mathbf{Ax} = \mathbf{b}$; $\mathbf{x} \geq 0$

Where **x** is an *n*-dimensional column vector, **c** is an *n*-dimensional row vector, **A** is an *m* x *n* matrix, and **b** is an *m*-dimensional column vector.

2.2. Non-Linear Programming

With the advent of more sophisticated non-linear optimization algorithms, it is becoming increasingly feasible to solve complex non-linear problems without having to linearize the problem.

In the non-linear programming case, we drop the linear requirements and simply re-write the standard problem as

Minimize	$f(\mathbf{x})$
Subject to	$\mathbf{x} \in \Omega$

where f is a real-valued function and the Ω feasible set.

2.3. Concepts of Optimization

2.3.1. Full Rank and Condition Number

For the linear optimization case, how can we be assured that a solution exists? How do we know that the "optimal" value found is a global optimal, if such one exists?

In general, a solution to the equation $\mathbf{Ax} = \mathbf{b}$ may not exist. Can you conceptualize what conditions would exist such that no solution exists? Or, the solution may exist but is "unstable."

From linear algebra, you may recall that the solution for **x** is $\mathbf{x}=\mathbf{A}^{-1}\mathbf{b}$. However, the matrix **A** may not always be invertible. When? The first condition on the matrix **A** is that the number of variables exceeds the number of equality constraints (i.e., n > m). Second, each row in **A** is linearly independent. A linear dependency of the rows of **A** would lead either to contradictory results or to a redundancy that could be eliminated. The *rank* of a *m x n* matrix **A** is equal to the maximum number of linearly independent rows or columns. The matrix is said to be of *full rank* when the rank of A is equal to the minimum of *m* and *n*.

Let us suppose that the numbers in **A** cannot be exactly represented in a computer due to a limitation of significant digits, or perhaps the parameters represent measurements which cannot be made to any higher level of precision or accuracy. (Thought question: What is the difference between "precision" and "accuracy?") What effect does this have on the numerical solution of **x** obtained by a linear equation solver?

To start, suppose that **A** can be exactly represented, but the vector **b** can not be. Let:
$\mathbf{b}' = \mathbf{b} - \delta\mathbf{b}$
$\mathbf{x}' = \mathbf{x} - \delta\mathbf{x}$

where

$\mathbf{b}'$, $\mathbf{x}'$ = computer representation of b and x, respectively
$\delta\mathbf{b}$,$\delta\mathbf{x}$ = error in the computer representation of **b** and **x**, respectively

The linear system is then

$\mathbf{A}(\mathbf{x}' + \delta\mathbf{x}) = \mathbf{b}' + \delta\mathbf{b}$

Solving for $\delta\mathbf{x}$ yields

$\mathbf{A}\mathbf{x}' + \mathbf{A}\delta\mathbf{x} = \mathbf{b}' + \delta\mathbf{b}$

Substituting $\mathbf{A}\mathbf{x}' = \mathbf{b}'$

$\delta\mathbf{x} = \mathbf{A}^{-1}\delta\mathbf{b}$

Using the Cauchy-Schwarz Inequality,

Cauchy-Schwarz Inequality: $\|\mathbf{AB}\| \le \|\mathbf{A}\| \cdot \|\mathbf{B}\|$

we can derive the inequality that $\|d\mathbf{x}\| \le \|\mathbf{A}^{-1}\|\|d\mathbf{b}\|$. Since $\mathbf{b}=\mathbf{A}\mathbf{x}$, and applying the Cauchy-Schwarz inequality to derive $\|\mathbf{b}\| \le \|\mathbf{A}\|\|\mathbf{x}\|$. Multiplying the two inequalities we get

$$\|\mathbf{b}\| \cdot \|d\mathbf{x}\| \le \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\| \cdot \|\mathbf{x}\|\|d\mathbf{b}\|$$

Assuming only that $\mathbf{b} \neq \mathbf{0}$, we get that

$$\frac{\|d\mathbf{x}\|}{\|\mathbf{x}\|} \le \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\| \cdot \frac{\|d\mathbf{b}\|}{\|\mathbf{b}\|}$$

This is the marginal error in **x**.

For any non-singular matrix **A**, we define the *condition number* of **A** to be the number:

cond ($\mathbf{A}$) = $\|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\| = {}^{l_1}\!/\!_{l_n}$

where λ_1 and λ_n are the largest and smallest eigenvalues of $\mathbf{A}$ respectively.

