Introduction to Numerical Analysis for Engineers

- Systems of Linear Equations
  - Cramer's Rule
  - Gaussian Elimination
  - Numerical implementation
    - Numerical stability
      - Partial Pivoting
      - Equilibration
      - Full Pivoting
    - Multiple right hand sides
    - Computation count
    - LU factorization
    - Error Analysis for Linear Systems
      - Condition Number
    - Special Matrices
  - Iterative Methods
    - Jacobi's method
    - Gauss-Seidel iteration
    - Convergence

Systems of Linear Equations
Cramer's Rule

Linear System of Equations

$$
\begin{array}{ccccccc}
a_{11}x_1 & a_{12}x_2 & \cdot & \cdot & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & a_{22}x_2 & \cdot & \cdot & a_{2n}x_n & = & b_2 \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}x_1 & \cdot & \cdot & \cdot & a_{nn}x_n & = & b_n
\end{array}
$$

Cramer's Rule, n=2

$$
\begin{aligned}
D &= a_{11}a_{22} - a_{21}a_{12} \\
D_1 &= b_1a_{22} - b_2a_{12} \\
D_2 &= b_2a_{11} - b_1a_{21}
\end{aligned}
$$

$$x_1 = \frac{D_1}{D} = \frac{b_1a_{22} - b_2a_{12}}{a_{11}a_{22} - a_{21}a_{12}}$$

$$x_2 = \frac{D_2}{D} = \frac{b_2a_{11} - b_1a_{21}}{a_{11}a_{22} - a_{21}a_{12}}$$

Example, n=2

$$
\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix}
\left\{ \begin{array}{c} x_1 \\ x_2 \end{array} \right\}
=
\left\{ \begin{array}{c} 1.0 \\ 1.0 \end{array} \right\}
$$

$$
\begin{aligned}
x_1 &= \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} &= \quad 1.0099 \\
x_2 &= \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} &= -0.9899
\end{aligned}
$$

Cramer's rule inconvenient for n>3

Systems of Linear Equations
Gaussian Elimination

Linear System of Equations

$$
\begin{array}{ccccccc}
a_{11}x_1 & a_{12}x_2 & \cdot & \cdot & a_{1n}x_n & = & b_1 \\
a_{21}x_1 & a_{22}x_2 & \cdot & \cdot & a_{2n}x_n & = & b_2 \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}x_1 & \cdot & \cdot & \cdot & a_{nn}x_n & = & b_n
\end{array}
$$

Reduction
Step 0

$$a_{ij}^{(1)} = a_{ij}, \quad b_i^{(1)} = b_i$$

$$
\begin{array}{ccccccc}
a_{11}^{(1)}x_1 & a_{12}^{(1)}x_2 & \cdot & \cdot & a_{1n}^{(1)}x_n & = & b_1^{(1)} \\
a_{21}^{(1)}x_1 & a_{22}^{(1)}x_2 & \cdot & \cdot & a_{2n}^{(1)}x_n & = & b_2^{(1)} \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\
a_{n1}^{(1)}x_1 & \cdot & \cdot & \cdot & a_{nn}^{(1)}x_n & = & b_n^{(1)}
\end{array}
$$

Systems of Linear Equations
Gaussian Elimination

Reduction
Step 1

$$\left.\begin{aligned} m_{i1} &= \frac{a_{i1}^{(1)}}{a_{11}^{(1)}} \\ a_{ij}^{(2)} &= a_{ij}^{(1)} - m_{i1} a_{1j}^{(1)}, \quad j = 1, \cdots n \\ b_i^{(2)} &= b_i^{(1)} - m_{i1} b_1^{(1)} \end{aligned}\right\} i = 2, \cdots n$$

$$\begin{array}{c|cccccccc} & & & j \longrightarrow & & & & & \\ & a_{11}^{(1)} x_1 & a_{12}^{(1)} x_2 & \cdot & \cdot & a_{1n}^{(1)} x_n & = & b_1^{(1)} \\ & 0 & a_{22}^{(2)} x_2 & \cdot & \cdot & a_{2n}^{(2)} x_n & = & b_2^{(2)} \\ i \downarrow & \cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\ & \cdot & \cdot & \cdot & \cdot & \cdot & = & \cdot \\ & 0 & a_{n2}^{(2)} x_2 & \cdot & \cdot & a_{nn}^{(2)} x_n & = & b_n^{(2)} \end{array}$$

