Formulating an Optimization Problem

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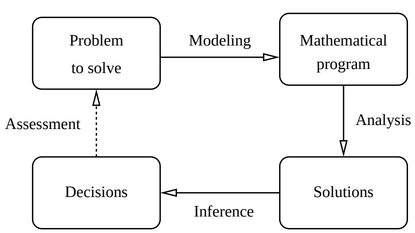
ChE 4G03: Optimization in Chemical Engineering

Outline

The Importance of a Good Formulation

Model-based Optimization Procedure:



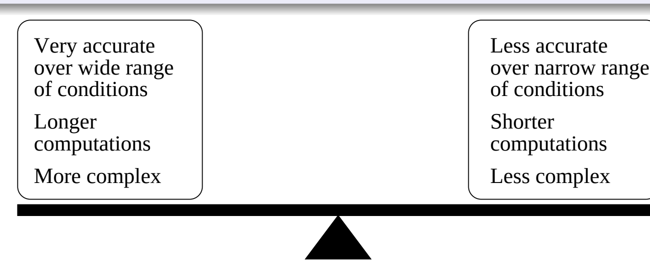
1. The conclusions are drawn from the model (mathematical program), not from the problem!
2. An inadequate model typically leads to false conclusions
3. The model must be computationally tractable: its analysis must be practical!

Dofasco:
"We find it useful to formulate the optimization problem even if we cannot solve it..."

Validity vs. Tractability

1. The validity of a model is the degree to which inferences drawn from the model hold for the real system
2. The tractability of a model is the degree to which this model admits convenient analysis – How much analysis is practical

Tradeoff:
Decision makers almost always confront a tradeoff between validity of optimization models and their tractability to analysis



Optimization Model Formulation

Standard Model:

Optimization models (also called mathematical programs) represent problem choices as decision variables and seek values that maximize (or minimize) objective functions of the decision variables subject to constraints on variable values expressing the limits on possible decision choices

$\max_{\mathbf{x}} f(\mathbf{x})$	$\longleftarrow$	Objective function
s.t.		
$\mathbf{h}(\mathbf{x}) = \mathbf{0}$	$\longleftarrow$	Equality constraints
$\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$	$\longleftarrow$	Inequality constraints
$\mathbf{x}_{\min} \leq \mathbf{x} \leq \mathbf{x}_{\max}$	$\longleftarrow$	Variable bounds

Decision Variables, $\mathbf{x}$

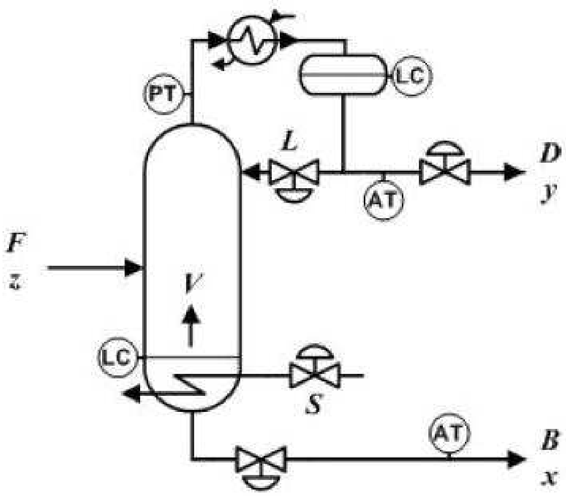
1. At the **formulation stage**, decision variables can be grouped into two categories:
   - Independent variables, whose values can be changed *independently* to modify the behavior of the system
   - Dependent variables, whose behavior is determined by the values selected for the independent variables

   Such a grouping helps understanding!
2. At the **solution stage**, independent and dependent variables need not be distinguished: the solution method just sees an optimization problem involving many variables

Examples of Decision Variables:

- Design: reactor volume, number of trays, heat exchanger area, etc.
- Operations: temperature, flow, pressure, valve opening, etc.
- Management: feed type, purchase price, sales price, etc.

