Mathematical modelling

Lecture notes

Faculty of Computer and Information Science
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Chapter 0:

What is Mathematical Modelling?

- Types of models
- Modelling cycle
- Numerical errors

Introduction

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

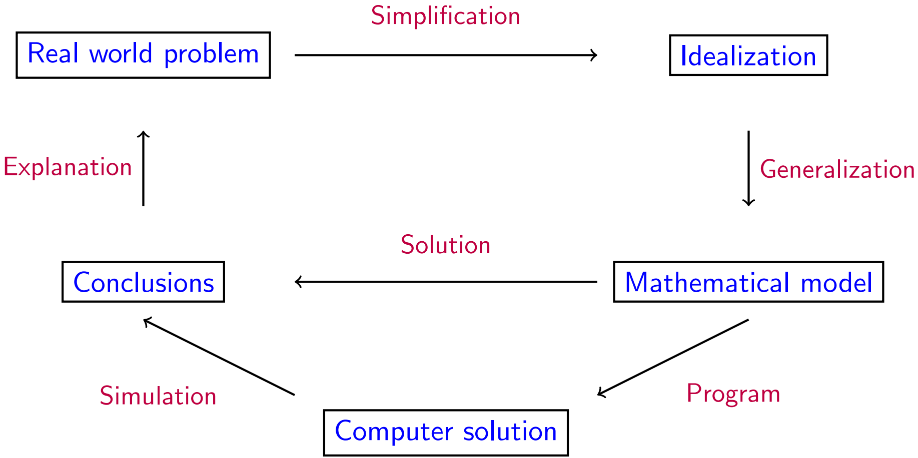
In this course we will introduce some (by far not all) mathematical tools that are used in setting up and solving mathematical models.

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 nonhomogeneous geometric object, angle and rotation in the initial thrust, ...)
- Choice of the 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

Chapter 1:

Linear model

- Definition
- Systems of linear equations
- Generalized inverses
- The Moore-Penrose (MP) inverse
- Singular value decomposition
- Principal component analysis
- MP inverse and solving linear systems

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 $A = [a_1, \ldots, a_n]$, 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 $\mathcal{C}(A)$ of A, i.e., $b \in \mathcal{C}(A)$.

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., $r = n$.

A generic 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 coefficient 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. $\square$

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

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

Plugging this into the left side of (9) we get exactly (7), 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 $\underline{A^+ = (A^TA)^{-1}A^T}$.

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

Case 3: $\Sigma \in \mathbb{R}^{n \times m}$ *is a diagonal matrix of the form*

$$\Sigma = \begin{bmatrix} \sigma_1 & & & & \\ & \sigma_2 & & & \\ & & \ddots & & \\ & & & \sigma_n & \\ & & & & \end{bmatrix} \quad \text{or} \quad \widetilde{\Sigma} = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_m \\ & & & \\ & & & \end{bmatrix}.$$

The MP inverse is

$$\Sigma^+ = \begin{bmatrix} \sigma_1^+ & & & \\ & \sigma_2^+ & & \\ & & \ddots & \\ & & & \sigma_n^+ \\ & & & \\ & & & \end{bmatrix} \quad \text{or} \quad \widetilde{\Sigma}^+ = \begin{bmatrix} \sigma_1^+ & & & & \\ & \sigma_2^+ & & & \\ & & \ddots & & \\ & & & \sigma_m^+ & \end{bmatrix},$$

where $\sigma_i^+ = \begin{cases} \frac{1}{\sigma_i}, & \sigma_i \neq 0, \\ 0, & \sigma_i = 0. \end{cases}$

Case 4: *A general matrix A. (using SVD)*

Theorem (Singular value decomposition - SVD)

Let $A \in \mathbb{R}^{n \times m}$ *be a matrix. Then it can be expressed as a product*

$$A = U \Sigma V^T,$$

where

- $U \in \mathbb{R}^{n \times n}$ *is an orthogonal matrix with left singular vectors* u_i *as its columns,*
- $V \in \mathbb{R}^{m \times m}$ *is an orthogonal matrix with right singular vectors* v_i *as its columns,*
- $\Sigma = \left[\begin{array}{ccc|c} \sigma_1 & & & 0 \\ & \ddots & & \vdots \\ & & \sigma_r & 0 \\ \hline & 0 & & 0 \end{array}\right] = \begin{bmatrix} S & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{n \times m}$ *is a diagonal matrix*

with singular values

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$$

on the diagonal.

