

MS-E2122 - Nonlinear Optimization

Lecture 1

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Outline of this lecture

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What is optimisation?

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

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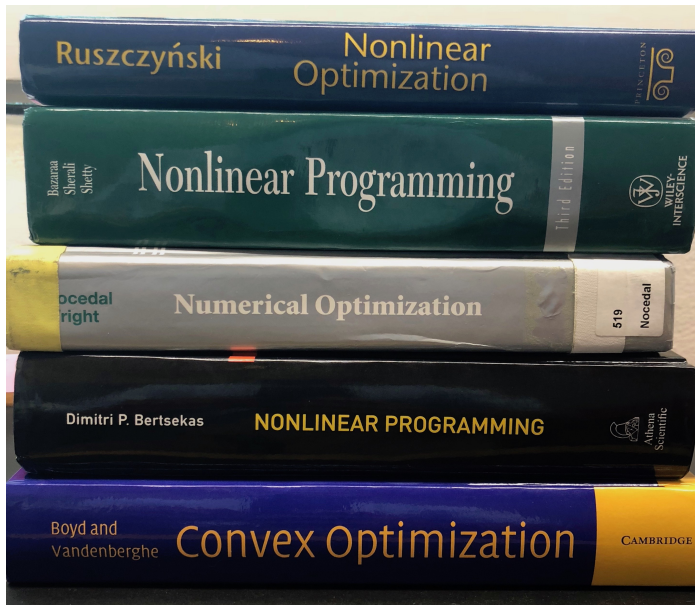
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However, math. programming has many applications in fields other than OR, **which causes some confusion**;

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 $i = 1, \dots, l$ - equality constraints.

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

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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 $a_i \in \mathbb{R}^n$, $b \in \mathbb{R}$); $X = \{x \in \mathbb{R}^n : x_j \geq 0, j = 1, \dots, n\}$.

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

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Resource allocation and portfolio optimisation

Problem statement. Plan production that maximises return. Let

- ▶ $I = \{1, \dots, i, \dots, M\}$ 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 $j \in J$;
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- ▶ notice that $\max. f(x) = \min. -f(x)$;
- ▶ 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

- ▶ $J = \{1, \dots, j, \dots, N\}$ assets;
- ▶ μ_j - expected relative return of asset $j \in J$;
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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;
- ▶ Several possible configurations;
- ▶ **Product property specifications** must be met;



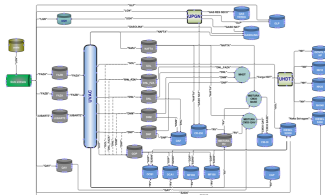
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Model characteristics:

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

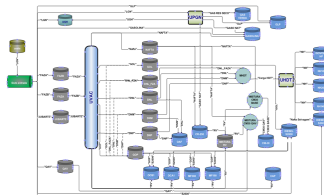


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Objective: maximize profit

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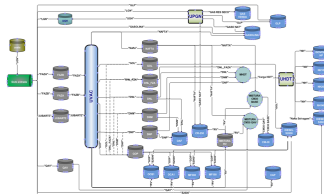
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Constraints

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

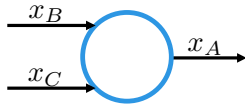


Refinery Operations Planning Problem

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



$$x_A = x_B + x_C$$

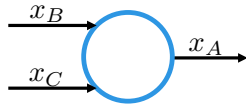
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Remarks:

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

Robust optimisation

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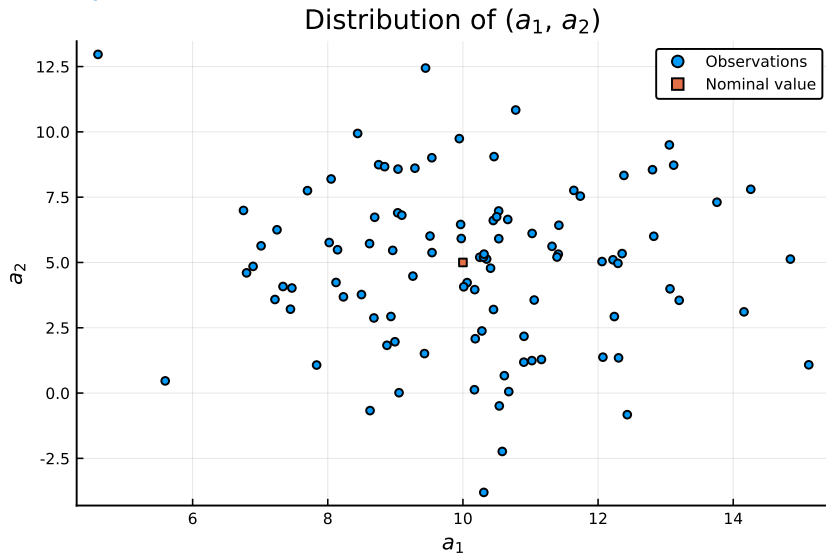
It's a risk-averse perspective that seeks **protection against variability**.

