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Chapter 1

Vectors and Matrices

1.1 Intuition for Dot product, Cosine formula, Schwarz and Triangle inequalities

Intuition for dot product

The unit vectors $\boldsymbol{v} = (\cos\alpha, \sin\alpha)$ and $\boldsymbol{w} = (\cos\beta, \sin\beta)$ are plotted as follows

Figure 1.5: Unit vectors: $\boldsymbol{u} \cdot \boldsymbol{i} = \cos\theta$. The angle between the vectors is θ.

See first that when fixed in this form, the magnitude of both vectors is 1, with an angle $\beta - \alpha$ between them. These unit vectors have dot product

$$\boldsymbol{v} \cdot \boldsymbol{w} = \cos\alpha \cos\beta + \sin\alpha \sin\beta = \cos(\beta - \alpha)$$

We have θ as the angle between the two vectors; see that the sign of $\boldsymbol{v} \cdot \boldsymbol{w}$ tells us whether θ is below or above a right angle (due to the cosine function being negative for its argument $> \pi/2$ and positive for $< \pi/2$):

Figure 1.6: Small angle $\boldsymbol{v} \cdot \boldsymbol{w_1} > 0$. Right angle $\boldsymbol{v} \cdot \boldsymbol{w_2} = 0$. Large angle $\boldsymbol{v} \cdot \boldsymbol{w_3} < 0$.

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Cont.
The idea here is that the dot product reveals the exact angle θ; for unit vectors $\boldsymbol{u}$ and $\boldsymbol{U}$, the dot product $\boldsymbol{u} \cdot \boldsymbol{U}$ is the cosine of θ. Ths remains true in n dimensions (not shown).

See that any $\boldsymbol{u}$ and $\boldsymbol{v}$ can be fixed in the above form by normalising their lengths to get $\boldsymbol{u} = \boldsymbol{v}/||\boldsymbol{v}||$ and $\boldsymbol{U} = \boldsymbol{w}/||\boldsymbol{w}||$. After which their dot product would give $\cos\theta$. This leads us to the *cosine formula*:

$$\textbf{Cosine formula}: \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{||\boldsymbol{v}|| \, ||\boldsymbol{w}||} = \cos\theta \quad \text{if } \boldsymbol{v} \text{ and } \boldsymbol{w} \text{ are nonzero vectors}$$

Perpendicular vectors
See that when the angle between $\boldsymbol{v}$ and $\boldsymbol{w}$ is $90°$, its cosine is 0; this gives us a way to test this. Also see that for perpendicular vectors:

$$||\boldsymbol{v} + \boldsymbol{w}||^2 = ||\boldsymbol{v}||^2 + ||\boldsymbol{w}||^2$$

because

$$||\boldsymbol{v} + \boldsymbol{w}||^2 = (\boldsymbol{v} + \boldsymbol{w}) \cdot (\boldsymbol{v} + \boldsymbol{w}) = \boldsymbol{v} \cdot \boldsymbol{v} + \boldsymbol{v} \cdot \boldsymbol{w} + \boldsymbol{w} \cdot \boldsymbol{v} + \boldsymbol{w} \cdot \boldsymbol{w}$$

where $\boldsymbol{v} \cdot \boldsymbol{w} = 0$.

Schwarz and Triangle inequalities
First, see from the cosine formula that the dot product of $\boldsymbol{v}/||\boldsymbol{v}||$ and $\boldsymbol{w}/||\boldsymbol{w}||$ never exceeds one (since $\cos\theta$ never exceeds one). This is the the *Schwarz inequality*:

$$\textbf{Schwarz inequality}: |\boldsymbol{v} \cdot \boldsymbol{w}| \leq ||\boldsymbol{v}|| \, ||\boldsymbol{w}||$$

The *Triangle inequality* comes directly from the Schwarz inequality:

$$\textbf{Triangle inequality}: ||\boldsymbol{v} + \boldsymbol{w}|| \leq ||\boldsymbol{v}|| + ||\boldsymbol{w}||$$

This can be seen from

$$||\boldsymbol{v} + \boldsymbol{w}||^2 = \boldsymbol{v} \cdot \boldsymbol{v} + \boldsymbol{v} \cdot \boldsymbol{w} + \boldsymbol{w} \cdot \boldsymbol{v} + \boldsymbol{w} \cdot \boldsymbol{w} \leq ||\boldsymbol{v}||^2 + 2||\boldsymbol{v}|| \, ||\boldsymbol{w}|| + ||\boldsymbol{w}||^2$$

The square root gives us the triangle equality (side 3 cannot exceed side 1 + side 2).

1.2 Intuition for column rank being equal to row rank

If all columns are in the same direction, why does it happen that all the rows are the same direction?

Consider the matrix, see that column 2 is m times column 1:

$$A = \begin{bmatrix} a & ma \\ b & mb \end{bmatrix}$$

See that the second row is just b/a times the first row—if the column rank is 1, then the row rank is 1. See that transposing the matrix, we have

$$A = \begin{bmatrix} a(1) & b(1) \\ a(m) & b(m) \end{bmatrix}$$

which still has one independent column. Now consider the 3x3 case:

$$A = \begin{bmatrix} a & ma & pa \\ b & mb & pb \\ c & mc & pc \end{bmatrix}$$

See that a similar deduction can also be made in this case, where the row rank of A is equal to its column rank.

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An informal proof

Consider any matrix A, suppose we go from left to right, looking for independent columns of A using the following procedure:

1. If column 1 of A is not zero, put it in matrix C

2. If column 2 of A is not a multiple of column 1, put it in into C

3. If column 3 of A is not a combination of columns 1 and 2, put it into C. *continue*

See that at the end C will have r columns taken from A, where r is the rank of A and C. While the n columns of A are dependent, the r columns of C will surely be independent.

