Mathematical modelling

Lecture notes, version February 22, 2022

Faculty of Computer and Information Science
University of Ljubljana

2021/22

Introduction

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

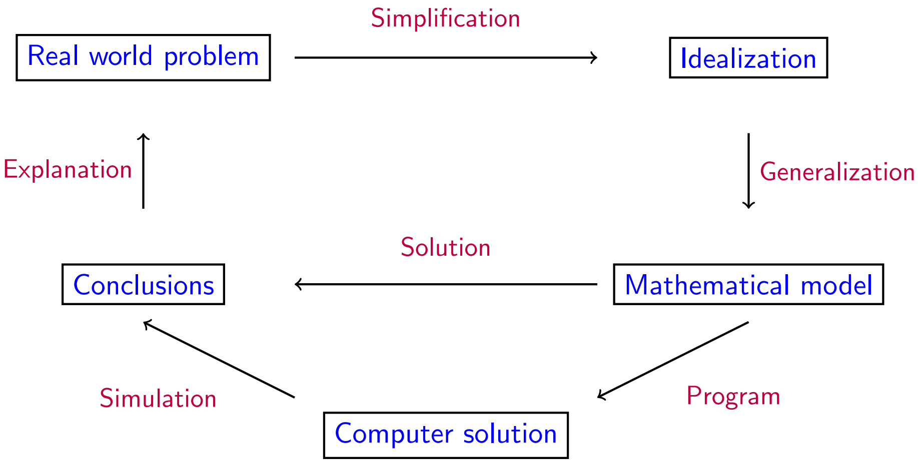
In this course we will introduce some (by far not all) mathematical tools that are used in setting up and solving mathematical models.

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

$$x_2 = -a^2 + \sqrt{a^4 + q} = \frac{(-a^2 + \sqrt{a^4 + q})(a^2 + \sqrt{a^4 + q})}{a^2 + \sqrt{a^4 + q}}$$

$$= \frac{q}{a^2 + \sqrt{a^4 + q}}.$$

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:

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

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

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

4. frequency or spectral analysis:

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

(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 $A = [a_1, \ldots, a_n]$, 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

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

Remark

Note that the dimension of A and its generalized inverse are transposed to each other. This is the only way which enables the multiplication $A \cdot * \cdot A$.

Proposition

If A is invertible, it has a unique generalized inverse, which is equal to A^{-1}.

Proof.

Let G be a generalized inverse of A, i.e., (1) holds. Multiplying (1) with A^{-1} from the left and the right side we obtain:

$$\begin{aligned} \text{Left hand side (LHS):} \quad & A^{-1}AGAA^{-1} = IGI = G, \\ \text{Right hand side (RHS):} \quad & A^{-1}AA^{-1} = IA^{-1} = A^{-1}, \end{aligned}$$

where I is the identity matrix. The equality LHS=RHS implies that $G = A^{-1}$. □

Theorem

Every matrix $A \in \mathbb{R}^{n\times m}$ has a generalized inverse.

Proof.

Let r be the rank of A.

Case 1. $\operatorname{rank} A = \operatorname{rank} A_{11}$, where

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

and $A_{11} \in \mathbb{R}^{r\times r}, A_{12} \in \mathbb{R}^{r\times(m-r)}, A_{21} \in \mathbb{R}^{(n-r)\times r}$, $A_{22} \in \mathbb{R}^{(n-r)\times(m-r)}$.
We claim that

$$G = \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix},$$

where 0s denote zero matrices of appropriate sizes, is the generalized inverse of A. To prove this claim we need to check that

$$AGA = A.$$

$$AGA = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} A_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} I & 0 \\ A_{21}A_{11}^{-1} & 0 \end{bmatrix} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

$$= \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{21}A_{11}^{-1}A_{12} \end{bmatrix}.$$

For AGA to be equal to A we must have

$$A_{21}A_{11}^{-1}A_{12} = A_{22}. \tag{2}$$

It remains to prove (2). Since we are in Case 1, it follows that every column of $\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix}$ is in the column space of $\begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix}$. Hence, there is a cofficient matrix $W \in \mathbb{R}^{r\times(m-r)}$ such that

$$\begin{bmatrix} A_{12} \\ A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix} W = \begin{bmatrix} A_{11}W \\ A_{21}W \end{bmatrix}.$$

We obtain the equations $A_{11}W = A_{12}$ and $A_{21}W = A_{22}$. Since A_{11} is invertible, we get $W = A_{11}^{-1}A_{12}$ and hence $A_{21}A_{11}^{-1}A_{12} = A_{22}$, which is (2).

