Basic mathematical question: existence and uniqueness

For Ax=b, one solution, no solution or infinitely many?

All start with "Elimination"

### **Gaussian Elimination**

**Example:** 

$$2 u + v + w = 5$$
  
 $4 u - 6 v = -2$   
 $-2 u + 7 v + 2 w = 9$ 

<u>Subtracting multiples</u> of the first equation from the others, so as to eliminate u from the last two equations.

2: the first pivot

-8: the second pivot

We continue to eliminate v from the third equation.

Pivots: 2, -8, 1

Back-substitution: solve w then v then u.

### **Breakdown of Gaussian Elimination**

- n equations  $\rightarrow n$  pivots: <u>nonsingular</u>, only one solution
- a zero appears in a pivot position → some problem! May be curable or incurable.
- Curable case (cured by row exchange): <u>nonsingular</u> case

$$u + v + w =$$
  $u + v + w =$   $u + v + w =$   $2u + 2v + 5w =$   $\Rightarrow$   $3w =$   $\Rightarrow$   $2v + 4w =$   $4u + 6v + 8w =$   $2v + 4w =$   $3w =$ 

• Incurable case: singular case

$$u+v+w= \qquad u+v+w=$$

$$2u+2v+5w= \rightarrow 3w=$$

$$4u+4v+8w= 4w=$$

Why is this system singular?

If 3w=6 and 4w=7 then inconsistent  $\rightarrow$  no solution If 3w=6 and 4w=8 then u+v= constant  $\rightarrow$  many solutions

### **Cost of Gaussian Elimination**

- How many separate arithmetical operations (cost) does elimination require, for *n* equations in *n* unknowns?
- Operations: division and multiply-subtract
- To produce a zero in the first column: 1 division and n-1 multiply-subtract are needed  $\rightarrow$  total n operations needed
- There are n-1 rows in the first column to be operated on:  $n(n-1)=n^2-n$  operations are needed to produce zeros in the first column
- For the second column:  $(n-1)^2$ -(n-1) .....and so on
- There are n columns:

$$(n^2 + \dots + 1^2) - (n + \dots + 1) = \frac{n(n+1)(2n+1)}{6} - \frac{n(n+1)}{2} = \frac{n^3 - n}{3}$$

- When n is large,  $n^3/3$  is a pretty good estimate
- For the right side: about  $n^2/2$  is required. Why?
- Operations required in back-substitution:

$$1+2+\cdots+n=\frac{n(n+1)}{2}\approx\frac{n^2}{2}$$

Why?

- The right side is responsible for a total of  $n^2$  operations
- Minimum operations required?  $Cn^{\log_2^7} = Cn^{2.8}$  ( $\log_2^7 \approx 2.8$ ). IBM research center has find some the power of n below 2.5!!

### Multiplication of a Matrix and a Vector

• Inner product of two vectors:

$$\begin{bmatrix} 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 2u + v + w \end{bmatrix}$$

• By rows:

$$Ax = \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 2u + v + w \\ 4u - 6v \\ -2u + 7v + 2w \end{bmatrix}$$

• Let  $a_{ij}$  be the entry in the *i*th row and *j*th column and  $x_j$  be the jth component of x

$$\sum_{i=1}^{n} a_{ij} x_{j}$$
 is the *i*th component of  $Ax$ 

Each row is the linear combination of components of x

• By columns:

$$Ax = u \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} + v \begin{bmatrix} 1 \\ -6 \\ 7 \end{bmatrix} + w \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}$$

Ax is a combination of the columns of A. The coefficients which multiply the columns are the components of x.