Systems of Linear Equations
Gaussian Elimination

Reduction Step k

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

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

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

$$
\begin{array}{rcl}
x_n & = & b_n^{(n)} / a_{nn}^{(n)} \\
x_{n-1} & = & \left(b_{n-1}^{(n-1)} - a_{n-1,n}^{(n-1)} x_n \right) / a_{n-1,n-1}^{(n-1)} \\
& \cdot \; \cdot \; \cdot & \\
& \cdot \; \cdot \; \cdot & \\
x_k & = & \left(b_k^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)} x_j \right) / a_{kk}^{(k)} \\
& \cdot \; \cdot \; \cdot & \\
x_1 & = & \left(b_1^{(1)} - \sum_{j=2}^{n} a_{1j}^{(1)} x_j \right) / a_{11}^{(1)}
\end{array}
$$

Systems of Linear Equations
Gaussian Elimination

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

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

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

Required at each step!

Partial Pivoting by Columns

$$
\begin{array}{l}
\\ \\ \\ \text{Row k} \\ \\ \text{Row i} \\ \\ \\
\end{array}
\begin{bmatrix}
\times & & & & & & \\
0 & \times & & & & & \\
\cdot & \cdot & \times & & & & \\
\cdot & & 0 & 0 & \times & \times & \times \\
\cdot & & \cdot & \times & & & \\
\cdot & & \cdot & \times & & & \\
\cdot & & \cdot & \times & & & \\
0 & \cdot & 0 & \times & & &
\end{bmatrix}
\cdot \bar{\mathbf{x}} =
\begin{Bmatrix}
\times \\ \cdot \\ \cdot \\ \times \\ \cdot \\ \cdot \\ \cdot \\ \times
\end{Bmatrix}
$$

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

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

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

Required at each step!

Partial Pivoting by Columns

New Row k

New Row i

$$\begin{bmatrix} \times & & & & & & \\ 0 & \times & & & & & \\ \cdot & \cdot & \times & & & & \\ \cdot & & 0 & \times & \times & \times & \times \\ \cdot & & \cdot & \times & & & \\ \cdot & & \cdot & 0 & & & \\ \cdot & & \cdot & \times & & & \\ 0 & \cdot & 0 & \times & & & \end{bmatrix} \cdot \bar{\mathbf{x}} = \begin{Bmatrix} \times \\ \cdot \\ \cdot \\ \times \\ \cdot \\ \cdot \\ \cdot \\ \times \end{Bmatrix}$$

Systems of Linear Equations
Gaussian Elimination

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Gaussian Elimination

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{cases} x_1 = 1.01 \\ x_2 = -0.99 \end{cases}$$

2-digit Arithmetic

100% error

1% error

$$m_{21} = 100$$

$$a_{21}^{(2)} = 0$$

$$a_{22}^{(2)} = \boxed{0.01} + 10\boxed{0} \simeq 100$$

$$b_2^{(2)} = \boxed{1} - 10\boxed{0} \simeq -100$$

$$x_2 = \boxed{-1}$$

$$x_1 = (1.0 - 1.0)/0.01 = \boxed{0}$$

```
n=3
a = [ [0.01 1.0]' [-1.0 0.01]']
b= [1 1]'
r=a^(-1) * b
x=[0 0];
m21=a(2,1)/a(1,1);
a(2,1)=0;
a(2,2) = radd(a(2,2),-m21*a(1,2),n);
b(2)   = radd(b(2),-m21*b(1),n);
x(2)   = b(2)/a(2,2);
x(1)   = (radd(b(1), -a(1,2)*x(2),n))/a(1,1);
x'
```

tbt.m

tbt.m

Systems of Linear Equations
Gaussian Elimination

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$x_1 = \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099$$

$$x_2 = \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899$$

Partial Pivoting by Columns
Interchange Rows

$$\begin{bmatrix} 1.0 & 0.01 \\ 0.01 & -1.0 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

2-digit Arithmetic

$$\begin{aligned} m_{21} &= 0.01 \\ a_{22}^{(2)} &= -1 - 0.0\boxed{001} \simeq -1.0 \\ b_2^{(2)} &= 1 - 0.0\boxed{1} \simeq 1.0 \\ x_2 &= \boxed{-1} \\ x_1 &= 1 + 0.01 \simeq \boxed{1.0} \end{aligned}$$

1% error

1% error

Systems of Linear Equations
Gaussian Elimination

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$\begin{aligned} x_1 &= \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = 1.0099 \\ x_2 &= \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} = -0.9899 \end{aligned}$$

