Contents

Estimation

Intermediate Value Theorem

For a continuous function $f(x)$ over the interval $[a, b]$, $\forall M, f(a) \leq M \leq f(b), \exists\, c$ such that $f(c) = M$.

Taylor Series

For a function $f(x)$, $n + 1$ times differentiable in an interval containing x_0, the Taylor Series is

$$T(x) = \sum_{i=0}^{n} \frac{(x - x_0)^i}{i!} f^{(i)}(x_0)$$

Solving Nonlinear Equations

Bisection Method

1. Choose points a and b with the solution between this domain
2. $x_{ns} = \frac{a+b}{2}$
3. Calculate $f(a)$, $f(b)$ and $f(x_{ns})$
4. Determine if the solution if between $[a, x_{ns}]$ or $[b, x_{ns}]$
5. Go to step two

Regula Falsi Method

1. Choose points a and b with the solution between this domain
2. $x_{ns} = \frac{af(b) - bf(a)}{f(b) - f(a)}$
3. Calculate $f(a)$, $f(b)$ and $f(x_{ns})$
4. Determine if the solution if between $[a, x_{ns}]$ or $[b, x_{ns}]$
5. Go to step two

Newton Method

1. Choose $(x_1, f(x_1))$ as a starting point near the solution
2. $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$
3. Repeat step two with the result

Secant Method

1. Choose $(x_1, f(x_1)), (x_2, f(x_2))$ as starting points new the solution
2. $x_3 = x_2 - \frac{f(x_2)(x_1 - x_2)}{f(x_1) - f(x_2)}$
3. Repeat step two with $(x_2, f(x_2)), (x_3, f(x_3))$

Fixed Point Iteration Method

1. Write $x = g(x)$ in the different ways
   - E.g. $xe^{0.5x} + 1.2x - 5 = 0$
   - Case a: $x = \frac{5 - xe^{0.5x}}{1.2}$
   - Case b: $x = \frac{5}{e^{0.5x} + 1.2}$
   - Case c: $x = \frac{5 - 1.2x}{e^{0.5x}}$
2. Work out $g'(x)$ for the edge values of where the root lies and use the equation where $\mid g'(x) \mid < 1$

3. Use this equation and start with one of the edge values and iterate using each result to the desired accuracy

Systems of Nonlinear Equations

Newton Method

1. Choose points x_1, y_2
2. Solve for the Jacobian determinant

$$J(f_1, f_2) = \det \begin{pmatrix} \frac{\delta f_1}{\delta x} & \frac{\delta f_1}{\delta y} \\ \frac{\delta f_2}{\delta x} & \frac{\delta f_2}{\delta y} \end{pmatrix}$$

3.

$$\Delta x = \frac{f_2(x_1, y_1)\frac{\delta f_1}{\delta y} - f_1(x_1, y_1)\frac{\delta f_2}{\delta y}}{J(f_1, f_2)}$$

4.

$$\Delta y = \frac{f_1(x_1, y_1)\frac{\delta f_2}{\delta x} - f_2(x_1, y_1)\frac{\delta f_1}{\delta x}}{J(f_1, f_2)}$$

5. Solve $x_2 = x_1 + \Delta x$ and $y_2 = y_1 \Delta y$
6. Repeat from step 3

Fixed Point Iteration Method

1. Choose points x_1, y_1
2. Get f_1 and f_2 in terms of x and y
3. Solve for x_2, y_2
4. Repeat from step 2

Systems of Linear Equations

Gaussian Elimination Method

Given:

$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 = b_1$

$a_{21}x_2 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4 = b_2$

$a_{31}x_3 + a_{32}x_3 + a_{33}x_3 + a_{34}x_4 = b_3$

$a_{41}x_4 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 = b_4$

1. Take the first equation (the pivot equation and a_{11} is called the pivot coefficient)
2. Multiply the first equation by $m_{21} = \frac{a_{21}}{a_{11}}$ and subtract this from the second equation (elminitating x_1)
3. Repeat for each equation with $m_{i1} = \frac{a_{i1}}{a_{11}}$
4. Repeat the process, taking the subsequent equations are the pivot equations.
    - Example: a_{22} becomes the pivot element, removing x_2 from equations