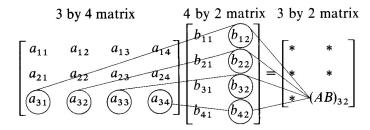
• Identity matrix I leaves every vector unchanged.

$$Ib = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 5 \\ -2 \\ 9 \end{bmatrix} = \begin{bmatrix} 5 \\ -2 \\ 9 \end{bmatrix}$$

### **Matrix Multiplication**

• Most common and least used: Each entry of AB is the product of a row and a column:  $(AB)_{ij} = inner\ product\ of\ row\ i\ of\ A\ and\ column\ j\ of\ B$ 

Example: Multiplication of matrix  $A_{3\times4}$  and matrix  $B_{4\times2}$ 



• Each column of AB is the product of A and a column of BColumn j of AB = A times column j of B

**Example:** 

$$AB = \begin{bmatrix} 1 & 0 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} a & b \\ 2a + 3c & 2b + 3d \end{bmatrix} \Rightarrow$$

Each column of AB is a combination of the columns of A with coefficients coming from each column of B

• Each row of AB is the product of a row of A and B:

Row i of AB = row i of A times  $B \Rightarrow$ 

Each row of AB is a combination of the rows of B with coefficients coming from each row of A

### **Elimination Steps and Elementary Matrices**

An Elimination step can be a Matrix: <u>Elementary Matrix</u>
 HOW? Subtracting 2 times the first row of A from the second row of A

$$EA = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 \\ 0 & -8 & -2 \\ -2 & 7 & 2 \end{bmatrix}$$

The matrix that subtracts a multiple  $l_{ij}$  of row j from row i is the elementary matrix  $E_{ij}$  with 1's on the diagonal and the number  $-l_{ii}$  in row i, column j.

Example:  $E_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -l_{31} & 0 & 1 \end{bmatrix}$ 

• Gaussian elimination for

$$Ax = \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 5 \\ -2 \\ 9 \end{bmatrix} = b$$

Step 1: Subtract 2 times the 1st equation from the  $2^{nd}$  (E)

Step 2: Subtract –1 times the 1st equation from the 3rd (F)

Step 2: Subtract –1 times the 2nd equation from the 3rd (G)

• Matrix form of Gaussian elimination: GFEA=U

$$GFE = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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## **Matrix Multiplication (Cont'd)**

- Matrix multiplication is associative (AB)C=A(BC)
- Matrix multiplication is distributive

$$A(B+C)=AB+AC$$
 and  $(B+C)D=BD+CD$ 

• Matrix multiplication is not commutative. Usually,

 $AB \neq BA$ 

Example: let G be the elementary matrix that adds row 2 to row 3 and E be the matrix that subtracts 2 times row 1 from row 2. Then,

$$EG = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \neq GE = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -2 & 1 & 1 \end{bmatrix}$$

That is, the order of elimination steps matters

### **Inverse of Elimination Steps**

$$Ax = \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 5 \\ -2 \\ 9 \end{bmatrix} = b$$

• Gaussian elimination leads to:

$$GFEAx = Ux = \begin{bmatrix} 2 & 1 & 1 \\ 0 & -8 & -2 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = GFEb = \begin{bmatrix} 5 \\ -12 \\ 2 \end{bmatrix} = c$$

*U* is called *upper triangular* 

After Gaussian elimination  $Ax=b \Rightarrow Ux=c$ 

• Undo the steps of Gaussian elimination:

Example: 
$$E = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
 then  $E^{-1} = ?$ 

$$E^{-1}E = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

If the elementary matrix E has the number  $-l_{ij}$  in the (i,j) position, then its inverse has  $+l_{ij}$  in that position

The 3<sup>rd</sup> step (G) was last in going from A to U. Its matrix
G must be the first to be inverted in the reverse direction.
That is:

$$E^{-1}F^{-1}G^{-1}U=A$$

### **Inverse of Elimination Steps in Matrix Form:** L

#### • The matrix that takes U back to $A: L \Rightarrow LU=A$

$$E^{-1}F^{-1}G^{-1} = \begin{bmatrix} I & 0 & 0 \\ 2 & I & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{2I} & 1 & 0 \\ l_{3I} & l_{32} & 1 \end{bmatrix} = L$$

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ l_{31} & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & l_{32} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}$$

