Mathematical modelling

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Introduction

Tha task of mathematical modelling is to find and evaluate solutions to real world problems with the use of mathematical concepts and tools.

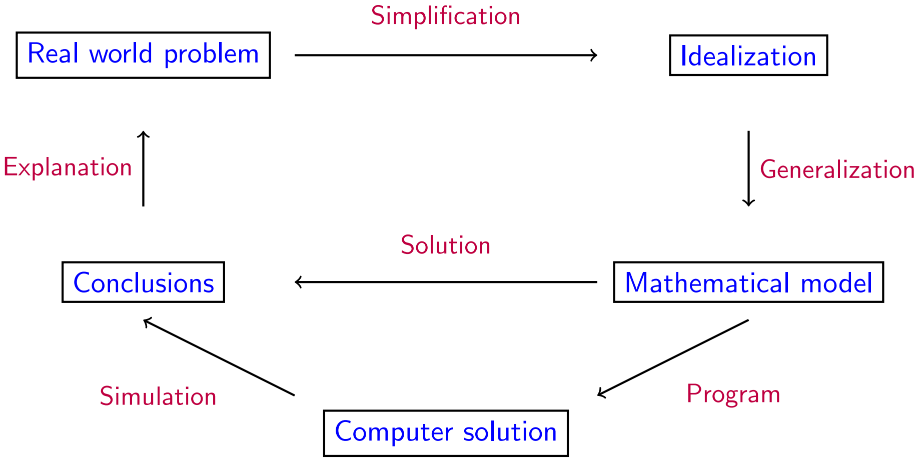
In this course we will introduce some (by far not all) mathematical tools that are used in setting up and solving mathematical models.

We will (together) also solve specific problems, study examples and work on projects.

Contents

- Introduction
- Linear models: systems of linear equations, matrix inverses, SVD decomposition, PCA
- Nonlinear models: vector functions, linear approximation, solving systems of nonlinear equations
- Geometric models: curves and surfaces
- Dynamical models: differential equations, dynamical systems

Modelling cycle



What should we pay attention to?

- Simplification: relevant assumptions of the model (distinguish important features from irrelevant)
- Generalization: choice of mathematical representations and tools (for example: how to represent an object - as a point, a geometric shape, . . .)
- Solution: as simple as possible and well documented
- Conclusions: are the results within the expected range, do they correspond to "facts" and experimantal results?

A mathematical model is not universal, it is an approximation of the real world that works only within a certain scale where the assumptions are at least approximately realistic.

Example

An object (ball) with mass m is thrown vertically into the air. What should we pay attention to when modelling its motion?

- The assumptions of the model: relevant forces and parameters (gravitation, friction, wind, ...), how to model the object (a point, a homogeneous or nonhomeogeneous geometric object, angle and rotation in the initial thrust, ...)
- Choice of mathematical model: differential equation, discrete model, ...
- Computation: analytic or numeric, choice of method,...
- Do the results make sense?

Errors

An important part of modelling is estimating the errors!

Errors are an integral part of every model.

Errors come from: assumptions of the model, imprecise data, mistakes in the model, computational precision, errors in numerical and computational methods, mistakes in the computations, mistakes in the programs, ...

Absolute error = Approximate value - Correct value

$$\Delta x = \bar{x} - x$$

Relative error $= \frac{\text{Absolute error}}{\text{Correct value}}$

$$\delta_x = \frac{\Delta x}{x}$$

Example: quadratic equation

$$x^2 + 2a^2x - q = 0$$

Analytic solutions are

$$x_1 = -a^2 - \sqrt{a^4 + q} \quad \text{and} \quad x_2 = -a^2 + \sqrt{a^4 + q}.$$

What happens if $a^2 = 10000$, $q = 1$? Problem with stability in calculating x_2.

More stable way for computing x_2 (so that we do not subtract numbers which are nearly the same) is

$$\begin{aligned} x_2 = -a^2 + \sqrt{a^4 + q} &= \frac{(-a^2 + \sqrt{a^4 + q})(a^2 + \sqrt{a^4 + q})}{a^2 + \sqrt{a^4 + q}} \\ &= \frac{q}{a^2 + \sqrt{a^4 + q}}. \end{aligned}$$

Example of real life disasters

- Disasters caused because of numerical errors: (http://www-users.math.umn.edu/~arnold//disasters/)
  - **The Patriot Missile failure, Dharan, Saudi Arabia, February 25 1991**, 28 deaths: bad analysis of rounding errors.
  - **The explosiong of the Ariane 5 rocket, French Guiana, June 4, 1996**: the consequence of overflow in the horizontal velocity.
    https://www.youtube.com/watch?v=PK_yguLapgA
    https://www.youtube.com/watch?v=W3YJeoYgozw
    https://www.arianespace.com/vehicle/ariane-5/
  - **The sinking of the Sleipner offshore platform, Stavanger, Norway, August 12, 1991**, billions of dollars of the loss: inaccurate finite element analysis, i.e., the method for solving partial differential equations.
    https://www.youtube.com/watch?v=eGdiPs4THW8

1. Linear mathematical models

Given points

$$\{(x_1, y_1), \ldots, (x_m, y_m)\}, \quad x_i \in \mathbb{R}^n,\ y_i \in \mathbb{R},$$

the task is to find a function $F(x, a_1, \ldots, a_p)$ that is a good fit for the data.

