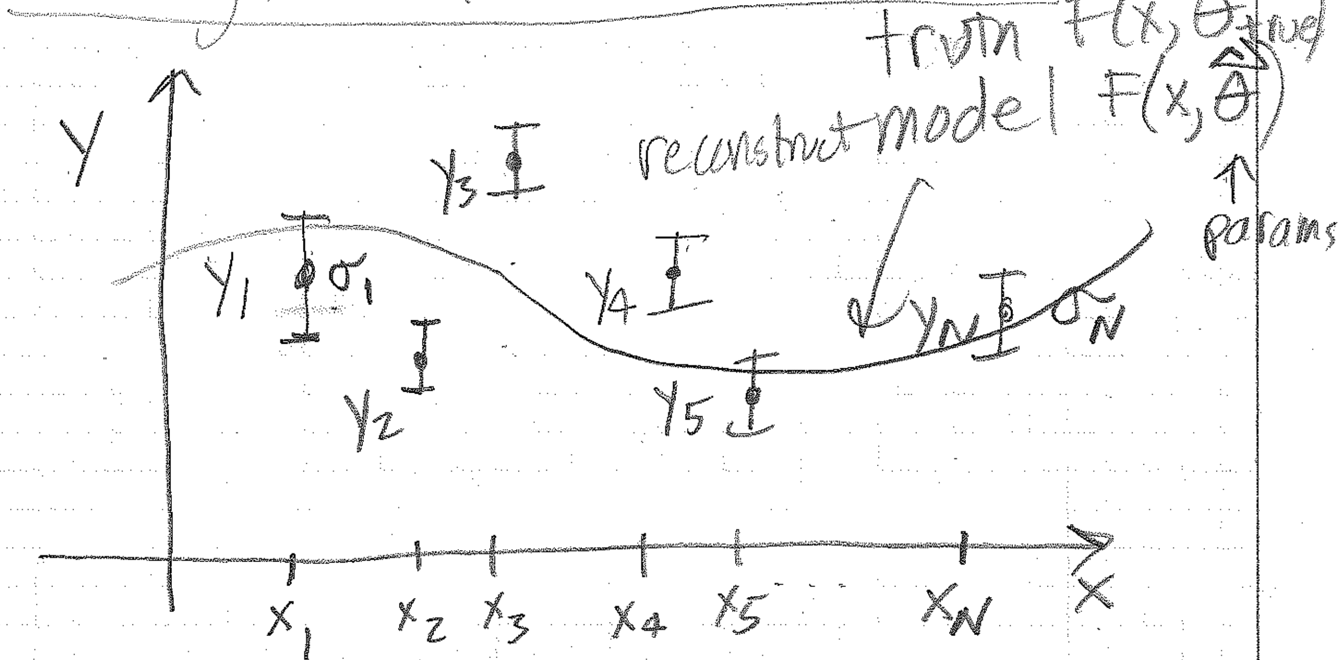
Fitting / Independant Variables



Imagine a model with "m" parameters

$N \geq m$ (obviously, otherwise under ~~under~~ constrained)

$(\theta_1, \theta_2, \ldots, \theta_m)$ — vector of m parameters

$N = m$ can work if invertible!

really $L(\vec{\theta}|\{y_i\})$ Bayes

if you knew

$$L(\vec{\theta}) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_i}} e^{-\frac{(y_i - F(x_i, \vec{\theta}))^2}{2\sigma_i^2}}$$

$$\left\langle \frac{(y_i - F(x_i, \vec{\theta}_{true}))^2}{\sigma_i^2} \right\rangle = 1$$

Gaussian? Central Limit Thereom.

$$-\ln L(\vec{\theta}) = \text{constant} + \frac{1}{2}\sum_{i=1}^{N} \frac{(y_i - F(x_i,\vec{\theta}))^2}{\sigma_i^2}$$

$$\underbrace{-2\ln L(\vec{\theta})}_{\text{"log likelihood" more general}} = \text{constant} + \underbrace{\sum_{i=1}^{N} \frac{(y_i - F(x_i,\vec{\theta}))^2}{\sigma_i^2}}_{\text{called } \chi^2(\vec{\theta})}$$

$$\langle \chi^2(\vec{\theta}_{true}) \rangle = N$$

Step #1 ... find $\vec{\theta}$ that minimizes (maximizes $L(\theta)$)

$\hat{\vec{\theta}} \Rightarrow$ m of them.