Decision Variables, $\mathbf{x}$ (cont'd)



Exercise:
Identify independent and dependent variables

Decision Variables, $\mathbf{x}$ (cont'd)

Discrete vs. Continuous Decision Variables:

1. A variable is discrete if it is limited to a fixed or countable set of values (e.g., all-or-nothing, either-or decisions)
2. A variable is continuous if it can take on any value in a specified interval

Problems with both discrete and continuous variables are called mixed-integer programs

Heuristics:

When there is an option, modeling with continuous variables is preferred to discrete variables (for tractability reasons)

Example: Variable magnitudes are likely to be large enough that fractions have no practical importance

Decision Variables, $\mathbf{x}$ (cont'd)

Exercise: Decide whether a discrete or a continuous variable would be best employed to model each of the following quantities:

1. the optimal temperature of a chemical process
2. the warehouse slot assigned a particular product
3. whether a capital project is selected for investment
4. ball bearings in a plant that manufactures 10,000+/day
5. the number of aircraft produced on a defense contract

Decision Variables, $\mathbf{x}$ (cont'd)

Indexing:

In real applications, optimization models quickly grow to thousands, sometimes millions, of variables: indexed notational schemes are needed to keep large models manageable!

1. Indexes (or subscripts) permit representing collections of similar quantities with a single symbol, e.g.

$$\{x_i : i = 1, \ldots, 100\}$$

   represents 100 similar values with the same x name, distinguishing them with the index i
2. The first step in formulating a large optimization model is to choose appropriate indexes for the different dimensions of the problem; multiple indexes are extremely common!

Decision Variables, $\mathbf{x}$ (cont'd)

Exercise:

A large manufacturer of corn seed operates $\ell = 20$ facilities producing seeds of $m = 25$ hybrid corn varieties and distributes them to customers in $n = 30$ regions. The optimization problem is to carry out these production and distribution operations at minimum cost.

Let the three main dimensions in this problem be denoted as:

- f = production facility number ($f = 1, \ldots, \ell$)
- v = hybrid variety number ($v = 1, \ldots, m$)
- r = sales region number ($r = 1, \ldots, n$)

Questions:

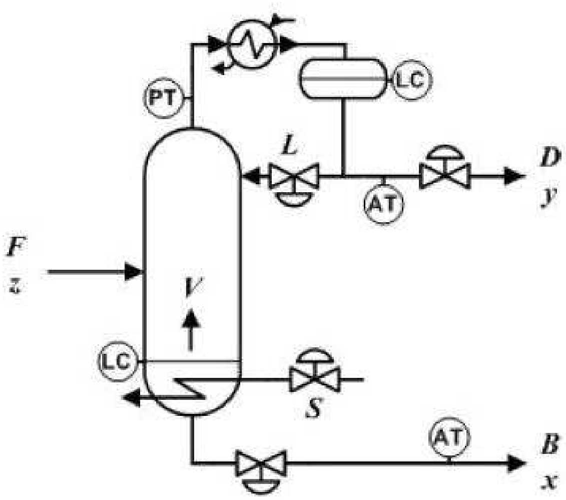
1. Choose appropriate decision variables for a model of this problem (use indexing).
2. What is the total number of decision variables for this model?

Variable Bounds, $\mathbf{x}_{\min}$, $\mathbf{x}_{\max}$

Variable bounds specify the domain of definition for decision variables: the set of values for which the variables have meaning

1. Setting the min and max values equal sets the variable to a constant value:
$$x_{\min,i} = x_{\max,i} = x_i, \quad \text{for some } i \in \{1, \ldots, n\}$$
2. The most common variable bound constraint is non-negativity, e.g.
$$x_i \geq 0, \quad \forall i = 1, \ldots, n$$

Variable Bounds, $\mathbf{x}_{\min}$, $\mathbf{x}_{\max}$ (cont'd)



Exercise:
Propose bounds for variables in the process

Main constraints, $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$, $\mathbf{h}(\mathbf{x}) = \mathbf{0}$

Main constraints of optimization models specify the restrictions and interactions, other than variable bounds, that limit decision variable values.

Inequality Constraints:

$$\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$$

1. These are one-way limits on the system and are essential for optimization
2. Inequality constraints of the form ≥ 0 and ≤ 0 are equivalent. Do you see why?
3. There can be many of these inequalities, so that $\mathbf{g}(\mathbf{x})$ is a vector (indexing is used for constraints too!)
4. We must be careful to prevent defining a problem incorrectly with no feasible region or an unbounded solution

Main constraints, $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$, $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ (cont'd)

What limits the possible solutions to the problem?