For instance consider A with rank 2

$$A = \begin{bmatrix} 2 & 6 & 4 \\ 4 & 12 & 8 \\ 1 & 3 & 5 \end{bmatrix} \quad \text{leads to} \quad C = \begin{bmatrix} 2 & 4 \\ 4 & 8 \\ 1 & 5 \end{bmatrix}$$

Now consider another matrix R to be multiplied by C such that $A = CR$. The first and third columns of A are already in C, so those respective columns in R make up a *identity matrix*; the second column of A is a multiple of the first, so we have

$$A = CR \quad \text{is} \quad \begin{bmatrix} 2 & 6 & 4 \\ 4 & 12 & 8 \\ 1 & 3 & 5 \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 4 & 8 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} 1 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

(See that the ith row of A can be seen as a linear combination of the rows of R specified the ith row of C. (or just consider $A^T = R^T C^T$). We know that

1. C contains the full set of r independent columns of A.

2. $R = [I \, F]$ contains the identity matrix I in the same r columns that held C.

3. The dependent columns of A are combinations of CF of the independent columns in C.

Where the matrix F goes into the other $n - r$ columns of $R = [I \, F]$. ($A = CR$ becomes $A = C[I, F] = [C, CF] = $ [indep cols of A, dep cols of A] (in correct order).

See that C has the same column space as A, and R *has the same row space* as A (every row of A is a combination of the rows of R).
(next page)

Cont.
We had the example

$$\boldsymbol{A} = \boldsymbol{CR} \quad \text{is} \quad \begin{bmatrix} 2 & 6 & 4 \\ 4 & 12 & 8 \\ 1 & 3 & 5 \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 4 & 8 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} 1 & 3 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Here is an informal proof that the row rank of $\boldsymbol{A}$ equals the column rank of $\boldsymbol{A}$ (based from facts we already know)

1. The r columns of $\boldsymbol{C}$ are independent (chosen that way from $\boldsymbol{A}$)

2. Every column of $\boldsymbol{A}$ is a combination of those r columns of $\boldsymbol{C}$ (since $\boldsymbol{A} = \boldsymbol{CR}$)

3. The r rows of $\boldsymbol{R}$ are independent (they contain the r by r matrix $\boldsymbol{I}$)

4. Every row of $\boldsymbol{A}$ is a combination of the $\boldsymbol{r}$ rows of $\boldsymbol{R}$

See that for every column of $\boldsymbol{A}$ that goes into $\boldsymbol{C}$, a column of $\boldsymbol{I}$ goes into $\boldsymbol{R}$, where each column of $\boldsymbol{I}$ in $\boldsymbol{R}$ adds an independent row.

This means that the column rank of $\boldsymbol{C}$ (column space of $\boldsymbol{A}$) is always equal to the row rank of $\boldsymbol{R}$ (row space of $\boldsymbol{A}$)—the column rank of $\boldsymbol{A}$ is equal to the row rank of $\boldsymbol{A}$.

More examples
Rank 2:
$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 4 & 5 \\ 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \end{bmatrix}$$

Rank 2:
$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 4 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & 4 \end{bmatrix} \begin{bmatrix} 1 & 2 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

Rank 1:
$$\begin{bmatrix} 1 & 2 & 10 & 100 \\ 3 & 6 & 30 & 300 \\ 2 & 4 & 20 & 200 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} \begin{bmatrix} 1 & 2 & 10 & 100 \end{bmatrix}$$

1.3   Ways to multiply $AB = C$

Multiplcation by columns of A and rows of B
A lesser known way to multiply AB is through considering the columns of A and the rows of B (contrary to the usual ideas where each entry of the result is a dot product of a row of A and column of B):

$$AB = \begin{bmatrix} | & & | \\ a_1 & \cdots & a_n \\ | & & | \end{bmatrix} \begin{bmatrix} - & b_1^* & - \\ & \vdots & \\ - & b_n^* & - \end{bmatrix} = a_1 b_1^* + a_2 b_2^* + \cdots + a_n b_n^*.$$

columns a_k \quad rows b_k^* \quad **Add columns a_k times rows b_k^***

We multiply each column of A by each row of B; this gives us n rank 1 matrices, which we then sum together; these matrices are called *outer products*

(usually we see the ith column of the result as a linear combination of the columns of A specified by the ith column of B. However in this case the ith outer product is a matrix of the same size as the result, that contains all the contributions of the ith column of A to the final product. By summing this over all n columns of A we get the result.)

Summary of methods

(3 by 2) (2 by 4) = (3 by 4)   **Four Ways to Multiply $AB = C$**

(**Row i of A**) · (**Column k of B**) = **Number C_{ik}**
$i = 1$ to 3 \qquad $k = 1$ to 4 \qquad **12 numbers**

A times (**Column k of B**) \qquad = **Column k of C**
$k = 1$ to 4 \qquad **4 columns**

(**Row i of A**) times B \qquad = **Row i of C**
$i = 1$ to 3 \qquad **3 rows**

(**Column j of A**) (**Row j of B**) = **Rank 1 Matrix**
$j = 1$ to 2 \qquad **2 matrices**

Dot product way, Column way, Row way, Columns times rows

(A nice way to intuit the the third method is to consider $(AB)^T = B^T A^T$; where the columns of $(AB)^T$ are the rows of AB)

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Chapter 2

Solving linear equations
$Ax = b$

2.1   Solutions to $Ax = b$

Given a nxn matrix A and an nx1 column vector b, there are three outcomes for the vector x that solves $Ax = b$.

First there may be *no vector* x that solves $Ax = b$, or there may be exactly *one* solution, or there may be *infinitely many* solution vectors x. Here are the possibilities:

1. **Exactly one solution** to $Ax = b$ means that A has independent columns (only one particular linear combination of the columns of A leads to b. That combination is specified by x). A is full rank and the only solution to $Ax = 0$ is $x = 0$. A *has an inverse matrix* A^{-1} (given b, we can work backward to get x since only one x leads to b).

2. **No solution** to $Ax = b$ means that b is not in the column space of A, so A is not full rank.

3. **Infinitely many solutions**. See that when the columns of A are not independent (not full rank), then there are infinitely many ways to produce the zero vector $b = 0$ (this is the meaning of dependent columns), and so there are infinitely many solutions to $AX = 0$.

Also see that if A is not full rank it means that its column space is some subspace, where solutions only exist for b within that subspace.

As such, if there so happens to be a solution to $Ax = b$ then we can add any solution to $AX = 0$:

$$A(x + \alpha X) = Ax + \alpha AX = b + 0 = b$$

For some constant α, which gives us b again—we have infinitely many solutions.

