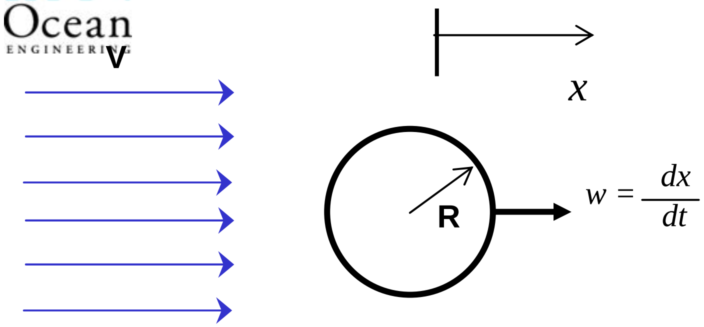
Numerical Marine Hydrodynamics Summary

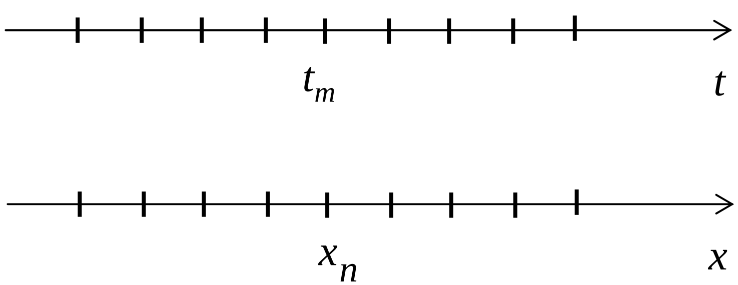
- Fundamentals of Digital Computing
- Error Analysis
- Roots of Non-linear Equations
- Systems of Linear Equations
  - Gaussian Elimination
  - Iterative Methods
- Optimization, Curve Fitting
- Interpolation
  - Numerical Integration
  - Numerical Differentiation
- Ordinary Differential Equations
  - Initial Value Problems
  - Boundary Value Problems
- Partial Differential Equations
- Finite Element and Spectral Methods
- Boundary Integral – Panel Methods

Digital Computer Models

Continuum Model



Discrete Model



$$t_m = t_0 + m\Delta t \ , \quad m = 0, 1, \dots M-1$$
$$x_n = x_0 + n\,\Delta x \ , \quad n = 0, 1, \dots N-1$$

$$\frac{dw}{dx} \simeq \frac{\Delta w}{\Delta x} \ , \quad \frac{dw}{dt} \simeq \frac{\Delta w}{\Delta t}$$

Differential Equation

$$L(p, w, x, t) = 0$$

Differentiation
Integration

Difference Equation

$$L_{mn}(p_{mn}, w_{mn}, x_n, t_m) = 0$$

System of Equations

$$\sum_{j=0}^{N-1} F_i(w_j) = B_i$$

Linear System of Equations

$$\sum_{j=0}^{N-1} A_{ij} w_j = B_i$$

Solving linear equations

Eigenvalue Problems

$$\bar{\bar{\mathbf{A}}}\mathbf{u} = \lambda \mathbf{u} \Leftrightarrow (\bar{\bar{\mathbf{A}}} - \lambda \bar{\bar{\mathbf{I}}})\mathbf{u} = \mathbf{0}$$

Non-trivial Solutions

$$\det(\bar{\bar{\mathbf{A}}} - \lambda \bar{\bar{\mathbf{I}}}) = 0$$

Root finding

Accuracy and Stability => Convergence

Error Analysis

Number Representation

Absolute Error

$$\bar{\epsilon} = |\bar{m} - m| \leq \frac{1}{2} b^{-t}$$

Relative Error

$$\bar{\alpha} = \frac{|\bar{m} - m| b^e}{|m| b^e} \leq \frac{\frac{1}{2} b^{-t}}{b^{-1}} \leq \frac{1}{2} b^{1-t}$$

Addition and Subtraction

$$r_1 \pm r_2 = m_1 b^{e_1} \pm m_2 b^{e_2}$$

Shift mantissa of largest number

$$e_1 > e_2$$

Result has exponent of largest number

$$r_1 \pm r_2 = \left(m_1 \pm m_2 b^{e_2 - e_1} \right) b^{e_1} = m b^{e1}$$

Absolute Error

$$\bar{\epsilon} \leq \bar{\epsilon_1} + \bar{\epsilon_2}$$

Relative Error

$$\bar{\alpha} = \frac{|\bar{m} - m|}{|m|}$$

Unbounded

Multiplication and Division

$$r_1 \times r_2 = m_1 m_2 b^{e1+e2}$$

$$m = m1m2 < 1$$

$$0.1_2 \times 0.1_2 = 0.01_2$$

Relative Error

$$\bar{\alpha} \leq \bar{\alpha_1} + \bar{\alpha_2}$$

Bounded

Recursion
Heron's Device

Numerically evaluate square-root

$$\sqrt{s}\ , \quad s > 0$$

Initial guess

$$x_0 \simeq \sqrt{s}$$

Test

$$x_0^2 < s \;\Rightarrow\; x_0 < \sqrt{s} \;\Rightarrow\; \frac{s}{x_0} > \sqrt{s}$$

$$x_0^2 > s \;\Rightarrow\; x_0 > \sqrt{s} \;\Rightarrow\; \frac{s}{x_0} < \sqrt{s}$$

Mean of guess and its reciprocal

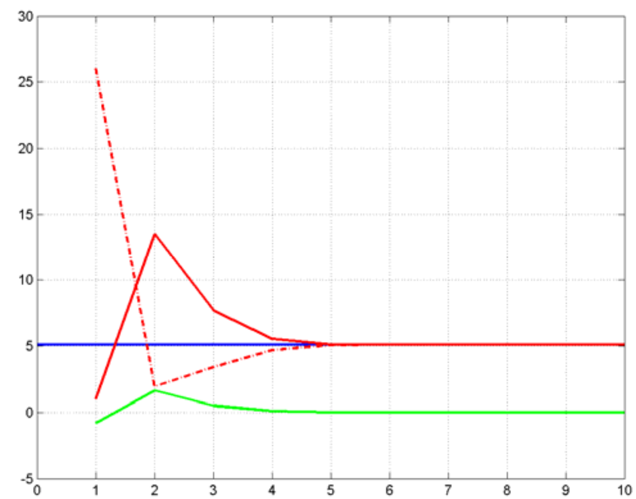
$$x_1 = \frac{1}{2}\left(x_0 + \frac{s}{x_0}\right)$$

Recursion Algorithm

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{s}{x_n}\right)$$

MATLAB script heron.m

```
a=26;
n=10;
g=1;
% Number of Digits
dig=5;
     sq(1)=g;
     for i=2:n
       sq(i)= 0.5*radd(sq(i-1),a/sq(i-1),dig);
     end
     hold off
     plot([0 n],[sqrt(a) sqrt(a)],'b')
     hold on
     plot(sq,'r')
     plot(a./sq,'r-.')
     plot((sq-sqrt(a))/sqrt(a),'g')
     grid on
```



Spherical Bessel Functions

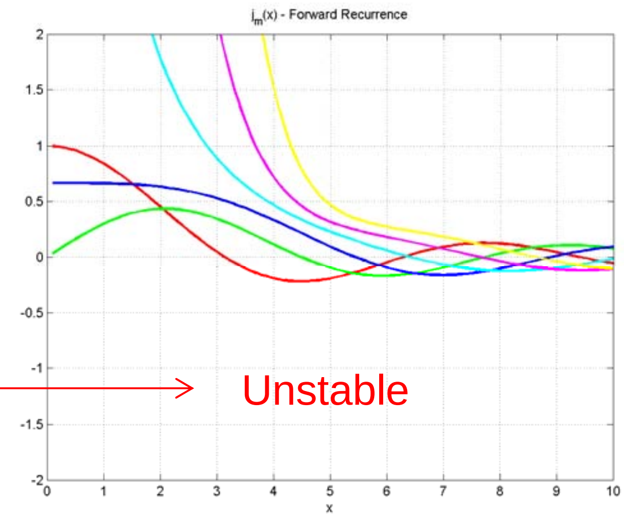
Generation by Recurrence Relations

Forward Recurrence

$$j_{n+1}(x) = \frac{2n+1}{x} j_n(x) - j_{n-1}(x)$$

Forward Recurrence

$$\frac{2n+1}{x} j_n(x) \simeq j_{n-1}(x)$$



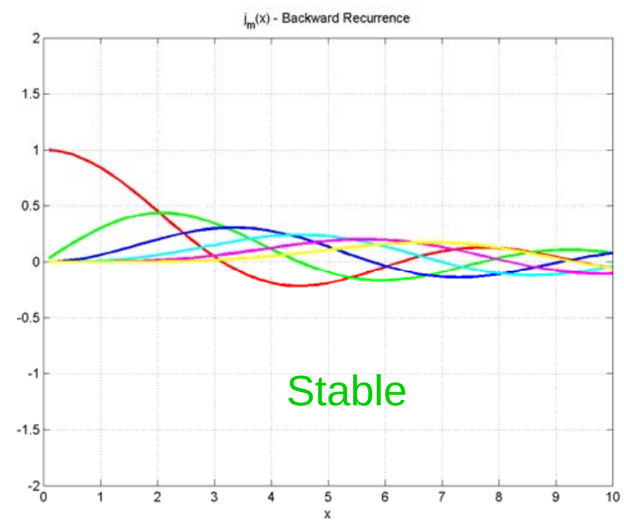
Backward Recurrence

$$j_{n-1}(x) = \frac{2n+1}{x} j_n(x) - j_{n+1}(x)$$

Miller's algorithm

$$j_N(x) = 1 \;,\; j_{N+1}(x) = 0 \;,\; j_0(x) = \frac{\sin x}{x}$$

$N \sim x+20$



Error Propagation

$$y = f(x_1, x_2, \ldots x_n)$$

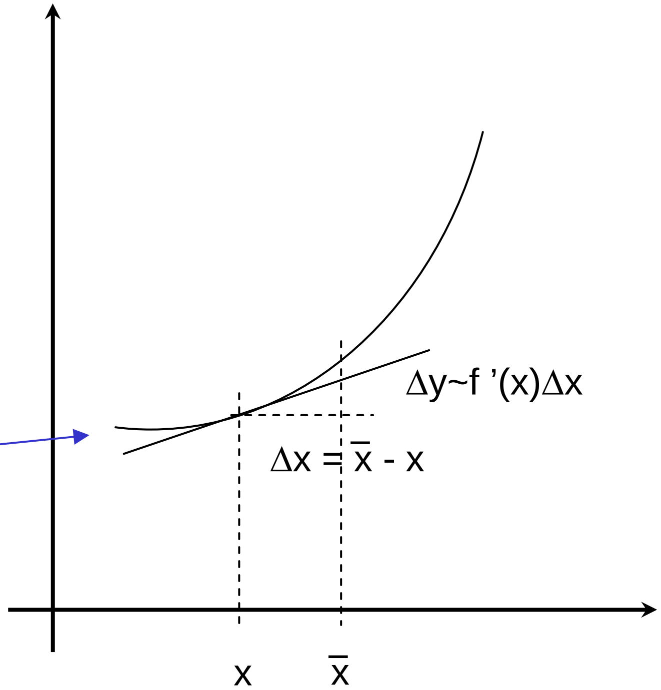
Absolute Errors

$$\epsilon_1, \epsilon_2, \ldots \epsilon_n$$

$$\epsilon_y$$

Function of one variable

$$y = f(x) \quad \bar{y} = f(\bar{x})$$

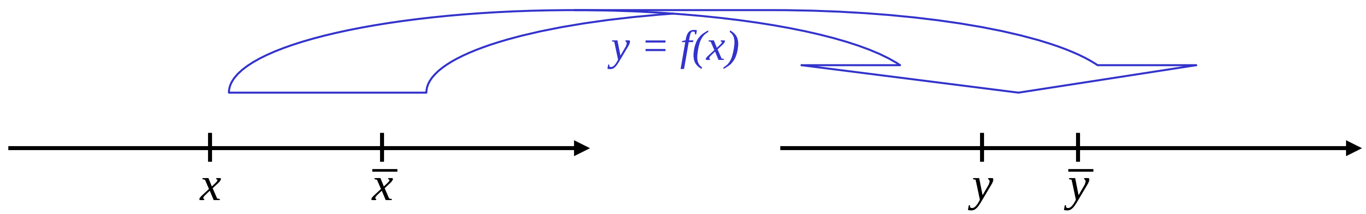


General Error Propagation Formula

$$\Delta y \simeq \sum_{i=1}^{n} \frac{\partial f(x_1, \ldots, x_n)}{\partial x_i} \Delta x_i$$

$$\epsilon_y \leq \sum_{i=1}^{n} \left| \frac{\partial f(x_1, \ldots, x_n)}{\partial x_i} \right| |\epsilon_i|$$

