Comp 260: Computational Models & Methods

Analytic Methods of Model Fitting – What do we mean by “best fit”?

Chebyshev Approximation Criterion
Sum of Absolute Differences
Least Squares

More Chebyshev: Minimize $\max\{|y_i - f(x_i)|\}$

Residual: $r_i = y_i - f(x_i)$

Minimize $r$ subject to the constraints $-r \leq r_i \leq r$ for $i = 1, 2, \ldots, m$.

Example: $f(x) = a \cdot x + b$ yields $-r \leq r_i \leq r$ for the system to minimize $r$ subject to the constraints ...

$r + y_i - a \cdot x_i - b \geq 0$

$r - y_i + a \cdot x_i + b \geq 0$

Solved by linear programming (Ch. 7)

Chebyshev Criterion: Given a set of data points $(x_i, y_i)$ find the model $f(x)$ that minimizes the largest deviation $|y_i - f(x_i)|$

Chebyshev: $\min \max \{ |y_i - f(x_i)| \}$

Sum of Absolute Differences: $\sum |y_i - f(x_i)|$

Least Squares: $\sum (y_i - f(x_i))^2$

Relating the Criteria: Chebyshev & Least Squares

Let $c_i = |y_i - f_i(x_i)|$ for $i = 1, 2, 3 \ldots m$ (Chebyshev $f_i$)

Define $c_{\text{max}} = \max(c_i)$

Let $d_i = |y_i - f_i(x_i)|$ for $i = 1, 2, 3 \ldots m$ (Least Squares $f_i$)

Define $d_{\text{max}} = \max(d_i)$. Therefore $c_{\text{max}} \leq d_{\text{max}}$.

$\sum_i d_i^2 \leq \sum_i c_i^2 \leq m \cdot c_{\text{max}}$ or $D = \sqrt{\frac{d_1^2 + d_2^2 + \ldots + d_m^2}{m}} \leq c_{\text{max}}$

Therefore: $D \leq c_{\text{max}} \leq d_{\text{max}}$

Least Squares – Fitting a Straight Line $y = Ax + B$

$S = \sum_i (y_i - f(x_i))^2 = \sum_i (y_i - ax_i - b)^2$

A necessary condition for optimization is $\frac{\partial S}{\partial a} = 0 = \frac{\partial S}{\partial b}$

$\frac{\partial S}{\partial a} = -2 \sum_i (y_i - ax_i - b) x_i = 0$

$\frac{\partial S}{\partial b} = -2 \sum_i (y_i - ax_i - b) = 0$

A linear system:

$\sum_i x_i \cdot a + b \sum_i x_i = \sum_i y_i$

$\sum_i x_i + m \cdot b = \sum_i y_i$

Least Squares - Fitting a Straight Line

$a = \frac{m \sum_i y_i - \sum_i x_i \sum_i y_i}{m \sum_i x_i^2 - (\sum_i x_i)^2}$

$b = \frac{\sum_i x_i y_i - \sum_i x_i \sum_i y_i}{m \sum_i x_i^2 - (\sum_i x_i)^2}$

Least Squares – Fitting a Power Curve

$S = \sum_i (y_i - ax_i^2)^2$

$\frac{\partial S}{\partial a} = -2 \sum_i x_i^4 (y_i - ax_i^2) = 0$

$a = \frac{\sum_i x_i^3 y_i}{\sum_i x_i^3}$
Transformed Least Squares Fit

\[ S = \sum_{i=1}^{n} (y_i - ae^{bx_i})^2 \]

\[ \frac{\partial S}{\partial a} = ? \quad \frac{\partial S}{\partial b} = ? \]

Instead take \( \ln(y) = \ln(ae^{bx}) = \ln(a) + ln(e^{bx}) = \ln(a) + b \cdot x \)

Do least squares linear approximation

For Monday: Ch. 3.3 – Ch. 3.4