PHYS 232 March 7, 2025

Assignment #4 on course website
→ due Wed. March 12 @ 09:00

Last time: Used method of maximum likelihood to find the weighted mean & its uncertainty.

If measure:

$$x_1 \pm \sigma_1$$
$$x_2 \pm \sigma_2$$
$$\vdots$$
$$x_N \pm \sigma_N$$

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

when $\sigma_1 = \sigma_2 = \ldots = \sigma_N \equiv \sigma$, these results reduce to:

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

<u>Today</u>: Use the method of maximum likelihood to, given a set of linear data $(x_i, y_i \pm \sigma_i)$, determine the best possible slope & intercept of a line that passes through the data.

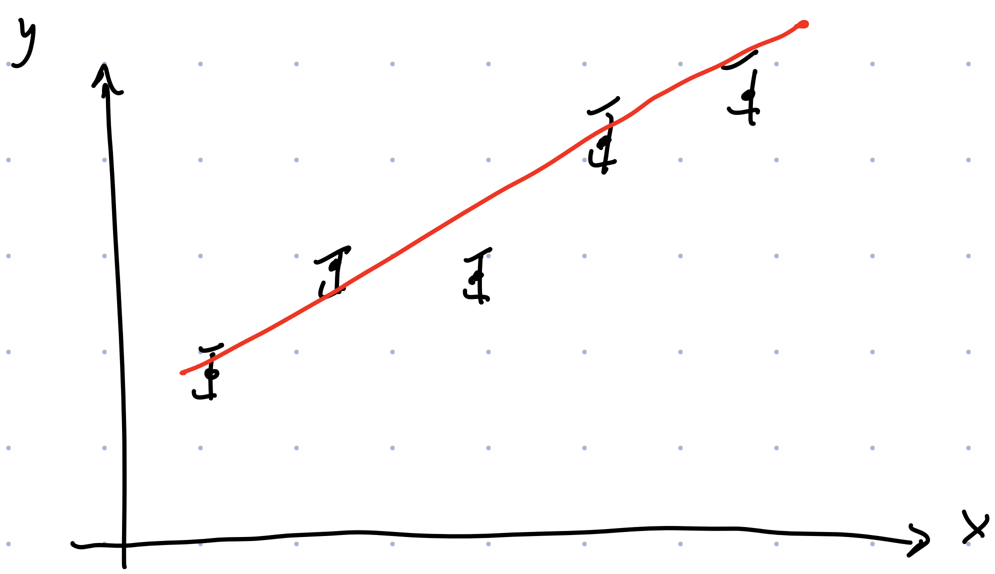
consider linear fcns:

$$\text{eg. } \ln I = \ln I_0 + \left(\frac{e}{k_B T}\right) V$$

$$y = \ln I \quad \text{vs} \quad x = V$$

$$a = \ln I_0 \quad \text{(intercept)}$$

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



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

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

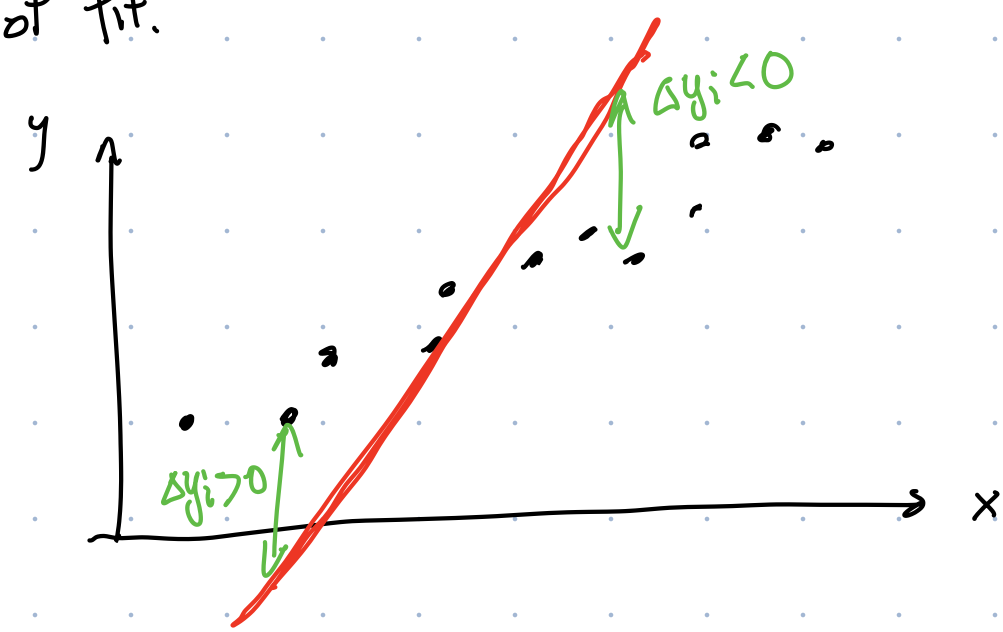
$$\Delta y_i = y_i - y(x_i) = y_i - \underbrace{(a + b x_i)}$$