Error Propagation
Condition Number



$\bar{x} = x(1 + \alpha)$ $\bar{y} = y(1 + \beta)$

Problem Condition Number

$$
\begin{aligned}
K_P &= \frac{|\beta|}{|\alpha|} \\
&= \left|\frac{f(\bar{x}) - f(x)}{f(x)}\right| / \left|\frac{\bar{x} - x}{x}\right| \\
&= \left|\frac{f(\bar{x}) - f(x)}{\bar{x} - x}\right| \times \left|\frac{x}{f(x)}\right| \\
&\simeq \left|x\frac{f'(x)}{f(x)}\right|
\end{aligned}
$$

$$K_P \gg 1$$

Problem ill-conditioned

Error cancellation example

$$y = f(x) \;=\; \sqrt{x^2 + 1} - x + 200; \quad x = 100 \pm 4$$

$$K_P \;=\; \left|100\,\frac{-10^{-4}}{200.005}\right| = 0.5\ 10^{-4}$$

Well-conditioned problem

Roots of Nonlinear Equations
General Method

Non-linear Equation

$$f(x) = 0$$

Goal: Converging series

$$x_0, x_1, \ldots x_n \to x^e \;, \quad n \to \infty$$

Rewrite Problem

$$f(x) = 0 \Leftrightarrow g(x^e) = x^e$$

Example

$$g(x) = x + c \cdot f(x)$$

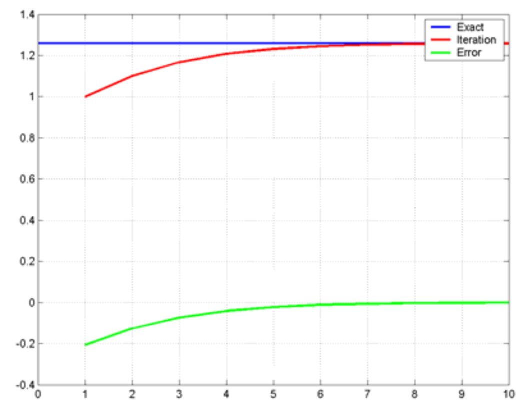
Iteration

$$x_n = g(x_{n-1})$$

Example: Cube root

cube.m

```
% f(x) = x^3 - a = 0
% g(x) = x + C*(x^3 - a)
a=2;
n=10;
g=1.0;
C=-0.1;
     sq(1)=g;
     for i=2:n
      sq(i)= sq(i-1) + C*(sq(i-1)^3 -a);
     end
     hold off
     plot([0 n],[a^(1./3.) a^(1/3.)],'b')
     hold on
     plot(sq,'r')
     plot( (sq-a^(1./3.))/(a^(1./3.)),'g')
     grid on
```



Roots of Nonlinear Equations
General Method

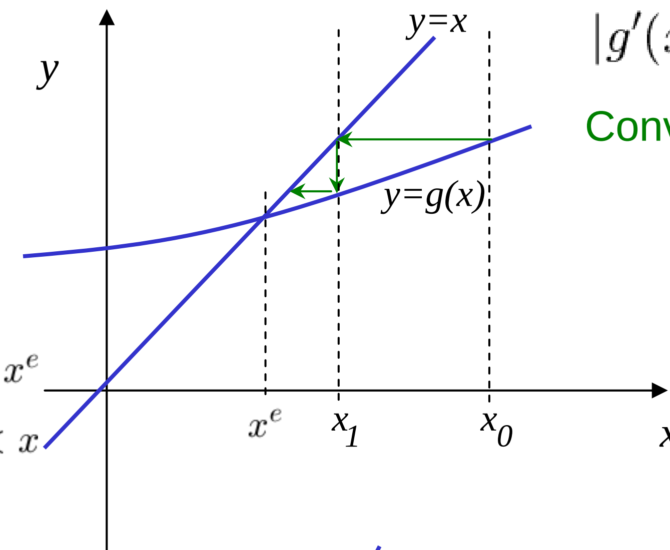
Convergence

Mean-value Theorem

$$\{\exists \xi \in [x, x^e] \mid g(x) - g(x^e) = g'(\xi)(x - x^e)\} \begin{cases} x < \xi < x^e \\ x^e < \xi < x \end{cases}$$

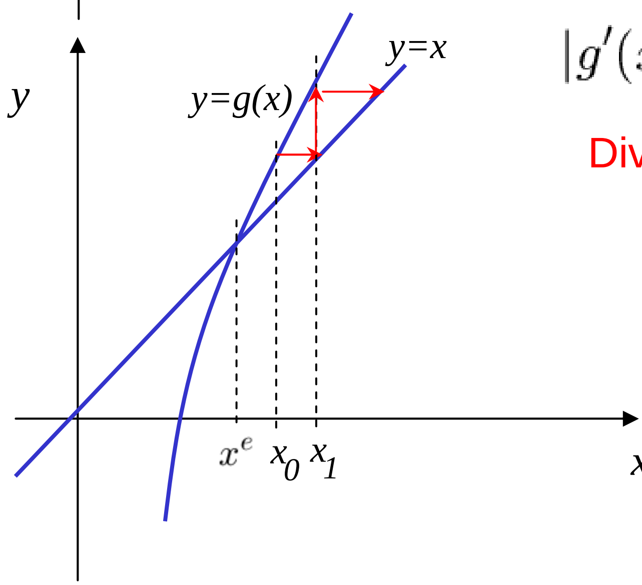
Convergence

$$|g'(x)|_{x \in I} \leq k < 1 \Rightarrow |g(x) - x^e| \leq k|x - x^e|$$



$|g'(x)| < 1$

Convergent



$|g'(x)| > 1$

Divergent

Systems of Linear Equations
Gaussian Elimination

Reduction Step k

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik} b_k^{(k)} \end{aligned}\right\} i = k+1, \cdots n$$

$$\begin{array}{cccccccc} a_{11}^{(1)} x_1 & a_{12}^{(1)} x_2 & \cdot & \cdot & a_{1n}^{(1)} x_n & = & b_1^{(1)} \\ 0 & a_{22}^{(2)} x_2 & \cdot & \cdot & a_{2n}^{(2)} x_n & = & b_2^{(2)} \\ 0 & \cdot & a_{kk}^{(k)} x_k & \cdot & \cdot & = & \cdot \\ 0 & \cdot & 0 & \cdot & \cdot & = & \cdot \\ 0 & \cdot & 0 & \cdot & a_{nn}^{(k+1)} x_n & = & b_n^{(k+1)} \end{array}$$

Reduction Step n-1

$$\begin{array}{ccccccc} a_{11}^{(1)} x_1 & a_{12}^{(1)} x_2 & \cdot & \cdot & a_{1n}^{(1)} x_n & = & b_1^{(1)} \\ 0 & a_{22}^{(2)} x_2 & \cdot & \cdot & a_{2n}^{(2)} x_n & = & b_2^{(2)} \\ 0 & \cdot & \cdot & \cdot & \cdot & = & \cdot \\ 0 & \cdot & 0 & a_{n-1,n-1}^{(n-1)} x_{n-1} & a_{n-1,n}^{(n-1)} x_n & = & b_{n-1}^{(n-1)} \\ 0 & \cdot & \cdot & 0 & a_{nn}^{(n)} x_n & = & b_n^{(n)} \end{array}$$

Back-Substitution

$$x_n = b_n^{(n)} / a_{nn}^{(n)}$$

$$x_{n-1} = \left(b_{n-1}^{(n-1)} - a_{n-1,n}^{(n-1)} x_n \right) / a_{n-1,n-1}^{(n-1)}$$

$$\cdot \quad \cdot \quad \cdot$$

$$\cdot \quad \cdot \quad \cdot$$

$$x_k = \left(b_k^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)} x_j \right) / a_{kk}^{(k)}$$

$$\cdot \quad \cdot \quad \cdot$$

$$x_1 = \left(b_1^{(1)} - \sum_{j=2}^{n} a_{1j}^{(1)} x_j \right) / a_{11}^{(1)}$$

Systems of Linear Equations
Gaussian Elimination

Reduction
Step k

$$\left.\begin{aligned} m_{ik} &= \frac{a_{ik}^{(k)}}{a_{kk}^{(k)}} \\ a_{ij}^{(k+1)} &= a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad j = k, \cdots n \\ b_i^{(k+1)} &= b_i^{(k)} - m_{ik} b_k^{(k)} \end{aligned}\right\} i = 2, \cdots n$$

Pivotal Elements

$$a_{11}^{(1)}, a_{22}^{(2)}, \ldots, a_{nn}^{(n)}$$

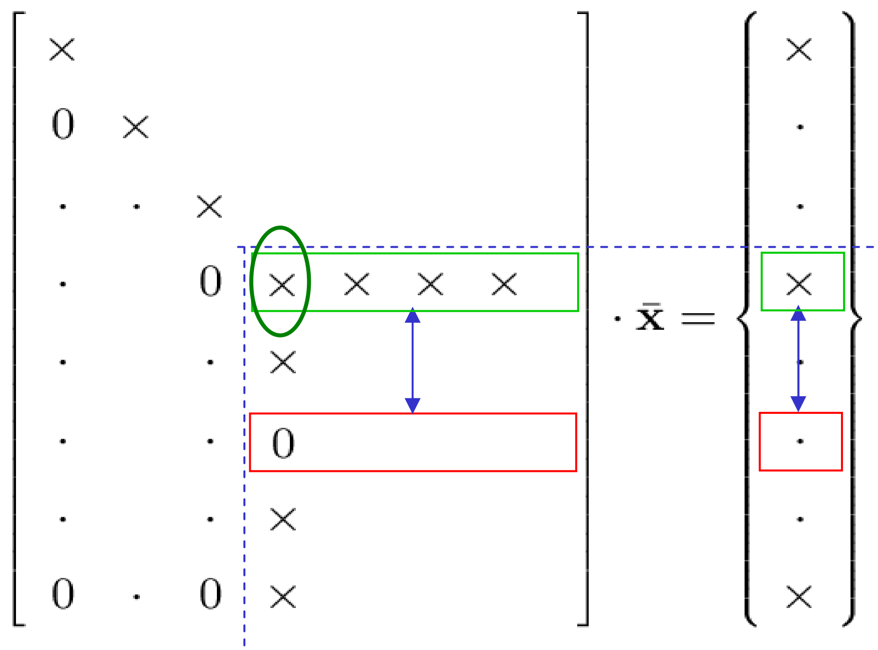
$$a_{kk}^{(k)} \neq 0$$

Required at each step!

Partial Pivoting by Columns

New Row k

New Row i



Systems of Linear Equations
Gaussian Elimination

Numerical Stability

- Partial Pivoting
  - Equilibrate system of equations
  - Pivoting by Columns
  - Simple book-keeping
    - Solution vector in original order
- Full Pivoting
  - Does not require equilibration
  - Pivoting by both row and columns
  - More complex book-keeping
    - Solution vector re-ordered

Partial Pivoting is simplest and most common

Neither method guarantees stability

Systems of Linear Equations
Gaussian Elimination

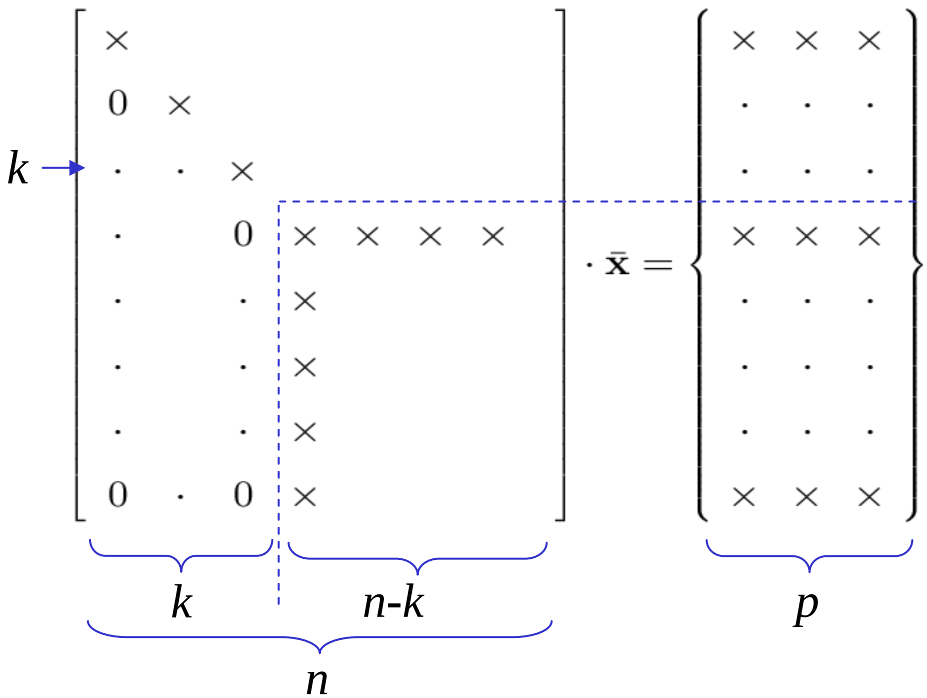
How to Ensure Numerical Stability

- System of equations must be well conditioned
  - Investigate condition number
    - Tricky, because it requires matrix inversion (next class)
  - Consistent with physics
    - E.g. don't couple domains that are physically uncoupled
  - Consistent units
    - E.g. don't mix meter and μm in unknowns
  - Dimensionless unknowns
    - Normalize all unknowns consistently
- Equilibration and Partial Pivoting, or Full Pivoting

Systems of Linear Equations
Gaussian Elimination

Multiple Right-hand Sides

Reduction
Step k



Computation Count
Reduction Step k

$(n-k)(n-k+p)$ Operations

Total Computation Count

$n \gg 1$

Reduction

$$N_r = \sum_{k=1}^{n-1}(n-k)(n-k+p) \simeq \frac{1}{3}n^3 + \frac{1}{2}n^2(p-1)$$

Back Substitution

$$N_b = \sum_{k=1}^{n-1}(n-k)p \simeq \frac{1}{2}n^2 p$$

Reduction for each right-hand side inefficient.
However, RHS may be result of iteration and unknown a priori
(e.g. Euler's method) -> LU Factorization

$n \gg 1 \Rightarrow N_r \gg N_b$

Systems of Linear Equations
LU Factorization

The coefficient Matrix $\overline{\overline{\mathbf{A}}}$ is decomposed as

$$\overline{\overline{\mathbf{A}}} = \overline{\overline{\mathbf{L}}} \cdot \overline{\overline{\mathbf{U}}}$$

where $\overline{\overline{\mathbf{L}}}$ is a lower triangular matrix
and $\overline{\overline{\mathbf{U}}}$ is an upper triangular matrix

$$\overline{\overline{\mathbf{L}}} = [l_{ij}] = \begin{bmatrix} l_{11} & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ l_{21} & l_{22} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & & & & \cdot \\ \cdot & & \cdot & l_{kk} & \cdot & & \cdot \\ & & & & \cdot & \cdot & 0 \\ l_{n1} & \cdot & \cdot & \cdot & \cdot & l_{n,n-1} & l_{nn} \end{bmatrix}$$

Then the solution is performed in two simple steps

1. $\overline{\overline{\mathbf{L}}}\vec{y} = \vec{b}$ Forward substitution
2. $\overline{\overline{\mathbf{U}}}\vec{x} = \vec{y}$ Back substitution

$$\overline{\overline{\mathbf{U}}} = [u_{ij}] = \begin{bmatrix} u_{11} & u_{12} & \cdot & \cdot & \cdot & \cdot & u_{1n} \\ 0 & u_{22} & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & & & & \\ \cdot & & \cdot & u_{kk} & \cdot & & \\ \cdot & & & & \cdot & \cdot & u_{n-1,n} \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & u_{nn} \end{bmatrix}$$

How to determine $\overline{\overline{\mathbf{L}}}$ and $\overline{\overline{\mathbf{U}}}$?