Concept: N little gaussians (measurements)

$$\langle \chi^2(\theta_{true}) \rangle = \langle \chi^2(\hat{\theta}) \rangle + m$$

$$N = \langle \chi^2(\hat{\theta}) \rangle + m$$

think of 1 point (measurement) 2

m gaussians $\longrightarrow$ "Residuals are like $N-m$ gaussians distributed like

$$e^{-\frac{z_1^2}{2}}\, e^{-\frac{z_2^2}{2}} \cdots e^{-\frac{z_{(N-m)}^2}{2}}$$

$$(\chi^{N-m-1})\, e^{-\frac{\chi^2}{2}}$$

$$\langle (\hat{\vec{\theta}} - \vec{\theta}_{true}) \rangle = m$$

$$(\hat{\vec{\theta}} - \vec{\theta}_{true})^2 \sim \begin{pmatrix} \sigma_1^2 & & \\ \sigma_1\sigma_2\rho_{12} & \sigma_2^2 & \\ & & \ddots \\ & & & \sigma_m^2 \end{pmatrix}$$

not necessarily

$n = N - m \equiv \text{DOF}$

meaning?

or $\underbrace{\dfrac{1}{2^{(n/2)}\Gamma\left(\frac{n}{2}\right)} \xi^{\frac{n}{2}-1} e^{-\xi/2}}$

peaks at $\chi^2 \sim n$

Large χ^2 means "bad ~~fit~~"

how big for how bad?

1992 RPP

$\dfrac{\chi^2}{N-m}$

obvious first choice, one variable

$$F(x_i, \theta_1) = \theta_1 \times 1$$

1 variable

(Quadratic Form)

$$\chi^2(\theta_1) = \sum_{i=1}^{N} \frac{(y_i - \theta_1)^2}{\sigma_i^2}$$

$$= \sum_{i=1}^{N} \frac{y_i^2}{\sigma_i^2} - 2\theta_1 \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} + \theta_1^2 \sum_{i=1}^{N} \frac{1}{\sigma_i^2}$$

$$\frac{\partial \chi^2}{\partial \theta_1} = -2 \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2} + 2\theta_1 \sum_{i=1}^{N} \frac{1}{\sigma_i^2} = 0$$

$$\hat{\theta}_1 = \frac{\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}}$$ (weighted mean)

$$\frac{\partial^2 \chi^2}{\partial \theta_1^2} = 2 \sum_{i=1}^{N} \frac{1}{\sigma_i^2}$$

$$\chi^2(\theta_1) \cong \underbrace{\chi^2(\hat{\theta}_1)}_{\text{goodness of fit}} + \overbrace{\frac{1}{2} \frac{\partial^2 \chi^2}{\partial \theta_1^2} (\theta_1 - \hat{\theta}_1)^2}^{\text{error on } \theta_1}$$

$$\sum_{i=1}^{N} \frac{y_i^2}{\sigma_i^2} - 2 \frac{\left(\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}\right)^2}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}} + \frac{\left(\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}\right)^2 \sum_{i=1}^{N} \frac{1}{\sigma_i^2}}{\left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2}\right)^2}$$

$$= \sum_{i=1}^{N} \frac{y_i^2}{\sigma_i^2} - \frac{\left(\sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}\right)^2}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}}$$

$$+ (\theta_1 - \hat{\theta}_1)^2 \sum_{i=1}^{N} \frac{1}{\sigma_i^2}$$

$$e^{-\frac{1}{2}(\theta_1 - \hat{\theta}_1)^2 \sum \frac{1}{\sigma_i^2}}$$

$$\sigma_{\theta_1}^2 = \frac{1}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}}$$

$$y_i = \theta_t + \delta y_i \qquad \langle \delta y_i \rangle = 0$$

$$\langle \delta y_i \, \delta y_j \rangle = \sigma_i^2 \delta_{ij}$$

$$\sum_{i=1}^{N}\frac{(\theta_t+\delta y_i)^2}{\sigma_i^2}-\frac{\left(\sum_{i=1}^{N}\left(\frac{\theta_t+\delta y_i}{\sigma_i^2}\right)\right)^2}{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}$$

$$\theta_t^2\sum_{i=1}^{N}\frac{1}{\sigma_i^2}+2\theta_t\sum_{i=1}^{N}\frac{\delta y_i}{\sigma_i^2}+\sum_{i=1}^{N}\frac{\delta y_i^2}{\sigma_i^2}\rightarrow\sum_{i=1}^{N}\frac{\langle\delta y_i^2\rangle}{\sigma_i^2}=N$$

$$-\frac{\theta_t^2\left(\sum_{i=1}^{N}\frac{1}{\sigma_i^2}\right)^2}{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}-\frac{2\theta_t\left(\sum_{i=1}^{N}\frac{1}{\sigma_i^2}\right)\left(\sum_{i=1}^{N}\frac{\delta y_i}{\sigma_i^2}\right)}{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}\qquad\langle\delta y_i\rangle=0$$

these cancel

$$-\frac{\left(\sum_{i=1}^{N}\frac{\delta y_i}{\sigma_i^2}\right)^2}{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}$$

