Numerical methods

Approximation of functions

OUTLINE

1. Approximation and interpolation
2. Least-square method
   - basis functions
   - design matrix
   - residual
   - weighted least squares
   - normal equation
   - Gramian matrix
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   - solution of overdetermined systems
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Approximation and interpolation

To approximate function $f(x)$ means

to substitute it by a function $\varphi(x)$,

which is in some sense close to function $f(x)$.

We will deal with two basic types of approximation:
interpolation and **least-square method**

Definition: **Interpolation** is such approximation,

in which the function $\varphi(x)$ goes exactly through given points $[x_i, y_i]$, where $y_i = f(x_i)$.

Sometimes we also require that

functions f and φ have the same derivatives

in points x_i.

Approximation and interpolation

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We will deal with two basic types of approximation:
interpolation and **least-square method**

Definition: **Least-square method** is such approximation,

in which $\varphi(x)$ is „interlaced"

between given points $[x_i, y_i]$ in such a way,

that the „distance" between functions f and φ is

in some sense minimal.

Usually the function $\varphi(x)$ does not go through

points $[x_i, y_i]$.

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Least-square method

means procedure
for approximate solution of overdetermined equations
or inaccurately defined linear systems
based on minimization of quadrate of residuals

Curve fitting is an important group of problem,
which could be solved by least-square method

We will describe what is it about.

Least-square method

Let t is an independent variable, e.g. time,
and $y(t)$ is an unknown function of variable t
we want to approximate.

Suppose that we performed m **measurements**,
i.e. values y were measured for specified values of t:

$$y_i = y(t_i)\,, \qquad i = 1, 2, \ldots, m\,.$$

Our aim is to model $y(t)$
using linear combination of n **basis functions**
for some $n \leq m$:

$$y(t) \approx x_1\varphi_1(t) + x_2\varphi_2(t) + \cdots + x_n\varphi_n(t) := R_n(t)\,.$$

We propose basis function based on
expected course of unknown function $y(t)$.
Then we have to estimate parameters $x_1, x_2, \ldots, x_n$.

Function $R_n(t)$ is called (in statistics)
linear regression function.

Design matrix

Design matrix A of a model is an rectangular matrix, which has m rows and n columns:

$$\mathbf{A} = \begin{pmatrix} \varphi_1(t_1) & \varphi_2(t_1) & \dots & \varphi_n(t_1) \\ \varphi_1(t_2) & \varphi_2(t_2) & \dots & \varphi_n(t_2) \\ \vdots & \vdots & & \vdots \\ \varphi_1(t_m) & \varphi_2(t_m) & \dots & \varphi_n(t_m) \end{pmatrix} \equiv (\boldsymbol{\varphi}_1, \boldsymbol{\varphi}_2, \dots, \boldsymbol{\varphi}_n),$$

where $\boldsymbol{\varphi}_i = (\varphi_i(t_1), \varphi_i(t_2), \dots \varphi_i(t_m))^T$ is i-th column of $\mathbf{A}$.

Matrix formulation of a model is

$$\mathbf{y} \approx \mathbf{A}\mathbf{x},$$

where $\mathbf{y} = (y_1, y_2, \dots, y_m)^T$ are measured data and

$\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ is a vector of unknown parameters.

Least-square method

Residuals are differences between measured and modelled data:

$$r_i = y_i - R_n(t_i) = y_i - \sum_{j=1}^{n} \varphi_j(t_i) x_j \equiv y_i - \sum_{j=1}^{n} a_{ij} x_j \,, \qquad i = 1, 2, \ldots, n \,,$$

where $a_{ij} = \varphi_j(t_i)$.

