Linear Least Squares Fitting

square of sum of residuals $R^2 = \sum_i (y_i - y_{fit})^2$

in linear case $R^2 = \sum_i (y_i - \underbrace{(\alpha x_i + \beta)}_{\text{yields } y_{fit}})^2$

Maximum Likelihood Estimation

$$\mathcal{L}(x_1, x_2 \dots x_N) = \prod^N f(x_i | param) \quad \text{likelihood function}$$

to obtain best param we maximize likelihood

$$\frac{\partial \mathcal{L}}{\partial param} = 0 \quad \text{or} \quad \frac{\partial \ln \mathcal{L}}{\partial param} = 0$$

In case of linear fit:

$$\mathcal{L} = \prod e^{-\chi_i^2/2\sigma^2} \quad \text{where} \quad \chi_i^2 = (y_i - (\alpha x_i + \beta))^2$$

$$\ln \mathcal{L} = \sum_i -\chi_i^2 \frac{1}{2\sigma^2} = \frac{-1}{2\sigma^2} \sum (y_i - (\alpha x_i + \beta))^2$$

$$\frac{\partial \ln \mathcal{L}}{\partial \alpha} = 0 \qquad \frac{\partial \ln \mathcal{L}}{\partial \beta} = 0$$

$$-\frac{1}{2}(2) \sum_i (y_i - (\alpha x_i + \beta))(-x_i) = 0 \qquad -\frac{1}{2}(2) \sum_i (y_i - (\alpha x_i + \beta))(-1) = 0$$

$$\sum_i (y_i - (\alpha x_i + \beta)) x_i = 0 \qquad \sum_i (y_i - (\alpha x_i + \beta)) = 0$$

Eq 1
$$\sum_i (y_i x_i) - \alpha \sum_i x_i^2 - \beta \sum_i x_i = 0$$

Eq 2
$$\sum_i y_i - \alpha \sum_i x_i - N\beta = 0$$

multiply eq 1 by N & eq 2 by $\sum x_i$

$$N \sum y_i x_i - N\alpha \sum x_i^2 - N\beta \sum x_i = 0 \qquad \sum x_i \sum y_i - \alpha \sum x_i \sum x_i - N\beta \sum x_i = 0$$

$$N \sum (x_i y_i) - N\alpha \sum (x_i)^2 = \sum x_i \sum y_i - \alpha (\sum x_i)^2$$

$$\alpha (\sum x_i)^2 - N\alpha \sum (x_i^2) = \sum x_i \sum y_i - N \sum x_i y_i$$

$$\alpha = \frac{\sum x_i \sum y_i - N \sum (x_i y_i)}{(\sum x_i)^2 - N \sum (x_i)^2}$$

divide top & bottom by N^2

$$\alpha = \frac{\frac{1}{N^2}(\sum x_i \sum y_i) - \frac{1}{N}\sum(x_i y_i)}{\frac{1}{N^2}(\sum x_i \sum x_i) - \frac{1}{N}\sum(x_i^2)} = \frac{\bar{x}\,\bar{y} - \overline{xy}}{\bar{x}\,\bar{x} - \overline{(x^2)}}$$

from eq 2

$$N\beta = \sum y_i - \alpha \sum x_i \quad \beta = \frac{1}{N}\sum y_i - \frac{\alpha}{N}\sum x_i$$

$$\beta = \bar{y} - \alpha\bar{x}$$

Uncertainty on parameters

can analytically solve for linear least squares case:

$$\sigma_\alpha = \sqrt{\frac{\frac{1}{(n-2)}(R^2)}{\sum_i (x_i - \bar{x})^2}} \qquad \sigma_\beta = \sqrt{\frac{1}{n-2} R^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum(x_i - \bar{x})^2}\right)}$$

more generally MLE parameter uncertainties can be measured through determining the covariance matrix, which is the inverse of the Hessian matrix

$$H = \begin{pmatrix} \frac{\partial^2 \ln(\mathcal{L})}{\partial \alpha^2} & \frac{\partial^2 \ln(\mathcal{L})}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \ln(\mathcal{L})}{\partial \beta \partial \alpha} & \frac{\partial^2 \ln(\mathcal{L})}{\partial \beta^2} \end{pmatrix} \qquad C = H^{-1}$$

Bayesian

"likelihood" $\sim \mathcal{L}(D|M)$

$$P(M|D) = \frac{P(D|M)P(M)}{P(D)}$$

"prior" what we know about model

"posterior" prob of model given data

"data probability" essentially normalization