2.2 Elimination and Back Substitution

Elimination

We want to produce an *upper triangular* matrix U from a square matrix A. This is done through elimination; the procedure (for a 3x3 matrix) is as follows (assuming no row exchanges):

1. Use the first equation(row) to produce zeros in column 1 below the first pivot.

2. Use the new second equation(row) to clear out column 2 below pivot 2 in row 2.

3. *Continue to column 3.* The expected result is an upper triangular matrix U.

These steps can be carried out using elimination matrices E.

Consider A and b

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

E_{21} multiplies equation 1 by 2 and subtracts that from equation 2 to get a zero in the first column below the first pivot:

$$E_{21} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \implies E_{21}A = \begin{bmatrix} 2 & 3 & 4 \\ 0 & 5 & 6 \\ 2 & 8 & 17 \end{bmatrix}, \quad E_{21}b = \begin{bmatrix} 19 \\ 17 \\ 50 \end{bmatrix}$$

(For intuition on the elimination matrices, consider the row perspective of matrix multiplication) This produced the desired zero in column 1. It changed equation 2. To make the first pivot column zero, we subtract row 1 from row 3 using E_{31}

$$E_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \implies E_{31}E_{21}A = \begin{bmatrix} 2 & 3 & 4 \\ 0 & 5 & 6 \\ 0 & 5 & 13 \end{bmatrix}, \quad E_{31}E_{21}b = \begin{bmatrix} 19 \\ 17 \\ 31 \end{bmatrix}$$

This completes elimination in column 1. Moving on to column 2 row 2 (the second pivot row). We use E_{32} to subtract equation 2 from equation 3

$$E_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \implies U = \begin{bmatrix} 2 & 3 & 4 \\ 0 & 5 & 6 \\ 0 & 0 & 7 \end{bmatrix}, \quad c = \begin{bmatrix} 19 \\ 17 \\ 14 \end{bmatrix}$$

$E_{32}E_{31}E_{21}A = U$ is triangular. See that the same steps were applied to the right hand side b to produce a new right hand side c.

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Possible breakdown of elimination

Elimination might fail. This occurs when zero appears in a pivot position—subtracting that zero from lower rows will not clear out the column below that pivot. For example:

$$\boldsymbol{A} = \begin{bmatrix} 2 & 3 & 4 \\ 4 & 6 & 14 \\ 2 & 8 & 17 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 3 & 4 \\ 0 & 0 & 6 \\ 0 & 5 & 13 \end{bmatrix} = \boldsymbol{B}$$

A possible way to get around this would be to *exchange* row 2 (with the zero pivot) for row (with the nonzero in that column), then carry out elimination as per usual. This exchange is carried out using the permuation matrix $\boldsymbol{P}$:

$$\boldsymbol{PB} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 3 & 4 \\ 0 & 0 & 6 \\ 0 & 5 & 13 \end{bmatrix} = \begin{bmatrix} 2 & 3 & 4 \\ 0 & 5 & 13 \\ 0 & 0 & 6 \end{bmatrix}$$

In this example the exchange produced $\boldsymbol{U}$ with nonzero pivots; normally there may be more columns eliminate before $\boldsymbol{U}$ is reached.

At times this exchange strategy may not work. This occurs when there is no pivot is available. Consider $\boldsymbol{A}'$:

$$\boldsymbol{A}' = \begin{bmatrix} 2 & 3 & 4 \\ 4 & 6 & 14 \\ 2 & 3 & 17 \end{bmatrix} \rightarrow \begin{bmatrix} 2 & 3 & 4 \\ 0 & 0 & 6 \\ 0 & 0 & 13 \end{bmatrix} = \boldsymbol{U}'$$

There is no second pivot in this case. This tells us that the matrix $\boldsymbol{A}'$ *did not have full rank* (intuitively see that the non-pivot row can be expressed as a linear combination of the other pivot rows, so the row space (which is equal to the row space of the original $\boldsymbol{A}'$ since the elimination steps are just linear combinations of the existing rows) is not full rank, and so the column space of the original $\boldsymbol{A}'$ is also not full rank.

In this case there will be nonzero solutions $\boldsymbol{X}$ to $\boldsymbol{A}'\boldsymbol{X} = 0$. The columns of $\boldsymbol{U}'$ (and $\boldsymbol{A}'$) are not independent.

Augmented matrix

During elimination, in order to make sure that the operations on the matrix $\boldsymbol{A}$ are also executed on $\boldsymbol{b}$, one can *include $\boldsymbol{b}$ as an extra column of $\boldsymbol{A}$*; this combination $[\boldsymbol{A}, \boldsymbol{b}]$ is called an *augmented matrix*:

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{b} \end{bmatrix} = \begin{bmatrix} 2 & 3 & 4 & 19 \\ 4 & 11 & 14 & 55 \\ 2 & 8 & 17 & 50 \end{bmatrix} \xrightarrow{E} \begin{bmatrix} 2 & 3 & 4 & 19 \\ 0 & 5 & 6 & 17 \\ 0 & 0 & 7 & 14 \end{bmatrix} = \begin{bmatrix} \boldsymbol{U} & \boldsymbol{c} \end{bmatrix}$$

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Back Substitution to solve $Ux = c$

Elimination (ideally) produces an upper triangular matrix U that has all zeros below the diagonal, with nonzero pivots. For instance we had, for some x

$$Ax = b, \quad A = \begin{bmatrix} 2 & 3 & 4 \\ 4 & 11 & 14 \\ 2 & 8 & 17 \end{bmatrix} \quad b = \begin{bmatrix} 19 \\ 55 \\ 50 \end{bmatrix}$$

undergo elimination to to become

$$Ux = c, \quad U = \begin{bmatrix} 2 & 3 & 4 \\ 0 & 5 & 6 \\ 0 & 0 & 7 \end{bmatrix} \quad c = \begin{bmatrix} 19 \\ 17 \\ 14 \end{bmatrix}$$

See that this form allows us to easily solve the equations by going from bottom to top in a procedural manner, finding x_3, then x_2, then x_1:

1. *Back substitution*: The last equation $7x_3 = 14$ gives $x_3 = 2$

2. *Work upwards*: The next equation $5x_2 + 6(2) = 17$ gives $x_2 = 1$

3. *repeat*: The first equation $2x_1 + 3(1) + 4(2) = 19$ gives $x_1 = 4$

giving us the only solution to this example $x = (4, 1, 2)$. Remember the pivots need to be nonzero(full rank) for a single specific solution to be found.

