NUMERICAL METHODS

LEAST SQUARES SCORE (SSE)

(GOAL: MINIMIZE THE SUM OF THE SQUARE OF THE RESIDUAL ERROR)

$$S_r = \sum e_i^2 = \sum (z_i - a_0 - a_1 x_i)^2$$

$$a_1 = \frac{n\sum(x_i y_i) - \sum x_i \sum y_i}{n\sum(x_i^2) - (\sum x_i)^2}$$

$$a_0 = \frac{\sum y}{n}, \quad a_1 = \frac{\sum x}{n} \Rightarrow a_0 = \bar{y} - a_1 \bar{x}$$

$$\bar{y} = a_0 + a_1 \bar{x}$$

STANDARD ERROR:

$$S_y = \sqrt{\frac{S_r}{n-2}} \qquad S_{y/x} = \sqrt{\frac{\sum(z_i - y_i^a)^2}{n-2}}$$

STND DEVIATION:

$$S = \sqrt{\frac{S_r}{n-1}} \qquad S_y = \sqrt{\frac{\sum(y_i - \bar{y})^2}{n-1}}$$

POLYNOMIAL / QUADRATIC REGRESSION:

$$S_r = \sum (y_i - a_0 - a_1 x_i - a_2 x_i^2)^2$$

$$\frac{\partial S_r}{\partial a_0} = -2\left(\sum y_i - \sum a_0 - a_1 \sum x_i - a_2 \sum x_i^2\right) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\left(\sum y_i x_i - \sum a_0 x_i - a_1 \sum x_i^2 - a_2 \sum x_i^3\right) = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2\left(\sum y_i x_i^2 - \sum a_0 x_i^2 - a_1 \sum x_i^3 - a_2 \sum x_i^4\right) = 0$$

$$\sum a_i = a_0 n$$

$$[A][X] = [B]$$

$$S_y = \sqrt{\frac{S_r}{n-1}}$$

COEFFICIENT OF DETERMINATION:

$$r^2 = \frac{S_t - S_r}{S_t}$$

INTERPOLATION

USE A POLYNOMIAL FIT:

DEGREE 1: 2 PTS
DEGREE 2: 3 PTS
DEGREE 3: 4 PTS
DEGREE n: n+1 PTS

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

ORDER — TURNS
n = 1 : 0
n = 2 : 1
n = 3 : 2
n = n : n-1

SPLINES:

$$m_i = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

ODE'S

EULER'S METHOD:

$$\frac{dy}{dx} = f(x,y) \qquad y_{i+1} = y_i + f(x_i, y_i) h$$

HEUN'S METHOD:

$$\frac{dy}{dx} = f(x,y)$$

$$x_{i+1} - y_i = f(x_i, y_i)\, \Delta x$$

$$\frac{dy}{dx} = y_i' = f(x_i, y_i)$$

$$\frac{dy}{dx} = y_i' = f(x_i, y_i)$$

$$y_i' = \frac{y_i' + y_{i+1}'}{2} = \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^0)}{2}$$

$$y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y_{i+1}^0)}{2}\, \Delta x$$

TAYLOR SERIES

$$y(x + \Delta x) = y(x) + \frac{dy}{dx}(x_0)\,\Delta x$$

$$y(x + \Delta x) = y(x) + f(x_0, y_0)\,\Delta x$$

CLASSIC 4TH ORDER RUNGE-KUTTA:

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)\,\Delta x$$

$$k_1 = f(x_i, y_i)$$

$$k_2 = f\left(x_i + \tfrac{1}{2}\Delta x,\; y_i + \tfrac{1}{2}k_1 \Delta x\right)$$

$$k_3 = f\left(x_i + \tfrac{1}{2}\Delta x,\; y_i + \tfrac{1}{2}k_2 \Delta x\right)$$

$$k_4 = f\left(x_i + \Delta x,\; y_i + k_3 \Delta x\right)$$

DORMAND-PRINCE RUNGE-KUTTA

$$y_{i+1} = y_i + \Delta x \sum a_i k_i$$

$$y_{i+1} = y_i + \Delta x \sum a_i k_i$$

EIGEN VALUES

λ = EIGEN VALUE

SOLVE 2x2:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{\det(A)}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

$$[X] = \frac{1}{\det(A)}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}[B]$$

$$\begin{bmatrix} a-\lambda & b \\ c & d-\lambda \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\lambda = \frac{(a+d) \pm \sqrt{(a+d)^2 - 4(ad - bc)}}{2}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$X_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$[X_2] = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

PDE'S

FINITE DIFFERENCE METHOD:

CENTRAL DIFFERENCE

$$u_{xx}(x,y) = \frac{u(x - \Delta x, y) - 2u(x, y) + u(x + \Delta x, y)}{\Delta x^2}$$

$$u_{yy}(x,y) = \frac{u(x, y - \Delta y) - 2u(x, y) + u(x, y + \Delta y)}{\Delta y^2}$$

TEMPERATURE

DIRICHLET:

BC:
- TEMP KNOWN @ BOUNDARY

COUPLED HEAT EQN:

$$u_t = k(u_{xx} + u_{yy}) + q$$

$$u_x = u_{yy} = 0$$

NEUMANN:

BC:
- TEMP DERIVATIVE KNOWN ON BOUNDARY

CENTRAL DIFFERENCE:

$$\frac{\partial u}{\partial x} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$

$$\frac{\partial u}{\partial y} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y}$$

5TH ROW OF A MATRIX:

$$[0 \;\; -1 \;\; 0 \;\; -1 \;\; 4 \;\; -1 \;\; 0 \;\; -1 \;\; 0][u] = 0$$

RIGHT NEUMANN B.C.

$$\frac{\partial u}{\partial x} = g_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$

$$u_{i+1,j} = u_{i-1,j} + 2\Delta x\, g_{i,j}$$

BOTTOM NEUMANN B.C.

$$\frac{\partial u}{\partial y} = g_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y}$$

$$u_{i,j-1} = u_{i,j+1} - 2\Delta y\, g_{i,j}$$

TOP NEUMANN B.C.

$$\frac{\partial u}{\partial y} = g_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y}$$

$$u_{i,j+1} = u_{i,j-1} + 2\Delta y\, g_{i,j}$$

LEFT NEUMANN B.C.

$$u_{i-1,j} = u_{i+1,j} - 2\Delta x\, g_{i,j}$$

[A] MATRIX:

LEFT:

$$-2u_{i-1,j} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1} = -2\Delta x\, g_{i,j}$$

RIGHT:

$$-2u_{i+1,j} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1} = -2\Delta x\, g_{i,j}$$

BOTTOM:

$$-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} - 2u_{i,j+1} = -2\Delta y\, g_{i,j}$$

TOP:

$$-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} - 2u_{i,j-1} = -2\Delta y\, g_{i,j}$$

MISC EQN'S:

CENTERED FINITE DIVIDED DIFFERENCE:

FIRST:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$$

Numerical Methods In Smog Prediction

Michael Seilmaier

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