Least squares

Sample Subtitle

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Example

Showing why least squares

We have a variable y. We know that it's dependent of another variable x in some way. But we don't know how, exactly.
So we go to the field and measure certain points. Those that we can reach. Six of them.

$$(2, 5), (5, 5), (7, 8), (11, 7), (14, 9), (18, 7)$$

That is: at $x = 2$ we measure $y = 5$, at $x = 5$ we measure $y = 5$ again, but at $x = 7$ we got $y = 8$, and so on.

Example

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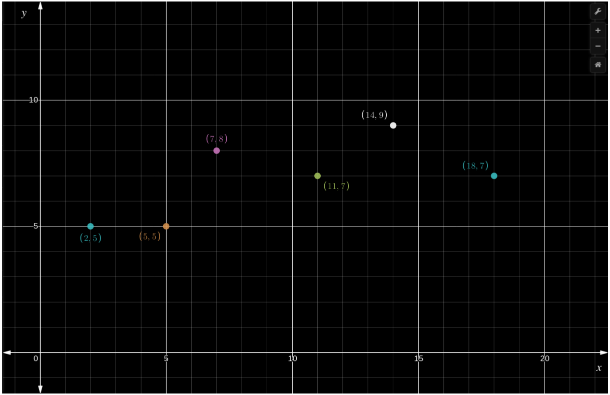
Back to desk we plot these points.



There is a model lurking in these points? A line perhaps?

Example

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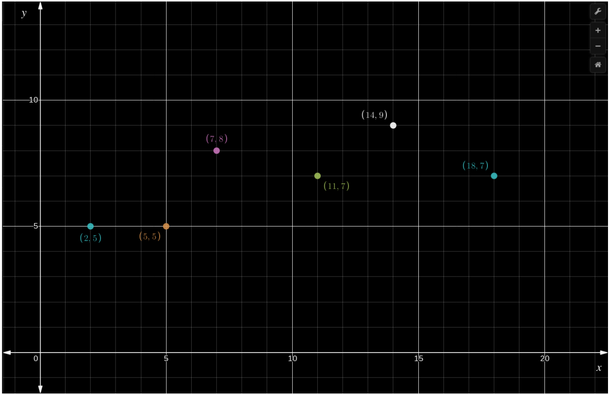
Let's start by tracing a line wich "best fit" that data



Why a line? To warm the modeling machine in our minds we are considering a line, a one degree polynomial.

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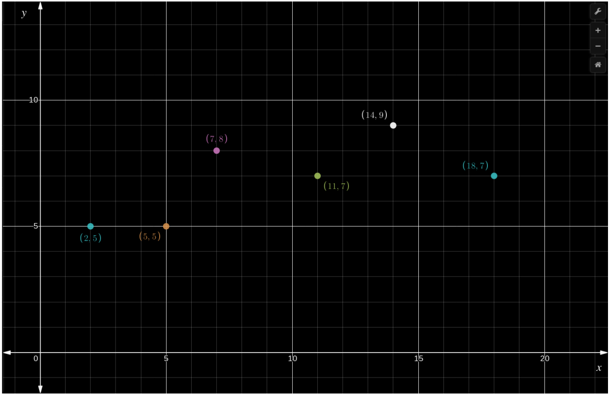
What line to plot? How to choose that line?



Enter the math...

Example

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A very common way to express a line in the plane is isolating y as a polynomial function of x:

$$y = mx + b$$

From this equation we can see that m is the *slope* of the line and b is the *y-intercept* (the value of y when $x = 0$).

Will be handy for us to write this equation using vector notation:

$$y = \begin{bmatrix} x & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix}$$

And switching terms:

$$\begin{bmatrix} x & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = y$$

Example

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Ok. Fine. This form

$$\begin{bmatrix} x & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = y$$

will be a useful one because we know x and y in six points. For example take the first point $(2, 5)$

$$\begin{bmatrix} 2 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = 5$$

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And yes, your guess is true. We can incorporate the second point $(5, 5)$ and get

$$\begin{bmatrix} 2 & 1 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$$

Doing the product you can workout m and b from this equation. $m = 0$ and $b = 5$. Because the matrix is square. And invertible by the way.

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Going further, incorporate the third point.

$$\begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \\ 8 \end{bmatrix}$$

This invalidate the previous result. m cannot be 0 more. Neither b with 5.
Actually, henceforth the equation is over-determined and have no solution.

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Fourth point.

$$\begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \end{bmatrix}$$

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Fifth point.

$$\begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \\ 9 \end{bmatrix}$$

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Sixth and last point.

$$\begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \\ 18 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \\ 9 \\ 7 \end{bmatrix}$$

This is the equation derived from our measurement.

