



# 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

## Gaussian Elimination

Reduction  
Step k

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

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

Reduction  
Step n-1

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

Back-Substitution

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

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

...

...

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

...

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

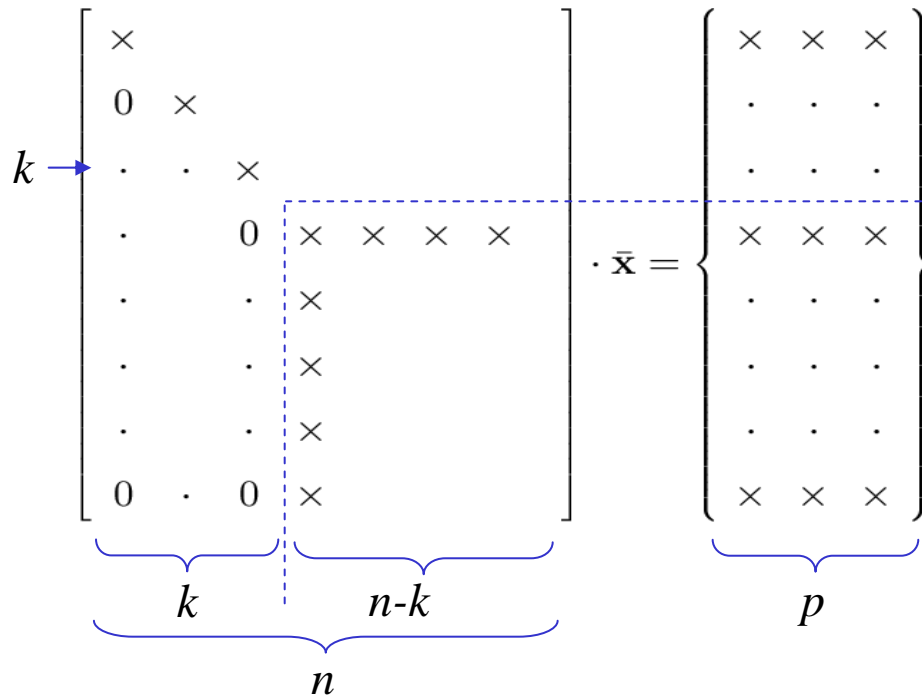


# Systems of Linear Equations

## Gaussian Elimination

### Multiple Right-hand Sides

Reduction  
Step  $k$



Computation Count  
Reduction Step  $k$

$$(n - k)(n - k + p) \text{ Operations}$$

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

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

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  $\bar{\bar{A}}$  is decomposed as