Linear Systems of Equations
Error Analysis

Vector and Matrix Norm

$$||\overline{\mathbf{x}}||_\infty = \max_i |x_i|$$

$$\left|\left|\overline{\overline{\mathbf{A}}}\right|\right|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$$

Properties

$$\overline{\overline{\mathbf{A}}} \neq \overline{\overline{\mathbf{0}}} \Rightarrow \left|\left|\overline{\overline{\mathbf{A}}}\right|\right| > 0$$

$$\left|\left|\alpha\overline{\overline{\mathbf{A}}}\right|\right| = |\alpha| \left|\left|\overline{\overline{\mathbf{A}}}\right|\right|$$

$$\left|\left|\overline{\overline{\mathbf{A}}} + \overline{\overline{\mathbf{B}}}\right|\right| \leq \left|\left|\overline{\overline{\mathbf{A}}}\right|\right| + \left|\left|\overline{\overline{\mathbf{B}}}\right|\right|$$

$$\left|\left|\overline{\overline{\mathbf{A}}}\,\overline{\overline{\mathbf{B}}}\right|\right| \leq \left|\left|\overline{\overline{\mathbf{A}}}\right|\right| \left|\left|\overline{\overline{\mathbf{B}}}\right|\right|$$

$$\left|\left|\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}\right|\right| \leq \left|\left|\overline{\overline{\mathbf{A}}}\right|\right| ||\overline{\mathbf{x}}||$$

Perturbed Right-hand Side

$$\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}} = \overline{\mathbf{b}}$$

$$\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}} + \delta\overline{\mathbf{x}}) = \overline{\mathbf{b}} + \delta\overline{\mathbf{b}}$$

Subtract original equation

$$\begin{aligned} \overline{\overline{\mathbf{A}}}\delta\overline{\mathbf{x}} &= \delta\overline{\mathbf{b}} \\ \delta\overline{\mathbf{x}} &= \overline{\overline{\mathbf{A}}}^{-1}\delta\overline{\mathbf{b}} \end{aligned}$$

$$\left.\begin{aligned} ||\delta\overline{\mathbf{x}}|| &\leq \left|\left|\overline{\overline{\mathbf{A}}}^{-1}\right|\right| \, ||\delta\overline{\mathbf{b}}|| \\ ||\overline{\mathbf{b}}|| = \left|\left|\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}\right|\right| &\leq \left|\left|\overline{\overline{\mathbf{A}}}\right|\right| \, ||\overline{\mathbf{x}}|| \end{aligned}\right\} \Rightarrow$$

Relative Error Magnification

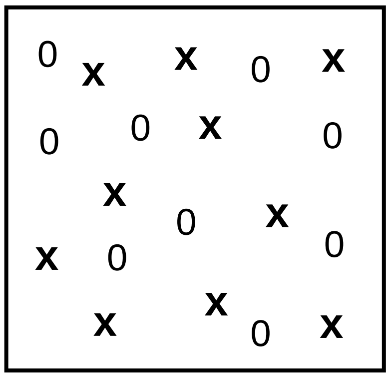
$$\frac{||\delta\overline{\mathbf{x}}||}{||\overline{\mathbf{x}}||} \leq \left|\left|\overline{\overline{\mathbf{A}}}^{-1}\right|\right| \left|\left|\overline{\overline{\mathbf{A}}}\right|\right| \frac{||\delta\overline{\mathbf{b}}||}{||\overline{\mathbf{b}}||}$$

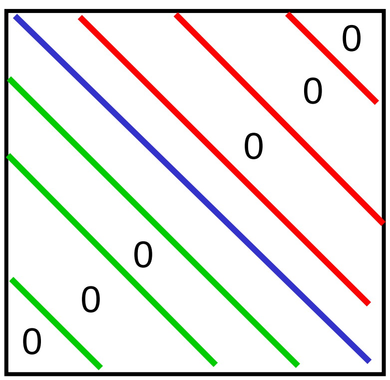
Condition Number

$$K(\overline{\overline{\mathbf{A}}}) = \left|\left|\overline{\overline{\mathbf{A}}}^{-1}\right|\right| \left|\left|\overline{\overline{\mathbf{A}}}\right|\right|$$

Linear Systems of Equations
Iterative Methods

Sparse, Full-bandwidth Systems





Rewrite Equations

$$\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}} = \overline{\mathbf{b}} \quad \Leftrightarrow \quad \sum_{j=1}^{n} a_{ij} x_j = b_i$$

$$a_{ii} \neq 0 \Rightarrow x_i = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j - \sum_{j=i+1}^{n} a_{ij} x_j}{a_{ii}} \;, \; i = 1, \ldots n$$

Iterative, Recursive Methods

Jacobi's Method

$$x_i^{(k+1)} = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)}}{a_{ii}} \;, \; i = 1, \ldots n$$

Gauss-Seidels's Method

$$x_i^{(k+1)} = \frac{b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k)}}{a_{ii}} \;, \; i = 1, \ldots n$$

Linear Systems of Equations
Iterative Methods

Convergence

$$\left\|\overline{\mathbf{x}}^{(k+1)} - \overline{\mathbf{x}}\right\| \rightarrow 0 \;\; \text{for} \;\; k \rightarrow \infty$$

Iteration – Matrix form

$$\overline{\mathbf{x}}^{(k+1)} = \overline{\overline{\mathbf{B}}}\overline{\mathbf{x}}^{(k)} + \overline{\mathbf{c}}\;,\;\; k = 0, \ldots$$

Decompose Coefficient Matrix

$$\overline{\overline{\mathbf{A}}} = \overline{\overline{\mathbf{D}}}\left(\overline{\overline{\mathbf{L}}} + \overline{\overline{\mathbf{I}}} + \overline{\overline{\mathbf{U}}}\right)$$

with

$$\overline{\overline{\mathbf{D}}} = \text{diag}\; a_{ii}$$

$$\overline{\overline{\mathbf{L}}} = \begin{cases} a_{ij}/a_{ii}\;, & i > j \\ 0, & i \leq j \end{cases}$$

Note: NOT LU-factorization

$$\overline{\overline{\mathbf{U}}} = \begin{cases} a_{ij}/a_{ii}\;, & i < j \\ 0, & i \geq j \end{cases}$$

Jacobi's Method

$$\overline{\mathbf{x}}^{(k+1)} = -\left(\overline{\overline{\mathbf{L}}} + \overline{\overline{\mathbf{U}}}\right)\overline{\mathbf{x}}^{(k)} + \overline{\overline{\mathbf{D}}}^{-1}\overline{\mathbf{b}}$$

Iteration Matrix form

$$\begin{aligned} \overline{\overline{\mathbf{B}}} &= -\left(\overline{\overline{\mathbf{L}}} + \overline{\overline{\mathbf{U}}}\right) \\ \overline{\mathbf{c}} &= \overline{\overline{\mathbf{D}}}^{-1}\overline{\mathbf{b}} \end{aligned}$$

Convergence Analysis

$$\begin{aligned} \overline{\mathbf{x}}^{(k+1)} &= \overline{\overline{\mathbf{B}}}\overline{\mathbf{x}}^{(k)} + \overline{\mathbf{c}} \\ \overline{\mathbf{x}} &= \overline{\overline{\mathbf{B}}}\overline{\mathbf{x}} + \overline{\mathbf{c}} \\ \hline \overline{\mathbf{x}}^{(k+1)} - \overline{\mathbf{x}} &= \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right) \\ &= \overline{\overline{\mathbf{B}}} \cdot \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k-1)} - \overline{\mathbf{x}}\right) \\ &\;\;. \\ &= \overline{\overline{\mathbf{B}}}^{k+1}\left(\overline{\mathbf{x}}^{(0)} - \overline{\mathbf{x}}\right) \end{aligned}$$

$$\left\|\overline{\mathbf{x}}^{(k+1)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\overline{\mathbf{B}}}^{k+1}\right\| \left\|\overline{\mathbf{x}}^{(0)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\overline{\mathbf{B}}}\right\|^{k+1} \left\|\overline{\mathbf{x}}^{(0)} - \overline{\mathbf{x}}\right\|$$

Sufficient Convergence Condition

$$\boxed{\left\|\overline{\overline{\mathbf{B}}}\right\| < 1}$$

Linear Systems of Equations
Iterative Methods

Sufficient Convergence Condition

$$\left\|\overline{\overline{\mathbf{B}}}\right\| < 1$$

Jacobi's Method

$$b_{ij} = -\frac{a_{ij}}{a_{ii}}\,,\; i \neq j$$

$$\left\|\overline{\overline{\mathbf{B}}}\right\|_\infty = \max_i \sum_{j=1, j\neq i}^{n} \frac{|a_{ij}|}{|a_{ii}|}$$

Sufficient Convergence Condition

$$\sum_{j=1, j\neq i}^{n} |a_{ij}| < |a_{ii}|$$

Diagonal Dominance

Stop Criterion for Iteration

$$\begin{aligned}\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}} &= \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k-1)} - \overline{\mathbf{x}}\right) \qquad \pm\overline{\overline{\mathbf{B}}}\,\overline{\mathbf{x}}^{(k)} \\ &= -\overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right) + \overline{\overline{\mathbf{B}}}\left(\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right)\end{aligned}$$

$$\left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\overline{\mathbf{B}}}\right\| \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right\| + \left\|\overline{\overline{\mathbf{B}}}\right\| \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\|$$

$$\left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\| \leq \frac{\left\|\overline{\overline{\mathbf{B}}}\right\|}{1 - \left\|\overline{\overline{\mathbf{B}}}\right\|} \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right\|$$

$$\left\|\overline{\overline{\mathbf{B}}}\right\| < 1/2 \Rightarrow \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}\right\| \leq \left\|\overline{\mathbf{x}}^{(k)} - \overline{\mathbf{x}}^{(k-1)}\right\|$$

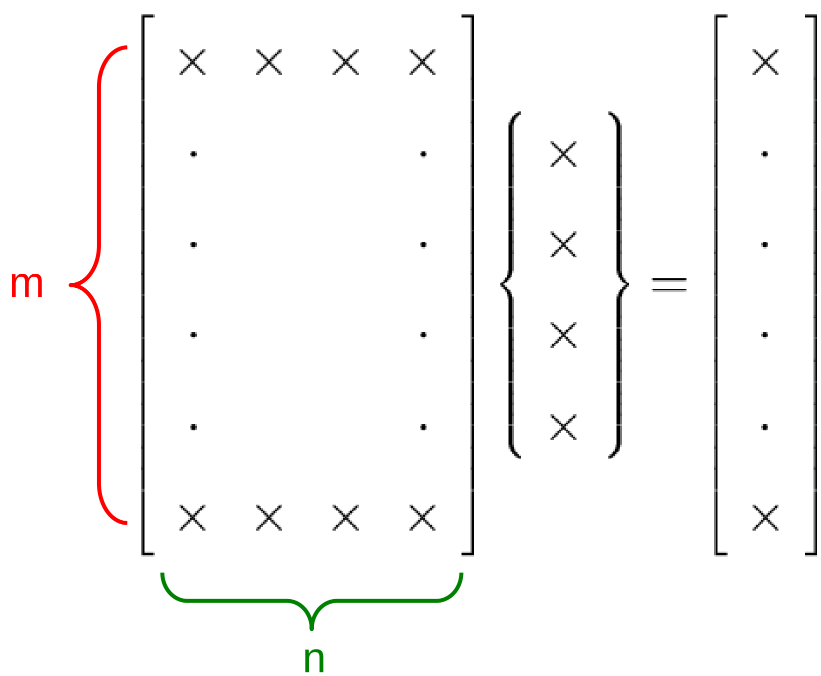
Least Square Approximation

Linear Measurement Model

n model parameters

$$\overline{\overline{\mathbf{A}}}\,\overline{\mathbf{x}} = \overline{\mathbf{b}}$$

m measurements



Overdetermined System

m measurements
n unknowns
m > n

Least Square Solution

Minimize Residual Norm

$$\overline{\mathbf{r}} = \overline{\mathbf{b}} - \overline{\overline{\mathbf{A}}}\,\overline{\mathbf{x}}$$

$$||r||_2 = (\overline{\mathbf{r}}^T \overline{\mathbf{r}})^{1/2}$$

Least Square Approximation

Theorem

If $\overline{\overline{\mathbf{A}}}^T\left(\overline{\mathbf{b}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}\right)=0 \Rightarrow \forall y \mid \left\|\overline{\mathbf{b}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}\right\|_2 \leq \left\|\overline{\mathbf{b}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{y}}\right\|_2$

