Linear Regression – Linear Least Squares

EAS 199A Notes

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Introduction

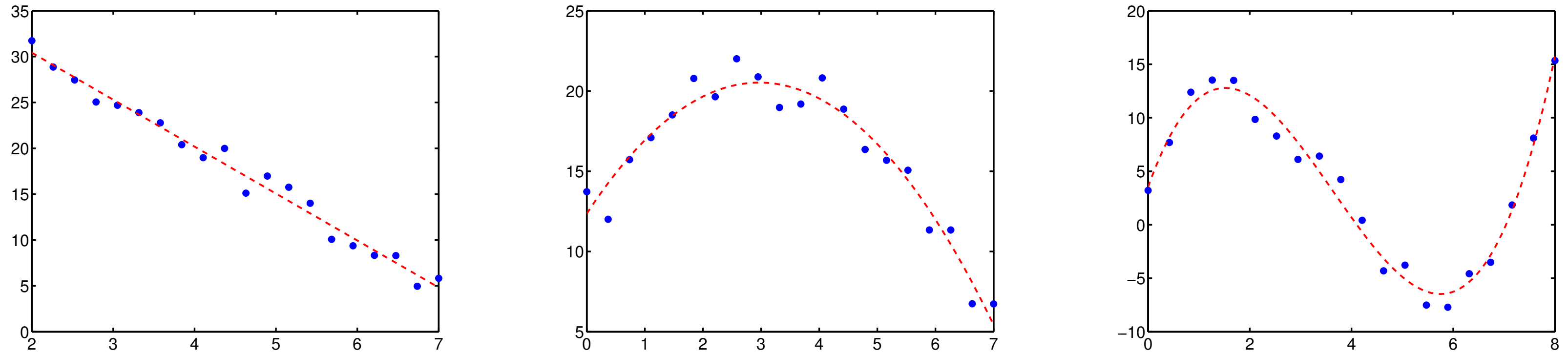
Engineers and Scientists work with lots of data.

Scientists try to undersand the way things behave in the physical world.

Engineers try to use the discoveries of scientists to produce useful products or services.

Given data from a measurement, how can we obtain a simple mathematical model that fits the data? By "fit the data", we mean that the function follows the trend of the data.

Polynomial Curve Fits



Basic Idea

- Given data set (x_i, y_i), $i = 1, \ldots, n$
- Find a function $y = f(x)$ that is *close* to the data

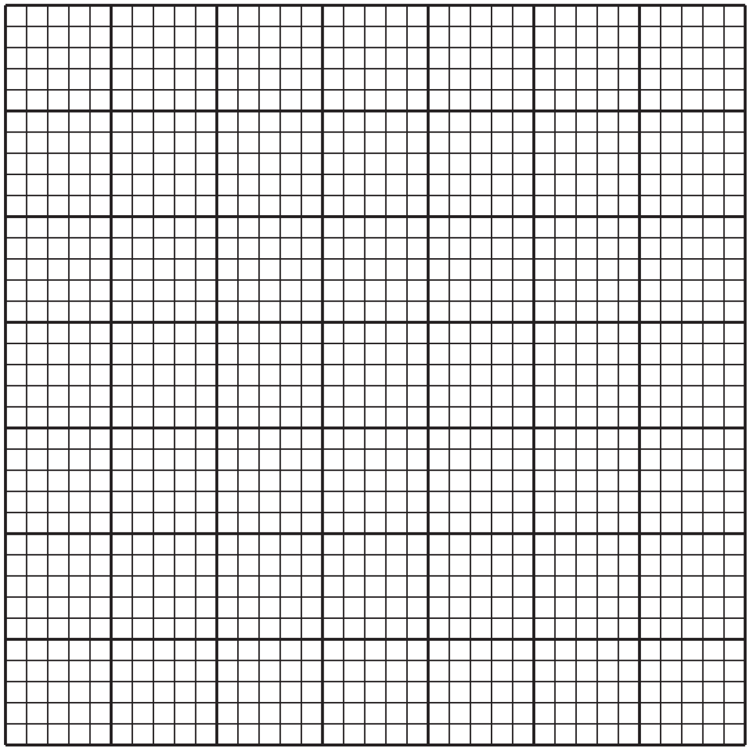
The process avoids guesswork.

Some sample data

x	y
(time)	(velocity)
1	9
2	21
3	28
4	41
5	47

It is aways important to visualize your data.
You should be able to plot this data by hand.