Using the definition of the condition number, we can now re-write the marginal error in $\mathbf{x}$ as:

$$\frac{\|d\mathbf{x}\|}{\|\mathbf{x}\|} \leq cond(\mathbf{A}) \cdot \frac{\|d\mathbf{b}\|}{\|\mathbf{b}\|}$$

Suppose now that $\mathbf{A}$ can not be precisely represented but $\mathbf{b}$ can.

The linear system is then

$$(\mathbf{A} + \delta\mathbf{A})(\mathbf{x} + \delta\mathbf{x}) = \mathbf{b}$$

Solving for $\delta\mathbf{x}$

$$\mathbf{x} + \delta\mathbf{x} = (\mathbf{A} + \delta\mathbf{A})^{-1} \cdot \mathbf{b}$$
$$\delta\mathbf{x} = (\mathbf{A} + \delta\mathbf{A})^{-1} \cdot \mathbf{b} - \mathbf{x}$$

Substituting $\mathbf{Ax}$=$\mathbf{b}$

$$\delta\mathbf{x} = [(\mathbf{A} + \delta\mathbf{A})^{-1} - \mathbf{A}^{-1}] \cdot \mathbf{b}$$

Using the identity that $\mathbf{B}^{-1} - \mathbf{A}^{-1} = \mathbf{A}^{-1}(\mathbf{A}\text{-}\mathbf{B})\mathbf{B}^{-1}$, then this reduces to:

$$\delta\mathbf{x} = -\mathbf{A}^{-1}(\delta\mathbf{A})(\mathbf{A} + \delta\mathbf{A})^{-1} \cdot \mathbf{b}$$
$$\delta\mathbf{x} = -\mathbf{A}^{-1}(\delta\mathbf{A})(\mathbf{x} + \delta\mathbf{x})$$

Taking the norms of both sides gives,

$$\|\delta\mathbf{x}\| \leq \|\mathbf{A}^{-1}\| \cdot \|\delta\mathbf{A}\| \cdot \|\mathbf{x} + \delta\mathbf{x}\|$$

It follows then that

$$\frac{\|d\mathbf{x}\|}{\|\mathbf{x} + d\mathbf{x}\|} \leq \|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\| \cdot \frac{\|d\mathbf{A}\|}{\|\mathbf{A}\|}$$
$$\frac{\|d\mathbf{x}\|}{\|\mathbf{x} + d\mathbf{x}\|} \leq cond(\mathbf{A}) \cdot \frac{\|d\mathbf{A}\|}{\|\mathbf{A}\|}$$

Thus, the error in **x** taken relative to **x** and $\delta\mathbf{x}$ is bounded by the relative error in **A** multiplied by the cond(**A**). Use the Matlab functions `eig` and `cond`.

Let us take a look at an example.

$$\mathbf{A} = \begin{bmatrix} 1.00 & 0.99 \\ 0.99 & 0.98 \end{bmatrix}$$

Using an application such as Matlab, one can find the maximum and minimum values of the eigenvalues of the matrix.

λ_{min} = -5.050376230775200e-005
λ_{max} = 1.980050503762308e+000

The condition number is 3.9206e+004.

Thus, we can expect any linear system involving A to give us trouble.

Consider the system

$$\begin{bmatrix} 1.00 & 0.99 \\ 0.99 & 0.98 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.99 \\ 1.97 \end{bmatrix}$$

The exact solution is $\mathbf{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$. But, due to the large condition number, if **b** cannot be represented accurately, then the error in **x** can be large. For example, $d\mathbf{b} = \begin{bmatrix} -0.00097 \\ 0.000106 \end{bmatrix}$ gives a $d\mathbf{x} = \begin{bmatrix} 10.555 \\ -10.663 \end{bmatrix}$. For this example, a 0.005% error in **b** produces a 100% error in the solution.

The "take home lesson" for this example is those numerical techniques that require computation of the matrix inverse can lead to erroneous results if the matrices involved are ill conditioned. In general, numerical techniques that do not require computing the matrix inverse are preferred. If they do, however, most numerical packages will warn you if the matrix is ill conditioned or not full rank.

2.3.2. Convex/Concave

Take a look at the four graphs below and decide whether or not a global optimal, and what kind of optimum, exists.