Multiply Equation 1 by 200

$$\begin{bmatrix} 2.0 & -200 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 200.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{cases} x_1 = 1.01 \\ x_2 = -0.99 \end{cases}$$

2-digit Arithmetic

$$\begin{aligned} m_{21} &= 0.5 \\ a_{21}^{(2)} &= 0 \\ a_{22}^{(2)} &= 0.01 + 100 \simeq 100 \\ b_2^{(2)} &= 1 - 0.5 \cdot 200 \simeq -100 \\ x_2 &= -1 \\ x_1 &= (200 - 200)/2 = \boxed{0} \end{aligned}$$

100% error

Equations must be normalized for partial pivoting to ensure stability

This **Equilibration** is made by normalizing the matrix to unit norm

Infinity-Norm Normalization

$$||a_{ij}||_\infty = \max_j |a_{ij}| \simeq 1, \quad i = 1, \ldots n$$

Two-Norm Normalization

$$||a_{ij}||_2 = \sum_{j=1}^{n} a_{ij}^2 \simeq 1, \quad i = 1, \ldots n$$

Systems of Linear Equations
Gaussian Elimination

Example, n=2

$$\begin{bmatrix} 2.0 & -200 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 200.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$\begin{aligned} x_1 &= \frac{1.0\cdot 0.01 - 1.0\cdot(-1.0)}{0.01\cdot 0.01 - 1.0\cdot(-1.0)} &= 1.0099 \\ x_2 &= \frac{1.0\cdot 0.01 - 1.0\cdot 1.0}{0.01\cdot 0.01 - 1.0\cdot(-1.0)} &= -0.9899 \end{aligned}$$

Interchange Unknowns

$$\begin{aligned} x_1 &= \tilde{x}_2 \\ x_2 &= \tilde{x}_1 \end{aligned}$$

Pivoting by Rows

$$\begin{bmatrix} -200 & 2.0 \\ 0.01 & 1.0 \end{bmatrix} \begin{Bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{Bmatrix} = \begin{Bmatrix} 200.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{cases} \tilde{x}_1 = -0.99 \\ \tilde{x}_2 = 1.01 \end{cases}$$

2-digit Arithmetic

$$\begin{aligned} m_{21} &= -0.00005 \\ a_{21}^{(2)} &= 0 \\ a_{22}^{(2)} &= 0.01 + 1.0 \simeq 1.0 \\ b_2^{(2)} &= 1 + 0.01 \simeq 1 \\ \tilde{x}_2 &\simeq \boxed{1} \\ \tilde{x}_1 &= (200 - 2)/(-200) \simeq \boxed{-1} \end{aligned}$$

1% error

Full Pivoting

Find largest numerical value in same row and column and interchange

Affects ordering of unknowns

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

Example, n=2

$$\begin{bmatrix} 0.01 & -1.0 \\ 1.0 & 0.01 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 1.0 \\ 1.0 \end{Bmatrix}$$

Cramer's Rule - Exact

$$\begin{aligned} x_1 &= \frac{1.0 \cdot 0.01 - 1.0 \cdot (-1.0)}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} &=& \quad 1.0099 \\ x_2 &= \frac{1.0 \cdot 0.01 - 1.0 \cdot 1.0}{0.01 \cdot 0.01 - 1.0 \cdot (-1.0)} &=& \quad -0.9899 \end{aligned}$$

Variable Transformation

$$\begin{aligned} x_1 &= \tilde{x}_1 \\ x_2 &= 0.01 \cdot \tilde{x}_2 \end{aligned}$$

$$\begin{bmatrix} 1.0 & -1.0 \\ 1.0 & 0.0001 \end{bmatrix} \begin{Bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{Bmatrix} = \begin{Bmatrix} 100.0 \\ 1.0 \end{Bmatrix} \Rightarrow \begin{Bmatrix} \tilde{x}_1 &=& 1.01 \\ \tilde{x}_2 &=& -99 \end{Bmatrix}$$

2-digit Arithmetic

$$\begin{aligned} m_{21} &= 1.0 \\ a_{21}^{(2)} &= 0 \\ a_{22}^{(2)} &= 0.0001 + 1.0 \simeq 1.0 \\ b_2^{(2)} &= 1 - 100 \simeq -100 \\ \tilde{x}_2 &= \boxed{-100} \\ \tilde{x}_1 &= 100 - 100 = \boxed{0} \end{aligned}$$

1% error

100% error

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