In matrix form

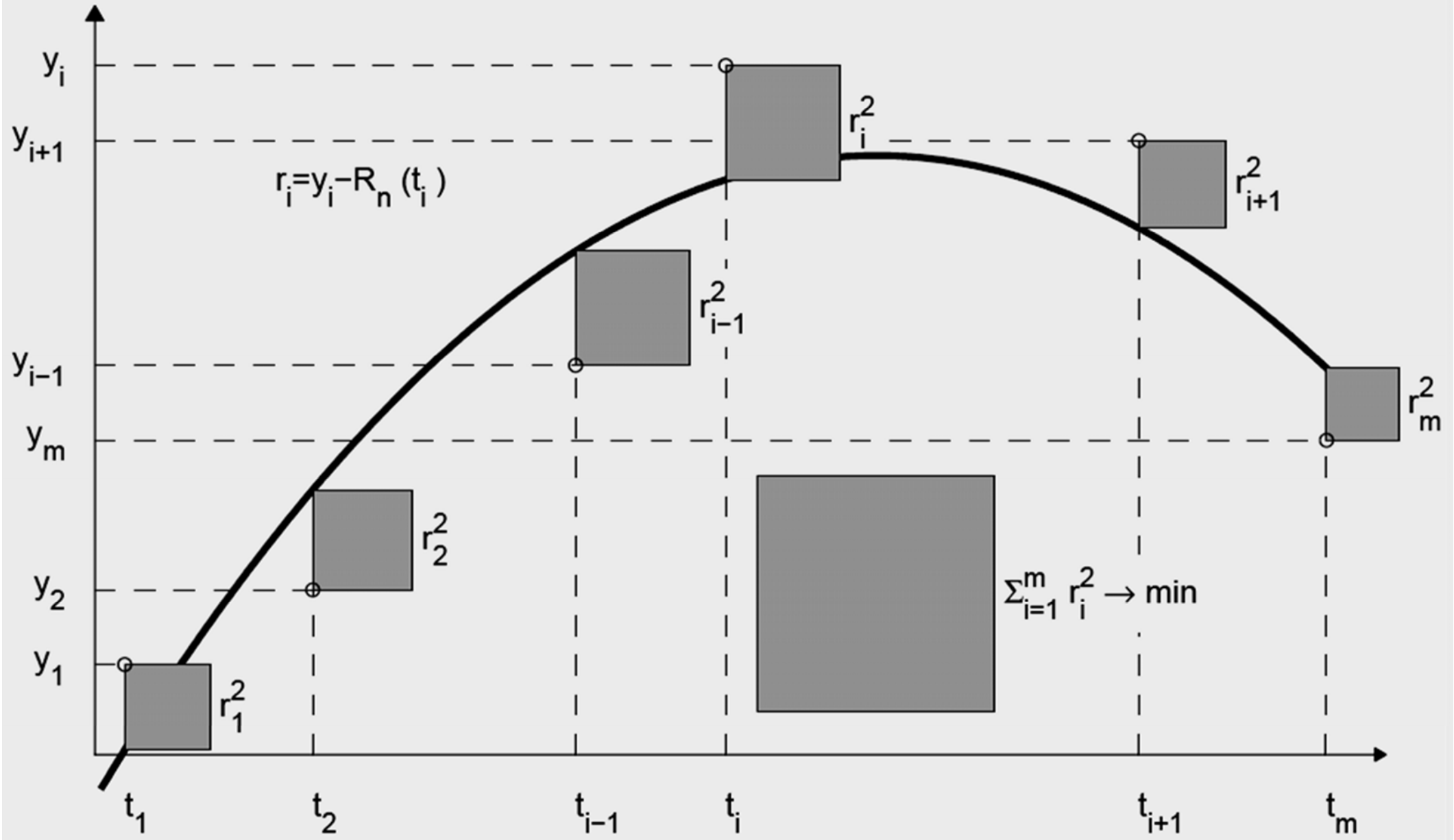
$$\mathbf{r} = \mathbf{y} - \mathbf{A}\mathbf{x} \,.$$

We want to determine the parameters x_j in such a way, that the residual will be minimal.