On diagonal terms only non-zero.

$$\frac{\sum_{i=1}^{N}\frac{\langle\delta y_i^2\rangle}{\sigma_i^4}}{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}=\frac{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}{\sum_{i=1}^{N}\frac{1}{\sigma_i^2}}=1$$

$$\boxed{\langle\chi^2(\hat{\theta}_1)\rangle=N-1}$$

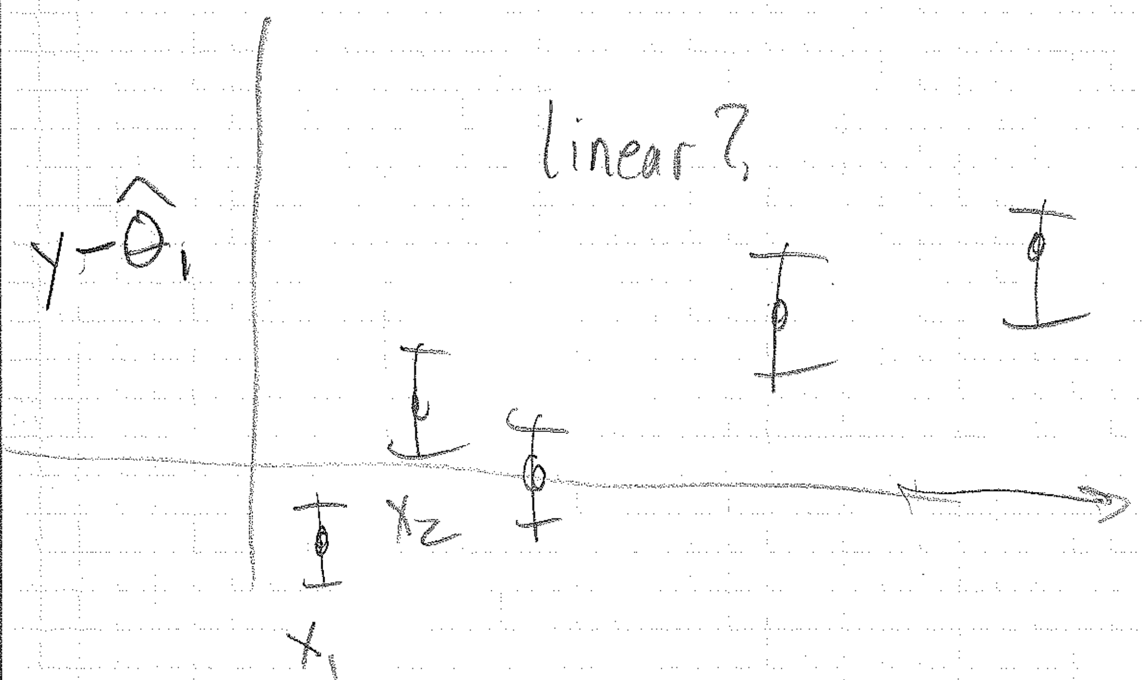
if $\chi^2(\hat{\theta}_1) >> N-1$

or $\dfrac{\chi^2(\hat{\theta}_1)}{N-1} >> 1$

or $CL(\chi^2(\hat{\theta}_1), N-1) < 1\%$ or 0.1%

→ add a second variable

→ good idea to look at residuals



!!!

Most Likely $F(x_i, \theta_1, \theta_2) = \theta_1 \cdot 1 + \theta_2(x_i - x_0)$

correct picking will

$$\chi^2(\theta_1, \theta_2) = \sum_{i=1}^{N} \frac{\left(y_i - \underbrace{\theta_1 - \theta_2(x - x_0)}_{\text{"}f_0\text{"}}\right)^2}{\sigma_i^2}$$

$$\frac{\partial \chi^2}{\partial \theta_1} = \cancel{2} \sum_{i=1}^{N} \frac{(y_i - \theta_1 - \theta_2(x_i - x_0))\,(-1)}{\sigma_i^2} = 0$$

$$\text{or} \quad \theta_1 \sum_{i=1}^{N} \frac{1}{\sigma_i^2} + \theta_2 \underbrace{\sum_{i=1}^{N} \frac{(x_i - x_0)}{\sigma_i^2}} = \sum_{i=1}^{N} \frac{y_i}{\sigma_i^2}$$

θ_1 + θ_2 "uncouple" if $\displaystyle\sum_{i=1}^{N} \frac{(x_i - x_0)}{\sigma_i^2} = 0$

or $\displaystyle x_0 = \frac{\sum_{i=1}^{N} \frac{x_i}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}}$

actually, important!

