

Part I: Highlights of Linear Algebra

I.1 Multiplication Ax Using Columns of A

We hope you already know some linear algebra. It is a beautiful subject—more useful to more people than calculus (in our quiet opinion). But even old-style linear algebra courses miss basic and important facts. This first section of the book is about *matrix-vector* multiplication Ax .

We always use examples to make our point clear.

Example 1 Multiply A times x using the three rows of A and then using the two columns :

$$\begin{array}{l} \text{By rows} \\ \text{By columns} \end{array} \quad \begin{array}{l} \begin{bmatrix} 2 & 3 \\ 2 & 4 \\ 3 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2x_1 + 3x_2 \\ 2x_1 + 4x_2 \\ 3x_1 + 7x_2 \end{bmatrix} \\ \begin{bmatrix} 2 & 3 \\ 2 & 4 \\ 3 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = x_1 \begin{bmatrix} 2 \\ 2 \\ 3 \end{bmatrix} + x_2 \begin{bmatrix} 3 \\ 4 \\ 7 \end{bmatrix} \end{array} \quad \begin{array}{l} = \text{inner products} \\ = \text{of the rows} \\ \text{with } x = (x_1, x_2) \\ \\ = \text{combination} \\ = \text{of the columns} \\ \mathbf{a}_1 \text{ and } \mathbf{a}_2 \end{array}$$

You see that both ways give the same result. The first way (a row at a time) produces 3 inner products. Those are also known as “dot products” because of the dot notation :

$$\text{row} \cdot \text{column} = (\mathbf{2}, \mathbf{3}) \cdot (x_1, x_2) = \mathbf{2}x_1 + \mathbf{3}x_2 \quad (1)$$

This is the way to find the three separate components of Ax . We use this for computing—but not for understanding. It is low level. Understanding is higher level, staying with vectors.

The vector approach sees Ax as a “linear combination” of \mathbf{a}_1 and \mathbf{a}_2 . This is the fundamental operation of linear algebra! A linear combination of vectors \mathbf{a}_1 and \mathbf{a}_2 includes two steps :

- (1) Multiply \mathbf{a}_1 and \mathbf{a}_2 by “scalars” x_1 and x_2
- (2) Add vectors $x_1\mathbf{a}_1 + x_2\mathbf{a}_2$.

Thus Ax is a linear combination of the columns of A . This is fundamental.

This thinking leads us to the **column space** of A . The key idea is to take **all combinations** of the columns. All real numbers x_1 and x_2 are allowed—the space includes Ax for all vectors x . In this way we get infinitely many output vectors Ax . And we can see those outputs geometrically.

In our example, each $A\mathbf{x}$ is a vector in 3-dimensional space. That 3D space is called \mathbf{R}^3 . (The \mathbf{R} indicates real numbers. Vectors with three complex components lie in the space \mathbf{C}^3 .) We stay with real vectors and we ask this key question:

All combinations $A\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2$ produce what part of the full 3D space?

Answer: Those vectors produce a **plane**. The plane contains the complete line in the direction of $\mathbf{a}_1 = (2, 2, 3)$, since every vector $x_1\mathbf{a}_1$ is included. The plane also includes the infinite line of all vectors $x_2\mathbf{a}_2$ in the direction of \mathbf{a}_2 . And it includes the *sum* of any vector on one line plus any vector on the other line. **This addition fills out an infinite plane containing the two lines.** But it does not fill out the whole 3-dimensional space \mathbf{R}^3 :

Definition **The combinations of the columns** fill out (“span”) the **column space** of A .

Here the column space is a plane. That plane includes the zero point $(0, 0, 0)$ which is produced when $x_1 = x_2 = 0$. The plane includes $(5, 6, 10) = \mathbf{a}_1 + \mathbf{a}_2$ and $(-1, -2, -4) = \mathbf{a}_1 - \mathbf{a}_2$. With probability 1 it does **not** include the random point **rand** $(3, 1)$! Which points are in the plane?

