Lecture #23: Models vs. Data 2: Bayesian view.

**Models vs. Data**

Theorem 83: As \( N_{\text{expt}} \to \infty \), the distribution of data, \( <Y_{\text{data}}>_N \) \( \to \) Normal \( \Rightarrow \) 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 \( \theta \)
3) We assume we know the uncertainties in data \( \sigma_{\text{mean}}, \sigma(<Y_{\text{data}}>) \)

\[
P(Y_{\text{data}}) = \text{const} \prod_{i=1}^{N_{\text{expt}}} \exp \left( -\frac{<Y_{\text{data}}>_i - Y_{\text{model}}_i}{\sigma_i} \right)^2
\]

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

\( \chi^2 \) collapses \( P(Y) \) to 1D

\[
\chi^2 = \sum_{i=1}^{N_{\text{expt}}} \left( \frac{Y_{\text{data}}_i - Y_{\text{model}}_i}{\sigma_i} \right)^2
\]

\( \sigma_i = \text{S.D.}/\sqrt{N_{\text{expt}}} \)

S.D. is the standard deviation of \( N_{\text{expt}} \) at condition \( i \).

![Chi-squared distribution](image)

**Figure 1.** Chi-squared distribution.

**Linear (in parameters) Models**

\( Y_{\text{model}} = M(x) \cdot \theta \)

to find best fit \( \theta \)

\[
\min_\theta \chi^2(\theta) = \min_\theta \sum_i \frac{(Y_{\text{data}}_i - M \cdot \theta)_i}{\sigma_i}^2
\]

such that \( \theta \in \{ \text{possible} \} \)

where \( (Y_{\text{data}})_i = \frac{Y_i}{\sigma_i} \)

\[
\sum_j \frac{M_{ij} \cdot \theta_j}{\sigma_j} = (\bar{M} \theta)_i
\]

\[
\frac{\partial \chi^2}{\partial \theta_j} = 0 = 2(Y - \bar{M} \theta)^T M_j
\]

Cite as: William Green, Jr., course materials for 10.34 Numerical Methods Applied to Chemical Engineering, Fall 2006. MIT OpenCourseWare (http://ocw.mit.edu), Massachusetts Institute of Technology. Downloaded on [DD Month YYYY].
\[
\chi^2 = \sum_i \left( \frac{Y_i - \sum_j M_{ij} \theta_j}{\sigma_i} \right)^2
\]

\[
0 = \frac{\partial \chi^2}{\partial \theta_n} = \sum_i \frac{1}{\sigma_i^2} \left( Y_i - \sum_j M_{ij} \theta_j \right) \left( -M_{en} \right)
\]