We can derive least-square method by solving quadratic minimization problem:

$$\|\mathbf{r}\|^2 := \sum_{i=1}^{m} r_i^2 \to \min \,.$$

Least-square method



Principle of least squares

Least-square method

Approximate solution of overdetermined system **A x = y**
(i.e. we have more equations than unknowns),
which minimize the residual **r = y – Ax**,
is called
solution of linear system
by least squares.

Least-square method

Sometimes we have to use
weighted linear least squares:

If measurements are
not equally reliable,
then we can assign
to each measurement
the weight $w_i > 0$ and
then we minimize sum of weighted quadrates

$$\|\mathbf{r}\|_w^2 := \sum_{i=1}^{m} w_i r_i^2 \to \min .$$

If, e.g. the error of i-th measurement
is approximately equal to e_i, we will choose $w_i = 1/e_i$.

Each method for solving unweighted LSM
is possible to use also for weighted LSM:
it is enough to multiply y_i and i-th row of $\mathbf{A}$ by $\sqrt{w_i}$.

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Normal equations

Solution of minimization problem

$$\|\mathbf{r}\|^2 := \sum_{i=1}^{m} r_i^2 \to \min$$

have to fulfill the necessary condition for extrema:

$$\frac{\partial \|\mathbf{r}\|^2}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{m} \left(y_i - \sum_{j=1}^{n} a_{ij} x_j \right)^2 = 0\,, \qquad k = 1, 2, \ldots, n\,.$$

After derivation we obtain

$$\frac{\partial \|\mathbf{r}\|^2}{\partial x_k} = 2 \sum_{i=1}^{m} \left(y_i - \sum_{j=1}^{n} a_{ij} x_j \right) (-a_{ik}) = 0$$

and then

$$\sum_{j=1}^{n} \left(\sum_{i=1}^{m} a_{ik} a_{ij} \right) x_j = \sum_{i=1}^{m} a_{ik} y_i\,, \qquad k = 1, 2, \ldots, n\,,$$

which could be written in matrix form as $\mathbf{A}^T \mathbf{A}\mathbf{x} = \mathbf{A}^T \mathbf{y}$.

Normal equations

Linear system $\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{y}$ is known as **normal equations.**

If the columns of matrix **A** are linearly independent, then the matrix $\mathbf{G} := \mathbf{A}^T\mathbf{A}$ is positive definite and solution $\mathbf{x}^*$ of normal equations is the only solution of minimization problem, i.e. it holds

$$\|\mathbf{y} - \mathbf{A}\mathbf{x}^*\|^2 = \min_{\mathbf{x}} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|^2 .$$

Normal equations

If we express the normal equations
using vectors φ_i, we get

$$\begin{pmatrix} (\varphi_1,\varphi_1) & (\varphi_1,\varphi_2) & \dots & (\varphi_1,\varphi_n) \\ (\varphi_2,\varphi_1) & (\varphi_2,\varphi_2) & \dots & (\varphi_2,\varphi_n) \\ \vdots & \vdots & \dots & \vdots \\ (\varphi_n,\varphi_1) & (\varphi_n,\varphi_2) & & (\varphi_n,\varphi_n) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} (\varphi_1,\mathbf{y}) \\ (\varphi_2,\mathbf{y}) \\ \vdots \\ (\varphi_n,\mathbf{y}) \end{pmatrix},$$

where

$$(\varphi_k,\varphi_j) = \sum_{i=1}^{m} \varphi_k(t_i)\varphi_j(t_i) \qquad \text{and} \qquad (\varphi_k,\mathbf{y}) = \sum_{i=1}^{m} \varphi_k(t_i)y_i$$

are scalar products of vectors φ_k, φ_i and $\varphi_k, \mathbf{y}$.

Matrix **G** of this system is called
Gramian matrix of a set of vectors $\varphi_j, j = 1, 2, \dots, n$.