$\mathbf{b} = (b_1, b_2, b_3)$ is in the column space of A exactly when $A\mathbf{x} = \mathbf{b}$ has a solution (x_1, x_2)

When you see that truth, you understand the column space $\mathbf{C}(A)$: The solution \mathbf{x} shows how to express the right side \mathbf{b} as a combination $x_1\mathbf{a}_1 + x_2\mathbf{a}_2$ of the columns. For some \mathbf{b} this is impossible.

Example 2 $\mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ is not in $\mathbf{C}(A)$ because $A\mathbf{x} = \begin{bmatrix} 2x_1 + 3x_2 \\ 2x_1 + 4x_2 \\ 3x_1 + 7x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ is unsolvable.

The first two equations force $x_1 = \frac{1}{2}$ and $x_2 = 0$. Then equation 3 fails: $3\left(\frac{1}{2}\right) + 7(0) = 1.5$ (**not 1**).

This means that $\mathbf{b} = (1, 1, 1)$ is not in the column space—the plane of \mathbf{a}_1 and \mathbf{a}_2 .

Example 3 What are the column spaces of $A_2 = \begin{bmatrix} 2 & 3 & 5 \\ 2 & 4 & 6 \\ 3 & 7 & 10 \end{bmatrix}$ and $A_3 = \begin{bmatrix} 2 & 3 & 1 \\ 2 & 4 & 1 \\ 3 & 7 & 1 \end{bmatrix}$?

Solution. The column space of A_2 is the same plane as before. The new column $(5, 6, 10)$ is the sum of column 1 + column 2. So $\mathbf{a}_3 =$ column 3 is already in the plane and adds nothing new. By including this “*dependent*” column we don’t go beyond the original plane $\mathbf{C}(A)$.

The column space of A_3 is the whole 3D space \mathbf{R}^3 . Example 2 showed us that the new third column $(1, 1, 1)$ is not in the plane $\mathbf{C}(A)$. Our column space $\mathbf{C}(A_3)$ has grown bigger. But there is nowhere to stop between a plane and the full 3D space. Visualize the $x - y$ plane and a third vector (x_3, y_3, z_3) out of the plane (meaning that $z_3 \neq 0$). They combine to give **every vector in \mathbf{R}^3** .

Here is a total and exclusive list of all possible column spaces inside \mathbf{R}^3 . Dimensions 0, 1, 2, 3:

Subspaces of \mathbf{R}^3

- The **zero vector** $(0, 0, 0)$ by itself
- A **line** of all vectors $x_1\mathbf{a}_1$
- A **plane** of all vectors $x_1\mathbf{a}_1 + x_2\mathbf{a}_2$
- The **whole \mathbf{R}^3** with all vectors $x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$

In that list we need the vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ to be “**independent**”. The only combination that gives the zero vector is $0\mathbf{a}_1 + 0\mathbf{a}_2 + 0\mathbf{a}_3$. So \mathbf{a}_1 by itself gives a line, \mathbf{a}_1 and \mathbf{a}_2 give a plane, \mathbf{a}_1 and \mathbf{a}_2 and \mathbf{a}_3 give every vector \mathbf{b} in \mathbf{R}^3 . The zero vector is in every subspace! In linear algebra language:

- Three independent columns in \mathbf{R}^3 produce an **invertible** 3×3 matrix: $AA^{-1} = A^{-1}A = I$.
- $A\mathbf{x} = \mathbf{0}$ requires $\mathbf{x} = (0, 0, 0)$. $A\mathbf{x} = \mathbf{b}$ has exactly one solution $\mathbf{x} = A^{-1}\mathbf{b}$ for every \mathbf{b} .

You see the picture for the columns of an n by n invertible matrix. Their combinations fill all of \mathbf{R}^n . Then the n rows will also be independent. We needed those ideas and that language to go further.

