UCD Physics 9A Lab Manual

The Staff of the UCD Physics Dep't
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THE METHOD OF LEAST SQUARES

The name "Least Squares" is associated with a broad range of analytical techniques that share a value judgment that the "best" result is the one that will leave errors (deviations) δ_i whose squares have as small a sum as possible:

$$\sum_i (\delta_i)^2 = \text{minimum.} \qquad (1)$$

A. EXAMPLE

Let us see how this criterion is used to determine the slope *m* and intercept *b* of a straight line

$$y(x) = mx + b \qquad (2)$$

which fits three data points

$$y(1) = 1 \pm 0.2,\ y(2) = 3 \pm 0.2,\ y(3) = 4 \pm 0.2 \qquad (3)$$

as closely as possible, as in Fig. 1.

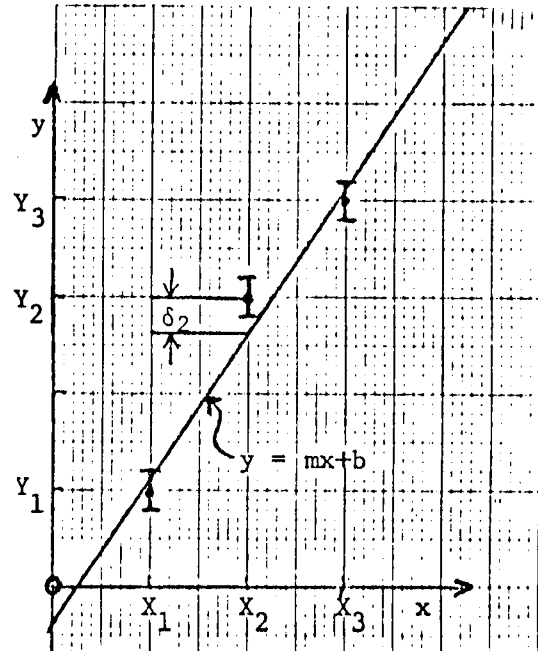

Fig. 1. Least Squares Fit

The deviations are the vertical distances

$$\delta_i = Y_i - (mX_i + b) \qquad (4)$$

between the data points and the straight line. We wish to find the values of *m* and *b* which yield the smallest possible sum of squared deviations

$$\sum_{i=1}^{n} \delta_i^2 = \sum_{i=1}^{3} (Y_i - mX_i - b)^2 \qquad (5a)$$

$$= (1 - m - b)^2 + (3 - 2m - b)^2 + (4 - 3m - b)^2 \qquad (5b)$$

$$= 26 + 14m^2 - 38m + 3b^2 - 16b + 12mb \qquad (5c)$$

$$= \frac{1}{6} + 2(m - \frac{3}{2})^2 + 3[(b + \frac{1}{3}) + 2(m - \frac{3}{2})]^2 \qquad (5d)$$

The final form (5d) is not easy to derive (Question 1), but has been chosen so that the following features are obvious: the smallest possible sum of squared deviations is $\frac{1}{6}$ and the "best" values of m and b are $m_o = \frac{3}{2}$ and $b_o = -\frac{1}{3}$ since any other values will yield $\Sigma\delta^2$ larger than $\frac{1}{6}$.

A more straightforward way to find the values of m and b that minimize (5c) is simply to set the derivatives

$$\frac{\partial}{\partial m}\sum\delta^2 = 28m - 38 + 12b = 0 \qquad (6a)$$

and

$$\frac{\partial}{\partial b}\sum\delta^2 = 6b - 16 + 12m = 0 \qquad (6b)$$

equal to zero and solve. The b equation yields the best b value

$$b = \frac{16 - 12m}{6} = \frac{8}{3} - 2m \qquad (7)$$

for arbitrary m, as seen in the last term in (5d). If we substitute (7) into (6a), we find

$$28m - 38 + 12(\frac{8}{3} - 2m) = 4m - 6 = 0 \qquad (8a)$$

or

$$m_o = \frac{6}{4} = \frac{3}{2} \qquad (8b)$$

and then substitute this back into (7) to find

$$b_o = \frac{8}{3} - 2m_o = \frac{8}{3} - 3 = -\frac{1}{3} \qquad (9)$$

as before. Thus, the "best fit" line is

$$y = m_o x + b_o = \frac{3}{2}x - \frac{1}{3}, \qquad (10)$$

as shown in Fig. 1, since any other line would have a larger sum of squared deviations (5).

Before obtaining general forms for m_o and b_o and their uncertainties, let us consider unequal uncertainties in the data.