Definition: A point x in a convex set *C* is said to be an extreme point of *C* if there are no two distinct points x_1 and x_2 in *C* such that $x = \alpha x_1 + (1-\alpha)x_2$ for some α, $0 < \alpha < 1$. One can conceptualize a convex set in two dimensions in the following graphs.

The first two sets are convex sets whereas the last set is not convex. If f(**x**) is a strictly convex set, what do you think we can say about the minimum point? Conversely, if f(**x**) is a strictly concave set, what do you think we can say about the maximum point?

2.4. Unconstrained Optimization

2.4.1. Problem Formulation

The general unconstrained optimization problem can be represented as

$$\text{Minimize} \quad f(\mathbf{x}), \quad \mathbf{x} \in \Omega$$

Note that Ω represents all possible points of **x** in real space rather than any constraints on **x**.

The *local* (relative) minimum $\mathbf{x}^*$ is a local minimum of f(**x**) over Ω if $\exists\ \varepsilon$ such that $f(\mathbf{x}) \geq f(\mathbf{x}^*)$ for all $\mathbf{x} \in \Omega$ such that $|\ \mathbf{x} - \mathbf{x}^*\ | < \varepsilon$.

The *global* minimum $\mathbf{x}^*$ is a global minimum of f(**x**) over Ω if $f(\mathbf{x}) \geq f(\mathbf{x}^*)$ for all $\mathbf{x} \in \Omega$. If $f(\mathbf{x}) > f(\mathbf{x}^*)$ for all $\mathbf{x} \in \Omega$ then $\mathbf{x}^*$ is a *strict global minimum.*

What are the conditions that govern whether or not the solution is truly a minimum point?

2.4.2. First-Order Necessary Conditions (FONC)

Let Ω be a subset of E^n and let $f \in C^1$ be a function on Ω. If $\mathbf{x}^*$ is a relative minimum point of f over Ω, then for any $\mathbf{d} \in E^n$ that is a feasible direction at $\mathbf{x}^*$, we have Ñ$f(\mathbf{x}^*)\mathbf{d} \geq 0$. One would have to check the feasible direction if the solution occurs on the boundary of Ω. An important special case occurs when $\mathbf{x}^*$ is an interior point. In this case, there are feasible directions emanating in every direction from $\mathbf{x}^*$. In this case, then the FONC reduces to Ñ$f(\mathbf{x}^*) = 0$. We often deal with this latter condition since the former condition would typically be treated as a constrained optimization case.

2.4.3. Second-Order Necessary Conditions (SONC)

Let Ω be a subset of E^n and let $f \in C^2$ be a function on Ω. If $\mathbf{x}^*$ is a relative minimum point of f over Ω, then for any $\mathbf{d} \in E^n$ that is a feasible direction at $\mathbf{x}^*$, we have

i) $\nabla f(\mathbf{x}^*)\mathbf{d} \geq 0$
ii) if $\nabla f(\mathbf{x}^*)\mathbf{d} = 0$, then $\mathbf{d}^T \nabla f(\mathbf{x}^*)\mathbf{d} \geq 0$

If $\mathbf{x}^*$ is an interior local minimum of $f(\mathbf{x}^*)$ over Ω then we have

i) $\nabla f(\mathbf{x}^*) = 0$
ii) $\nabla^2 f(\mathbf{x}^*) > 0$

which are the second-order sufficiency conditions (SOSC). Note that the SOSC find interior optimal points, but not necessarily all optimal values. You will need to check boundary values also and check the SONC when FONC is flat at the boundary.

2.5. Constrained Optimization

2.5.1. Problem Formulation

The general constrained optimization problem can be represented as

Minimize	$f(\mathbf{x})$
Subject to	$\mathbf{x} \in \Omega$

where f is a real-valued function and the Ω feasible set.

It is often convenient to write the constraints in terms of equality and inequality constraints.

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

where

n = number of variables in $\mathbf{x}$
$m \leq n$ is the number of equality constraints
p = number of inequality constraints

A point $\mathbf{x}$ that satisfied all of the function constraints is said to be feasible or a *feasible point*.

An inequality constraint $g_j(\mathbf{x}) \leq 0$ is said to be *active* at a feasible point $\mathbf{x}'$ if $g_j(\mathbf{x}') = 0$ and *inactive* if $g_j(\mathbf{x}') < 0$.

