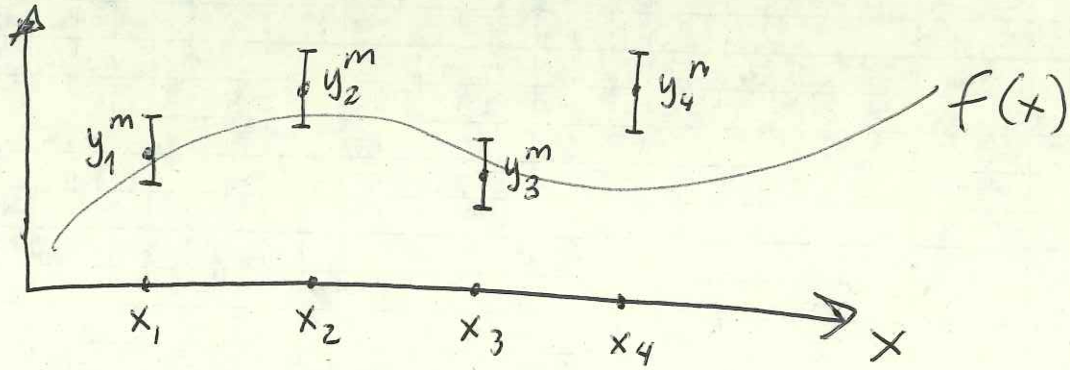
χ^2 Fit (Least Square)

χ^2-1



~~N points~~ N measurements y_i^m with uncertainty σ_i at different values of x_i

We think that some function $f(x)$ may be a good fit. This function has some parameters $\vec{\alpha}$ — M parameters

eg quadratic would be $y = \alpha_1 + \alpha_2 x + \alpha_3 x^2$

For a given ~~set~~ $\vec{\alpha}$ we can predict $y_i(\vec{\alpha})$

In the ~~quartic~~ quadratic case it would be

$y_i = \alpha_1 + \alpha_2 x_i + \alpha_3 x_i^2$

Define $$\chi^2 = \sum_{i=1}^{N} \frac{\left(y_i^m - y_i(\vec{\alpha})\right)^2}{\sigma_i^2}$$

Want to find $\vec{\alpha}$ such that χ^2 is minimized

Start with a guess $\vec{\alpha} = \vec{\alpha}^0$ — Want to find $\delta\vec{\alpha} = \vec{\alpha} - \vec{\alpha}_0$

$\vec{y}^0 = \vec{y}(\vec{\alpha}^0)$ in other words $y_i^0 = y_i(\alpha_1 \dots \alpha_m)$

Expand in Taylor series

$$y_i = y_i^0 + \sum_j \frac{\partial y_i}{\partial \alpha_j} \delta\alpha_j = y_i^0 + \sum_{j=1}^{M} A_{ij}\, \delta\alpha_j$$

Note: if the model is linear in the α_j this is exact. For example

$$y_i = \alpha_1 + \alpha_2 x_i + \alpha_3 x_i^2$$

$$\frac{\partial y_i}{\partial \alpha_1} = 1 \quad \frac{\partial y_i}{\partial \alpha_2} = x_i$$

$$\frac{\partial y_2}{\partial \alpha_3} = x_i^2$$

Then $$\chi^2 = \sum_{i=1}^{N} \frac{\left(y_i^m - y_i^0 - \sum_{j=1}^{M} A_{ij}\, \delta\alpha_j\right)^2}{\sigma_i^2}$$

Want to find $\delta\vec{\alpha}$ such that χ^2 is minimized

Set $\frac{\partial \chi^2}{\partial \alpha_k} = 0$ for all k's (between 1 and M)

χ^2-3

Some simple algebra gives $(\delta y_i = y_i^m - y_i^o)$

$$\sum_{i=1}^{N}\sum_{j=1}^{M} \frac{A_{ij} A_{ik}\,\delta\alpha_j}{\sigma_i^2} = \sum_{i=1}^{N} \frac{A_{ik}\,\delta y_i}{\sigma_i^2}$$