B. UNEQUAL WEIGHTING

So far, we have treated each data point as having equal uncertainty σ and, therefore, equal importance. With unequal uncertainties, the more certain data points (those with small uncertainties) should have more importance. In particular, we should try to get deviations δ_i as small as their uncertainties σ_i. That is, a deviation/uncertainty ratio (δ_i/σ_i) smaller than 1 should be expected for most (68%) of the points, with ratios larger than 1 as seldom as possible. The quantity we wish to minimize is then the sum of squared <u>relative</u> deviations,

$$\boxed{\chi^2 \equiv \sum\left(\frac{\delta_i}{\sigma_i}\right)^2 = \text{minimum.}} \qquad (11)$$

If the theory has no adjustable parameters, and the uncertainties have been chosen appropriately (as in the section on Errors and Uncertainties), then we expect the deviations (δ_i) to be about equal to the uncertainties (σ_i), and χ^2 to be about equal to the number of data points (n). If we can reduce χ^2 by adjusting some parameters (such as adjusting m and b to m_o and b_o) then we expect χ^2 to be about n-p, where p is the number of adjusted parameters (p=2 for m and b). If one of the adjustable parameters (say m) changes from its optimum value (m_o), χ^2 must increase, and we can define the uncertainty (σ_m) to be the amount of change that will increase χ^2 by exactly 1:

$$\chi^2(m_o \pm \sigma_m) = \chi^2(m_o) + 1.$$

When χ^2 is a quadratic function of m (as it is in a straight-line y=mx+b fit), we thus expect to have exactly

$$\chi^2(m) = \chi^2(m_o) + \left(\frac{m - m_o}{\sigma_m}\right)^2. \qquad (12)$$

Example: Weighted Averages.

Suppose we have a number of independent measurements $(q_1 \pm \sigma_1, q_2 \pm \sigma_2, ..., q_n \pm \sigma_n)$ of some quantity q, and we wish to calculate the "best" value of q and its uncertainty (σ_q). To minimize

$$\chi^2 = \sum_{i=1}^{n}\left(\frac{q_i - q}{\sigma_i}\right)^2 = \sum_i \left(\frac{q_i^2}{\sigma_i^2}\right) - 2q\sum_i\left(\frac{q_i}{\sigma_i^2}\right) + q^2\sum_i\left(\frac{1}{\sigma_i^2}\right), \qquad (13)$$

we use the vanishing derivative

$$\frac{\partial\chi^2}{\partial q} = -2\sum_i\left(\frac{q_i}{\sigma_i^2}\right) + 2q\sum_i\left(\frac{1}{\sigma_i^2}\right) = 0 \qquad (14)$$

to solve for the best value

$$q_o = \frac{\Sigma_i\left(q_i / \sigma_i^2\right)}{\Sigma_i\left(1/\sigma_i^2\right)} \equiv \bar{q}, \qquad (15)$$

which we find to be the weighted average,

$$\bar{q} \equiv \frac{\Sigma_i q_i w_i}{\Sigma_i w_i} \qquad (16)$$

where the weighting, $w_i \quad 1/\sigma_i^2$, is inversely proportional to the square of the uncertainty.

In terms of $\bar{q}$ *, we can rewrite eq. (13) in the form of eq. (12) as*

$$\chi^2 = \sum_i\left(\frac{q_i^2}{\sigma_i^2}\right) + (q^2 - 2q\bar{q})\sum_i\left(\frac{1}{\sigma_i^2}\right)$$
$$= (q - \bar{q})^2\sum_i\left(\frac{1}{\sigma_i^2}\right) - \bar{q}^2\sum_i\left(\frac{1}{\sigma_i^2}\right) + \sum_i\left(\frac{q_i^2}{\sigma_i^2}\right)$$
$$= \left(\frac{q - q_o}{\sigma_q}\right)^2 + \chi^2_{min} \qquad (17)$$

so that we can easily identify $q_o = \bar{q}$ *and its uncertainty* σ_q *in*

$$\frac{1}{\sigma_q^2} = \sum_i\left(\frac{1}{\sigma_i^2}\right), \qquad (18)$$

and relate the minimized mean square deviation $\overline{\delta^2} \equiv \overline{(q - \bar{q})^2}$ *to*

$$\chi^2_{min} = \sum_i\left(\frac{q_i^2}{\sigma_i^2}\right) - \bar{q}^2\sum_i\left(\frac{1}{\sigma_i^2}\right)$$
$$= (\overline{q^2} - \bar{q}^2)\sum_i\left(\frac{1}{\sigma_i^2}\right) \qquad (19)$$
$$= \overline{(q - \bar{q})^2}\sum_i\left(\frac{1}{\sigma_i^2}\right) = \overline{\delta^2}\sum_i\left(\frac{1}{\sigma_i^2}\right).$$