meas. value y_i @ x_i

value of y on best-fit line at $x = x_i$

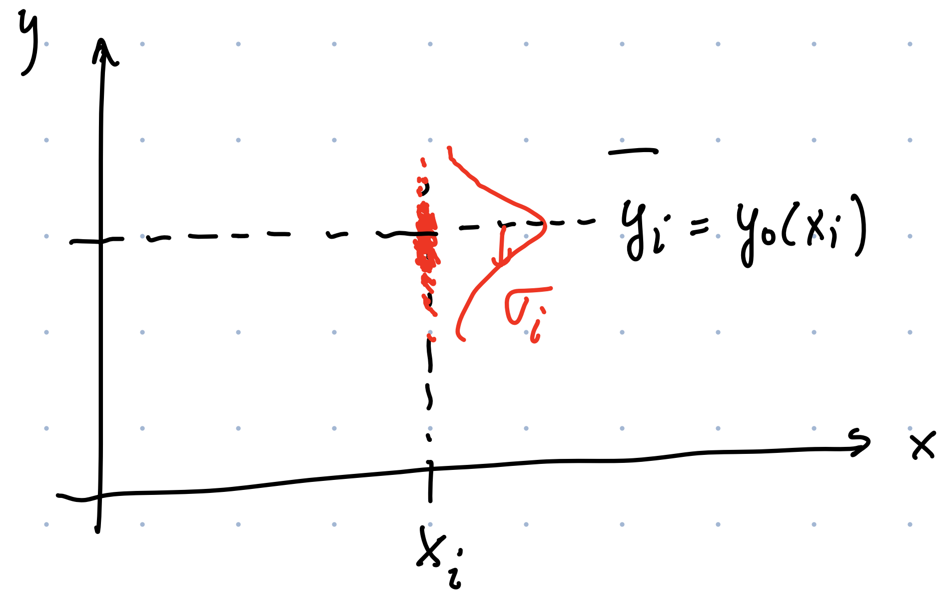
Expect Δy_i to be small for good choices of a & b.

Δy_i, on its own, is <u>not</u> a good meas of quality of fit.



In the example above, $\sum_{i=1}^{N} \Delta y_i$ would be small even though the deviations are large.

Better approach: Assume that y_i meas. are 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 the true parameters that describe the best-fit line (a_0 & b_0 are unknown). The dist'n also has a std. dev. σ_i

Prob. of meas. a value of y between y_i & $y_i + \Delta y$ is:

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

$y_0(x_i) = a - b x_i \Rightarrow$ determine best values for a & b to try & est. a_0 & b_0.

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

$$P(a,b) = \prod_{i=1}^{N} P_i$$

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

To find the best estimates of a_0 & b_0, we will maximize $P(a, b)$ by minimizing

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

Chi-squared → a "goodness of fit" parameter

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

Simultaneously minimize χ^2 w.r.t. a & b.

$$\left.\begin{aligned}
&① \quad \frac{\partial \chi^2}{\partial a} = 0 = -\cancel{2} \sum_{i=1}^{N} \left[\frac{y_i - a - bx_i}{\sigma_i}\right] \frac{1}{\sigma_i} \\
&② \quad \frac{\partial \chi^2}{\partial b} = 0 = -\cancel{2} \sum_{i=1}^{N} \frac{x_i}{\sigma_i} \left[\frac{y_i - a - bx_i}{\sigma_i}\right]
\end{aligned}\right\} \text{system of 2 eq'ns \& two unknowns } (a, b).$$

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

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

Solve system of 2 eq'ns & 2 unknowns using Matrices

of the form:

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

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

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

For a 2x2 matrix

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

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

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

$$\Downarrow$$

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

intercept.

$$\boxed{b = \frac{-v_a u + u_a v}{u_a v_b - v_a u_b}}$$

slope.

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

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

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

intercept

Likewise:

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

slope.

Best-fit parameters for a weighted linear fit.

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

(Note: Δ is indep. of y_i values)