Metabolic Modelling

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A very short introduction to linear programming

What is Linear Programming (LP)

- (One of) the most important methods for solving real-world computational problems

- Powerful and general optimization tool
  - Resource allocation, shortest path, maxflow, matching, 2-person zero sum games...
  - Approximations to NP-complete problems
  - Applications in agriculture, computer science, telecommunications, medicine, logistics, management, economics . . .
  - Dozens of software tools (including MATLAB) and text books, hundreds of resarch papers . . .

Principle of LP

- Encode the problem as minimization (maximization) task with *linear obejctive function* and *linear constraints*
- Exploit the linearity to get an optimal solution efficiently
  - Can use linear algebra and local search strategies to reach a global optimum
- Suitable for extremely large problems
  - Hundreds of thousands of variables
  - Thousands of constraints

Forms of LP

- Objective function

  $y = \min(\max) \sum_i c_i x_i$

  – x_i's are decision variables, c_i's their weights

- Constrains

  – subject to:

$$
\begin{gathered}
a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n \le (=\ge) b_1 \\
a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n \le (=\ge) b_2 \\
\vdots \\
a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n \le (=\ge) b_m
\end{gathered}
$$

- Sometimes nonnegative variables

Forms of LP

- Easy to convert from one form to another
- (The most) common formulation:

$$
\begin{array}{ll}
\min & \mathbf{c}^T\mathbf{x} \\
\texttt{subject to} & \\
 & \mathbf{A}\mathbf{x} \geq \mathbf{b} \\
 & \mathbf{x} \geq \mathbf{0}
\end{array}
$$

Forms of LP

- MATLAB formulation (function *linprog*)

$$\begin{aligned} \min \quad & \mathbf{c}^T\mathbf{x} \\ \texttt{subject to} \quad & \\ \mathbf{Ax} \quad & \leq \mathbf{b} \\ \mathbf{A_{eq}x} \quad & = \mathbf{b_{eq}} \\ \mathbf{lb} \quad & \leq \mathbf{x} \\ \mathbf{ub} \quad & \geq \mathbf{x} \end{aligned}$$

Example

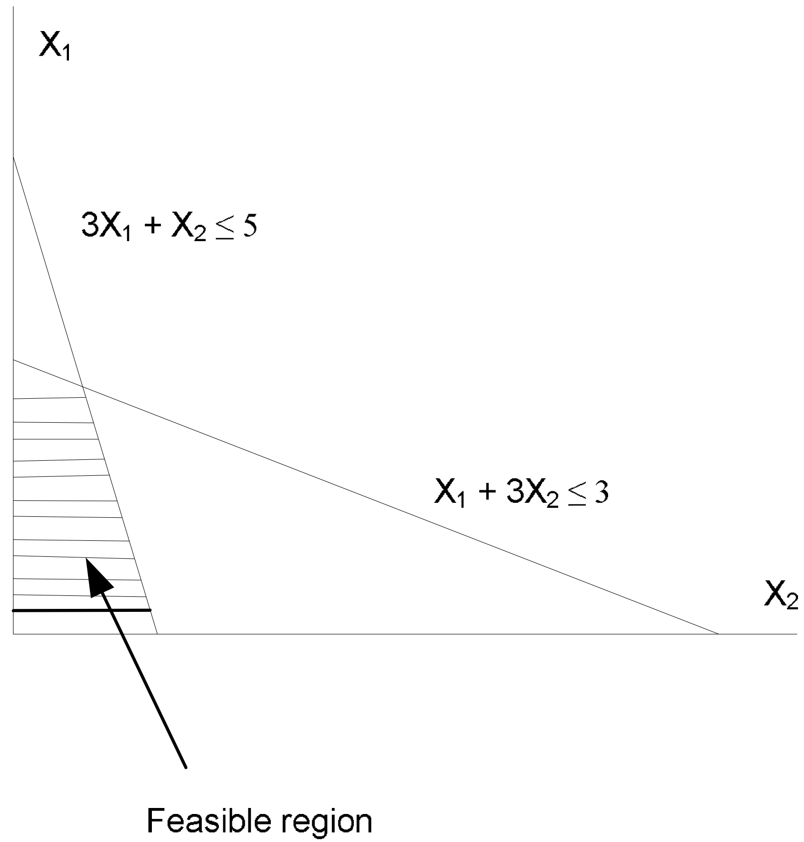
- Transportation problem: minimize the cost of moving paper from mills to shops
  c_{ij} = cost of moving a ton of paper from mill i to shop j

$$
\begin{array}{lll}
\min \sum_{ij} & c_{ij} x_{ij} & \\
\texttt{subject to} & & \\
& \sum_j x_{ij} \leq s_i & \texttt{Mill } i \texttt{ produces at most } s_i \texttt{ tons} \\
& \sum_i x_{ij} \geq s_j & \texttt{Transport at least } s_j \texttt{ tons to shop } j
\end{array}
$$

Geometric interpretation

$$\begin{aligned} \max \quad & x_1 + x_2 \\ \texttt{subject to} \quad & \\ x_1 + 3x_2 \quad & \leq 3 \\ 3x_1 + x_2 \quad & \leq 5 \\ x_1 \quad & \geq 0 \\ x_2 \quad & \geq 0 \end{aligned}$$

Geometric interpretation



Solving LP problems

- Because of the linear constraints the feasible region is convex
- Linear objective function $\rightarrow$ solutions lie on the edge of the feasible region
- Edges are linear $\rightarrow$ a solution lies on the corner point of the feasible region
  - Corners can be found by solving linear equation systems
- Can have multiple optima!

Solving LP problems

- General solution strategy:
  1. Find a corner point
  2. Proceed to a better corner point
  3. Halt if no better corner point found
- Simplex method: Move around in the surface of the polytope
- Interior point methods: Move inside the polytope
  - Polynomial time complexity
- More information at the course of combinatorial optimization

Solving LP problems

- Available packages solve LP's efficiently, you can concentrate on describing your problem as an LP task!