

# Ordinary least squares

## Introduction

A system of linear equations is considered *overdetermined* if there are more equations than unknown variables. If all equations of an overdetermined system are linearly independent, the system has no exact solution.

A *linear least-squares problem* is the problem of finding an approximate solution to an overdetermined linear system. It often arises in applications where a theoretical model is fitted to experimental data.

## Linear least-squares problem

Consider a linear system

$$\mathbf{A}\mathbf{c} = \mathbf{b} , \tag{1}$$

where  $\mathbf{A}$  is an  $n \times m$  matrix,  $\mathbf{c}$  is an  $m$ -component vector of unknown variables and  $\mathbf{b}$  is an  $n$ -component vector of the right-hand side terms. If the number of equations  $n$  is larger than the number of unknowns  $m$ , the system is overdetermined and generally has no solution.

However, it is still possible to find an approximate solution—the one where  $\mathbf{A}\mathbf{c}$  is only approximately equal  $\mathbf{b}$ —in the sense that the Euclidean norm of the difference between  $\mathbf{A}\mathbf{c}$  and  $\mathbf{b}$  is minimized,

$$\mathbf{c} : \min_{\mathbf{c}} \|\mathbf{A}\mathbf{c} - \mathbf{b}\|^2 . \tag{2}$$

The problem (2) is called the ordinary least-squares problem and the vector  $\mathbf{c}$  that minimizes  $\|\mathbf{A}\mathbf{c} - \mathbf{b}\|^2$  is called the *least-squares solution*.

## Solution via QR-decomposition

The linear least-squares problem can be solved by QR-decomposition. The matrix  $\mathbf{A}$  is factorized as  $\mathbf{A} = \mathbf{Q}\mathbf{R}$ , where  $\mathbf{Q}$  is  $n \times m$  matrix with orthogonal columns,  $\mathbf{Q}^T\mathbf{Q} = \mathbf{1}$ , and  $\mathbf{R}$  is an  $m \times m$  upper triangular matrix. The Euclidean norm  $\|\mathbf{A}\mathbf{c} - \mathbf{b}\|^2$  can then be rewritten as

$$\begin{aligned} \|\mathbf{A}\mathbf{c} - \mathbf{b}\|^2 &= \|\mathbf{Q}\mathbf{R}\mathbf{c} - \mathbf{b}\|^2 \\ &= \|\mathbf{R}\mathbf{c} - \mathbf{Q}^T\mathbf{b}\|^2 + \|(1 - \mathbf{Q}\mathbf{Q}^T)\mathbf{b}\|^2 \geq \|(1 - \mathbf{Q}\mathbf{Q}^T)\mathbf{b}\|^2 . \end{aligned} \tag{3}$$

The term  $\|(1 - \mathbf{Q}\mathbf{Q}^T)\mathbf{b}\|^2$  is independent of the variables  $\mathbf{c}$  and can not be reduced by their variations. However, the term  $\|\mathbf{R}\mathbf{c} - \mathbf{Q}^T\mathbf{b}\|^2$  can be reduced down to zero by solving the  $m \times m$  system of linear equations

$$\mathbf{R}\mathbf{c} = \mathbf{Q}^T\mathbf{b} . \tag{4}$$

The system is right-triangular and can be readily solved by back-substitution. Thus the solution to the ordinary least-squares problem (2) is given by the solution of the triangular system (4).

## Ordinary least-squares curve fitting

Ordinary least-squares curve fitting is a problem of fitting  $n$  (experimental) data points  $\{x_i, y_i \pm \Delta y_i\}$ , where  $\Delta y_i$  are experimental errors, by a linear combination,  $F$ , of  $m$  functions  $\{f_k(x) \mid k = 1, \dots, m\}$ ,

$$F_{\mathbf{c}}(x) = \sum_{k=1}^m c_k f_k(x) . \tag{5}$$

The objective of the least-squares fit is to minimize the square deviation, called  $\chi^2$ , between the fitting function  $F(x)$  and the experimental data,

$$\chi^2 = \sum_{i=1}^n \left( \frac{F(x_i) - y_i}{\Delta y_i} \right)^2 . \tag{6}$$

Individual deviations from experimental points are weighted with their inverse errors in order to promote contributions from the more precise measurements.

Minimization of  $\chi^2$  with respect to the coefficient  $c_k$  in (5) is apparently equivalent to the least-squares problem (2) where

$$A_{ik} = \frac{f_k(x_i)}{\Delta y_i}, \quad b_i = \frac{y_i}{\Delta y_i}. \quad (7)$$

If  $\mathbf{QR} = \mathbf{A}$  is the QR-decomposition of the matrix  $\mathbf{A}$ , the formal least-squares solution to the fitting problem is

$$\mathbf{c} = R^{-1}Q^T\mathbf{b}. \quad (8)$$

However, in practice one has to back-substitute the system  $\mathbf{Rc} = \mathbf{Q}^T\mathbf{b}$ .

