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Lecture 5 start

Least-Squares Fit to a Straight Line

(Ch 6 Bevington)

Collect data $\{y_i\}$ - ~~the independe~~ ~~that depend on~~ that depend on some other quantity $\{x_i\}$. Hypothesize the relationship b/w these quantities is

$$y(x) = a+bx$$

where a and b are "model parameters".

Our goal is to determine the most likely ~~mode~~ values for a and b together with their errors.

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Errors on the data

In addition to $\{y_i\}$, $\{x_i\}$, we will need the errors $\{\sigma_{y_i}^2\}$ and $\{\sigma_{x_i}^2\}$. Generally you can try to measure y_i many times and then compute the sample variance, as we've done.

Often times the error in x_i is neglected. This is justified if

$$\sigma_y \gg \frac{\partial y}{\partial x}\sigma_x$$

(Something to estimate for the speed of light lab) If this is not the case, an approximate treatment is to compute the "indirect" error from x on y_i

$$\sigma_{yI} = \frac{\partial y}{\partial x}\sigma_x$$

Then the total error on y is increased accordingly

$$\sigma_{y,new}^2 = \sigma_{y,old}^2 + \sigma_{yI}^2$$

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Method of Maximum Likelihood

Want $\mathcal{L}(a, b \mid d) = P(d \mid a, b)$

$\uparrow$ data

$d = \{y_i\}$

$$P(y_i \mid a, b) = \frac{1}{\sqrt{2\pi\sigma_{y_i}^2}}\, e^{-\frac{1}{2}\frac{(y_i - \overset{\text{model}}{y(x_i)})^2}{\sigma_{y_i}^2}}$$

$$P(\{y_i\} \mid a, b) = \left[\prod_i^N \left(\frac{1}{\sqrt{2\pi\sigma_{y_i}^2}}\right)\right] e^{-\frac{1}{2}\sum_i^N \frac{(y_i - y(x_i))^2}{\sigma_{y_i}^2}}$$

assumes an independent errors

$$-2\ln(\mathcal{L}) = \underbrace{\sum_i^N \ln 2\pi\sigma_{y_i}^2}_{\text{independent of model}} + \underbrace{\sum_i^N \frac{[y_i - y(x_i)]^2}{\sigma_{y_i}^2}}_{\chi^2}$$

Maximize likelihood $\longleftrightarrow$ Minimize χ^2

$$\chi^2 = \sum_i^N \frac{[y_i - (a + bx_i)]^2}{\sigma_{y_i}^2}$$

Called "least squares"

b/c model is linear in the parameters this is called "linear least squares"

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$$\frac{\partial\chi^2}{\partial a} = -2\sum_i^N \frac{(y_i - (a + bx_i))}{\sigma_{y_i}^2} = 0$$

$$\frac{\partial\chi^2}{\partial b} = -2\sum_i^N \frac{(y_i - (a + bx_i))x_i}{\sigma_{y_i}^2} = 0$$

2 coupled equations

$$\sum \frac{y_i}{\sigma_{y_i}^2} = a\sum \frac{1}{\sigma_{y_i}^2} + b\sum \frac{x_i}{\sigma_{y_i}^2}$$

$$\sum \frac{x_i y_i}{\sigma_{y_i}^2} = a\sum \frac{x_i}{\sigma_{y_i}^2} + b\sum \frac{x_i^2}{\sigma_{y_i}^2}$$

Write as matrix eqn — note symmetric

$$\begin{bmatrix} \sum \frac{y_i}{\sigma_{y_i}^2} \\ \sum \frac{x_i y_i}{\sigma_{y_i}^2} \end{bmatrix} = \begin{bmatrix} \sum \frac{1}{\sigma_{y_i}^2} & \sum \frac{x_i}{\sigma_{y_i}^2} \\ \sum \frac{x_i}{\sigma_{y_i}^2} & \sum \frac{x_i^2}{\sigma_{y_i}^2} \end{bmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

To find ~~gra~~ most likely a and b, just need to invert a 2×2 matrix

$$\begin{pmatrix} e & f \\ g & h \end{pmatrix}^{-1} = \frac{1}{eh - gf}\begin{pmatrix} h & -f \\ -g & e \end{pmatrix}$$

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

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

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

Uncertainties on Parameters

$$\sigma_a = \sum_i^N \left(\frac{\partial a}{\partial y_i}\right)^2 \sigma_{y_i}^2$$

$$= \frac{1}{\Delta^2} \sum_i \left[\left(\sum_j \frac{x_j^2}{\sigma_{y_j}^2}\right)\frac{1}{\sigma_{y_i}^2} - \left(\sum_j \frac{x_j}{\sigma_{y_j}^2}\right)\frac{x_i}{\sigma_{y_i}^2}\right]^2 \sigma_{y_i}^2$$

...

$$= \frac{1}{\Delta} \sum \frac{x_i^2}{\sigma_i^2}$$

$$\sigma_b = \sum_i^N \left(\frac{\partial b}{\partial y_i}\right)^2 \sigma_{y_i}^2$$

$$= \frac{1}{\Delta^2} \sum_i \left[\left(\sum_j \frac{1}{\sigma_{y_j}^2}\right)\frac{x_i}{\sigma_{y_i}^2} - \left(\sum_j \frac{x_j}{\sigma_{y_j}^2}\right)\frac{1}{\sigma_{y_i}^2}\right]^2 \sigma_i^2$$

...

$$= \frac{1}{\Delta} \sum \frac{1}{\sigma_i^2}$$

Common Errors

$$\sigma_i^2 = \sigma^2$$

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

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

$$\sigma_a^2 = \left(\frac{\sum x_i^2}{N\sum x_i^2 - (\sum x_i)^2}\right)\sigma^2$$

$$\sigma_b^2 = \frac{\sigma^2}{N\sum x_i^2 - (\sum x_i)^2}$$

⑦

χ^2 goodness of fit

Given the best fit model we can use the χ^2 distribution to evaluate how well the data are described by gaussian ~~ra~~ variables distributed about that model

$$\chi^2 = \sum_i^N \frac{[y_i - (a+bx)]^2}{\sigma_{y_i}^2}$$

expect $\chi^2 \simeq \nu = N - N_{param} = N - 2$

a & b

Compute ~~PTA~~ PTE:

$$\int_{\chi^2}^{\infty} P_\chi(\chi^{2\prime}, \nu)\, d\chi^{2\prime}$$

expect $0.95 > PTE > 0.05$

If PTE doesn't fall in the "reasonable" interval, then it may be the case $\sigma_{y_i}^2$ are misestimated

$PTE > 0.95$: $\sigma_{y_i}^2$ too big

$PTE < 0.05$: $\sigma_{y_i}^2$ too small

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One principal problem with misestimating $\sigma_{y_i}^2$ is that σ_a^2 and σ_b^2 - parameter errors - will also be misestimated.

Consider a readjustment:

$$\sigma_{y_i}'^2 = \sigma_{y_i}^2 \frac{\chi^2}{\nu} = \sigma_{y_i}^2 \chi_\nu^2$$

"reduced" χ^2

then

$$\chi'^2 = \sum \frac{(y_i - y(x))^2}{\sigma_{y_i}'^2}$$

$$= \frac{1}{\chi^2/\nu} \underbrace{\sum \frac{(y_i - y(x))^2}{\sigma_{y_i}^2}}_{\chi^2}$$

$$= \nu$$

$\Rightarrow$ need to in principle ~~re~~ recompute all $\sigma_{y_i}^2$ dependent quantities...