In the graph shown below, which one of the three constraints $g_1(\mathbf{x})$, $g_2(\mathbf{x})$ and $g_3(\mathbf{x})$ are active constraints?

2.5.2. First-Order Necessary Conditions

Let $\mathbf{x}^*$ be a feasible point under the set of m constraints $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ and the local minimum of **f** subject to these constraints. Then there exists a vector $\lambda \in E^m$ such that:

$$\nabla f(\mathbf{x}^*) + \lambda^T \nabla \mathbf{h}(\mathbf{x}^*) = \mathbf{0}.$$

This equation is often known as the *Lagrangian* and the multipliers of the equality constraints λ as the *Lagrange multipliers*. The Lagrangian function is defined as follows:

$$\mathcal{L}(\mathbf{x}, \lambda) = f(\mathbf{x}^*) + \lambda^T \mathbf{h}(\mathbf{x})$$

The FONC for a local minimum is then a set of n+m equations with n unknown variables **x** and m unknown multiplier variables λ.

$$\nabla_x \mathcal{L}(\mathbf{x}, \lambda) = \mathbf{0} \quad \Rightarrow \quad \nabla_x f(\mathbf{x}^*) + \lambda^T \mathbf{h}(\mathbf{x}^*) = \mathbf{0}$$

$$\nabla_\lambda \mathcal{L}(\mathbf{x}, \lambda) = \mathbf{0} \quad \Rightarrow \quad \mathbf{h}(\mathbf{x}) = \mathbf{0}$$

The Lagrange multiplier is best interpreted as a sensitivity parameter of the minimum point to the active constraint. The Lagrange multiplier represents the "cost of the constraint" and shows how much improvement can be obtained in the objective by loosening that constraint. Without proof, the sensitivity (rate of change) of f with respect to the magnitude of the change in the constraint is $-\lambda^T$.

2.5.3. Second-Order Necessary Conditions

I will not delve deeply into the SONC for constrained minimization since a complete treatment is beyond the scope of this course. This is but a brief explanation of the requirements.

Assume that the gradient vectors of the non-linear equality constraints **h**(**x**) are linearly independent and thus the constraints form an n-m hyperplane "S" in E^n. The tangent plane to the S hyperplane at a feasible point **x*** will be referred to as:

M = { **y**: Ñ**h**(**x***)**y** = **0** } (read: the vector **y** which satisfies the following condition)

Then, the matrix

L(**x***) = **F**(**x***) + l ^{T}**H**(**x***)

is positive semi-definite; that is, **y**^{T}Ñ^2£(**x**, l)**y** ≥ 0 for all **y** ∈ M.

If the point **x*** also satisfies the FONC and if the matrix of second partial derivatives of the Lagrangian is positive definite on M, that is:

y^{T}Ñ^2£(**x**, l)**y** > 0 for all **y** ∈ M

then **x*** is a strict local minimum of **f** subject to **h**(**x**) = **0**.

In the extension to inequality constraints, one adds another slack parameter μ to the inequality constraints. The local minimum must satisfy the Karush-Kuhn-Tucker Conditions (KKT):

Let **x*** be a relative minimum point for the problem

Minimize	f(**x**)
Subject to	**h**(**x**) = **0**
	g(**x**) ≤ **0**

and suppose **x*** is a regular point for the constraints. Then, there is a vector l ∈ E^m and a vector m ∈ E^p with m ≥ **0** such that

Ñf(**x***) + l ^{T}**h**(**x***) + m^T**g**(**x***)= **0**
and
m^T**g**(**x**) = 0

These are the FONC. The SONC conditions deal with the second-order derivatives equivalently with the SONC for the equality constraints case.

L(**x***) = **F**(**x***) + l ^{T}**H**(**x***) + m^T**G**(**x***)

is positive semi-definite on the tangent subspace of the active constraints at **x***.

The sufficiency conditions state that **x*** is a strict local minimum if

m ≥ **0**
m^T**g**(**x**) = 0
Ñf(**x***) + l ^{T}**h**(**x***) + m^T**g**(**x***)= **0**

and the Hessian matrix $\mathbf{L}(\mathbf{x}^*) = \mathbf{F}(\mathbf{x}^*) + l^T\mathbf{H}(\mathbf{x}^*) + m^T\mathbf{G}(\mathbf{x}^*)$ is positive definite.

A positive definite matrix will have a positive (non-zero) determinant.