THE LEAST SQUARES METHOD

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Overview

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2. Fitting problem formulation
3. The general linear problem
4. Intersecting n lines in 2D
5. Intersecting n planes in 3D
6. Fitting a plane to n given points in 3D

Introduction (1/4)

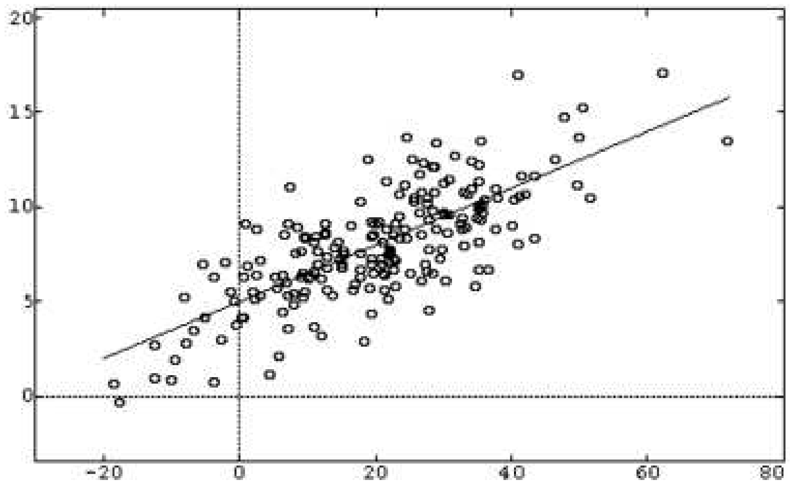
- The method of **least squares** is a standard approach to the approximate solution of overdetermined systems, i.e. sets of equations in which there are more equations than unknowns.
- *Least squares* means that the overall solution minimizes the sum of the squares of the errors made in solving every single equation.
- The most important application is in **data fitting**.
- The best fit in the least-squares sense minimizes the sum of squared residuals, a residual being the difference between an observed value and the fitted value provided by a model.

Introduction (2/4)

- Depending on whether or not the residuals are linear in all unknowns, Least squares problems fall into two categories:
  1. linear least squares
  2. nonlinear least squares

Introduction (3/4)

Linear least squares occurs in statistical regression analysis. It has a closed-form solution.



The approach is called **linear** least squares since the solution depends **linearly** on the data.

Introduction (4/4)

- The nonlinear least squares problem has no closed solution and is usually solved by iterative refinement.
- At each iteration the system is approximated by a linear one, thus the core calculation is similar in both cases.

Fitting Problem Formulation (1/3)

Given N points located at positions $\mathbf{x}_i$ in $\mathbb{R}^d$ with $i \in [1..N]$. We wish to obtain a globally defined function $f(\mathbf{x})$ that approximates the given scalar values f_i at points $\mathbf{x}_i$ in such a way that minimizes the error functional

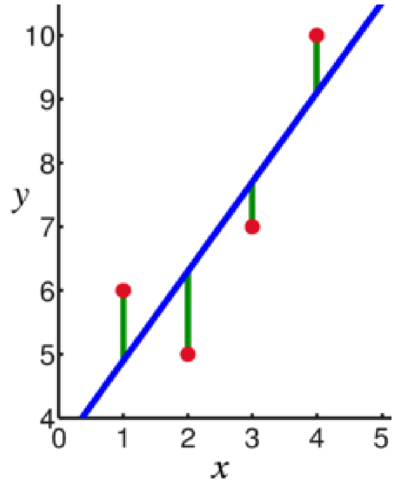
$$J_{LS} = \sum_i ||f(\mathbf{x}_i) - f_i||^2$$

Fitting Problem Formulation (2/3)

Illustrative example:

- Experimental data. Points shown in red in the picture

x	1	2	3	4
y	6	5	7	10



- It is desired to find a line $y = ax + b$ that fits "best" these four points. In other words, we would like to find the numbers a and b that approximately solve the overdetermined linear system

$$\begin{array}{rcccr} a & + & b & = & 6 \\ 2\,a & + & b & = & 5 \\ 3\,a & + & b & = & 7 \\ 4\,a & + & b & = & 10 \end{array}$$

