# April 21 Math 2335 sec 51 Spring 2016

#### Section 5.4: Numerical Differentiation

If we have a scheme to approximate the first derivative f'(x), we're using the notation

 $f'(x) \approx D_h f(x)$ , for step size h.

If we want to approximate f''(x), we'll use a superscript with parentheses

$$f''(x) \approx D_h^{(2)} f(x)$$
 for step size *h*.

For an *n*<sup>th</sup> derivative, we write

$$f^{(n)}(x) \approx D_h^{(n)} f(x)$$
 for step size *h*.

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# Some First Derivative Rules Forward, Backward, and Central Difference

For h > 0 we have the names:

Forward Difference: 
$$D_h f(x) = \frac{f(x+h) - f(x)}{h}$$

Backward Difference: 
$$D_h f(x) = \frac{f(x) - f(x - h)}{h}$$

Central Difference: 
$$D_h f(x) = \frac{f(x+h) - f(x-h)}{2h}$$

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#### Errors: Order of a Rule

Definition: If the error for a particular rule satisfies

 $Err = Ch^{p}$ , for some constants *C* and *p*,

we will say that the rule is of **order** *p*.

- The forward and backward difference rules are order p = 1.
- The central difference rule is order p = 2.

We confirmed both of these using Taylor's theorem.

# The Method Undetermined Coefficients

The use of Taylor series expansions can help us to define new numerical differentiation rules as well as analyze the error for a rule.

The Method of Undetermined Coefficients involves setting up a form the rule is to take, and then finding out what coefficients are needed.

## The Method Undetermined Coefficients an Example

Suppose we wish to approximate a second derivative

$$f''(x) \approx D_h^{(2)} f(x).$$

We begin by deciding how many points to use, such as x, x + h, and x - h (or x + 2h etc.), then write out a general form.

$$D_h^{(2)}f(x) = Af(x+h) + Bf(x) + Cf(x-h)$$

Then, we determine the values of the unknown coefficients A, B, and C using Taylor series.

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#### A Second Derivative Rule

We sought a rule to approximate f''(x) using three points x, x + h and x - h of the form

$$D^{(2)}f(x) = Af(x+h) + Bf(x) + Cf(x-h).$$

Writing out the Taylor expansions for Af(x + h) and Cf(x - h) we arrived at three equations for our three unknowns

with solution  $A = C = \frac{1}{h^2}$  and  $B = \frac{-2}{h^2}$ . This gives the rule

$$D_h^{(2)}f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Determine the Order of The Method Just Found

$$D_h^{(2)}f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

From the previous computations, since  $A = C = 1/h^2$ 

$$A\frac{h^3}{6}f'''(x) - C\frac{h^3}{6}f'''(x) = 0.$$

So we can use the Taylor expansions up to degree 3 with error:

$$\frac{1}{h^2}f(x+h) = \frac{1}{h^2}\left(f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_1)\right)$$
$$\frac{1}{h^2}f(x-h) = \frac{1}{h^2}\left(f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(c_2)\right)$$

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Sum  

$$\frac{1}{h^{2}}\left(f(x+h)+f(x-h)\right) = \frac{1}{h^{2}}\left(2f(x)+h^{2}f''(x)+\frac{h^{2}}{24}\left[f^{(u)}_{(c_{1})}+f^{(u)}_{(c_{2})}\right]\right)$$

$$= \frac{2}{h^2} f(x) + f''(x) + \frac{h^2}{2y} \left[ f^{(u)}_{(c_1)} + f^{(u)}_{(c_2)} \right]$$

$$\Rightarrow \frac{1}{h^{2}} \left[ f(x+h) + f(x-h) - 2f(x) \right] = f''(x) + \frac{h^{2}}{2u} \left[ f_{(c,1)}^{(u)} + f_{(cn)}^{(u)} \right]$$

