2 Solving Linear Equations $Ax = b$

2.1 Elimination and Back Substitution

2.2 Elimination Matrices and Inverse Matrices

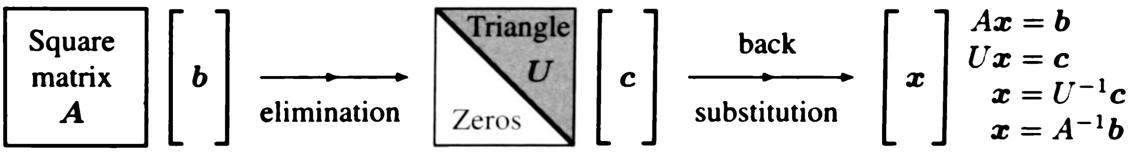
2.3 Matrix Computations and $A = LU$

2.4 Permutations and Transposes

2.5 Derivatives and Finite Difference Matrices

The matrices in this chapter are square: n by n. $\boldsymbol{Ax = b}$ **gives $\boldsymbol{n}$ equations** (one from each row of A). Those equations have $\boldsymbol{n}$ **unknowns** in the vector $\boldsymbol{x}$. Often but not always there is one solution $\boldsymbol{x}$ for each $\boldsymbol{b}$. In this case A has an **inverse** $\boldsymbol{A^{-1}}$ with $A^{-1}A = I$ and $AA^{-1} = I$. Multiplying $A\boldsymbol{x} = \boldsymbol{b}$ by A^{-1} produces the symbolic solution $\boldsymbol{x} = A^{-1}\boldsymbol{b}$.

This chapter aims to find that solution $\boldsymbol{x}$. **But we don't compute $\boldsymbol{A^{-1}}$.** (That would solve $A\boldsymbol{x} = \boldsymbol{b}$ for every possible $\boldsymbol{b}$.) We go forward column by column, assuming that A has independent columns. We only stop if this proves wrong. At the end $A\boldsymbol{x} = \boldsymbol{b}$ has changed to a **triangular system** $\boldsymbol{U x = c}$, and now the solution $\boldsymbol{x}$ is easy to find.



Here is an idea that goes back thousands of years (to China). Each step of "elimination" produces a zero in the matrix. The original A changes slowly into an **upper triangular** $\boldsymbol{U}$. We may need row exchanges. This is not exciting, it is just the natural way to simplify A.

To describe all the steps we need matrices. This is the point of linear algebra! A simple elimination matrix E_{ij} produces a zero where row $\boldsymbol{i}$ meets column $\boldsymbol{j}$ ($\boldsymbol{i} > \boldsymbol{j}$). Overall, an elimination matrix E multiplies A to give $EA = U$. And we multiply U by an **inverse matrix** $L = E^{-1}$ to come back to A. Here are key matrices in this chapter:

Coefficient matrix $\boldsymbol{A}$	Upper triangular $\boldsymbol{U}$	Lower triangular $\boldsymbol{L}$
Elimination matrix $\boldsymbol{E_{ij}}$	Overall elimination $\boldsymbol{E}$	Inverse matrix $\boldsymbol{A^{-1}}$
Permutation matrix $\boldsymbol{P}$	Transpose matrix $\boldsymbol{A^{\mathrm{T}}}$	Symmetric matrix $\boldsymbol{S = S^{\mathrm{T}}}$

Our goal is to explain all the steps from $\boldsymbol{A}$ **to** $\boldsymbol{EA = U}$ **to** $\boldsymbol{A = E^{-1}U = LU}$ **to** $\boldsymbol{x}$. (If the steps fail, this signals that $A\boldsymbol{x} = \boldsymbol{b}$ has no solution for most $\boldsymbol{b}$.) Every computer system has a code to find the triangular U and then the solution $\boldsymbol{x}$. Those codes are used so often that elimination adds up to the greatest cost in all of scientific computing.

But the codes are highly engineered and we don't know a better way to solve $A\boldsymbol{x} = \boldsymbol{b}$. Section 2.5 introduces difference matrices from Computational Science and Engineering.