Fitting Problem Formulation (3/3)

- The least squares approach minimizes the sum of squares of **errors** or **residual values**, that is, to find the minimum of the function

$$R(a,b) = (6-(a+b))^2+(5-(2a+b))^2+(7-(3a+b))^2+(10-(4a+b))^2$$

- The minimum is determined by calculating the partial derivatives of $R(a,b)$ with respect to a and b and setting them to zero. This results in a system of two equations in two unknowns, called the normal equations.
- When solved, we have $a = 1.4$ and $b = 3.5$. Therefore, the line $y = 1.4x + 3.5$ is the best least squares fit.

Solution to the first degree problem

The common computational procedure to find a first-degree polynomial function approximation over n data points is as follows.

- The slope is given by

$$a = \frac{n \sum xy - \sum x \sum y}{n \sum x^2 - (\sum x)^2}$$

- The Y-intercept is given by

$$b = \frac{\sum y \sum x^2 - \sum x \sum xy}{n \sum x^2 - (\sum x)^2}$$

General Problem (1/10)

Consider an overdetermined system of m linear equations each with n unknowns such that $m > n$,

$$\sum_{j=1}^{n} a_j \mathbf{x}_{ij} = \mathbf{b}_j, \qquad (i = 1, 2, \ldots, m)$$

Written in matrix form

$$\mathbf{XA} = \mathbf{Y}$$

General Problem (2/10)

Where

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mn} \end{pmatrix} \qquad \mathbf{A} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \qquad \mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

General Problem (3/10)

Such a system usually has no solution, and the goal is then to find the coefficients **A** which fit the equations "best", in the sense of minimizing the residuals:

$$||\mathbf{Y} - \mathbf{XA}||^2$$

General Problem (4/10)

- This minimization problem has a unique solution, provided that the n columns of the matrix $\mathbf{X}$ are linearly independent
- The solution is given by solving the **normal equations**

$$(\mathbf{X}^\top \mathbf{X})\mathbf{A} = \mathbf{X}^\top \mathbf{Y}$$

General Problem (5/10)

- Solving the normal equations

$$(\mathbf{X}^\top\mathbf{X})\mathbf{A} = \mathbf{X}^\top\mathbf{Y}$$

  entails inverting $(\mathbf{X}^\top\mathbf{X})$.

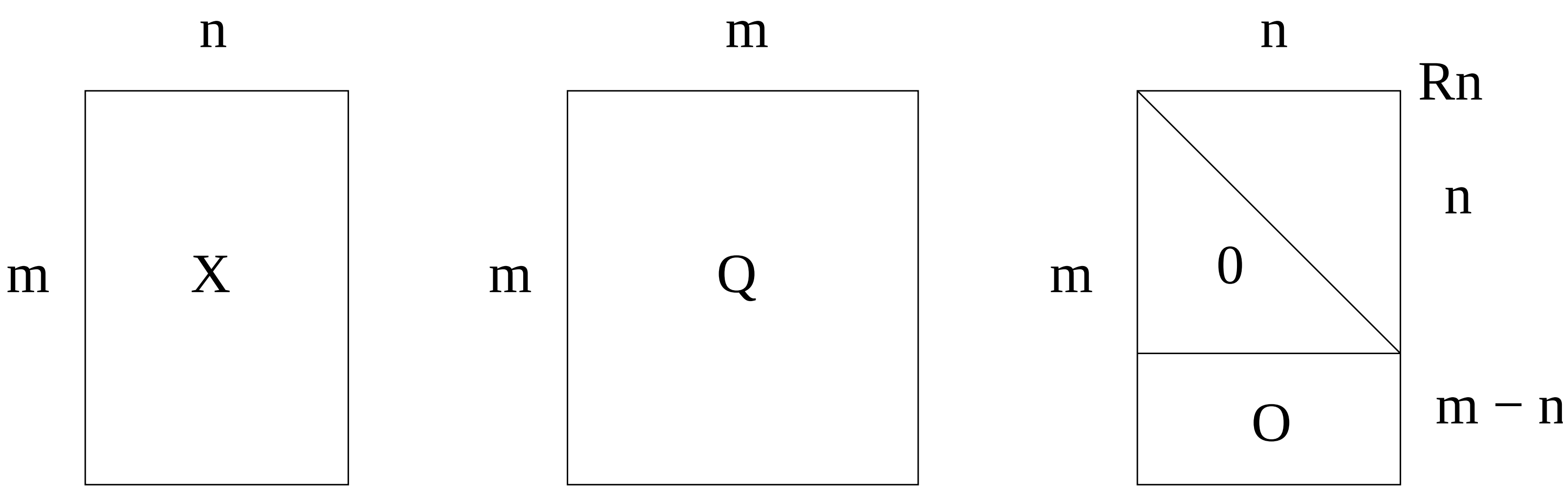
- However, for large values of m, matrix $(\mathbf{X}^\top\mathbf{X})$ is ill conditioned and thus the computation is numerically unstable.