Normal equations

During the design of approximation $R_n(t)$
we should select functions $\varphi_i(t)$ in such a way,
that columns φ_i of matrix **A** to be linearly independent.

If it to be the contrary
than it is possible to show that
the minimization problem
has infinite number of solutions
which is obviously not desirable.

Normal equations

Two important special cases,
for which the columns of matrix **A** are linearly independent:

1. $\varphi_j(t)$ is a polynomial of degree j-1, e.g. $\varphi_j(t) = t^{j-1}$, $j = 1, 2, \ldots, n$;
2. for n=2N+1, where N is a whole nonnegative integer, we chose

$$\begin{aligned} &\varphi_1(t) = 1, \\ &\varphi_{2k}(t) = \cos kt, \\ &\varphi_{2k+1}(t) = \sin kt, \quad k = 1, 2, \ldots, N, \end{aligned}$$

and „time of measurement" t_i we chose from interval $\langle c, c + 2\pi)$,
where c is an arbitrary number.

Approximation $R_n(t)$ is in the first case an **algebraic polynomial** and
in the second case a **trigonometric polynomial**.

Normal equations

If $m=n$ and the matrix $\mathbf{A}$ is regular,
then $\mathbf{x}^*=\mathbf{A}^{-1}\mathbf{y}$ and $\mathbf{r}=\mathbf{0}$,
i.e. $R_n(t_i) = y_i,\ i = 1, 2, \ldots, m.$

However if measured data y_i contains errors,
then it is not practical,
that function $R_n(t)$ follows those errors.

On the contrary, we want that $R_n(t)$ authentically
reconstructs the unknown function $y(t)$,
therefore it is desirable,
that $R_n(t)$ **smooths** measured data.

This is possible only if
the number of measurements m is much larger than
the number of design parameters n,
i.e. for $m \gg n$.

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Example

For data given by the table

t_i	0	0,5	1	1,5	2	2,5	3
y_i	3,57	2,99	2,62	2,33	2,22	2,10	2,05

estimate an approximation $R_2(t) = x_1 + x_2 e^{-t}$ using least squares.

Obviously $\varphi_1(t) = 1$ and $\varphi_2(t) = e^{-t}$.

Normal equations are

$$\begin{pmatrix} \sum_{i=1}^{7} 1 \cdot 1 & \sum_{i=1}^{7} 1 \cdot e^{-t_i} \\ \sum_{i=1}^{7} e^{-t_i} \cdot 1 & \sum_{i=1}^{7} e^{-t_i} \cdot e^{-t_i} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{7} 1 \cdot y_i \\ \sum_{i=1}^{7} e^{-t_i} \cdot y_i \end{pmatrix}.$$

Example

For data given by the table

t_i	0	0,5	1	1,5	2	2,5	3
y_i	3,57	2,99	2,62	2,33	2,22	2,10	2,05

estimate an approximation $R_2(t) = x_1 + x_2 e^{-t}$
using least squares.

After computations of sums,
we get system

$$\begin{pmatrix} 7 & 2{,}4647 \\ 2{,}4647 & 1{,}5805 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 17{,}88 \\ 7{,}4422 \end{pmatrix},$$

which solution is $x_1 \doteq 1{,}9879$ and $x_2 \doteq 1{,}6087$.

Seeking approximation is

$$R_2(t) \doteq 1{,}99 + 1{,}61 e^{-t} \text{ and } \|\mathbf{r}\| \doteq 0{,}0651.$$

Example

For data given by the table

t_i	0	0,5	1	1,5	2	2,5	3
y_i	3,57	2,99	2,62	2,33	2,22	2,10	2,05

gradually we will approximate the data by polynomials of the first, second and third degree.