Looks awful. But can write it in matrix notation

$$W^{-1} = \begin{pmatrix} 1/\sigma_1^2 & & & 0 \\ & 1/\sigma_2^2 & & \\ & & \ddots & \\ 0 & & & 1/\sigma_n^2 \end{pmatrix} \quad N\times N \text{ matrix}$$

$\delta\vec{y}$ = N-column vector

$\delta\vec{\alpha}$ = M-column vector

$$\underbrace{(\underset{M\times N}{A^T}\,\underset{N\times N}{W^{-1}}\,\underset{N\times M}{A})\,\underset{M\times 1}{\delta\vec{\alpha}}}_{M\text{-column vector}} = \underbrace{\underset{M\times N}{A^T}\,\underset{N\times N}{W^{-1}}\,\underset{N\times 1}{\delta\vec{y}}}_{M\text{-column vector}}$$

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

We can then ~~write~~ change our initial guess $\vec{\alpha}^0 \to \vec{\alpha}^0 + \delta\vec{\alpha}$ and iterate

$$\delta\vec{\alpha} = C\,\delta\vec{y}$$

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

If the model is not linear: <u>iterate</u>

Get a new set of α and $\vec{y}^0$

New $\vec{\alpha}^0 = \vec{\alpha}^0 + \delta\vec{\alpha}$, $\vec{y}^0 = \vec{y}(\vec{\alpha}^0)$

What is the uncertainty in $\vec{\alpha}$?

<u>Answer</u> covariance matrix for $\vec{\alpha}$ is $\boxed{V = (A^T W^{-1} A)^{-1}}$

<u>Proof</u> $\delta\vec{\alpha} = C\,\delta\vec{y}$ means $\delta\alpha_i = \sum_r C_{ir}\,\delta y_i$

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

If $\delta\vec{y}$ were uncorrelated, propagation of errors would give (remember, we took them as uncorrelated!!)

$$\sigma^2(\delta\alpha_i) = \sum_r (C_{ir})^2 \sigma^2(\delta y_r) = \sum_r C_{ir}^2 W_{rr}$$

W diagonal

This generalizes to

$$V_{ij} = \sigma^2(\delta\alpha_i\,\delta\alpha_j) = \sum_{r,s} C_{ir} C_{js} W_{rs}$$

W is covariance of y's

$$\boxed{V = C W C^T}$$

(This works also if W is <u>not diagonal</u>)

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

$V = C W C^T$ becomes

$$V = (G A^T \underbrace{W^{-1}) W}_{=1} [\underbrace{(W^{-1})^T}_{= W^{-1} \text{ since } W \text{ is diagonal}} A \, G^T]$$

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

$V = G^T$ $\quad \boxed{V = G} \leftarrow$ since V is symmetric G must also be symmetric

χ^2-6

Recipe

- Guess $\vec{\alpha}^0$ ← column vector $M \times 1$
- $\delta\vec{y} = \vec{y}^m - \vec{y}^0(\alpha_0)$ ← column vector $N \times 1$
- $W^{-1} = \begin{pmatrix} 1/\sigma_1^2 & & \\ & \ddots & \\ & & 1/\sigma_n^2 \end{pmatrix}$ ← $N \times N$ matrix
- $A_{ij} = \left.\dfrac{\partial y_i}{\partial \alpha_j}\right|_{\vec{y} = \vec{y}^0(\vec{\alpha}^0)}$ ← $N \times M$ matrix (calculate derivatives numerically if necessary)
- $C = \left(A^T W^{-1} A\right)^{-1} A^T W^{-1}$
- $\vec{\alpha} = \vec{\alpha}_0 + C\delta\vec{y}$
- Iterate if you like
- Covariance Matrix for $\vec{\alpha}$:

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