MS-E2122 - Nonlinear Optimization Lecture I

Fernando Dias

Department of Mathematics and Systems Analysis

Aalto University School of Science

Outline of this lecture

Context

Mathematical programming and optimisation

Types of mathematical optimisation models

Example of Applications

Resource allocation

The pooling problem: refinery operations planning

Robust optimisation

Combinatorial optimisation

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Example of Applications

- Resource allocation
- The pooling problem: refinery operations planning
- Robust optimisation
- Combinatorial optimisation

NonLinear (or Non-Linear):

adjective

not arranged in a straight line.

not sequential or straightforward.

Optimization (or Optimisation):

🕨 noun

the action of making the best or most effective use of a situation or resource.

Field of applied mathematics. The goal is to search values for variables in a given domain that maximise/minimise function values.

Can be achieved by:

 Analysing/Visualizing properties of functions / extreme points or



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Optimisation has important applications in fields such as

- operations research (OR);
- economics;
- statistics;
- bioinformatics;
- machine learning and artificial intelligence.

In this course, optimisation is viewed as the core element of mathematical programming.

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However, math. programming has many applications in fields other than OR, which causes some confusion;

We will study math. programming in its most general form: both constraints and objectives are nonlinear functions.

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• $h_i(x) = 0$ for i = 1, ..., l - equality constraints.

Our goal will be to solve variations of the general problem P:

$$\begin{array}{ll} (P): & \mbox{min.} & f(x)\\ \mbox{subject to:} & g_i(x) \leq 0, i=1,\ldots,m\\ & & h_i(x)=0, i=1,\ldots,l\\ & & x\in X. \end{array}$$

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▶ Linear programming (LP): linear $f(x) = c^{\top}x$ with $c \in \mathbb{R}^n$; constraint functions $g_i(x)$ and $h_i(x)$ are affine $(a_i^{\top}x - b_i)$, with $a_i \in \mathbb{R}^n$, $b \in \mathbb{R}$); $X = \{x \in \mathbb{R}^n : x_j \ge 0, j = 1, ..., n\}$.

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Mixed-integer nonlinear programming (MINLP): MIP+NLP.

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Problem statement. Plan production that maximises return. Let

- $I = \{1, \ldots, i, \ldots, M\}$ resources;
- $J = \{1, \dots, j, \dots, N\}$ products;
- ▶ c_j return per unit of product $j \in J$;
- ▶ a_{ij} resource $i \in I$ requirement for making product $j \in J$;
- \blacktriangleright b_i availability of resource $i \in I$;
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Remark:

• notice that max.
$$f(x) = \min(-f(x))$$
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Remark:

- notice that max. $f(x) = \min (-f(x));$
- the base of most practical optimisation problems; exploits mature LP technology.

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Portfolio optimization

Problem statement. Plan portfolio of assets to minimise exposition to risk. Let

- ▶ $J = \{1, \dots, j, \dots, N\}$ assets;
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$$\begin{array}{ll} \mathsf{min.} & x^\top \Sigma x\\ \mathsf{subject to:} & \mu^\top x \geq \epsilon\\ & 0 \leq x_j \leq 1, \forall j \in J \end{array}$$

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Remarks:

- The term $x^{\top}\Sigma x$ measures exposition to risk. It is credited to Harry Markowitz (1952).
- Another important class: quadratic programming (nonlinear).

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min.
$$x^{\top} \Sigma x$$

subject to: $\mu^{\top} x \ge \epsilon$
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Oil refinery operational planning

- Goal is to maximize profit;
- Several possible configurations;
- Product property specifications must be met;



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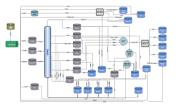
Oil refinery operational planning

- Goal is to maximize profit;
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Model characteristics:

- Bilinear (nonconvex) and mixed-integer;
- Large number of flows;
- Several nonlinear constraints.



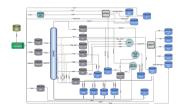


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Objective: maximize profit **Variables:**

- Stream Flows (crude, intermediate and final products);
- Storage;
- Stream properties.





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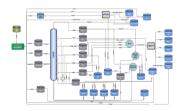
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Constraints

- Mass balance;
- Market features (supply and demand);
- Unit capacities;
- Stream property limits;
- Calculation of mix properties (nonlinear).





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Refinery Operations Planning Problem

The challenging aspect is how to model the calculation of product properties in a mix. Let:

▶ x_p be the volume of product $p \in P$ and

q_p the value of a given chemical property (sulphur content, octane content, viscosity...).

In a given mix, mass and property balances are calculated as:



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Remarks:

- More complex mixes (such as nonlinear balances) might need to be considered.
- These are bilinear programming problems (nonlinear).