Plot the Data

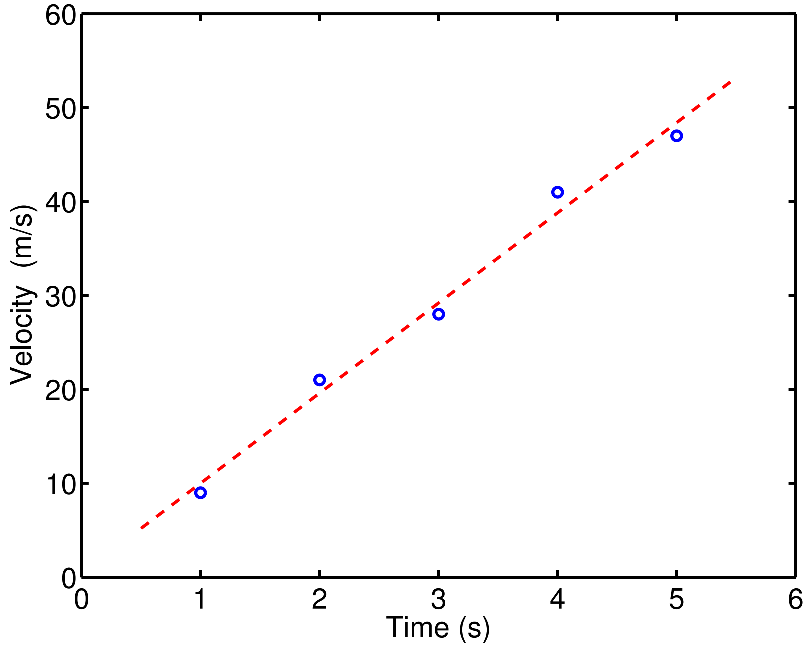


- Plot x on the horizontal axis, y on the vertical axis.
  - ▷ What is the range of the data?
  - ▷ Use the range to select an appropriate scale so that the data uses all (or most) of the available paper.
- In this case, x is the *independent* variable.
- y is the *dependent* variable.

Suppose that x is a measured value of time, and y is a measured velocity of a ball.

- Label the axes

Analyze the plot



An equation that represents the data is valuable

- A simple formula is more compact and reusable than a set of points.
- This data looks linear so our "fit function" will be

$$y = mx + b$$

- The value of slope or intercept may have physical significance.

Trial and Error: Not a good plan

Pick any two points (x_1, y_1) and (x_2, y_2), and solve for m and b

$$y_1 = mx_1 + b$$

$$y_2 = mx_2 + b$$

Subtract the two equations

$$\Longrightarrow y_1 - y_2 = mx_1 - mx_2 \qquad\qquad (b \text{ terms cancel})$$

Solve for m

$$m = \frac{y_1 - y_2}{x_1 - x_2} = \frac{y_2 - y_1}{x_2 - x_1} = \frac{\text{rise}}{\text{run}}$$

Trial and Error: Not a good plan

Now that we know m, we can use any one of the two original equations to solve for b.

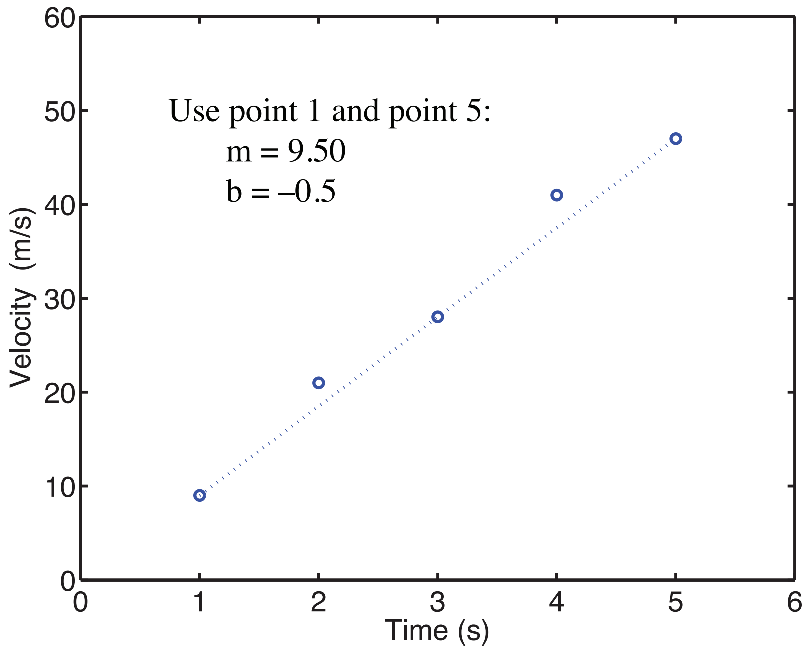
$$y_1 = mx_1 + b \quad \Longrightarrow \quad b = y_1 - mx_1$$

So, by picking two arbitrary data pairs, we can find the equation of a line that is at least related to our data set.