#### ⇒ Expressing Inverse of Elimination Steps is EASY!

How about Guassian Elimination in matrix form? It's NOT EASY!  $GFE=L^{-1}=$ 

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -l_{32} & 1 \end{bmatrix} \bullet \begin{bmatrix} 1 & 0 & 0 \\ -l_{21} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -l_{31} & 0 & 1 \end{bmatrix} \neq \begin{bmatrix} 1 & 0 & 0 \\ -l_{21} & 1 & 0 \\ -l_{31} & -l_{32} & 1 \end{bmatrix}$$

## Triangular Factorization of A: A=LU

#### • Example:

Step 1: Subtract 2 times the 1st equation from the  $2^{nd} \Rightarrow l_{21}=2$ 

Step 2: Subtract –1 times the 1st equation from the 3rd  $\Rightarrow l_{31} = -1$ 

Step 2: Subtract -1 times the 2nd equation from the 3rd  $\Rightarrow l_{32}$ = -1

$$GFEA = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 \\ 0 & -8 & -2 \\ 0 & 0 & 1 \end{bmatrix} = U$$

$$\boldsymbol{L} = \boldsymbol{E}^{-1} \boldsymbol{F}^{-1} \boldsymbol{G}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1 & 1 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 1 \\ 4 & -6 & 0 \\ -2 & 7 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & -8 & -2 \\ 0 & 0 & 1 \end{bmatrix} = \mathbf{L}\mathbf{U}$$

## • Triangular Factorization | A=LU

Without row exchanges required, the original matrix A can be written as a product A=LU. The matrix L is lower triangular, with 1's on the diagonal and the multipliers  $l_{ij}$  (taken from the elimination) below the diagonal. U is the upper triangular matrix which appears after forward elimination and before back-substitution; its diagonal entries are the pivots.

### **Examples of Triangular Factorization**

- The steps of elimination are actually  $L^{-1}$  that takes A to U and reduce L to I:  $L^{-1}A = L^{-1}LU = U$ .
- Another way of looking at it:

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} row \ l \ of \ U \\ row \ 2 \ of \ U \\ row \ 3 \ of \ U \end{bmatrix} = original \ A$$

The matrix L, applied to U, brings back A!

Example: When U is the identity then L is the same as A

$$A = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} I = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ l_{31} & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & l_{32} & 1 \end{bmatrix} I$$

### **Example:**

$$A = \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & 1 & -1 & \\ & & & 1 \end{bmatrix}$$

## **Solving a Linear System**

- c is the right side after Gaussian elimination. That is,  $c=L^{-1}b \Rightarrow c$  can be solved by Lc=b
- When A=LU and L and U are known,

$$Ax=b \Rightarrow \boxed{Lc=b \text{ and } Ux=c}$$

- Given A=LU
   One Linear System = Two Triangular Systems
- We first solve a lower triangular system for c (Lc=b) then the upper triangular system for x (Ux=c)
- Multiply Ux=c by L. We have  $LUx=Lc \Rightarrow Ax=b$ . Example: Band matrix in the previous example
- *U* can be further rewritten as:

$$U = \begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{bmatrix} \begin{bmatrix} 1 & u_{12}/d_1 & u_{13}/d_1 & \cdot \\ & 1 & u_{23}/d_2 & \cdot \\ & & \ddots & \cdot \\ & & & 1 \end{bmatrix}$$

The triangular factorization is often written A=LDU, where L and U have 1's on the diagonal and D is the diagonal matrix of pivots.

• Some freedom in the elimination steps and calculations, but absolutely no freedom in the final L, D and U. That is,

L, D and U are uniquely determined by A

## **Row Exchanges and Permutation Matrices**

- Remember what we do if a zero appears in the pivot location? Problem may be curable or incurable (singular)
- How can the problem be cured? Looking below the zero to seek out nonzero entry lower down in the same column. Then, a row exchange is carried out; the nonzero entry becomes the needed pivot and elimination can get going again.
- Row exchanges in matrix forms: Permutation matrices
   Example: an exchange of rows 1 and 3 and exchange of rows 2 and 3:

$$P_{13} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \qquad P_{23} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Why? A trick:  $P_{13}I = P_{13}$ 

• Do both of the row exchanges at once:

$$P_{23}P_{13} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} = P$$

- In a nonsingular case, Ax=b has a unique solution
  - (1) It is found by elimination with row exchanges
  - (2) With the rows reordered in advance, PA can be factored into LU.
- In a singular case, no reordering can produce a full set of pivots.