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^{2}} = f''(x) + (-c)h^{2}$$
where  $-(z) = \frac{1}{2u} \left[ f_{(c,1)}^{(u)} + f_{(cn)}^{(u)} \right]$ 

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$$D_{h}^{(z)}f(x) = f''(x) - Ch^{2}$$

$$\Rightarrow f''(x) - D'_{h}f(x) = Ch'^{2}$$

$$\operatorname{Err}\left(\mathcal{D}_{h}^{(2)}f(x)\right)=\operatorname{Ch}^{2}$$

Our rule is on order 2 method,

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# Section 6.1: Systems of Linear Equations

**Definition:** A linear equation in *n* variables  $x_1, \ldots, x_n$  is one of the form

$$a_1x_1+a_2x_2+\cdots+a_nx_n=b.$$

Here,  $a_1, \ldots, a_n$  are known constants called the **coefficients**, and b is a known constant.

#### **Examples:**

$$2x_1 + 3x_2 - x_3 = 7$$

or

$$x - 2y = 12$$

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# System of Linear Equations

A **system of linear equations** is two or more linear equations in the same variables—the equations are considered together.

For example:

$$3x + 2y = 9$$
  
 $x - 5y = -14$ 

or

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## Solution

A system of linear equations may have solutions. A **solution** is an *n*-tuple of numbers that satisfies all equation in the system simultaneously.

**Example:** Show that (x, y) = (1, 3) is a solution, and show that (x, y) = (3, 0) is **not** a solution of the system

$$3x + 2y = 9$$
  
 $x - 5y = -14$ 

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Check 
$$(3,0)$$
  $3.3 - 2.0 = 9 - 0 = 9 \sqrt{}$ 

#### Matrices

**Definition:** A matrix is a rectangular array of numbers. It's **size** (a.k.a. dimension/order) is  $m \times n$  (read "*m* by *n*") where *m* is the number of rows and *n* is the number of columns the matrix has.

Examples:

# General System and Matrix Formalism

A system of *n* equations in *n* variables has the form

We can equate two matrices with this system of equations, a **coefficient matrix** and an **augmented matrix**.

 $\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} & b_n \end{bmatrix}.$ 

The system is called **homogeneous** if  $b_1 = b_2 = \ldots = b_n = 0$ .

## Example Source of a Linear System

Find a linear system for the following problem and write the coefficient and augmented matrices.

Find a quadratic polynomial  $p(x) = ax^2 + bx + c$  through the points (0,2), (1,3), and (2,10).

$$P(0) = a \cdot 0^{2} + b \cdot 0 + c = 2 \qquad 0a + 0b + c = 2$$

$$P(1) = a \cdot 1^{2} + b \cdot 1 + c = 3 \qquad 1a + 1b + c = 3$$

$$P(2) = a \cdot 2^{2} + b \cdot 2 + c = 10 \qquad \forall a + 2b + c = 10$$

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The augmented motive is
$$\begin{bmatrix}
0 & 0 & | & 2 \\
| & 1 & | & 3 \\
| & 2 & | & |0
\end{bmatrix}$$

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#### Another Example: Cubic Spline

Suppose we have  $h_j = 1$ . The equations for the cubic spline numbers  $M_j$  were

$$\frac{M_{j-1}}{6} + \frac{2M_j}{3} + \frac{M_{j+1}}{6} = y_{j+1} - 2y_j + y_{j-1}, \quad j = 2, \ldots, n-1.$$

Multiply both sides by 6, and let  $b_{j-1} = 6(y_{j+1} - 2y_j + y_{j-1})$ . Then all equations can be written as

Coefficent Matrix for Cubic Spline Equations<sup>1</sup>

$$\begin{bmatrix} 1 & 4 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 4 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 4 & 1 & 0 & \cdots & 0 \\ & & & \ddots & \ddots & & \\ & & & & \ddots & & \\ 0 & & & & & 0 & 1 & 4 & 1 \end{bmatrix}$$
A
tridiagonal
matrix

<sup>1</sup>This structure is called *tri-diagonal*.