Example

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Time to name things.

Example

Showing why least squares

Call A to the matrix

$$A = \begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \\ 18 & 1 \end{bmatrix}$$

Example

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Call x to the column vector

$$x = \begin{bmatrix} m \\ b \end{bmatrix}$$

Example

Showing why least squares

Call b to the column vector

$$b = \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \\ 9 \\ 7 \end{bmatrix}$$

Example

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Thus, the equation

$$\begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \\ 18 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \\ 9 \\ 7 \end{bmatrix}$$

becomes

$$Ax = b$$

Example

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In other words: if you want to know the values m and b in the equation $y = mx + b$ of the line we are searching find the x such $Ax = b$.

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$$\|Ax - b\| \neq 0$$

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Showing why least squares

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$$\|Ax - b\| \neq 0$$

We need the least squares approximate solution

Example

Showing why least squares

In the least squares approximate solution of $Ax = b$ we, provided that $\|Ax - b\| \neq 0$, select x that the *norm* of the *residual* $r = Ax - b$ is minimal.

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Let's see it.

Example

Showing why least squares

All start with our equation $Ax = b$.

Example

Showing why least squares

Take the original matrix A:

$$A = \begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \\ 18 & 1 \end{bmatrix}$$

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Take the original matrix A:

$$A = \begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \\ 18 & 1 \end{bmatrix}$$

Transpose it, and get $A^\intercal$:

$$A^\intercal = \begin{bmatrix} 2 & 5 & 7 & 11 & 14 & 18 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

Example

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Multiply $A^\intercal$ by A

$$A^\intercal A = \begin{bmatrix} 2 & 5 & 7 & 11 & 14 & 18 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 11 & 1 \\ 14 & 1 \\ 18 & 1 \end{bmatrix} = \begin{bmatrix} 719 & 57 \\ 57 & 6 \end{bmatrix}$$

Example

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Invert the product

$$(A^\intercal A)^{-1} = \begin{bmatrix} 719 & 57 \\ 57 & 6 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{2}{355} & -\frac{19}{355} \\ -\frac{19}{355} & \frac{719}{1065} \end{bmatrix}$$

Example

Showing why least squares

Multiply inverse and transpose

$$(A^\intercal A)^{-1}A^\intercal = \begin{bmatrix} \frac{2}{355} & -\frac{19}{355} \\ -\frac{19}{355} & \frac{719}{1065} \end{bmatrix} \begin{bmatrix} 2 & 5 & 7 & 11 & 14 & 18 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} -\frac{3}{71} & -\frac{9}{355} & -\frac{1}{71} & \frac{3}{355} & \frac{9}{355} & \frac{17}{355} \\ \frac{121}{213} & \frac{434}{1065} & \frac{64}{213} & \frac{92}{1065} & -\frac{79}{1065} & -\frac{307}{1065} \end{bmatrix}$$

Let's call this product $(A^\intercal A)^{-1}A^\intercal$ the *pseudo-inverse*

Example

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Finally multiply the pseudo-inverse by b

$$x = (A^\intercal A)^{-1} A^\intercal b \tag{1}$$

$$= \begin{bmatrix} -\frac{3}{71} & -\frac{9}{355} & -\frac{1}{71} & \frac{3}{355} & \frac{9}{355} & \frac{17}{355} \\ \frac{121}{213} & \frac{434}{1065} & \frac{64}{213} & \frac{92}{1065} & -\frac{79}{1065} & -\frac{307}{1065} \end{bmatrix} \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \\ 9 \\ 7 \end{bmatrix} \tag{2}$$

$$= \begin{bmatrix} \frac{61}{355} \\ \frac{5539}{1065} \end{bmatrix} \tag{3}$$

$$= \begin{bmatrix} 0.171831 \\ 5.20094 \end{bmatrix} \tag{4}$$

Example

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That's it

$$x = \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} \frac{61}{355} \\ \frac{5539}{1065} \end{bmatrix} \text{ or } \begin{bmatrix} 0.171831 \\ 5.20094 \end{bmatrix}$$

and $m = 0.171831$
and $b = 5.20094$
and the line is

$$y = 0.171831x + 5.20094$$

and **that** is the line which **best fit** our data points.

