Introduction to Numerical Analysis for Engineers

- Systems of Linear Equations
  Mathews
  - Cramer's Rule
  - Gaussian Elimination 3.3-3.5
    - Numerical implementation
      3.3-3.4
    - Numerical stability
      - Partial Pivoting
      - Equilibration
      - Full Pivoting
    - Multiple right hand sides
    - Computation count
    - LU factorization 3.5
    - Error Analysis for Linear Systems 3.4
      - Condition Number
    - Special Matrices
  - Iterative Methods 3.6
    - 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

$$
\begin{aligned}
D &= a_{11}a_{22} - a_{21}a_{12} \\
D_1 &= b_1 a_{22} - b_2 a_{12} \\
D_2 &= b_2 a_{11} - b_1 a_{21}
\end{aligned}
$$

$$x_1 = \frac{D_1}{D} = \frac{b_1 a_{22} - b_2 a_{12}}{a_{11}a_{22} - a_{21}a_{12}}$$

$$x_2 = \frac{D_2}{D} = \frac{b_2 a_{11} - b_1 a_{21}}{a_{11}a_{22} - a_{21}a_{12}}$$

Example, n=2

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

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

Cramer's rule inconvenient for n>3

Systems of Linear Equations
Gaussian Elimination

Linear System of Equations

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

Reduction
Step 0

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

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

Systems of Linear Equations
Gaussian Elimination

Reduction
Step 1

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

$j \longrightarrow$

$i \downarrow$

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

Systems of Linear Equations
Gaussian Elimination

Reduction Step k

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

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

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

Step k

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

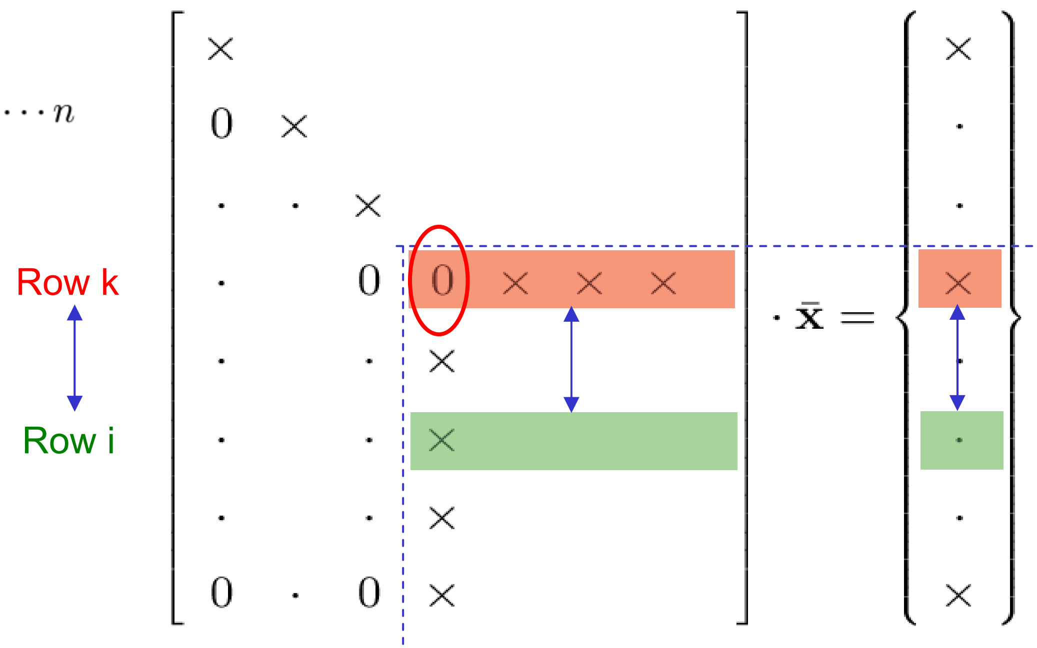
Pivotal Elements

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

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

Required at each step!