2.3 Elimination matrices and inverse matrices

Elimination matrices

The basic elimination step *subtracts* a multiple ℓ_{ij} of equation j from equation i. We always speak about *subtractions* as elimination proceeds. For instance even if the first pivot $a_{11} = 3$ and below it is $a_{21} = -3$ where we could just add equation 1 to 2, we *subtract* $\ell_{21} = -1$ *times equation 1 from equation 2* (which gives us the same result).

For instance here is the matrix that subtracts 2 times row 1 from row 3:

$$\boldsymbol{E}_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix}$$

If no row exchanges are needed, then three elimination matrices $\boldsymbol{E}_{21}, \boldsymbol{E}_{31}, \boldsymbol{E}_{32}$ will produce three zeros below the diagonal to change $\boldsymbol{A}$ to the upper triangular $\boldsymbol{U}$ (this just carries out elimination using matrices to represent each step).

Inverse

See that the *inverse* of each matrix $\boldsymbol{E}_{ij}$ just *adds back* $\ell_{ij} \cdot (\text{row } j)$ to row i. This leads to the inverse of their product $\boldsymbol{E} = \boldsymbol{E}_{32}\boldsymbol{E}_{31}\boldsymbol{E}_{21}$. We denote the inverse of $\boldsymbol{E}$ by $\boldsymbol{L}$. For instance, say some $\boldsymbol{E}$ subtracts 5 times row 1 from row 2, then $\boldsymbol{E}^{-1}$ adds 5 times row 1 to row 2:

$$\boldsymbol{E} = \begin{bmatrix} 1 & 0 & 0 \\ -5 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \boldsymbol{E}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 5 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

(See that sequential application of these matrices, in either order, to some vector leads to no net change—as if we had multiplied by the identity.)

Now lets consider $\boldsymbol{F}$ which subtracts 4 times row 2 from row 3 (which might be a next step during elimination), naturally $\boldsymbol{F}^{-1}$ adds it back:

$$\boldsymbol{F} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -4 & 1 \end{bmatrix}, \quad \boldsymbol{F}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 4 & 1 \end{bmatrix}$$

During elimination we would first apply $\boldsymbol{E}$ then $\boldsymbol{F}$, which is the same as applying $\boldsymbol{FE}$. Reversing the elimination would amount to $(\boldsymbol{FE})^{-1}$, which is the same as applying $\boldsymbol{E}^{-1}\boldsymbol{F}^{-1}$:

$$\boldsymbol{FE} = \begin{bmatrix} 1 & 0 & 0 \\ -5 & 1 & 0 \\ 20 & -4 & 1 \end{bmatrix} \quad \text{is inverted by} \quad \boldsymbol{E}^{-1}\boldsymbol{F}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 5 & 1 & 0 \\ 0 & 4 & 1 \end{bmatrix}$$

See that the product $\boldsymbol{FE}$ contains '20' but its inverse doesn't. In $\boldsymbol{FE}$, row 3 feels an effect of size 20 from row 1. However in $\boldsymbol{E}^{-1}\boldsymbol{F}^{-1}$ that doesn't happen. (next page)

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$\boldsymbol{L}$ is the inverse of $\boldsymbol{E}$

$\boldsymbol{E}$ is the product of all the elimination matrices $\boldsymbol{E}_{ij}$, it turns $\boldsymbol{A}$ into its upper triangular form $\boldsymbol{EA} = \boldsymbol{U}$ (assuming no row exchanges). The difficulty with $\boldsymbol{E}$ is multiplying all the separate elimination steps $\boldsymbol{E}_{ij}$ does not produce a good formula; illustrating $\boldsymbol{E} = \boldsymbol{E}_{32}\boldsymbol{E}_{31}\boldsymbol{E}_{21}$:

$$\boldsymbol{E} = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & -\ell_{32} & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ 0 & 1 & \\ -\ell_{31} & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ -\ell_{21} & 1 & \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & \\ -\ell_{21} & 1 & \\ (\ell_{32}\ell_{21} - \ell_{31}) & -\ell_{32} & 1 \end{bmatrix}.$$

See that the bottom left corner is dependent on multiple constants (since mutating the third row requries knowledge of the mutations that already occured to the second row).

Now consider the inverse $\boldsymbol{E}_{21}^{-1}\boldsymbol{E}_{31}^{-1}\boldsymbol{E}_{32}^{-1} = \boldsymbol{E}^{-1} = \boldsymbol{L}$ (see that inverses need to be applied in reverse):

$$\boldsymbol{E}^{-1} = \begin{bmatrix} 1 & & \\ \ell_{21} & 1 & \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ 0 & 1 & \\ \ell_{31} & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & \ell_{32} & 1 \end{bmatrix} = \begin{bmatrix} 1 & & \\ \ell_{21} & 1 & \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix} = \boldsymbol{L}$$

(In the inverse matrix, the mutation of each row doesn't depend on previous mutations, so the multipliers fall into place in the lower triangular $\boldsymbol{L}$. Also see that the final matrix is only lower triangular because the elimination algorithm specifies that we don't manipulate the first row, and that we don't manipulate the second row with the third row.)

This is why we might want to consider $\boldsymbol{A} = \boldsymbol{LU}$ to go back from triangular $\boldsymbol{U}$ to the original $\boldsymbol{A}$.

2.4   Gauss-Jordan elimination

How would one compute the inverse of an nxn matrix $\boldsymbol{A}$? Before answering that question, one might want to consider whether it is really necessary to know $\boldsymbol{A}^{-1}$; although it is possible to find the solution to $\boldsymbol{Ax} = \boldsymbol{b}$ using $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$, computing $\boldsymbol{A}^{-1}$ and taking $\boldsymbol{A}^{-1}\boldsymbol{b}$ is a very slow way to find $\boldsymbol{x}$.