Result:

$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 = b_1$

$a'_{22}x_2 + a'_{23}x_3 + a'_{24}x_4 = b'_2$

$a'_{33}x_3 + a'_{34}x_4 = b'_3$

$a'_{44}x_4 = b'_4$

With Pivoting

Given:

$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 = b_1$

$0 + 0 + a_{23}x_3 + a_{24}x_4 = b_2$

$0 + a_{32}x_3 + a_{33}x_3 + a_{34}x_4 = b_3$

$0 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 = b_4$

If a pivot element is 0, swap some equations:

$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 = b_1$

$0 + a_{32}x_3 + a_{33}x_3 + a_{34}x_4 = b_3$

$0 + 0 + a_{23}x_3 + a_{24}x_4 = b_2$

$0 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 = b_4$

Gauss-Jordan Elimination Method

The same as the Gaussian Elimination Method except

1. The pivot equation is normalised by dividing all the terms in the pivot equation by the pivot coefficient (making the pivot coefficient 1)
2. The pivot equation is used to eliminate the off-diagonal terms in **all** equations

LU Decomposition Method

1. Calculate first column of $[L]$; $L_{i1} = a_{i1}$
2. Substitute 1s in the diagonal of $[U]$; $U_{ii} = 1$
3. Calculate the elements in the first row of $[U]$ (Except U_{11}); $U_{1j} = \frac{a_{1j}}{L_{11}}$
4. Calculate the rest of the elements row after row where

$$a_{ij} = \sum_{k=1}^{k=j} L_{ik} U_{kj}$$

   - Example: $a_{33} = L_{31}U_{13} + L_{32}U_{23} + L_{33}U_{33} = L_{31}U13 + L_{32}U_{23} + L_{33}$ $(U_{ii} = 1)$

5. $[L][y] = [b]$ to solve for y
6. $[U][x] = [y]$ to solve for x

Norms

$$\begin{bmatrix} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1 \\ a_{21}x_2 + a_{22}x_2 + a_{23}x_3 = b_2 \\ a_{31}x_3 + a_{32}x_3 + a_{33}x_3 = b_3 \end{bmatrix}$$

1-Norm:

$|| a ||_1 = max[| a_{11} | + | a_{21} | + | a_{31} |, | a_{12} | + | a_{22} | + | a_{32} |, | a_{13} | + | a_{23} | + | a_{33} |]$

Infinity Norm:

$|| a ||_\infty = max[| a_{11} | + | a_{12} | + | a_{13} |, | a_{21} | + | a_{22} | + | a_{23} |, | a_{31} | + | a_{32} | + | a_{33} |]$

Condition Number: $|| [a] || \times || [a]^{-1} ||$

Eigenvalues and Eigenvectors

For a given square matrix $[a]$ the number of λ is an eigenvalue of the matrix if $[a][u] = \lambda[u]$. The vector $[u]$ is a column vector called the eigenvector associated with the eigenvalue λ. If should be noted that there are usually more than one eigenvalue and eigenvector. In fact, in an $n \times n$ matrix there are n eigenvalues and an infinite number of eigenvectors.

Characteristic Equation

$\det[a - \lambda I] = 0$ where $[a]$ is the matrix, I is the identity matrix, and λ is a polynomial equation whose roots are the eigenvalues. This can be used to solve $[a][u] = \lambda[u]$ for the eigenvectors.

Basic Power Method

$n \times n$ matrix $[a]$ with n distinct real eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ and n associated eigenvectores $[u]_1, [u]_2, \ldots, [u]_n$.

1. Choose a non-zero vector $[x]_1$.
2. Multiply by $[a]$
3. Factor out the largest element in the resulting vector to get $[x]_2$ and a factor
4. Go back to step one with $[x]_2$

$[x]_\infty = [u]_1$ where $[u]_1$ is the eigenvector corresponding to the largest eigenvalue.

