3750 Tutorial 2 – Least Square Calculations

Theory

for a given multi-variable function $f(x_1, x_2, \ldots, x_N)$,
a minimum occurs when: $\frac{\partial f}{\partial x_1} = 0$, $\frac{\partial f}{\partial x_2} = 0$, $\ldots$, $\frac{\partial f}{\partial x_N} = 0$

if we apply this same idea to an error function, we can minimize the error.

when defining the magnitude of a vector, we have 3 choices;
- i) 1-norm $\left(|\underline{x}| = \sum_i |x_i|\right)$
- ii) 2-norm $\left(|\underline{x}| = \sqrt{\sum_i |x_i|^2}\right)$
- iii) ∞-norm $\left(|\underline{x}|_\infty = \max |x_i|\right)$

↳ we choose to use the 2-norm squared, as this allows us to use calculus;

$$|x| = \sum_i |x_i|^2$$

Data Fitting: (approximation)

let $\underbrace{f(x)}_{LHS} = \underbrace{ax^2 + bx + c}_{RHS}$ where LHS = data 'y' value
RHS = function of data 'x' values with unknown constant coefficients a, b, c

i) for discrete data;

$$E(a,b,c) = \sum_{i=1}^{N} (RHS - LHS)^2 = \sum_{i=1}^{N} (ax_i^2 + bx_i + c - f(x_i))^2$$

(N ← num. data points)

→ error should be zero 'in an ideal world'
→ will always have error due to noise, etc.

ii) for continuous data;

$$E(a,b,c) = \int (ax^2 + bx + c - f(x))^2 \, dx$$

→ used to check error associated with a taylor approximation (not obtained data)

In each case, you want to minimize the error state, to find optimal selections for your constants.

ie. $E(a,b,c) = \sum_{i=1}^{N} (ax_i^2 + bx_i + c - f(x_i))^2$

find; $\frac{\partial E}{\partial a} = 0 = \ldots$ $\frac{\partial E}{\partial b} = 0 = \ldots$ $\frac{\partial E}{\partial c} = 0 = \ldots$

→ this will result in simultaneous equations, use matrices to solve for a, b, c... !

Why is approximation good? (vs. interpolation)

→ allows reasonable data fitting to imperfect data (all experimental data will be imperfect)

→ can easily expand general form to suit any relationship you want.

ie $f(x) = a\sqrt{x} + bx + c\ln(x) + d$.

Example
matrix representation for solving a, b in $f(x) = ax + b$

$E(a,b) = \sum_{i=1}^{N} (ax_i + b - f(x_i))^2$ i) error function

$\frac{\partial E}{\partial a} = 2\cancel{x_i} \sum_{i=1}^{N} x_i(ax_i + b - f(x_i))^{\cancel{2}} = 0$ [1] ii) find partials as required

$\frac{\partial E}{\partial b} = 2\sum_{i=1}^{N} (ax_i + b - f(x_i))^{\cancel{2}} = 0$ [2]

$[1] \rightarrow 2a\sum x_i^2 + 2b\sum x_i = 2\sum x_i f(x_i)$ iii) separate equations by unknown coefficients

$[2] \rightarrow 2a\sum x_i + 2b\sum 1 = 2\sum f(x_i)$

$$\begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & \sum 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum x_i f(x_i) \\ \sum f(x_i) \end{bmatrix}$$

iv) formulate as equations