Say we want to compute $\boldsymbol{A}^{-1}$. This is equivalent to solving for $\boldsymbol{AX} = \boldsymbol{I}$. In that sense, by performing the manipulations on $\boldsymbol{A}$ to make it look like $\boldsymbol{I}$. We essentially replicate the effect of $\boldsymbol{A}^{-1}$ on $\boldsymbol{A}$; by repeating those steps on the identity, it becomes as if we were taking $\boldsymbol{A}^{-1}\boldsymbol{I} = \boldsymbol{A}^{-1}$, allowing us to obtain the desired matrix.

This whole process can be done with an augmented matrix using *Gauss-Jordan elimination*, where we essentially take steps to reduce $\boldsymbol{A}$ to reduced row echelon form, while repeating said steps on the identity to obtain the inverse:

$$
\begin{bmatrix} \boldsymbol{A} & \boldsymbol{I} \end{bmatrix} = \left[\begin{array}{rrr|rrr} 1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 1 & 0 & 0 & 1 \end{array}\right] \rightarrow \left[\begin{array}{rrr|rrr} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 & 0 & 1 \end{array}\right]
$$

Gauss-Jordan elimination
Solve $AX = I \Rightarrow X = A^{-1}$
Slower than solving $A\boldsymbol{x} = \boldsymbol{b}$

$$
\rightarrow \left[\begin{array}{rrr|rrr} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 \end{array}\right] = \begin{bmatrix} \boldsymbol{I} & \boldsymbol{A}^{-1} \end{bmatrix}
$$

The Gauss-Jordan essentially turns $[\boldsymbol{A}, \boldsymbol{I}]$ into $[I, \boldsymbol{A}^{-1}]$, where the elimination steps are essentially equivalent to multiplicaiton by $\boldsymbol{A}^{-1}$.

2.5 Proving $A = LU$

Elimination is expressed by $EA = U$ and inverted by $LU = A$. It starts with A and ends with upper triangular U, with each elimination step being carried out by elimination matrices E_{ij}. To invert one elimination step we add rows instead of subtracting:

$$E_{31} = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ -\ell_{31} & 0 & 1 \end{bmatrix} \quad \text{and} \quad L_{31} = \text{inverse of } E_{31} = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ \ell_{31} & 0 & 1 \end{bmatrix}.$$

Recall that $E = E_{32}E_{31}E_{21}$ gives us a fairly messy result:

$$E = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & -\ell_{32} & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ 0 & 1 & \\ -\ell_{31} & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ -\ell_{21} & 1 & \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & \\ -\ell_{21} & 1 & \\ (\ell_{32}\ell_{21} - \ell_{31}) & -\ell_{32} & 1 \end{bmatrix}.$$

while the inverse, $E^{-1} = E_{21}^{-1}E_{31}^{-1}E_{32}^{-1} = L$ produces a much simpler result

$$E^{-1} = \begin{bmatrix} 1 & & \\ \ell_{21} & 1 & \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ 0 & 1 & \\ \ell_{31} & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0 & \ell_{32} & 1 \end{bmatrix} = \begin{bmatrix} 1 & & \\ \ell_{21} & 1 & \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix} = L$$

We then have a elegant expression in $A = E^{-1}U = LU$. We now show that this equation holds over larger matrices of size n.

Proof 1
Following each step in elimination, consider the pivot rows that are subtracted from lower rows; see that these rows are not original rows of A, since they have been mutated by the previous elimination steps; they are instead rows of U.

When computing the, say, third row of U, we subtract multiples of earlier rows of U:

$$\text{Row 3 of } U = (\text{Row 3 of } A) - \ell_{31}(\text{Row 1 of } U) - \ell_{32}(\text{Row 2 of } U)$$

Rewriting, see that

$$\text{Row 3 of } A = \ell_{31}(\text{Row 1 of } U) + \ell_{32}(\text{Row 2 of } U) + 1(\text{Row 3 of } U)$$

Row $[\ell_{31}, \ell_{32}, 1]$ is multiplying the matrix U. This is *exactly row 3 of $A = LU$*. All rows look like this regardless of the size of A. With no row exchanges, we have $A = LU$.
(next page)

Proof 2

Here is another proof. The idea here is to see elimination as removing one rank 1 matrix at a time—one column of L times one row of U from A; where the problem becomes one size smaller with each iteration.

Elimination begins with pivot row = row 1 of A. We multiply that pivot row by the numbers ℓ_{21}, then ℓ_{31}, and eventually ℓ_{n1}; we subtract the respective products from row 2, row 3, and eventually row n of A. By choosing $\ell_{21} = a_{21}/a_{11}$, $\ell_{31} = a_{31}/a_{11}$ and so on until $\ell_{n1} = a_{n1}/a_{11}$; now consider if we also subtracted away the pivot row away from itself—this subtraction leaves zeros in column 1:

$$\text{Step 1 removes} \begin{bmatrix} 1 \ (\text{row 1}) \\ \ell_{21}(\text{row 1}) \\ \ell_{31}(\text{row 1}) \\ \ell_{41}(\text{row 1}) \end{bmatrix} \text{ from } A \text{ to leave } A_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix}.$$

The idea here is that we *removed a rank 1 matrix* with columns made up of multiples of $\ell_1 = (1, \ell_{21}, \ell_{31}, \ell_{41}, \ldots)$, scaled by each respective entry of the first row of A, which is also the first pivot row u_1 of the final upper triangular matrix.

We continue with elimination in the second pivot column, using the second row as the pivot row; as before we also subtract the second pivot row from itself. See that this is again equivalent to subtracting a rank 1 matrix with basis $\ell_2 = (0, 1, \ell_{32}, \ell_{42}, \ldots)$. Recall that the second pivot row is the second row of the upper triangular matrix U in our factorisation.

$$\text{Step 2 removes} \begin{bmatrix} 0 \ (\text{row 2 of } A_2) \\ 1 \ (\text{row 2 of } A_2) \\ \ell_{32}(\text{row 2 of } A_2) \\ \ell_{42}(\text{row 2 of } A_2) \end{bmatrix} \text{ from } A_2 \text{ to leave } A_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \times & \times \\ 0 & 0 & \times & \times \end{bmatrix}.$$