As basis functions we chose

$$\varphi_j(t) = t^{j-1},\ j = 1, 2, \ldots, n \text{ and } n = 2, 3, 4.$$

Example

Polynomial of first degree

For $\varphi_1(t) = 1$ and $\varphi_2(t) = t$ we obtain normal equations

$$\begin{pmatrix} 7 & 10{,}5 \\ 10{,}5 & 22{,}75 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 17{,}88 \\ 23{,}45 \end{pmatrix},$$

which has solution

$x_1 \doteq 3{,}28$ and $x_2 \doteq -0{,}48$ therefore

$$R_2(t) \doteq 3{,}28 - 0{,}48t \qquad \|\mathbf{r}\| \doteq 0{,}4756.$$

Approximation by linear polynomial is not good.

Polynomial of second degree

Normal equations

$$\begin{pmatrix} 7 & 10{,}5 & 22{,}75 \\ 10{,}5 & 22{,}75 & 55{,}125 \\ 22{,}75 & 55{,}125 & 142{,}1875 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 17{,}88 \\ 23{,}45 \\ 49{,}0625 \end{pmatrix}$$

have solution

$$x_1 \doteq 3{,}53,\ x_2 \doteq -1{,}09\ ,\ x_3 \doteq 0{,}20,$$
$$R_3(t) \doteq 3{,}53 - 1{,}09t + 0{,}2t^2\ ,\ \|\mathbf{r}\| \doteq 0{,}1006.$$

The residual is smaller but still large than
in the previous example.

Example

Polynomial of the third degree

Normal equations

$$\begin{pmatrix} 7 & 10{,}5 & 22{,}75 & 55{,}125 \\ 10{,}5 & 22{,}75 & 55{,}125 & 142{,}1875 \\ 22{,}75 & 55{,}125 & 142{,}1875 & 381{,}2813 \\ 55{,}125 & 142{,}1875 & 381{,}2813 & 1049{,}5469 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 17{,}88 \\ 23{,}45 \\ 49{,}0625 \\ 116{,}78 \end{pmatrix}$$

have solution

$$x_1 \doteq 3{,}57,\ x_2 \doteq -1{,}35,\ x_3 \doteq 0{,}43\ ,\ x_4 \doteq -0{,}05,$$

$$R_4(t) \doteq 3{,}57 - 1{,}35t + 0{,}43t^2 - 0{,}05t^3\ ,\ \|\mathbf{r}\| \doteq 0{,}0360.$$

Example

If we enlarge the degree of the polynomial,
we could see that
polynomial $R_7(t)$ of the sixth degree
passes through all points $[t_i, y_i]$,
so we will obtain interpolating polynomial.

Notice the elements of Gramian matrices:
the larger degree, the larger maximal coefficient.

This means that the condition number
of Gramian matrices is growing.

Table shows the condition numbers $\kappa_2(\mathbf{G})$:

n	2	3	4	5	6	7
$\kappa_2(\mathbf{G})$	16	$4{,}27 \cdot 10^2$	$1{,}91 \cdot 10^4$	$1{,}20 \cdot 10^6$	$1{,}17 \cdot 10^8$	$2{,}31 \cdot 10^{10}$

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Solution of overdetermined systems

Normal equations are not suitable for solving
large overdetermined systems
because the condition number
of Gramian matrix is considerably larger than
condition number of design matrix **A**, because

$$\kappa_2(\mathbf{A}^T\mathbf{A}) = [\kappa_2(\mathbf{A})]^2 .$$

The better way is to use
singular value decomposition
or
QR decomposition.

Singular value decomposition - introduction

If the number of equations M is less than the number of unknowns N,
or if $M = N$ but equations are linearly dependent,
then the system has no solution
or
it has more than one solution.

In the later case the space of solutions is given by
a particular solution
added to the any linear combination of $N - M$ vectors.

The task to find the space of solution for matrix $\mathbf{A}$
is possible to solve using
singular value decomposition of matrix $\mathbf{A}$.

Singular value decomposition - introduction

If the number of equations M is greater than the number of unknowns N,
then in general there is no solution vector and
the system is called **overdetermined**.