Case 2. *The upper left $r \times r$ submatrix of A is not invertible.*

One way to handle this case is to use permutation matrices P and Q, such that $PAQ = \begin{bmatrix} \widetilde{A}_{11} & \widetilde{A}_{12} \\ \widetilde{A}_{21} & \widetilde{A}_{22} \end{bmatrix}$, $\widetilde{A}_{11} \in \mathbb{R}^{r \times r}$ and $\operatorname{rank} \widetilde{A}_{11} = r$. By Case 1 we have that the generalized inverse $(PAQ)^g$ of PAQ equals to $\begin{bmatrix} \widetilde{A}_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix}$.

Thus,

$$(PAQ) \begin{bmatrix} \widetilde{A}_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix} (PAQ) = PAQ. \tag{3}$$

Multiplying (3) from the left by P^{-1} and from the right by Q^{-1} we get

$$A \left(Q \begin{bmatrix} \widetilde{A}_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix} P \right) A = A.$$

So, $Q \begin{bmatrix} \widetilde{A}_{11}^{-1} & 0 \\ 0 & 0 \end{bmatrix} P = \left(P^T \begin{bmatrix} \left(\widetilde{A}_{11}^{-1}\right)^T & 0 \\ 0 & 0 \end{bmatrix} Q^T \right)^T$ is a generalized inverse of A. □

Algorithm for computing a generalized inverse of A

Let r be the rank of A.

1. Find any nonsingular submatrix B in A of order $r \times r$,
2. in A substitute
   - elements of the submatrix B for corresponding elements of $(B^{-1})^T$,
   - all other elements with 0,
3. the transpose of the obtained matrix is a generalized inverse G.

Example

Compute at least one generalized inverse of

$$A = \begin{bmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 1 & 0 \\ 2 & 0 & 1 & 4 \end{bmatrix}.$$

- Note that $\operatorname{rank} A = 2$. For B from the algorithm one of the possibilities is

$$B = \begin{bmatrix} 1 & 0 \\ 1 & 4 \end{bmatrix},$$

i.e., the submatrix in the right lower corner.

- Computing B^{-1} we get $B^{-1} = \begin{bmatrix} 1 & 0 \\ -\frac{1}{4} & \frac{1}{4} \end{bmatrix}$ and hence

$$\left(B^{-1}\right)^T = \begin{bmatrix} 1 & -\frac{1}{4} \\ 0 & \frac{1}{4} \end{bmatrix}.$$

- A generalized inverse of A is then

$$G = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -\frac{1}{4} \\ 0 & 0 & 0 & \frac{1}{4} \end{bmatrix}^T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{4} \end{bmatrix}.$$

Generalized inverses of a matrix A play a similar role as the usual inverse (when it exists) in solving a linear system $Ax = b$.

Theorem

Let $A \in \mathbb{R}^{n \times m}$ and $b \in \mathbb{R}^m$. If the system

$$Ax = b \tag{4}$$

is solvable (that is, $b \in \mathcal{C}(A)$) and G is a generalized inverse of A, then

$$x = Gb \tag{5}$$

is a solution of the system (4).

Moreover, all solutions of the system (4) are exaclty vectors of the form

$$x_z = Gb + (GA - I)z, \tag{6}$$

where z varies over all vectors from $\mathbb{R}^m$.

Proof.

We write A in the column form

$$A = \begin{bmatrix} a_1 & a_2 & \dots & a_m \end{bmatrix},$$

where a_i are column vectors of A. Since the system (4) is solvable, there exist real numbers $\alpha_1, \dots, \alpha_m \in \mathbb{R}$ such that

$$\sum_{i=1}^{m} \alpha_i a_i = b. \tag{7}$$

First we will prove that Gb also solves (4). Multiplying (7) with G we get

$$Gb = \sum_{i=1}^{m} \alpha_i G a_i. \tag{8}$$

Multiplying (9) with A the left side becomes $A(Gb)$, so we have to check that

$$\sum_{i=1}^{m} \alpha_i A G a_i = b. \tag{9}$$

Since G is a generalized inverse of A, we have that $AGA = A$ or restricting to columns of the left hand side we get

$$AGa_i = a_i \quad \text{for every } i = 1, \ldots, m.$$

Plugging this into the left side of (9) we get exactly (**??**), which holds and proves (9).

For the moreover part we have to prove two facts:

(i) Any x_z of the form (6) solves (4).

(ii) If $A\tilde{x} = b$, then $\tilde{x}$ is of the form x_z for some $z \in \mathbb{R}^m$.

(i) is easy to check:

$$\begin{aligned} Ax_z &= A\big(Gb + (GA - I)z\big) = AGb + A(GA - I)z \\ &= b + (AGA - A)z = b. \end{aligned}$$

To prove (ii) note that

$$A(\tilde{x} - Gb) = 0,$$

which implies that

$$\tilde{x} - Gb \in \ker A.$$

It remains to check that

$$\ker A = \{(GA - I)z \colon z \in \mathbb{R}^m\}. \tag{10}$$

The inclusion ($\supseteq$) of (10) is straightforward:

$$A((GA - I)z) = (AGA - A)z = 0.$$

For the inclusion ($\subseteq$) of (10) we have to notice that any $v \in \ker A$ is equal to $(GA - I)z$ for $z = -v$:

$$(GA - I)(-v) = -GAv + v = 0 + v = v. \quad \square$$

Example

Find all solutions of the system

$$Ax = b,$$

where $A = \begin{bmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 1 & 0 \\ 2 & 0 & 1 & 4 \end{bmatrix}$ and $b = \begin{bmatrix} 2 \\ 1 \\ 4 \end{bmatrix}$.