However, that is not the *best* way to solve the problem.

Before showing a better way, let's use this simplistic approach.

Simplistic line approximation: Use points 1 and 5



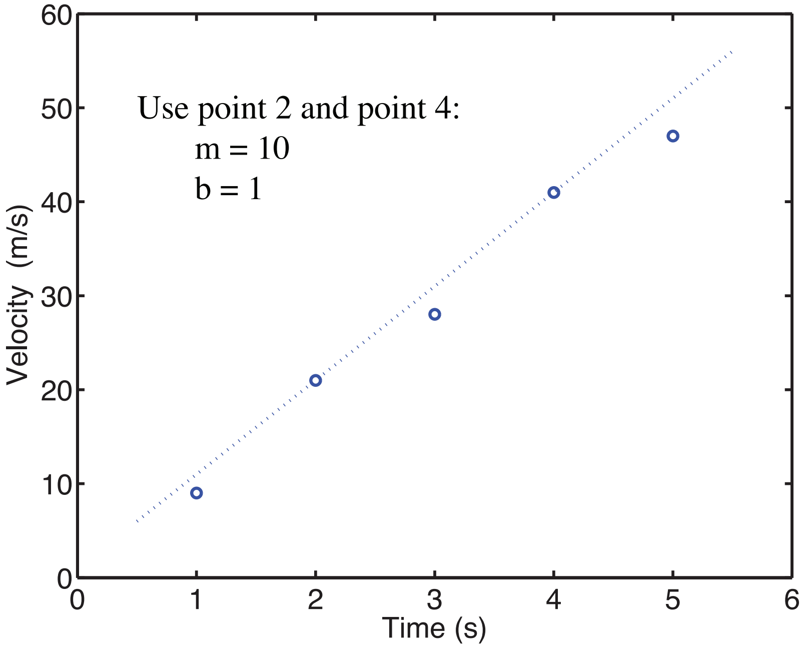
Compute slope and intercept using points 1 and 5

$$m = \frac{47 - 9 \text{ m/s}}{5 - 1 \text{ s}} = 9.5\,\frac{\text{m}}{\text{s}^2}$$

$$b = 47\,\frac{\text{m}}{\text{s}} - \left(9.5\,\frac{\text{m}}{\text{s}^2}\right)(5\,\text{s})$$

$$= -0.5\,\text{m/s}$$

Simplistic line approximation: Use points 2 and 4



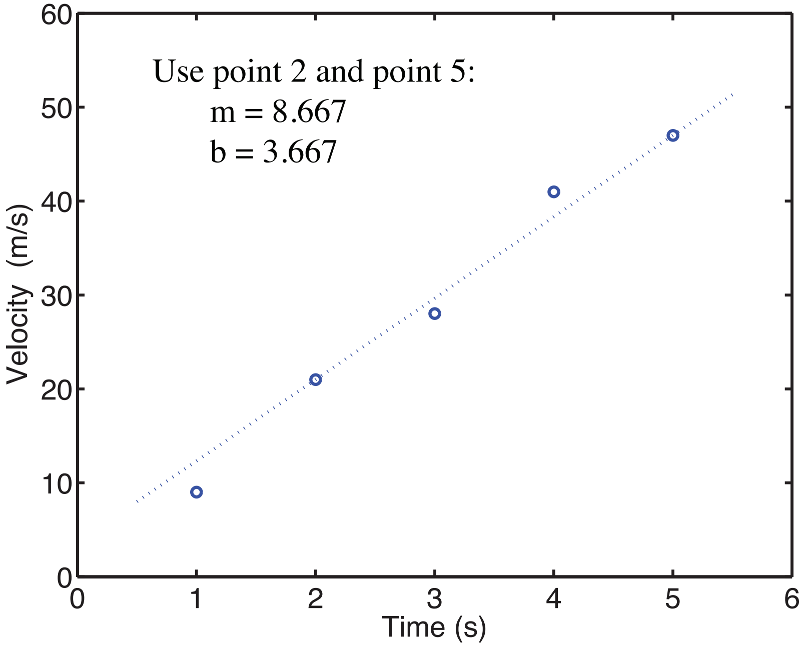
Compute slope and intercept using points 2 and 4