Notice that both ℓ_1 and ℓ_2 are columns of L. We removed a column ℓ_2 times the second pivot row. Continuing in the same way, we successively remove columns with each step removing a column ℓ_j of L times a pivot row u_j of U. See that this entire process can be depicted as

$$\boxed{\begin{aligned} A = \ell_1 u_1 + \ell_2 u_2 + \cdots + \ell_n u_n \ &= \begin{bmatrix} \ell_1 & \cdots & \ell_n \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix} = LU \\ \textbf{columns times rows} \quad & \end{aligned}}$$

Notice that U is upper triangular; the pivot row u_k begins with $k-1$ zeros. L is lower triangular with 1's on the main diagonal. Column ℓ_k also begins with $k-1$ zeros. (See that this proof makes use of the idea that matrix multiplication can be seen as a sum of rank 1 matrices)

2.6 Permutation matrices

Examples

Permutation matrices have a 1 in every row and a 1 in every column. All other entries are 0. When this matrix P multiplies a vector, it changes the order of its components; for instance:

$$
\begin{array}{l}
\textbf{P has the rows of } \textbf{\textit{I}} \\
\textbf{P\textit{x} = Circular shift of \textit{x}} \\
\textbf{1, 2, 3 to 3, 1, 2}
\end{array}
\qquad
P\boldsymbol{x} =
\begin{bmatrix}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
=
\begin{bmatrix}
x_3 \\
x_1 \\
x_2
\end{bmatrix}
$$

(A nonzero ith entry on row m of P means that row i of x goes on that row m in the result) Other examples include

$$
\begin{array}{l}
\textbf{P\textit{x} reverses} \\
\textbf{the order to} \\
x_4. x_3. x_2, x_1 \\
\boldsymbol{P^2 = I}
\end{array}
\begin{bmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{bmatrix}
\qquad
\begin{array}{l}
x_4 \textbf{ stays fixed} \\
\textbf{Input } x_1, x_2, x_3, x_4 \\
\textbf{output } x_3, x_1, x_2, x_4 \\
\boldsymbol{P^3 = I}
\end{array}
\begin{bmatrix}
0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
$$

$$
\begin{array}{l}
\textbf{Circular shift} \\
\textbf{Input } x_1, x_2, x_3, x_4 \\
\textbf{output } x_4, x_1, x_2, x_3 \\
\boldsymbol{P^4 = I}
\end{array}
\begin{bmatrix}
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0
\end{bmatrix}
\qquad
\begin{array}{l}
\textbf{Evens before odds} \\
x_0, x_2 \textbf{ before } x_1, x_3 \\
\textbf{Fast Fourier Transform} \\
\textbf{Number from 0 to 3}
\end{array}
\begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
$$

Recall that elimination may require row exchanges. If A is invertible, then there is a permuation P to order its rows in advance, so that elimination on PA meets no zeros in the pivot positions. Then $PA = LU$.

Inverse

We can intuit that the inverse of P is just its transpose:

$$
\begin{array}{l}
\textbf{The rows of any } \textbf{\textit{P}} \textbf{ are} \\
\textbf{the columns of } \boldsymbol{P^{-1} = P^{\mathrm{T}}} \\
\boldsymbol{P^{\mathrm{T}}} = \textbf{``transpose of } \boldsymbol{P}\textbf{''}
\end{array}
\quad
P^{\mathrm{T}}P =
\begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
0 & 0 & 1 \\
1 & 0 & 0 \\
0 & 1 & 0
\end{bmatrix}
=
\begin{bmatrix}
1 & & \\
& 1 & \\
& & 1
\end{bmatrix}
= I
$$

(For instance, a nonzero entry in row 1 column 2 means 'row 2 of x becomes row 1 of result'. Its transpose corresponds to a nonzero entry in row 2 column 1, so 'row 1 of x becomes row 2 in the result'—reversing the change. This logic can be extrapolated to every other row.)

(next page)

$PA = LU$ factorisation

Recall that elimination may require row exchanges; consider for instance

$$A = \begin{bmatrix} 1 & 2 & a \\ 2 & 4 & b \\ 3 & 7 & c \end{bmatrix} \xrightarrow{E} \begin{bmatrix} 1 & 2 & a \\ 0 & 0 & b-2a \\ 0 & 1 & c-3a \end{bmatrix} \xrightarrow{P} \begin{bmatrix} 1 & 2 & a \\ 0 & 1 & c-3a \\ 0 & 0 & b-2a \end{bmatrix} = U$$

To rescue elimination, P exchanged row 2 with 3, bringing 1 to the second pivot so elimination could continue.

See that we could order the rows in advance, first exchanging rows 2 and 3 to get PA, then LU factorisation becomes $PA = LU$; the matrix PA sails through elimination without seeing that zero pivot:

$$\underset{P}{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}} \underset{A}{\begin{bmatrix} 1 & 2 & a \\ 2 & 4 & b \\ 3 & 7 & c \end{bmatrix}} = \underset{PA}{\begin{bmatrix} 1 & 2 & a \\ 3 & 7 & c \\ 2 & 4 & b \end{bmatrix}} = \underset{L}{\begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 2 & 0 & 1 \end{bmatrix}} \underset{U}{\begin{bmatrix} 1 & 2 & a \\ 0 & 1 & c-3a \\ 0 & 0 & b-2a \end{bmatrix}}$$

We may require several row exchanges; in that case the an overall permutation P would include them all, still producing $PA = LU$. A useful way to keep track of the permutations might be to add a column of indices at the end of A so that the original indices are displayed:

$$\begin{bmatrix} 1 & 2 & a & 1 \\ 2 & 4 & b & 2 \\ 3 & 7 & c & 3 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & a & 1 \\ 0 & 0 & b-2a & 2 \\ 0 & 1 & c-3a & 3 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & a & 1 \\ 0 & 1 & c-3a & 3 \\ 0 & 0 & b-2a & 2 \end{bmatrix}. \ P_{132} \text{ is } \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

Column permutations

We know that we can reorder rows using

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \qquad PA = \begin{bmatrix} a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{11} & a_{12} & a_{13} \end{bmatrix}$$

See that we can also reorder columns by applying a permutation matrix on the right:

$$Q = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \qquad PAQ = \begin{bmatrix} a_{23} & a_{22} & a_{21} \\ a_{33} & a_{32} & a_{31} \\ a_{13} & a_{12} & a_{11} \end{bmatrix}$$

Note that these two operations don't cover all possible permutations of the 9 entries in A. The first index is constant on every row and the second index is constant on every column.