#### Theorem

**Theorem** For a linear system of equations, exactly one of the following is true.

- The system has exactly one solution  $(x_1, \ldots, x_n)$ .
- The system has no solution.
- The system has infinitely many solutions.

A homogeneous system (all right hand sides are zero) always has at least one solution

$$x_1 = x_2 = \ldots = x_n = 0$$

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called the trivial solution.

# Solving a System: Gaussian Elimination

**Definition:** Two systems are **equivalent** if they have the same solution set.

For example, the following are equivalent:

$$3x + 2y = 9$$
  

$$x - 5y = -14$$
, and 
$$3x + 2y = 9$$
  

$$y = 3$$
  
Note that the solution to the system on  
the right is fairly obvious.  
From y=3, we get  $3x = 9 - 2y = 9 - 2 \cdot 3 = 3$   

$$s, x = 1$$
  
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# Solving a System: Gaussian Elimination

We can try to solve a system by obtaining a convenient form for an equivalent system using an augmented matrix. We are allowed to perform three **row operations**.

The following Row Operations result in an equivalent system:

- i Swap any two rows. Devoled Ri and Ry
- ii Multiply a row by any nonzero number  $k R \rightarrow R'_{i}$
- iii Add a nonzero multiple of one row to another row and replace one of these rows with the result.  $R_{j} k R_{c} \rightarrow R_{j}$

# Example (a): Gaussian Elimination w/ Back Substitution

$$R_2 - ZR_1 \rightarrow R_2$$
  
$$R_3 - (-1)R_1 \rightarrow R_3$$

Scratch 2 2 3 3 -2 -4 -2 0 -1 -3 0 2 1 2 10

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

$$\begin{cases} 1 & 2 & 1 & 0 \\ 0 & -2 & 1 & 3 \\ 0 & -1 & 1 & 2 \\ \end{cases}$$

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$$R_{3} - (\frac{1}{2})R_{2} \rightarrow R_{3}$$

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

$$0 = 1 - \frac{1}{2} - \frac{3}{2}$$
The system for this Augmented metrix is equivalent. It is
$$X_{1} + 2X_{2} + X_{3} = 0$$

$$-2 \times 2 + X_{3} = 3$$

$$\frac{1}{2} \times 3 = \frac{1}{2}$$

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$$\begin{array}{cccc} \chi_{3} = & & -2\chi_{2} = 3 - \chi_{3} \\ & & \chi_{2} = & \frac{\chi_{3} - 3}{2} = \frac{1 - 3}{2} = - \\ & & \chi_{1} = -2\chi_{2} - \chi_{3} = -2(-1) - 1 = 1 \\ & & \left( \chi_{1,3} \chi_{2,3} \chi_{3} \right) = \left( 1, -1, 1 \right) \end{array}$$

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# **Triangular Matrix**

The matrix 
$$\begin{bmatrix} 1 & 2 & 1 \\ 0 & -2 & 1 \\ 0 & 0 & \frac{1}{2} \end{bmatrix}$$
 is called **upper triangular**. A matrix with only zero entries *above* the main diagonal is called **lower triangular**.

$$\begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix} \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix}$$
upper triangular Lower triangular

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#### Section 6.3: Gaussian Elimination: The Process

We begin with the system

$a_{11}x_1$	+	$a_{12}x_{2}$	+	<i>a</i> <sub>13</sub> <i>x</i> <sub>3</sub>	=	$b_1$
$a_{21}x_1$	+	$a_{22}x_{2}$	+	$a_{23}x_{3}$	=	b <sub>2</sub>
$a_{31}x_1$	+	$a_{32}x_{2}$	+	<i>a</i> <sub>33</sub> <i>x</i> <sub>3</sub>	=	b <sub>3</sub>

whose augmented matrix is

$$\left[\begin{array}{ccccc} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{array}\right]$$