Derivations for computing SVD

If $A = U\Sigma V^T$, then

$$A^TA = (V\Sigma^TU^T)(U\Sigma V^T) = V\Sigma^T\Sigma V^T = V\begin{bmatrix} S^2 & 0 \\ 0 & 0 \end{bmatrix} V^T \in \mathbb{R}^{m\times m},$$

$$AA^T = (U\Sigma V^T)(U\Sigma V^T)^T = U\Sigma\Sigma^TU^T = U\begin{bmatrix} S^2 & 0 \\ 0 & 0 \end{bmatrix} U^T \in \mathbb{R}^{n\times n}.$$

Let

$$V = \begin{bmatrix} v_1 & v_2 & \cdots & v_m \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix}$$

be the column decompositions of V and U.

Let $e_1, \ldots, e_m \in \mathbb{R}^m$ and $f_1, \ldots, f_n \in \mathbb{R}^n$ be the standard coordinate vectors of $\mathbb{R}^m$ and $\mathbb{R}^n$, i.e., the only nonzero component of e_i (resp. f_j) is the i-th one (resp. j-th one), which is 1. Then

$$A^TAv_i = V\Sigma^T\Sigma V^Tv_i = V\Sigma^T\Sigma e_i = \begin{cases} \sigma_i^2 v_i, & \text{if } i \le r, \\ 0, & \text{if } i > r, \end{cases}$$

$$AA^Tu_j = U\Sigma\Sigma^TU^Tu_j = U\Sigma\Sigma^Tf_j = \begin{cases} \sigma_i^2 u_j, & \text{if } j \le r, \\ 0, & \text{if } j > r. \end{cases}$$

Further on,

$$(AA^T)(Av_i) = A(A^TA)v_i = \begin{cases} \sigma_i^2 Av_i, & \text{if } i \leq r, \\ 0, & \text{if } i > r, \end{cases}$$
$$(A^TA)(A^Tu_j) = A^T(AA^T)u_j = \begin{cases} \sigma_j^2 A^Tu_j, & \text{if } j \leq r, \\ 0, & \text{if } j > r. \end{cases}$$

It follows that:

- $\Sigma^T\Sigma = \begin{bmatrix} S^2 & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{m\times m}$ (resp. $\Sigma\Sigma^T = \begin{bmatrix} S^2 & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{n\times n}$) is the diagonal matrix with eigenvalues σ_i^2 of A^TA (resp. AA^T) on its diagonal, so the singular values σ_i are their square roots.
- V has the corresponding eigenvectors (normalized and pairwise orthogonal) of A^TA as its columns, so the right singular vectors are eigenvectors of A^TA.
- U has the corresponding eigenvectors (normalized and pairwise orthogonal) of AA^T as its columns, so the left singular vectors are eigenvectors of AA^T.

- Av_i is an eigenvector of AA^T corresponding to σ_i^2 and so

$$u_i = \frac{Av_i}{\|Av_i\|} = \frac{Av_i}{\sigma_i}$$

is a left singular vector corresponding to σ_i, where in the second equality we used that

$$\|Av_i\| = \sqrt{(Av_i)^T(Av_i)} = \sqrt{v_i^T A^T A v_i} = \sqrt{\sigma_i^2 v_i^T v_i} = \sigma_i \|v_i\| = \sigma_i.$$

- $A^T u_j$ is an eigenvector of $A^T A$ corresponding to σ_j^2 and so

$$v_j = \frac{A^T u_j}{\|A^T u_j\|} = \frac{A^T u_j}{\sigma_j}$$

is a right singular vector corresponding to σ_j, where in the second equality we used that

$$\|A^T u_j\| = \sqrt{(A^T u_j)^T(A^T u_j)} = \sqrt{u_j^T A A^T u_j} = \sqrt{\sigma_j^2 u_j^T u_j} = \sigma_j \|u_j\| = \sigma_j.$$

