Optimization

What is optimization about?

- Typical problems in process design or plant operation have many (possibly infinite) solutions.
- Optimization is concerned with selecting the best alternative among the entire set by efficient quantitative methods.
- Computer methods are typically required to do the necessary calculations.

Optimization Problems Found in Industry

Problem 1: The rate of return on investment is given by

$$R = 100(1-t)\frac{[S-(V+F/n)]}{I/n}$$

$$\begin{aligned}
R &= \text{rate of return} \\
t &= \text{tax rate} \\
S &= \text{sales price} \\
V &= \text{variable cost of production} \\
F &= \text{fixed charge} \\
n &= \text{number of units produced} \\
I &= \text{total investment}
\end{aligned}$$

What is the maximum rate of return as a function of n?

Problem 2: A refinery has two crude oils that have yields and maximum allowable production rates as shown below:

	Crude 1	Crude 2	Rate
Gasoline	70	31	6,000
Kerosene	6	9	2,400
Fuel oil	24	60	12,000

The profit on processing crude 1 is \$1.00/bbl and on crude 2 is \$0.70/bbl.

What are the optimum daily feed rates of the two crudes to this plant?

Problem 3: A chemical company sells three products and has found that its revenue function is $f = 10x + 4.4y^2 + 2z$ where x, y and z are the monthly production rates of each chemical. Furthermore, limits on production rates are described by

$$
\begin{aligned}
x &\geq 2 \\
z^2 + 2y^2 &\geq 3 \\
x + 4y + 5z &\leq 32 \\
x + 3y + 2z &\leq 29
\end{aligned}
$$

What is the best production schedule for this company?

Course Outline

- Unconstrained Optimization
- Constrained Optimization
- Numerical Methods
- Linear Programming

UNCONSTRAINED OPTIMIZATION

Example 1: A non-elementary reaction $A \rightarrow B$ is occurring in a CSTR with the following rate kinetics:

$$r_A = \frac{k_1 C_A}{(k_2 + C_A)(k_3 + C_A)} \tag{1}$$

where

$$\begin{aligned} k_1 &= 0.25 \\ k_2 &= 0.50 \\ k_3 &= 500 \end{aligned}$$

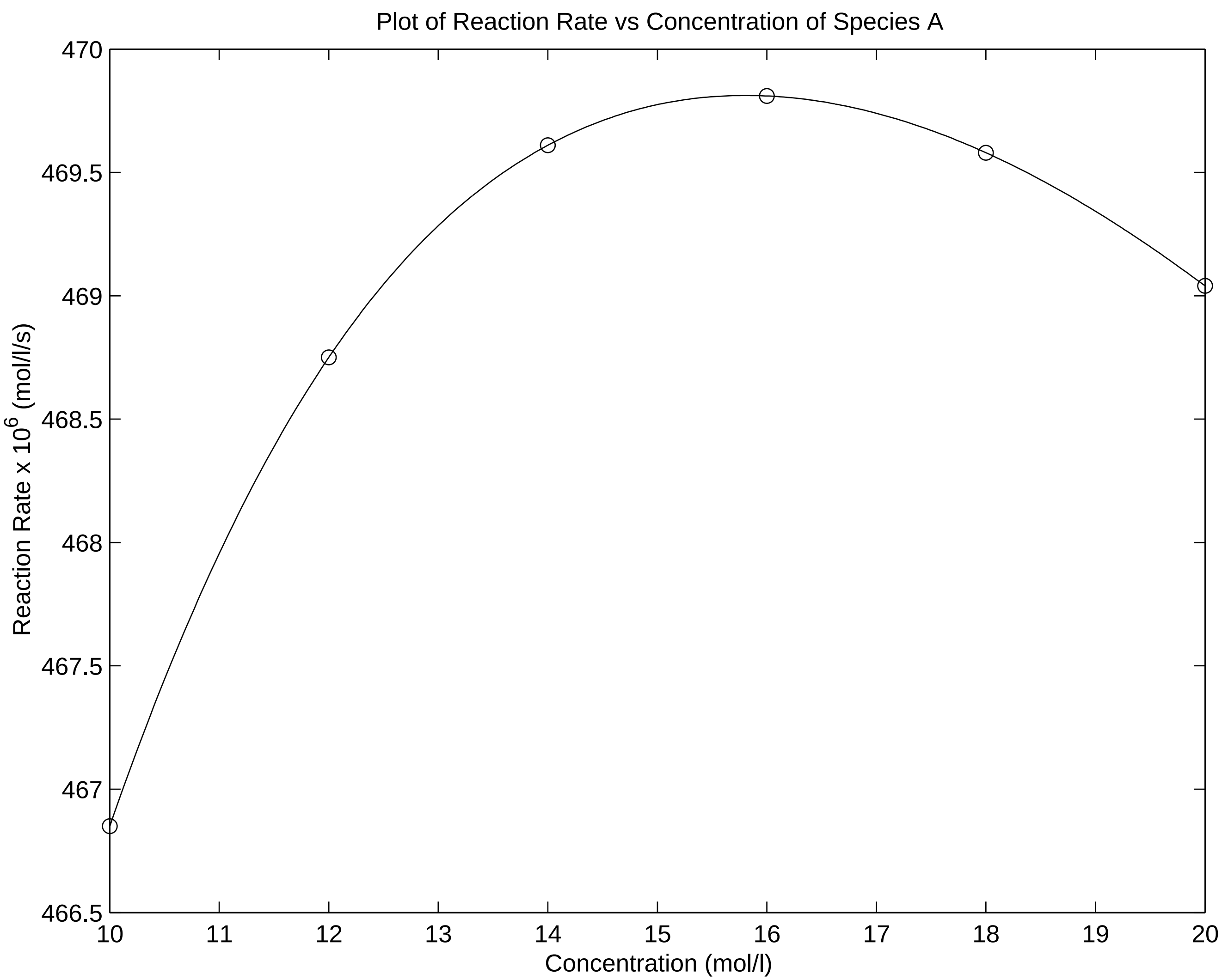
It is possible to operate the reactor at any concentration between $C_A = 10$ and $C_A = 20\ mol/l$.