However, we could find a best “compromise” solution,
which is “the closest” solution
that satisfy all equations.

If „the closest“ we define in a sense of least square,
i.e. the sum of square of residuals is the smallest possible,
then the overdetermined system is reduced to
solvable problem
called the **least square method**.

Singular value decomposition - introduction

Reduced system of equations could be written as
system N x N equation

$$\left(\mathbf{A}^T \cdot \mathbf{A}\right) \cdot \mathbf{x} = \left(\mathbf{A}^T \cdot \mathbf{b}\right) \ .$$

This equations we call **normal equations**
of a least square problem.

Singular value decomposition has many common features
with the least square method,
which we show later.

Direct solution of normal equations is in general
not the best way to find a solution of least square problem.

Singular value decomposition

SVD is based on the following theorem of linear algebra:

Each matrix $\mathbf{A}$ of type M x N,

which the number of rows M is greater or equal to the number of columns N,

could be decomposed to a product of

matrix with orthogonal columns $\mathbf{U}$ of type M x N,

diagonal matrix $\mathbf{W}$ of type N x N

with positive or zero entries (**singular values**)

and transpose orthogonal matrix $\mathbf{V}$ of type N x N.

$$\begin{pmatrix} \\ \mathbf{A} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{U} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} w_1 & & & \\ & w_2 & & \\ & & \cdots & \\ & & \cdots & \\ & & & w_N \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{V}^T \\ \\ \end{pmatrix}$$

Singular value decomposition

Orthogonality of matrices $\mathbf{U}$ and $\mathbf{V}$ could be written as

$$\begin{pmatrix} & \mathbf{U}^T & \end{pmatrix} \cdot \begin{pmatrix} & \mathbf{U} & \end{pmatrix} = \begin{pmatrix} & \mathbf{V}^T & \end{pmatrix} \cdot \begin{pmatrix} & \mathbf{V} & \end{pmatrix}$$

$$= \begin{pmatrix} & \mathbf{1} & \end{pmatrix}$$

SVD could be done also if $M < N$.

In such a case the singular values w_j for $j = M+1, \ldots, N$ are all zero

as well as corresponding columns of matrix $\mathbf{U}$.

There is a lot of algorithms of SVD,
proven is subroutine **svdcmp** from *Numerical Recipes*.

Singular value decomposition for more equations than unknowns

If we have more equations than unknowns
we are seeking solution
in a least square sense.

We are solving system written as:

$$\left(\mathbf{A} \right) \cdot \left(\mathbf{x} \right) = \left(\mathbf{b} \right)$$

Singular value decomposition for more equations than unknowns

After SVD of matrix $\mathbf{A}$ we have

the solution in a form

$$\begin{pmatrix} \\ \mathbf{x} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \mathbf{V} \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathrm{diag}(1/w_j) \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{U}^T \\ \\ \end{pmatrix} \cdot \begin{pmatrix} \\ \mathbf{b} \\ \\ \end{pmatrix}$$

In this case usually it is not necessary set to zero values w_j
however the unusually small values indicate
that the data are not sensitive to some parameters.

QR decomposition

Another useful method for solving least squares
is using QR decomposition
of $m \times n$ matrix A of normal equations, with $m \geq n$.

QR decomposition is the product of an $m \times m$ unitary matrix Q
and an $m \times n$ upper triangular matrix R
which can be computed using e.g. the Gram–Schmidt process.

As the bottom $(m-n)$ rows of matrix R
consist entirely of zeroes, it is often useful to partition R,
or both R and Q:

$$A = QR = Q \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = [\, Q_1, Q_2 \,] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1,$$

where R_1 is an $n \times n$ upper triangular matrix,
0 is an $(m - n) \times n$ zero matrix, Q_1 is $m \times n$, Q_2 is $m \times (m - n)$,
and Q_1 and Q_2 both have orthogonal columns.

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