Algorithm for SVD computation

- Compute the eigenvalues and an orthonormal basis consisting of eigenvectors of the symmetric matrix $A^T A$ or AA^T (depending on which is of them is of smaller size).
- The singular values of the matrix $A \in \mathbb{R}^{n \times m}$ are equal to $\sigma_i = \sqrt{\lambda_i}$, where λ_i are the nonzero eigenvalues of $A^T A$ (resp. AA^T).
- The left singular vectors are the corresponding orthonormal eigenvectors of AA^T.
- The right singular vector are the corresponding orthonormal eigenvectors of $A^T A$.
- If u (resp. v) is a left (resp. right) singular vector corresponding to the singular value σ_i, then $v = A^T u$ (resp. $u = Av$) is a right (resp. left) singular vector corresponding to the same singular value.
- The remaining columns of U (resp. V) consist of an orthonormal basis of the kernel (i.e., the eigenspace of $\lambda = 0$) of AA^T (resp. $A^T A$).

General algorithm for computation of A^+ (long version)

1. For $A^T A$ compute its eigenvalues
$$\lambda_1 \geq \lambda_2 \geq \cdots, \geq \lambda_r > \lambda_{r+1} = \ldots = \lambda_m = 0$$
and the corresponding orthonormal eigenvectors
$$v_1, \ldots, v_r, v_{r+1}, \ldots, v_m,$$
and form the matrices
$$\Sigma = \mathrm{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_m}) \in \mathbb{R}^{n \times m},$$
$$V_1 = \begin{bmatrix} v_1 & \cdots & v_r \end{bmatrix}, \quad V_2 = \begin{bmatrix} v_{r+1} & \cdots & v_m \end{bmatrix} \quad \text{and} \quad V = \begin{bmatrix} V_1 & V_2 \end{bmatrix}.$$
2. Let
$$u_1 = \frac{Av_1}{\sigma_1}, \quad u_2 = \frac{Av_2}{\sigma_2}, \quad \ldots \quad , \quad u_r = \frac{Av_r}{\sigma_r},$$
and $u_{r+1}, \ldots, u_n$ vectors, such that $\{u_1, \ldots, u_n\}$ is an ortonormal basis for $\mathbb{R}^n$. Form the matrices
$$U_1 = \begin{bmatrix} u_1 & \cdots & u_r \end{bmatrix}, \quad U_2 = \begin{bmatrix} u_{r+1} & \cdots & u_n \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}.$$
3. Then
$$A^+ = V\Sigma^+ U^T.$$

General algorithm for computation of A^+ (short version)

1. For $A^T A$ compute its **nonzero** eigenvalues

$$\lambda_1 \geq \lambda_2 \geq \cdots, \geq \lambda_r > 0$$

   and the corresponding orthonormal eigenvectors

$$v_1, \ldots, v_r,$$

   and form the matrices

$$S = \operatorname{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_r}) \in \mathbb{R}^{r \times r},$$
$$V_1 = \begin{bmatrix} v_1 & \cdots & v_r \end{bmatrix} \in \mathbb{R}^{m \times r}.$$

2. Put the vectors

$$u_1 = \frac{Av_1}{\sigma_1}, \quad u_2 = \frac{Av_2}{\sigma_2}, \quad \ldots \quad, \quad u_r = \frac{Av_r}{\sigma_r}$$

   in the matrix

$$U_1 = \begin{bmatrix} u_1 & \cdots & u_r \end{bmatrix}.$$

3. Then

$$A^+ = V_1 \Sigma^+ U_1^T.$$

Correctness of the computation of A^+

Step 1. $V\Sigma^+U^T$ is equal to A^+.

(i) $AA^+A = A$:

$$\begin{aligned} AA^+A &= (U\Sigma V^T)(V\Sigma^+U^T)(U\Sigma V^T) = U\Sigma(V^TV)\Sigma^+(U^TU)\Sigma V^T \\ &= U\Sigma\Sigma^+\Sigma V^T = U\Sigma V^T = A. \end{aligned}$$

(ii) $A^+AA^+ = A^+$: Analoguous to (i).

