NUMERICAL METHODS

LEAST SQUARES REGRESSION:

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

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

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

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

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

$$y = a_0 + a_1 x$$

POLYNOMIAL (QUADRATIC) REGRESSION:

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

TAKE DERIVATIVE OF S_r w.r.t. TO EACH PARAMETER

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

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

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

$$\sum a_0 = a_0 n$$

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

$$X = A \backslash B$$

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

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

STANDARD ERROR:

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

STAND. DEVIATION:

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

INTERPOLATION

USE A POLYNOMIAL FIT:

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

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

ORDER
n=1
n=2
n=3
n=n

TURNS
0
1
2
n-1

SPLINES:

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

ODE'S

EULER'S METHOD:

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

$$y_{i+1} = y_i + f(x_i, y_i)h$$

HEUN'S METHOD:

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

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

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

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

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

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

TAYLOR SERIES:

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

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

CLASSIC 4TH ORDER RUNGE-KUTTA:

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

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

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

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

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

DORMAND PRINCE RUNGE-KUTTA

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

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

EIGEN VALUES

λ = EIGEN VALUE

DAMPED:

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

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

SOLVE 2x2:

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

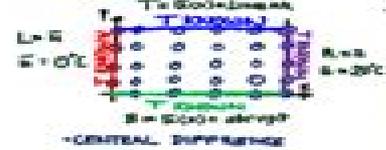$$[X] = \frac{1}{\det(A)}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}[B]$$

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

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

EIGENVECTOR:

$$X_1 = \begin{bmatrix} -b \\ a \end{bmatrix}$$

$$[X_2] = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

PDE'S

FINITE DIFFERENCE METHOD:

DIVIDED EVENLY THROUGHOUT

CONSTANT HEIGHT

TEMPERATURE

DIRICHLET:
$$L = 5$$
$$T_0 = 0°C$$

BC:
TEMP GRADIENT @ BOUNDARY

DERIVING HEAT EQN:
$$u_t = K(u_{xx} + u_{yy} + u_{zz}) + q$$
$$u_{xx} + u_{yy} = 0$$

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:

BC:
TEMP DERIVATIVE (NORMAL) ON BOUNDARY

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

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

5TH ROW OF A MATRIX:

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

RIGHT NEUMANN B.C.
$$\frac{\partial u}{\partial x} = q_x = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$
$$u_{i+1,j} = u_{i-1,j} + 2\Delta x q_x$$

BOTTOM NEUMANN B.C.
$$\frac{\partial u}{\partial y} = q_y = \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta y}$$
$$u_{i,j-1} = u_{i,j+1} - 2\Delta y q_y$$

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

LEFT NEUMANN B.C.
$$u_{i-1,j} = u_{i+1,j} - 2\Delta x q_x$$

[A] MATRIX:

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

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

BOTTOM:
THIS CHANGED
$$-2u_{i,j+1} + 4u_{i,j} - u_{i+1,j} - u_{i-1,j} = -2\Delta y q_y$$

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

THIS CHANGED

MISC EQN'S:

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 For Mathematics Science And Engineering](#)

Mark Steyvers

Numerical Methods For Mathematics Science And Engineering:

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benefits for solving complicate functions Several methods for analyzing both the ordinary and partial differential equations are then presented These methods are simple and work well for problems that have regular geometry For problems with complex geometry the finite element method is preferred The finite element method for analyzing one and two dimensional problems is explained in the last chapter Numerous examples are illustrated to increase understanding of these methods for analyzing different types of problems Computer programs corresponding to the computational procedures of these methods are provided The programs are written in MATLAB Fortran C and Pascal so that readers can use the preferred language for their study These computer programs can also be modified to use in other courses and research work **Numerical Methods for Solving Partial Differential Equations** George F. Pinder,2017-12-06 A comprehensive guide to numerical methods for simulating physical chemical systems This book offers a systematic highly accessible presentation of numerical methods used to simulate the behavior of physical chemical systems Unlike most books on the subject it focuses on methodology rather than specific applications Written for students and professionals across an array of scientific and engineering disciplines and with varying levels of experience with applied mathematics it provides comprehensive descriptions of numerical methods without requiring an advanced mathematical background Based on its author s more than forty years of experience teaching numerical methods to engineering students Numerical Methods for Solving Partial Differential Equations presents the fundamentals of all of the commonly used numerical methods for solving differential equations at a level appropriate for advanced undergraduates and first year graduate students in science and engineering Throughout elementary examples show how numerical methods are used to solve generic versions of equations that arise in many scientific and engineering disciplines In writing it the author took pains to ensure that no assumptions were made about the background discipline of the reader Covers the spectrum of numerical methods that are used to simulate the behavior of physical chemical systems that occur in science and engineering Written by a professor of engineering with more than forty years of experience teaching numerical methods to engineers Requires only elementary knowledge of differential equations and matrix algebra to master the material Designed to teach students to understand appreciate and apply the basic mathematics and equations on which Mathcad and similar commercial software packages are based Comprehensive yet accessible to readers with limited mathematical knowledge Numerical Methods for Solving Partial Differential Equations is an excellent text for advanced undergraduates and first year graduate students in the sciences and engineering It is also a valuable working reference for professionals in engineering physics chemistry computer science and applied mathematics

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