PHYS 232 March 21, 2025

- Assignment #5 due $\boxed{\text{today}}$
- Start working on your formal report
  - due April 7 @ 14:00 in SCI 241

Last time: Used the method of maximum likelihood to develop a technique to fit data $(x_i, y_i \pm \sigma_i)$ to a fcn of the form:

$$y(x) = a_1 f_1(x) + a_2 f_2(x) + \dots + a_m f_m(x)$$

$$= \sum_{k=1}^{m} a_k f_k(x)$$

Found that $\underline{a} = \underline{\underline{\varepsilon}}\, \underline{\beta} = \underline{\underline{\alpha}}^{-1} \underline{\beta}$

where

$$\beta_\ell = \sum_{i=1}^{N} \frac{1}{\sigma_i^2} y_i f_\ell(x_i)$$

$$\alpha_{\ell k} = \sum_{i=1}^{N} \left[\frac{1}{\sigma_i^2} f_\ell(x_i) f_k(x_i) \right]$$

$a_k = a_k$

Today: Apply prop. of errors to $a_k(y_1, y_2, \dots y_N)$ in order to find σ_k.

Will show that the diagonal elements of $\underline{\underline{\varepsilon}}$ give the square of the uncertainty. Specifically,

$$\varepsilon_{kk} = \alpha^{-1}_{kk} = \sigma_k^2$$

Apply prop. of errors to $a_\ell(y_1, y_2, \dots, y_N)$

$$\sigma_\ell^2 = \left(\frac{\partial a_\ell}{\partial y_1}\sigma_1\right)^2 + \left(\frac{\partial a_\ell}{\partial y_2}\sigma_2\right)^2 + \dots + \left(\frac{\partial a_\ell}{\partial y_N}\sigma_N\right)^2$$

$$= \sum_{i=1}^{N}\left(\frac{\partial a_\ell}{\partial y_j}\sigma_j\right)^2$$

If $m=3$, then

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \underbrace{\begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix}}_{\text{symmetric}} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}$$

depend on y_i

$$l = 1 \qquad a_1 = \varepsilon_{11} \beta_1 + \varepsilon_{12} \beta_2 + \varepsilon_{13} \beta_3$$

In general, can express

$$a_l = \sum_{k=1}^{m} \varepsilon_{kl} \beta_k$$

sub in for β_k expression:

$$a_l = \sum_{k=1}^{m} \varepsilon_{kl} \left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2} y_i f_k(x_i) \right)$$

indep. of y_i

$$\frac{\partial a_l}{\partial y_j} = \sum_{k=1}^{m} \varepsilon_{kl} \underbrace{\left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2} \underbrace{\frac{\partial y_i}{\partial y_j}}_{\delta_{ij}} f_k(x_i) \right)}_{\frac{f_k(x_j)}{\sigma_j^2}}$$

δ_{ij} "killer of sums"

$$\therefore \frac{\partial a_l}{\partial y_j} = \sum_{k=1}^{m} \varepsilon_{kl} \frac{f_k(x_j)}{\sigma_j^2}$$

To find the uncertainties in a_ℓ, we will need to know $\left(\frac{\partial a_\ell}{\partial y_j}\right)^2$

Define $$\sigma^2_{a_\ell a_{\ell'}} = \sum_{j=1}^{N} \left[\sigma_j^2 \frac{\partial a_\ell}{\partial y_j} \frac{\partial a_{\ell'}}{\partial y_j} \right]$$

With this definition, the uncertainty in a_ℓ is found by setting $\ell' = \ell$.

$$\sigma^2_{a_\ell a_\ell} = \sigma^2_{a_\ell} = \sum_{j=1}^{N} \sigma_j^2 \left(\frac{\partial a_\ell}{\partial y_j}\right)^2$$

$\ell' = \ell$

Start w/

$$\sigma^2_{a_\ell a_{\ell'}} = \sum_{j=1}^{N} \left[\cancel{\sigma_j^2} \left(\sum_{k=1}^{m} \varepsilon_{k\ell} \frac{f_k(x_j)}{\cancel{\sigma_j^2}} \right) \left(\sum_{p=1}^{m} \varepsilon_{p\ell'} \frac{f_p(x_j)}{\sigma_j^2} \right) \right]$$

$$\sigma^2_{a_l a_{l'}} = \sum_{k=1}^{m} \left\{ \varepsilon_{kl} \sum_{p=1}^{m} \left[\varepsilon_{pl'} \underbrace{\sum_{j=1}^{N} \left(\frac{1}{\sigma_j^2} f_k(x_j) f_p(x_j) \right)}_{\text{elements of the } \underline{\underline{\alpha}} \text{ matrix } \alpha_{kp}} \right] \right\}$$

$$\therefore \sigma^2_{a_l a_{l'}} = \sum_{k=1}^{m} \left\{ \varepsilon_{kl} \left(\sum_{p=1}^{m} \varepsilon_{pl'} \alpha_{kp} \right) \right\} \quad (*)$$