(iii) $(AA^+)^T = AA^+$:

$$\begin{aligned} (AA^+)^T &= \Big((U\Sigma V^T)(V\Sigma^+U^T)\Big)^T = \Big(U\Sigma\Sigma^+U^T\Big)^T \\ &= \left(U\begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}U^T\right)^T = U\begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix}U^T \\ &= (U\Sigma V^T)(V\Sigma^+U^T) = A^+. \end{aligned}$$

(iv) $(A^+A)^T = A^+A$: Analoguous to (iii).

Step 2. $V\Sigma^+U^T$ is equal to $V_1\Sigma^+U_1^T$.

$$V\Sigma U^T = \begin{bmatrix} V_1 & V_2 \end{bmatrix} \begin{bmatrix} S & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} U_1^T \\ U_2^T \end{bmatrix} = \begin{bmatrix} V_1 S & 0 \end{bmatrix} \begin{bmatrix} U_1^T \\ U_2^T \end{bmatrix} = V_1 S U_1^T.$$

Example

Compute the SVD and A^+ of the matrix $A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$.

- $AA^T = \begin{bmatrix} 17 & 8 \\ 8 & 17 \end{bmatrix}$ has eigenvalues 25 and 9.
- The eigenvectors of AA^T corresponding to the eigenvalues 25, 9 are

$$u_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}^T, \qquad u_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}^T.$$

- The left singular vectors of A are

$$v_1 = \frac{A^T u_1}{\sigma_1} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}^T, \qquad v_2 = \frac{A^T u_2}{\sigma_2} = \begin{bmatrix} \frac{1}{3\sqrt{2}} & -\frac{1}{3\sqrt{2}} & \frac{4}{3\sqrt{2}} \end{bmatrix}^T.$$

$$v_3 = v_1 \times v_2 = \begin{bmatrix} \frac{2}{\sqrt{3}} & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix}^T.$$

- $$A = U\Sigma V^T = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{3\sqrt{2}} & -\frac{1}{3\sqrt{2}} & \frac{4}{3\sqrt{2}} \\ \frac{2}{\sqrt{3}} & -\frac{2}{3} & -\frac{1}{3} \end{bmatrix}.$$
- $$\begin{aligned} A^+ = V\Sigma^+ U^T &= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{3\sqrt{2}} & \frac{2}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{3\sqrt{2}} & -\frac{2}{3} \\ 0 & \frac{4}{3\sqrt{2}} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} \frac{1}{5} & 0 \\ 0 & \frac{1}{3} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \\ &= \begin{bmatrix} \frac{7}{45} & \frac{2}{45} \\ \frac{2}{45} & \frac{7}{45} \\ \frac{2}{9} & -\frac{2}{9} \end{bmatrix}. \end{aligned}$$

1.3 The MP inverse and systems of linear equations

Let $A \in \mathbb{R}^{n\times m}$, where $m > n$. A system of equations $Ax = b$ that has more variables than constraints. Typically such system has infinitely many solutions, but it may happen that it has no solutions. We call such system an underdetermined system.

Theorem

1. *An underdetermined system of linear equations*

$$Ax = b \tag{11}$$

   is solvable if and only if $AA^{+}b = b$.

2. *If there are infinitely many solutions, the solution $A^{+}b$ is the one with the smallest norm, i.e.,*

$$\|A^{+}b\| = \min\{\|x\| \colon Ax = b\}.$$

   Moreover, it is the unique solution of smallest norm.

Proof of Theorem.

We already know that $Ax = b$ is solvable iff Gb is a solution, where G is any generalized inverse of A. Since A^+ is one of the generalized inverses, this proves the first part of the theorem.