### Inverse of A

The matrix A is <u>invertible</u> if there exists a matrix B such that BA=I and AB=I. There is at most one such B, called the inverse of A and denoted by  $A^{-1}$ :

$$A^{-1}A=I$$
 and  $AA^{-1}=I$ 

• There could not be two different inverses, because if BA=I and AC=I then

$$B=BI=B(AC)=(BA)C=IC=C$$

- $\bullet (A^{-1})^{-1} = A$
- $\bullet \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$

• if 
$$A = \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_n \end{bmatrix}$$
 then  $A^{-1} = \begin{bmatrix} 1/d_1 & & \\ & \ddots & \\ & & 1/d_n \end{bmatrix}$ 

•  $(A+B)^{-1}$ ? Nothing. No quick solution. But  $(AB)^{-1}$ ?

$$(AB)^{-1}=B^{-1}A^{-1}$$

Proof:

$$(AB)(B^{-1}A^{-1})=ABB^{-1}A^{-1}=AIA^{-1}=AA^{-1}=I$$
  
 $(B^{-1}A^{-1})(AB)=BAA^{-1}B^{-1}=BIB^{-1}=BB^{-1}=I$ 

- Similarly,  $(ABC)^{-1}=C^{-1}B^{-1}A^{-1}$
- Remember GFEA=U and  $A=E^{-1}F^{-1}G^{-1}U=LU$ !

#### Gauss-Jordan Method to Find A-1

• We first go from A to U using Gaussian elimination

$$[A \quad e_1 \quad e_2 \quad e_3] = \begin{bmatrix} 2 & 1 & 1 & 1 & 0 & 0 \\ 4 & -6 & 0 & 0 & 1 & 0 \\ -2 & 7 & 2 & 0 & 0 & 1 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 2 & 1 & 1 & 1 & 0 & 0 \\ 0 & -8 & -2 & -2 & 1 & 0 \\ 0 & 8 & 3 & 1 & 0 & 1 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 2 & 1 & 1 & 1 & 0 & 0 \\ 0 & -8 & -2 & -2 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} U \quad L^{-1} \end{bmatrix}$$

$$[A \quad I] \rightarrow L^{-1}[A \quad I] = \begin{bmatrix} L^{-1}A \quad L^{-1}I \end{bmatrix} = \begin{bmatrix} U \quad L^{-1} \end{bmatrix}$$

• Then from U to I: creating zeros above the pivots

$$\begin{bmatrix} U & L^{-1} \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 1 & 0 & 2 & -1 & -1 \\ 0 & -8 & 0 & -4 & 3 & 2 \\ 0 & 0 & 1 & -1 & 1 & 1 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 2 & 0 & 0 & \frac{12}{8} & -\frac{5}{8} & -\frac{6}{8} \\ 0 & -8 & 0 & -4 & 3 & 2 \\ 0 & 0 & 1 & -1 & 1 & 1 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 1 & 0 & 0 & \frac{12}{16} & -\frac{5}{16} & -\frac{6}{16} \\ 0 & 1 & 0 & \frac{4}{8} & -\frac{3}{8} & -\frac{2}{8} \\ 0 & 0 & 1 & -1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} I & U^{-1}L^{-1} \end{bmatrix}$$

$$\begin{bmatrix} U & L^{-1} \end{bmatrix} \rightarrow U^{-1} \begin{bmatrix} U & L^{-1} \end{bmatrix} = \begin{bmatrix} I & U^{-1}L^{-1} \end{bmatrix} = \begin{bmatrix} I & A^{-1} \end{bmatrix}$$

Operations required for calculating  $A^{-1}$ ?  $n^3/6+n^3/3+n(n^2/2)$  How?

