

- Assignment #4 due Wed., Mar. 13
- Sign up for Experiment #5

Last Time:

Weighted Mean:

$$\mu' = \frac{\sum_{i=1}^N \frac{x_i}{\sigma_i^2}}{\sum_{i=1}^N \frac{1}{\sigma_i^2}} \quad \sigma_{\mu'}^2 = \frac{1}{\sum_{i=1}^N \frac{1}{\sigma_i^2}}$$

If all σ_i equal to σ , then $\sum_{i=1}^N \frac{1}{\sigma_i^2} = \frac{N}{\sigma^2}$

∴ μ' & $\sigma_{\mu'}$ reduce to:

$$\mu' = \frac{1}{N} \sum_{i=1}^N x_i \quad \sigma_{\mu'} = \frac{\sigma}{\sqrt{N}}$$

Today: "Least-Squares" Fit to a Straight Line

often meas. a quantity y as a fn of x .

Instead of repeated meas. of a value x ,
make a series of meas. of pairs (x_i, y_i) .

Consider linear fns ...

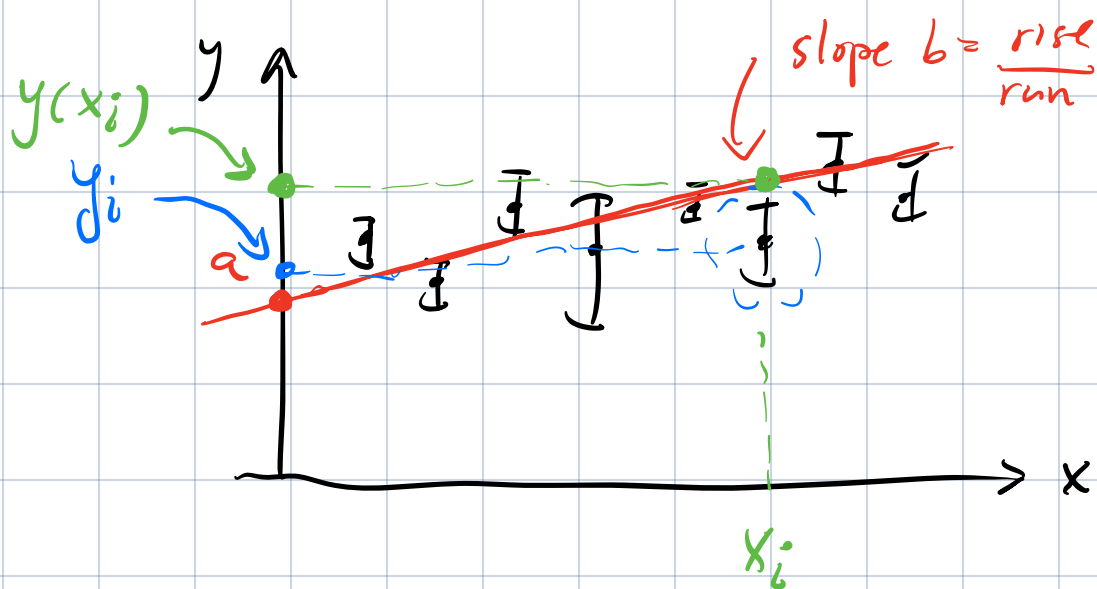
$$\text{eg. } \ln \bar{I} = \ln \bar{I}_0 + \left(\frac{e}{k_B T} \right) V$$

