L23: Least-Squares Linear Regression

Part 2: General approach

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Version: release

Announcements

Lab 08 is due on March 17 at 12 pm (noon)

Lecture slides of lecture L22 (March 13$^{\mathrm{th}}$ 2017) were updated

Today:

- Least-squares linear regression: general case

Friday:

- Least-squares linear regression: discussion and applications

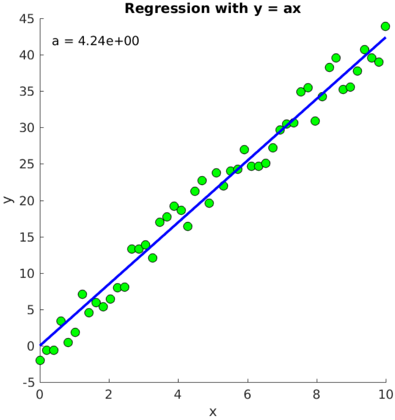
Next week:

- Monday: Interpolation (chapter 14)
- Wednesday: Series (chapter 15)
- Friday: Discussion
- Wednesday or Friday: presentation of the final programming project

Review of Monday's lecture (L22): $y = ax$

We fitted lines of equation $y = ax$, deriving the expression of a analytically:

$$a = \frac{\sum_{i=1}^{m} x_i y_i}{\sum_{i=1}^{m} x_i^2}$$



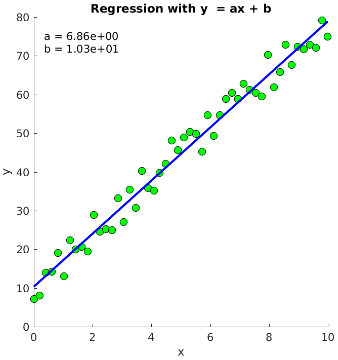

```
% Determine and plot the least-squares linear regression line
a = sum(x.*y) / sum(x.*x);
plot(x, a*x, 'b', 'LineWidth', 2)
```

Review of Monday's lecture (L22): $y = ax + b$

We fitted lines of equation $y = ax + b$, deriving the expressions of a and b analytically:

$$a = \frac{\sum_{i=1}^{m}(x_\mathrm{i} - \bar{x})(y_\mathrm{i} - \bar{y})}{\sum_{i=1}^{m}(x_\mathrm{i} - \bar{x})^2}$$

$$b = \bar{y} - a\bar{x}$$




```
% Determine and plot the least-squares linear regression line
x_mean = mean(x);
y_mean = mean(y);
a = sum((x-x_mean).*(y-y_mean)) / sum((x-x_mean).^2);
b = y_mean - a*x_mean;
plot(x, a*x+b, 'b', 'LineWidth', 2)
```

What type of function can be fitted using linear regression?

Answer: any function of the form:

$$y = a_1 f_1(x) + a_2 f_2(x) + \cdots + a_n f_n(x)$$

where:

- The a_i's are the coefficients to be determined using linear regression
- The f_i's are real-valued functions
- The f_i's are linearly independent of each other

(*i.e.* **linear** combinations of known functions $\rightarrow$ **linear** regression)

Examples:

- $y = ax$ (coefficient: a)
- $y = ax + b$ (coefficients: a and b)
- $y = a_0 + a_1 x + a_2 x^2 + a_3 x^3$ (coefficients: a_0, a_1, a_2, and a_3)
- $y = a\cos(x) + b\sin(x) + c$ (coefficients: a, b, and c)

Linear regression: practice question

Which of the functions below is of the form:

$$y = a_1 f_1(x) + a_2 f_2(x) + \cdots + a_n f_n(x)$$

where:

- The a_i's are the coefficients to be determined using linear regression
- The f_i's are real-valued functions
- The f_i's are linearly independent of each other

