OPTIMIZATION

Numerical methods in chemical engineering
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OVERVIEW

• In this lecture we get introduced to constrained and unconstrained optimization.
• We will use the simplex method to solve linear programming problems (LP)
• We will use the Lagrange multiplier method to solve nonlinear programming problems (NLP’s)
• And we will briefly discuss optimal control, using Pontryagin’s principle.
• Lastly we will play a little with another optimization platform (AMPL)
WHAT IS OPTIMIZATION?

• Optimization is minimization or maximization of an objective function (also called a performance index or goal function) that may be subject to certain constraints:

\[
\min f(x) \quad \text{Goal function}
\]

\[
s.t. \quad g(x) = 0 \quad \text{Equality constraints}
\]

\[
h(x) \geq 0 \quad \text{Inequality constraints}
\]

\[
\min f(x) = \max -f(x)
\]

(10-1)
## OPTIMIZATION SPECTRUM

### MATHEMATICAL PROGRAMMING

<table>
<thead>
<tr>
<th>Problem</th>
<th>Method</th>
<th>Solvers</th>
</tr>
</thead>
</table>
| LP      | Simplex method  
Barrier methods | Linprog (Matlab)  
CPLEX (GAMS, AIMMS, AMPL, OPB) |
| NLP     | Lagrange multiplier method  
Successive linear programming  
Quadratic programming | Fminsearch/fmincon (Matlab)  
MINOS (GAMS, AMPL)  
CONOPT (GAMS) |
| MIP     | Branch and bound  
Dynamic programming  
Generalized Benders Decomposition  
Outer Approximation method  
Disjunctive programming | Bintprog (Matlab)  
DICOPT (GAMS)  
BARON (GAMS) |
| MILP    |        |         |
| MINLP   |        |         |
| MIQP    |        |         |

### META HEURISTICS

- Neural networks, fuzzy modeling, genetic algorithms, expert systems, etc.

### ADVANCED TOPICS

- Constraint programming, stochastic programming, multi-objective programming, etc.
FACTORS OF CONCERN

- Continuity of the functions
- Convexity of the functions
- Global versus local optima
- Constrained versus unconstrained optima
LINEAR PROGRAMMING

• In linear programming the objective function and the constraints are linear functions!

• For example:

$$\text{max } z = f(x_1, x_2) = 40x_1 + 88x_2$$

$$s.t.$$

$$2x_1 + 8x_2 \leq 60$$

$$5x_1 + 2x_2 \leq 60$$

$$x_1 \geq 0$$

$$x_2 \geq 0$$

(10-2)

If the constraints are satisfied, but the objective function is not maximized/minimized we speak of a feasible solution.

If also the objective function is maximized/minimized, we speak of an optimal solution!
PLOTTING THE CONSTRAINTS

$5x_1 + 2x_2 = 60$

$2x_1 + 8x_2 = 60$

Feasible solutions
PLOTTING THE OBJECTIVE FUNCTION

Optimal solution
NORMAL FORM OF AN LP PROBLEM

\[
\max z = f(x_1, x_2) = 40x_1 + 80x_2 \\
\text{s.t.} \\
2x_1 + 8x_2 \leq 60 \\
5x_1 + 2x_2 \leq 60 \\
x_1 \geq 0 \\
x_2 \geq 0
\]

\[
\max f(x) = 40x_1 + 88x_2 \\
\text{s.t.} \\
2x_1 + 8x_2 + x_3 = 60 \\
5x_1 + 2x_2 + x_4 = 60 \\
x_i \geq 0 \{i = 1, ..., 4\}
\]

\[\text{(10-3)}\]

\(x_3\) and \(x_4\) are called \textbf{slack variables}, they are non auxiliary variables introduced for the purpose of converting inequalities into equalities.
THE SIMPLEX METHOD

• We can formulate our earlier example to the normal form and consider it as the following augmented matrix:

\[
\begin{bmatrix}
z & x_1 & x_2 & x_3 & x_4 & b \\
1 & -40 & -88 & 0 & 0 & 0 \\
0 & 2 & 8 & 1 & 0 & 60 \\
0 & 5 & 2 & 0 & 1 & 60 \\
\end{bmatrix}
\]

\( T_0 \) (10-4)

This matrix is called the (initial) simplex table.