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[ a <sub>11</sub>	<b>a</b> <sub>12</sub>	<b>a</b> 13	$b_1$
<i>a</i> <sub>21</sub>	<i>a</i> <sub>22</sub>	<i>a</i> <sub>23</sub>	<i>b</i> <sub>2</sub>
<i>a</i> <sub>31</sub>	<i>a</i> <sub>32</sub>	<i>a</i> <sub>33</sub>	<i>b</i> <sub>3</sub>

We introduce the multipliers

$$m_{21} = \frac{a_{21}}{a_{11}}$$
 and  $m_{31} = \frac{a_{31}}{a_{11}}$ 

and perform the row operations  $R_2 - m_{21}R_1$  and  $R_3 - m_{31}R_1$  to get new rows 2 and 3. (<sup>(2)</sup> means *second generation*.)

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & b_2^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & b_3^{(2)} \end{bmatrix}$$

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$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & b_2^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} & b_3^{(2)} \end{bmatrix}$$

Then we form another multiplier

$$m_{32} = rac{a_{32}^{(2)}}{a_{22}^{(2)}}$$

and perform  $R_3 - m_{32}R_2$  for a new row 3

$$\left[\begin{array}{cccc}a_{11}&a_{12}&a_{13}&b_{1}\\0&a_{22}^{(2)}&a_{23}^{(2)}&b_{2}^{(2)}\\0&0&a_{33}^{(3)}&b_{3}^{(3)}\end{array}\right]$$

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This leaves the augmented matrix for the equivalent system

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & b_2^{(2)} \\ 0 & 0 & a_{33}^{(3)} & b_3^{(3)} \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} & u_{13} & g_1 \\ 0 & u_{22} & u_{23} & g_2 \\ 0 & 0 & u_{33} & g_3 \end{bmatrix}$$

(a)

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which can be solved using back substitution.

**Word of Caution:** We've assumed that the numbers we divide by are nonzero! Trouble can occur if one of them is zero or even just *close to* zero.

We can side step the possible problem this causes by using **pivoting**.

#### Error: An Example

Consider solving the following system using a four digit computer.

6 <i>x</i> 1	+	2 <i>x</i> <sub>2</sub>	+	6 <i>x</i> 3	=	-2
<i>x</i> <sub>1</sub>	+	$\frac{1}{3}X_{2}$	+	1 <i>x</i> <sub>3</sub>	=	1
		$\tilde{2}x_2$				

The exact solution is  $x_1 = -1.6$ ,  $x_2 = 1.8$ ,  $x_3 = 2.0$ .

The augmented matrix in our computer is

ſ	6.000	2.000	2.000	-2.000	1
	1.000	.3333	1.000	1.000	
	1.000	2.000	-1.000	-2.000 1.000 0.000	

with  $m_{21} = 0.1667$  and  $m_{31} = 0.1667$ .

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## Error: An Example

The second generation in our computer is

Γ	6.000	2.000	2.000	-2.000	1
	0	0001	.6667	1.333	
L	0	1.667	-1.333	.3333	

The new multiplier is (much larger than the numbers we're working with)

$$m_{32}=\frac{1.667}{-.0001}=.16670.$$

The numerical solution we end up with is

$$x_1 = 3.444, \quad x_2 = -15.33, \quad x_3 = 3.998$$

which isn't even close!

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# **Pivoting**

A solution is to use swapping of rows called **pivoting**. At each step, look at all possible values for the denominator in our multipliers. Choose the largest one.

For example:

Γ	6.000	2.000	2.000	-2.000	
	1.000	.3333	1.000	1.000 0.000	
	1.000	2.000	-1.000	0.000	

The three possible denominators are 6, 1 and 1. Choose 6.

Γ	6.000	2.000	2.000	-2.000	٦
	0	0001	.6667	1.333	
L	0	1.667	-1.333	.3333	

The two possible denominators are -.0001 and 1.667. Choose 1.667, so swap rows 2 and 3 before proceeding.