Proof

$$\left.\begin{array}{l}\overline{\mathbf{r}}_x=\overline{\mathbf{b}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}\\ \overline{\mathbf{r}}_y=\overline{\mathbf{b}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{y}}\end{array}\right\}\Rightarrow$$

$$\overline{\mathbf{r}}_y=(\overline{\mathbf{b}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}})+(\overline{\overline{\mathbf{A}}}\overline{\mathbf{x}}-\overline{\overline{\mathbf{A}}}\overline{\mathbf{y}})=\overline{\mathbf{r}}_x+\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}}-\overline{\mathbf{y}})$$

$$\overline{\mathbf{r}}_y^T\overline{\mathbf{r}}_y=\overline{\mathbf{r}}_x^T\overline{\mathbf{r}}_x+(\overline{\mathbf{x}}-\overline{\mathbf{y}})^T\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}}-\overline{\mathbf{y}})+(\overline{\mathbf{x}}-\overline{\mathbf{y}})^T\overline{\overline{\mathbf{A}}}^T\overline{\mathbf{r}}_x+r_x^T\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}}-\overline{\mathbf{y}})$$

$$\overline{\overline{\mathbf{A}}}^T\overline{\mathbf{r}}_x = \overline{\mathbf{0}}$$

$$\overline{\mathbf{r}}_x^T\overline{\overline{\mathbf{A}}} = \left(\overline{\overline{\mathbf{A}}}^T\overline{\mathbf{r}}_x\right)^T=\overline{\mathbf{0}}$$

$$\overline{\mathbf{r}}_y^T\overline{\mathbf{r}}_y = \overline{\mathbf{r}}_x^T\overline{\mathbf{r}}_x+(\overline{\mathbf{x}}-\overline{\mathbf{y}})^T\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}}-\overline{\mathbf{y}})$$

$$\Rightarrow$$

$$||\overline{\mathbf{r}}_y||_2^2 = ||\overline{\mathbf{r}}_x||_2^2+\left\|\overline{\overline{\mathbf{A}}}(\overline{\mathbf{x}}-\overline{\mathbf{y}})\right\|_2^2 \geq ||\overline{\mathbf{r}}_x||_2^2$$

q.e.d

Normal Equation

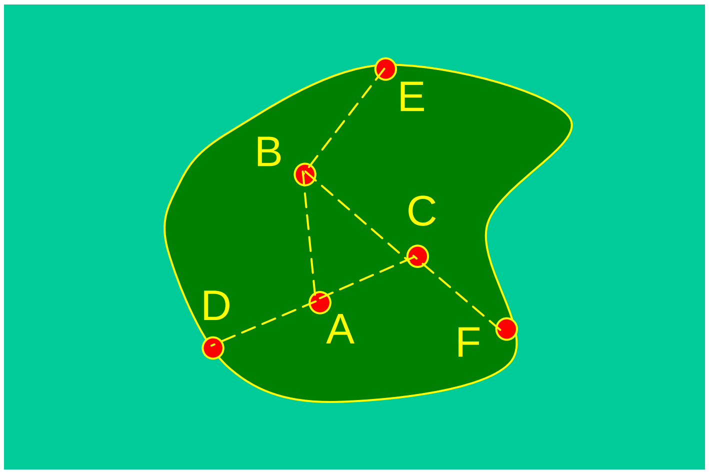
$$\left(\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}\right)\overline{\mathbf{x}}=\overline{\overline{\mathbf{A}}}^T\overline{\mathbf{b}}$$

$$\overline{\overline{\mathbf{C}}}=\overline{\overline{\mathbf{A}}}^T\overline{\overline{\mathbf{A}}}$$

Symmetric n x n matrix. Non-singular if columns of A are linearly independent

Least Square Approximation
Parameter estimation

Example
Island Survey



Points D, E, and F at sea level. Find altitude of inland points A, B, and C.

```
A=[ [1 0 0 -1 0 -1]' [0 1 0 1 -1 0]' [0 0 1 0 1 1]']
b=[1 2 3 1 2 1]';
C=A'*A
c=A'*b
% Least square solution
z=inv(C)*c
% Residual
r=b-A*z
rn=sqrt(r'*r)
```

lstsq.m

Measured Altitude Differences

$$h_{DA} = 1\ ,\ h_{EB} = 2\ ,\ h_{FC} = 3\ ,\ h_{AB} = 1\ ,\ h_{BC} = 2\ ,\ h_{AC} = 1$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ -1 & 0 & 1 \end{bmatrix} \begin{Bmatrix} z_A \\ z_B \\ z_C \end{Bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 1 \\ 2 \\ 1 \end{bmatrix}$$

Normal Equation

$$\begin{bmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{bmatrix} \begin{Bmatrix} z_A \\ z_B \\ z_C \end{Bmatrix} = \begin{bmatrix} -1 \\ 1 \\ 6 \end{bmatrix} \Rightarrow \begin{cases} z_A = \frac{5}{4} \\ z_B = \frac{7}{4} \\ z_C = 3 \end{cases}$$

Residual Vector

$$\bar{\mathbf{r}} = \frac{1}{4}[-1, 1, 0, 2, 3, -3]^T$$

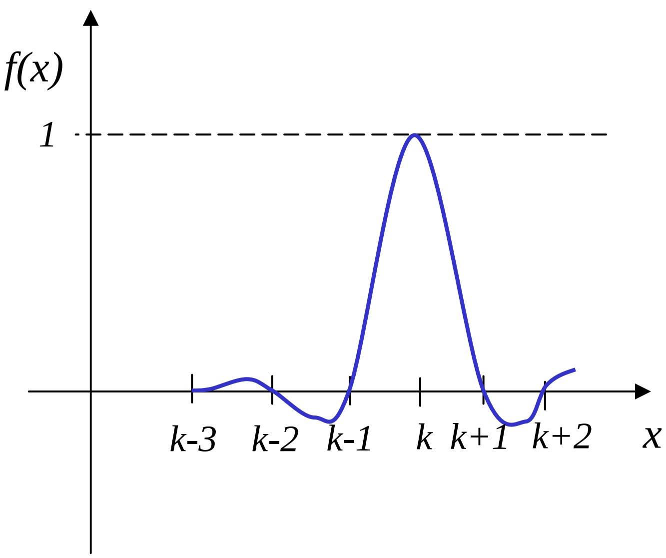
Numerical Interpolation
Lagrange Polynomials

$$p(x) = \sum_{k=0}^{n} L_k(x) f(x_k) = \sum_{k=0}^{n} L_k(x) f_k$$

$$L_k(x) = \sum_{i=0}^{n} \ell_{ik} x^i$$

$$L_k(x_i) = \delta_{ki} = \begin{cases} 0 & k \neq i \\ 1 & k = i \end{cases}$$

$$L_k(x) = \prod_{j=0, j\neq k}^{n} \frac{x - x_j}{x_k - x_j}$$



Difficult to program
Difficult to estimate errors
Divisions are expensive

Important for numerical integration

Numerical Integration

Lagrange Interpolation

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

$$f(x) \simeq p(x) = \sum_{k=0}^{n} L_k(x) f(x_k)$$

$$L_k(x) = \frac{(x-x_0)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_n)}{(x_k-x_0)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_n)}$$

Equidistant Sampling

$$x_k = x_0 + kh$$

$$x = x_0 + sh$$

$$L_k(x) = \frac{s(s-1)(s-2)\cdots(s-k+1)(s-k-1)\cdots(s-n)}{k(k-1)(k-2)\cdots(1)(-1)\cdots(k-n)}$$

$$I = \int_a^b f(x)dx \simeq \int_{x_0}^{x_n} p(x)dx = h\sum_{k=0}^{n} f(x_k)\int_0^n L_k(s)ds = nh\sum_{k=0}^{n} f(x_k)C_k^n$$

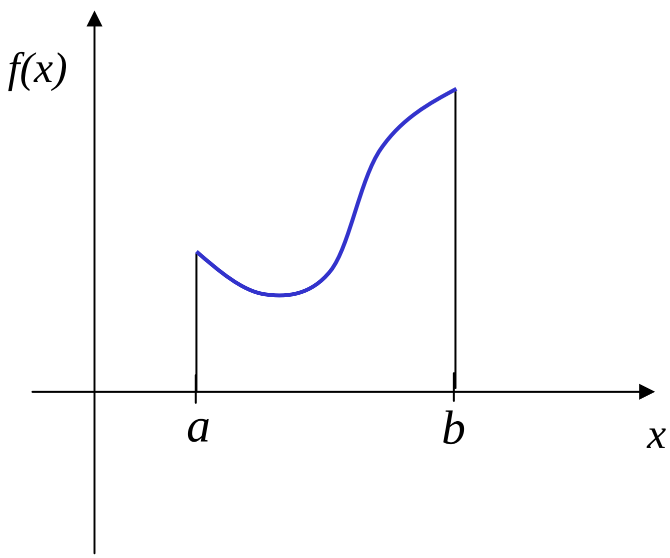
Integration Weights (Cote's Numbers)

$$C_k^n = \frac{1}{n}\int_0^n L_k(s)ds$$

Properties

$$C_k^n = C_{n-k}^n$$

$$\sum_{k=0}^{n} C_k^n = 1$$



Numerical Integration

$n = 1$

Trapezoidal Rule

$$k = 0: \quad C_0^1 = \int_0^1 \frac{s-1}{-1} ds = 1 - 1/2 = 0.5$$

$$k = 1: \quad C_1^1 = \int_0^1 \frac{s}{1} ds = 1/2 = 0.5$$

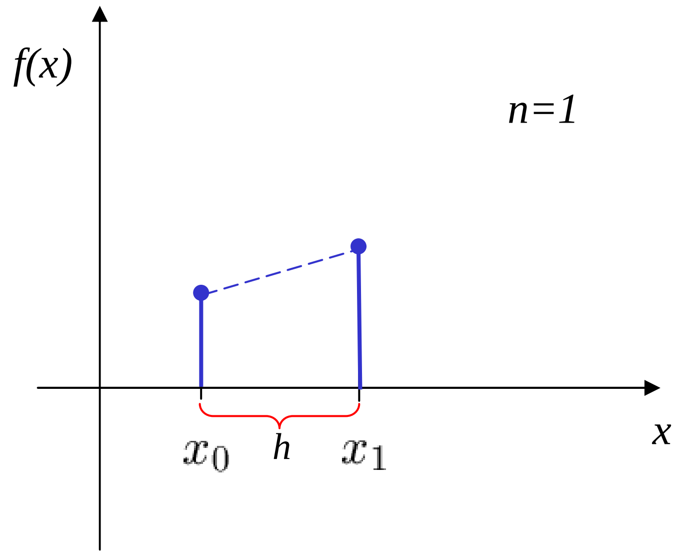
$$\int_{x_0}^{x_1} f(x)dx \simeq 1 \cdot (x_1 - x_0) \left(\frac{1}{2} f(x_0) + \frac{1}{2} f(x_1) \right) = \frac{1}{2}(x_1 - x_0)(f(x_0) + f(x_1))$$

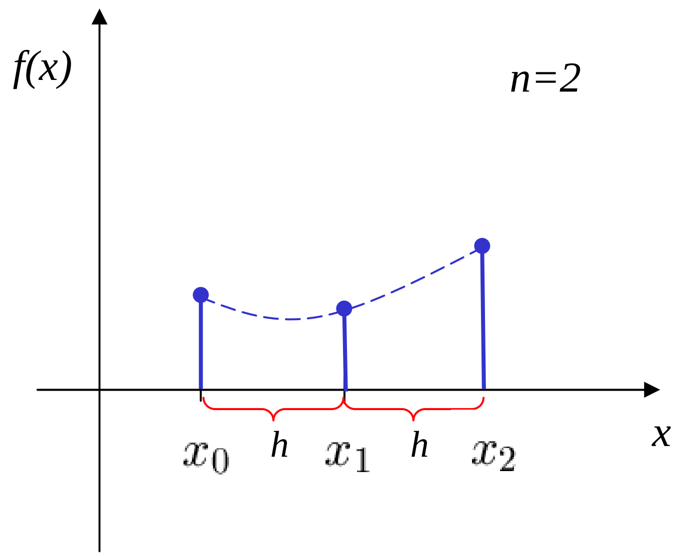
$n = 2$

Simpson's Rule

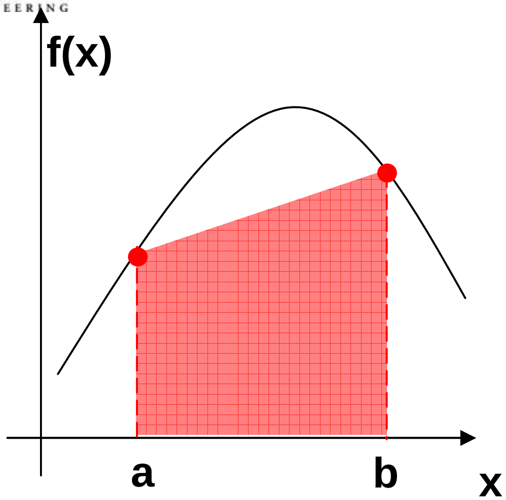
$$\begin{aligned}
k = 0: \quad C_0^2 &= \frac{1}{2} \int_0^2 \frac{(s-1)(s-2)}{(-1)(-2)} ds \\
&= \frac{1}{4} \int_0^2 (s^2 - 3s + 2) ds \\
&= \frac{1}{4} \left[\frac{s^3}{3} - \frac{3s^2}{2} + 2s \right] \\
&= \frac{1}{4} \left[\frac{8}{3} - \frac{12}{2} + 4 \right] = \frac{1}{4} \cdot \frac{4}{6} = \frac{1}{6} \\
k = 1: \quad C_1^2 &= \frac{1}{2} \int_0^2 \frac{s(s-2)}{(1)(-1)} ds \\
&= \frac{1}{2} \int_0^2 (2s - s^2) ds \\
&= \frac{1}{2} \left[s^2 - \frac{s^3}{3} \right] \\
&= \frac{1}{2} \left[4 - \frac{8}{3} \right] = \frac{2}{3} \\
k = 2: \quad C_2^2 &= C_0^2 = \frac{1}{6}
\end{aligned}$$

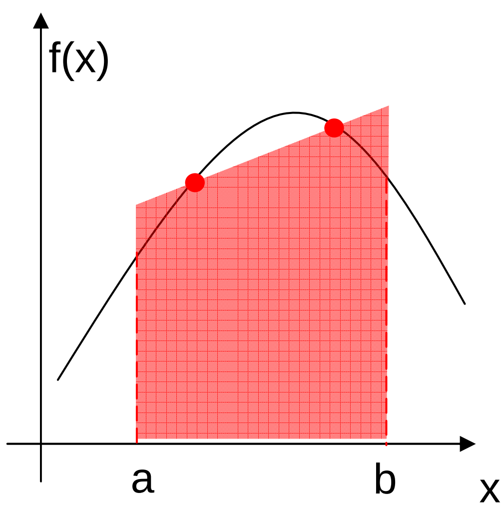
$$\int_{x_0}^{x_1} f(x)dx \simeq 2h \frac{1}{6} (f(x_0) + 4f(x_1) + f(x_2)) = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$$





Gaussian Quadrature





Trapezoidal Rule

$$I \simeq (b-a)\frac{f(a)+f(b)}{2}$$

$$I \simeq c_0 f(a) + c_1 f(b)$$

Exact Integration of const and linear f

$$c_0 + c_1 = \int_{-(b-a)/2}^{-(b-a)/2} 1 dx$$

$$-c_0\frac{b-a}{2} + c_1\frac{b-a}{2} = \int_{-(b-a)/2}^{-(b-a)/2} x dx$$

$$\begin{aligned} c_0 + c_1 &= b-a \\ -c_0\frac{a-b}{2} + c_1\frac{a-b}{2} &= 0 \\ &\Rightarrow \\ c_0 = c_1 &= \frac{b-a}{2} \end{aligned}$$

$$I \simeq \frac{b-a}{2}f(a) + \frac{b-a}{2}f(b)$$

Numerical Interpolation
Triangular Families of Polynomials

Ordered Polynimials

$$p(x) = c_0\phi_0(x) + c_1\phi_1(x) + \cdots + c_n\phi_n(x)$$

where

$$\begin{aligned}
\phi_0(x) &= a_{00} \\
\phi_1(x) &= a_{10} + a_{11}x \\
\phi_1(x) &= a_{20} + a_{21}x + a_{22}x^2 \\
&\cdot \\
&\cdot \\
\phi_n(x) &= a_{n0} + a_{n1}x + \cdots\cdots\cdots + a_{nn}x^n
\end{aligned}$$

Special form convenient for interpolation

$$\begin{aligned}
\phi_0(x) &= 1 \\
\phi_1(x) &= x - x_0 \\
\phi_2(x) &= (x - x_0)(x - x_1) \\
&\cdot \\
&\cdot \\
\phi_n(x) &= (x - x_0)(x - x_1)\cdots(x - x_{n-1})
\end{aligned}$$

Coefficients

$$\begin{aligned}
f(x_0) = p(x_0) &= c_0 \\
f(x_1) = p(x_1) &= c_0 + c_1(x_1 - x_0) \\
f(x_2) = p(x_2) &= c_0 + c_1(x_2 - x_0) + c_2(x_2 - x_0)
\end{aligned}$$

$c_0, \; c_1, \; \ldots c_n$ found by recursion

.