$$\bar{\bar{A}} = \bar{\bar{L}} \cdot \bar{\bar{U}}$$

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

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

Then the solution is performed in two simple steps

1.  $\bar{\bar{L}}\vec{y} = \vec{b}$  Forward substitution

2.  $\bar{\bar{U}}\vec{x} = \vec{y}$  Back substitution

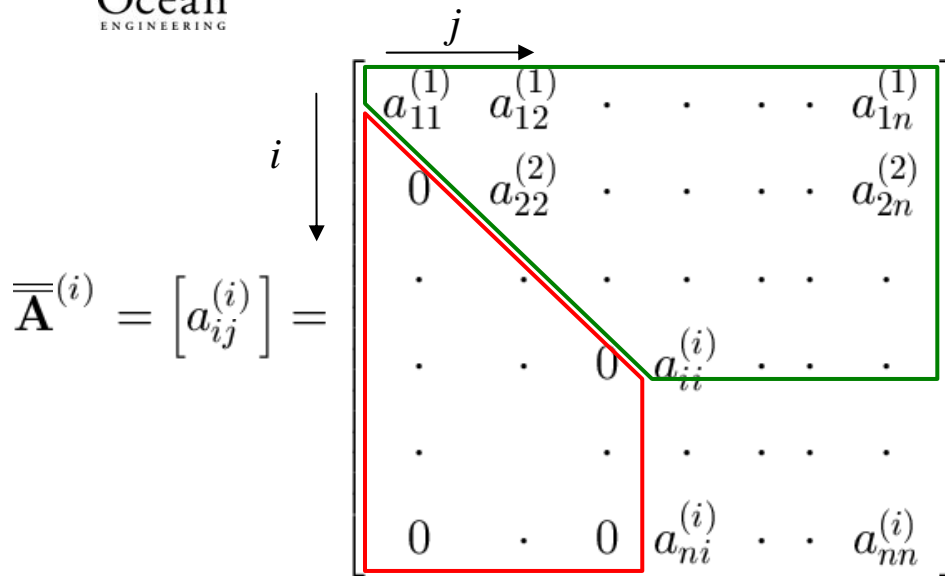
$$\bar{\bar{U}} = [u_{ij}] =$$

$$\begin{bmatrix} u_{11} & u_{12} & \cdot & \cdot & \cdot & \cdot & u_{1n} \\ 0 & u_{22} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & u_{kk} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & u_{n-1,n} \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & u_{nn} \end{bmatrix}$$

How to determine  $\bar{\bar{L}}$  and  $\bar{\bar{U}}$  ?

# Systems of Linear Equations

## LU Factorization



Change in reduction steps  $1 - i-1$ :

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - m_{ik} a_{kj}^{(k)}, \quad m_{ik} = a_{ik}^{(k)} / a_{kk}^{(k)}$$

Total change above diagonal

$$i \leq j : a_{ij}^{(i)} = a_{ij} - \sum_{k=1}^{i-1} m_{ik} a_{kj}^{(k)}$$

Total change below diagonal

$$i > j : a_{ij}^{(i)} = 0 = a_{ij} - \sum_{k=1}^j m_{ik} a_{kj}^{(k)}$$

Define

$$m_{ii} = 1, \quad i = 1, \dots, n$$

=>

$$i \leq j : a_{ij} = \sum_{k=1}^i m_{ik} a_{kj}^{(k)}$$

$$i > j : a_{ij} = \sum_{k=1}^j m_{ik} a_{kj}^{(k)}$$

$$\Rightarrow a_{ij} = \sum_{k=1}^{\min(i,j)} m_{ik} a_{kj}^{(k)}$$

After reduction step  $i-1$ :

Above and on diagonal

$$i \leq j$$

Unchanged after step  $i-1$

$$a_{ij}^{(n)} = \dots a_{ij}^{(i)}$$

Below diagonal

$$j < i$$

Become and remain 0 in step  $j$

$$a_{ij}^{(n)} = \dots a_{ij}^{(j+1)} = 0$$

# Systems of Linear Equations

## LU Factorization

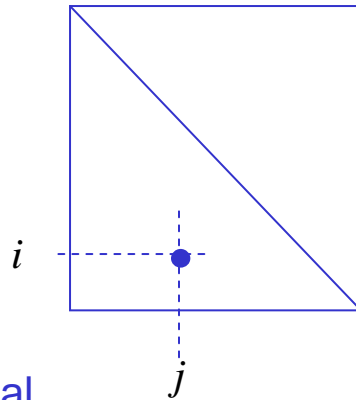
'Matrix product'

Sum stops at diagonal

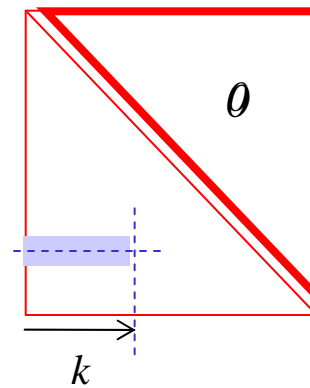
$$a_{ij} = \sum_{k=1}^{\min(i,j)} m_{ik} a_{kj}^{(k)}$$

Below diagonal

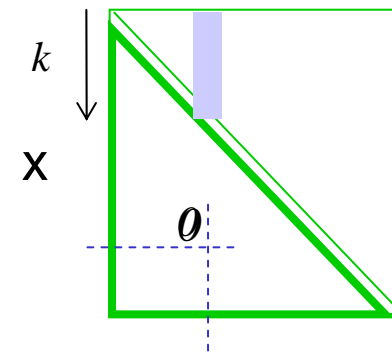
$i > j :$



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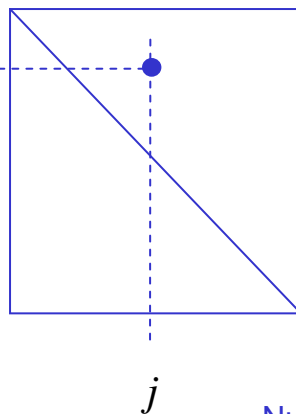


