PHYS 232 March 20, 2024

- Assignment #5 due Fri, Mar. 22
- Formal Report due Apr. 10 @ 11am

Last Time:

Fit data to:

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

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

Want to determine:

$$a_1 \pm \sigma_{a_1}, \; a_2 \pm \sigma_{a_2}, \; \ldots, \; a_m \pm \sigma_{a_m}$$

We found the a_k values from

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

where $\underline{\underline{\varepsilon}} = \underline{\underline{\alpha}}^{-1}$ & the elements of the various matrices are given by:

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

$$a_k = a_k$$

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

$\underline{\underline{\alpha}}$ is indep. of y_i values since $\underline{\underline{\varepsilon}} = \underline{\underline{\alpha}}^{-1}$, it is also indep. of y_i.

Today, the goal is to show that the diagonal elements of $\underline{\underline{\varepsilon}}$ (called the error matrix our covariance matrix) give the uncertainty in the best-fit parameters.

Apply prop. of errors to

$$a_\ell(y_1, y_2, \ldots, y_N)$$

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

$$= \sum_{j=1}^{N} \left(\frac{\partial a_l}{\partial y_j} \sigma_j \right)^2$$

If $m = 3$, then

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

depend on y_i.

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

In general, can express

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

subbing expression for β_k gives:

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

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

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

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

Define:

$$\sigma_{a_l a_{l'}}^2 = \sum_{j=1}^{N} \left[\sigma_j^2 \frac{\partial a_l}{\partial y_j} \frac{\partial a_{l'}}{\partial y_j} \right]$$

With this definity, the uncertainty in a_l is found by setting $l = l'$

$$\sigma_{a_l a_l}^2 \equiv \sigma_{a_l}^2 = \sum_{j=1}^{N} \sigma_j^2 \left(\frac{\partial a_l}{\partial y_j}\right)^2$$

$$\therefore \sigma_{a_l a_{l'}}^2 = \sum_{j=1}^{N} \left[\cancel{\sigma_j^2} \left(\sum_{k=1}^{m} \varepsilon_{kl} \frac{f_k(x_j)}{\cancel{\sigma_j^2}} \right) \left(\sum_{p=1}^{m} \varepsilon_{pl'} \frac{f_p(x_j)}{\sigma_j^2} \right) \right]$$

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

$$\therefore \quad \sigma^2_{a_\ell a_{\ell'}} = \sum_{k=1}^{m} \left\{ \varepsilon_{k\ell} \left(\sum_{p=1}^{m} \varepsilon_{p\ell'}\, \alpha_{kp} \right) \right\} \qquad \circledast$$

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

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

1st element

$$\varepsilon_{11}\alpha_{11} + \varepsilon_{12}\alpha_{12} + \varepsilon_{13}\alpha_{13} = 1 \quad (a)$$

2nd element

$$\varepsilon_{11}\alpha_{12} + \varepsilon_{12}\alpha_{22} + \varepsilon_{13}\alpha_{23} = 0 \quad (b)$$

$$\vdots$$

Compare to $\displaystyle\sum_{p=1}^{m=3} \varepsilon_{pl'}\alpha_{kp} = \varepsilon_{1l'}\alpha_{k1} + \varepsilon_{2l'}\alpha_{k2} + \varepsilon_{3l'}\alpha_{k3}$

try $l' = k = 1$

$$\varepsilon_{11}\alpha_{11} + \varepsilon_{21}\alpha_{12} + \varepsilon_{31}\alpha_{13} = 1 \quad \text{by } (a).$$

try $l' = 1,\ k = 2$

$$\varepsilon_{11}\alpha_{21} + \varepsilon_{21}\alpha_{22} + \varepsilon_{31}\alpha_{23} = 0 \quad \text{by } (b)$$

In general, $\displaystyle\sum_{p=1}^{m} \varepsilon_{pl'}\alpha_{kp} = \delta_{l'k}$

elements of the identity matrix.

Sub this result into ⊛

$$\sigma^2_{a_\ell a_{\ell'}} = \sum_{k=1}^{m} \varepsilon_{k\ell}\, \delta_{\ell' k} = \varepsilon_{\ell\ell'}$$

$$\boxed{\therefore \quad \sigma^2_{a_\ell a_{\ell'}} = \varepsilon_{\ell\ell'}}$$

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

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

$$\underline{\underline{\varepsilon}} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix}$$

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

Σ_{11} is σ_1^2 ... square of uncertainty in a_1

$\sigma_1^2 = \sigma_{a_1}^2 = \sigma_{a_1 a_1}^2$

Σ_{22} is σ_2^2 ... square of uncertainty in a_2

Σ_{33} is σ_3^2 ... square of uncertainty in a_3.

Off-diagonal terms give the covariances

$\sigma_{12} = \Sigma_{12} = \Sigma_{21}$ 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 $i = 1 .. N$

column matrix of best-fit values $\rightarrow$ $\underline{a} = \underline{\underline{\varepsilon}}\, \underline{\beta}$

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

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

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

2. Invert $\underline{\alpha}$ to find the error 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 parameters

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

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

$$\vdots$$

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