CHE 0426 Introduction to Optimization

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Why optimized?

- Improve the process to realize maximum system potential;
- Attain improved designs; maximize profits; reduce cost of productions.

Essential features of optimization problem

- An **objective function** is defined which needs to be either maximized or minimized. The objective function may be technical or economic. Examples of economic objective are profits, costs of production etc.. Technical objective may be the yield from the reactor that needs to be maximized, minimum size of an equipment etc.. Technical objectives are ultimately related to economics.
- **Underdetermined system**: If all the design variables are fixed. There is no optimization. Thus one or more variables is relaxed and the system becomes an underdetermined system which has at least in principle infinite number of solutions.

Essential features of optimization problem- Continued

- **Competing influences**: In most of the optimization problems, there would be some set of variables which has opposite influence on the objective function. Such competing influences require some balancing and hence result in typical optimization problems.

- **Restrictions**: Usually, the optimization is done keeping certain restrictions or constraints. Thus, the amount of row material may be fixed or there may be other design restrictions. Hence in most problems the absolute minimum or maximum is not needed but a restricted optimum i.e. the best possible in the given condition

Problem Statements

Given a design vector $\mathbf{x} = \left[x_1, x_2, \cdots, x_n \right]^T$

An objective function $f(\boldsymbol{x})$

A set of equality constraints $\boldsymbol{g}(x)=0$

A set of inequality constraints, $\boldsymbol{h}(x)\geq 0$

The general problem formulation:

$$\begin{aligned} &\min_{\mathbf{x}} \ f(\mathbf{x}) \\ &s.t. \quad \mathbf{g}(\mathbf{x}) = 0 \\ &\qquad\ \ \mathbf{h}(\mathbf{x}) \geq 0 \end{aligned}$$

Examples- An Inspector Problem (Linear Programming):

Assume that it is desired to hire some inspectors for monitoring a production line. A total amount of 1800 species of products are manufactured every day (8 working hours), while two grades of inspectors can be found. Maximum, 8 grade A inspector and 10 grade B inspector are available from the job market. Grade A inspectors can check 25 species/hour, with an accuracy of 98 percent. Grade B inspectors can check 15 species/hour, with an accuracy of 95 percent. The wage of a grade A inspector is $4.00/hour, and the wage of a grade B inspector is $3.00/hour. What is the optimum policy for hiring the inspectors?