2.1 Elimination and Back Substitution

1 Elimination subtracts ℓ_{ij} times row j from row i, leave a zero in row i.

2 $Ax = b$ becomes $Ux = c$ (or else $Ax = b$ is proved to have no solution).

3 Then $Ux = c$ is solved by **back substitution** because U is upper triangular.

This chapter explains a systematic way to solve $Ax = b$: *n equations for n unknowns.* The n by n matrix A is given and the n by 1 column vector b is given. There may be *no vector* $x = (x_1, x_2, \ldots, x_n)$ that solves $Ax = b$, or there may be exactly *one solution*, or there may be *infinitely many* solution vectors x. Our job is to decide among these three possibilities and to find all solutions. Here are the possibilities with $n = 2$.

1 **Exactly one solution to $Ax = b$.** In this case A has independent columns. The rank of A is 2. The only solution to $Ax = \mathbf{0}$ is $x = 0$. **A has an *inverse matrix* A^{-1}.**

$$\textbf{Example with one solution } (x, y) = (1, 1) \qquad \begin{aligned} 2x + 3y &= 5 \\ 4x + 2y &= 6 \end{aligned} \qquad \begin{bmatrix} 2 & 3 \\ 4 & 2 \end{bmatrix}$$
Independent columns $(2, 4)$ and $(3, 2)$

2 **No solution to $Ax = b$.** In this case b is not a combination of the columns of A. In other words b is not in the column space of A. The rank of A is 1.

$$\textbf{Example with no solution} \qquad \begin{aligned} 2x + 3y &= 6 \\ 4x + 6y &= 15 \end{aligned} \qquad \begin{bmatrix} 2 & 3 \\ 4 & 6 \end{bmatrix}$$
Dependent columns $(2, 4)$ and $(3, 6)$

Subtract 2 times the first equation from the second to get $0 = 3$. **No solution.**

3 There will be **infinitely many solutions** to $AX = \mathbf{0}$ when the columns of A are not independent. This is the meaning of **dependent columns**—many ways to produce the zero vector $b = \mathbf{0}$. We can multiply X by any number α.

If there is one solution to $Ax = b$ then we can add any solution to $AX = \mathbf{0}$. All the vectors $x + \alpha X$ solve the same equations, so we have many solutions.

For any number α $$A(x + \alpha X) = Ax + \alpha AX = b + \mathbf{0} = b. \qquad (1)$$

$$\textbf{Example with infinitely many solutions} \qquad \begin{aligned} 2x + 3y &= 6 \\ 4x + 6y &= 12 \end{aligned} \qquad \begin{bmatrix} 2 & 3 \\ 4 & 6 \end{bmatrix}$$
A has dependent columns: b is in $\mathbf{C}(A)$

Those equations $Ax = b$ are solved by $x = 0, y = 2$. But there are more solutions because $X = (3, -2)$ solves $AX = \mathbf{0}$. Then $2X = (6, -4)$ also solves $A(2X) = \mathbf{0}$. All vectors αX can be added to the particular solution $x = (0, 2)$ to produce more solutions:

$$x + \alpha X = (0 + 3\alpha, 2 - 2\alpha) \textbf{ is a line of solutions to our two equations } Ax = b.$$

This chapter will start with $Ux = c$: one solution, easy to find. Then we explain how $Ax = b$ leads to $Ux = c$. When this fails, a row exchange may save it. When row exchanges also fail, A has no inverse matrix A^{-1}. Its columns are dependent (cases **2 — 3**).

Back Substitution to Solve $Ux = c$

This chapter will give a systematic way to decide between those possibilities **1, 2, 3**: One solution, no solution, infinitely many solutions. This system is called **elimination.** It simplifies the matrix A without changing any solution x to the equation $Ax = b$. We do the same operations to both sides of the equation, and those operations are reversible. Elimination keeps all solutions x and creates no new ones.