At what concentration should it be operated so that the rate is maximum

Brute Force Solution Strategy

- Choose different values of C_A between 10 and 20 mol/l and calculate r_A at each value of C_A.
- Plot r_A vs C_A.
- Fit a curve through the points and find the C_A that corresponds to the maximum r_A.

C_A	$r_A \times 10^6$
10	466.85
12	468.75
14	469.61
16	469.81
18	469.58
20	469.04



Plot of Reaction Rate vs Concentration of Species A
Reaction Rate x 10^6 (mol/l/s)
Concentration (mol/l)
470
469.5
469
468.5
468
467.5
467
466.5
10
11
12
13
14
15
16
17
18
19
20

EXAMPLE 2

Suppose:

$$r_A = \frac{k_1 C_A C_B}{(k_2 + C_A)(k_3 + C_B)} \tag{2}$$

What are the optimal values of C_A and C_B?

Analysis of Brute Force Strategy

- Strategy is simple to use.
- However, it is tedious to use if there is more than one variable involved.
- Constraints are not handled explicitly.

Review of Material from Elementary Calculus

Given a function $f(x)$ that is continuous and twice differentiable, a *stationary point* x^* is defined by:

$$\frac{\partial f}{\partial x}|_{x=x^*} = 0 \tag{3}$$

- x^* is a minimum if $\frac{\partial^2 f}{\partial x^2}|_{x=x^*} > 0$
- x^* is a maximum if $\frac{\partial^2 f}{\partial x^2}|_{x=x^*} < 0$
- x^* is a saddle point if $\frac{\partial^2 f}{\partial x^2}|_{x=x^*} = 0$

EXAMPLE 1 REVISITED

A non-elementary reaction $A \rightarrow B$ is occurring in a CSTR with the following rate kinetics:

$$r_A = \frac{k_1 C_A}{(k_2 + C_A)(k_3 + C_A)} \tag{4}$$

where

$$\begin{aligned} k_1 &= 0.25 \\ k_2 &= 0.50 \\ k_3 &= 500 \end{aligned}$$

It is possible to operate the reactor at any concentration between $C_A = 10$ and $C_A = 20\ mol/l$.

At what concentration should it be operated so that the rate is maximum

$$r_A = \frac{k_1 C_A}{(k_2 + C_A)(k_3 + C_A)} \tag{5}$$

$$\frac{\partial r_A}{\partial C_A} = 0 => C_A = 15.81 \tag{6}$$

It can be easily shown that the second derivative is negative and so $C_A = 15.81$ is a maximum.

Analysis of Analytical Approach

- Provides explicit formulae to determine optimal values.
- However, it requires the funciton to be differentiated twice.
- Constraints are not handled explicitly.

Sign Convention

We will consider only minimization problems from now on with the knowledge that *maximizing* a function is the same as *minimizing* the *negative* of that function.

For example,

$$Max(-2x^2 - 2x + 1) \tag{7}$$

is the same as

$$Min(+2x^2 + 2x - 1) \tag{8}$$

Multivariable Version of Analytical Approach

Problem without Constraints

Consider a scalar function $f(x)$ where x is a vector.

$$x = [x_1 \; x_2 \; ... \; x_n]^T$$

Then, the necessary conditions for a local minimum are:

$$\frac{\partial f}{\partial x}|_{x=x^*} = 0 \tag{9}$$

The sufficient conditions for a local minimum are:

$$\frac{\partial^2 f}{\partial x^2}|_{x=x^*} > 0 \tag{10}$$

The necessary conditions for a local minima imply that we need to solve:

$$\begin{aligned}
\frac{\partial f}{\partial x_1} &= 0 \\
\frac{\partial f}{\partial x_2} &= 0 \\
&\cdot \\
&\cdot \\
\frac{\partial f}{\partial x_n} &= 0
\end{aligned} \tag{11}$$

The solution of the above n nonlinear equations results in the vector x^*.

The <u>sufficient</u> conditions for a local minima imply that the following matrix has all positive eigenvalues.

$$\begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ . & . & \cdots & \\ . & . & \cdots & \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \Big|_{x=x^*} \tag{12}$$

If some eigenvalues are positive and some are negative, the point $x = x^*$ is called a saddlepoint.

If one or more eigenvalues are zero, the point $x = x^*$ is called a singular point and more information is needed to determine if the point is a minimum point or not.

EXAMPLE 2:

Find the stationary points for the following functions and determine if the stationary points are a minimum, saddlepoint or singular points.

1. $f(x) = x_1^2 - 2x_1x_2 + 4x_2^2$
2. $f(x) = -x_1^2 + 2x_1x_2 + 3x_2^2$
3. $f(x) = x_1^2 - 4x_1x_2^2 + 3x_2^4$

EXAMPLE 3

A chemical company produces two products and has determined that its cost function is given by:

$$f(x) = x_1^4 - 2x_1^2 x_2 + x_2^2 + x_1^2 - 2x_1 + 5$$

where x_1 is the production rate of the first product and x_2 is the production rate of the second product. Determine the production rates of x_1 and x_2 at which the cost function is minimized.