$$m = \frac{41 - 21\ \mathrm{m/s}}{4 - 2\ \mathrm{s}} = 10\ \frac{\mathrm{m}}{\mathrm{s}^2}$$

$$b = 41\,\frac{\mathrm{m}}{\mathrm{s}} - \left(10\,\frac{\mathrm{m}}{\mathrm{s}^2}\right)(5\,\mathrm{s})$$

$$= 1\,\mathrm{m/s}$$

Simplistic line approximation: Use points 2 and 5



Compute slope and intercept using points 2 and 5

$$m = \frac{47 - 21 \text{ m/s}}{5 - 2 \text{ s}} = 8.667 \, \frac{\text{m}}{\text{s}^2}$$

$$b = 47 \, \frac{\text{m}}{\text{s}} - \left(8.667 \, \frac{\text{m}}{\text{s}^2} \right) (5 \, \text{s})$$

$$= 6.667 \, \text{m/s}$$

Simplistic line approximation: So far . . .

Computing the m and b from any two points gives values of m and b that depend on the points you choose.

Data	m	b
(x_1, y_1), (x_5, y_5)	9.50	-0.5
(x_2, y_2), (x_4, y_4)	10.0	1.0
(x_2, y_2), (x_5, y_5)	8.67	3.7

Don't use the simplistic approach because m and b depend on the choice of data.

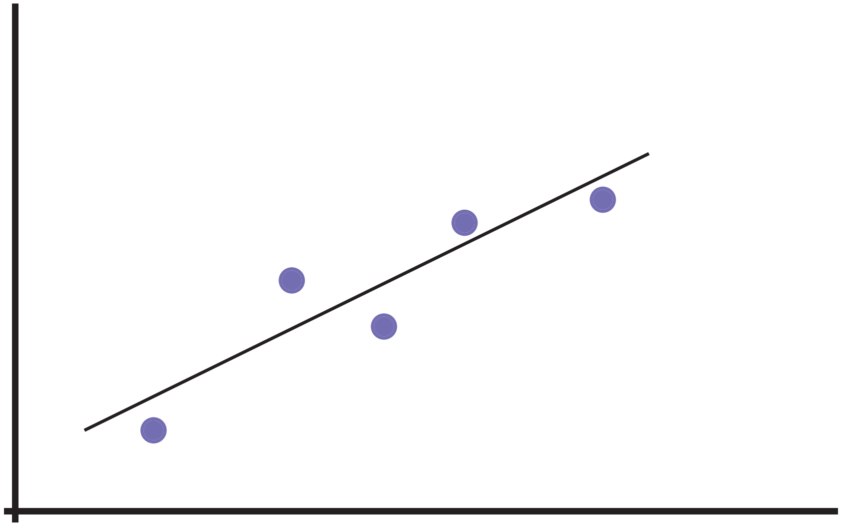
Instead use the *least squares* method that will give only one slope and one intercept for a given set of data.

Least Squares Method

- Compute slope and intercept in a way that minimizes an error (to be defined).
- Use calculus or linear algebra to derive equations for m and b.
- There is only one slope and intercept for a given set of data.

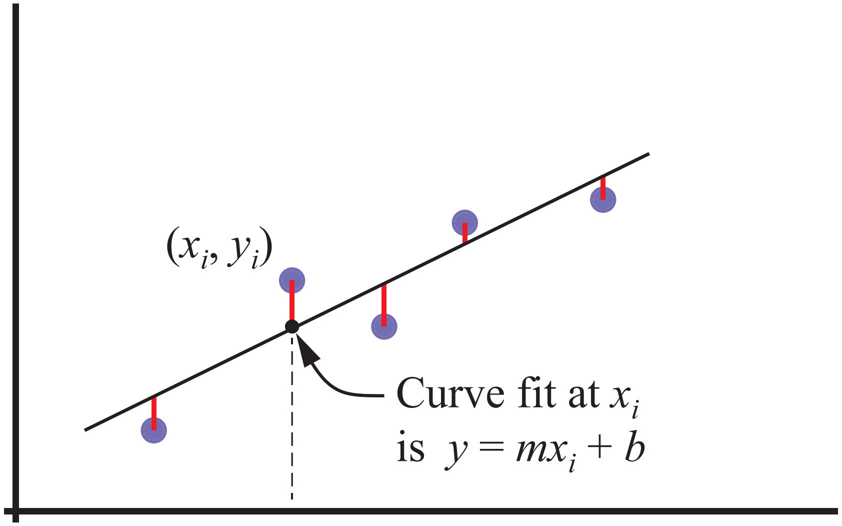
Do not guess m and b. Use least squares.