Problem Set I.1

- 1 Give an example where a combination of three nonzero vectors in \mathbf{R}^4 is the zero vector. Then write your example in the form $A\mathbf{x} = \mathbf{0}$. What are the shapes of A and \mathbf{x} and $\mathbf{0}$?
- 2 Suppose a combination of the columns of A equals a different combination of those columns. Write that statement as $A\mathbf{x} = A\mathbf{y}$. Find a combination of the columns of A that equals the zero vector (in matrix language, find a solution to $A\mathbf{z} = \mathbf{0}$). Then find a second solution \mathbf{z}_2 .
- 3 (Practice with subscripts) The vectors $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ are in m -dimensional space \mathbf{R}^m , and a combination $c_1\mathbf{a}_1 + \dots + c_n\mathbf{a}_n$ is the zero vector. That statement is at the vector level.
 - (1) Write that statement at the matrix level. Use the matrix A with the \mathbf{a} 's in its columns and use the column vector $\mathbf{c} = (c_1, \dots, c_n)$.
 - (2) Write that statement at the scalar level using subscripts and sigma notation to add up numbers. The column vector \mathbf{a}_j has components $a_{1j}, a_{2j}, \dots, a_{mj}$.
- 4 Suppose A is the 3 by 3 matrix $\mathbf{ones}(3, 3)$ of all ones. Find two independent vectors \mathbf{x} and \mathbf{y} that solve $A\mathbf{x} = \mathbf{0}$ and $A\mathbf{y} = \mathbf{0}$. Write that first equation $A\mathbf{x} = \mathbf{0}$ (with numbers) as a combination of the columns of A . Why don't I ask for a third independent vector with $A\mathbf{z} = \mathbf{0}$?
- 5 The linear combinations of $\mathbf{v} = (1, 1, 0)$ and $\mathbf{w} = (0, 1, 1)$ fill a plane in \mathbf{R}^3 .
 - (a) Find a vector \mathbf{z} that is perpendicular to \mathbf{v} and \mathbf{w} . Then \mathbf{z} is perpendicular to every vector $c\mathbf{v} + d\mathbf{w}$ on the plane: $(c\mathbf{v} + d\mathbf{w})^T \mathbf{z} = c\mathbf{v}^T \mathbf{z} + d\mathbf{w}^T \mathbf{z} = 0 + 0$.
 - (b) Find a vector \mathbf{u} that is not on the plane. Check that $\mathbf{u}^T \mathbf{z} \neq 0$.
- 6 In the xy plane mark all nine of these linear combinations:

$$c \begin{bmatrix} 2 \\ 1 \end{bmatrix} + d \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \text{with } c = 0, 1, 2 \quad \text{and } d = 0, 1, 2.$$
- 7 If three corners of a parallelogram are $(1, 1)$, $(4, 2)$, and $(1, 3)$, what are all three of the possible fourth corners? Draw two of them.
- 8 Draw two vectors \mathbf{v} and \mathbf{w} coming out from the center point $(0, 0)$.
 - (a) Mark the points $\frac{1}{2}\mathbf{v} + \frac{1}{2}\mathbf{w}$ and $\frac{1}{4}\mathbf{v} + \frac{1}{4}\mathbf{w}$.
 - (b) Draw a line containing all the points $c\mathbf{v} + (1 - c)\mathbf{w}$ (all c).
 - (c) Draw the "cone" of all combinations $c\mathbf{v} + d\mathbf{w}$ with $c \geq 0$ and $d \geq 0$.
- 9 How many corners does a cube have in 4 dimensions? How many 3D faces? How many edges? An edge goes between two adjacent corners.
- 10 Describe the column space of $A = [\mathbf{v} \ \mathbf{w} \ \mathbf{v} + 2\mathbf{w}]$. Describe the nullspace of A : all vectors $\mathbf{x} = (x_1, x_2, x_3)$ that solve $A\mathbf{x} = \mathbf{0}$. Add the "dimensions" of that plane and that line:

dimension of column space + dimension of nullspace = number of columns
- 11 Suppose the column space of an m by n matrix is all of \mathbf{R}^3 . What can you say about m ? What can you say about n ?