Inverse Power Method

This method is used to find the smallest eigenvalue. Apply the power method using $[a]^{-1}$

QR Factorisation

Step 1

1. Choose $[c]$ to be the first column of $[a]$
2. The first element in vector $[e]$ is 1 is the first element of $[c]$ is postivie, otherwise is it negative. The rest is 0
3. Calculate $[H]^{(1)} = [I] - \frac{2}{[v]^T[v]}[v][v]^T$ where $[v] = [c] + \| [c] \|_2 [e]$ where $\| [c] \|_2 = \sqrt{c_1^2 + c_2^2 + \cdots + c_n^2}$
4. $[Q]^{(1)} = [H]^{(1)}$ and $[R]^{(1)} = [H]^{(1)}[a]$

Step 2

1. Vector $[c]$ is now defined as the second column of $[R]^{(1)}$
2. The second element in vector $[e]$ is 1 is the first element of $[c]$ is postivie, otherwise is it negative. The rest is 0
3. Calculate $H^{(2)}$
4. $[Q]^{(2)} = [Q]^{(1)}[H]^{(2)}$ and $[R]^{(2)} = [R]^{(1)}[H]^{(2)}$

Continue on, taking $[c]$ as the third column of $[R]^{(2)}$, $[Q]^{(3)} = [Q]^{(2)}[H]^{(3)}$ and $[R]^{(3)} = [R]^{(2)}[H]^{(3)}$

Curve Fitting and Interpolation

Linear Equation

$$y = a_1 x + a_0$$

$$\text{Error} = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n} (y_i - f(x_i))^2 = \sum_{i=1}^{n} (y_i - (a_1 x_i + a_0))^2$$

Linear Least-Squares Regression:

1. Calculate
   - $S_x = \sum_{i=1}^{n} x_i$
   - $S_y = \sum_{i=1}^{n} y_i$
   - $S_{xy} = \sum_{i=1}^{n} x_i y_i$
   - $S_{xx} = \sum_{i=1}^{n} x_i^2$
2. $a_1 = \frac{n S_{xy} - S_x S_y}{n S_{xx} - (S_x)^2}$
3. $a_0 = \frac{S_{xx} S_y - S_{xy} S_x}{n S_{xx} - (S_x)^2}$

Nonlinear Equation in Linear Form

Nonlinear Equation	Linear Form
$y = bx^m$	$\ln(y) = m \ln(x) + \ln(b)$
$y = be^{mx}$	$\ln(y) = mx + \ln(b)$
$y = b10^{mx}$	$\log(y) = mx + \log(b)$
$y = \frac{1}{mx+b}$	$\frac{1}{y} = mx + b$
$y = \frac{mx}{b+x}$	$\frac{1}{y} = \frac{b}{m}\frac{1}{x} + \frac{1}{m}$

Use least-squares regression on a nonlinear equation's linear form.

Quadratic and Higher-Order Polynomials

If the polynomial, of order m, that is used for the curve fitting is:

$$f(x) = a_n x^m + a_{m-1} x^{m-1} + \cdots + a_1 x + a_0$$

then, for a given set of n data points, (where $m < n-1$), then total error is given by

$$\text{Error} = \sum_{i=1}^{n}(y_i - (a_n x^m + a_{m-1}x^{m-1} + \cdots + a_1 x + a_0))^2$$

Example of a second order polynomial:

1. $na_0 + (\sum_{i=1}^{n} x_i)a_1 + (\sum_{i=1}^{n} x_i^2)a_2 = \sum_{i=1}^{n} y_i$
2. $(\sum_{i=1}^{n} x_i)a_0 + (\sum_{i=1}^{n} x_i^2)a_1 + (\sum_{i=1}^{n} x_i^3)a_2 = \sum_{i=1}^{n} x_i y_i$
3. $(\sum_{i=1}^{n} x_i^2)a_0 + (\sum_{i=1}^{n} x_i^3)a_1 + (\sum_{i=1}^{n} x_i^4)a_2 = \sum_{i=1}^{n} x_i^2 y_i$