- Recall from the example a few slides above that $G = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{4} & \frac{1}{4} \end{bmatrix}$.
- Calculating Gb and $GA - I$ we get

$$Gb = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \frac{3}{4} \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \end{bmatrix}.$$

- Hence,

$$x_z = \begin{bmatrix} -z_1 & -z_2 & 1 & \frac{3}{4} + \frac{1}{2} z_1 \end{bmatrix}^T$$

where z_1, z_2 vary over $\mathbb{R}$.

1.2 The Moore-Penrose generalized inverse

Among all generalized inverses of a matrix A, one has especially nice properties.

Definition

The Moore-Penrose generalized inverse, or shortly the MP inverse of $A \in \mathbb{R}^{n\times m}$ is any matrix $A^+ \in \mathbb{R}^{m\times n}$ satifying the following four conditions:

1. A^+ is a generalized inverse of A: $AA^+A = A$.
2. A is a generalized inverse of A^+: $A^+AA^+ = A^+$.
3. The square matrix $AA^+ \in \mathbb{R}^{n\times n}$ is symmetric: $(AA^+)^T = AA^+$.
4. The square matrix $A^+A \in \mathbb{R}^{m\times m}$ is symmetric: $(A^+A)^T = A^+A$.

Remark

There are two natural questions arising after defining the MP inverse:

- *Does every matrix admit a MP inverse? Yes.*
- *Is the MP inverse unique? Yes.*

Theorem

The MP inverse A^+ of a matrix A is unique.

Proof.

Assume that there are two matrices M_1 and M_2 that satisfy the four conditions in the definition of MP inverse of A. Then,

$$\begin{aligned} AM_1 &= (AM_2A)M_1 && \text{by property (1)} \\ &= (AM_2)(AM_1) = (AM_2)^T(AM_1)^T && \text{by property (3)} \\ &= M_2^T(AM_1A)^T = M_2^TA^T && \text{by property (1)} \\ &= (AM_2)^T = AM_2 && \text{by property (3)} \end{aligned}$$

A similar argument involving properties (2) and (4) shows that

$$M_1A = M_2A,$$

and so

$$M_1 = M_1AM_1 = M_1AM_2 = M_2AM_2 = M_2.$$

□

Remark

Let us assume that A^+ exists (we will shortly prove this fact). Then the following properties are true:

- *If A is a square invertible matrix, then it $A^+ = A^{-1}$.*
- $(A^+)^+ = A$.
- $(A^T)^+ = (A^+)^T$.

In the rest of this chapter we will be interested in two obvious questions:

- How do we compute A^+?
- Why would we want to compute A^+?

To answer the first question, we will begin by three special cases.

Construction of the MP inverse of $A \in \mathbb{R}^{n\times m}$:

Case 1: $A^TA \in \mathbb{R}^{m\times m}$ *is an invertible matrix. (In particular, $m \leq n$.)*

In this case $A^+ = (A^TA)^{-1}A^T$.

To see this, we have to show that the matrix $(A^TA)^{-1}A^T$ satisfies properties (1) to (4):

1. $AMA = A(A^TA)^{-1}A^TA = A(A^TA)^{-1}(A^TA) = A.$
2. $MAM = (A^TA)^{-1}A^TA(A^TA)^{-1}A^T = (A^TA)^{-1}A^T = M.$
3. $$(AM)^T = \left(A(A^TA)^{-1}A^T\right)^T = A\left(\left(A^TA\right)^{-1}\right)^T A^T =$$ $$= A\left(\left(A^TA\right)^T\right)^{-1} A^T = A(A^TA)^{-1}A^T = AM.$$
4. Analoguous to the previous fact.

Case 2: AA^T *is an invertible matrix. (In particular, $n \leq m$.)*

In this case A^T satisfies the condition for Case 1, so $(A^T)^+ = (AA^T)^{-1}A$.

Since $(A^T)^+ = (A^+)^T$ it follows that

$$\begin{aligned} A^+ &= \left((A^+)^T\right)^T = \left((AA^T)^{-1}A\right)^T = A^T\left((AA^T)^{-1}\right)^T \\ &= A^T\left((AA^T)^{-T}\right)^{-1} = A^T(AA^T)^{-1}. \end{aligned}$$

Hence, $\underline{A^+ = A^T(AA^T)^{-1}}$.