MS-E2122 - Nonlinear Optimization
Lecture 1

Fabricio Oliveira

Systems Analysis Laboratory
Department of Mathematics and Systems Analysis

Aalto University
School of Science

Outline of this lecture

What is optimisation?

Mathematical programming and optimisation

Types of mathematical optimisation models

Applications

Resource allocation

The pooling problem: refinery operations planning

Robust optimisation

Classification: support vector machines

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

Can be achieved by

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Optimisation has important applications in fields such as

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

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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.
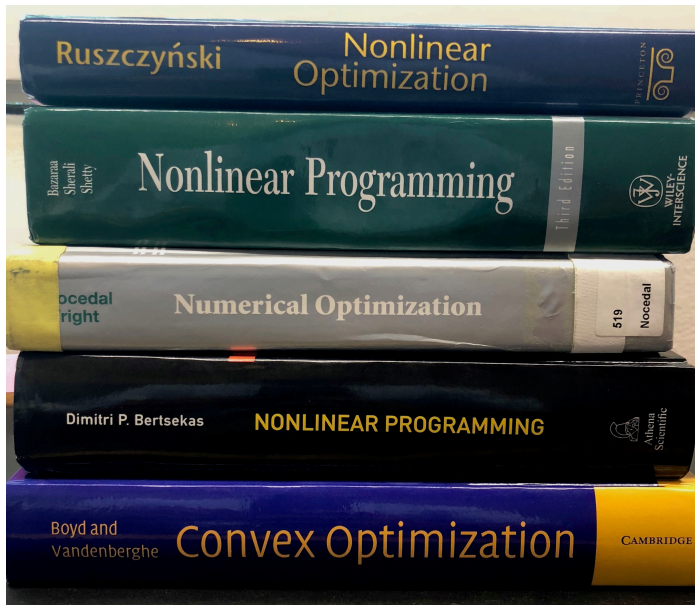
Types of programming

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

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

Outline of this lecture

Resource allocation and portfolio optimisation

Problem statement. Plan production that maximises return. Let

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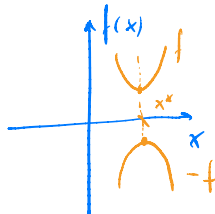
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Remark:

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

Portfolio optimization

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

- $J = \{1, \ldots, j, \ldots, N\}$ assets;
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min. $x^\top \Sigma x$

subject to: $\mu^\top x \geq \epsilon$

$0 \leq x_j \leq 1, \forall j \in J$

$$\Sigma_{ij}\, x_i\, x_j$$

$$\overline{\Sigma}_j\, \mu_j\, x_j$$

$$\frac{\sum_{ij=1}^{n} (R_i - \mu_i)(R_j - \mu_j)}{n}$$

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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).
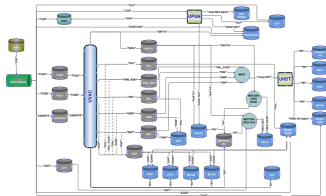
Refinery Operations Planning Problem

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.
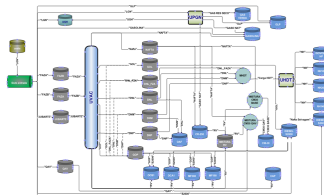
$x \cdot x = x^2$

$x \cdot y$

Refinery Operations Planning Problem

Objective: maximize profit

Variables:

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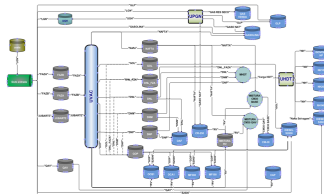- ▶ Stream properties.

Refinery Operations Planning Problem

Objective: maximize profit

Variables:

- ▶ Stream Flows (crude, intermediate and final products);
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Constraints

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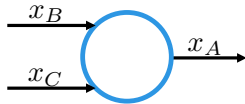- ▶ Calculation of mix properties (nonlinear).

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:

$$x_A = x_B + x_C$$

$$q_A = \frac{q_B x_B + q_C x_C}{x_A}$$

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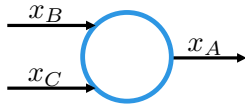$$x_A = x_B + x_C$$
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Remarks:

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

Robust optimisation

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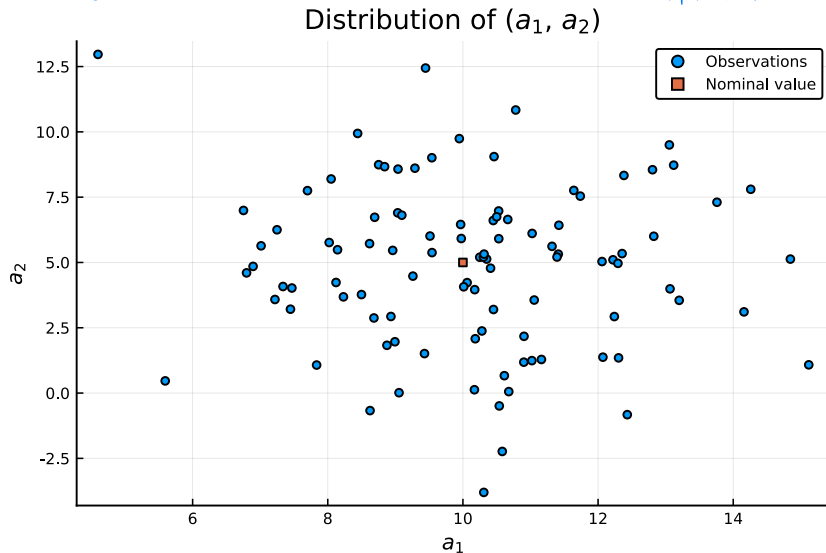Consider the resource allocation problem under uncertainty:

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

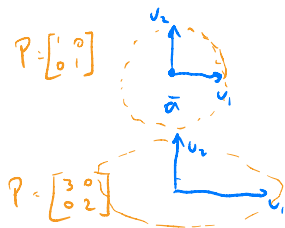where $\tilde{a}_i$ is a random variable.

Robust optimisation

$a_1 x_1 + a_2 x_2 \leq b$

Distribution of (a_1, a_2)

Robust optimisation

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

- ▶ $\overline{a}_i$ is the nominal (average) value;
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Then, the robust counterpart can be stated as

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Notice that

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

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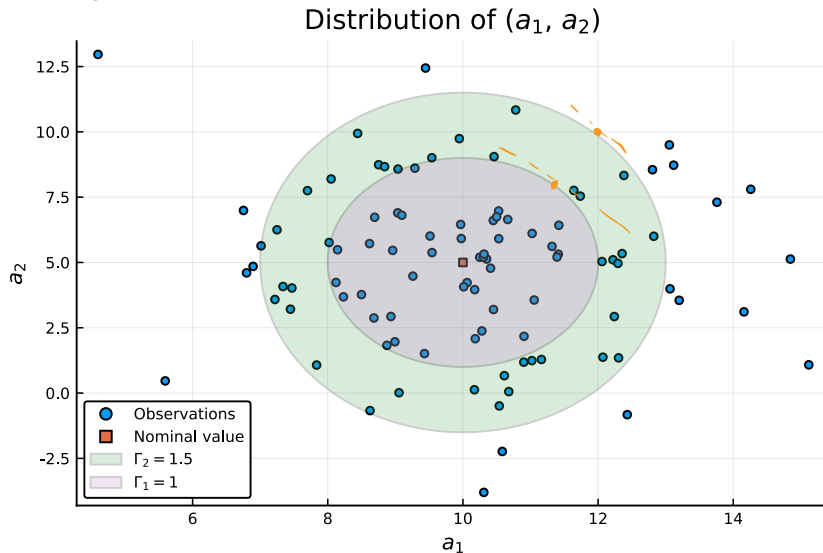
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▶ Values of Γ_i can be drawn, for example, from a Chi-squared distribution. Γ_i is sometimes called the budget of uncertainty.

Robust optimisation

Distribution of (a_1, a_2)

Legend:
- Observations
- Nominal value
- $\Gamma_2 = 1.5$
- $\Gamma_1 = 1$

Classification

Suppose we are given some data $D \subset \mathbb{R}^n$ that can be separated into two sets in $\mathbb{R}^n$: $I^- = \{x_1, \dots, x_N\}$ and $I^+ = \{x_1, \dots, x_M\}$.

Each element in D is an observation of a given set of features; belonging to either I^- or I^+ defines a classification.

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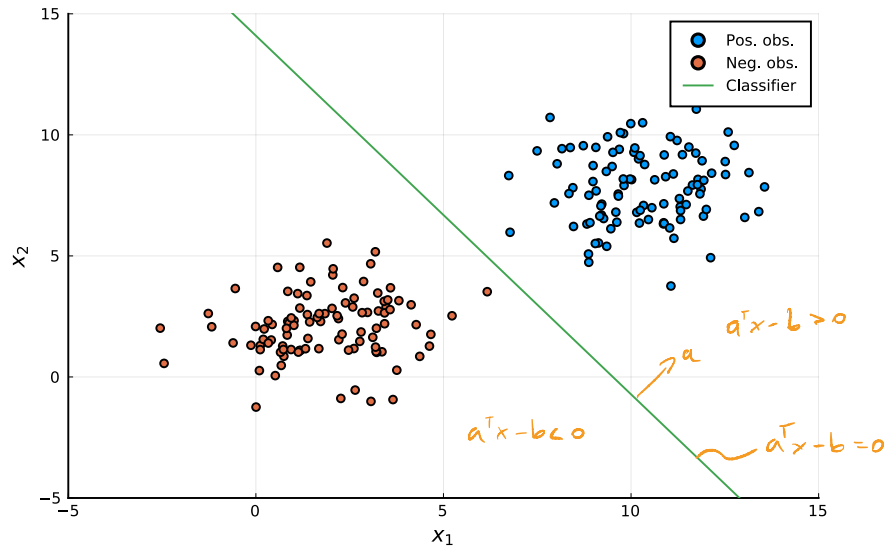
Our task is to select a function $f : \mathbb{R}^n \to \mathbb{R}$ from a given family of functions such that