For equal uncertainties, $\sigma_i = \sigma$, *eq. (18) becomes*

$$\frac{1}{\sigma_q^2} = \sum_{i=1}^{n}\left(\frac{1}{\sigma^2}\right) = \frac{n}{\sigma^2} \text{ (equal uncertainties)} \qquad (20)$$

or $\sigma_q = \sigma/\sqrt{n}$ *as in UNC eq. (16); eq. (19) becomes*

$$\chi^2 = \overline{\delta^2}\,\frac{n}{\sigma^2} \text{ (equal uncertainties)} \qquad (21)$$

and we see the consistency between the expected values $\chi^2 \quad n$ *and* $\sigma^2 \quad \overline{\delta^2}$.

C. GENERAL FORMULAS FOR STRAIGHT LINE FITS

If we wish to fit a straight line *y(x) = mx+b* to *n* data points

$$Y(X_1) = Y_1 \pm \sigma_1, \quad Y(X_2) = Y_2 \pm \sigma_2, ..., \quad Y(X_n) = Y_n \pm \sigma_n, \qquad (22)$$

we must choose *m* and *b* to minimize

$$\chi^2 = \sum_{i=1}^{n}\left(\frac{Y_i - mX_i - b}{\sigma_i}\right)^2 = \overline{\delta^2}\sum_i\left(\frac{1}{\sigma_i^2}\right). \quad (23)$$

This is most easily done in terms of weighted averages, by minimizing

$$\overline{\delta^2} = \overline{(Y - mX - b)^2} = b^2 + 2mb\overline{X} - 2b\overline{Y} + m^2\overline{X^2} - 2m\overline{XY} + \overline{Y^2}. \quad (24)$$

Here we find the vanishing derivative (for constant m)

$$\frac{\partial\overline{\delta^2}}{\partial b} = 2b + 2m\overline{X} - 2\overline{Y} = 0 \quad (25a)$$

will give the "best" b (for any constant m) so that <u>the line will pass through the average data point ($\overline{X},\overline{Y}$) as</u>

$$\boxed{\overline{Y} = m\overline{X} + b.} \quad (25b)$$

This result alone is a very helpful guide in drawing a line through graphs of data points, since it is relatively easy to calculate and plot the average data point. We then only need to adjust the slope (m) of the line through the average data point until we obtain the best fit line.

If we use this as a guide to rewrite eq. (24) in terms of $b + m\overline{X} - \overline{Y}$, we get

$$\overline{\delta^2} = (b + m\overline{X} - \overline{Y})^2 + m^2(\overline{X^2} - \overline{X}^2) - 2m(\overline{XY} - \overline{X}\overline{Y}) + \overline{Y^2} - \overline{Y}^2 \quad (26a)$$

$$= (b + m\overline{X} - \overline{Y})^2 + (m - m_o)^2(\overline{X^2} - \overline{X}^2) + \overline{Y^2} - \overline{Y}^2 - m_o^2(\overline{X^2} - \overline{X}^2). \quad (26b)$$

Now we can see that

$$\boxed{m_o = \frac{\overline{XY} - \overline{X}\,\overline{Y}}{\overline{X^2} - \overline{X}^2}} \quad (27)$$

is the best-fit slope[1] and

$$\boxed{b_o = \overline{Y} - m_o\overline{X}} \quad (29)$$

is the best-fit intercept.

For uncertainties σ_m and σ_b in m_o and b_o, we multiply eq. (26b) by $\sum_i\left(1/\sigma_i^2\right)$ to get

$$\chi^2 = \left(\frac{b + m\overline{X} - \overline{Y}}{\sigma_b}\right)^2 + \left(\frac{m - m_o}{\sigma_m}\right)^2 + \chi_o^2. \quad (30)$$

Now the intercept uncertainty σ_b is seen to be given by

$$\frac{1}{\sigma_b^2} = \sum_i\left(\frac{1}{\sigma_i^2}\right) \quad (31)$$

and the slope uncertainty σ_m is seen to be given by

$$\frac{1}{\sigma_m^2} = (\overline{X^2} - \overline{X}^2)\sum_i\left(\frac{1}{\sigma_i^2}\right) = \frac{\sigma_x^2}{\sigma_b^2} \quad or \quad \sigma_m = \frac{\sigma_b}{\sigma_x}, \quad (32)$$

where σ_x is the RMS variation of the X_i points, as given in eq. (28) (refer to footnote 1.)