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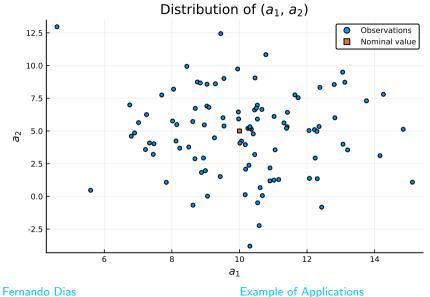
Consider the resource allocation problem under uncertainty:

max.
$$c^{\top}x$$

subject to: $\tilde{a}_i^{\top}x \leq b_i, \forall i \in I$
 $x_j \geq 0, \forall j \in J,$

where \tilde{a}_i is a random variable.

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Assume that, for any $i \in I$, $\tilde{a}_i \in \epsilon_i = \{\overline{a}_i + P_i u : ||u||_2 \le \Gamma_i\}$, where

- $\triangleright \overline{a}_i$ is the nominal (average) value;
- > P_i is the characteristic matrix of the ellipsoid ϵ ;
- \triangleright Γ_i is risk-aversion control parameter.

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Then, the robust counterpart can be stated as

$$\begin{array}{ll} \max & c^{\top}x\\ \text{subject to:} & \max_{a_i \in \epsilon_i} \ \left\{a_i^{\top}x\right\} \leq b_i, \forall i \in I\\ & x_j \geq 0, \forall j \in J. \end{array}$$

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Notice that

$$\max_{a_i \in \epsilon_i} \left\{ a_i^\top x \right\} = \overline{a}_i^\top x + \max_u \left\{ u^\top P_i x : ||u||_2 \le \Gamma_i \right\} = \overline{a}_i^\top x + \Gamma_i ||P_i x||_2$$

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The robust counterpart can be equivalently stated as:

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In case data is available, P_i can be obtained from the empirical covariance matrix;

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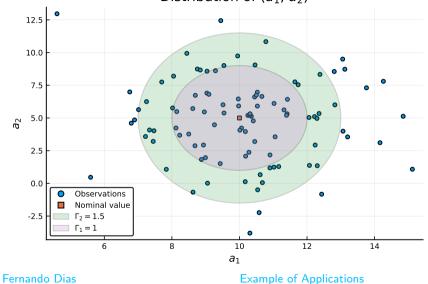
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Remarks:

- In case data is available, P_i can be obtained from the empirical covariance matrix;
- Values of Γ_i can be drawn, for example, from a Chi-squared distribution. Γ_i is sometimes called the budget of uncertainty.

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Distribution of (a_1, a_2)



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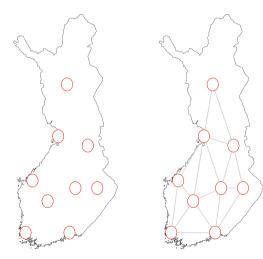
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One of most classic problems is Travelling Salesman Problem (TSP)



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Assume a number of cities labeled with numbers $1, \dots, n$, and the distance (or any cost) between two cities i and j is defined as c_{ij} .

The main variable is x_{ij} such that:

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 x_{ij} is binary variable \leftarrow integer programming

The goal can be stated as:

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The objective function is:

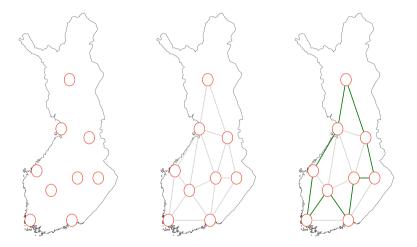
$$\min\sum_{i=1}^{n}\sum_{j\neq i,j=1}^{n}c_{ij}x_{ij}$$
(1)

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The constraints can be written as:

$$\sum_{\substack{i \neq j, i=1 \\ j \neq i, j=1}}^{n} x_{ij} = 1 \qquad \forall j = 1, \cdots, n \qquad (2)$$
$$\sum_{\substack{j \neq i, j=1 \\ j \neq i, j=1}}^{n} x_{ij} = 1 \qquad \forall j = 1, \cdots, n \qquad (3)$$

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Reference

Sahinidis, Nikolaos V. "Mixed-integer nonlinear programming 2018." Optimization and Engineering 20 (2019): 301-306.

Floudas, Christodoulos A. Nonlinear and mixed-integer optimization: fundamentals and applications. Oxford University Press, 1995.

Tawarmalani, Mohit, and Nikolaos V. Sahinidis. Convexification and global optimization in continuous and mixed-integer nonlinear programming: theory, algorithms, software, and applications. Vol. 65. Springer Science & Business Media, 2013.