Each simplex table has two kinds of variables, the **basic variables** (columns having only one nonzero entry) and the **nonbasic variables**
THE SIMPLEX METHOD

Every simplex table has a feasible solution. It can be obtained by setting the nonbasic variables to zero: $x_1 = 0$, $x_2 = 0$, $x_3 = 60/1$, $x_4 = 60/1$, $z = 0$
THE OPTIMAL SOLUTION?

• The optimal solution is now obtained stepwise by pivoting in such way that $z$ reaches a maximum.

• The big question is, how to choose your pivot equation …
STEP 1: SELECTION OF THE PIVOT COLUMN

- Select as the column of the pivot, the first column with a negative entry in Row 1. In our example, that’s column 2 (-40)

\[
T_0 = \begin{bmatrix}
z & x_1 & x_2 & x_3 & x_4 & b \\
1 & -40 & -88 & 0 & 0 & 0 \\
0 & 2 & 8 & 1 & 0 & 60 \\
0 & 5 & 2 & 0 & 1 & 60 \\
\end{bmatrix}
\]
**STEP 2: SELECTION OF THE PIVOT ROW**

- Divide the right sides by the corresponding column entries of the selected pivot column. In our example that is $60/2 = 30$ and $60/5 = 12$.

\[
\begin{array}{cccccc}
  z & x_1 & x_2 & x_3 & x_4 & b \\
 1 & -40 & -88 & 0 & 0 & 0 \\
 0 & 2 & 8 & 1 & 0 & 60 \\
 0 & 5 & 2 & 0 & 1 & 60 \\
\end{array}
\]

\[T_0 = \begin{bmatrix}
  1 & -40 & -88 & 0 & 0 & 0 \\
  0 & 2 & 8 & 1 & 0 & 60 \\
  0 & 5 & 2 & 0 & 1 & 60 \\
\end{bmatrix}
\]

(10-6)

- Take as the pivot equation the equation that gives the smallest quotient, so $60/5$
STEP 3: ELIMINATION BY ROW OPERATIONS

\[
T_1 = \begin{bmatrix}
1 & 0 & -72 & 0 & 8 & 480 \\
0 & 0 & 7.2 & 1 & -0.4 & 36 \\
0 & 5 & 2 & 0 & 1 & 60
\end{bmatrix}
\]

Row 1 + 8*Row 3
Row 2 + 0.4*Row 3
(10-7)

• The basic variables are now \(x_1, x_3\) and the nonbasic variables are \(x_2, x_4\). Setting the nonbasic variables to zero will give a new feasible solution: \(x_1 = 60/5, x_2 = 0, x_3 = 36/1, x_4 = 0, z = 480\)
THE SIMPLEX METHOD

• We moved from $z = 0$ to $z = 480$. The reason for the increase is because we eliminated a negative term from the equation, so: elimination should only be applied to negative entries in Row 1, but no others.

• Although we found a feasible solution, we did not find the optimal solution yet (the entry of -72 in our simplex table) → so we repeat step 1 to 3.
THE SECOND ITERATION

• Step 1: select column 3
• Step 2: $36/7.2 = 5$ and $60/2 = 30 \rightarrow$ select 7.2 as the pivot
• Elimination by row operations:

$$T_2 = \begin{bmatrix} 1 & 0 & 0 & 10 & 4 & 840 \\ 0 & 0 & 7.2 & 1 & -0.4 & 36 \\ 0 & 5 & 0 & -1/36 & 1/0.9 & 50 \end{bmatrix}$$

Row 1 + 10*Row 2
Row 3 – (2/7.2)*Row 2

• The basic feasible solution: $x_1 = 50/5$, $x_2 = 36/7.2$, $x_3 = 0$, $x_4 = 0$, $z = 840$ (no more negative entries: so this solution is also the optimal solution)
• We are going to solve the following LP problem:
  \[ \min f(x) = -5x_1 - 4x_2 - 6x_3 \]
  \[ \text{s.t.} \]
  \[ x_1 - x_2 + x_3 \leq 20 \]
  \[ 3x_1 + 2x_2 + 4x_3 \leq 42 \]
  \[ 3x_1 + 2x_2 \leq 30 \]
  \[ 0 \leq x_1, 0 \leq x_2, 0 \leq x_3 \]

  \[ \text{(10-9)} \]