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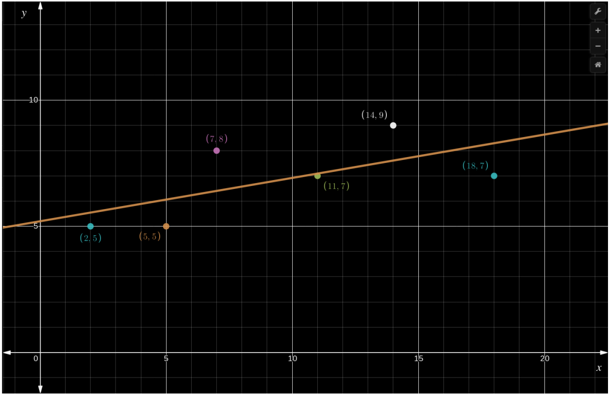
And the best fit is



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Recapitulation

You have a bunch of data points and suspect that a polynomial function $y = Ax + B$ from this points is a good model.
You build a matrix A and a vector b from the polynomial and the points.
The polynomial coefficients are a vector x so $Ax = b$
Then $x = (A^{\intercal}A)^{-1}A^{\intercal}b$

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Don't worry, its XXI century

So the key is calculate $x = (A^\intercal A)^{-1} A^\intercal b$.
But you don't need to do this by hand like Gauss did.
See the code, in this case Javascript code, using the mathjs package.

```
const { multiply, transpose, inv, matrix, format } =
    require( "mathjs")

const solve = (A, b) => {
   const transposed   = transpose(A)
   const product      = multiply(transposed, A)
   const inverse      = inv(product)
   const pseudoInverse = multiply(inverse,transposed)
   const x            = multiply(pseudoInverse, b)
   return x
}

const A = matrix([[2,1],[5,1],[7,1],[11,1],[14,1],[18,1]])
const b = matrix([5,5,8,7,9,7])

console.log(format(solve(A, b),5))
```

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The polynomial function

Get a terminal and do the magic

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The polynomial function

Get a terminal and do the magic

```
$ node ls.js
[0.17183, 5.2009]
```

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Going further

Mind blowing is coming

To avert catastrophic damage in our brains it's time to rename things

In the example we found a line $y = mx + b$, now:

m becomes a_1

b becomes a_0

x becomes x_1

y remains the same

The found line, then, becomes

$$y = a_1 x_1 + a_0 = 0.17183 x_1 + 5.2009$$

Nothing has changed, only the names.

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The polynomial function

In the example we picked a line for regression.
A line in a plane can be expressed as a polynomial function $P(x_1)$ where y (the dependent variable, a real number) is a function of x_1 (the independent variable, a real number)

$$y\colon \mathbb{R} \to \mathbb{R} = P(x_1) = a_1 x_1 + a_0$$

But there are others $P(x_1)$s, for example:

$$y\colon \mathbb{R} \to \mathbb{R} = P(x_1) = a_2 x_1^2 + a_1 x_1 + a_0$$

What about using that quadratic function as the model for the measured points?

Let's see...

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A curve as a model

That is the curve: $y = a_2x_1^2 + a_1x_1 + a_0$
And those are the points: $(2,5),(5,5),(7,8),(11,7),(14,9),(18,7)$
Replacing x_1 and y in each point, and rearranging:

$$4a_2 + 2a_1 \quad + a_0 = 5 \tag{5}$$
$$25a_2 + 5a_1 \quad + a_0 = 5 \tag{6}$$
$$49a_2 + 7a_1 \quad + a_0 = 8 \tag{7}$$
$$121a_2 + 11a_1 \quad + a_0 = 7 \tag{8}$$
$$196a_2 + 14a_1 \quad + a_0 = 9 \tag{9}$$
$$324a_2 + 18a_1 \quad + a_0 = 7 \tag{10}$$

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A curve as a model

The curve: $y = a_2 x_1^2 + a_1 x_1 + a_0$
In matrix form:

$$\begin{bmatrix} 4 & 2 & 1 \\ 25 & 5 & 1 \\ 49 & 7 & 1 \\ 121 & 11 & 1 \\ 196 & 14 & 1 \\ 324 & 18 & 1 \end{bmatrix} \begin{bmatrix} a_2 \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \\ 8 \\ 7 \\ 9 \\ 7 \end{bmatrix}$$