Numerical Interpolation
Newton's Iteration Formula

Standard triangular family of polynomials

$$
\begin{aligned}
f(x) &= p(x) + r(x) \\
&= c_0 + c_1(x - x_0) \cdots + c_n(x - x_0)\cdots(x - x_{n-1}) \\
&\quad + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)\cdots(x - x_n)
\end{aligned}
$$

Divided Differences

$$f(x_0) = c_0 \Rightarrow c_0 = \boxed{f(x_0)}$$

$$f(x_1) = c_0 + c_1(x_1 - x_0) \Rightarrow c_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \boxed{f[x_0, x_1]}$$

$$f(x_2) = c_0 + c_1(x_2 - x_0) + c_2(x_2 - x_0)(x_2 - x_1)$$

$$c_2 = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0} = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} = \boxed{f[x_0, x_1, x_2]}$$

$$c_n = \boxed{f[x_0, x_1, \ldots, x_n]} = \frac{f[x_1, \ldots, x_n] - f[x_0, \ldots x_{n-1}]}{x_n - x_0}$$

Newton's Computational Scheme

$c_0 = f(x_0)$, $c_1 = f[x_0, x_1]$, $c_2 = f[x_0, x_1, x_2]$, $c_3 = f[x_0, x_1, x_2, x_3]$

$x_0 \quad f(x_0)$

$\qquad f[x_0, x_1]$

$x_1 \quad f(x_1) \qquad f[x_0, x_1, x_2]$

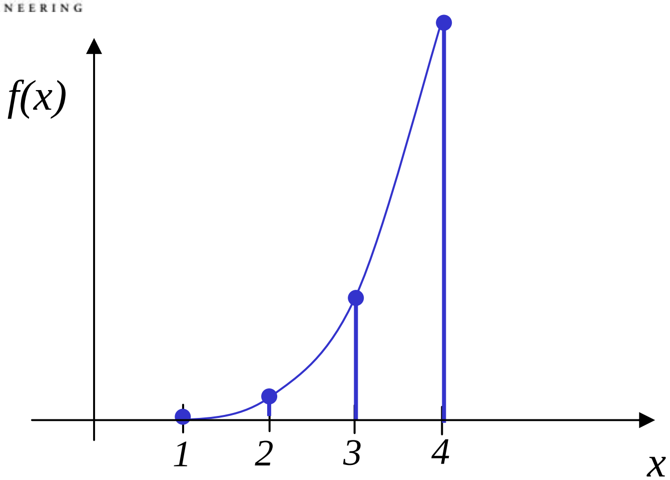
$\qquad f[x_1, x_2] \qquad f[x_0, x_1, x_2, x_3]$

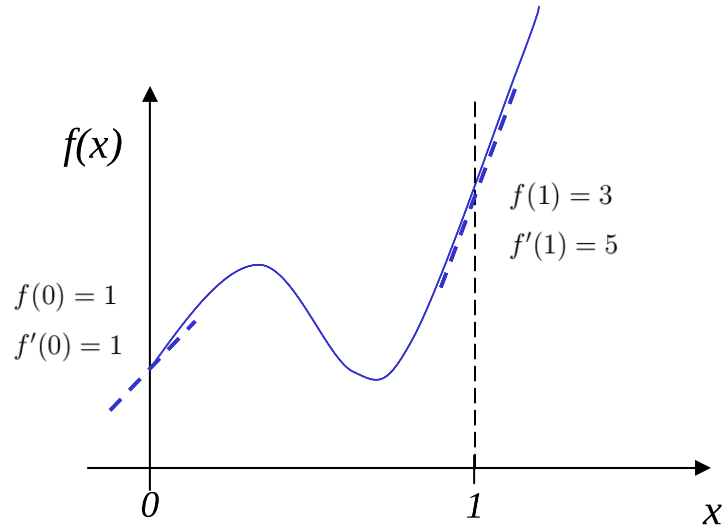
$x_2 \quad f(x_2) \qquad f[x_1, x_2, x_3]$

$\qquad f[x_2, x_3]$

$x_3 \quad f(x_3)$

Numerical Interpolation
Newton's Iteration Formula





i	x_i	$f(x_i)$
0	1	0
1	2	4
2	3	20
3	4	60

$$(4-0)/1 = 4 \qquad (20-4)/1 = 16 \qquad (60-20)/1 = 40$$

$$(16-4)/2 = 6 \qquad (40-16)/2 = 12$$

$$(12-6)/3 = 2$$

$$p(x) = 4(x-1) + 6(x-1)(x-2) + 2(x-1)(x-2)(x-3)$$

$$\lim_{\epsilon \to 0} f[x_0, x_0+\epsilon] = f'(x_0)$$

i	x_i	$f(x_i)$
0	0	1
1	$0(+\epsilon)$	$1(+\epsilon f'(0))$
2	$1(-\epsilon)$	$3(-\epsilon f'(1))$
3	1	60

$$f'(0) = 1 \qquad (3-1)/1 = 2 \qquad f'(1) = 5$$

$$(2-1)/1 = 1 \qquad (5-2)/1 = 3$$

$$(3-1)/1 = 2$$

$$p(x) = 1 + x + x^2 + 2x^2(x-1) = 1 + x - x^2 + 2x^3$$

Numerical Interpolation
Equidistant Newton Interpolation

Equidistant Sampling

$$x_i = x_0 + ih$$

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1}{h}(f_1 - f_0) = \frac{1}{h}\Delta f_0$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} = \frac{1}{1 \cdot 2 \cdot h^2}(f_2 - 2f_1 + f_0) = \frac{1}{2!h^2}\Delta^2 f_0$$

$$f[x_0, x_1, x_2, x_3] = \frac{1}{3! \cdot h^3}(f_3 - 3f_2 + 3f_1 - f_0) = \frac{1}{3!h^3}\Delta^3 f_0$$

Divided Differences
Stepsize Implied

$x_0 \quad f_0$

$f_1 - f_0 = \Delta f_0$

$x_1 \quad f_1$

$f_2 - 2f_1 + f_0 = \Delta^2 f_0$

$f_2 - f_1 = \Delta f_1$

$f_3 - 3f_2 + 3f_1 - f_0 - = \Delta^3 f_0$

$x_2 \quad f_2$

$f_3 - 2f_2 + f_1 = \Delta^2 f_1$

$f_3 - f_2 = \Delta f_2$

$x_3 \quad f_3$

$$c_0 = f_0$$
$$c_1 = \frac{1}{h}\Delta f_0$$
$$c_2 = \frac{1}{2!h^2}\Delta^2 f_0$$
$$c_3 = \frac{1}{3!h^3}\Delta^3 f_0$$

Triangular Family of Polynomials
Equidistant Sampling

$$f(x) = f_0 + \frac{\Delta f_0}{h}(x - x_0) + \frac{\Delta^2 f_0}{2!h^2}(x - x_0)(x - x_1) + \cdots$$
$$+ \frac{\Delta^n f_0}{n!h^n}(x - x_0)(x - x_1)\cdots(x - x_{n-1}) + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)\cdots(x - x_n)$$

Numerical Differentiation

Second order

$n = 2$

$$f(x) = f_0 + \frac{\Delta f_0}{h}(x-x_0) + \frac{\Delta^2 f_0}{2!h^2}(x-x_0)(x-x_1) + \frac{f'''(\xi)}{3!}(x-x_0)(x-x_1)(x-x_2) + \cdots$$

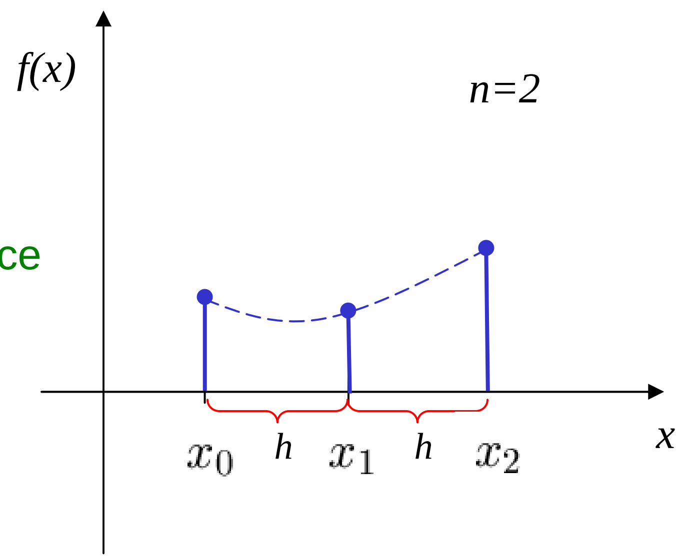
$$f'(x) = \frac{\Delta f_0}{h} + \frac{\Delta^2 f_0}{h}(x-x_0) + \frac{\Delta^2 f_0}{h}(x-x_1) + O(h^2)$$

$$\begin{aligned} f'(x_0) &= \frac{f_1 - f_0}{h} - \frac{1}{2h}(f_2 - 2f_1 + f_0) + O(h^2) \\ &= \frac{2f_1 - 2f_0 - f_2 + 2f_1 - f_0}{2h} + O(h^2) \\ &= \boxed{\frac{1}{h}(-\frac{3}{2}f_0 + 2f_1 - \frac{1}{2}f_2) + O(h^2)} \end{aligned}$$

Forward Difference

$$\begin{aligned} f'(x_1) &= \frac{f_1 - f_0}{h} + \frac{1}{2h}(f_2 - 2f_1 + f_0) + O(h^2) \\ &= \boxed{\frac{1}{2h}(f_2 - f_0) + O(h^2)} \end{aligned}$$

Central Difference



Second Derivatives

n=2 $$f''(x_0) = \frac{\Delta^2 f_0}{h^2} + O(h) = \boxed{\frac{1}{h^2}(f_0 - 2f_1 + f_2) + O(h)}$$ Forward Difference

n=3 $$f''(x_1) = \boxed{\frac{1}{h^2}(f_0 - 2f_1 + f_2) + O(h^2)}$$ Central Difference

Ordinary Differential Equations
Initial Value Problems

Euler's Method

Differential Equation

$$\frac{dy}{dx} = f(x,y) \ , \ y_0 = p$$

Example

$$f(x,y) = x \ (y = x^2/2 + p)$$

Discretization

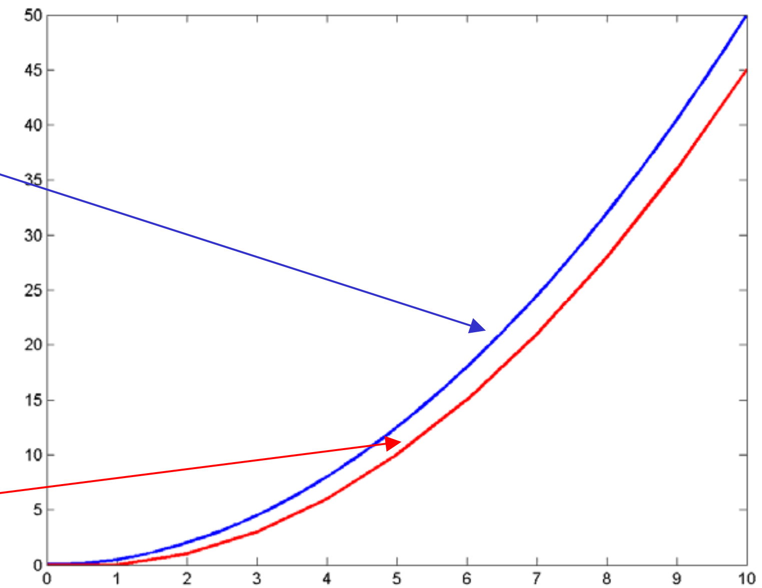
$$x_n = nh$$

Finite Difference (forward)

$$\frac{dy}{dx}|_{x=x_n} \simeq \frac{y_{n+1} - y_n}{h}$$

Recurrence

$$y_{n+1} = y_n + hf(nh, y_n)$$



euler.m

Initial Value Problems
Runge-Kutta Methods

Initial Value Problem

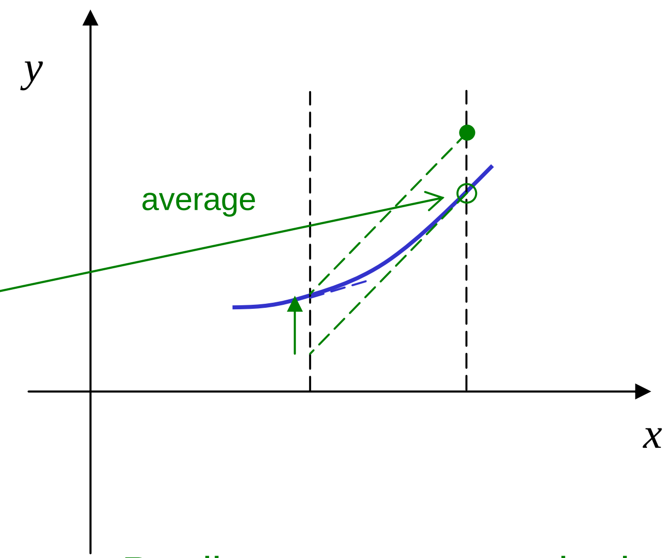
$$y' = f(x,y)$$
$$y(x_0) = y_0$$
$$x_n = x_0 + nh$$