#### **Operation Count**

To solve the linear system of *n* equations  $A\mathbf{x} = \mathbf{b}$  by Gaussian elimination with back substitution, we had two general processes:

$$A \longrightarrow U$$
, and  $b \longrightarrow g \longrightarrow x$ 

We can count the number of multiplications, additions, subtractions, divisions involved (# of operations):

$$A \longrightarrow U: \quad rac{4n^3 + 9n^2 - 7n}{6} \quad ext{operations}$$
  
 $b \longrightarrow g \longrightarrow x: \quad 2n^2 \quad ext{operations}$ 

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#### Operation Count

For example: If A is  $5 \times 5$ , it takes

#### 115 + 50 = 165 operations

If A is  $10 \times 10$ , it takes

Suppose we wish to solve the system  $A\mathbf{x} = \mathbf{b}_k$  for k = 1, 2, ..., N. If

A is  $10 \times 10$ , and N = 25

total # of operations = 25, 125

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# **Operation Count**

If we can do  $A \longrightarrow U$  only once, and  $b \longrightarrow g \longrightarrow x$  25 times, then the total number of operations drops to

5805 (about 1/4 as many).

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# Section 6.4: LU Decomposition

Suppose we wish to solve the linear system  $A\mathbf{x} = \mathbf{b}$ , and we happen to know that

A = LU

where L is lower triangular, and U is upper triangular.

$$LU\mathbf{x} = \mathbf{b} \iff L\mathbf{g} = \mathbf{b}$$
 and  $U\mathbf{x} = \mathbf{g}$ 

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#### Example

We wish to solve the system

And we know that

A=LU

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & -1 & 3 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

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Solve  $L\mathbf{g} = \mathbf{b}$  and then  $U\mathbf{x} = \mathbf{g}$  where  $\mathbf{b} = \begin{vmatrix} 12 \\ 23 \\ -19 \end{vmatrix}$ .

 $L\mathbf{g} = \mathbf{b}$ 

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} g_1 \\ g_2 \\ g_3 \end{bmatrix} = \begin{bmatrix} 12 \\ 23 \\ -19 \end{bmatrix}$$
  
$$g_1 = 12 \qquad 2g_1 + g_2 = 23 \qquad g_2 = 23 - 2g_1 = 23 - 24 = -1$$
  
$$= g_1 + g_2 + g_3 = -19 \qquad g_3 = -19 \qquad g_3 = -19 + g_1 - g_2 = -19 + 12 - (-1) = -6$$
  
$$= g_3 = -19 + g_1 - g_2 = -19 + 12 - (-1) = -6$$
  
$$= g_3 = -19 + g_1 - g_2 = -19 + 12 - (-1) = -6$$

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 $U\mathbf{x} = \mathbf{g}$ 

$$\begin{array}{c} 2 & -1 & 3 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{array} \right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{array} \right] = \begin{bmatrix} 12 \\ -1 \\ -6 \end{bmatrix}$$

$$\begin{array}{c} -2x_3 = -6 \quad \Rightarrow \quad X_3 = 3 \\ X_2 + 0X_3 = -1 \quad \Rightarrow \quad X_2 = -1 \\ 2x_1 - x_2 + 3X_3 = 12 \\ X_1 = \frac{1}{2} \left( 12 + X_2 - 3X_3 \right)^{-\frac{1}{2}} \left( 12 - 1 - 9 \right) = 1$$

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$$x = \begin{bmatrix} 1 \\ -1 \\ 3 \end{bmatrix}$$

## The LU Factorization

Let *A* be an  $n \times n$  matrix, and suppose that we can do Gaussian elimination with *A* without any pivoting.

That is, we are able to form the necessary multipliers  $m_{ij}$  without swapping any rows.

Then we can write *A* as the product A = LU where

$$U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & u_{1n} \end{bmatrix} \text{ and } L = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ m_{n1} & \cdots & m_{nn-1} & 1 \end{bmatrix}$$

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