The values of the parameters $a_1, \ldots, a_p$ should be chosen so that the equations

$$y_i = F(x, a_1, \ldots a_p), \quad i = 1, \ldots, m,$$

are satisfied or, if this is not possible, that the error is as small as possible.

Least squares method: the parameters are determined so that the sum of squared errors

$$\sum_{i=1}^{m} (F(x_i, a_1, \ldots a_p) - y_i)^2$$

is as small as possible.

The mathematical model is linear, when the function F is a linear function of the parameters:

$$F(x, a_1, \ldots, a_p) = a_1\varphi_1(x) + \varphi_2(x) + \cdots + a_p\varphi_p(x),$$

where $\varphi_1, \varphi_2, \ldots \varphi_p$ are functions of a specific type.

Examples of linear models:

1. linear regression: $x, y \in \mathbb{R}$, $\varphi_1(x) = 1, \varphi_2(x) = x$,
2. polynomial regression: $x, y \in \mathbb{R}$, $\varphi_1(x) = 1, \ldots, \varphi_p(x) = x^{p-1}$,
3. multivariate linear regression: $x = (x_1, \ldots, x_n) \in \mathbb{R}^n, y \in \mathbb{R}$,

$$\varphi_1(x) = 1, \varphi_2(x) = x_1, \ldots, \varphi_n(x) = x_n,$$

4. frequency or spectral analysis:

$$\varphi_1(x) = 1, \varphi_2(x) = \cos\omega x, \varphi_3(x) = \sin\omega x, \varphi_4(x) = \cos 2\omega x, \ldots$$

(there can be infinitely many functions $\varphi_i(x)$ in this case)

Examples of nonlinear models: $F(x, a, b) = ae^{bx}$ and $F(x, a, b, c) = \dfrac{a + bx}{c + x}$.

Given the data points $\{(x_1, y_1), \ldots, (x_m, y_m)\}$, $x_i \in \mathbb{R}^n$, $y_i \in \mathbb{R}$, the parameters of a linear model

$$y = a_1\varphi_1(x) + a_2\varphi_2(x) + \cdots + a_p\varphi_p(x)$$

should satisfy the system of linear equations

$$y_i = a_1\varphi_1(x_i) + a_2\varphi_2(x_i) + \cdots + a_p\varphi_p(x_i), \quad i = 1, \ldots, m,$$

or, in a matrix form,

$$\begin{bmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \ldots & \varphi_p(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \ldots & \varphi_p(x_2) \\ \ldots & \ldots & \ldots & \ldots \\ \varphi_1(x_m) & \varphi_2(x_m) & \ldots & \varphi_p(x_m) \end{bmatrix} \begin{bmatrix} a_1 \\ a_1 \\ \vdots \\ a_p \end{bmatrix} = \begin{bmatrix} y_1 \\ y_1 \\ \vdots \\ y_p \end{bmatrix}.$$

1.1 Systems of linear equations and generalized inverses

A system of linear equations in the matrix form is given by

$$Ax = b,$$

where

- A is the matrix of coefficients of order $m \times n$ where m is the number of equations and n is the number of unknowns,
- x is the vector of unknowns and
- b is the right side vector.

Existence of solutions:

Let $A = [a_1, \dots, a_n]$, where a_i are vectors representing the columns of A.

For any vector $x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$ the product Ax is a linear combination

$$Ax = \sum_i x_i a_i.$$

The system is **solvable** if and only if the vector b can be expressed as a linear combination of the columns of A, that is, it is in the column space of A, $b \in \mathcal{C}(A)$.

By adding b to the columns of A we obtain the extended matrix of the system

$$[A \mid b] = [a_1, \ldots, a_n \mid b],$$

Theorem

The system $Ax = b$ is solvable if and only if the rank of A equals the rank of the extended matrix $[A \mid b]$, i.e.,

$$\text{rank } A = \text{rank } [A \mid b] =: r.$$

The solution is unique if the rank of the two matrices equals the number of unknowns, i.e., $r = n$.

An especially nice case is the following:

If A is a square matrix ($n = m$) that has an inverse matrix A^{-1}, the system has a unique solution

$$x = A^{-1}b.$$

Let $A \in \mathbb{R}^{n \times n}$ be a square matrix. The following conditions are equivalent and characterize when a matrix A is invertible or nonsingular:

- The matrix A has an inverse.
- The rank of A equals n.
- $\det(A) \neq 0$.
- The null space $N(A) = \{x : Ax = 0\}$ is trivial.
- All eigenvalues of A are nonzero.
- For each b the system of equations $Ax = b$ has precisely one solution.

A square matrix that does not satisfy the above conditions does not have an inverse.

Example

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & 1 & 0 \end{bmatrix}$$

A is invertible and is of rank 3, B is not invertible and is of rank 2.

For a rectangular matrix A of dimension $m \times n$, $m \neq n$, its inverse is not defined (at least in the above sense...).

Definition

A generalized inverse of a matrix $A \in \mathbb{R}^{n \times m}$ is a matrix $G \in \mathbb{R}^{m \times n}$ such that

$$AGA = A. \tag{1}$$