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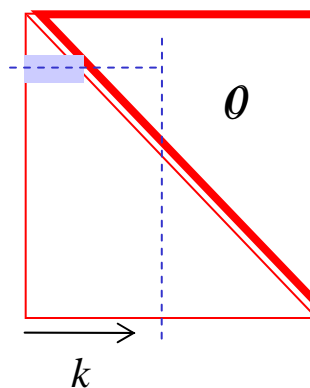


Above diagonal

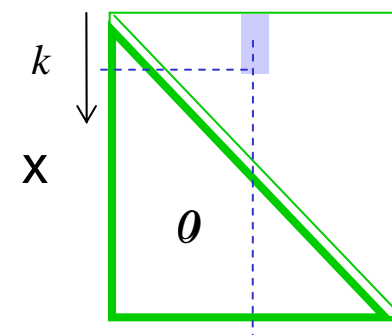
$i \leq j :$



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# Systems of Linear Equations LU Factorization

GE Reduction directly yields LU factorization

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

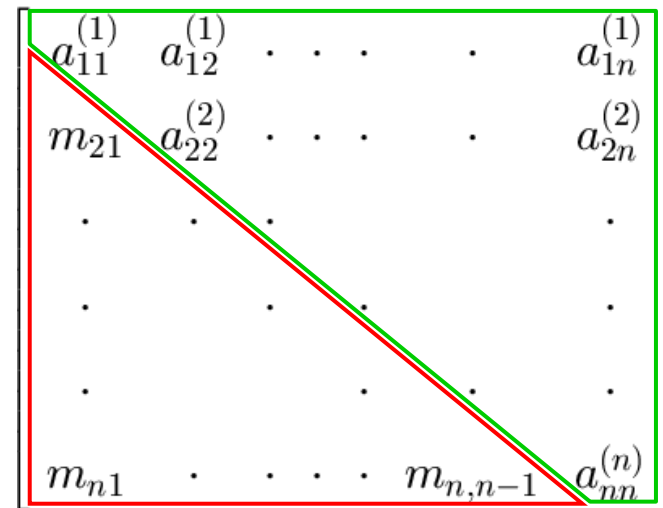
Lower triangular

$$\bar{\bar{\mathbf{L}}} = l_{ij} = \begin{cases} 0 & i < j \\ 1 & i = j \\ m_{ij} & i > j \end{cases}$$

Upper triangular

$$\bar{\bar{\mathbf{U}}} = u_{ij} = \begin{cases} a_{ij}^{(i)} & i \leq j \\ 0 & i > j \end{cases}$$

Compact storage



Lower diagonal implied

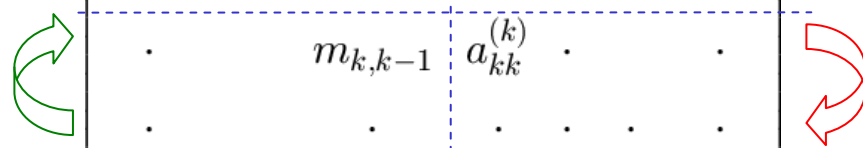
$$m_{ii} = 1, \quad i = 1, \dots, n$$



# Systems of Linear Equations

## Pivoting in LU Factorization

Before reduction, step  $k$

$$\begin{bmatrix}
 a_{11}^{(1)} & a_{12}^{(1)} & \cdot & \cdot & \cdot & \cdot & a_{1n}^{(1)} \\
 m_{21} & a_{22}^{(2)} & \cdot & \cdot & \cdot & \cdot & a_{2n}^{(2)} \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & m_{k,k-1} & a_{kk}^{(k)} & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 m_{n1} & \cdot & m_{n,k-1} & a_{nk}^{(k)} & \cdot & \dots & a_{nn}^{(n)}
 \end{bmatrix}$$


Pivoting if

$$|a_{ik}^{(k)}| \gg |a_{kk}^{(k)}|, \quad i > k$$

Interchange rows  $i$  and  $k$

$$p_k = i$$

else

$$p_k = k$$

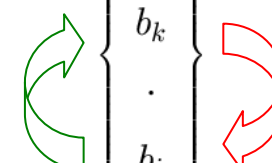
Pivot element vector

$$p_i, \quad i = 1, \dots, n$$

Forward substitution, step  $k$

$$\bar{\bar{L}}\vec{y} = \vec{b}$$

Interchange rows  $i$  and  $k$

$$\begin{bmatrix}
 b_1 \\
 \cdot \\
 \cdot \\
 b_k \\
 \cdot \\
 b_i \\
 \cdot \\
 b_n
 \end{bmatrix}$$


$$p_k = i \Rightarrow \begin{cases} b_i^{(k)} = b_k \\ b_k = b_i \\ b_i = b_i^{(k)} \end{cases}$$