The solution of the system of equations give the values a_0, a_1, a_2

Single Polynomial

Lagrange Polynomials

First-order polynomial:

$$f(x) = \frac{x - x_2}{x_1 - x_2}y_1 + \frac{x - x_1}{x_2 - x_1}y_2$$

Second-order polynomial:

$$f(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}y_3$$

And it goes on…

Sneaky fourth-order polynomial:

$f(x) = \frac{(x-x_2)(x-x_3)(x-x_4)(x-x_5)}{(x_1-x_2)(x_1-x_3)(x_1-x_4)(x_1-x_5)}y_1 + \frac{(x-x_1)(x-x_3)(x-x_4)(x-x_5)}{(x_2-x_1)(x_2-x_3)(x_2-x_4)(x_2-x_5)}y_2 + \frac{(x-x_1)(x-x_2)(x-x_4)(x-x_5)}{(x_3-x_1)(x_3-x_2)(x_3-x_4)(x_3-x_5)}y_3 + \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_5)}{(x_4-x_1)(x_4-x_2)(x_4-x_3)(x_4-x_5)}y_4 + \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_5-x_1)(x_5-x_2)(x_5-x_3)(x_5-x_4)}y_5$

Newton's Polynomials

First-order polynomial:

$$f(x) = a_1 + a_2(x - x_1)$$

1. $a_1 = y_1$

2. $a_2 = \frac{y_2 - y_1}{x_2 - x_1}$

Second-order polynomial:

$$f(x) = a_1 + a_2(x - x_1) + a_3(x - x_1)(x - x_2)$$

1. $a_1 = y_1$
2. $a_2 = \frac{y_2 - y_1}{x_2 - x_1}$
3. $a_3 = \frac{\frac{y_3 - y_2}{x_3 - x_2} - \frac{y_2 - y_1}{x_2 - x_1}}{x_3 - x_1}$

And it goes on…

Piecewise Interpolation

Linear Splines

$$f_i(x) = \frac{(x - x_{i+1})}{(x_i - x_{i+1})} y_i + \frac{(x - x_i)}{(x_{i+1} - x_i)} y_{i+1}$$

for $i = 1, 2, \ldots, n - 1$

Numerical Differentation

Finite Difference Approximation of the Derivative

$f'(x)$ of a functi(on $f(x)$ at point $x = a$ is defined by

$$\left. \frac{df(x)}{dx} \right|_{x=a} = f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a}$$

Forward difference:

$$\left. \frac{df(x)}{dx} \right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

Backward difference:

$$\left. \frac{df(x)}{dx} \right|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

Central difference:

$$\left. \frac{df(x)}{dx} \right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$

Finite Difference Formulas using Taylor Series Expansion

Taylor series:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \dots$$

Truncation error: $O(h)$

Derivation

Two point forward difference formula for first derivative

The value of a function at point x_{i+1} can be approximated by a Taylor series in terms of the value of the function and its derivates at point x_i

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1}-x_i) + \frac{f''(x_i)}{2!}(x_{i+1}-x_i)^2 + \frac{f'''(x_i)}{3!}(x_{i+1}-x_i)^3 + \dots$$

By using two-term Taylor series expansion with a remainder, this can be written as

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

where ξ is a value between x_i and x_{i+1}. This can be solved for $f'(x_i)$ giving

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

where $h = x_{i+1} - x_i$

Two point backward difference formula for first derivative

Likewise, the function at point x_{i-1} is approximated by a Taylor series in terms of the value of the function and its derivates at point x_i

$$f(x_{i-1}) = f(x_i) - f'(x_i)(x_i-x_{i-1}) + \frac{f''(x_i)}{2!}(x_i-x_{i-1})^2 - \frac{f'''(x_i)}{3!}(x_i-x_{i-1})^3 + \dots$$

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

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

where $h = x_i - x_{i-1}$

Two point central difference formula for first derivative

$f(x_{i+1})$ and $f(x_{i-1})$ can be derived using three terms in the Taylor series expansion.

