Linear Least Squares Line Fitting Calculus

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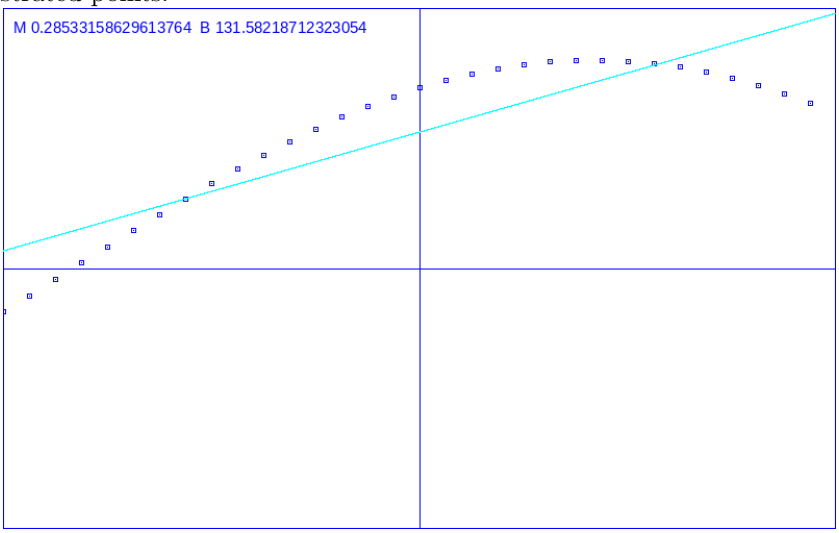
1 Introduction

This is a description of fitting a line to a collection of two dimensional points (x, y) by minimizing the error defined as the square of the differences between the line $y = mx + b$ and each y_i for every x_i in the point set, when added together. Below is an example of a solution of the best fitting line given the illustrated points.



To find the line, we define our error function. Described below, it is sometimes called the sum of residuals. The important idea is that it is a function, and thus has parameters and a derivative.

To find the minimum, we take the derivative, or gradient, and set it to zero. This is possible because the function $z = (x - y)^2$ is convex and increases as x and y differ, the minimum value has gradient zero. This is like our error function which is a sum of squares.

2 The error function

The error function is defined as the differences between the line's y values and the y values of the data set squared for each pair.

$$\sum_{i=1}^{n} \left(mx_i + b - y_i\right)^2 \tag{1}$$

We can see this as a function f taking two variables, m and b:

$$f(m,b) = \sum_{i=1}^{n} \left(mx_i + b - y_i\right)^2 \tag{2}$$

3 Finding the minimum: Simplfy

The current definition of $f(m,b)$ would require the chain rule for a derivative, in a sum, things we can avoid by trying to isolate our terms by carrying out the square, isolating the sums from our parameters **m** and **b** and separating constants from our variables.

Dropping the sum for the moment, we expand:

$$\begin{aligned} f(m,b) &= \left(mx_i + b - y_i\right)^2 \\ &= \left(mx_i + b - y_i\right)\left(mx_i + b - y_i\right) \\ &= mx_i\left(mx_i + b - y_i\right) + b\left(mx_i + b - y_i\right) - y_i\left(mx_i + b - y_i\right) \\ &= mx_imx_i + mx_ib - mx_iy_i + bmx_i + b^2 - by_i - y_imx_i - y_ib + y_i^2 \\ &= m^2x_i^2 + mbx_i - mx_iy_i + mbx_i + b^2 - by_i - my_ix_i - by_i + y_i^2 \\ &= m^2x_i^2 + 2mbx_i - 2mx_iy_i - 2by_i + b^2 + y_i^2 \end{aligned} \tag{3}$$

If we add the sum back we get:

$$f(m,b) = \sum_{i=1}^{n} \left(m^2x_i^2 + 2mbx_i - 2mx_iy_i - 2by_i + b^2 + y_i^2\right) \tag{4}$$

Expanding the sums, carefully:

$$f(m,b) = \sum_{i=1}^{n} m^2x_i^2 + \sum_{i=0}^{n} 2mbx_i - \sum_{i=0}^{n} 2mx_iy_i - \sum_{i=0}^{n} 2by_i + \sum_{i=0}^{n} b^2 + \sum_{i=0}^{n} y_i^2 \tag{5}$$

Then factoring and simplifying:

$$f(m,b) = m^2\sum_{i=1}^{n} x_i^2 + 2mb\sum_{i=0}^{n} x_i - 2m\sum_{i=0}^{n} x_iy_i - 2b\sum_{i=0}^{n} y_i + nb^2 + \sum_{i=0}^{n} y_i^2 \tag{6}$$

4 Summed Constants

We know the sums of x_i and x_i^2 are constant, that is, we cannot change them, we using them to define our gradient. So let's rename them to simplify our calculations.

$$\chi = \sum_{i=1}^{n} x_i \tag{7}$$

And

$$\Omega = \sum_{i=1}^{n} x_i^2 \tag{8}$$

With

$$\upsilon = \sum_{i=1}^{n} y_i \tag{9}$$

And finally

$$\phi = \sum_{i=1}^{n} x_i y_i \tag{10}$$

The equation above becomes more simple:

$$f(m,b) = m^2\Omega + 2mb\chi - 2m\phi - 2b\nu + nb^2 + \sum_{i=0}^{n} y_i^2 \tag{11}$$

The final sum does not involve our parameters m or b so we don't simplify it, we will ignore it.