Problem Formulation

Assume that the x_1 grade A inspectors, x_2 grade B inspects are hired, then

- total cost to be minimized

  $4(8)x_1 + 3(8)x_2 + 25(8)(0.02)(2)x_1 + 15(8)(0.05)(2)\, x_2$

  $= 40\, x_1 + 36\, x_2$

- manufacturing constraint

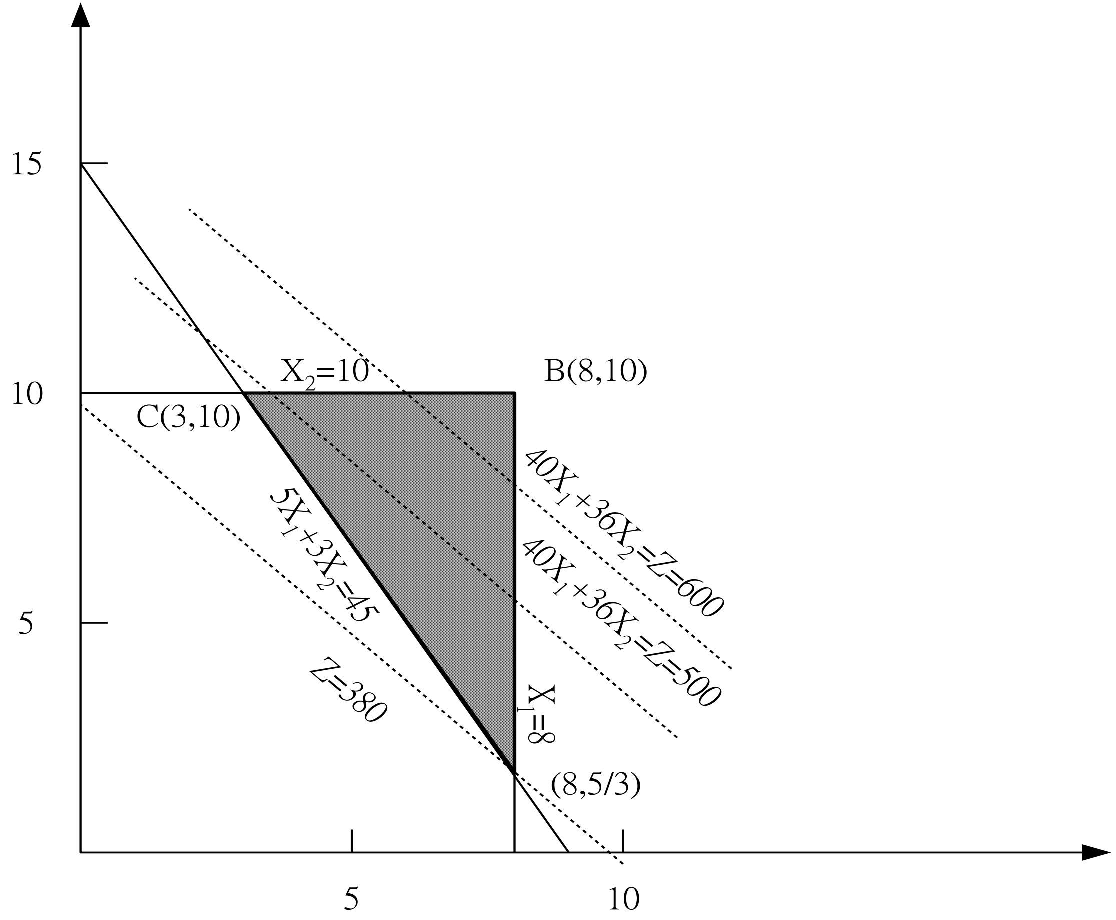
  $25(8)\, x_1 + 15(8)\, x_2 \geq 1{,}800 \;\rightarrow\; 200\, x_1 + 120\; x_2 \geq 1{,}800$

- no. of inspectors available:

  $0 \leq x_1 \leq 8$

  $0 \leq x_2 \leq 10$

The Graphical Solution



Example – optimal pipe diameter

In a chemical plant, the cost of pipes, their fittings, and pumping are important investment cost. Consider a design of a pipeline L feet long that should carry fluid at the rate of Q gpm. The selection of economic pipe diameter D(in.) is based on minimizing the annual cost of pipe, pump, and pumping. Suppose the annual cost of a pipeline with a standard carbon steel pipe and a motor-driven centrifugal pump can be expressed as:

$$f = 0.45L + 0.245LD^{1.5} + 3.25(hp)^{1/2} + 61.6(hp)^{0.925} + 102$$

$$\textit{where}$$

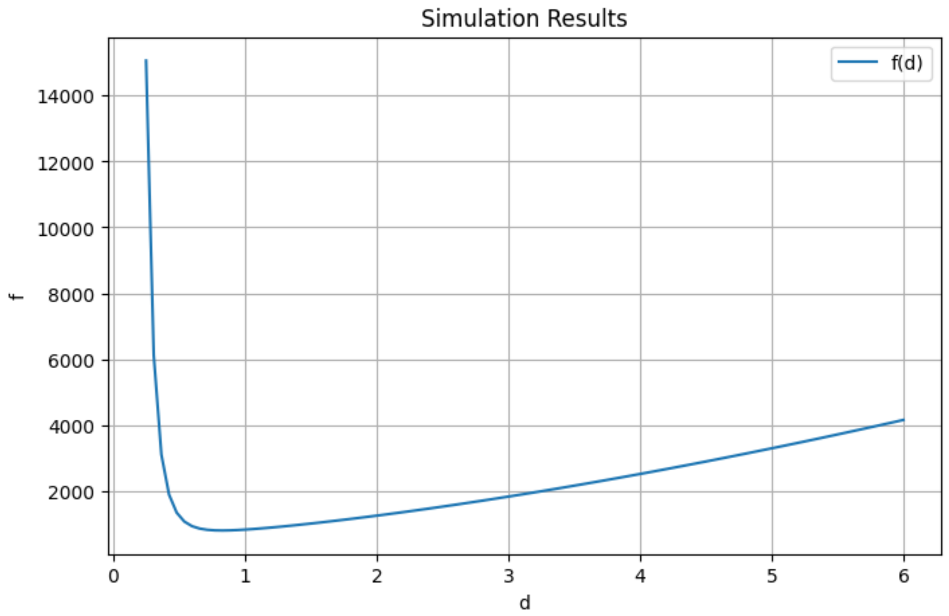
$$hp = 4.4\times10^{-8}\,\frac{LQ^3}{D^5} + 1.92\times10^{-9}\,\frac{LQ^{2.68}}{D^{4.68}}$$

Formulate the appropriate single-variable optimization problem for designing a pipe of length 1000ft with a fluid rate of 20gpm. The diameter of the pipe should be between 0.25 to 6 in.

Python Code

https://colab.research.google.com/drive/1YcFnrEFjGIefFn9C8MHTS7PWEMMql11g?usp=sharing

```
import numpy as np
import matplotlib.pyplot as plt

# 1. Setup the variables
d = np.linspace(0.25, 6, 100)

l = 1000
q = 20

# 2. Perform Calculations
hp = 4.4e-8 * (l * q**3) / d**5 + 1.92e-9 * (l * q**2.68) / d**4.68


f = 0.45 * l + 0.245 * l * d**1.5 + 3.25 * hp**0.5 + 61.6 * hp**0.925 + 102

# 3. Output the results
# Printing the first few values to verify
print("First 5 values of f:")
print(f[:5])

# Optional: Plotting the data
plt.figure(figsize=(8, 5))
plt.plot(d, f, label='f(d)')
plt.xlabel('d')
plt.ylabel('f')
plt.title('Simulation Results')
plt.grid(True)
plt.legend()
plt.show()
```



Example - A Chemical Reactor Design Problem

$$A \underset{k_1}{\longrightarrow} B \underset{k_2}{\longrightarrow} C$$

$$k_1 = k_{10} e^{-E_1/RT}$$

$$k_2 = k_{20} e^{-E_2/RT}$$

Material Balances:

$$\frac{dC_A}{dt} = -k_1 C_A$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$

$$\frac{dC_C}{dt} = k_2 C_B$$

Energy Balances:

$$\rho V C_P \frac{dT}{dt} = (-\Delta H_1) k_1 C_A V + (-\Delta H_2) k_2 C_B V - UA(T - T_J)$$

Example - A Chemical Reactor Design Problem

Problem: Assume that C_0, T_J, t_f can be designed, it is our objective to find good settings such that $C_B(t_f)$ can be maximized

Special Types of Optimization problems

❑ Unconstrained optimization

$$\min_{\mathbf{x}} f(\mathbf{x})$$

- In here, neither equality nor inequality constraint exists

❑ Linear Programming (LP)

$$\max_{\mathbf{x}} f(\mathbf{x}) = \mathbf{c}^T \mathbf{x} = c_1 x_1 + c_2 x_2 + \cdots + c_n x_n$$

$$s.t. \sum_{i=1}^{n} a_{ij} x_i - b_j \geq 0 \qquad j = 1, \cdots, m$$

$$x_i \geq 0$$

- In here, all the objective function and constraints are linear functions to **x**