- Safety
- Product quality (contracts)
- Equipment damage (long term)
- Equipment operation
- Legal/ethical considerations

Examples:

- Max. investment available
- Max. flow rate due to pump limit
- Min. liquid flow rate on trays $t = 1, \ldots, N_t$
- Max. pressure in a closed vessel
- Max. region within which an approximation/simplification is acceptable

Main constraints, $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$, $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ (cont'd)

Equality Constraints:

$$\mathbf{h}(\mathbf{x}) = \mathbf{0}$$

1. These describe interactions between the variables in the model
2. Equality constraints are written with a zero right-hand side by convention
3. There can be many of these inequalities, so that $\mathbf{h}(\mathbf{x})$ is a vector (indexing is used for equality constraints too!)
4. There cannot be more (independent) equality constraints than decision variables in the model! Do you see why?

Main constraints, $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$, $\mathbf{h}(\mathbf{x}) = \mathbf{0}$ (cont'd)

Examples of Equality Constraints:

- material, energy, current, etc. balances, e.g. for conserved quantity q:

$$\left\{ \begin{array}{c} \text{accumulation} \\ \text{of } q \end{array} \right\} = \left\{ \begin{array}{c} \text{rate of} \\ q \text{ in} \end{array} \right\} - \left\{ \begin{array}{c} \text{rate of} \\ q \text{ out} \end{array} \right\} + \left\{ \begin{array}{c} \text{generate} \\ \text{rate of } q \end{array} \right\}$$

- constitutive relations, e.g.

$$Q = hA\Delta T$$
$$r_A = k_0 \exp(-\tfrac{E}{RT})$$

- equilibrium relations, e.g. VLE
- decisions by the engineer, e.g. $F_A - 2F_B = 0$
- behavior enforced by controllers, e.g. temperature set-point $T_s = 231\ \mathrm{K}$

Objective Function, $f(\mathbf{x})$

Objective functions in optimization models tell us how to rate decisions

1. We need a quantitative measure; a qualitative measure such as "good" or "bad" is not adequate!
2. A scalar objective function is preferred for solving, even though multiple objectives are typical in real life!
3. There is no fundamentale or practical difference between max and min problems:

$$\max_{\mathbf{x}} f(\mathbf{x}) \quad \Leftrightarrow \quad \min_{\mathbf{x}} -f(\mathbf{x})$$

Objective Function, $f(\mathbf{x})$

How do we define a scalar that represents performance?

- Maximize profit (or mininize cost) – Economics
- Maximize product quality
- Mininize energy use
- Minimize polluting effluents
- Maximize safety
- etc.

Exercise: Write the expression for an objective function $f(\mathbf{x})$ that depends on *all* variables x_i, $i = 1, \ldots, n$, and the cost associated with each variable is c_i.

1. Express the answer as a summation of indexed variables
2. Express the answer as a product of vectors

Case Study: Model Formulation

A refinery distills crude petroleum from two sources, Saudi Arabia and Venezuela, into three main products: gasoline, jet fuel and lubricants. The two crudes differ in chemical composition and thus yield different product mixes (the remaining 10% of each barrel is lost to refining):

- Each barrel of Saudi crude yields 0.3 barrel of gasoline, 0.4 barrel of jet fuel, and 0.2 barrel of lubricants;
- Each barrel of Venezuelan crude yields 0.4 barrel of gasoline, 0.2 barrel of jet fuel, and 0.3 barrel of lubricants.

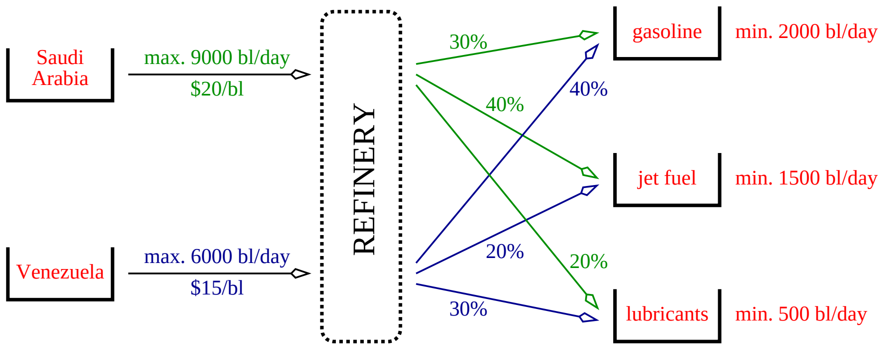
The crudes also differ in cost and availability:

- Up to 9,000 barrels per day of Saudi crude are available at the cost \$20 per barrel;
- Up to 6,000 barrels per day of Saudi crude are also available at the lower cost \$15 per barrel.