Are Gauss-Jordan method the only order of elimination?
 We could have produced zeros above and below a pivot!

### **Invertible = Nonsingular**

- Nonsingular → Invertible
  - A matrix has a full set of n pivots  $\rightarrow$  nonsingular by definition. (There exists a unique solution for any b)
  - $AA^{-1}=I$  can then be viewed as n separate  $Ax_i=e_i$  systems where  $x_i$ 's are columns of  $A^{-1}$ .
  - $x_i$ 's can be solved because A is nonsingular and therefore  $A^{-1}$  can be determined uniquely.
  - A<sup>-1</sup>A=I? A<sup>-1</sup> is actually the multiplication of many elementary matrices formed by the Gauss-Jordan steps.
- Invertible → Nonsingular
  - If A has an inverse, Gauss-Jordan method must not break down. That is, the following should not occur.

$$A' = \begin{bmatrix} d_1 & x & x & x & x \\ 0 & d_2 & x & x & x \\ 0 & 0 & 0 & x & x \\ 0 & 0 & 0 & x & x \\ 0 & 0 & 0 & x & x \end{bmatrix}$$

- No matter what x's are, the Gauss-Jordan method cannot be carried out. That is, A must have a full set of pivots and is nonsingular.

A square matrix is invertible if and only if it is nonsingular

# **Transposes**

- The transpose of  $A = A^T$
- The *i*th row of A becomes the *i*th column of  $A^T$
- The entry  $(A^T)_{ij}=A_{ji}$

$$\left( \begin{bmatrix} 2 & 1 & 4 \\ 0 & 0 & 3 \end{bmatrix} \right)^T = \begin{bmatrix} 2 & 0 \\ 1 & 0 \\ 4 & 3 \end{bmatrix}$$

 $\bullet$   $(AB)^T = B^T A^T$ 

$$AB = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 3 & 3 & 3 \\ 2 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 3 & 3 & 3 \\ 5 & 5 & 5 \end{bmatrix}$$

$$B^{T} A^{T} = \begin{bmatrix} 3 & 2 \\ 3 & 2 \\ 3 & 2 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 5 \\ 3 & 5 \\ 3 & 5 \end{bmatrix}$$

- $(A^{-1})^T = (A^T)^{-1}$  not trivial!  $(A^{-1})^T A^T = (AA^{-1})^T = I^T = I$  and  $A^T (A^{-1})^T = (A^{-1}A)^T = I^T = I$
- A <u>symmetric matrix</u>:  $A^T = A$  or  $a_{ij} = a_{ji}$
- A symmetric matrix's inverse, if there is one, is also symmetric
- If A is symmetric and can be factored into LDU without row exchanges to destroy the symmetry, then the upper triangular U is the transpose of the lower triangular L.
   That is, the factorization becomes <u>A=LDL</u><sup>T</sup>

$$A = LDU = A^T = U^TD^TL^T$$

### **Roundoff Error**

• A typical computer round-off:

 $.345+.00123 \rightarrow .346$  (keep three digits)

- Roundoff error: the digits lost (0.00023)
- Example:

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1.0001 \end{bmatrix}$$
 and  $A' = \begin{bmatrix} .0001 & 1 \\ 1 & 1 \end{bmatrix}$ 

• Some matrices are extremely sensitive to small changes and others are not. The matrix A is ill-conditioned (sensitive) and A' is well-conditioned. In A, if  $a_{ij}$  (in A) becomes 1 due to roundoff error the system becomes singular

**Example** 

Original: 
$$u+v=2$$
 Roundoff:  $u+v=2$   
 $u+1.0001v=2.0001$   $u+1.0001v=2$ 

solution: u=v=1, solution: u=2 v=0

A change in the fifth digit of b was amplified to a change in the first digit of the solution!!

# **Partial Pivoting**

• Even a well-conditioned matrix can be ruined by a poor algorithm. Straightforward Gaussian elimination is among the poor algorithms!!