I.2 Matrix-Matrix Multiplication AB

Inner products (*rows times columns*) produce each of the numbers in $AB = C$:

$$\begin{array}{l} \text{row 2 of } A \\ \text{column 3 of } B \\ \text{give } c_{23} \text{ in } C \end{array} \begin{bmatrix} \cdot & \cdot & \cdot \\ a_{21} & a_{22} & a_{23} \\ \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} \cdot & \cdot & b_{13} \\ \cdot & \cdot & b_{23} \\ \cdot & \cdot & b_{33} \end{bmatrix} = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & c_{23} \\ \cdot & \cdot & \cdot \end{bmatrix} \quad (1)$$

That dot product $c_{23} = (\text{row 2 of } A) \cdot (\text{column 3 of } B)$ is a sum:

$$c_{23} = a_{21} b_{13} + a_{22} b_{23} + a_{23} b_{33} = \sum_{k=1}^3 a_{2k} b_{k3} \quad \text{and} \quad c_{ij} = \sum_{k=1}^n a_{ik} b_{kj}. \quad (2)$$

This is how we usually compute each number in $AB = C$.

There is another way to multiply AB : **columns of A times rows of B** . We need to see this! I start with numbers to make two key points: one column \mathbf{u} times one row \mathbf{v}^T produces a *matrix*. Concentrate first on that piece of AB . This matrix $\mathbf{u}\mathbf{v}^T$ is especially simple:

$$\begin{array}{l} \text{Outer} \\ \text{product} \end{array} \quad \mathbf{u}\mathbf{v}^T = \begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix} \begin{bmatrix} 3 & 4 & 6 \end{bmatrix} = \begin{bmatrix} 6 & 8 & 12 \\ 6 & 8 & 12 \\ 3 & 4 & 6 \end{bmatrix} = \text{“rank one matrix”}$$

An m by 1 matrix (a column \mathbf{u}) times a 1 by p matrix (a row \mathbf{v}^T) gives an m by p matrix. Notice what is special about the rank one matrix $\mathbf{u}\mathbf{v}^T$:

$$\text{All columns of } \mathbf{u}\mathbf{v}^T \text{ are multiples of } \mathbf{u} = \begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix}. \text{ All rows are multiples of } \mathbf{v}^T = \begin{bmatrix} 3 & 4 & 6 \end{bmatrix}.$$

The column space of $\mathbf{u}\mathbf{v}^T$ is one-dimensional: *the line in the direction of \mathbf{u}* . The dimension of the column space (the number of independent columns) is the **rank of the matrix**—a key number. **All nonzero matrices $\mathbf{u}\mathbf{v}^T$ have rank one.** They are the perfect building blocks for every matrix.

Notice also: **The row space of $\mathbf{u}\mathbf{v}^T$ is the line through \mathbf{v}** . By definition, the row space of any matrix A is the column space $\mathbf{C}(A^T)$ of its transpose A^T . That way we stay with column vectors. In the example, we transpose $\mathbf{u}\mathbf{v}^T$ (**exchange rows with columns**) to get the matrix $\mathbf{v}\mathbf{u}^T$:

$$(\mathbf{u}\mathbf{v}^T)^T = \begin{bmatrix} 6 & 8 & 12 \\ 6 & 8 & 12 \\ 3 & 4 & 6 \end{bmatrix}^T = \begin{bmatrix} 6 & 6 & 3 \\ 8 & 8 & 4 \\ 12 & 12 & 6 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ 6 \end{bmatrix} \begin{bmatrix} 2 & 2 & 1 \end{bmatrix} = \mathbf{v}\mathbf{u}^T.$$

We are seeing the clearest possible example of the first great theorem in linear algebra:

Row rank = Column rank r independent columns $\Leftrightarrow r$ independent rows
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A nonzero matrix $\mathbf{u}\mathbf{v}^T$ has one independent column and one independent row! All columns are multiples of \mathbf{u} and all rows are multiples of \mathbf{v}^T . The rank is $r = 1$ for this matrix.

