# Least square fit of a line/polynomial to input/output data

Prashant Dave

Chemical Engg., Indian Institute of Technology Bombay

Jan, 2012

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへで

#### Outline





Prashant Dave Least square fit

・ロト ・回ト ・ヨト ・ヨト

æ

#### • Scilab is free.

・ロン ・雪と ・雨と

æ

- Scilab is free.
- Matrix/loops syntax is same as for Matlab.

▲□→ < □→</p>

문 문 문

- Scilab is free.
- Matrix/loops syntax is same as for Matlab.
- Scilab provides all basic and many advanced tools.

**A** ►

- Scilab is free.
- Matrix/loops syntax is same as for Matlab.
- Scilab provides all basic and many advanced tools.
- Today: best fit: line and polynomial : reglin command

#### Linear fit

Given *n* samples of (x, y) pairs:  $x_i$  and  $y_i$  for i = 1, ..., n, we expect following equation is satisfied

$$y_i = a_1 x_i + a_0$$
 for  $i = 1, ..., n$  (1)

▲□→ < □→</p>

for some constants  $a_1$  and  $a_0$ .

#### Linear fit

Given *n* samples of (x, y) pairs:

 $x_i$  and  $y_i$  for  $i = 1, \ldots, n$ , we expect following equation is satisfied

$$y_i = a_1 x_i + a_0$$
 for  $i = 1, ..., n$  (1)

for some constants  $a_1$  and  $a_0$ .

- x: independent variable (exactly known),
- y: dependent variable (some error in measuring it)

 $x_i$  and  $y_i$  fall on some line with slope  $a_1$  and 'y-intercept'= $a_0$ . The 'line fit' problem:

Find these constants  $a_1$  and  $a_0$ .

'Best' fit?

#### Best fit

The true relationship is  $y_i = a_{0a} + a_{1a}x_i$ , but due to noise (for example in measurements), the available  $x_i, y_i$  pairs will not satisfy the equation exactly.

A ■

#### Best fit

The true relationship is  $y_i = a_{0a} + a_{1a}x_i$ , but due to noise (for example in measurements), the available  $x_i, y_i$  pairs will not satisfy the equation exactly. Least-square-fit problem: Given *n* samples of  $(x_i, y_i)$  pairs,

#### Best fit

The true relationship is  $y_i = a_{0a} + a_{1a}x_i$ , but due to noise (for example in measurements), the available  $x_i$ ,  $y_i$  pairs will not satisfy the equation exactly.

- Least-square-fit problem:
- Given *n* samples of  $(x_i, y_i)$  pairs,

find constants  $a_1$  and  $a_0$  such that the 'total square error'

$$\sum_{i=1}^{n} (y_i - a_1 x_i - a_0)^2$$
 (2)

#### is least.

# Scilab Tool: reglin

[a1,a0,sig] = reglin(x,y)

- x:  $1 \times n$  vector (for *n* data points)
- y:  $1 \times n$  vector (for *n* data points)
- a1: slope, a0: intercept
- sig: standard deviation of fit error: lower is "better"

# Straight line fit example

Generate data using known (actual) values of a0 and a1. Add noise to dependent variable.

Using noisy data, estimate a0 and a1.

- True data generation: y = 5 + 2x for x = 0: 10.
- 2 Noise addition: y = y + e where e is normally distributed noise with mean 0 and standard deviation 2.
- Least squares fit: [a1, a0, sig] = reglin(x, y).
- O Plot: (xi,yi) pairs, true (noise free) line, fitted line

Generate a vector of length n from a normal distribution with mean a and standard deviation b.

▲ □ ► < □ ►</p>

문 문 문

Generate a vector of length n from a normal distribution with mean a and standard deviation b.

rand('seed',10): get repeatable random numbers by initializing seed.

A 1

æ

Generate a vector of length n from a normal distribution with mean a and standard deviation b.

- rand('seed',10): get repeatable random numbers by initializing seed.
- **2** rand('normal'): generate from a normal distribution.

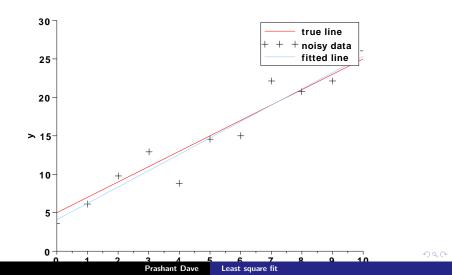
Generate a vector of length n from a normal distribution with mean a and standard deviation b.

- rand('seed',10): get repeatable random numbers by initializing seed.
- I rand('normal'): generate from a normal distribution.
- rand(x): generate a vector of same length as x.

Generate a vector of length n from a normal distribution with mean a and standard deviation b.