In this case

$$x = \begin{bmatrix} -0.028205 \\ 0.73633 \\ 3.2181 \end{bmatrix}$$

and the curve is $y = -0.028205 x_1^2 + 0.73633 x_1 + 3.2181$

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Adding one dimension

Until now we were working with polynomials whis one independent variable (x_1) and one dependent variable (y)

$$y\colon \mathbb{R} \to \mathbb{R} = P(x_1)$$

What about a polynomial with two independent variables?
Nothing, the least squares method stays the same. Note that is all about finding coefficients. So for example take

$$y\colon \mathbb{R}^2 \to \mathbb{R} = P(x_1, x_2)$$

where

$$y = a_5 x_1^2 + a_4 x_2^2 + a_3 x_1 x_2 + a_2 x_1 + a_1 x_2 + a_0$$

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Adding one dimension

That function ($y = a_5 x_1^2 + a_4 x_2^2 + a_3 x_1 x_2 + a_2 x_1 + a_1 x_2 + a_0$) is useful when you need a model to represent height at a certain point given with two coordinates (x_1, x_2).
In this case we are looking for six coefficients

$$x = \begin{bmatrix} a_5 \\ a_4 \\ a_3 \\ a_2 \\ a_1 \\ a_0 \end{bmatrix}$$

so we need at least six points (x_1, x_2, y) to uniquely determinate those coefficients.

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Adding one dimension

If you have more points than six you form the matrix A, form the vector b as usual, and resolve x using the least squares approximate solution:

$$x = (A^\intercal A)^{-1} A^\intercal b$$

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Multidimensional input

Of course you can extend the application of least squares to problems where the input have more than two dimension

$$y\colon \mathbb{R}^n \to \mathbb{R} = P(x_1, x_2, \ldots, x_n)$$

Take for example a set of measured temperatures in certain points (ten or more) (x_1, x_2, x_3, t) in the interior of a body. If we want a quadratic model then the polynomial will be:

$$y = f(x_1, x_2, x_3) : \mathbb{R}^3 \to \mathbb{R} \tag{11}$$

$$y = a_9 x_1^2 + a_8 x_2^2 + a_7 x_3^2 + a_6 x_1 x_2 + a_5 x_1 x_3 + \tag{12}$$

$$a_4 x_2 x_3 + a_3 x_1 + a_2 x_2 + a_1 x_3 + a_0 \tag{13}$$

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Multidimensional input

Take the measurements, build the matrix A evaluating x_1, x_2, x_3, their products and their squares, build the column vector b evaluating y. Be aware that x (in $Ax = b$) will be

$$x = \begin{bmatrix} a_9 \\ a_8 \\ a_7 \\ a_6 \\ a_5 \\ a_4 \\ a_3 \\ a_2 \\ a_1 \\ a_0 \end{bmatrix}$$

evaluate $x = (A^\intercal A)^{-1} A^\intercal b$ and you are done.

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Multidimensional output

What about $\mathbb{R}^n \to \mathbb{R}^m$?

Almost the same, with certain precautions.

Take the case of $y : \mathbb{R}^3 \to \mathbb{R}^3$
where

$$y_1 : \mathbb{R}^3 \to \mathbb{R} = P_1(x_1, x_2, x_3) \tag{14}$$
$$y_2 : \mathbb{R}^3 \to \mathbb{R} = P_2(x_1, x_2, x_3) \tag{15}$$
$$y_3 : \mathbb{R}^3 \to \mathbb{R} = P_3(x_1, x_2, x_3) \tag{16}$$

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Multidimensional output

We can isolate and resolve each function e.g., taking the first coordinate of $y(y_1)$:

from the measurements and the selected polynomial model form the matrix A_1 so:

$$A_1 x = b_1$$

$$x = (A_1^\intercal A_1)^{-1} A_1^\intercal b_1$$

x here denotes $\begin{bmatrix} a_{11} & a_{21} & \dots & a_{n1} \end{bmatrix}^T$ (the second subscript indicates that those are the coefficients of P_1, the polynomial of y_1)

Doing the same for y_2 and y_3 the model for the transformation $y : \mathbb{R}^3 \to \mathbb{R}^3$ is complete.
But these results came from isolated functions. What if I want a least squares solution for the transformation as a whole?
Let's see it.

Least squares

Multidimensional output

What if I want a least squares solution for the transformation as a whole?
Instead of calculate

$$(A_1^\intercal A_1)^{-1} A_1^\intercal b_1 \text{ for } P_1$$

$$(A_2^\intercal A_2)^{-1} A_2^\intercal b_2 \text{ for } P_2$$

$$(A_3^\intercal A_3)^{-1} A_3^\intercal b_3 \text{ for } P_3$$

We cant integrate the evaluation of the column vector x (the coefficients) using the following calculation:

$$x = (A_1^T A_1 + A_2^T A_2 + A_3^T A_3)^{-1}(A_1^T b_1 + A_2^T b_2 + A_3^T b_3)$$

And that is the way to map, for example, from one color to another given a set of example points.