$y = \ln \bar{I}$ depends linearly on V

$$y = a + bx$$

$$a = \ln \bar{I}_0 \quad (\text{intercept})$$

$$b = \frac{e}{k_B T} \quad (\text{slope})$$



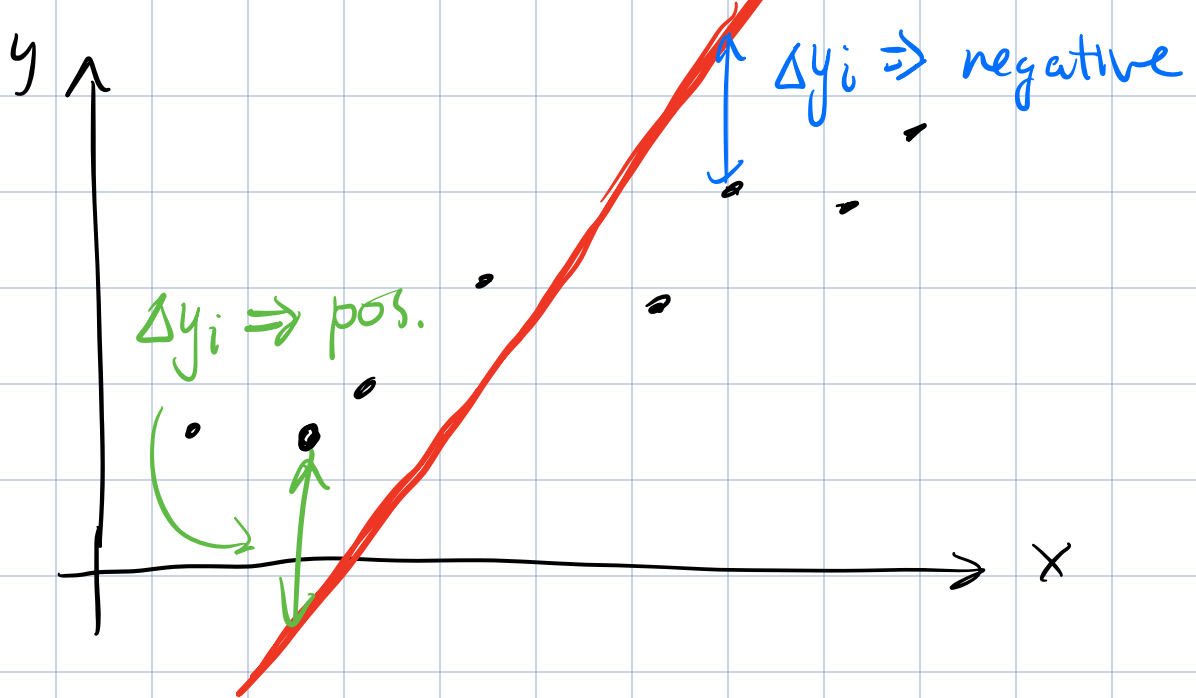
given a set of data $(x_i, y_i \pm \sigma_i)$, what are the most probable values of a & b ?

In our approach, we will assume uncertainty in x_i values negligible w.t. uncertainty in y_i measurements.

We will examine the deviations between meas. y_i & y calculated from x_i :

$$\Delta y_i = y_i - y(x_i) = y_i - (a + b x_i)$$

Expect Δy_i to be small for good choices of a & b values.

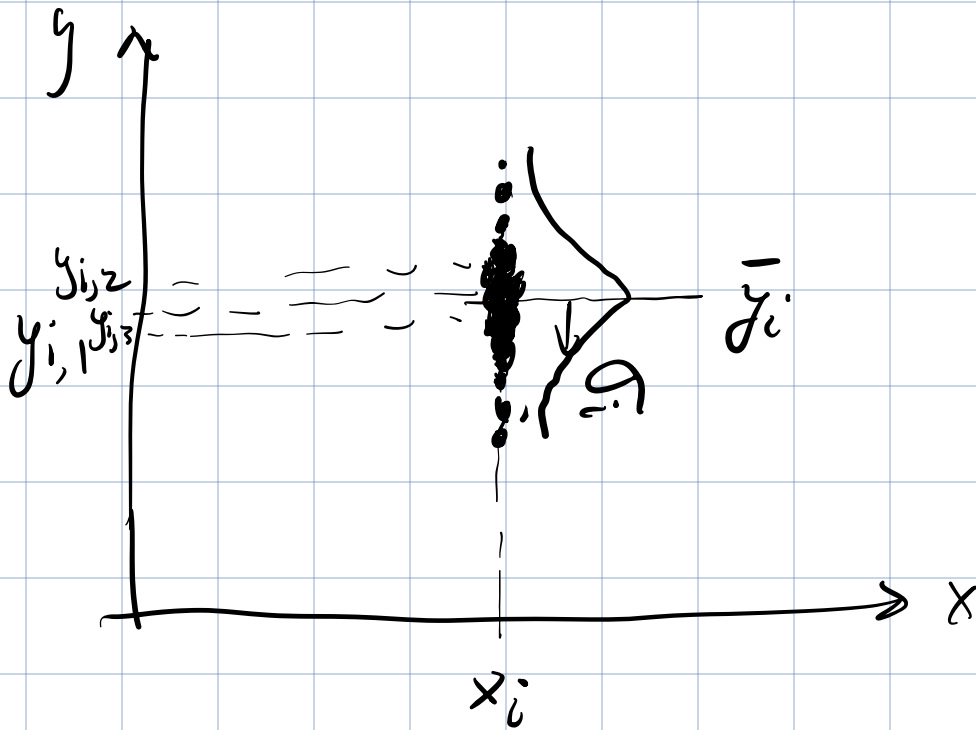


Δy_i on its own is not a good meas.
of quality of fit.