- rand('seed',10): get repeatable random numbers by initializing seed.
- I rand('normal'): generate from a normal distribution.
- rand(x): generate a vector of same length as x.
- **(**) a+b\*rand(x): generate with mean a and standard deviation b.

# Plots for example



Suppose we expect  $y_i$  satisfies the following equation:

$$y_i = a_2 x_i^2 + a_1 x_i + a_0$$

● ▶ < ミ ▶

Suppose we expect  $y_i$  satisfies the following equation:

$$y_i = a_2 x_i^2 + a_1 x_i + a_0$$

Points  $(x_i, y_i)$  are sitting on a parabola.

Suppose we expect  $y_i$  satisfies the following equation:

$$y_i = a_2 x_i^2 + a_1 x_i + a_0$$

Points  $(x_i, y_i)$  are sitting on a parabola. Problem (more generally):

Suppose we expect  $y_i$  satisfies the following equation:

$$y_i = a_2 x_i^2 + a_1 x_i + a_0$$

Points  $(x_i, y_i)$  are sitting on a parabola. Problem (more generally): Given *n* samples of  $(x_i, y_i)$  pairs and some choice of degree *d*.

$$y_i = a_d x_i^d + a_{d-1} x_i^{d-1} + \dots + a_1 x_i + a_0$$

Suppose we expect  $y_i$  satisfies the following equation:

$$y_i = a_2 x_i^2 + a_1 x_i + a_0$$

Points  $(x_i, y_i)$  are sitting on a parabola. Problem (more generally): Given *n* samples of  $(x_i, y_i)$  pairs and some choice of degree *d*.

$$y_i = a_d x_i^d + a_{d-1} x_i^{d-1} + \dots + a_1 x_i + a_0$$

Find constants  $a_d, \ldots a_1$  and  $a_0$  such that the 'total square error'

$$\sum_{i=1}^{n} (a_d x_i^d + a_{d-1} x_i^{d-1} + \dots + a_1 x_i + a_0 - y_i)^2$$
(3)

is least.

# Still a linear regression problem

The unknowns  $a_i$  enter the problem linearly.

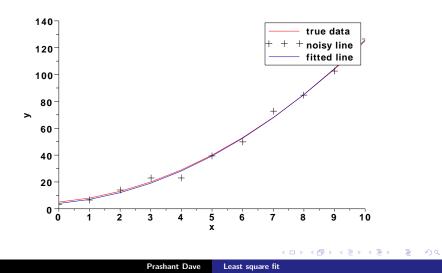
▲ □ ► < □ ►</p>

э.

# Still a linear regression problem

The unknowns  $a_i$  enter the problem linearly. (i.e.  $a_i$ 's are not getting squared, or multiplied to each other.) [slopes, intercept] = reglin(X,y) where  $X = [x; x^2]$ : a matrix with two regressors (one in each row) y: a row vector with same number of columns as X. slopes: the coefficients a1,a2 intercept: the coefficient a0 sig : standard deviation of the residual.

#### Second order fit example



#### More than one independent variables

Suppose y depends on independent variables  $x_1$ ,  $x_2$ , etc.

$$y_i = a_0 + a_1 x_{1i} + a_2 x_{2i} + \dots + a_p x_{pi}$$

A multiple linear regression problem (coefficients  $a_i$  still appear linearly)

#### More than one independent variables

Suppose y depends on independent variables  $x_1$ ,  $x_2$ , etc.

$$y_i = a_0 + a_1 x_{1i} + a_2 x_{2i} + \dots + a_p x_{pi}$$

A multiple linear regression problem (coefficients  $a_i$  still appear linearly)

[slopes, intercept] = reglin(X, y)

where X and y are matrix/vector with same number of columns.

#### More than one independent variables

Suppose y depends on independent variables  $x_1$ ,  $x_2$ , etc.

$$y_i = a_0 + a_1 x_{1i} + a_2 x_{2i} + \dots + a_p x_{pi}$$

A multiple linear regression problem (coefficients  $a_i$  still appear linearly)

[slopes,intercept]=reglin(X,y)

where X and y are matrix/vector with same number of columns. (but X has many rows.) Components in slopes = number of rows of X

(number of independent variables.)

# Nonlinear Least Squares

The parameters to be estimated appear non-linearly in the model: y = f(x)Example,  $y_i = a/(b + x_i)$ 

・ 同・ ・ ヨ・

# Nonlinear Least Squares

The parameters to be estimated appear non-linearly in the model: y = f(x)Example,  $y_i = a/(b + x_i)$ 

- Want to choose parameters so as to minimize  $\sum_{i=1}^{n} (y_i f(x_i))^2$ .
- Analytical solution usually not available.
- Use a numerical optimization technique.
- Scilab functions: Isqrsolve, leastsq (front end to optim function)

#### Thank You

Prashant Dave Least square fit

▲口> ▲圖> ▲注> ▲注>

æ