2.7   Transposes and symmetric matrices

2.7.1   The transpose of AB is $B^T A^T$: Intuition

We have
$$(AB)^T = B^T A^T$$

Consider AB. Computing the first *row* of the result (the first column of $(AB)^T$); this can be seen as a linear combination of the *rows* of B (the columns of B^T) specified by the entries in the first *row* of A (the first column of A^T).

2.7.2   Showing $(A^T)^{-1} = (A^{-1})^T$

Consider taking the transpose of $A^{-1}A$,

Transpose of inverse $A^{-1}A = I$ is transposed to $A^T(A^{-1})^T = I.$

Similarly, transposing $AA^{-1} = I$ leads to $(A^{-1})^T A^T = I$. Notice especially that A^T *is invertible exactly when A is invertible.*

2.7.3 $A^T A$ is symmetric

Choose any matrix A, probably rectangular. Multiply A^T times A, then the product $S = A^T A$ is automatically a square symmetric matrix:

The transpose of $A^T A$ is $A^T(A^T)^T$ which is $A^T A$ again.

The matrix AA^T is also symmetric (see that their shapes permit multiplication in either order), note howerver that AA^T *is a different matrix* from $A^T A$.

Chapter 3

The Four Fundamental Subspaces

3.1   Reduced Row Echelon Form

Motivation

Consider reducing a 2x4 matrix A to its reduced row echelon form R:

$$A = \begin{bmatrix} 1 & 2 & 11 & 17 \\ 3 & 7 & 37 & 57 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & 11 & 17 \\ 0 & 1 & 4 & 6 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 3 & 5 \\ 0 & 1 & 4 & 6 \end{bmatrix} = R$$

See how the added upward elimination essentially inverted the a portion W of A:

$$W = \begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

to turn that part of the matrix into the identity:

Multiply $W^{-1}A = W^{-1}\begin{bmatrix} W & H \end{bmatrix}$ **to produce** $R = \begin{bmatrix} I & W^{-1}H \end{bmatrix} = \begin{bmatrix} I & F \end{bmatrix}$.

We have $H = WF$, where H refers to the other parts of A, and W the portion that was inverted—we can combine the components of W (the first independent columns) to produce the other (dependent) columns. The matrix F specifies the parameters to do this:

$$\textbf{Dependent columns } H = \begin{bmatrix} 11 & 17 \\ 37 & 57 \end{bmatrix} = WF = \begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix} \text{ times } \begin{bmatrix} 3 & 5 \\ 4 & 6 \end{bmatrix}.$$

See that the first r independent columns of A locate the columns of R containing I. Also see that the last $m - r$ rows of R will be rows of zeros (the dependent columns in the reduced form can be expressed in terms of the identity contained within that form, so there can't be any additional nonzero rows).

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Algorithm

Elimination goes a column at a time from left to right; after k columns, that part of the matrix is in the reduced form, and we move to the $(k+1)$th column; this new column has an upper part u and a lower part ℓ:

$$\textbf{First } k+1 \textbf{ columns} \qquad \begin{bmatrix} I_k & F_k \\ 0 & 0 \end{bmatrix} P_k \textbf{ followed by } \begin{bmatrix} u \\ \ell \end{bmatrix}.$$

The idea here is to decide whether this $(k+1)$th column joins I_k or F_k.

See that if ℓ is *all zeros*, the new column is *dependent* on the first k columns; then u joins with F_k to produce F_{k+1}.

If ℓ is *not* all zero, then the column is *independent* of the first k columns. Pick any nonzero in ℓ as the pivot, move that row of A up into row $k + 1$, then subtract multiples of that pivot row to zero out all the rest of column $k + 1$ (eliminate up and down). If necessary, divide the row by its first nonzero entry to have a pivot of 1. Column $k+1$ joins I_k (see that it adds a new nonzero row to the identity) to produce I_{k+1}.

Repeat for the next column and so on.

Row operations

There are three row operations allowed in elimination from A to R:

1. Subtract a multiple of one row from another (below or above)

2. Divide a row by its first nonzero entry (to reach pivot 1)

3. Exchange rows (to move all zero rows to the bottom)

A different series of steps could be used reach the same R. But the result R can't change.

3.2 $A = CR$ factorisation

We can apply elimination to reduce A to R_0 (reduced echelon form with zero rows); then I in R_0 locates the matrix C of *independent columns* in A. Removing any zero rows from R_0 produces the row matrix R such that $A = CR$. For instance,

$$
A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 5 \\ 3 & 6 & 9 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & 1 \\ 0 & 0 & 3 \\ 0 & 0 & 6 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 2 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} = R_0 \text{ with rank 2}
$$

where the independent columns of A are 1 and 3, and

$$
R = \begin{bmatrix} 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 1 \\ 2 & 5 \\ 3 & 9 \end{bmatrix}
$$

so

$$
A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 5 \\ 3 & 6 & 9 \end{bmatrix} = CR = \begin{bmatrix} 1 & 1 \\ 2 & 5 \\ 3 & 9 \end{bmatrix} \begin{bmatrix} 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{array}{cc} \text{(column basis)} & \text{(row basis)} \\ \text{in } C & \text{in } R \end{array}
$$

3.3 Systematic nullspace computation

Elimination gives us a systematic way to find a basis for the nullspace. Say we have

$$A = \begin{bmatrix} 1 & 7 & 3 & 35 \\ 2 & 14 & 6 & 70 \\ 2 & 14 & 9 & 97 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 7 & 3 & 35 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 27 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 7 & 0 & 8 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 27 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 7 & 0 & 8 \\ 0 & 0 & 1 & 9 \\ 0 & 0 & 0 & 0 \end{bmatrix} = R_0$$

Consider attempting to find a basis for the nullspace, meaning a basis for the solutions of $Ax = 0$; say that $W^{-1}A = R_0$, then for some x,

$$Ax = 0 \implies W^{-1}Ax = W^{-1}0 \implies R_0 x = 0$$

See that the elimination process doesn't change the space of solutions that satisfy $Ax = 0$. Also see that using R instead of R_0 only removes the redundant zero rows without removing any solutions.