2nd Order Runge-Kutta

$$\begin{aligned} y_{n+1} &= y_n + \tfrac{1}{2}(k_1 + k_2) \\ k_1 &= hf(x_n, y_n) \\ k_2 &= hf(x_n + h, y_n + k_1) \end{aligned}$$

4th Order Runge-Kutta

$$\begin{aligned} y_{n+1} &= y_n + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\ k_1 &= hf(x_n, y_n) \\ k_2 &= hf(x_n + \tfrac{h}{2}, y_n + \tfrac{k_1}{2}) \\ k_3 &= hf(x_n + \tfrac{h}{2}, y_n + \tfrac{k_2}{2}) \\ k_4 &= hf(x_n + h, y_n + k_3) \end{aligned}$$



Predictor-corrector method

Second-order RK methods

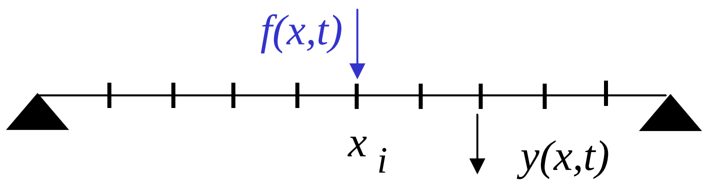
b = ½, a = ½ : Heun's method

b= 1, a = 0 : Midpoint method

b =2/3, a = 1/3 : Ralston's Method

Boundary Value Problems
Finite Difference Methods

Forced Vibration of a String



Harmonic excitation

$$f(x,t) = f(x)\cos(\omega t)$$

Differential Equation

$$\frac{d^2y}{dx^2} + k^2 y = f(x)$$

Boundary Conditions

$$y(0) = 0\,, \quad y(L) = 0$$

Finite Difference

$$\left.\frac{d^2y}{dx^2}\right|_{x_i} \simeq \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}$$

Discrete Difference Equations

$$y_{i-1} + \left((kh)^2 - 2\right) y_i - y_{i+1} = f(x_i)h^2$$

Matrix Form

$$\begin{bmatrix} (kh)^2-2 & 1 & \cdot & \cdot & \cdot & \cdot & 0 \\ 1 & (kh)^2-2 & 1 & & & & \cdot \\ \cdot & & \cdot & \cdot & & & \cdot \\ \cdot & & 1 & (kh)^2-2 & 1 & & \cdot \\ \cdot & & & \cdot & \cdot & & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & 1 & (kh)^2-2 \end{bmatrix} \overline{\mathbf{x}} = \begin{Bmatrix} f(x_1)h^2 \\ \cdot \\ \cdot \\ f(x_i)h^2 \\ \cdot \\ \cdot \\ f(x_n)h^2 \end{Bmatrix}$$

Tridiagonal Matrix

$kh < 1$ Symmetric, positive definite: No pivoting needed

Partial Differential Equations

Quasi-linear PDE

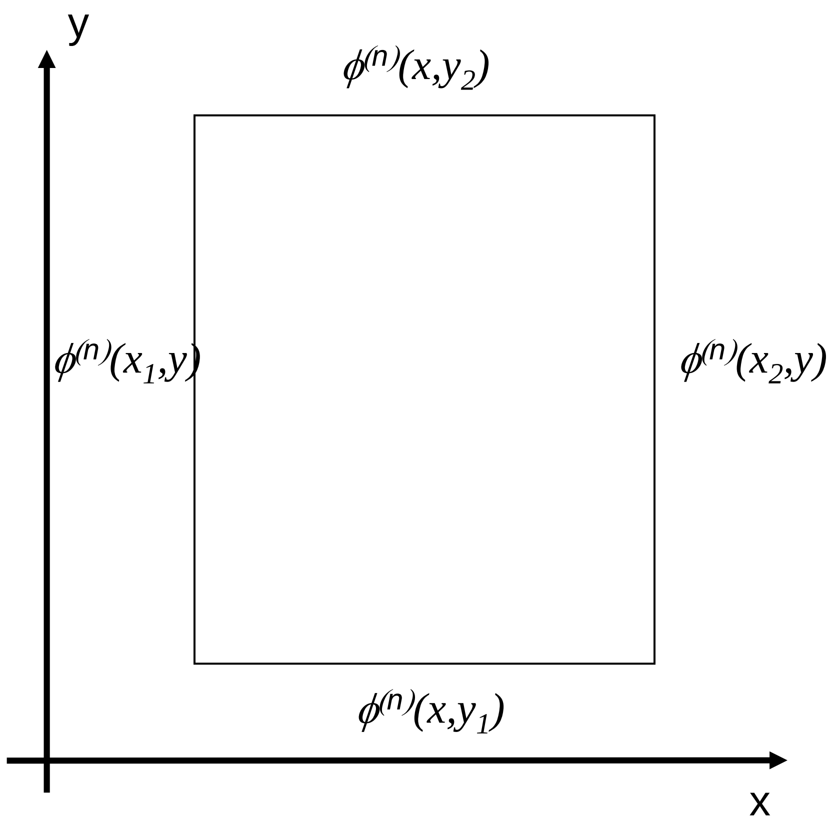
$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} = F(x, y, \phi, \phi_x, \phi_y)$$

A,B and C Constants

$$B^2 - 4AC > 0$$ Hyperbolic

$$B^2 - 4AC = 0$$ Parabolic

$$B^2 - 4AC < 0$$ Elliptic



Partial Differential Equations
Hyperbolic PDE

Waves on a String

$$\rho u^{tt}(x,t) = T u_{xx}(x,t),\ \ 0 < x < L\ ,\ 0 < t < \infty$$

Initial Conditions

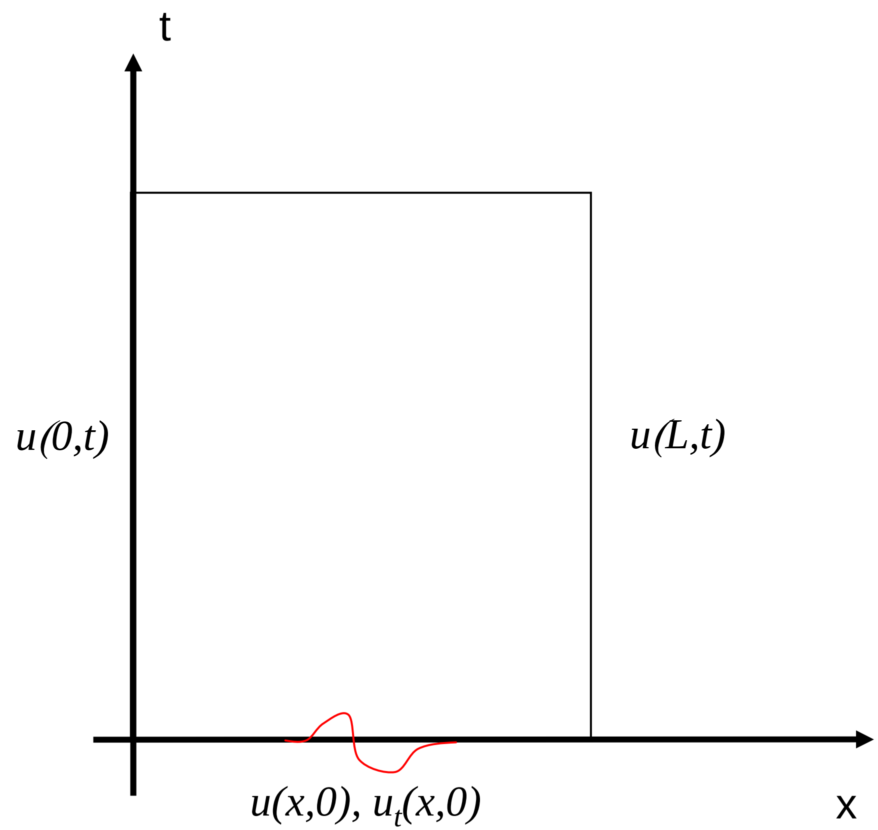
$$\begin{aligned} u(x,0) &= f(x),\ \ 0 \le x \le L \\ u_t(x,0) &= g(x),\ \ 0 < x < L \end{aligned}$$

Boundary Conditions

$$\begin{aligned} u(0,t) &= 0,\ ,\ 0 < t < \infty \\ u(L,t) &= 0,\ ,\ 0 < t < \infty \end{aligned}$$

Wave Solutions

$$u = \begin{cases} F(x-ct) & \text{Forward propagating wave} \\ G(x+ct) & \text{Backward propagating wave} \end{cases}$$



Typically Initial Value Problems in Time, Boundary Value Problems in Space
Time-Marching Solutions – Explicit Schemes Generally Stable

Partial Differential Equations
Hyperbolic PDE

Dimensionless Wave Speed

$$C = \frac{ck}{h}$$

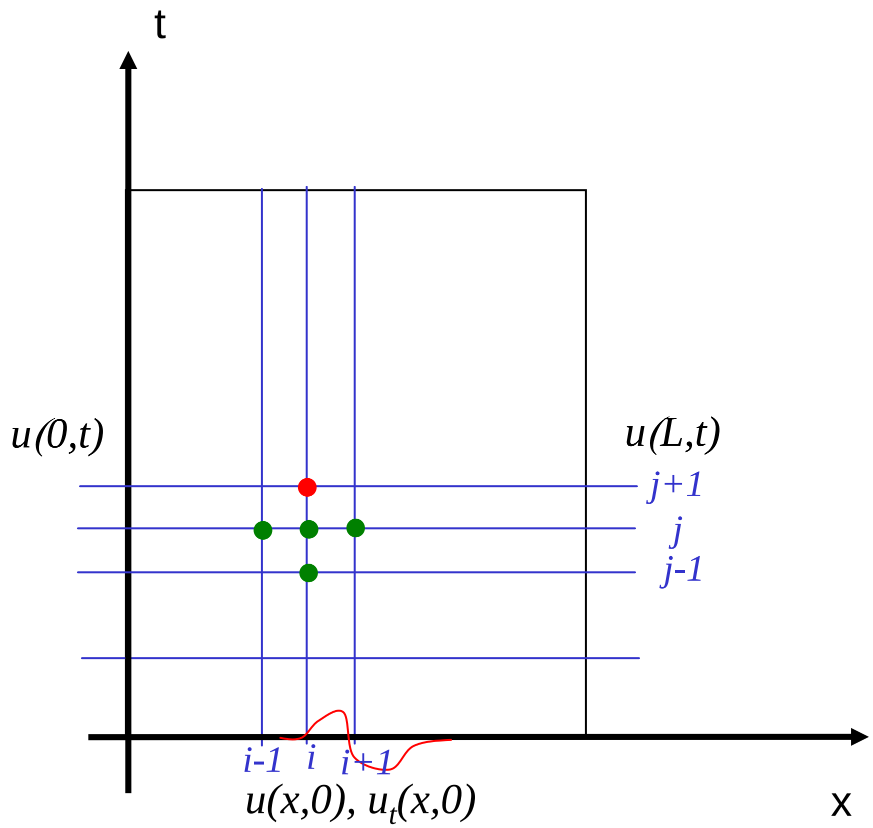
$$u_{i,j-1} - 2u_{i,j} + u_{i,j+1} = C^2(u_{i-1,j} - 2u_{i,j} + u_{i+1,j})$$

Explicit Finite Difference Scheme

$$u_{i,j+1} = (2 - 2C^2)u_{i,j} + C^2(u_{i+1,j} + u_{i-1,j}) - u_{i,j-1}, \quad i = 2, \ldots n-1$$