(A) $x \mapsto \cos(ax) + \sin^2(bx)$ $\quad a, b \in \mathbb{R}$

(B) $\boxed{x \mapsto a\cos(x) + b\sin^2(x) \quad a, b \in \mathbb{R}}$

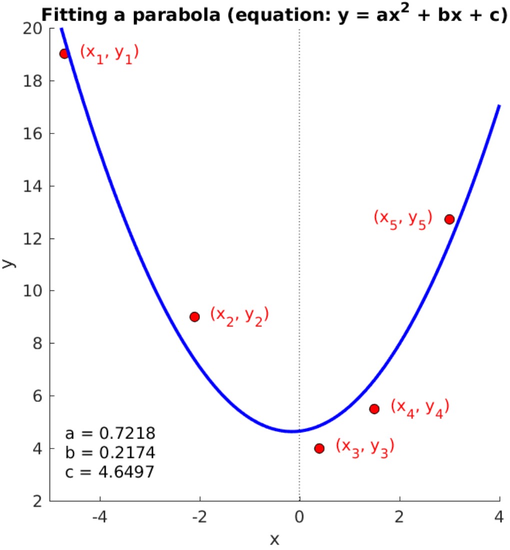
(C) $\boxed{x \mapsto a + b\exp(x) + c\log(x^2 + 1) \quad a, b, c \in \mathbb{R}}$

(D) $x \mapsto \exp(a + x/b)$ $\quad a, b \in \mathbb{R}$

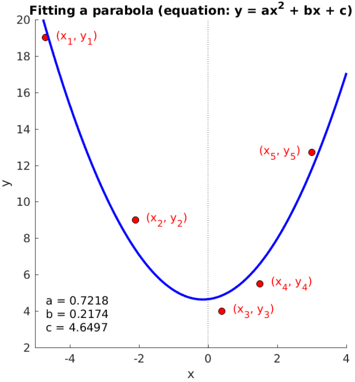
(E) $\boxed{x \mapsto a \quad a \in \mathbb{R}}$

Introduction to the general approach

Let us try to fit a parabola through the following points:



Introduction to the general approach



If the fit is perfect:

The line passes through point 1 *i.e.*

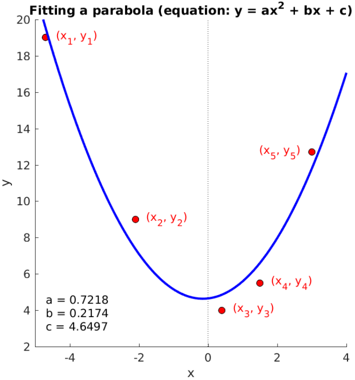
$$ax_1^2 + bx_1 + c = y_1$$

And the line passes through point 2 *i.e.*

$$ax_2^2 + bx_2 + c = y_2$$

Same with the other points:

$$ax_3^2 + bx_3 + c = y_3$$
$$ax_4^2 + bx_4 + c = y_4$$
$$ax_5^2 + bx_5 + c = y_5$$



If the fit is perfect:

The line passes through all the points:

$$
\begin{aligned}
ax_1^2 + bx_1 + c &= y_1 \\
ax_2^2 + bx_2 + c &= y_2 \\
ax_3^2 + bx_3 + c &= y_3 \\
ax_4^2 + bx_4 + c &= y_4 \\
ax_5^2 + bx_5 + c &= y_5
\end{aligned}
$$

In matrix form (tip: write the unknowns first):

$$
\begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \\ x_4^2 & x_4 & 1 \\ x_5^2 & x_5 & 1 \end{bmatrix}
\begin{bmatrix} a \\ b \\ c \end{bmatrix}
=
\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix}
$$

Introduction to the general approach

If the fit is perfect: $M\beta = y$, with:

$$M = \begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \\ x_4^2 & x_4 & 1 \\ x_5^2 & x_5 & 1 \end{bmatrix}; \qquad \beta = \begin{bmatrix} a \\ b \\ c \end{bmatrix}; \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix}$$

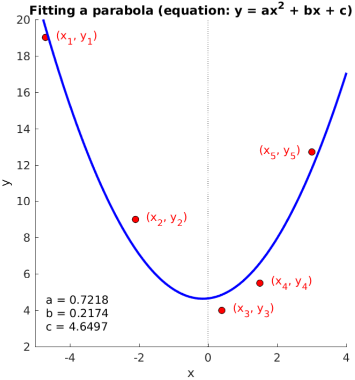
Note: the vector of unknowns β is the vector of the coefficients to fit