Partial Pivoting by Columns



Systems of Linear Equations
Gaussian Elimination

Reduction
Step k

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

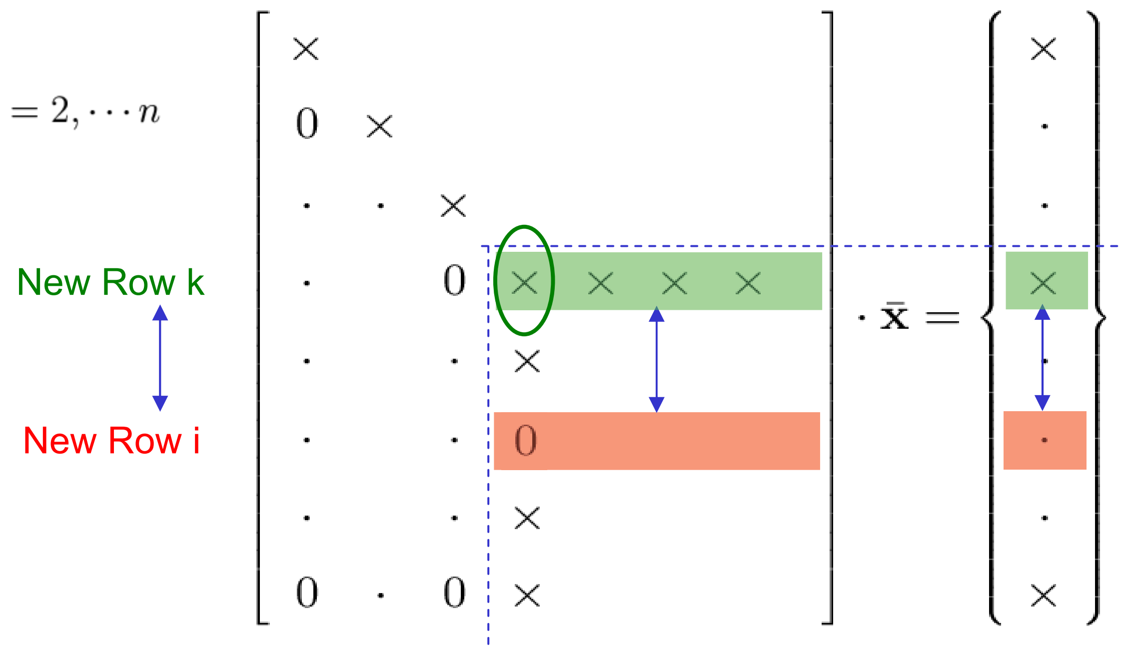
Pivotal Elements

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

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

Required at each step!

Partial Pivoting by Columns



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

$$m_{21} = 100$$

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

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

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

$$x_2 = -1$$

$$x_1 = (1.0 - 1.0)/0.01 = 0$$

100% error (Cramer's $x_1 = 1.0099$ vs. Gaussian $x_1 = 0$)

1% error (Cramer's $x_2 = -0.9899$ vs. Gaussian $x_2 = -1$)

```
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

$$m_{21} = 0.01$$

$$a_{22}^{(2)} = -1 - 0.0001 \simeq -1.0$$

$$b_2^{(2)} = 1 - 0.01 \simeq 1.0$$

$$x_2 = -1$$

$$x_1 = 1 + 0.01 \simeq 1.0$$

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

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

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

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

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

100% error (x_1)

1% error (x_2)

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

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

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

Interchange Unknowns

$$x_1 = \tilde{x}_2$$

$$x_2 = \tilde{x}_1$$

Pivoting by Rows

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

2-digit Arithmetic

$$m_{21} = -0.00005$$

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

$$a_{22}^{(2)} = 0.01 + 1.0 \simeq 1.0$$

$$b_2^{(2)} = 1 + 0.01 \simeq 1$$

$$\tilde{x}_2 \simeq 1$$

$$\tilde{x}_1 = (200 - 2)/(-200) \simeq -1$$

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

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

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

Variable Transformation

$$x_1 = \tilde{x}_1$$

$$x_2 = 0.01 \cdot \tilde{x}_2$$

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

2-digit Arithmetic

$$m_{21} = 1.0$$

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

$$a_{22}^{(2)} = 0.0001 + 1.0 \simeq 1.0$$

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

$$\tilde{x}_2 = -100$$

$$\tilde{x}_1 = 100 - 100 = 0$$

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