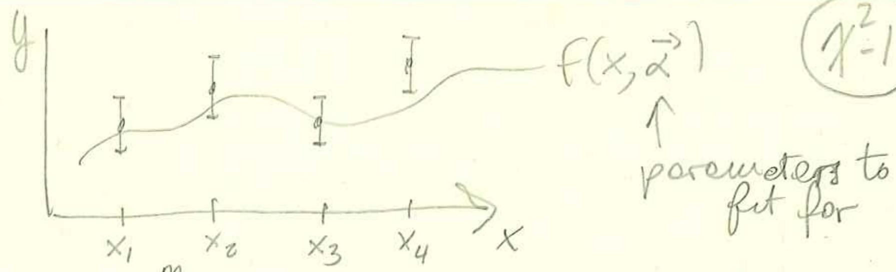
$\boxed{\chi^2 \text{ FiT}}$

χ^2-1

eg



N measurements $\vec{y}^m$ $\begin{pmatrix} y_1^m \\ \vdots \\ y_N^m \end{pmatrix}$ M parameters $\vec{\alpha}$ $\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_M \end{pmatrix}$

Fitted values $\vec{y}(\vec{\alpha})$

$$\chi^2 = \underbrace{\left[\vec{y}^m - \vec{y}(\vec{\alpha})\right]^T}_{1\times N} \underbrace{W^{-1}}_{N\times N} \underbrace{\left[\vec{y}^m - \vec{y}(\vec{\alpha})\right]}_{N\times 1}$$

In case of no correlations $W^{-1} = \begin{pmatrix} 1/\sigma_1^2 & & 0 \\ & 1/\sigma_2^2 & \\ 0 & & 1/\sigma_n^2 \end{pmatrix}$

Guess solution $\vec{\alpha}_0 \Rightarrow \delta\vec{\alpha} = \vec{\alpha} - \vec{\alpha}_0$

Expand in Taylor series $\quad y_i(\vec{\alpha}) = y_i(\vec{\alpha}_0) + \sum_{j=1}^{M} \frac{\partial y_i}{\partial \alpha_j} \delta\alpha_j$

Note: this is exact for linear problem, eg

$$y(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 \frac{x}{x-1} \quad \text{etc}$$

Write Taylor expansion compactly as

$$\vec{y} = \vec{y}_0 + A\delta\vec{\alpha} \qquad A_{ij} = \frac{\partial y_i}{\partial \alpha_j} \text{ is } N \times M \text{ matrix}$$

$$\vec{y}_0 = \vec{y}(\alpha_0)$$

$$\vec{y}_m - \vec{y}(\vec{\alpha}) = \vec{y}_m - \vec{y}_0 - A\delta\vec{\alpha} = \delta\vec{y} - A\delta\vec{\alpha}$$

$$\chi^2 = \left[\delta\vec{y} - A\delta\vec{\alpha}\right]^T W^{-1} \left[\delta\vec{y} - A\delta\vec{\alpha}\right]$$

$$\chi^2 = \delta y^T W^{-1} \delta y - \delta y^T W^{-1} A \delta\vec{\alpha} - \delta\vec{\alpha}^T A^T W^{-1} \delta\vec{y} + \delta\alpha^T A^T W^{-1} A \delta\vec{\alpha}$$

note: since W^{-1} is $N \times N$ symmetric, $(W^{-1})^T = W^{-1}$
Also, all terms are obviously (1×1), so the 2nd and 3rd term are the same

$$\chi^2 = \delta y^T W^{-1} \delta y - 2\, \delta y^T W^{-1} A\, \delta\vec{\alpha} + \delta\alpha^T A^T W^{-1} A\, \delta\vec{\alpha}$$

$\dfrac{\partial \chi^2}{\partial \alpha_j} = 0$ results in $\quad -\delta\vec{y}^T W^{-1} A + \delta\vec{\alpha}^T A^T W^{-1} A = 0 \quad (1)$