### Variations and correlations of fitting parameters

Suppose  $\delta y_i$  is a small deviation of the measured value of the physical observable at hand from its exact value. The corresponding deviation  $\delta c_k$  of the fitting coefficient is then given as

$$\delta c_k = \sum_i \frac{\partial c_k}{\partial y_i} \delta y_i. \quad (9)$$

In a good experiment the deviations  $\delta y_i$  are statistically independent and distributed normally with the standard deviations  $\Delta y_i$ . The deviations (9) are then also distributed normally with *variances*

$$\langle \delta c_k \delta c_k \rangle = \sum_i \left( \frac{\partial c_k}{\partial y_i} \Delta y_i \right)^2 = \sum_i \left( \frac{\partial c_k}{\partial b_i} \right)^2. \quad (10)$$

The standard errors in the fitting coefficients are then given as the square roots of variances,

$$\Delta c_k = \sqrt{\langle \delta c_k \delta c_k \rangle} = \sqrt{\sum_i \left( \frac{\partial c_k}{\partial b_i} \right)^2}. \quad (11)$$

The variances are diagonal elements of the *covariance matrix*,  $\Sigma$ , made of *covariances*,

$$\Sigma_{kq} \equiv \langle \delta c_k \delta c_q \rangle = \sum_i \frac{\partial c_k}{\partial b_i} \frac{\partial c_q}{\partial b_i}. \quad (12)$$

Covariances  $\langle \delta c_k \delta c_q \rangle$  are measures of to what extent the coefficients  $c_k$  and  $c_q$  change together if the measured values  $y_i$  are varied. The normalized covariances,

$$\frac{\langle \delta c_k \delta c_q \rangle}{\sqrt{\langle \delta c_k \delta c_k \rangle \langle \delta c_q \delta c_q \rangle}} \quad (13)$$

are called *correlations*.

Using (12) and (8) the covariance matrix can be calculated as

$$\Sigma = \left( \frac{\partial \mathbf{c}}{\partial \mathbf{b}} \right) \left( \frac{\partial \mathbf{c}}{\partial \mathbf{b}} \right)^T = R^{-1} (R^{-1})^T = (R^T R)^{-1} = (A^T A)^{-1}. \quad (14)$$

The square roots of the diagonal elements of this matrix provide the estimates of the errors  $\Delta \mathbf{c}$  of the fitting coefficients,

$$\Delta c_k = \sqrt{\Sigma_{kk}} \Big|_{k=1 \dots m}, \quad (15)$$

and the (normalized) off-diagonal elements provide the estimates of their correlations.

A C implementation of the ordinary least squares fit with QR-decomposition is shown in Table (1).

An illustration of a fit is shown on Figure (1) where a polynomial is fitted to a set of data.

Table 1: C implementation of ordinary least squares fit with QR-decomposition.

```

#include <matrix.h>
#include <gc.h> // garbage collector
#include <qr.h> // qr-decomposition
typedef struct {vector*c; matrix*S;} lsfit;
lsfit* lsfit_alloc(vector*x,vector*y,vector*dy,
int nf,double f(int k,double x))
{ int n=x->size, m=nf;
  matrix *A = matrix_alloc(n,m), *R = matrix_alloc(m,m);
  vector *b = vector_copy(y); vector_div(b,dy);
  for(int i=0;i<n;i++)
  { double xi=vector_get(x,i), dyi=vector_get(dy,i);
    for(int k=0;k<m;k++) matrix_set(A,i,k,f(k,xi)/dyi);
  }
  qrdec(A,R);
  lsfit* fit = (lsfit*)GC_MALLOC(sizeof(lsfit));
  fit->c = qrback(A,R,b);
  fit->S = qrinverse(matrixT_times_matrix(R,R));
  return fit;
}

```

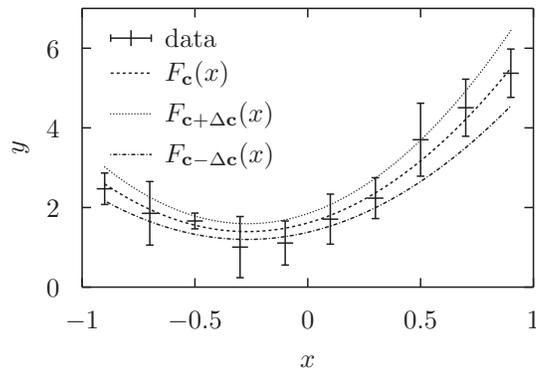


Figure 1: Ordinary least squares fit of  $F_{\mathbf{c}}(x) = c_1 + c_2x + c_3x^2$  to a set of data. Shown are fits with optimal coefficients  $\mathbf{c}$  as well as with  $\mathbf{c} + \Delta\mathbf{c}$  and  $\mathbf{c} - \Delta\mathbf{c}$ .