$AB = \text{Sum of Rank One Matrices}$

We turn to the full product AB , using columns of A times rows of B . Let $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n$ be the columns of A . Let $\mathbf{b}_1^*, \mathbf{b}_2^*, \dots, \mathbf{b}_n^*$ be the rows of B . Notice the same number n (or we couldn't multiply A times B). **Then the product AB is the sum of columns \mathbf{a}_k times rows \mathbf{b}_k^* :**

Column-row multiplication of matrices

$$AB = \left[\begin{array}{c|ccc|} & & & \\ \mathbf{a}_1 & \dots & \mathbf{a}_n & \\ & & & \end{array} \right] \left[\begin{array}{c} \text{--- } \mathbf{b}_1^* \text{ ---} \\ \vdots \\ \text{--- } \mathbf{b}_n^* \text{ ---} \end{array} \right] = \mathbf{a}_1 \mathbf{b}_1^* + \mathbf{a}_2 \mathbf{b}_2^* + \dots + \mathbf{a}_n \mathbf{b}_n^*. \quad (3)$$

Here is a 2 by 2 example to show the $n = 2$ pieces (column times row) and their sum AB :

$$\begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 \\ 0 & 5 \end{bmatrix} = \begin{bmatrix} \mathbf{1} \\ \mathbf{3} \end{bmatrix} \begin{bmatrix} \mathbf{2} & \mathbf{4} \end{bmatrix} + \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{5} \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 6 & 12 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 5 \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 6 & 17 \end{bmatrix}. \quad (4)$$

Can you count the multiplications of number times number? Four multiplications to get 2, 4, 6, 12. Four more to get 0, 0, 0, 5. A total of $2^3 = 8$ multiplications. Always there are n^3 multiplications when A and B are n by n . And mnp multiplications when $AB = (m \text{ by } n)$ times $(n \text{ by } p)$: n rank one matrices, each of those matrices is m by p .

The count is the same for the usual inner product way! Row of A times column of B needs n multiplications. We do this for every number in AB : mp dot products when AB is m by p . The total count is again mnp for $(m \text{ by } n)$ times $(n \text{ by } p)$.

 mp inner products, n multiplications each OR n outer products, mp multiplications each

When you look closely, they are exactly the same multiplications $a_{ik} b_{kj}$ in different orders. Here is the algebra proof that c_{ij} is the same by outer products in (3) as by inner products in (2):

The i, j entry of $\mathbf{a}_k \mathbf{b}_k^*$ is $a_{ik} b_{kj}$. Add for $k = 1$ to n . Then $c_{ij} = \sum_{k=1}^n a_{ik} b_{kj} = \text{row } i \cdot \text{column } j$.

Insight from Column times Row

Why is the outer product approach essential in data science? The short answer is: *We are looking for the important part of a matrix C .* We don't usually want the biggest number in C (though that could be important). What we want more is the largest piece of C . **And those pieces are rank one matrices uv^T .** A dominant theme in applied linear algebra is:

Factor C into AB and look at the pieces $\mathbf{a}_k \mathbf{b}_k^*$ of $AB = C$.

Factoring C into AB is the reverse of multiplying $AB = C$. Factoring takes longer, especially if the pieces involve *eigenvalues* or *singular values*. But those numbers have inside information about the matrix C . That information is not visible until you factor.

Here are five important factorizations, written with the standard choice of letters (usually A , not C) for the original product matrix and then for its factors. This book will explain all five.

$$A = LU \quad A = QR \quad S = Q\Lambda Q^T \quad A = X\Lambda X^{-1} \quad A = U\Sigma V^T$$

At this point we simply list key words and properties for each of these factorizations.