Consider, for example, the 3x3 case of $\underline{\underline{\varepsilon}}\,\underline{\underline{\alpha}}$

$$\underbrace{\begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix}}_{\underline{\underline{\varepsilon}} = \underline{\underline{\alpha}}^{-1}} \underbrace{\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{12} & \alpha_{22} & \alpha_{23} \\ \alpha_{13} & \alpha_{23} & \alpha_{33} \end{pmatrix}}_{\underline{\underline{\alpha}}} = \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}}_{\underline{\underline{I}} \text{ identity matrix}}$$

1st Element: $\varepsilon_{11}\alpha_{11} + \varepsilon_{12}\alpha_{12} + \varepsilon_{13}\alpha_{13} = 1$ (a)

2nd Element: $\varepsilon_{11}\alpha_{12} + \varepsilon_{12}\alpha_{22} + \varepsilon_{13}\alpha_{23} = 0$ (b)

$\vdots$ $\vdots$ $\vdots$

Compare to $\sum_{p=1}^{m=3} \varepsilon_{pl'} \alpha_{kp}$

try $l' = k = 1$: $\varepsilon_{11}\alpha_{11} + \varepsilon_{12}\alpha_{12} + \varepsilon_{13}\alpha_{13} = 1$ by ⓐ

try $l' = 1$, $k = 2$: $\varepsilon_{11}\alpha_{12} + \varepsilon_{12}\alpha_{22} + \varepsilon_{13}\alpha_{23} = 0$ by ⓑ

$\vdots \qquad \vdots \qquad \vdots$

In general, $\sum_{p=1}^{m} \varepsilon_{pl'} \alpha_{kp} = \delta_{l'k}$ ← Kroneker-delta → just the elements of the identity matrix $\underline{\underline{I}}$

Sub this result into ⊛

$$\sigma^2_{a_l a_{l'}} = \sum_{k=1}^{m} \varepsilon_{kl} \delta_{l'k} = \varepsilon_{ll'}$$

"killer of sums"

$\Rightarrow k = l'$

$$\boxed{\therefore \ \sigma^2_{a_l a_{l'}} = \varepsilon_{ll'}}$$

The diagonal elements of $\underline{\underline{\varepsilon}}$ give the squares of the uncertainties in the best-fit parameters.

To get the uncertainty in a_l parameter, set $l' = l$:

$$\sigma_{a_l a_l}^2 \equiv \boxed{\sigma_{a_l}^2 = \mathcal{E}_{ll}}$$

Eg. For 3 parameters (a_1, a_2, a_3)

$$\underline{\mathcal{E}} = \begin{pmatrix} \mathcal{E}_{11} & \mathcal{E}_{12} & \mathcal{E}_{13} \\ \mathcal{E}_{12} & \mathcal{E}_{22} & \mathcal{E}_{23} \\ \mathcal{E}_{13} & \mathcal{E}_{23} & \mathcal{E}_{33} \end{pmatrix}$$

called <u>error</u> or covariance matrix.

$\mathcal{E}_{11}$ is σ_1^2 ... square of uncertainty in a_1
$\mathcal{E}_{22}$ " σ_2^2 ... " " " " a_2
$\mathcal{E}_{33}$ " σ_3^2 ... " " " " a_3

The off-diagonal terms give the covariance

$\sigma_{12} = \mathcal{E}_{12} = \mathcal{E}_{21}$ covariance between a_1 & a_2.

Summary

Fits to fcns of the form:

$$y = a_1 f_1(x) + a_2 f_2(x) + \dots + a_m f_m(x)$$
$$= \sum_{k=1}^{m} a_k f_k(x)$$

Have measured $(x_i, y_i \pm \sigma_i)$ for $i = 1..N$

$$\underline{a} = \underline{\underline{\varepsilon}}\, \underline{\beta}$$

column matrix of the best-fit parameters.

$(x_i, y_i \pm \sigma_i)$ fully determine all of $\underline{\underline{\alpha}}$, $\underline{\underline{\varepsilon}} = \underline{\underline{\alpha}}^{-1}$, & $\underline{\beta}$

There is <u>no</u> guess work involved when fitting data to a fcn of the form $y = \sum_{k=1}^{M} a_k f_k(x)$.

1. Calculate the elements of the $\underline{\beta}$ column matrix & the $\underline{\underline{\alpha}}$ square matrix.

$$\beta_l = \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} f_l(x_i) \qquad l = 1..m$$

$$\alpha_{lk} = \sum_{i=1}^{N} \left[\frac{1}{\sigma_i^2} f_l(x_i) f_k(x_i) \right] \qquad \begin{array}{l} l=1..m \\ k=1..m \end{array}$$

2. Invert $\underline{\underline{\alpha}}$ to find the error or covariance matrix:

$$\underline{\underline{\varepsilon}} = \underline{\underline{\alpha}}^{-1} \quad \text{(software)}$$

3. Calculate the best-fit parameters using

$$\underline{a} = \underline{\underline{\varepsilon}}\, \underline{\beta}$$

4. The diagonal elements of $\underline{\underline{\varepsilon}}$ give the square of the uncertainties in the best-fit parameters.

$$\sigma_{a_1} = \sqrt{\varepsilon_{11}}$$

$$\sigma_{a_2} = \sqrt{\varepsilon_{22}}$$

$$\vdots$$

$$\sigma_{a_m} = \sqrt{\varepsilon_{mm}}$$

no additonal calculation required!