# Linear Systems of Equations Error Analysis

Function of one variable

$$y = f(x)$$

Condition number

$$\left| \frac{f(\bar{x}) - f(x)}{f(x)} \right| = K \left| \frac{\bar{x} - x}{x} \right|, \quad \bar{x} = x + \delta x$$

$$\left| \frac{\delta y}{y} \right| = K \left| \frac{\delta x}{x} \right|$$

The condition number  $K$  is a measure of the **amplification** of the **relative error** by the function  $f(x)$

Linear systems

How is the relative error of  $\bar{\mathbf{x}}$  dependent on errors in  $\bar{\mathbf{b}}$ ?

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

Example

$$\bar{\mathbf{A}} = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 1.0001 \end{bmatrix}, \quad \det(\bar{\mathbf{A}}) = 0.0001$$

$$\bar{\mathbf{b}} = \begin{Bmatrix} 2 \\ 2 \end{Bmatrix} \Rightarrow \bar{\mathbf{x}} = \begin{Bmatrix} 2 \\ 0 \end{Bmatrix}$$

$$\bar{\mathbf{b}} = \begin{Bmatrix} 2 \\ 2.0001 \end{Bmatrix} \Rightarrow \bar{\mathbf{x}} = \begin{Bmatrix} 1 \\ 1 \end{Bmatrix}$$

Small changes in  $\bar{\mathbf{b}}$  give large changes in  $\bar{\mathbf{x}}$   
The system is **ill-Conditioned**

# Linear Systems of Equations Error Analysis

## Vector and Matrix Norm

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

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

### Properties

$$\bar{\mathbf{A}} \neq \bar{\mathbf{0}} \Rightarrow \|\bar{\mathbf{A}}\| > 0$$

$$\|\alpha \bar{\mathbf{A}}\| = |\alpha| \|\bar{\mathbf{A}}\|$$

$$\|\bar{\mathbf{A}} + \bar{\mathbf{B}}\| \leq \|\bar{\mathbf{A}}\| + \|\bar{\mathbf{B}}\|$$

$$\|\bar{\mathbf{A}}\bar{\mathbf{B}}\| \leq \|\bar{\mathbf{A}}\| \|\bar{\mathbf{B}}\|$$

$$\|\bar{\mathbf{A}}\bar{\mathbf{x}}\| \leq \|\bar{\mathbf{A}}\| \|\bar{\mathbf{x}}\|$$

## Perturbed Right-hand Side

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



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

Subtract original equation

$$\bar{\mathbf{A}}\delta\bar{\mathbf{x}} = \delta\bar{\mathbf{b}}$$

$$\delta\bar{\mathbf{x}} = \bar{\mathbf{A}}^{-1}\delta\bar{\mathbf{b}}$$



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

Relative Error Magnification

$$\frac{\|\delta\bar{\mathbf{x}}\|}{\|\bar{\mathbf{x}}\|} \leq \|\bar{\mathbf{A}}^{-1}\| \|\bar{\mathbf{A}}\| \frac{\|\delta\bar{\mathbf{b}}\|}{\|\bar{\mathbf{b}}\|}$$

Condition Number

$$K(\bar{\mathbf{A}}) = \|\bar{\mathbf{A}}^{-1}\| \|\bar{\mathbf{A}}\|$$

# Linear Systems of Equations Error Analysis

## Vector and Matrix Norm

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

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

### Properties

$$\bar{\mathbf{A}} \neq \bar{\mathbf{0}} \Rightarrow \|\bar{\mathbf{A}}\| > 0$$

$$\|\alpha \bar{\mathbf{A}}\| = |\alpha| \|\bar{\mathbf{A}}\|$$

$$\|\bar{\mathbf{A}} + \bar{\mathbf{B}}\| \leq \|\bar{\mathbf{A}}\| + \|\bar{\mathbf{B}}\|$$

$$\|\bar{\mathbf{A}}\bar{\mathbf{B}}\| \leq \|\bar{\mathbf{A}}\| \|\bar{\mathbf{B}}\|$$

$$\|\bar{\mathbf{A}}\bar{\mathbf{x}}\| \leq \|\bar{\mathbf{A}}\| \|\bar{\mathbf{x}}\|$$