- 1 $A = LU$ comes from **elimination**. Combinations of rows take A to U and U back to A . L is lower triangular and U is upper triangular as in equation (4)
- 2 $A = QR$ comes from **orthogonalizing** the columns \mathbf{a}_1 to \mathbf{a}_n as in “Gram-Schmidt”. Q has orthonormal columns ($Q^T Q = I$) and R is upper triangular
- 3 $S = Q\Lambda Q^T$ comes from the **eigenvalues** $\lambda_1, \dots, \lambda_n$ of a symmetric matrix $S = S^T$. Eigenvalues on the diagonal of Λ and **orthonormal eigenvectors** in the columns of Q
- 4 $A = X\Lambda X^{-1}$ is **diagonalization** when A is n by n with n independent eigenvectors. Eigenvalues of A are on the diagonal of Λ . Eigenvectors of A are in the columns of X
- 5 $A = U\Sigma V^T$ is the **Singular Value Decomposition** of any matrix A (square or not). The **singular values** $\sigma_1, \dots, \sigma_r$ are in Σ . The orthonormal **singular vectors** are in U and V

Let me pick out a favorite (number 3) to illustrate the idea. This special factorization $Q\Lambda Q^T$ starts with a symmetric matrix S . That matrix has orthogonal unit eigenvectors $\mathbf{q}_1, \dots, \mathbf{q}_n$. Those eigenvectors go into the columns of Q . S and Q are the kings and queens of linear algebra:

$$\begin{aligned} \text{Symmetric matrix } S \quad S^T &= S \quad \text{when all } s_{ij} = s_{ji} \\ \text{Orthogonal matrix } Q \quad Q^T &= Q^{-1} \quad \text{when all } \mathbf{q}_i \cdot \mathbf{q}_j = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases} \end{aligned}$$

The diagonal matrix Λ contains real eigenvalues λ_1 to λ_n . Every real symmetric matrix S has n orthonormal eigenvectors \mathbf{q}_1 to \mathbf{q}_n . When multiplied by S , they keep the same direction:

$$\boxed{\text{Eigenvector } \mathbf{q} \text{ and eigenvalue } \lambda \quad S\mathbf{q} = \lambda\mathbf{q}} \quad (5)$$

Finding λ and \mathbf{q} is not easy for a big matrix. But n pairs always exist when S is symmetric. Our purpose here is to see how $SQ = Q\Lambda$ comes column by column from $S\mathbf{q} = \lambda\mathbf{q}$:

$$SQ = S \begin{bmatrix} \mathbf{q}_1 & \dots & \mathbf{q}_n \end{bmatrix} = \begin{bmatrix} \lambda_1 \mathbf{q}_1 & \dots & \lambda_n \mathbf{q}_n \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 & \dots & \mathbf{q}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} = Q\Lambda \quad (6)$$

Multiply $SQ = Q\Lambda$ by $Q^{-1} = Q^T$ to get $S = Q\Lambda Q^T$ = a symmetric matrix. Each eigenvalue λ_k and each eigenvector \mathbf{q}_k contribute a rank one piece $\lambda_k \mathbf{q}_k \mathbf{q}_k^T$ to S .

$$\text{Always symmetric} \quad (Q\Lambda Q^T)^T = Q^{TT} \Lambda^T Q^T = Q\Lambda Q^T \quad (\text{diagonal } \Lambda^T = \Lambda) \quad (7)$$

$$\text{Rank one pieces} \quad S = (Q\Lambda)Q^T = (\lambda_1 \mathbf{q}_1) \mathbf{q}_1^T + (\lambda_2 \mathbf{q}_2) \mathbf{q}_2^T + \dots + (\lambda_n \mathbf{q}_n) \mathbf{q}_n^T \quad (8)$$

Please notice that the columns of $Q\Lambda$ are $\lambda_1 \mathbf{q}_1$ to $\lambda_n \mathbf{q}_n$. When you multiply a matrix on the right by the diagonal matrix Λ , you multiply its *columns* by the λ 's.