Let me show you the ideal result. Elimination produces an upper triangular matrix. That matrix is called U. **Then $Ax = b$ leads to $Ux = c$**, which we easily solve:

Apply elimination to $Ax = b$ (next page)
The result is $Ux = c$ (here)
Back substitution now finds x

$$Ux = c \quad \text{is} \quad \begin{bmatrix} 2 & 3 & 4 \\ 0 & 5 & 6 \\ 0 & 0 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 19 \\ 17 \\ 14 \end{bmatrix}$$

That letter U stands for **upper triangular**. The matrix has all zeros below its diagonal. Highly important: **The "pivots" 2, 5, 7 on that main diagonal of U are not zero.** Then we can solve the equations by going from bottom to top: **find x_3 then x_2 then x_1.**

Back substitution	The last equation $7x_3 = 14$ gives $x_3 = 2$
Work upwards	The next equation $5x_2 + 6(2) = 17$ gives $x_2 = 1$
Upwards again	The first equation $2x_1 + 3(1) + 4(2) = 19$ gives $x_1 = 4$
Conclusion	The only solution to this example $Ux = c$ is $\boxed{x = (4, 1, 2).}$
Special note	In solving for x_1, x_2, x_3 we needed to divide by the pivots $2, 5, 7$.

These pivots were probably not on the diagonal of the original matrix A (which we haven't seen). The pivots 2, 5, 7 were discovered when "elimination" produced the lower triangular zeros in U. This crucial step from A to U is still to be explained! We have displayed the final back substitution step, next we explain elimination.

Equations $Ax = b$ Elimination to $Ux = c$ Back substitution to $x = U^{-1}c = A^{-1}b$

Note We would not allow the number zero to be a pivot. That would destroy our plan because an equation like $0x_1 = 2$ or $0x_2 = 5$ or $0x_3 = 8$ has no solution. Back substitution will break down with a zero in any pivot position (on the diagonal of U). **The test for independent columns in A is n nonzero pivots in U (after possible row exchanges).**

Every square matrix A with independent columns (full rank) can be reduced to a triangular matrix U with nonzero pivots. *This is our job.* It is possible that we may need to put the equations $Ax = b$ in a different order. We start with the usual case when elimination goes from A to U. Then back substitution as above finds the solution vector x to $Ax = b$.

From A to U and b to c: Elimination in Each Column

First comes a matrix A (independent columns) that will require no row exchanges. We will apply elimination matrices E_{21} then E_{31} then E_{32}. A and b will change to U and c.

The starting matrix is A
The first pivot is 2
The right side is b

$$A = \begin{bmatrix} \mathbf{2} & 3 & 4 \\ 4 & 11 & 14 \\ 2 & 8 & 17 \end{bmatrix} \qquad b = \begin{bmatrix} 19 \\ 55 \\ 50 \end{bmatrix} \tag{2}$$

E_{21} multiplies equation 1 by 2 and subtracts from equation 2. You see the new zero.

$$E_{21} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \boldsymbol{E_{21}A} = \begin{bmatrix} \mathbf{2} & 3 & 4 \\ \mathbf{0} & 5 & 6 \\ 2 & 8 & 17 \end{bmatrix} \qquad \boldsymbol{E_{21}b} = \begin{bmatrix} 19 \\ \mathbf{17} \\ 50 \end{bmatrix} \tag{3}$$

This produced the desired zero in column 1. It changed equation 2. To produce another zero, *we subtract row* 1 *from row* 3 *using* E_{31}. This completes elimination in column 1:

$$E_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \qquad \boldsymbol{E_{31}E_{21}A} = \begin{bmatrix} \mathbf{2} & 3 & 4 \\ \mathbf{0} & \mathbf{5} & 6 \\ \mathbf{0} & 5 & 13 \end{bmatrix} \qquad \begin{bmatrix} 19 \\ 17 \\ \mathbf{31} \end{bmatrix} \tag{4}$$

Move now to column 2 and row 2 (the second pivot row). The pivot is 5, on the diagonal. To eliminate the 5 below it, multiply row 2 by the number 1 and subtract from row 3.

