NUMERICAL METHODS

r/KAPPY | EXAM 2 | 11/14/2022 | [illegible]

LEAST SQUARES REGRESSION:

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

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

MINIMIZE → DERIVATIVES

S_t = [illegible]

S_r = [illegible]

SLOPE:

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

INTERCEPT:

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

MEAN:

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

$$y = a_0 + a_1 x$$

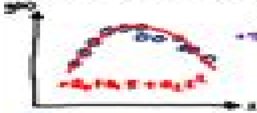
STANDARD ERROR:

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

STAND DEVIATION:

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

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 a_i TO [illegible]

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

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

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

$$\sum_{1}^{n} a_0 = a_0 n$$

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

MATLAB: $x = A \backslash B$

$$S_{y/x} = \sqrt{\frac{S_r}{n - (m+1)}}$$

data points

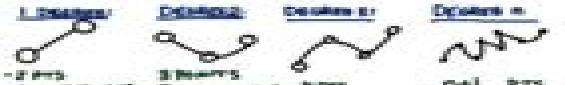
estimated coefficients

COEFFICIENT OF DETERMINATION:

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

INTERPOLATION

-USE A POLYNOMIAL FIT:



LINEAR: -2 PTS, -2 UNKNOWNS

DEGREE 2: 3 POINTS, 3 UNKNOWNS

DEGREE 3: 4 PTS, 4 UNKNOWNS

DEGREE n: n+1 PTS, n+1 [illegible]

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

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

SPLINES:

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

ODE'S

-EULER'S METHOD:

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

• TAYLOR SERIES:

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

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

• HEUN'S METHOD:

[illegible]

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

$$y^p_{i+1} = y_i + f(x_i, y_i)\Delta x \quad \text{(predictor)}$$

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

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

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

$$y_{i+1} = y_i + \frac{f(x_i, y_i) + f(x_{i+1}, y^p_{i+1})}{2}\Delta x \quad \text{(corrector)}$$

CLASSIC 4TH ORDER RUNGE-KUTTA:

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

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

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

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

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

DORMAND PRINCE RUNGE-KUTTA

$$y_{i+1} = y_i + \Delta x \sum_{j=1}^{7} a_j k_j \quad \text{LOWER ORDER}$$

$$y_{i+1} = y_i + \Delta x \sum_{j=1}^{7} b_j k_j \quad \text{HIGHER ORDER}$$

EIGEN VALUES eig( )

λ = EIGEN VALUE

EXAMPLE:

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

TO SOLVE:

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

SIMPLE 2x2:

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

$$[x] = \frac{1}{\det(A)}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}\begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

NOTE: [illegible]

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

[illegible]

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

PLUG [illegible] INTO [illegible]

$$[\;][\;] = [\;]$$

$1x_1 + 1x_2 = 0$

$1x_1 + 1x_2 = 0$

$x_1 = -x_2$

$x_1 = -x_2$

SET $x_2 = 1$

$x_1 = -1$

- EIGEN VECTOR

$$x_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$[\;][\;] = [\;]$$

$-1x_1 + 1x_2 = 0$

$1x_1 + -1x_2 = 0$

$x_1 = x_2$

$x_2 = 1$

$x_1 = 1$

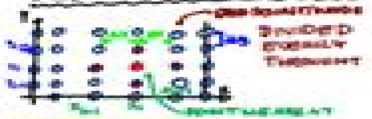
- 2ND EIGENVECTOR

$$[x_2] = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

PDE'S

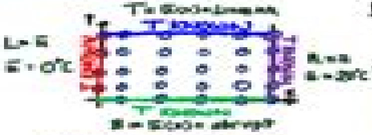
[illegible]

FINITE DIFFERENCE METHOD:



TEMPERATURE

DIRICHLET:



BC: [illegible]

- TEMP KNOWN @ BOUNDARY

SIMPLIFIED HEAT EQN:

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

IF $q = 0$ + $k = 1$

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

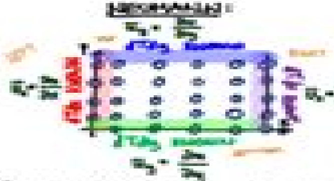
LAPLACE'S EQUATION

-CENTRAL DIFFERENCE

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

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

NEUMANN:



$G_y = \frac{\partial u}{\partial y}$
$G_x = \frac{\partial u}{\partial x}$
$G_x = \frac{\partial u}{\partial x}$
$G_y = \frac{\partial u}{\partial y}$

BC: [illegible]

- TEMP DERIVATIVE KNOWN ON BOUNDARY

CENTRAL DIFFERENCE:

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

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

5TH ROW OF A MATRIX

[illegible] POINT NOT ADJACENT TO BOUNDARY

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

RIGHT NEUMANN B.C.

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

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

BOTTOM NEUMANN B.C.

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

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

TOP NEUMANN BC

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

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

LEFT NEUMANN B.C.

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

[A] MATRIX:

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

LEFT:

$$\underbrace{-2u_{i+1,j}}_{\text{THIS CHANGED}} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1} = -2\Delta x G_x$$

RIGHT:

$$\underbrace{-2u_{i-1,j}}_{\text{THIS CHANGED}} + 4u_{i,j} - u_{i,j-1} - u_{i,j+1} = -2\Delta x G_x$$

BOTTOM:

$$-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} \underbrace{- 2u_{i,j+1}}_{\text{THIS CHANGED}} = -2\Delta x G_y$$

TOP:

$$-u_{i-1,j} - u_{i+1,j} + 4u_{i,j} \underbrace{- 2u_{i,j-1}}_{\text{THIS CHANGED}} = -2\Delta x G_y$$

MISC EQNS:

CENTERED FINITE-DIVIDED DIFF. FORMULAS:

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 Of Reactor Analysis

M Lipman

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