Contracts with independent distributors require that the refinery produce 2,000 barrels per day of gasoline, 1,500 barrels per day of jet fuel, and 500 barrels per day of lubricants.

Case Study: Model Formulation (cont'd)

Question:
Formulate an optimization model in standard form so as to fulfill the requirements in the most efficient manner.



Graphing Constraints

1. Very simple graphic solution have enough power to deal with tiny models, such as 2- or 3-variable models
2. The first issue in graphic solution is the feasible set:

The feasible set S (or feasible region) of an optimization model is the collection of choices for decision variables satisfying *all* model constraints:

$$S \triangleq \{\mathbf{x} : \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \mathbf{h}(\mathbf{x}) = \mathbf{0}, \mathbf{x}_{\min} \leq \mathbf{x} \leq \mathbf{x}_{\max}\}$$

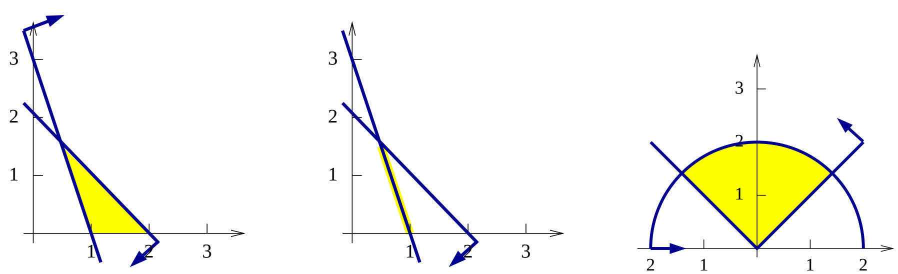
- The set of all points satisfying an equality constraint plots as a line or a curve (in 2-d)
- The set of all points satisfying an inequality constraint plots as a boundary line or curve, where the constraint holds with equality, along with all points on whichever side of the boundary satisfy the constraint as an inequality

Examples of Feasible Regions

$$x_1 + x_2 \leq 2 \qquad 3x_1 + x_2 \geq 3 \qquad x_1, x_2 \geq 0$$

$$x_1 + x_2 \leq 2 \qquad 3x_1 + x_2 = 3 \qquad x_1, x_2 \geq 0$$

$$(x_1)^2 + (x_2)^2 \leq 4 \qquad |x_1| - x_2 \leq 0$$



Exercise: Plot the feasible region in the two-crude case study.

Graphing Objective Functions

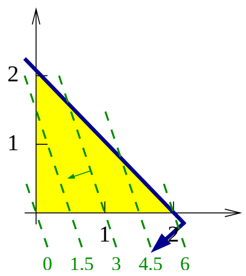
1. To find out the best feasible point, the objective function must be introduced into a plot
2. Objective functions are normally plotted in the same coordinate system as the feasible set by introducing contours:

The contour C_z of an objective function (in the decision variable space) is the line or curve passing through points having equal objective values z:

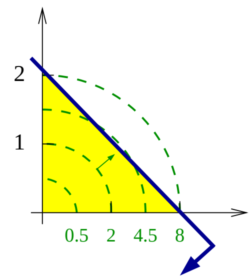
$$C_z \triangleq \{\mathbf{x} : f(\mathbf{x}) = z\}$$

Examples of Graphic Solutions

$$\min_{x_1,x_2} \; 3x_1 + x_2$$
$$\text{s.t. } x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$



$$\max_{x_1,x_2} \; (x_1)^2 + (x_2)^2$$
$$\text{s.t. } x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$



Exercise: Plot the objective function contours in the two-crude case study.

Optimization Outcomes

Optimum

An optimal solution $\mathbf{x}^*$ is a feasible choice for decision variables with objective function value at least equal to that of any other solution satisfying all constraints. For a minimization problem:

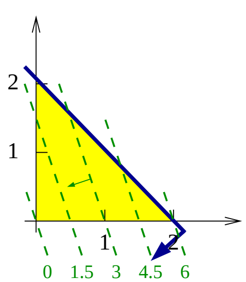
$$f(\mathbf{x}^*) \leq f(\mathbf{x}), \quad \forall \mathbf{x} \in S$$

1. Optimal solutions show graphically as points lying on the best objective function contour that intersects the feasible region
2. The optimal value f^* in an optimization model is the objective function value of any optimal solutions: $f^* = f(\mathbf{x}^*)$
3. An optimization model can have only one optimal value
4. An optimization model may have:
   - a unique optimal solution
   - several alternative optimal solutions
   - no optimal solutions (unbounded or infeasible models)