Using the function LINPROG:

\[ f = [-5; -4; -6] \]
\[ A = [1 -1 1 3 2 4 3 2 0]; \]
\[ b = [20; 42; 30]; \]
\[ lb = zeros(3,1); \]
\[ [x,fval,exitflag,output,lambda] = \text{linprog}(f,A,b,[],[],lb); \]

Gives:

\[ x = 0.00 \ 15.00 \ 3.00 \]
\[ \text{lambda.ineqlin} = 0 \ 1.50 \ 0.50 \]
\[ \text{lambda.lower} = 1.00 \ 0 \ 0 \]
NONLINEAR PROGRAMMING

• In **nonlinear programming** the objective function and the constraints are **nonlinear functions**!

• For example:

\[ \begin{align*}
\min f(x) &= 5x_1^2 + 3x_2^2 \\
\text{s.t.} \\
g(x) &= 2x_1 + x_2 - 5
\end{align*} \]

(10-10)
LAGRANGE MULTIPLIER METHOD

• Consider the general problem:

\[
\min f(x) \\
\text{s.t.} \\
g(x) = 0
\]  

(10-11)

• A Lagrangian function can be defined as:

\[
L(x, \nu) = f(x) + \nu g(x)
\]  

(10-12)

• To find the optimum, differentiate \( L \) with respect to \( x \) and \( \nu \) and set the equations to zero:

\[
\frac{\partial L}{\partial x} = \frac{\partial f}{\partial x} + \nu \frac{\partial g}{\partial x} = 0, \quad g(x) = 0
\]  

(10-13)
\begin{align*}
\text{min } f(x) &= 5x_1^2 + 3x_2^2 \\
\text{s.t.}
\quad g(x) &= 2x_1 + x_2 - 5 \\
L &= 5x_1^2 + 3x_2^2 + \nu(2x_1 + x_2 - 5) \\
\frac{\partial L}{\partial x_1} &= 10x_1 + 2\nu = 0 \\
\frac{\partial L}{\partial x_2} &= 6x_2 + \nu = 0 \\
\frac{\partial L}{\partial \nu} &= g(x) = 2x_1 + x_2 - 5 = 0
\end{align*}
\hspace{1cm} (10-14)
LMM FOR NLPs WITH INEQUALITY CONSTRAINTS

• When the problem has the following shape:

\[
\begin{align*}
\text{min } f(x) \\
\text{s.t.} \\
h_j(x) &= 0 \quad \{ j = 1, \ldots, m \} \\
g_i(x) &\geq 0 \quad \{ i = m + 1, \ldots, p \}
\end{align*}
\]  

(10-16)

• The Lagrangian function is defined as:

\[
L(x,u,v) = f(x) + \sum_{j=1}^{m} v_j h_j(x) + \sum_{j=m+1}^{p} u_j g_j(x)
\]  

(10-17)

\[
\nabla f(x) + \sum_{j=1}^{m} v_j \nabla h_j(x) + \sum_{j=m+1}^{p} u_j \nabla g_j(x) = 0
\]

(10-18)

This condition, known as the Karush-Kuhn-Tucker condition for optimality should be satisfied.
We are going to solve the following NLP problem:

\[ \min f(x) = -x_1 x_2 x_3 \]

s.t.

\[ 0 \leq x_1 + 2x_2 + 2x_3 \leq 72 \]

Using the function \texttt{FMINCON}:

```matlab
function f = myfun(x)
    f = -x(1) * x(2) * x(3);
end
```

\[ A = \begin{bmatrix} -1 & -2 & -2; 1 & 2 & 2 \end{bmatrix}; b = \begin{bmatrix} 0 72 \end{bmatrix}; \]

\[ x_0 = \begin{bmatrix} 10; 10; 10 \end{bmatrix}; \]

\[ \text{solution } [x,fval] = \text{fmincon(@myfun,x0,A,b)} \]

Gives:

\[ x = 24.00 \ 12.00 \ 12.00 \]
SOME TIPS FOR SOLVING NLPPs

• Avoid nonlinearity if possible
• Better nonlinearities in the objective function than in the constraints
• Better inequalities than equalities
• Supply good starting guesses to a solver
• Don’t blame the solver if you don’t find a solution, take a critical look at the problem formulation