$$E_{32} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \qquad \boldsymbol{U} = \begin{bmatrix} \mathbf{2} & 3 & 4 \\ \mathbf{0} & \mathbf{5} & 6 \\ \mathbf{0} & \mathbf{0} & \mathbf{7} \end{bmatrix} \qquad \boldsymbol{c} = \begin{bmatrix} 19 \\ 17 \\ 14 \end{bmatrix} \tag{5}$$

$E_{32}E_{31}E_{21}A = U$ is triangular. $\boldsymbol{x} = (4, 1, 2)$ solved $U\boldsymbol{x} = \boldsymbol{c}$ on page 41 and $\boldsymbol{x} = (4, 1, 2)$ solves $A\boldsymbol{x} = \boldsymbol{b}$ here. Since U has $2, 5, 7$ on its diagonal we know that back substitution will succeed. The columns of U are independent (and therefore the columns of the original A were independent, as we will see). The matrices A and U have full rank.

We can summarize the elimination steps when no row exchanges are involved.

> Use the first equation to produce zeros in column 1 below the first pivot.
>
> Use the new second equation to clear out column 2 below pivot 2 in row 2.
>
> *Continue to column* 3. The expected result is an upper triangular matrix U.

Elimination on A produces U. **The same steps were applied to the right hand side b.** Those steps produce a new right hand side c. The new equations $U\boldsymbol{x} = \boldsymbol{c}$ (equivalent to the old equations $A\boldsymbol{x} = \boldsymbol{b}$) are solved by back substitution (previous page): $\boldsymbol{x} = (\mathbf{4}, \mathbf{1}, \mathbf{2})$.

Possible Breakdown of Elimination

Elimination might fail. *Zero can appear in a pivot position.* Subtracting that zero from lower rows will not clear out the column below the unwanted zero. Here is an example:

Zero in pivot 2 from elimination in column 1
$$A = \begin{bmatrix} 2 & 3 & 4 \\ 4 & 6 & 14 \\ 2 & 8 & 17 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 3 & 4 \\ 0 & 0 & 6 \\ 0 & 5 & 13 \end{bmatrix} = B$$

The cure is simple if it works. **Exchange row 2 with the zero for row 3 with the 5.** Then the second pivot is **5** and we can clear out the second column below that pivot. Elimination continues to U as normal after the row exchange by the matrix P.

Row exchange Successful
$$PB = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 3 & 4 \\ 0 & \mathbf{0} & 6 \\ 0 & \mathbf{5} & 13 \end{bmatrix} = \begin{bmatrix} 2 & 3 & 4 \\ 0 & \mathbf{5} & 13 \\ 0 & \mathbf{0} & \mathbf{6} \end{bmatrix}$$

For this small example, the row exchange is all we need. It produced U with nonzero pivots $2, 5, 6$. Normally there are more columns and rows to work on, before we reach U.

Caution! That row exchange was a success. This is what we hope for, to reach U with no zeros on its main diagonal. (The pivots $2, 5, 6$ are on the diagonal.) But a slightly different matrix A^* would lead to a bad situation: **no pivot is available in column 2.**

Dependent columns
U^* is not invertible
A^* is not invertible
$$\rightarrow \quad A^* = \begin{bmatrix} 2 & 3 & 4 \\ 4 & \mathbf{6} & 14 \\ 2 & \mathbf{3} & 17 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 3 & 4 \\ 0 & \mathbf{0} & 6 \\ 0 & \mathbf{0} & 13 \end{bmatrix} = U^* \quad (6)$$

At this point elimination is helpless in column 2. *No second pivot.* This misfortune tells us that **the matrix A^* did not have full rank.** Column 2 of U^* is in the same direction as column 1 of U^*. Column 2 of A^* is in the same direction as column 1 of A^*.

You see how dependent columns are systematically identified by elimination. They can't escape a zero in the pivot. Then there will be nonzero solutions $\boldsymbol{X}$ to $A^*\boldsymbol{X} = \mathbf{0}$. The columns of U^* (and A^*) are not independent.