## Perturbed Coefficient Matrix

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

Subtract unperturbed equation

$$\bar{\mathbf{A}}\delta\bar{\mathbf{x}} + \delta\bar{\mathbf{A}}(\bar{\mathbf{x}} + \delta\bar{\mathbf{x}}) = \bar{\mathbf{0}}$$

$$\delta\bar{\mathbf{x}} = -\bar{\mathbf{A}}^{-1} \delta\bar{\mathbf{A}}(\bar{\mathbf{x}} + \delta\bar{\mathbf{x}}) \simeq -\bar{\mathbf{A}}^{-1} \delta\bar{\mathbf{A}}\bar{\mathbf{x}}$$

$$\|\delta\bar{\mathbf{x}}\| \leq \|\bar{\mathbf{A}}^{-1}\| \|\delta\bar{\mathbf{A}}\| \|\bar{\mathbf{x}}\|$$

Relative Error Magnification

$$\frac{\|\delta\bar{\mathbf{x}}\|}{\|\bar{\mathbf{x}}\|} \leq \|\bar{\mathbf{A}}^{-1}\| \|\bar{\mathbf{A}}\| \frac{\|\delta\bar{\mathbf{A}}\|}{\|\bar{\mathbf{A}}\|}$$

Condition Number

$$K(\bar{\mathbf{A}}) = \|\bar{\mathbf{A}}^{-1}\| \|\bar{\mathbf{A}}\|$$



## Ill-Conditioned System

$$\begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 1.0001 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\det(\overline{\overline{\mathbf{A}}}) = 0.0001$$

$$a_{11} = \frac{1.0001}{0.0001} = 10,001$$

$$a_{12} = \frac{-1}{0.0001} = -10,000$$

$$a_{21} = \frac{-1}{0.0001} = -10,000$$

$$a_{22} = \frac{1.0}{0.0001} = 10,000$$

$$\left. \begin{array}{l} \|\overline{\overline{\mathbf{A}}}\|_{\infty} = 2.0001 \\ \|\overline{\overline{\mathbf{A}}}^{-1}\|_{\infty} = 20,001 \end{array} \right\} \Rightarrow K(\overline{\overline{\mathbf{A}}}) \simeq \boxed{40,000}$$

Ill-conditioned system

```
n=4
a = [ [1.0 1.0]' [1.0 1.0001] ] tbt6.m
b= [1 2]'

ai=inv(a);
a_nrm=max( abs(a(1,1)) + abs(a(1,2)) ,
           abs(a(2,1)) + abs(a(2,2)) )
ai_nrm=max( abs(ai(1,1)) + abs(ai(1,2)) ,
           abs(ai(2,1)) + abs(ai(2,2)) )
k=a_nrm*ai_nrm

r=ai * 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'
```



# Well-Conditioned System

$$\begin{bmatrix} 0.0001 & 1.0 \\ 1.0 & 1.0 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\det(\overline{\mathbf{A}}) = 0.9999$$

$$a_{11} = \frac{-1}{0.9999} = -1.0001$$

$$a_{12} = \frac{1}{0.9999} = 1.0001$$

$$a_{21} = \frac{1}{0.9999} = 1.0001$$

$$a_{22} = \frac{-0.0001}{0.9999} = -0.0001$$

4-digit Arithmetic

```
n=4
a = [ [0.0001 1.0]' [1.0 1.0] ] tbt7.m
b= [1 2]'

ai=inv(a);
a_nrm=max( abs(a(1,1)) + abs(a(1,2)) ,
           abs(a(2,1)) + abs(a(2,2)) )
ai_nrm=max( abs(ai(1,1)) + abs(ai(1,2)) ,
           abs(ai(2,1)) + abs(ai(2,2)) )
k=a_nrm*ai_nrm

r=ai * 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'
```

$$\left. \begin{aligned} \|\overline{\mathbf{A}}\|_{\infty} &= 2.0 \\ \|\overline{\mathbf{A}}^{-1}\|_{\infty} &= 2.0002 \end{aligned} \right\} \Rightarrow K(\overline{\mathbf{A}}) \simeq \boxed{4}$$

Well-conditioned system

Algorithmically ill-conditioned