**Example:** the well-condition matrix A' (symmetric)

$$0.0001u+v=1$$
  
 $u+v=2$ 

after elimination: 
$$-9999v = -9998 \rightarrow v = .99990$$

original: 
$$.0001u + .9999 = 1 \rightarrow u = 1.0$$

round-off: 
$$v = .99990 \rightarrow v \sim 1.0$$

$$.0001u + 1 = 1 \rightarrow u \sim 0 !!!$$

$$A' = \begin{bmatrix} 1 & 0 \\ 10,000 & 1 \end{bmatrix} \begin{bmatrix} .0001 & 0 \\ 0 & -9999 \end{bmatrix} \begin{bmatrix} 1 & 10,000 \\ 0 & 1 \end{bmatrix} = LDU$$

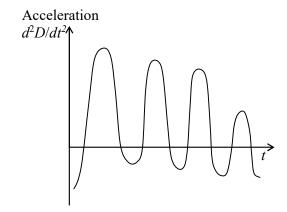
- The small pivot 0.0001 brought instability!!
- Remedy: row exchanges to remove small pivots.
- A computer must compare each pivot with all the other possible pivots in the same column. Choosing the largest of these candidates, and exchanging the corresponding rows so as to make this largest value the pivot is called Partial Pivoting.

$$A'' = \begin{bmatrix} 1 & 1 \\ .0001 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ .0001 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & .9999 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} = LDU$$

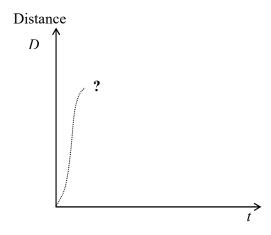
A symmetric A' is not necessarily better for a computer!!

## An Application: Differential Equation

- A continuous problem cannot be solved by computers.
   Computer can only approximate a continuous problem by a discrete problem
- Example: riding motorcycles with only acceleration known as a function of time



Question: distance as a function of time?



### **Continuous**→**Discrete**

$$\frac{d^2D}{dt^2} = f(t), \qquad 0 \le t \le 1 \implies D(t) = ?$$

- Uncertainty in the problem since a+bt for any a and b after second derivative contributes nothing to f(t).
- Usually, initial conditions, such as D(0)=0 (starting from the origin) and dD(0)/dt=0 (initial speed is zero), are added to remove the uncertainty.
- Discrete approximation of differentiation:

$$\frac{dD}{dt} \approx \frac{D(t+h) - D(t)}{h} \Rightarrow \frac{d^2D}{dt^2} = \frac{d\binom{dD}{dt}}{dt} \approx \frac{\frac{D(t+h) - D(t)}{h} - \frac{D(t) - D(t-h)}{h}}{h}$$
$$\approx \frac{D(t+h) - 2D(t) + D(t-h)}{h^2} = f(t)$$

Let time interval= $h \Rightarrow D_{i+1} - 2D_i + D_{i-1} = h^2 f(jh) \ j=1,...,n$ 

• Let n=5,  $D_0=0$  and  $dD_0/dt=0 \Rightarrow (D_1-D_0)/h=0 \Rightarrow D_1=D_0=0$ 

$$D_0 - 2D_1 + D_2 = D_2 = h^2 f(h)$$

$$D_1 - 2D_2 + D_3 = -2D_2 + D_3 = h^2 f(2h)$$

$$D_{i-1}-2D_i+D_{i+1}=h^2f(jh)$$
 for  $j=3,...,5$ 

$$\begin{bmatrix} 1 & 0 & & & \\ -2 & 1 & 0 & & \\ 1 & -2 & 1 & 0 & \\ & 1 & -2 & 1 & 0 \\ & & 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} D_2 \\ D_3 \\ D_4 \\ D_5 \\ D_6 \end{bmatrix} = h^2 \begin{bmatrix} f(h) \\ f(2h) \\ f(3h) \\ f(4h) \\ f(5h) \end{bmatrix} \Rightarrow \textbf{Lower Triangular}$$