In the example above,

$\sum_{i=1}^N \Delta y_i$ would be small
even though the "fit" is poor.

Better approach: Assume that y_i meas. drawn from a Gaussian dist'n.



Our Gaussian dist'n of y_i values would have a mean $y_0(x_i) = a_0 + b_0 x_i$

where a_0 & b_0 are true parameters that describe our line (unknown).

The dist'n also has a st. dev. σ_i

Prob. of meas. a value of y between

y_i and $y_i + \Delta y$ is:

$$P_i = \frac{\Delta y}{\sigma_i \sqrt{2\pi}} \exp \left\{ -\frac{1}{2} \left[\frac{y_i - y_0(x_i)}{\sigma_i} \right]^2 \right\}$$

Prob. of making set of meas. $(x_1, y_1 \pm \sigma_1)$
 $(x_2, y_2 \pm \sigma_2)$
 \vdots
 $(x_N, y_N \pm \sigma_N)$

is:

$$P(a_0, b_0) = \prod_{i=1}^N P_i$$

$$= \left[\prod_{i=1}^N \left(\frac{\Delta y}{\sigma_i \sqrt{2\pi}} \right) \right] \exp \left\{ -\frac{1}{2} \sum_{i=1}^N \left[\frac{y_i - y_0(x_i)}{\sigma_i} \right]^2 \right\}$$

To find the best estimates of a_0 & b_0 from meas. data, we will maximize $P(a_0, b_0)$ by minimizing

$$\chi^2 \equiv \sum_{i=1}^N \left[\frac{y_i - y(x_i)}{\sigma_i} \right]^2$$

Chi-squared \rightarrow a "goodness of fit" parameter

$$\chi^2 = \sum_{i=1}^N \left[\frac{y_i - a - b x_i}{\sigma_i} \right]^2$$

Minimize χ^2 w.r.t. a & b .

2 eq's
& 2 unknowns
(a, b)

$$\begin{cases} \frac{\partial \chi^2}{\partial a} = 0 = -2 \sum_{i=1}^N \left[\frac{y_i - a - b x_i}{\sigma_i^2} \right] \\ \frac{\partial \chi^2}{\partial b} = 0 = -2 \sum_{i=1}^N \left[\frac{x_i (y_i - a - b x_i)}{\sigma_i^2} \right] \end{cases}$$

$$\therefore \sum \frac{y_i}{\sigma_i^2} = a \underbrace{\sum \frac{1}{\sigma_i^2}}_{u_a} + b \underbrace{\sum \frac{x_i}{\sigma_i^2}}_{u_b}$$

$$\sum \frac{x_i y_i}{\sigma_i^2} = a \underbrace{\sum \frac{x_i}{\sigma_i^2}}_{v_a} + b \underbrace{\sum \frac{x_i^2}{\sigma_i^2}}_{v_b}$$

solve system of 2 eq'ns for 2 unknowns a & b .

Of the form:

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u_a & u_b \\ v_a & v_b \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} a u_a + b u_b \\ a v_a + b v_b \end{pmatrix} \quad \checkmark$$

$$\text{If } \begin{pmatrix} u \\ v \end{pmatrix} = \overbrace{\begin{pmatrix} u_a & u_b \\ v_a & v_b \end{pmatrix}}^A \begin{pmatrix} a \\ b \end{pmatrix}$$

then
$$\begin{pmatrix} a \\ b \end{pmatrix} = A^{-1} \begin{pmatrix} u \\ v \end{pmatrix}$$

For 2×2 matrix

$$A^{-1} = \frac{1}{\det A} \begin{pmatrix} v_b & -u_b \\ -v_a & u_a \end{pmatrix}$$

$$\therefore \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\det A} \begin{pmatrix} v_b & -u_b \\ -v_a & u_a \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\det A = (u_a v_b - v_a u_b)$$

$$a = \frac{v_b u - u_b v}{u_a v_b - v_a u_b}$$

$$b = \frac{-V_a U + U_a V}{U_a V_b - V_a U_b}$$

Subbing in for our definitions of u, v
 u_a, v_a, u_b, v_b we get:

$$a = \frac{\sum \frac{x_i^2}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2}}{\sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2}$$

$$a = \frac{1}{\Delta} \left(\sum \frac{x_i^2}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} \right)$$

$$\Delta = \sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2$$

In the same way, find

$$b = \frac{1}{\Delta} \left(\sum \frac{1}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} \right)$$

Best-fit parameters for a weighted linear fit.

Next time, use prop. of errors to find σ_a & σ_b .