$\llcorner$ kernel

$$f(x_i) < 0, \ \forall x_i \in I^- \text{ and } f(x_i) > 0, \ \forall x_i \in I^+.$$

Typically, f is selected as a linear classifier, i.e., $f(x_i) = a^\top x_i - b$.

Of course, there is always the possibility of misclassification and, therefore, we want to determine the best possible classifier.

Classification

Classification

Let us define the following error measures:

$$e^-(x_i \in I^-; a, b) := \begin{cases} 0, & \text{if } a^\top x_i - b \leq 0, \\ a^\top x_i - b, & \text{if } a^\top x_i - b > 0. \end{cases}$$

$$e^+(x_i \in I^+; a, b) := \begin{cases} 0, & \text{if } a^\top x_i - b \geq 0, \\ b - a^\top x_i, & \text{if } a^\top x_i - b < 0. \end{cases}$$

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Using slack variables u_i, $i = 1, \ldots, M$, and v_i, $i = 1, \ldots, N$, to represent e^- and e^+, the optimal classifier is obtained from:

$$(LC): \quad \text{min.} \quad \sum_{i=1}^{M} u_i + \sum_{i=1}^{N} v_i$$

subject to: $a^\top x_i - b - u_i \leq 0, i = 1, \ldots, M$ $a^\top x - b \leq 0$

$a^\top x_i - b + v_i \geq 0, i = 1, \ldots, N$ $-2 \quad 4$ -3

$\|a\|_2 = 1$

$u_i \geq 0, i = 1, \ldots, M; v_i \geq 0, i = 1, \ldots, N; a \in \mathbb{R}^n, b \in \mathbb{R}.$
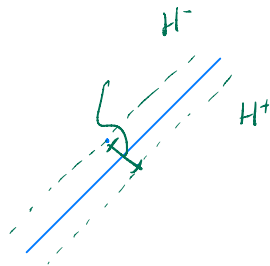
Classification

In practice, we can enforce a slab $S = \left\{ -1 \leq a^\top x_i - b \leq 1 \right\}$ as a buffer to trade off the robustness of the classifier to outliers.

Accordingly, we redefine our error measures as follows.

$$e^-(x_i \in I^-; a, b) := \begin{cases} 0, & \text{if } a^\top x_i - b \leq -1, \\ |a^\top x_i - b|, & \text{if } a^\top x_i - b > -1. \end{cases}$$

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Classification

In practice, we can enforce a slab $S = \left\{ -1 \leq a^\top x_i - b \leq 1 \right\}$ as a buffer to trade off the robustness of the classifier to outliers.
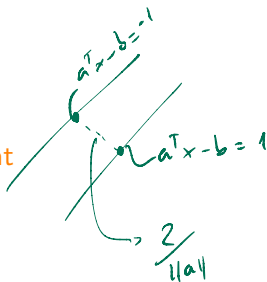
Accordingly, we redefine our error measures as follows.

$$e^-(x_i \in I^-; a, b) := \begin{cases} 0, \text{ if } a^\top x_i - b \leq -1, \\ |a^\top x_i - b|, \text{ if } a^\top x_i - b > -1. \end{cases}$$

$$e^+(x_i \in I^+; a, b) := \begin{cases} 0, \text{ if } a^\top x_i - b \geq 1, \\ |b - a^\top x_i|, \text{ if } a^\top x_i - b < 1. \end{cases}$$

e^- and e^+ include misclassifications and correct classifications that lie within S. The latter are know as support vectors.

The width of S is given by $2/||a||_2$, which is the distance between the hyperplanes $a^\top x_i - b = -1$ and $a^\top x_i - b = 1$.

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The robust version of LC incorporating this buffer becomes

$$\text{min.} \quad \sum_{i=1}^{M} u_i + \sum_{i=1}^{N} v_i + \gamma \|a\|_2^2$$

$$\text{subject to:} \quad a^\top x_i - b - u_i \leq -1, \ i = 1, \dots, M$$

$$a^\top x_i - b + v_i \geq 1, \ i = 1, \dots, N$$

$$u_i \geq 0, i = 1, \dots, M; v_i \geq 0, i = 1, \dots, N;$$

$$a \in \mathbb{R}^n, b \in \mathbb{R}.$$

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▶ The parameter γ controls the trade-off between the width of the slab S and the number of observations within the slab.

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▶ This quadratic programming problem is known in the machine learning literature as support vector machine (SVM).

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