10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #23: Models vs. Data 2: Bayesian view.

Models vs. Data

Theorem 83: As $N_{expt} \rightarrow \infty$, the distribution of data, $<Y_{data}>_{Nexpts} \rightarrow$ Normal ➔ Gaussian

1) Assume Central Limit Theorem (Theorem 83)

2) We assume we have the true model (always wrong)

a) We assume we have the true model parameters, or at least the best possible fit $\underline{\theta}$

3) We assume we know the uncertainties in data σ_{mean}, $\sigma(<\underline{Y}_{data}>)$

$$P(\underline{Y}_{data}) = \text{const} \prod_{i=1}^{N_{\exp}} \exp\left(-\left(\frac{<Y_{i\,data}> - Y_{i\,model}}{\sigma_i}\right)^2\right)$$

Since we have the probability density, need to integrate over some $\Delta\underline{Y}$ = const $\exp(-\chi^2)$.

χ^2 collapses $P(\underline{Y})$ to 1D

$$\chi^2 = \sum_{i=1}^{N_{\exp}} \left(\frac{Y_{i\,data} - Y_{i\,model}}{\sigma_i}\right)^2 \qquad \sigma_i = S.D. \Big/ \sqrt{N_{expts}}$$

S.D. is the standard deviation of N_{expts} at condition i.

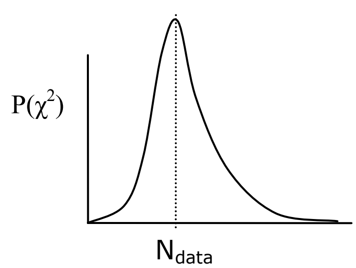

Figure 1. Chi-squared distribution.

Linear (in parameters) Models

$\underline{Y}_{model} = \underline{\underline{M}}(\underline{x}) \cdot \underline{\theta}$

to find best fit $\underline{\theta}$ $\qquad \min_{\underline{\theta}} \chi^2(\underline{\theta})$

$\min \|\underline{Y}_{data} - \underline{\underline{M}} \cdot \underline{\theta}\|^2$ $\qquad$ such that $\underline{\theta} \in$ {possible}

$$\text{where} \left(Y_{data}\right)_i \equiv \frac{Y_i}{\sigma_i} \qquad \sum_j \frac{M_{ij}}{\sigma_i}\theta_i = \left(\underline{\underline{M}}\,\underline{\theta}\right)_i$$

$$\frac{\partial \chi^2}{\partial \theta_j} = 0 = 2\left(\underline{Y} - \underline{\underline{M}}\,\underline{\theta}\right)^T M_j$$

$$\chi^2 = \sum_i \left(\frac{Y_i - \sum_j M_{ij}\theta_j}{\sigma_i} \right)^2$$

$$0 = \frac{\partial X^2}{\partial \theta_n} = \sum_i \frac{1}{\sigma^2} 2\left(Y_i - \sum_j M_{ij}\theta_j \right)\left(-M_{cn}\right)$$