Consider the resource allocation problem under uncertainty:

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

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

Robust optimisation



Robust optimisation

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

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

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Then, the **robust counterpart** can be stated as

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Notice that

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

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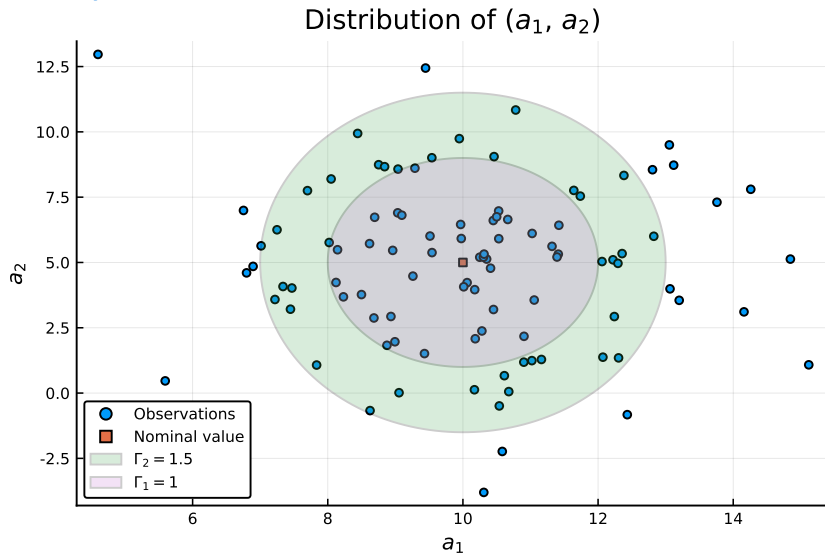
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Remarks:

- ▶ 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**.

Robust optimisation



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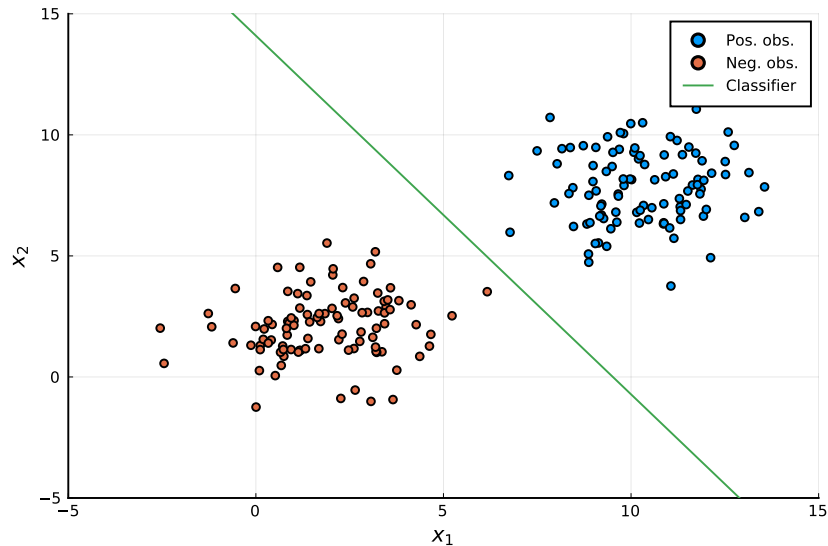
Our task is to select a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ from a given family of functions such that

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

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**:

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

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

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

$$\text{subject to: } a^\top x_i - b - u_i \leq 0, i = 1, \dots, M$$

$$a^\top x_i - b + v_i \geq 0, i = 1, \dots, N$$

$$\|a\|_2 = 1$$

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

Classification

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

Accordingly, we redefine our error measures as follows.

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

e^- and e^+ include **misclassifications** and **correct classifications that lie within S** . The latter are known 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 $a^\top x_i - b = 1$.

Classification

The robust version of LC incorporating this buffer becomes

$$\begin{aligned} \min. \quad & \sum_{i=1}^M u_i + \sum_{i=1}^N v_i + \gamma \|a\|_2^2 \\ \text{subject to: } & a^\top x_i - b - u_i \leq -1, \quad i = 1, \dots, M \\ & a^\top x_i - b + v_i \geq -1, \quad i = 1, \dots, N \\ & u_i \geq 0, i = 1, \dots, M; v_i \geq 0, i = 1, \dots, N; \\ & a \in \mathbb{R}^n, b \in \mathbb{R}. \end{aligned}$$

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Remarks:

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

Classification

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Remarks:

- ▶ The parameter γ controls the **trade-off** between the width of the slab S and the number of observations within the slab.
- ▶ This quadratic programming problem is known in the machine learning literature as **support vector machine** (SVM).

Classification

