NUMERICAL METHODS

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LEAST SQUARES REGRESSION

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

$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$

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

$a_0 = \frac{\sum y_i}{n} - a_1 \frac{\sum x_i}{n} \rightarrow a_0 = \bar{y} - a_1 \bar{x}$

STANDARD ERROR:

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

STND DEVIATION:

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

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

$y = a_0 + a_1 x$

INTERPOLATION

- USE A POLYNOMIAL FIT!

LINEAR	DEGREE 2	DEGREE 3	DEGREE 4
2 PTS	3 PTS	4 PTS	n+1 PTS
2 UNKNOWNS	3 UNKNOWNS	4 UNKNOWNS	n+1 UNKNOWNS

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

ORDER	TURNS
n=1	0
n=2	1
n=3	2
n=4	3
n=n	n-1

SPLINES:

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

POLYNOMIAL (QUADRATIC) REGRESSION:

$S_r = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i - a_2 x_i^2)^2$

- TAKE DERIVATIVE OF S_r TO FIND MIN ERROR

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

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

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

$\sum a_0 = a_0 n$

$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{bmatrix} \rightarrow [A][X] = [B]$

[A] [X] [B]

$S_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$ — data points; m = order of polynomial

$r^2 = \frac{S_t - S_r}{S_t}$ — coefficient of determination

ODE'S

- EULER'S METHOD (FORWARD EULER)

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

- HEUN'S METHOD:

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

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

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

$\frac{dy_{i+1}}{dx} = y'_{i+1} = f(x_{i+1}, y_{i+1}^0)$

$\frac{dy_i}{dx} = y'_i = f(x_i, y_i)$

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

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

- TAYLOR SERIES:

$y(x+\Delta x) = y(x) + \sum_{n=1}^{\infty} \frac{f^n(x)}{n!}(\Delta x)^n$

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

CLASSIC 1ST ORDER RUNGE-KUTTA:

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

$k_1 = f(x_i, y_i)$

$k_2 = f(x_i + \frac{1}{2}\Delta x, y_i + \frac{1}{2}k_1 \Delta x)$

$k_3 = f(x_i + \frac{1}{2}\Delta x, y_i + \frac{1}{2}k_2 \Delta x)$

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

DORMAND-PRINCE RUNGE-KUTTA:

$y_{n+1} = y_n + \Delta x \sum_{i=1}^{s} b_i k_i$ (ORDER 5 METHOD)

$y_{n+1} = y_n + \Delta x \sum_{i=1}^{s} a_i k_i$ (ORDER 4 METHOD)

PDE'S

- FINITE DIFFERENCE METHOD:

DIRICHLET BOUNDARY CONDITIONS

INSULATED OR CONVECTIVE THERMOCOUPLE

TEMPERATURE

EIGEN VALUES

λ = EIGEN VALUE

EXAMPLE:

$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$

THE SAME!

$\begin{bmatrix} a_{11}-\lambda & a_{12} & a_{13} \\ a_{21} & a_{22}-\lambda & a_{23} \\ a_{31} & a_{32} & a_{33}-\lambda \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$

SIMPLE 2x2:

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

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

NOTE: $\det(A) \neq 0$

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

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

FIND EIGEN VALUES FIRST

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

$1x_1 + 1x_2 = 0$

$1x_1 + 1x_2 = 0$

$x_1 = -x_2$

$x_2 = -x_1$

$x_1 = x_2$

- EIGEN VECTOR

$x_1 = \begin{bmatrix} : \\ : \end{bmatrix}$

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

$-1x_1 + 1x_2 = 0$

$1x_1 + -1x_2 = 0$

$x_1 = x_2$

$x_2 = x_1$

- ZERO EQUATION

$[x_1] = \begin{bmatrix} : \\ : \end{bmatrix}$

PROJECT:

THE SOLID + LIQUID

T_{BOTTOM}

T_{TOP}

$L = 5$

$T = 0°C$

$R_{in} = 2$

$R_{out} = 3°C$

$k = 500 \frac{W}{m \cdot K}$ (STEEL)

- CENTRAL DIFFERENCE

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

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

BC:

- TEMP KNOWN AT BOUNDARY

SIMPLIFIED HEAT EQN:

$0 = k(u_{xx} + u_{yy} + u_{zz}) + q$

IF $q = 0$ & $k = 1$

$u_{xx} + u_{yy} = 0$

NEUMANN:

BC:

- TEMP DERIVATIVE KNOWN AT BOUNDARY

CENTRAL DIFFERENCE:

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

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

RIGHT NEUMANN B.C.

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

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

BOTTOM NEUMANN B.C.

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

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

TOP NEUMANN BC

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

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

LEFT NEUMANN B.C.

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

5TH ROW OF A MATRIX

- RESULT MUST BE EQUAL TO ZERO!

$\begin{bmatrix} 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \end{bmatrix} [u] = 0$

LEFT | BELOW | MIDDLE | ABOVE | RIGHT

[A] MATRIX:

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

LEFT:

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

THIS CHANGED

RIGHT:

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

THIS CHANGED

BOTTOM:

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

THIS CHANGED

TOP:

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

THIS CHANGED

FDC EQNS:

CENTERED FINITE-DIFFERENCE APPROXIMATION

FIRST:

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

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

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