Least Squares: The Basic Idea



The best fit line goes near the data, but not through them.

Least Squares: The Basic Idea



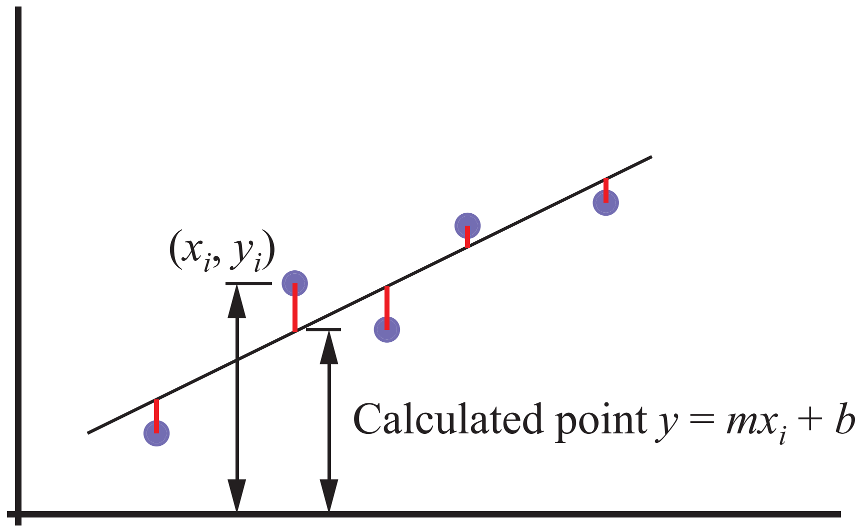
The best fit line goes near the data, but not through them.

The equation of the line is

$$y = mx + b$$

The data (x_i, y_i) are known.
m and b are unknown.

Least Squares: The Basic Idea



The best fit line goes near the data, but not through them.

The discrepancy between the known data and the unknown fit function is taken as the *vertical distance*

$$y_i - (mx_i + b)$$

But the error can be positive or negative, so we use the *square of the error*

$$[y_i - (mx_i + b)]^2$$

Least Squares Computational Formula

Use calculus to *minimize the sum of squares* of the errors

$$\text{Total error in the fit} = \sum_{i=1}^{n} \left[y_i - (mx_i + b) \right]^2$$

Minimizing the total error with respect to the two parameters m and b to get

$$m = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - \left(\sum x_i \right)^2} \qquad\qquad b = \frac{\sum y_i - m \sum x_i}{n}$$

Notice that b depends on m, so solve for m first.

Subscript and Summation Notation

Suppose we have a set of numbers

$$x_1, x_2, x_3, x_4$$

We can use a variable for the subscript

$$x_i, \quad i = 1, \ldots, 4$$

To add the numbers in a set we can write

$$s = x_1 + x_2 + x_3 + x_4$$

as

$$s = \sum_{i=1}^{n} x_i$$

Subscript and Summation Notation

We can put any formula with subscripts inside the summation notation.

Therefore

$$\sum_{i=1}^{4} x_i y_i = x_1 y_1 + x_2 y_2 + x_3 y_3 + x_4 y_4$$

$$\sum_{i=1}^{4} x_i^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2$$

The result of a sum is a number, which we can then use in other computations.

Subscript and Summation Notation

The order of operations matters. Thus,

$$\sum_{i=1}^{4} x_i^2 \neq \left(\sum_{i=1}^{4} x_i \right)^2$$

$$x_1^2 + x_2^2 + x_3^2 + x_4^2 \neq (x_1 + x_2 + x_3 + x_4)^2$$

Subscript and Summation: Lazy Notation

Sometimes we do not bother to write the range of the set of data.

Thus,

$$s = \sum x_i$$

implies

$$s = \sum_{i=1}^{n} x_i$$

where n is understood to mean, “however many data are in the set”

Subscript and Summation: Lazy Notation

So, in general

$$x_i$$

implies that there is a set of x values

$$x_1, x_2, \ldots, x_n$$

or

$$x_i, \ i = 1, \ldots, n$$

Subscript and Summation Notation

Practice!

Given some data (x_i, y_i), $i = 1, \ldots, n$.

1. *Always plot your data first!*
2. Compute the slope and intercept of the least squares line fit.

$$m = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - \left(\sum x_i\right)^2}$$

$$b = \frac{\sum y_i - m \sum x_i}{n}$$

Sample Data:

x (time)	y (velocity)
1	9
2	21
3	28
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