Special Types of Optimization problems

❑Quadratic Programming (QP)

$$\max_{\mathbf{x}} f(\mathbf{x}) = a_0 + \mathbf{a}_1\mathbf{x} + \mathbf{x}^{\mathrm{T}}\mathbf{Q}\mathbf{x}$$

$$s.t. \sum_{i=1}^{n} a_{ij}x_i - b_j \geq 0 \qquad j = 1, \cdots, m$$

$$x_i \geq 0$$

In here, only the objective function is quadratic,
but the constraints are linear

Special Types of Optimization problems

- **Optimization with respect to a continuous variable (Calculus of Variation)**

Find *x(t)* such that

$$y = \int_a^b F(t, x, x')\,dt$$

is minimized

Special Types of Optimization problems

Dynamic Programming (DP)

Here, x_i represents the state of the system in the *ith* stage and u_i is some decision variable, i.e. some decision taken at the *ith* stage. The values of x_i and u_i determine uniquely x_{i+1}:

$$x_{i+1} = f(x_i, u_i, i)$$

Here, it is assumed that *x0* is known, when the state of the system changes from *xi* to *xi+1*, there is an improvement or degradation in an objective function as cost or profit. Let this be $J=f(x_i,u_i,i)$, then the cumulative profit over N stages is:

$$J_C = \sum_{i=1}^{N} J(x_i, u_i, i)$$

Special Types of Optimization problems

As x_0 is fixed the magnitude of the cumulative profit is determined only by the various decisions taken u_i (i=0 to N-1). Hence Jc is to be optimized with respect to u_i.

Now, constraints may be imposed on x_i and u_i. This constitutes a dynamic programming (DP)

Special Types of Optimization problems

- **Integer Programming (IP):**

Some of the variables are constrained to take integer values

The Iterative Optimization Procedure – A Basic Idea

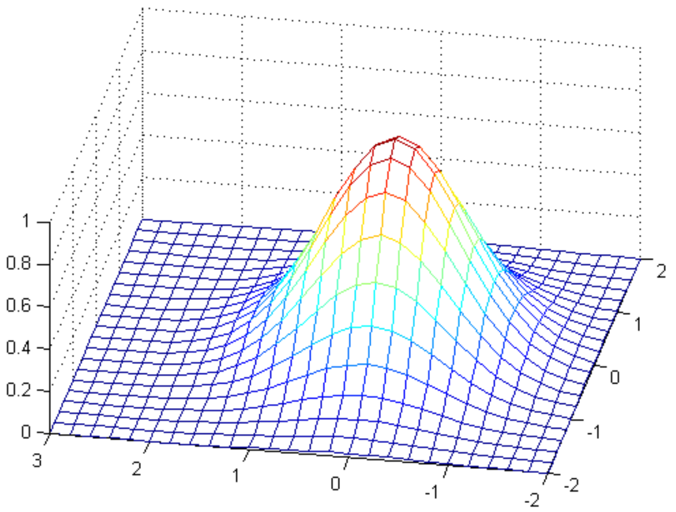
Optimization is basically performed in a fashion of iterative optimization. We give an initial point **x**0, and a direction **s**, and then perform the following line search:

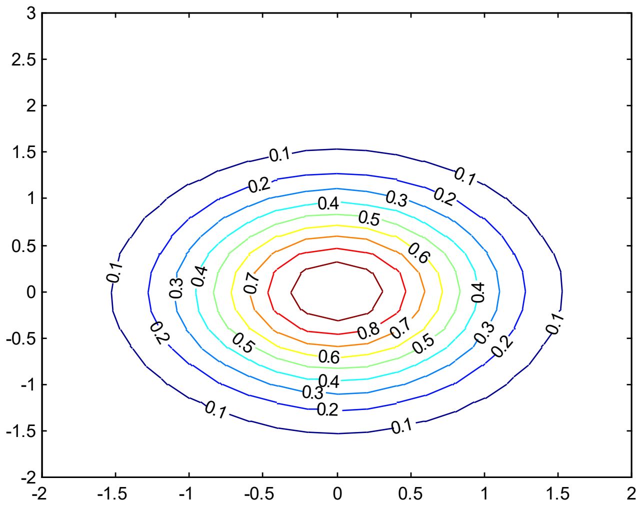
$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha^* \mathbf{s}$$

where α^* is the optimal point for the objective function and satisfies all the constraints. Then we start from **x**1 and find the other direction **s**', and perform a new line search until the optimum is reached.