This example has column 2 $= \frac{3}{2}$ column 1. The solution vector $\boldsymbol{X}$ is $(3, -2, 0)$. *The equation $A^*\boldsymbol{x} = \boldsymbol{b}$ may or may not be solvable, depending on $\boldsymbol{b}$*: probably not.

Dependent or Independent Columns

This A^* looks like a failure of elimination: No second pivot. But it was a success because the problem was identified: dependent columns. The beauty of aiming for a triangular matrix U or U^* is that the diagonal entries tell us everything.

A triangular matrix U has full rank exactly when its main diagonal has no zeros.

In that case (square matrix with nonzero pivots) the columns of U are independent. Also the rows are independent. We can see this directly because elimination has simplified the original A to the triangular U.

How do we know that a zero on the diagonal of U^* leads to dependent columns?

$$U^* = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & 0 & * \\ 0 & 0 & 0 & * \end{bmatrix} = \begin{matrix} \text{Upper triangular with an extra zero on its diagonal} \\ \text{This matrix is } \textbf{singular} \text{ (not full rank 4) (no inverse)} \\ \text{The first three columns are dependent} \\ \text{The last two rows are dependent} \end{matrix}$$

The Row Picture and the Column Picture

The next pictures will show the three possibilities for $Ax = b$: **No solution or a line of solutions or one solution.** There are two ways to see this. We start with the *rows of A* and we graph the two equations: **the row picture.** We have trouble if the lines don't meet.

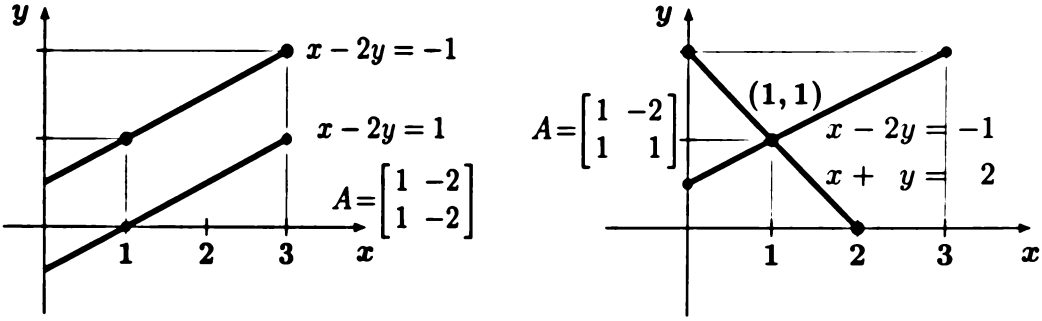


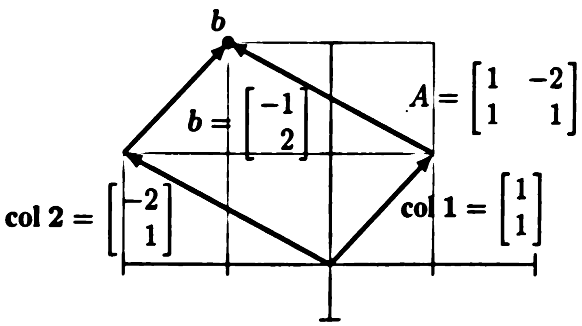
Figure 2.1: Parallel lines mean **no solution.** One line twice means **a line of solutions.**

Intersecting lines give **one solution.** The solution is where the lines meet.

If we had three equations for x, y, and z, those two lines would change to three planes. The three planes meet at a single point in 3-dimensional space. This row picture becomes hard to draw. The column picture is much easier in three or more dimensions.

The **column picture** just shows column vectors: columns of A and also the vector b. We are not looking for points where these vectors meet. The goal of $Ax = b$ is to **combine the columns of A** so as to produce the vector b.

This is always possible when the columns of A (n vectors in n-dimensional space) are *independent.* Then the column space of A contains all vectors b in $\mathbf{R}^n$. There is exactly one combination Ax of the columns that equals b. Elimination finds that solution x.