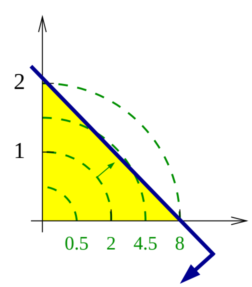
Examples of Graphic Solutions

What is the **optimal solution**? What is the **optimal value**?

$$\min_{x_1,x_2} \; 3x_1 + x_2$$
$$\text{s.t. } x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$



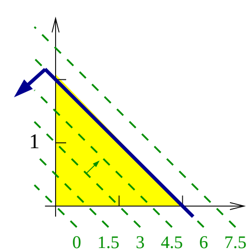
$$\max_{x_1,x_2} \; (x_1)^2 + (x_2)^2$$
$$\text{s.t. } x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$



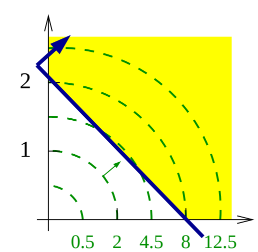
Examples of Graphic Solutions

What is the **optimal solution**? What is the **optimal value**?

$$\max_{x_1,x_2} \; 3x_1 + 3x_2$$
$$\text{s.t. } x_1 + x_2 \leq 2$$
$$x_1, x_2 \geq 0$$



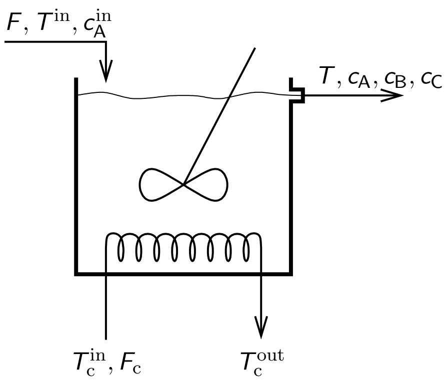
$$\max_{x_1,x_2} \; (x_1)^2 + (x_2)^2$$
$$\text{s.t. } x_1 + x_2 \geq 2$$
$$x_1, x_2 \geq 0$$



Exercise: Determine a graphic solution to the two-crude case study.

Recognizing Optimization Opportunity

Class Exercise: What is optimum for the following process system?



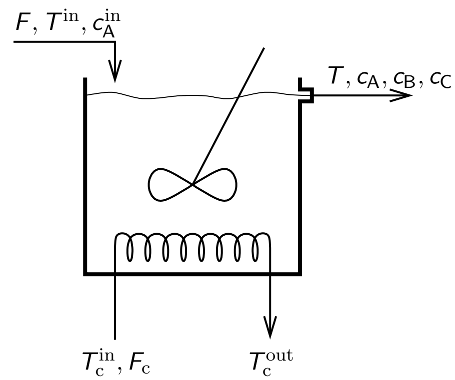
This is an isothermal CFSTR with the series reaction:

$$A \rightarrow B \rightarrow C$$

- The goal is to maximize C_B in the effluent at steady state
- Only the flow rate of feed F can be adjusted

Recognizing Optimization Opportunity

Class Exercise: What is optimum for the following process system?



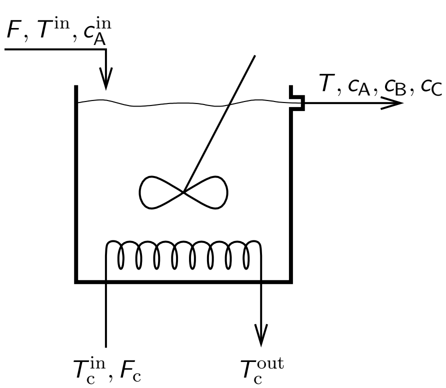
This is an isothermal CFSTR with the series reaction:

$$A \rightarrow B \rightarrow C$$

- The goal is to maximize C_C in the effluent at steady state
- Only the flow rate of feed F can be adjusted

Recognizing Optimization Opportunity

Class Exercise: What is optimum for the following process system?



This is an isothermal CFSTR with the parallel reaction:

$$A \rightarrow B \qquad A \rightarrow C$$

- The goal is to maximize C_B in the effluent at steady state
- Only the flow rate of feed F can be adjusted
- What other variable would you like to adjust?