$\hat{\theta}_1 \rightarrow$ same as before!

$$\frac{\partial \chi^2}{\partial \theta_2} = 2 \sum_{i=1}^{N} \frac{(y_i - \theta_1 - \theta_2(x_i - x_0))\overbrace{(x_i - x_0)}^{\text{"}f_1\text{"}}}{\sigma_i^2} = 0$$

$$\theta_1 \cancel{\sum_{i=1}^{N} \frac{(x_i - x_0)}{\sigma_i^2}} + \theta_2 \sum_{i=1}^{N} \frac{(x_i - x_0)^2}{\sigma_i^2} = \sum_{i=1}^{N} \frac{(x_i - x_0)\,y_i}{\sigma_i^2}$$

0 if x_0 chosen above

$$\boxed{\hat{\theta}_2 = \frac{\sum_{i=1}^{N} \frac{(x_i - x_0)\,y_i}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{(x_i - x_0)^2}{\sigma_i^2}}}$$

$$\frac{\partial^2 \chi^2}{\partial\theta_1 \partial\theta_1} = 2\sum_{i=1}^{N} \frac{1}{\sigma_i^2}$$

$$\left.\frac{\partial^2 \chi^2}{\partial\theta_2 \partial\theta_1}\right| = 0 \text{ if } x_0 = \frac{\sum_{i=1}^{N} \frac{x_i^2}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{1}{\sigma_i^2}} \; !$$

$$= \frac{\partial^2 \chi}{\partial\theta_1 \partial\theta_2}$$

$$\frac{\partial^2 \chi^2}{\partial\theta_2^2} = 2 \sum_{i=1}^{N} \frac{(x_i - x_0)^2}{\sigma_i^2}$$

so,

on average, $N-2$

$$\chi^2(\theta_1, \theta_2) = \chi^2(\hat{\theta}_1, \hat{\theta}_2)$$

$$+ \left(\sum_{i=1}^{N} \frac{1}{\sigma_i^2}\right)(\theta_1 - \hat{\theta}_1)^2 + \left(\sum_{i=1}^{N} \frac{(x_i - x_0)^2}{\sigma_i^2}\right)(\theta_2 - \hat{\theta}_2)^2$$

$$\sigma_{\theta_1}^2 = 1 \Big/ \sum_{i=1}^{N} \frac{1}{\sigma_i^2} \qquad \sigma_{\theta_2}^2 = 1 \Big/ \sum_{i=1}^{N} \frac{(x_i - x_0)^2}{\sigma_i^2}$$

VARIANCE OF X!!!

maybe χ^2 still too bad

(F-test actually can be used here!).

$$F(x_i;\theta_1,\theta_2,\theta_3)$$
$$= \theta_1 \cdot 1 + \theta_2(x_i - x_0) + \theta_3(x_i^2 - ax_i - b)$$

equations decouple when ..

$$\underbrace{\sum_{i=1}^{N} \frac{(x_i^2 - ax_i - b)\cdot 1}{\sigma_i^2} = 0 \qquad \sum_{i=1}^{N} \frac{(x_i^2 - ax_i - b)\cdot(x_i - x_0)}{\sigma_i^2} = 0}$$

solve for $a + b$, then ---

$\hat{\theta}_1$ same

$\hat{\theta}_2$ same

$$\hat{\theta}_3 = \frac{\sum_{i=1}^{N} \frac{(x_i^2 - ax_i - b)y_i}{\sigma_i^2}}{\sum_{i=1}^{N} \frac{(x_i^2 - ax_i - b)^2}{\sigma_i^2}}$$

$$\sigma_{\theta_3}^2 = \frac{1}{\sum_{i=1}^{N} \frac{(x_i^2 - ax_i - b)^2}{\sigma_i^2}}$$

the error envelope ...

$$F(x_i, \theta_1, \theta_2, \theta_3, \ldots)$$

$$= \theta_1 + \theta_2(x_i - x_0) + \theta_3(x_i^2 - ax_i - b)$$

$$\delta F = \delta\theta_1 + \delta\theta_2(x_i - x_0) + \delta\theta_3(x_i^2 - ax_i - b)$$

$$\langle \delta F^2 \rangle \Rightarrow \langle \delta\theta_1 \delta\theta_2 \rangle = 0 \quad \text{(by choice!)}$$

etc!

$$= \langle \delta\theta_1^2 \rangle + \langle \delta\theta_2^2 \rangle (x_i - x_0)^2 + \langle \delta\theta_3^2 \rangle (x_i^2 - ax_i - b)^2$$

$$= \frac{1}{\sum \frac{1}{\sigma_i^2}} + \frac{(x - x_0)^2}{\sum \frac{(x_i - x_0)^2}{\sigma_i^2}} + \frac{(x^2 - ax - b)^2}{\sum \frac{(x_i - ax_i - b)^2}{\sigma_i^2}}$$

dominates near $x = x_0$