The columns of A are independent
Column 1 + Column 2 = b
Then the solution is $x_1 = 1, x_2 = 1$
Construct b from the columns!
The bottom point is $(0, 0)$

Figure 2.2: **Column picture.** The vector b is a combination Ax of the columns of A.

Examples of Elimination and Permutation

This chapter will go on to express the whole process using matrices. An elimination matrix E will act on $A\boldsymbol{x} = \boldsymbol{b}$. In case zero appears in a pivot position, use a permutation matrix P. The final result is an upper triangular U and a new right hand side $\boldsymbol{c}$. Then $U\boldsymbol{x} = \boldsymbol{c}$ is solved by back substitution.

In reality a computer takes those steps ($\boldsymbol{x} = A\backslash \boldsymbol{b}$ in MATLAB). But it is good to solve a few examples—*not too many*—by hand. You see the steps to $U\boldsymbol{x} = \boldsymbol{c}$ and then to the solution $\boldsymbol{x}$. This page contains a variety of examples, hopefully to show the way.

$$\boldsymbol{A} = \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} \xrightarrow{E_{21}} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ -2 & -3 & 7 \end{bmatrix} \xrightarrow{E_{31}} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix} \xrightarrow{E_{32}} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} = \boldsymbol{U}$$

Those elimination steps E_{21} and E_{31} and E_{32} produced zeros in positions $(2, 1)$ and $(3, 1)$ and $(3, 2)$. The matrices E have -2 and $+1$ and -1 in those positions. The same steps E_{21}, E_{31}, E_{32} must be applied to the right hand side $\boldsymbol{b}$, to keep the equations correct.

$$\boldsymbol{b} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix} \to E_{21}\boldsymbol{b} = \begin{bmatrix} 2 \\ 4 \\ 10 \end{bmatrix} \to E_{31}E_{21}\boldsymbol{b} = \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix} \to E_{32}E_{31}E_{21}\boldsymbol{b} = E\boldsymbol{b} = \boldsymbol{c} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

There is a simple way to make sure that operations on the matrix A (left side of equations) are also executed on $\boldsymbol{b}$ (right side of equations). The good way is to **include $\boldsymbol{b}$ as an extra column with $\boldsymbol{A}$**. The combination $\begin{bmatrix} A & \boldsymbol{b} \end{bmatrix}$ is called an **augmented matrix**.

$$\begin{bmatrix} A & \boldsymbol{b} \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 & 2 \\ 4 & 9 & -3 & 8 \\ -2 & -3 & 7 & 10 \end{bmatrix} \xrightarrow{E} \begin{bmatrix} 2 & 4 & -2 & 2 \\ 0 & 1 & 1 & 4 \\ 0 & 0 & 4 & 8 \end{bmatrix} = \begin{bmatrix} U & \boldsymbol{c} \end{bmatrix}. \quad (7)$$

Now we include an example that requires a permutation matrix P. It will exchange equations and avoid zero in the pivot. The new matrix A needs P to improve column 2.

Exchange rows 2 and 3
$$A = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 2 & 3 \\ 0 & 4 & 5 \end{bmatrix} \xrightarrow{E} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 4 & 5 \end{bmatrix} \xrightarrow{P} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 4 & 5 \\ 0 & 0 & 1 \end{bmatrix} = \boldsymbol{U}$$

That permutation P_{23} exchanged rows 2 and 3 when it was needed to avoid a zero pivot. But we could have exchanged rows 2 and 3 at the start. Then E_{21} and E_{31} change places.

In the final description $PA = LU$ of elimination on A, all the E's will be moved to the right side. **Each matrix in $\boldsymbol{E_{32}E_{31}E_{21}}$ is inverted.** Those inverses come in **reverse order $\boldsymbol{L} = E_{21}^{-1}E_{31}^{-1}E_{32}^{-1}$.** The overall equation is $\boldsymbol{PA = LU}$. Often no permutations are needed and elimination produces $\boldsymbol{A = LU}$: the best equation of all, in Section 2.2.

Section 2.4 will return to understand all the possible permutations of n rows. *There are $n\,!$ permutation matrices P, including $P = I$ for no row exchanges.*