Matrix

### **Continuous**→**Discrete**

• Let n=5,  $D_0=0$  and  $dD_5/dt=0 \Rightarrow (D_6-D_5)/h=0 \Rightarrow$   $D_0 - 2D_1 + D_2 = -2D_1 + D_2 = h^2 f(h)$   $D_{j-1} - 2D_j + D_{j+1} = h^2 f(jh) \text{ for } j=2,...,4$   $D_4 - 2D_5 + D_6 = D_4 - 2D_5 + D_5 = D_4 - D_5 = h^2 f(5h)$   $\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 \\ & & 1 & -1 \end{bmatrix} \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \end{bmatrix} = h^2 \begin{bmatrix} f(h) \\ f(2h) \\ f(3h) \\ f(4h) \\ f(5h) \end{bmatrix}$ 

- ⇒ Tri-diagonal Matrix
- Let n=5,  $D_0=0$  and  $D_6=0$  (Boundary Conditions)

$$D_0 - 2D_1 + D_2 = -2D_1 + D_2 = h^2 f(h)$$

$$D_{i-1} - 2D_i + D_{i+1} = h^2 f(jh)$$
 for  $j=2,...,4$ 

$$D_4 - 2D_5 + D_6 = D_4 - 2D_5 = h^2 f(5h)$$

$$\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \end{bmatrix} = h^2 \begin{bmatrix} f(h) \\ f(2h) \\ f(3h) \\ f(4h) \\ f(5h) \end{bmatrix}$$

#### ⇒ Tri-diagonal Matrix

# **Tridiagonal Matrices**

$$\begin{bmatrix} 2 & -1 \\ -1 & 2 & -1 \\ & -1 & 2 & -1 \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}$$

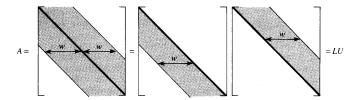
- Tridiagonal matrix:  $a_{ij}=\theta$  if |i-j|>1; that is, all nonzero entries lie on the main diagonal and the two adjacent diagonals.
- Symmetric matrix:  $U=L^T$
- Positive definite matrix: all pivots are positive. A symmetric matrix with all positive pivots does not require row exchanges.
- For a tridiagonal matrix,
  - (a) only one nonzero entry below the pivot
  - (b) operations are carried out on a very short row.

$$A = \begin{bmatrix} \frac{1}{-1} & & & \\ \frac{-1}{2} & 1 & & & \\ & \frac{-2}{3} & 1 & & \\ & & \frac{-3}{4} & 1 & \\ & & & \frac{-4}{5} & 1 \end{bmatrix} \begin{bmatrix} \frac{2}{1} & & & \\ & \frac{3}{2} & & & \\ & & \frac{4}{3} & & \\ & & & \frac{5}{4} & \\ & & & & \frac{6}{5} \end{bmatrix} \begin{bmatrix} 1 & \frac{-1}{2} & & & \\ & 1 & \frac{-2}{3} & & \\ & & & 1 & \frac{-3}{4} & \\ & & & & 1 & \frac{-4}{5} \\ & & & & 1 \end{bmatrix}$$

L and U are bi-diagonal. The pivots are converging to +1.

## **Operations Required by Band Matrices**

- For a tridiagonal matrix, every forward elimination stage requires 2 multiply-subtract operations and there are n such stages  $\rightarrow$  we need only 2n operations instead of the usual  $n^3/3$ .
- Back-substitution: again only 2n, instead of  $n^2/2$ , operations are needed.
- No. of operations for a tridiagonal matrix is proportional to n instead of to a higher power of n.



- In general, a band matrix with nonzero entries only on the band  $|i-j| \le w$ . A tridiagonal matrix has w=2.
- Each stage of elimination requires w(w-1) operations
- A total of about  $w^2n$  operations are needed.
- The exact number of divisions and multiply-subtracts is w(w-1)(3n-2w+1)/3 = (n(n-1)(n+1)/3 when w=n)
- In band matrix problems, calculating  $A^{-1}$  to solve  $x=A^{-1}b$  is not more efficient than calculating L and U to solve Lc=b and Ux=c