If a perfect fit does not exist, then this system of linear algebraic equations has zero solution, BUT the set of coefficients (β) that yields the smallest possible square error is given by:

$$\beta = \mathrm{pinv(M)} \times y$$

$\mathrm{pinv(M)} = (M^T M)^{-1} M^T$ = pseudo-inverse of M

Introduction to the general approach



$$M = \begin{bmatrix} x_1^2 & x_1 & 1 \\ x_2^2 & x_2 & 1 \\ x_3^2 & x_3 & 1 \\ x_4^2 & x_4 & 1 \\ x_5^2 & x_5 & 1 \end{bmatrix}$$

```
>> x = [-4.7; -2.1; 0.4; 1.5; 3];
>> y = [19; 9; 4; 5.5; 12.7];

>> m = [x.^2, x, ones(size(x))];
```

```
>> coeffs = pinv(m)*y
coeffs =
    0.7218
    0.2174
    4.6497
```

```
>> coeffs = m\y
coeffs =
    0.7218
    0.2174
    4.6497
```

Remember that when a system has zero solution, the backslash operator gives the least-squares approximation

General approach to least-squares linear regression

Objective: Fit the following function:

$$y = a_1 f_1(x) + a_2 f_2(x) + \cdots + a_n f_n(x)$$

to a set of x- and y-data, corresponding to m data points

If the fit is perfect, the line passes through all the points:

$$\begin{aligned}
&a_1 f_1(x_1) + a_2 f_2(x_1) + \cdots + a_n f_n(x_1) = y_1 \\
&a_1 f_1(x_2) + a_2 f_2(x_2) + \cdots + a_n f_n(x_2) = y_2 \\
&\dots \\
&a_1 f_1(x_m) + a_2 f_2(x_m) + \cdots + a_n f_n(x_m) = y_m
\end{aligned}$$

General approach to least-squares linear regression

If the fit is perfect, the line passes through all the points:

$$
\begin{aligned}
&a_1 f_1(x_1) + a_2 f_2(x_1) + \cdots + a_n f_n(x_1) = y_1 \\
&a_1 f_1(x_2) + a_2 f_2(x_2) + \cdots + a_n f_n(x_2) = y_2 \\
&\ldots \\
&a_1 f_1(x_m) + a_2 f_2(x_m) + \cdots + a_n f_n(x_m) = y_m
\end{aligned}
$$

If the fit is not perfect, the square error E_2 is non-zero

$$
\begin{aligned}
E_2 &= \sum_{i=1}^{m} (y_{\mathrm{i,predicted}} - y_{\mathrm{i}})^2 \\
&= \sum_{i=1}^{m} (a_1 f_1(x_i) + a_2 f_2(x_i) + \cdots + a_n f_n(x_i) - y_{\mathrm{i}})^2
\end{aligned}
$$

General approach to least-squares linear regression

If the fit is perfect, the line passes through all the points:

$$
\begin{aligned}
&a_1 f_1(x_1) + a_2 f_2(x_1) + \cdots + a_n f_n(x_1) = y_1 \\
&a_1 f_1(x_2) + a_2 f_2(x_2) + \cdots + a_n f_n(x_2) = y_2 \\
&\dots \\
&a_1 f_1(x_m) + a_2 f_2(x_m) + \cdots + a_n f_n(x_m) = y_m
\end{aligned}
$$

In matrix form: $M\beta = y$ (tip: write the unknowns first)

$$
M = \begin{bmatrix} f_1(x_1) & f_2(x_1) & \dots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \dots & f_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_m) & f_2(x_m) & \dots & f_n(x_m) \end{bmatrix} \qquad \beta = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}
$$

General approach to least-squares linear regression

In matrix form: $M\beta = y$

$$M = \begin{bmatrix} f_1(x_1) & f_2(x_1) & \dots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \dots & f_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_m) & f_2(x_m) & \dots & f_n(x_m) \end{bmatrix} \qquad \beta = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

Most often, the system is very over-determined (i.e. $m \gg n$), and has zero solution. Least-squares linear regression consists of finding the values of the coefficients (β) such that the square error is minimum. These coefficients are given by:

$$\beta = \mathrm{pinv(M)} \times y$$

$\mathrm{pinv(M)} = (M^T M)^{-1} M^T =$ pseudo-inverse of M

General approach to least-squares linear regression

Steps to perform least-squares linear regression:

1. **Choose the shape of the function to fit**
   (*e.g.*, straight line? sinusoid? cubic polynomial?)
   (This step will often be done for you in E7 lab assignments)

2. **Write the system of linear algebraic equations to "solve"**
   (the unknowns are the coefficients of the linear regression)

3. **Write this system in matrix form**

4. **Find the values of the coefficients that minimize the square error**
   (use the pseudo-inverse of the matrix of the system)

Vocabulary: "linear" and "least-squares"

When doing least-squares linear regression:

"linear" means that the function to fit is of the form:

$$y = a_1 f_1(x) + a_2 f_2(x) + \cdots + a_n f_n(x)$$

where:

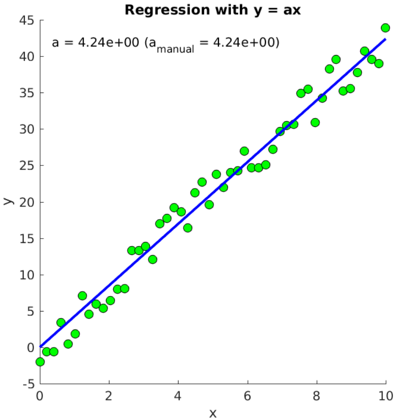
- The a_i's are the coefficients to be determined using regression
- The f_i's are real-valued functions
- The f_i's are linearly independent of each other

"least-squares" means that we determine the values of the coefficients that minimize the square error E_2

One can also do least-squares non-linear regression (not taught in E7) and linear non-least-squares regression (the error metric being minimized is not the square error, see one example in lab 09)

Least-squares linear regression example: $y = ax$

$$M = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

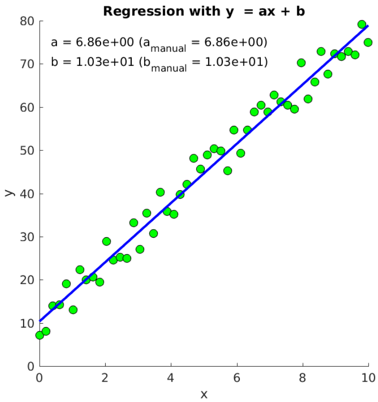



```
% Determine and plot the least-squares linear regression line
m = x;
a_manual = sum(x.*y) / sum(x.*x);
a = pinv(m) * y;
plot(x, a*x, 'b', 'LineWidth', 2)
```

Here, "manual" values are values calculated using analytical expressions derived in lecture L22 (March 13$^{\text{th}}$ 2017)

Least-squares linear regression example: $y = ax + b$

$$M = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \\ x_m & 1 \end{bmatrix}$$

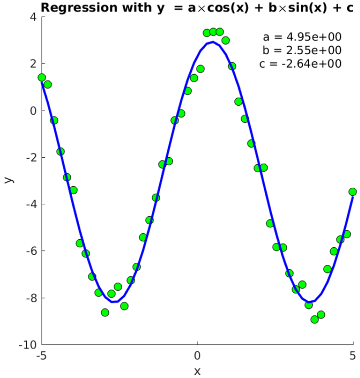



```
% Determine and plot the least-squares linear regression line
m = [x, ones(size(x))];
coefficients = pinv(m) * y;
a = coefficients(1);
b = coefficients(2);
plot(x, a*x+b, 'b', 'LineWidth', 2)
```

Here, “manual” values are values calculated using analytical expressions derived in lecture L22 (March 13^{th} 2017)

Least-sq. lin. reg. example: $y = a\cos(x) + b\sin(x) + c$

$$M = \begin{bmatrix} \cos(x_1) & sin(x_1) & 1 \\ \cos(x_2) & sin(x_2) & 1 \\ \vdots & & \\ \cos(x_m) & sin(x_m) & 1 \end{bmatrix}$$




```
% Determine and plot the least-squares linear regression line
m = [cos(x), sin(x), ones(size(x))];
coefficients = pinv(m) * y;
a = coefficients(1);
b = coefficients(2);
c = coefficients(3);
plot(x, m*coefficients, 'b', 'LineWidth', 2)
```

"manual" values are values calculated using analytical expressions derived in lecture L22 (March 13th 2017)