(the factor of two cancels because there are effectively two $\delta\vec{\alpha}$ terms in the last term)

$$A^T W^{-1} A\, \delta\vec{\alpha} = A^T W^{-1} \delta\vec{y}$$

$$\boxed{\delta\vec{\alpha} = (A^T W^{-1} A)^{-1} A^T W^{-1}\, \delta\vec{y}} \quad \boxed{\delta\vec{\alpha} = C\, \delta\vec{y}}$$

If the problem is not perfectly linear, change initial guess $\vec{\alpha}^0 \to \vec{\alpha}^0 + \delta\vec{\alpha}$ and <u>iterate</u>

with $C = (A^T W^{-1} A)^{-1} A^T W^{-1}$

What about the covariance matrix? χ^2-3

<u>Answer</u>: $V = \left(A^T W^{-1} A\right)^{-1}$

Remember we said last time that for MLE in the case of one parameter a

$$\sigma(\hat{a}) = -\frac{1}{\left\langle \frac{\partial^2 \log \mathcal{L}}{\partial a^2} \right\rangle} \quad (2)$$

and that $-\log \mathcal{L} = \frac{1}{2}\chi^2$

Going back to an expression that we (almost) wrote down for $\frac{\partial \chi^2}{\partial \alpha_j}$

eqtn (1) on page χ^2-2

$$\frac{\partial \chi^2}{\partial \alpha_j} = -2\left(\vec{\delta y}^T W^{-1} A\right)_{1j} + 2\left(\vec{\delta \alpha}^T A^T W^{-1} A\right)_{1j}$$

independent of α's

$(1\times M)(M\times N)(N\times N)(N\times M)$

$$= \delta\alpha_i \left(A_T W^{-1} A\right)_{ij}$$

$$\frac{\partial^2 \chi}{\partial \alpha_i \partial \alpha_j} = 2 A_T W^{-1} A = -2 \frac{\partial^2 \log \mathcal{L}}{\partial \alpha_i \partial \alpha_j}$$

which generalizing equation (2) gives $\boxed{V = \left(A^T W^{-1} A\right)^{-1}}$

Can get the same answer by propagation of errors

$$\delta\vec{\alpha} = C\,\delta\vec{y} \qquad C = \left(A^T W^{-1} A\right)^{-1} A^T W^{-1}$$

$$\delta\alpha_i = C_{ir}\,\delta y_r$$

$$\frac{\partial\left(\delta\alpha_i\right)}{\partial\left(\delta y_r\right)} = C_{ir}$$

$$V^2_{ij} = \sum_{r,s} C_{ir} W_{rs} C_{sj} \qquad V = C W C^T$$

Let $G = \left(A^T W^{-1} A\right)^{-1}$ $\quad C = G A^T W^{-1}$

$V = C W C^T$ becomes

$$V = G A^T \underbrace{W^{-1} W}_{=1} \underbrace{\left(W^{-1}\right)^T}_{=W^{-1}} A G^T$$

$$V = G \underbrace{A^T W^{-1} A}_{G^{-1}} G^T = G^T = G$$

↑ since V is symmetric, G also symmetric

χ^2-5

Receipe

- Guess $\vec{\alpha}^0$ ← column vector $M \times 1$
- $\delta\vec{y} = \vec{y}^m - y(\vec{\alpha}_0)$ ← column vector $N \times 1$
- $W^{-1} = (\quad)$ (cov matrix)$^{-1}$ of measurements $N \times N$
- $A_{ij} = \left.\frac{\partial y_i}{\partial \alpha_j}\right|_{\vec{y} = y(\vec{\alpha}_0)}$ ← $N \times M$ matrix (numerically if necessary)
- $C = (A^T W^{-1} A)^{-1} A^T W^{-1}$
- $\vec{\alpha} = \vec{\alpha}_0 + C\,\delta\vec{y}$
- Iterate
- Covariance Matrix for $\vec{\alpha}$ $\quad V = (A^T W^{-1} A)^{-1}$