Terminology

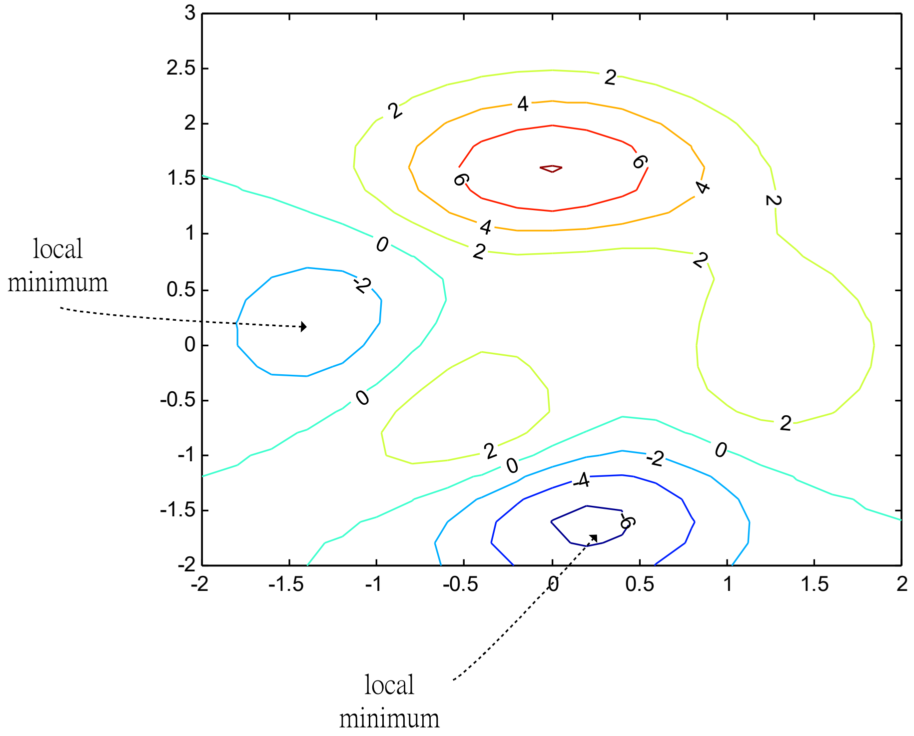
Contour Plot





Terminology - Continued

Global optimum v.s. Local optimum



Terminology - Continued

Convex v.s. Concave functions

- A function $\phi(x)$ is called convex over the domain R if for all x1, x2$\in$R, and 0<θ<1, then

$$\phi\left[\theta x_1 + (1-\theta)x_2\right] \le \theta\phi(x_1) + (1-\theta)\phi(x_2)$$

- If the inequality holds, the function is called strictly convex. A concave function is a function that cannot have a value smaller than that obtained by a linear approximation.

Terminology - Continued

Unimodal function

- If the function increases up to a maximum then decreases for all other values, it is called a unimodal function

Gradient and Hessian of a function

- Gradient of a function $f(\mathbf{x})$ is defined by a column vector of the first partial derivatives of $f(\mathbf{x})$ with respect to each variables $x1$ to xn evaluated at some $\mathbf{x}$
- Hessian matrix of $f(\mathbf{x})$ is defined as the symmetric square matrix of second partial derivatives

Terminology - Continued

Feasible Regions-

- Region of search.
- The region bounded by the inequality and equality constraints.

Convex region of search (not convex function):

- A convex region is one region such that a line joining any two points lying in the region.

Thank you