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1}-x_i) + \frac{f''(x_i)}{2!}(x_{i+1}-x_i)^2 + \frac{f'''(\xi_1)}{3!}(x_{i+1}-x_i)^3$$

where ξ_1 is a value between x_{i+1} and x_i and

$$f(x_{i-1}) = f(x_i) - f'(x_i)(x_i - x_{i-1}) + \frac{f''(x_i)}{2!}(x_i - x_{i-1})^2 - \frac{f'''(\xi_2)}{3!}(x_i - x_{i-1})^3$$

where ξ_2 is a value between x_i and x_{i-1}

Subtracting these gives us

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3$$

this can be solved for $f'(x_i)$

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

x-point difference formula for first derivative The 3-point forward difference formula uses $f(x_{i+2})$, $f(x_{i+1})$ and $f(x_i)$ to calculate $f'(x_i)$. This can be continued for x-points, using forward, backward and central differences.

x-point difference formula for nth derivative The Taylor series can be expanded with any number of points to get a higher order derivative.

Differentiation Formulas using Lagrange Polynomials

The two-point central, three-point forward and three-point backward difference formulas are obtained by considering points $(x_i, y_i), (x_{i+1}, y_{i+2}).(x_{i+2}, y_{i+2})$. The polynomial passing through the points can be obtained in Lagrange form, and differentiated.

Richardson's Extrapolation

$$D = \frac{1}{3}(4D\frac{h}{2} - D(h)) + O(h^4)$$

where h is the spacing between points

A more accurate approximationg:

$$D = \frac{1}{15}(16D\frac{h}{2} - D(h)) + O(h^6)$$

Numerical Integration

$$I(f) = \int_a^b f(x)dx$$

Rectangle Method

$$I(f) = \int_a^b f(a)dx = f(a)(b-a)$$

or

$$I(f) = \int_a^b f(b)dx = f(b)(b-a)$$

Composite:

$$I(f) = \int_a^b f(x)dx \approx h\sum_{i=1}^{N} f(x_i)$$

where $h = x_{i+1} - x_i$

Midpoint Method

$$I(f) = \int_a^b f(x)dx \approx_i nt_a^b f(\frac{a+b}{2})dx = f(\frac{a+b}{2})(b-a)$$

Composite:

$$I(f) = \int_a^b f(x)dx \approx h\sum_{i=1}^{N} f(\frac{x_i + x_{i+1}}{2})$$

Trapezoidal Method

$$I(f) \approx \frac{[f(a) + f(b)]}{2}(b-a)$$

Composite:

$$I(f) \approx \frac{h}{2}[f(a) + f(b)] + h\sum_{i=2}^{N} f(x_i)$$

Simpson's Method (hinting to come up)

Simpson's 1/3 Method (quadratic)

$$I = \int_{x_i}^{x_3} f(x)dx \approx \int_{x_1}^{x_3} p(x)dx = \frac{h}{3}[f(x_1)+4f(x_2)+f(x_3)] = \frac{h}{3}[f(a)+4f(\frac{a+b}{2})+f(b)]$$

Composite:

$$I(f) \approx \frac{h}{3}[f(a) + 4\sum_{i=2,4,6}^{N} f(x_i) + 2\sum_{j=3,5,7}^{N-1} f(x_j) + f(b)]$$

Can only be used if

- The subinterval must be equally spaced
- The number of subintervals within $[a, b]$ must be an even number

Simpson's 3/8 Method (cubic)

$$I = \int_a^b f(x)dx \approx \int_a^b p(x)dx = \frac{3}{8}h[f(a) + 3f(x_2) + 3f(x_3) + f(b)]$$

Composite:

$$I(f) \approx \frac{3h}{8}[f(a) + 3\sum_{i=2,5,8}^{N-1} [f(x_i) + f(x_{i+1})] + 2\sum_{j=4,7,10}^{N-2} f(x_j) + f(b)]$$

Can only be used if

- The subinterval must be equally spaced
- The number of subintervals within $[a, b]$ must be divisible by 3