PHYS 232 March 15, 2024

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

Last Time When it's not possible to linearize data, need to develop alternative fitting methods.

Eg. Calibration of a thermocouple over a large span of temperatures is non-linear

→ Fitting T vs V to a polynomial.

$$T = a_0 + a_1 V + a_2 V^2$$ ← not linearizable.

Want to fit data to $y(x) = a_0 + a_1 x + a_2 x^2 + \dots a_m x^m$

In fact, the technique that we'll develop can be further generalized.

Want to fit data to a fcn of the form:

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

where $f_k(x)$ are fcns of x that do not involve the unknown parameters $a_1, a_2, \dots, a_m$ that we're trying to find.

For example, for a polynomial:

$$f_1 = 1 \quad f_2 = x, \quad f_3 = x^2$$

Use the same method of maximum likelihood that was developed for linear fits.

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

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

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

$\therefore$ Minimize

$$\chi^2 = \sum_{i=1}^{N} \left[\frac{1}{\sigma_i} \left\{ y_i - \sum_{k=1}^{m} a_k f_k(x_i) \right\} \right]^2$$

w.r.t. $a_1, a_2, a_3, \ldots, a_m$

Involves partial derivatives of χ^2 w.r.t. parameters a_ℓ. $\Rightarrow$ End up w/ system of m eq'ns & m unknowns.

$$\frac{\partial \chi^2}{\partial a_\ell} = \frac{\partial}{\partial a_\ell} \sum_{i=1}^{N} \left[\frac{1}{\sigma_i} \left\{ y_i - \sum_{k=1}^{m} a_k f_k(x_i) \right\} \right]^2$$

$$= 2 \sum_{i=1}^{N} \left(\left[\frac{1}{\sigma_i} \left\{ y_i - \sum_{k=1}^{m} a_k f_k(x_i) \right\} \right] \cdot \underbrace{\frac{\partial}{\partial a_\ell} \left[\frac{1}{\sigma_i} \left\{ y_i - \sum_{k=1}^{m} a_k f_k(x_i) \right\} \right]}_{-\frac{1}{\sigma_i} f_\ell(x_i) \text{ from } \otimes} \right)$$

consider

indep. of a parameters

$$\frac{\partial}{\partial a_l}\left[\frac{1}{\sigma_i}\left\{y_i - \sum_{k=1}^{m} a_k f_k(x_i)\right\}\right]$$

$$= -\frac{1}{\sigma_i}\frac{\partial}{\partial a_l}\sum_{k=1}^{m} a_k f_k(x_i)$$

$$= -\frac{1}{\sigma_i}\sum_{k=1}^{m}\underbrace{\frac{\partial a_k}{\partial a_l}}_{\delta_{kl}} f_k(x_i) = -\frac{1}{\sigma_i}\underbrace{\sum_{k=1}^{m}\delta_{kl} f_k(x_i)}_{f_l(x_i)}$$

$$= \boxed{-\frac{1}{\sigma_i} f_l(x_i)} \quad (*)$$

$$\therefore \frac{\partial \chi^2}{\partial a_l} = -2\sum_{i=1}^{N}\left[\frac{f_l(x_i)}{\sigma_i^2}\left\{y_i - \sum_{k=1}^{m} a_k f_k(x_i)\right\}\right]$$

$$= 0$$

$$\boxed{\therefore \sum_{i=1}^{N} y_i \frac{f_l(x_i)}{\sigma_i^2} = \sum_{i=1}^{N}\frac{f_l(x_i)}{\sigma_i^2}\sum_{k=1}^{m} a_k f_k(x_i)} \quad (\#)$$

This result represents a system of m eq'ns & m unknowns $(a_1, a_2, \dots a_m)$ since $l = 1, 2, 3, \dots m$.

Eg. $y = a_1 + a_2 x + a_3 x^2$

$$f_1 = 1 \quad f_2 = x \quad f_3 = x^2$$

$l=1$, $f_1 = 1$: $$\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} = \sum_{i=1}^{N} \frac{1}{\sigma_i^2}\left[a_1 + a_2 x_i + a_3 x_i^2\right]$$

$l=2$, $f_2 = x$: $$\sum_{i=1}^{N} \frac{y_i x_i}{\sigma_i^2} = \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2}\left[a_1 + a_2 x_i + a_3 x_i^2\right]$$

$l=3$, $f_3 = x^2$: $$\sum_{i=1}^{N} \frac{y_i x_i^2}{\sigma_i^2} = \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}\left[a_1 + a_2 x_i + a_3 x_i^2\right]$$

system of 3 eq'ns.

Can represent (#) as a Matrix eq'n.

$$\underline{\beta} = \underline{\underline{\alpha}}\ \underline{a}$$

column matrix $m \times 1$

column matrix $m \times 1$

square matrix $m \times m$

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

$$a_k = a_k$$

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

Note that $\underline{\underline{\alpha}}$ is symmetric

$$\alpha_{\ell k} = \alpha_{k \ell}$$

Eg. $y = a_1 + a_2 x + a_3 x^2 \qquad f_1 = 1,\ f_2 = x,\ f_3 = x^2$

$$\underbrace{\begin{pmatrix} \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} \\ \sum_{i=1}^{N} \frac{y_i x_i}{\sigma_i^2} \\ \sum_{i=1}^{N} \frac{y_i x_i^2}{\sigma_i^2} \end{pmatrix}}_{\beta} = \underbrace{\begin{pmatrix} \sum_{i=1}^{N} \frac{1}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} \\ \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i^3}{\sigma_i^2} \\ \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i^3}{\sigma_i^2} & \sum_{i=1}^{N} \frac{x_i^4}{\sigma_i^2} \end{pmatrix}}_{\underline{\underline{\alpha}}} \underbrace{\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}}_{\underline{a}}$$

Check the first Eq'n.

$$\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} = a_1 \sum_{i=1}^{N} \frac{1}{\sigma_i^2} + a_2 \sum_{i=1}^{N} \frac{x_i}{\sigma_i^2} + a_3 \sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}$$

$$= \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \left(a_1 + a_2 x_i + a_3 x_i^2 \right)$$

this is the $l=1$ eq'n that we previously wrote down.

Back to $\quad \underline{\beta} = \underline{\underline{\alpha}}\ \underline{a}$

want to solve for the unknown parameters a_k

$$\therefore \quad \underline{\underline{\alpha}}^{-1}\underline{\beta} = \underbrace{\underline{\underline{\alpha}}^{-1}\underline{\underline{\alpha}}}_{\underline{\underline{I}}}\ \underline{a} = \underline{\underline{I}}\ \underline{a} = \underline{a}$$

$\underline{\underline{I}}$ ← identity matrix.

$$\boxed{\therefore \quad \underline{a} = \underline{\underline{\alpha}}^{-1}\underline{\beta}}$$

know everything to calc. $\underline{\underline{\alpha}}$ & $\underline{\beta}$

$\therefore$ we can find $\underline{a}$.

In general, it is not easy to manually invert a large $m \times m$ matrix, but it can be done easily in software.

Usually $\underline{\underline{\alpha}}^{-1} \equiv \underline{\underline{\varepsilon}}$ which is called the error matrix or the covariance matrix.

We will show that the diagonal elements of $\underline{\underline{\varepsilon}}$ give the square of the uncertainties in the best-fit parameters a_k.

$$\varepsilon_{kk} = \sigma_k^2$$