To prove the second part of the theorem, first recall that all the solutions of the system are precisely the set

$$\{A^+b + (A^+A - I)z \colon z \in \mathbb{R}^m\}.$$

So we have to prove that for every $z \in \mathbb{R}^m$,

$$\|A^+b\| \leq \|A^+b + (A^+A - I)z\|.$$

We have that:

$$\|A^+b + (A^+A - I)z\|^2 =$$
$$= \left(A^+b + (A^+A - I)z\right)^T \left(A^+b + (A^+A - I)z\right)$$
$$= \left(A^+b\right)^T \left(A^+b\right) + 2\left(A^+b\right)^T (A^+A - I)z + \left((A^+A - I)z\right)^T \left((A^+A - I)z\right)$$
$$= \|A^+b\|^2 + 2\left(A^+b\right)^T (A^+A - I)z + \|(A^+A - I)z\|^2$$

Now,

$$\begin{aligned}
\left(A^+b\right)^T(A^+A - I)z &= b^T(A^+)^T(A^+A - I)z \\
&= b^T(A^+)^T(A^+A)^T z - b^T(A^+)^T z \\
&= b^T\left((A^+A)A^+\right)^T z - b^T(A^+)^T z \\
&= b^T\left(A^+AA^+\right)^T z - b^T(A^+)^T z \\
&= b^T(A^+)^T z - b^T(A^+)^T z = 0,
\end{aligned}$$

where we used the fact $(A^+A)^T = A^+A$ in the second equality.

Thus,

$$\|A^+b + (A^+A - I)z\|^2 = \|A^+b\|^2 + \|(A^+A - I)z\|^2 \geq \|A^+b\|^2,$$

with the equality iff $(A^+A - I)z = 0$. This proves the second part of the theorem. $\square$

Example

- The solutions of the underdetermined system $x + y = 1$ geometrically represent an affine line. Matricially, $A = \begin{bmatrix} 1 & 1 \end{bmatrix}$, $b = 1$. Hence, $A^+ b = A^+ 1$ is the point on the line, which is the nearest to the origin. Thus, the vector of this point is perpendicular to the line.
- The solutions of the underdetermined system $x + 2y + 3z = 5$ geometrically represent an affine hyperplane. Matricially, $A = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$, $b = 5$. Hence, $A^+ b = A^+ 5$ is the point on the hyperplane, which is the nearest to the origin. Thus, the vector of this point is normal to the hyperplane.
- The solutions of the underdetermined system $x + y + z = 1$ and $x + 2y + 3z = 5$ geometrically represent an affine line in $\mathbb{R}^3$. Matricially, $A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix}$, $b = \begin{bmatrix} 1 \\ 5 \end{bmatrix}$. Hence, $A^+ b$ is the point on the line, which is the nearest to the origin. Thus, the vector of this point is perpendicular to the line.

Example

Find the point on the plane $3x + y + z = 2$ closest to the origin.

- In this case,
$$A = \begin{bmatrix} 3 & 1 & 1 \end{bmatrix} \quad \text{and} \quad b = [2].$$
- We have that $AA^T = [11]$ and hence its only eigenvalue is $\lambda = 11$ with eigenvector $u = [1]$, implying that
$$U = [1] \quad \text{and} \quad \Sigma = \begin{bmatrix} \sqrt{11} & 0 & 0 \end{bmatrix}.$$
- Hence,
$$v_1 = \frac{A^T u}{\|A^T u\|} = \frac{A^T u}{\sigma_1} = \frac{1}{\sqrt{11}} \begin{bmatrix} 3 & 1 & 1 \end{bmatrix}^T.$$
- $$A^+ = V\Sigma^+ U^T = \frac{1}{\sqrt{11}} \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix} \frac{1}{\sqrt{11}} [1] = \begin{bmatrix} \frac{3}{11} \\ \frac{1}{11} \\ \frac{1}{11} \end{bmatrix}.$$
- $$x^+ = A^+ b = \begin{bmatrix} \frac{6}{11} & \frac{2}{11} & \frac{2}{11} \end{bmatrix}^T.$$

Overdetermined systems

Let $A \in \mathbb{R}^{n \times m}$, where $n > m$. This system is called overdetermined, since here are more constraints than variables. Such a system typically has no solutions, but it might have one or even infinitely many solutions.