Stability Requirement

$$C = \frac{ck}{h} < 1$$



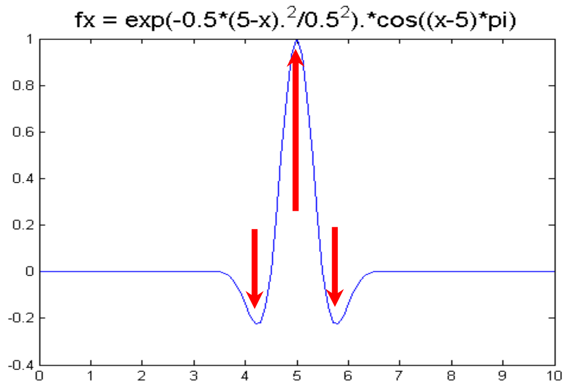
Waves on a String

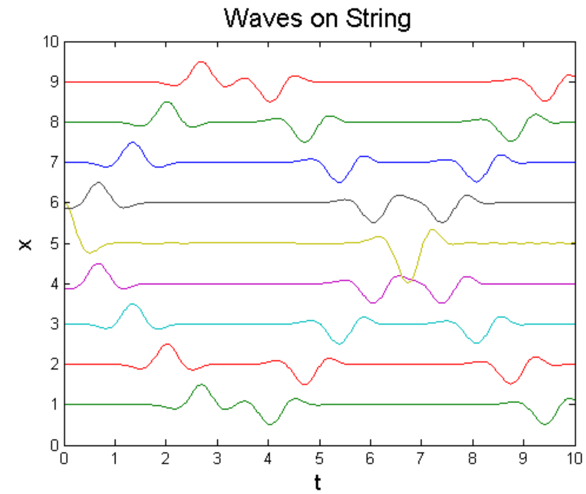
waveeq.m

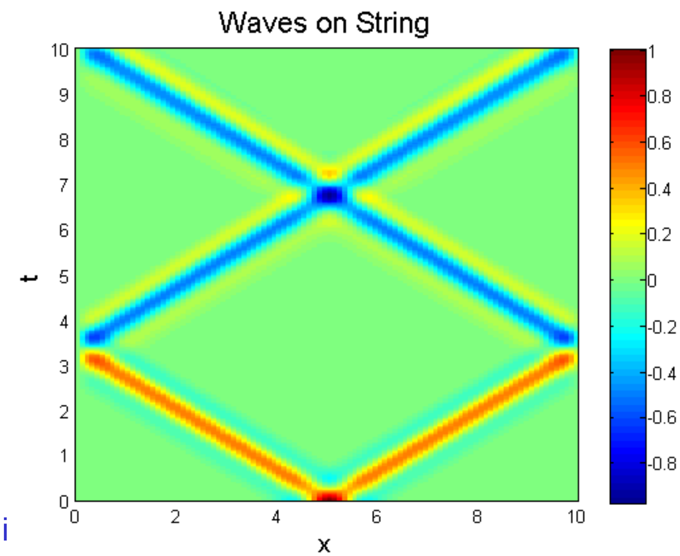
```
L=10;
T=10;
c=1.5;
N=100;
h=L/N;
M=400;
k=T/M;
C=c*k/h
Lf=0.5;
x=[0:h:L]';
t=[0:k:T];
%fx=['exp(-0.5*(' num2str(L/2) '-x).^2/(' num2str(Lf) ').^2)'];
%gx='0';
fx='exp(-0.5*(5-x).^2/0.5^2).*cos((x-5)*pi)';
gx='0';
f=inline(fx,'x');
g=inline(gx,'x');

n=length(x);
m=length(t);
u=zeros(n,m);
u(2:n-1,1)=f(x(2:n-1));
for i=2:n-1
 u(i,2) = (1-C^2)*u(i,1) + k*g(x(i)) +C^2*(u(i-1,1)+u(i+1,1))/2;
end

for j=2:m-1
   for i=2:n-1
u(i,j+1)=(2-2*C^2)*u(i,j) + C^2*(u(i+1,j)+u(i-1,j)) - u(i,j-1);
   end
end
```







Partial Differential Equations
Parabolic PDE

Heat Flow Equation

$$\kappa u_{xx}(x,t) = \sigma\rho u_t(x,t),\ 0 < x < L\ ,\ 0 < t < \infty$$

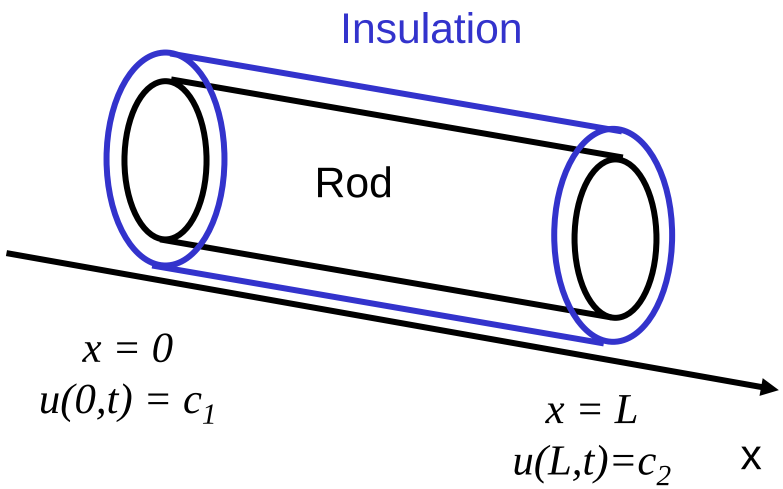
Initial Condition

$$u(x,0) = f(x),\ 0 \leq x \leq L$$

Boundary Conditions

$$\begin{aligned} u(0,t) &= c_1\ ,\ 0 < t < \infty \\ u(L,t) &= c_2\ ,\ 0 < t < \infty \end{aligned}$$

κ Thermal conductivity
σ Specific heat
ρ Density
u Temperature



IVP in one dimension, BVP in the other
Marching, Explicit or Implicit Schemes

Partial Differential Equations
Parabolic PDE

Dimensionless Flow Speed

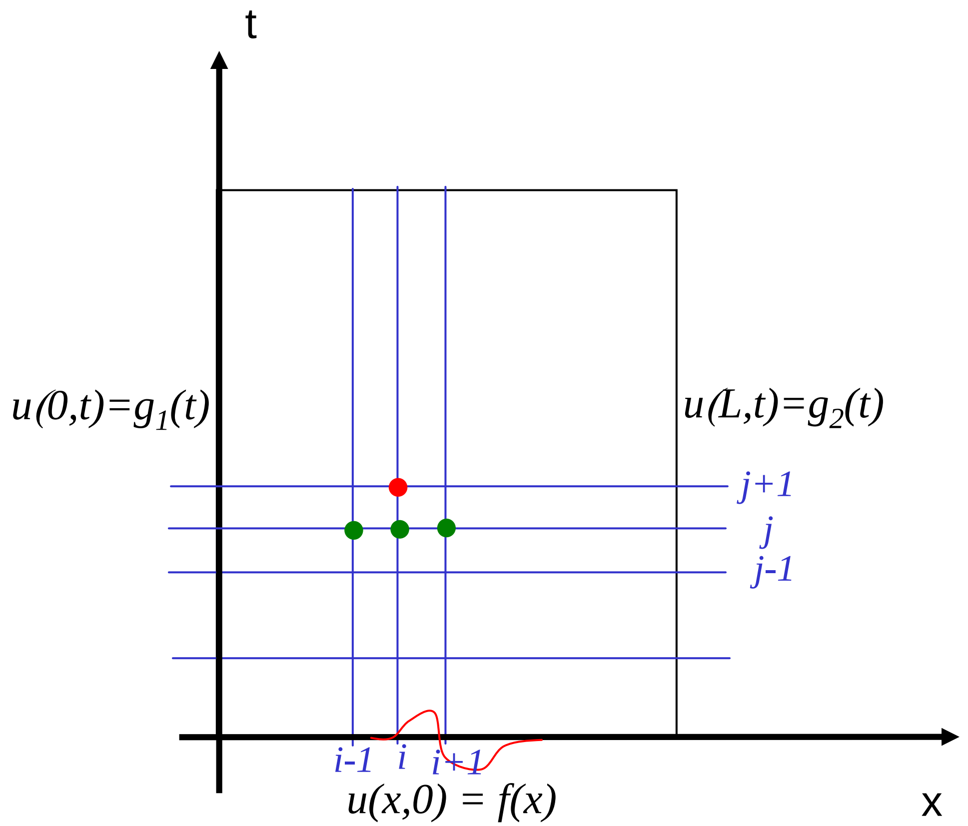
$$r = \frac{c^2 k}{h^2}$$

Explicit Finite Difference Scheme

$$u_{i,j+1} = (1 - 2r)u_{i,j} + r(u_{i-1,j} + u_{i+1,j})$$

Stability Requirement

$r <= 0.5$



Heat Flow Equation
Explicit Finite Differences

heat_fw.m

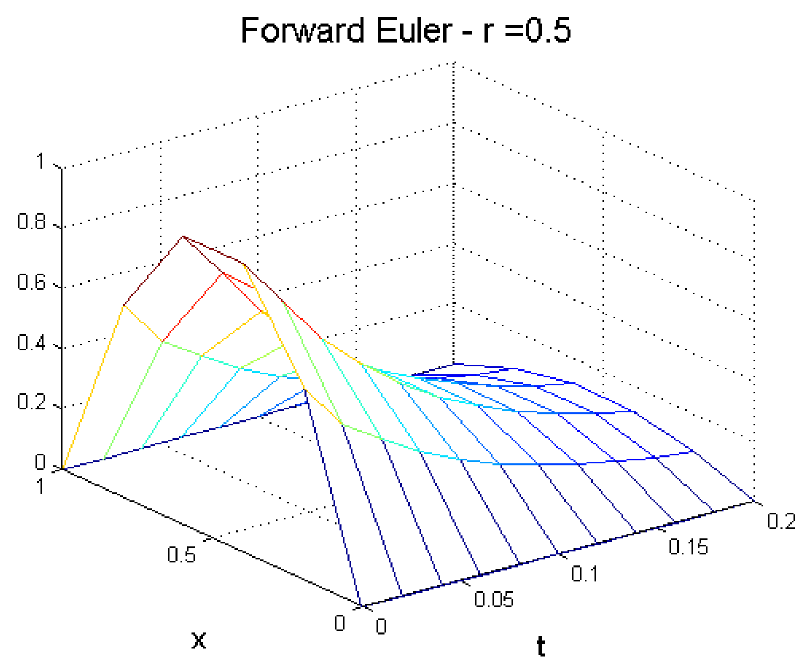
```
L=1; T=0.2; c=1;
N=5; h=L/N;
M=10; k=T/M;
r=c^2*k/h^2

x=[0:h:L]';
t=[0:k:T];
fx='4*x-4*x.^2';
g1x='0';
g2x='0';
f=inline(fx,'x');
g1=inline(g1x,'t');
g2=inline(g2x,'t');
n=length(x);
m=length(t);
u=zeros(n,m);
u(2:n-1,1)=f(x(2:n-1));
u(1,1:m)=g1(t);
u(n,1:m)=g2(t);
for j=1:m-1
    for i=2:n-1
u(i,j+1)=(1-2*r)*u(i,j) + r*(u(i+1,j)+u(i-1,j));
    end
end
 .
figure(4)
mesh(t,x,u);
a=ylabel('x');
set(a,'Fontsize',14);
a=xlabel('t');
set(a,'Fontsize',14);
a=title(['Forward Euler - r =' num2str(r)]);
set(a,'Fontsize',16);
```

$$u_t(x,t) = u_{xx}(x,t)\ ,\quad 0 < x < 1\ ,\quad 0 < t < 0.0$$

$$u(x,0) = f(x) = 4x - 4x^2$$

$$\begin{aligned} u(0,t) &= g_1(t) \equiv 0 \\ u(1,t) &= g_2(t) \equiv 0 \end{aligned}$$



Partial Differential Equations
Elliptic PDE

Laplace Equation

$$\nabla^2 u = \frac{u(x_{i-1},y_j) + u(x_i,y_{j-1}) - 4u(x_i,y_j) + u(x_{i+1},y_j) + u(x_i,y_{j+1})}{h^2} = 0$$

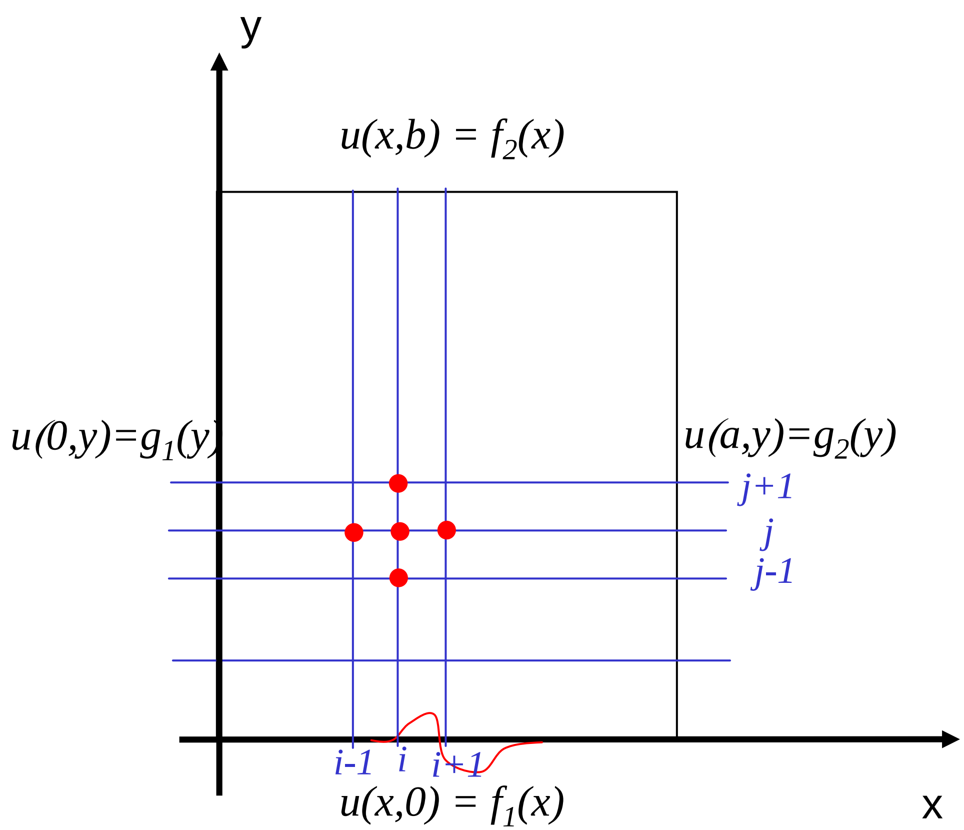
$$u_{i,j} = u(x_i, t_j)$$

Finite Difference Scheme

$$u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = 0$$

Boundary Conditions

$$\begin{aligned}
u(x_1,y_j) &= u_{1,j}\ ,\quad 2 \le j \le m-1 \\
u(x_n,y_j) &= u_{n,j}\ ,\quad 2 \le j \le m-1 \\
u(x_i,y_1) &= u_{i,1}\ ,\quad 2 \le j \le n-1 \\
u(x_i,y_n) &= u_{i,n}\ ,\quad 2 \le j \le n-1
\end{aligned}$$