General Problem (6/10)

- It is preferable to apply orthogonal decomposition methods.
- The residuals are $\mathbf{r} = \mathbf{Y} - \mathbf{XA}$
- Apply QR decomposition to get $\mathbf{X} = QR$
- Q is an $m \times m$ orthogonal matrix and R is an $m \times n$ which is partitioned into an $n \times n$ upper triangular matrix block, say R_n, and a $(m - n) \times n$ zero block, say O.

$$\begin{pmatrix} R_n \\ O \end{pmatrix}$$

General Problem (7/10)



General Problem (8/10)

- Therefore, residuals $\mathbf{r} = \mathbf{Y} - QR\mathbf{A}$ can be written as

$$
\begin{aligned}
Q^\top \mathbf{r} &= Q^\top \mathbf{Y} - (Q^\top Q)R\mathbf{A} \\
&= \begin{pmatrix} (Q^\top \mathbf{Y})_n - R_n\mathbf{A} \\ (Q^\top \mathbf{Y})_{m-n} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}
\end{aligned}
$$

- $\mathbf{v}$ doesn't depend on $\mathbf{A}$. Then the minimum residual value is attained when the upper block, $\mathbf{u}$, is zero.

General Problem (9/10)

- Therefore the parameters are found by solving

$$R_n\mathbf{A} = \left(Q^\top \mathbf{Y}\right)_n$$

- These equations are easily solved as R_n is upper triangular.

General Problem (10/10)

HOMEWORK

Search for numerical libraries to perform the compuations so far discussed

Intersecting n lines in 2D

- Set of given line equations

$$\left.\begin{array}{lcl} a_1x + b_1y + c_1 & = & 0 \\ a_2x + b_2y + c_2 & = & 0 \\ \ldots & & \\ a_nx + b_ny + c_n & = & 0 \end{array}\right\}$$

- Residuals are $r_i = a_ix + b_iy - c_i, \quad 1 \leq i \leq n$
- Apply what has been said in the solution to the first degree problem considering as unknowns x and y.

Intersecting n planes in 3D

- Set of given plane equations

$$\left.\begin{array}{lcl} a_1x + b_1y + c_1z + d_1 & = & 0 \\ a_2x + b_2y + c_2z + d_2 & = & 0 \\ \dots & & \\ a_nx + b_ny + c_nz + d_n & = & 0 \end{array}\right\}$$

- Residuals are $r_i = a_ix + b_iy + c_iz - d_i, \quad 1 \leq i \leq n$
- Apply what has been said in the solution to the general problem considering as unknowns x, y and z.

Fitting a plane to n points in 3D

- Set of given 3D points

$$\begin{array}{lll} x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \\ \dots & & \\ x_n & y_n & z_n \end{array}$$

- Plane equation to be fit $ax + by + cz + d = 0$
- We want to find values for a, b, c and d that approximately solve the system of equations

$$\left.\begin{array}{rcl} x_1a + y_1b + z_1c + d & = & 0 \\ x_2a + y_2b + z_2c + d & = & 0 \\ \dots & & \\ x_na + y_nb + z_nc + d & = & 0 \end{array}\right\}$$

- Apply what has been said in the solution to the general problem considering as unknowns a, b, c and d.

This is it concerning Least Squares fitting