Least squares approximation problem: if the system $Ax = b$ has no solutions, then a best fit for the solution is a vector x such that the error $||Ax - b||$ or, equivalently in the row decomposition

$$A = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix},$$

its square

$$||Ax - b||^2 = \sum_{i=1}^{n} (\alpha_i x - b_i)^2,$$

is the smallest possible.

Theorem

If the system $Ax = b$ has no solutions, then

$$x^{+} = A^{+} b$$

is the solution to the least squares approximation problem:

$$\min\{\|Ax - b\| \colon x \in \mathbb{R}^n\}. \tag{12}$$

Moreover, if $\operatorname{rank} A = m$, *then* (12) *has a unique solution. If* $\operatorname{rank} A < m$, *then x^{+} has the smallest second norm $\|x^{+}\|_2$ among all solution to* (12).

Proof.

Let $A = U\Sigma V^T$ be the SVD decomposition of A. We have that

$$\|Ax - b\| = \|U\Sigma V^T x - b\| = \|\Sigma V^T x - U^T b\|,$$

where we used that

$$\|U^T v\| = \|v\|$$

in the second equality (which holds since U^T is an orthogonal matrix).

Let

$$\Sigma = \begin{bmatrix} S & 0 \\ 0 & 0 \end{bmatrix}, \quad U = \begin{bmatrix} U_1 & U_2 \end{bmatrix}, \quad V = \begin{bmatrix} V_1 & V_2 \end{bmatrix}, \quad \text{where}$$

$S \in \mathbb{R}^{r\times r}$, $U_1 \in \mathbb{R}^{n\times r}, U_2 \in \mathbb{R}^{n\times(n-r)}$, $V_1 \in \mathbb{R}^{m\times r}$, $V_2 \in \mathbb{R}^{m\times(m-r)}$. Thus,

$$\begin{aligned} \|\Sigma V^T x - U^T b\| &= \left\| \begin{bmatrix} S & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1^T \\ V_2^T \end{bmatrix} x - \begin{bmatrix} U_1^T \\ U_2^T \end{bmatrix} b \right\| \\ &= \left\| \begin{bmatrix} S V_1^T x - U_1^T b \\ U_2^T b \end{bmatrix} \right\|. \end{aligned}$$

But this norm is minimal iff

$$S V_1^T x - U_1^T b = 0$$

or equivalently

$$V_1^T x = S^{-1} U_1^T b. \tag{13}$$

Further on,

$$V^T V = \begin{bmatrix} V_1^T V_1 & V_1^T V_2 \\ V_2^T V_1 & V_2^T V_2 \end{bmatrix} = I_n,$$

implies that $V_1^T V_1 = I_r$ and $V_2^T V_1 = 0$, where I_k stands for the $k \times k$ identity matrix.

If $\operatorname{rank} A = m$, then $V_1 \in \mathbb{R}^{m\times m}$ is invertible with the inverse V_1^T and hence,

$$V_1 S^{-1} U_1^T b = A^+ b$$

is the unique solution to (12).
If $r = \operatorname{rank} A < m$, then all x which solve (13) are of the form $A_1^+ b + z$, for $z \in \ker V_1^T$. Since $\ker V_1^T = \operatorname{im} V_2$ and $V_2^T V_1 = 0$, it follows that the norm of $A_1^+ b + z$ is minimal for $z = 0$. □

Remark

The closest vector to b in the column space $C(A) = \{Ax \colon x \in \mathbb{R}^m\}$ of A is the orthogonal projection of b onto $C(A)$. It follows that $A^+ b$ is this projection. Equivalently, $b - (A^+ b)$ is orthogonal to any vector Ax, $x \in \mathbb{R}^m$, which can be proved also directly.

Example

Given points $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ in the plane, we are looking for the line $ax + b = y$ which is the least squares best fit.

If $n > 2$, we obtain an overdetermined system

$$\begin{bmatrix} x_1 & 1 \\ \vdots & \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}.$$

The solution of the least squares approximation problem is given by

$$\begin{bmatrix} a \\ b \end{bmatrix} = A^+ \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}.$$

The line $y = ax + b$ in the regression line.

An application of SVD: principal component analysis or PCA

PCA is a very well-known and efficient method for data compression, dimension reduction, ...