5 Finding the minimum: derivatives of $f(m,b)$

Now let's get the gradient by taking partial derivatives using our two knobs: m and b: Let us first solve for m.

$$\frac{\partial f(m,b)}{\partial m} = 2m\Omega + 2b\chi - 2\phi \tag{12}$$

Then, by b

$$\frac{\partial f(m,b)}{\partial b} = 2m\chi - 2\nu + 2nb \tag{13}$$

Setting both to zero, and dividing by two, we get:

$$\frac{\partial f(m,b)}{\partial m} = m\Omega + b\chi - \phi = 0 \tag{14}$$

And

$$\frac{\partial f(m,b)}{\partial b} = m\chi + nb - \nu = 0 \tag{15}$$

Find a common factor for $\mathbf{b}$ by multiplying (14) by $\mathbf{n}$ and (15) by $-\chi$

$$m\mathbf{n}\Omega + b\chi\mathbf{n} - \phi\mathbf{n} = 0 \tag{16}$$

And

$$-m\chi^{\mathbf{2}} - b\chi n + \upsilon\chi = 0 \tag{17}$$

Adding them and removing the $-b\chi n$ term.

$$\mathbf{m}\left(n\Omega - \chi^2\right) + \upsilon\chi - \phi n = 0 \tag{18}$$

Move $\nu\chi$ and ϕn to the other side, and divide by $n\Omega - \chi^2$ and we get the first half of our solution, m

$$\mathbf{m} = \frac{\phi n - \upsilon\chi}{n\Omega - \chi^2} \tag{19}$$

Should we divide by zero, the slope will become ∞! We deal with that in the next section. Should $n\Omega - \chi^2$ not be zero, we can find b with:

$$\mathbf{b}\chi = \phi - m\Omega \tag{20}$$

Finally:

$$\mathbf{b} = \frac{\phi - m\Omega}{\chi} \tag{21}$$

6 Corner cases

Notice the two pitfalls: $\chi = 0$ and $n\Omega - \chi^2 = 0$! What do these mean? $\chi = 0$ implies:

$$\sum_{i=0}^{n} x_i = 0 \tag{22}$$

This is not difficult. Consider the points: $(-1, 1), (0, 2), (1, 3)$. Starting at $(-1, 1)$, the line has slope 1 and y intercept of 2. Nevertheless, the sum of $\mathbf{x_i}$ is zero i.e. χ is zero and the equation for $\mathbf{b}$ fails.

Hence we try an alternate strategy: solve for $\mathbf{b}$ instead of $\mathbf{m}$. Find a common factor for $\mathbf{m}$ by multiplying (14) by χ and (15) by $-\mathbf{\Omega}$

$$m\Omega\chi + b\chi^2 - \phi\chi = 0 \tag{23}$$

$$-m\chi\Omega - nb\Omega + \nu\Omega = 0 \tag{24}$$

Add them up, and we get:

$$b\chi^2 - nb\Omega + \nu\Omega - \phi\chi = 0 \tag{25}$$

Collecting $\mathbf{b}$ and moving constants to the other side:

$$b(\chi^2 - n\Omega) = \phi\chi - \nu\Omega \tag{26}$$

We are in a contingency, where $\chi = 0$, so let us exploit this to simplify.

$$n\Omega b = \nu\Omega \tag{27}$$

Immediately:

$$b = \frac{\nu\Omega}{n\Omega} = \frac{\nu}{n} \tag{28}$$

Things get even more weird using (15) with $\chi = 0$ to find $\mathbf{m}$:

$$m\Omega - \phi = 0 \tag{29}$$

And hence:

$$m = \frac{\phi}{\Omega} \tag{30}$$

Now to deal with pitfall two: $n\Omega - \chi^2 = 0$, or:

$$n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=0}^{n} x_i\right)^2 = 0 \tag{31}$$

For example, a single point will create that problem, and a single point has no solution. Let's see what we can do.

$$n\left(\sum_{i=1}^{n} x_i^2\right) = \left(\sum_{i=0}^{n} x_i\right)^2 \tag{32}$$

$$\sqrt{n}\sqrt{\sum_{i=1}^{n} x_i^2} = \sum_{i=0}^{n} x_i \tag{33}$$

Note the square root of squares is actually vector length, if we treat each $\mathbf{x_i}$ as a vector $\vec{x}$.

$$\sqrt{n}\,|\vec{x}| = \sum_{i=0}^{n} x_i \tag{34}$$

And then we end up with a normalized vector:

$$\sqrt{n} = \frac{\sum_{i=0}^{n} x_i}{|\vec{x}|} \tag{35}$$

I'm not sure what to do with this, but my efforts to find an example where this is true have failed. The python code prints an error should this occur.

7 Code

A function to obtain $\mathbf{m}$ and $\mathbf{b}$ is given below, as you can see, it is quite short.

```
def FindLine(points=[]):
    """points is a 2-D array
       [[x, y], [x, y], ...]"""
    chi = 0.0
    omega = 0.0
    nu = 0.0
    phi = 0.0

    n = len(points)
    for x, y in points:
      chi += x
      omega += x * x
      nu += y
      phi += x * y

    if chi == 0.0:  # special case.
      m = phi / omega
      b = nu / n
      return (m, b)

    d = n * omega - chi * chi
    if d == 0.0:
      print("Highly unlikely!")
      return (1, 1)
    m = (chi + phi * n - nu * chi) / d
    b = (phi - m * omega) / chi
    return (m, b)
```

8 Conclusion

By using partial derivatives and some algebra, it is fairly easy to understand how to fit a line to a collection of points. This is called Gradient Descent and is used in Inverse Kinematics and Artificial Intelligence.