<u>NON- LINEAR FITS</u>

There are two different generalizations that might be called non-linear. The first simply replaces the straight line (2) with a parabola or higher order polynomial, such as

$$y(x) = a + bx + cx^2 + dx^3, \quad (33)$$

or a non-linear function like

[1] The denominator

$$\overline{X^2} - \overline{X}^2 = \overline{X^2 - 2X\overline{X} + \overline{X}^2} = \overline{(X - \overline{X})^2} \equiv \sigma_x^2 \quad (28)$$

is a sum of positive squares, $(X_i - \overline{X})^2$, and thus is never zero (unless all the data were at the same value of $X_i = \overline{X}$); σ_x is the RMS variation of the X_i values.

$$y(x) = a\cos(x) + b\sin(x). \tag{34}$$

However, this is still linear in the parameters a, b, c, d to be determined, so the sum of squared deviations, like (5), (13) or (23), can still be reduced to quadratic functions of those parameters, and the minimization equations, like (6) or (25b), are still linear in those parameters. The only difficulty is the straightforward but tedious algebra involved in solving those p minimization equations for the p parameters. There is no difference in principle from what we have done for p = 2, so this is usually called a p-parameter linear fit.

A distinctively non-linear fit involves functions y(x) that are non-linear functions of the parameters to be determined, such as

$$y(x) = a\sin(bx) \tag{35}$$

which is non-linear in the parameter b and is not really linear for parameter a since that parameter multiplies a function of b. The behavior of χ^2 *as a function of such non-linear parameters can be quite complicated, possibly with more than one minimum. However, near any one of these minima, say* (a_o, b_o) *we can use a differential approximation (see the Supplement by that name) to linearize the function. For our example (35), we would expect*

$$\begin{aligned} y(x) \quad & a_c\sin(b_c x) + (a - a_c)\sin(b_c x) \\ & +(b - b_c)a\cos(bx) \end{aligned} \tag{36}$$

to be a good approximation for a and b close to a_o *and* b_o *if* a_c *and* b_c *are constant values close to the undetermined minimum* a_o, b_o. *Now y(x) is an approximately linear function of the parameters a and b, and* χ^2 *(a,b) is approximately quadratic, so we can use standard methods to find values of a and b to minimize this* χ^2; *these values may be expected to be good approximations to* a_o *and* b_o. *Instead of adding more terms to (36), we may improve the approximation by selecting new values of* a_c and b_c *closer to* a_o *and* b_o, *usually selecting them equal to the previous approximate values found for* a_o *and* b_o. *Such a sequence of successive approximations usually converges quite rapidly (once we are fairly close to a minimum) but each step can be a bit tedious.*

QUESTIONS / EXERCISES

1. Show that (5c) and (5d) are algebraically identical.

2. Using calculations like those in (28), show that (27) can be written as

$$m_o = \frac{\overline{(Y-\overline{Y})(X-\overline{X})}}{\overline{(X-\overline{X})^2}}. \tag{37}$$

   Note that this result shows that a positive slope m_o is associated with positive correlation: above-average values of Y occurring for above-average values of X, and below-average values also occurring together.

3. For the data points (3), calculate the average values in (27) and (29), and show that they yield the same m_o and b_o as (8) and (9).

4. Find the best straight line through the four equally weighted data points

$$\begin{aligned} &Y(1) = -1,\ \ Y(2) = 1, \\ &Y(3) = 2,\ \ Y(4) = 4, \end{aligned} \tag{38}$$

   first graphically, then using the results of this supplement,

5. Use the data points in (3), but halve the uncertainty in the second to $y(2)=3\pm 0.1$. (It should then be weighted four times as heavily as either the first or third point.)

   (a) Find the new values of m_o and b_o. (You will find that m_o is the same. Can you see why?)

   (b) Find the new deviations $\delta_1, \delta_2, \delta_3$ and show that δ_{RMS} has been unchanged even though δ_1 and δ_3 are larger than before and are larger than δ_{RMS}. Note that this is still consistent with expectations, since we effectively have 6 points (1,3, and four of 2) and 68% (4/6) of them have a deviation (δ_2) smaller than δ_{RMS}.

6. At one second intervals a cart's position is measured along a meter stick (in cm). The results were 0.1, 5.3, 10.9, 15.8, 21.5, and 25.9 centimeters (see UNC-Question 16).

   (a) Using the method of Least Squares calculate the "best" velocity (i.e., the slope of the "best" line through the data). You may want to compare your result with those obtained in UNC-Question 16.

   (b) Calculate the root-mean-square deviation. If the uncertainty in each position was ± 0.3 cm would you say the line fits the data reasonably well? Why?

   (c) If the uncertainty in each position was ± 0.1 cm what could this possibly mean?