Due to its importance in different fields, it has many other names: discrete Karhunen-Loève transform (KLT), Hotelling transform, empirical orthogonal functions (EOF), ...

Let $\{X_1, \ldots, X_m\}$ be a sample of vectors from $\mathbb{R}^n$.

In applications, often $m << n$, where n is very large, for example, $X_1, \ldots, X_m$ can be

- vectors of gene expressions in m tissue samples or
- vectors of grayscale in images
- bag of words vectors, with components corresponding to the numbers of certain words from some dictionary in specific texts, ...,

or $n << m$ for example if the data represents a point cloud in a low dimensional space $\mathbb{R}^n$ (for example in the plane).

We will assume that $m << n$. Also assume that the data is centralized, i.e., the centeroid is in the origin

$$\mu = \frac{1}{m} \sum_{i=1}^{m} X_i = 0 \in \mathbb{R}^n.$$

If not, we substract μ from all vectors in the data set.

A matrix norm $\| \cdot \| : \mathbb{R}^{n \times m} \to \mathbb{R}$ is a function, which generalizes the notion of the absolute value for numbers to matrices. It is used to measure a distance between matrices. In contrast with the absolute value, which is unique up to multiplication with a positive constant, there are many different matrix norms.

Two important matrix norms are the following:

1. Spectral norm $\| \cdot \|_2$:

$$\|A\|_2 := \max_{\|x\|_2=1} \|Ax\|_2 = \max_{j=1,\ldots,\min(n,m)} \sigma_j(A).$$

2. Frobenius norm $\| \cdot \|_F$:

$$\|A\|_F := \sqrt{\sum_{i,j} a_{i,j}^2} = \sqrt{\sum_{j=1,\ldots,\min(n,m)} \sigma_j(A)^2}.$$

Let

$$X = \begin{bmatrix} X_1 & X_2 & \cdots & X_m \end{bmatrix}^T$$

be the matrix of dimension $m \times n$ with data in the rows.

Let $X^T X \in \mathbb{R}^{m \times m}$ and $XX^T \in \mathbb{R}^{n \times n}$ be the covariance matrices of the data.

- The principal values of the data set $\{X_1, \ldots, X_r\}$ are the nonzero eigenvalues $\lambda_i = \sigma_i^2$ of the covariance matrices (where σ_i are the singular values of X).
- The principal directions in $\mathbb{R}^n$ are corresponding eigenvectors $v_1, \ldots, v_r$, i.e. the columns of the matrix V from the SVD of X. The remaining clolumns of V (i.e. the eigenvectors correspondong to 0) form a basis of the null space of X.
- The first column v_1, the first principal direction, corresponds to the direction in $\mathbb{R}^n$ with the largest variance in the data X_i, that is, the most informative direction for the data set, the second the second most important, ...
- The principal directions in $\mathbb{R}^m$ are the columns $u_1, \ldots, u_r$ of the matrix U and represent the coefficients in the linear decomposition of the vectors $X_1, \ldots, X_m$ along the orthonormal basis $v_1, \ldots v_n$ of $\mathbb{R}^n$.

PCA provides a linear dimension reduction method based on a projection of the data from the space $\mathbb{R}^n$ into a lower dimensional subspace spanned by the first few principal vectors $v_1, \ldots, v_k$ in $\mathbb{R}^n$.

The idea is to approximate

$$X_i = \sigma_1 u_{1,i} v_1 + \cdots + \sigma_m u_{m,i} v_m \cong \sigma_1 u_{1,i} v_1 + \cdots + \sigma_k u_{k,i} v_k$$

with the first k most informative directions in $\mathbb{R}^n$ and supress the last $m-k$.

PCA has the following amazing property:

Theorem

Among all possible projections of $p\colon \mathbb{R}^n \to \mathbb{R}^k$ onto a k-dimensional subspace, PCA provides the best in the sense that the errors

$$\|X - p(X)\|_F^2 \qquad \textit{and} \qquad \|X - p(X)\|_2^2,$$

where $p(X) = \begin{bmatrix} p(X_1) & \cdots & p(X_m) \end{bmatrix}^T$, are the smallest possible.