ENGR 4/695 Advanced Topics in Engineering Mathematics Fall 2026

Lecture Outline for Wednesday, Sept. 9

1. Curve-fitting and the method of least squares: How to find the "best" solution to an inconsistent overdetermined system

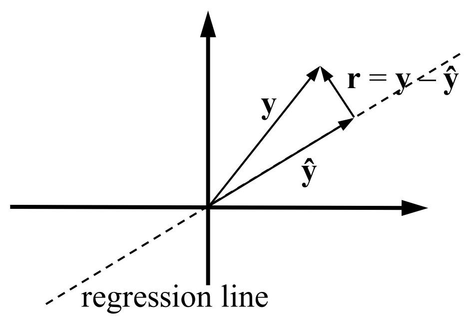
    a. Given a data set: (x_i, y_i), $i = 1$ to M $\rightarrow$ data vectors $\mathbf{x}$ and $\mathbf{y}$
    b. Define model: a set of functions $\{f_j(x_i)\}_{j=1 \text{ to } N}$ and coefficients $\{c_j\}_{j=1 \text{ to } N}$ that yield the best approximations to $\{y_i\}_{i=1 \text{ to } M}$:

    $y(x) \approx \hat{y}(x) = \sum_{j=1}^{N} c_j f_j(x)$ $\qquad$ $\hat{y}(x)$ is the best fit to the actual curve $y(x)$

    c. In matrix form, $\hat{\mathbf{y}} = F\mathbf{c}$, where $F_{ij} = f_j(x_i)$ and $\hat{\mathbf{y}}$ contains best fit
    d. Functions $\{f_j(x)\}$ (often called basis functions) can be almost anything; popular choices are 1 and x (linear fit), polynomials (including quadratic and cubic), sin/cos, exponentials, and logarithms
    e. Least squares approach:
        i. Residual vector: $\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}}$ (r_i = distance from actual y_i to approximation $\hat{y}_i$ for each data point i; $\mathbf{r}$ has M rows)
        ii. Minimize $|\mathbf{r}|^2 = \mathbf{r}^T\mathbf{r}$ or make residual orthogonal to approximation ($\mathbf{r}^T\hat{\mathbf{y}} = 0$)
        iii. Either way, the *normal equation* results (LS solution)
        iv. See supplemental reading "Constrained Least-Squares Optimization Using Minimized Coefficient Magnitudes" for derivation based on minimizing $|\mathbf{r}|^2$

2. Derivation of normal equation from setting $\mathbf{r}^T\hat{\mathbf{y}} = 0$:

$$\mathbf{r}^T\hat{\mathbf{y}} = (\mathbf{y} - \hat{\mathbf{y}})^T \hat{\mathbf{y}} = 0$$
$$(\mathbf{y} - F\mathbf{c})^T F\mathbf{c} = 0$$
$$\left[\mathbf{y}^T - (F\mathbf{c})^T\right] F\mathbf{c} = 0$$
$$\left(\mathbf{y}^T - \mathbf{c}^T F^T\right) F\mathbf{c} = 0$$
$$\left(\mathbf{y}^T F - \mathbf{c}^T F^T F\right)\mathbf{c} = 0$$



The elements of $\mathbf{c}$ should not be zero, so

$$\mathbf{y}^T F - \mathbf{c}^T F^T F = 0$$
$$\left(\mathbf{y}^T F - \mathbf{c}^T F^T F\right)^T = 0$$
$$F^T\mathbf{y} - F^T F\mathbf{c} = 0$$
$$F^T F\mathbf{c} = F^T\mathbf{y} \quad \rightarrow \quad \mathbf{c} = \left(F^T F\right)^{-1} F^T\mathbf{y}$$

(*continued on next page*)

This result is called the *normal equation* (sometimes the plural *normal equations*) because it is derived from the fact that $\mathbf{r}$ is normal (orthogonal) to $\hat{\mathbf{y}}$. Since it is equivalent to the result obtained by minimizing $|\mathbf{r}|^2 = \mathbf{r}^T\mathbf{r}$, it is also sometimes called a *least squares* solution.

3. Practical considerations:

   a. In *Matlab*, use: `c = F\y`; automatically forms solution using normal equation (or its functional equivalent)
   b. Could also use: `c = (F'F)\(F'y)` (academic interest only)
   c. F^TF is symmetric and nonsingular if there are no repeated data points
   d. F is $M \times N$, so F^TF is $N \times N$

4. Back to the simple data set example: Apply the normal equation

   a. Find quadratic fit $y = c_0 + c_1 x + c_2 x^2$ to the following small data set. Note that $f_0(x) = 1, f_1(x) = x, f_2(x) = x^2$.

i	x_i	y_i
1	1.0	1.1
2	2.0	3.2
3	4.0	5.2

   Form matrix F and data vector $\mathbf{y}$, then solve normal equation:

$$F = \begin{bmatrix} 1 & 1.0 & 1.0 \\ 1 & 2.0 & 4.0 \\ 1 & 4.0 & 16.0 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 1.1 \\ 3.2 \\ 5.2 \end{bmatrix} \quad \rightarrow \quad \mathbf{c} = \begin{bmatrix} -1.7333 \\ 3.2000 \\ -0.3667 \end{bmatrix}$$

   Same solution as those obtained with standard solution methods for square systems like Gaussian elimination.

   b. Find linear fit $y = d_0 + d_1 x$ to the data set. Note that $f_0(x) = 1, f_1(x) = x$.

   Form matrix F and data vector $\mathbf{y}$, then solve normal equation:

$$F = \begin{bmatrix} 1 & 1.0 \\ 1 & 2.0 \\ 1 & 4.0 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 1.1 \\ 3.2 \\ 5.2 \end{bmatrix} \quad \rightarrow \quad \mathbf{d} = \begin{bmatrix} 0.1000 \\ 1.3143 \end{bmatrix}$$