Global Solution Required

Elliptic PDEs
Iterative Schemes

Finite Difference Scheme

$$u_{n+1,j} + u_{n-1,j} + u_{n,j+1} + u_{n,j-1} - 4u_{n,j} = 0$$

Liebman Iterative Scheme

$$u_{i,j}^{k+1} = u_{i,j}^{k} + r_{i,j}^{k}$$

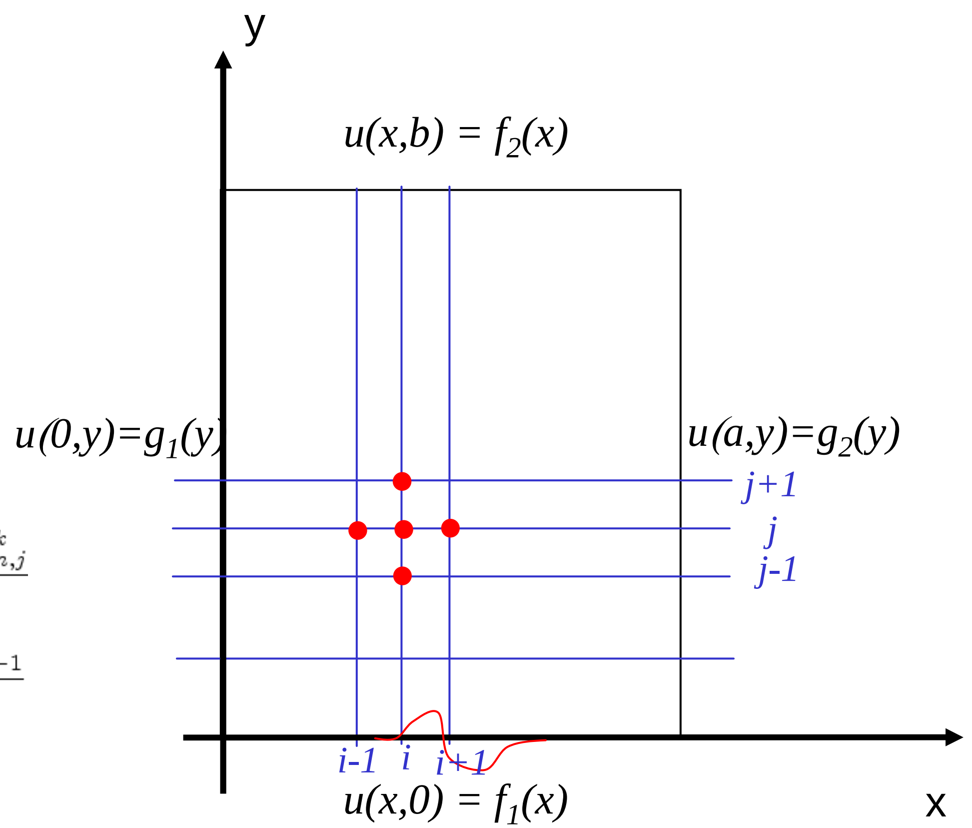
$$r_{i,j} = \frac{u_{n+1,j} + u_{n-1,j} + u_{n,j+1} + u_{n,j-1} - 4u_{n,j}}{4}$$

SOR Iterative Scheme

$$\begin{aligned} u_{i,j}^{k+1} &= u_{i,j}^{k} + \omega r_{i,j}^{k} \\ &= u_{i,j}^{k} + \omega \frac{u_{n+1,j}^{k} + u_{n-1,j}^{k} + u_{n,j+1}^{k} + u_{n,j-1}^{k} - 4u_{n,j}^{k}}{4} \\ &= (1-\omega)u_{i,j}^{k} + \omega \frac{u_{n+1,j}^{k} + u_{n-1,j}^{k} + u_{n,j+1}^{k} + u_{n,j-1}^{k}}{4} \end{aligned}$$

Optimal SOR

$$\omega = \frac{4}{2 + \sqrt{4 - \left[\cos\left(\frac{\pi}{n-1}\right) + \cos\left(\frac{\pi}{m-1}\right)\right]^2}}$$



Galerkin's Method
Viscous Flow in Duct

Remainder

$$R = -\left[\sum_{i=1,3,5\ldots}^{N}\sum_{j=1,3,5\ldots}^{N} a_{ij}\cos i\frac{\pi}{2}x\cos j\frac{\pi}{2}y\left\{\left(i\frac{\pi}{2}\right)^2+\left(j\frac{\pi}{2}\right)^2\right\}-1\right]$$

Inner product

$$\left(R,\cos k\frac{\pi}{2}x\cos \ell\frac{\pi}{2}y\right)\ ,\ i,j=1,3,5,\ldots$$

Analytical Integration

$$a_{ij}=\left(\frac{8}{\pi^2}\right)^2\frac{(-1)^{(i+j)/2-1}}{ij(i^2+j^2)}$$

Galerkin Solution

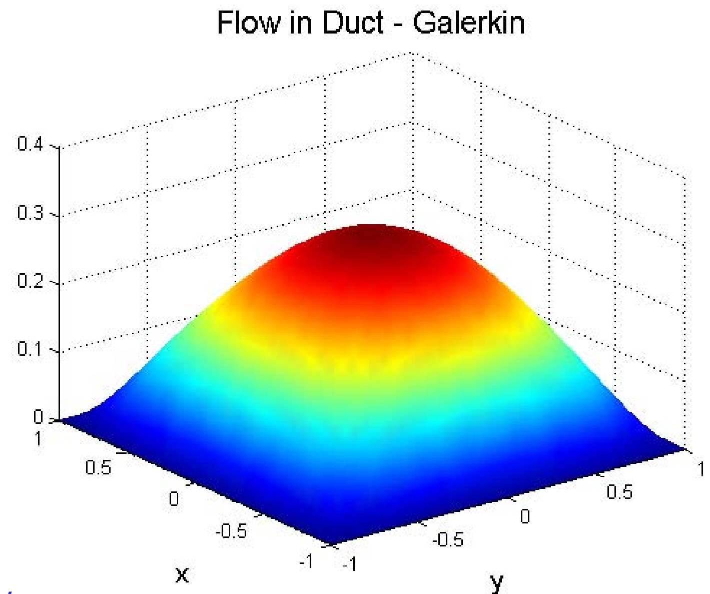
$$\tilde{w}=\left(\frac{8}{\pi^2}\right)^2\sum_{i=1,3,5\ldots}^{N}\sum_{j=1,3,5\ldots}^{N}\frac{(-1)^{(i+j)/2-1}}{ij(i^2+j^2)}\cos i\frac{\pi}{2}x\cos j\frac{\pi}{2}y$$

Flow Rate

$$\begin{aligned}\dot{q} &= \int_{-1}^{1}\int_{-1}^{1}\tilde{w}(x,y)dxdy\\ &= 2\left(\frac{8}{\pi^2}\right)^3\sum_{i=1,3,5\ldots}^{N}\sum_{j=1,3,5\ldots}^{N}\frac{1}{i^2j^2(i^2+j^2)}\end{aligned}$$

duct_galerkin.m

```
x=[-1:h:1]';
y=[-1:h:1];
n=length(x); m=length(y); u=zeros(n,m);
Nt=5;
for j=1:n
 xx(:,j)=x; yy(j,:)=y;
end
for i=1:2:Nt
    for j=1:2:Nt
        u=u+(8/pi^2)^2*
          (-1)^((i+j)/2-1)/(i*j*(i^2+j^2))
          *cos(i*pi/2*xx).*cos(j*pi/2*yy);
    end
end
```



Finite Elements
2-dimensional Elements

$$\tilde{u} = \sum_{i=1}^{N}\sum_{j=1}^{N} N_{ij}(x)\overline{u}_{ij}$$

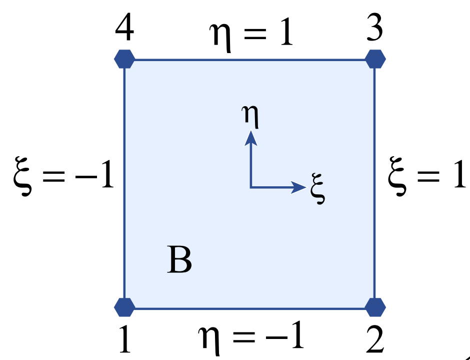


Figure by MIT OCW.

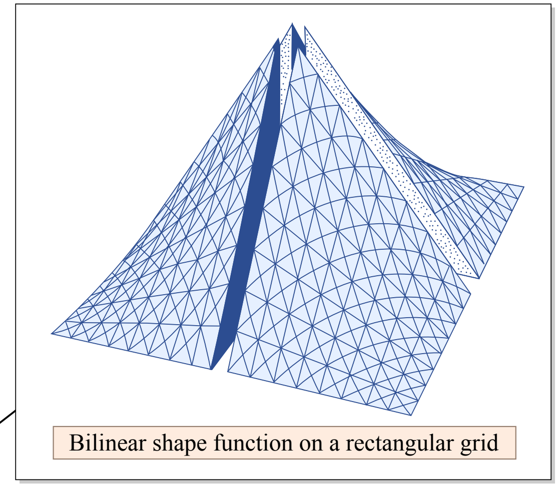


Figure by MIT OCW.

$$\tilde{u} = \sum_{\ell=1}^{4} N_\ell(\xi,\eta)\overline{u}_\ell$$

Linear Interpolation Functions

$$\begin{aligned}
N_1 &= 0.25(1-\xi)(1-\eta) \\
N_2 &= 0.25(1+\xi)(1-\eta) \\
N_3 &= 0.25(1+\xi)(1+\eta) \\
N_4 &= 0.25(1+\xi)(1+\eta)
\end{aligned}$$

$$N_\ell = 0.25(1+\xi_\ell\xi)(1+\eta_\ell\eta)$$

Quadratic Interpolation Functions

$$\prod_{r\neq i} \frac{(\xi-\xi_r)(\eta-\eta_r)}{(\xi_i-\xi_r)(\eta_i-\eta_r)}$$

$$\begin{aligned}
N_i &= 0.25\xi_i\xi(1+\xi_i\xi)\eta_i\eta(1+\eta_i\eta) \\
N_i &= 0.5(1-\xi^2)\eta_i\eta(1+\eta_i\eta)\ ,\ \xi_i = 0 \\
N_i &= 0.5(1-\eta^2)\xi_i\xi(1+\xi_i\xi)\ ,\ \eta_i = 0 \\
N_i &= (1-\xi^2)(1-\eta^2)
\end{aligned}$$

Two-Dimensional Finite Elements
Flow in Duct

Finite Element Solution

$$\tilde{w} = \sum_{j=1}^{N} \overline{w}_j N_j(x,y)$$

$$N_j = 0.25(1 + \xi_j \xi)(1 + \eta_j \eta)$$

$$\left(\frac{\partial^2 \tilde{w}}{\partial x^2}, N_k \right) + \left(\frac{\partial^2 \tilde{w}}{\partial x^2}, N_k \right) = (-1, N_k)$$

Integration by Parts

$$(\frac{\partial^2 w}{\partial x^2}, N_k) \equiv \int_{-1}^{1} \frac{\partial^2 w}{\partial x^2} N_k = \left[\frac{\partial w}{\partial x} N_k \right]_{-1}^{1} - \int_{-1}^{1} \frac{\partial w}{\partial x} \frac{dN_k}{dx}$$

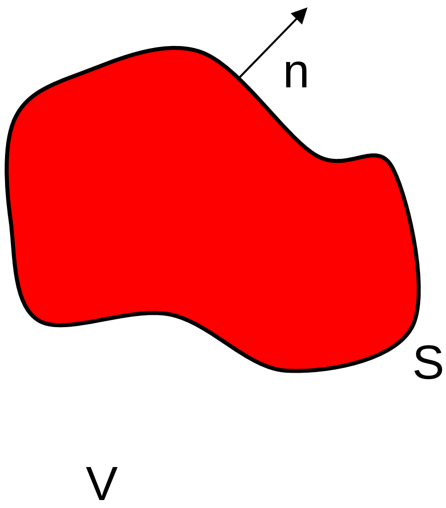
$$\left(\frac{\partial^2 \tilde{w}}{\partial x^2}, N_k \right) = - \left(\frac{\partial \tilde{w}}{\partial x}, \frac{\partial N_k}{\partial x} \right)$$

Algebraic Equations

$$-\sum_{j=1}^{N} \left(\int_{-1}^{1} \int_{-1}^{1} \frac{\partial N_j}{\partial x} \frac{\partial N_k}{\partial x} + \frac{\partial N_j}{\partial y} \frac{\partial N_k}{\partial y} \ dxdy \right) \overline{w}_j = - \int_{-1}^{1} \int_{-1}^{1} 1 N_k dxdy, k = 1, \ldots N$$

Potential Flow

Boundary Integral Equations



Green's Theorem

$$\int_S \left[G(\mathbf{x},\mathbf{x}_0)\frac{\partial \phi(\mathbf{x}_0)}{\partial n} - \phi(\mathbf{x}_0)\frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial n}\right] dS_0$$

$$= \int_V \left[\phi(\mathbf{x}_0)\nabla^2 G(\mathbf{x},\mathbf{x}_0) - G(\mathbf{x},\mathbf{x}_0)\nabla^2\phi(\mathbf{x}_0)\right] dV_0$$

Green's Function

$$G(\mathbf{x},\mathbf{x}_0) = \frac{1}{r} = \frac{1}{\sqrt{(x-x_0)^2+(y-y_0)^2+(z-z_0)^2}} + \psi(\mathbf{x})$$

Homogeneous Solution

$$\nabla^2\psi = 0$$

$$\nabla^2 G((\mathbf{x},\mathbf{x}_0) = -\delta(\mathbf{x}-\mathbf{x}_0)$$

Boundary Integral Equation

$$\phi(\mathbf{x}) = \int_S \left[G(\mathbf{x},\mathbf{x}_0)\frac{\partial \phi(\mathbf{x}_0)}{\partial n} - \phi(\mathbf{x}_0)\frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial n}\right] dS_0 - \int_V \left[G(\mathbf{x},\mathbf{x}_0)\nabla^2\phi(\mathbf{x}_0)\right] dV_0$$

Discretized Integral Equation

$$\sum_{j=0}^{N-1} A_{ij} w_j = B_i$$

Linear System of Equations

$$\overline{\overline{\mathbf{A}}}\mathbf{u} = \mathbf{b}$$

Panel Methods