Given some R, we have a systematic way to find a basis for the nullspace: considering all the indices of x corresponding to dependent indices, by letting one of those indices be 1 and the rest 0, we have a simple solution for $Rx = 0$:

$$Rs_1 = 0 \qquad \begin{bmatrix} 1 & 7 & 0 & 8 \\ 0 & 0 & 1 & 9 \end{bmatrix} \begin{bmatrix} -7 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \begin{matrix} \text{Put 1 and 0} \\ \text{in positions 2 and 4} \end{matrix}$$

$$Rs_2 = 0 \qquad \begin{bmatrix} 1 & 7 & 0 & 8 \\ 0 & 0 & 1 & 9 \end{bmatrix} \begin{bmatrix} -8 \\ 0 \\ -9 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \begin{matrix} \text{Put 0 and 1} \\ \text{in positions 2 and 4} \end{matrix}$$

See that if we were to write R as $[I, F]$, the solutions can be found in an algorithmic manner:

The two special solutions to $\begin{bmatrix} I & F \end{bmatrix} x = 0$ are the columns of $\begin{bmatrix} -F \\ I \end{bmatrix}$ in Example 1

The special solutions to $\begin{bmatrix} I & F \end{bmatrix} P x = 0$ are the columns of $P^T \begin{bmatrix} -F \\ I \end{bmatrix}$ in Example 2

The second case occurs should we have to permute R to reorder the independent columns. Recall that $PP^T = I$, and so

$$Rx = 0 \qquad \begin{bmatrix} I & F \end{bmatrix} P \text{ times } P^T \begin{bmatrix} -F \\ I \end{bmatrix} \text{ reduces to } \begin{bmatrix} I & F \end{bmatrix} \begin{bmatrix} -F \\ I \end{bmatrix} = \begin{bmatrix} 0 \end{bmatrix}$$

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Cont.

To put these two ideas together, suppose the $m \mathrm{x} n$ matrix $\boldsymbol{A}$ has rank r. To find the $n - r$ special solutions to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$, compute the reduced row echelon form $\boldsymbol{R}_0$ of $\boldsymbol{A}$; remove the $m - r$ zero rows of $\boldsymbol{R}_0$ to produce $\boldsymbol{R} = [\boldsymbol{I}, \boldsymbol{F}]\boldsymbol{P}$, where $\boldsymbol{A} = \boldsymbol{C}\boldsymbol{R}$.

Then the special solutions to $\boldsymbol{A}\boldsymbol{x} = 0$ are the $n - r$ columns of $\boldsymbol{P}^T \begin{bmatrix} -\boldsymbol{F} \\ \boldsymbol{I} \end{bmatrix}$.

3.4 The complete solution to $Ax = b$

Finding a particular solution

We can reduce $Ax = b$ to a simpler system $R_0 x = d$ with the same solutions (if any). A useful aid here is to augment A with b to produce an augmented matrix $[A, b]$:

$$\begin{bmatrix} 1 & 3 & 0 & 2 \\ 0 & 0 & 1 & 4 \\ 1 & 3 & 1 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 6 \\ 7 \end{bmatrix} \quad \begin{matrix} \text{has the} \\ \text{augmented} \\ \text{matrix} \end{matrix} \quad \begin{bmatrix} 1 & 3 & 0 & 2 & 1 \\ 0 & 0 & 1 & 4 & 6 \\ 1 & 3 & 1 & 6 & 7 \end{bmatrix} = \begin{bmatrix} A & b \end{bmatrix}.$$

Applying elimination to reach R_0, the augmented part also undergoes the same elimination steps to produce a d:

$$\begin{bmatrix} 1 & 3 & 0 & 2 \\ 0 & 0 & 1 & 4 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 6 \\ 0 \end{bmatrix} \quad \begin{matrix} \text{has the} \\ \text{augmented} \\ \text{matrix} \end{matrix} \quad \begin{bmatrix} 1 & 3 & 0 & 2 & 1 \\ 0 & 0 & 1 & 4 & 6 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} R_0 & d \end{bmatrix}.$$

For an easy solution x_p we can *choose the free variables to be 0*. In this case $x_2 = x_4 = 0$, then the pivot variables can just be read off from d:

$$R_0 x_p = \begin{bmatrix} 1 & 3 & 0 & 2 \\ 0 & 0 & 1 & 4 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 6 \\ 0 \end{bmatrix} = d \quad \begin{matrix} \textbf{Pivot variables 1, 6} \\ \textbf{Free variables 0, 0} \\ \boldsymbol{x}_{\textbf{particular}} = (1, 0, 6, 0). \end{matrix}$$

See that for a solution to exist, the zero rows in R_0 must also be zero in d.

This procedure allows us to come up with a particular solution. For a complete solution, we consider any sum of the particular solution x_p with any nullspace vectors x_n:

$$\begin{matrix} \text{One } \boldsymbol{x}_{\textbf{particular}} & \textit{The particular solution solves} & A\boldsymbol{x}_p = \boldsymbol{b} \\ \text{All } \boldsymbol{x}_{\textbf{nullspace}} & \textit{The } \boldsymbol{n-r} \textit{ special solutions solve} & A\boldsymbol{x}_n = \mathbf{0} \end{matrix}$$

$$\begin{matrix} \textbf{Complete solution} \\ \textbf{one } \boldsymbol{x}_p\textbf{+many } \boldsymbol{x}_n \\ \textbf{particular } \boldsymbol{x}_p \\ \textbf{nullspace vectors } \boldsymbol{x}_n \end{matrix} \qquad \boldsymbol{x} = \boldsymbol{x}_p + \boldsymbol{x}_n = \begin{bmatrix} 1 \\ 0 \\ 6 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} -3 \\ 1 \\ 0 \\ 0 \end{bmatrix} + x_4 \begin{bmatrix} -2 \\ 0 \\ -4 \\ 1 \end{bmatrix}.$$

The nullspace can be found as per outlined earlier (setting one variable to one and the rest to zero to get each nullspace basis vector). See that the complete solution includes all nullspace basis vectors, and that if the nullspace is just the zero vector then every particular solution x_p is the only solution to that b.
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3.4.1   Rank and solution

Full column rank

In the case where A has *full column rank*, every column has a pivot and the rank is $r = n$. The matrix is tall and thin ($m \geq n$). Row reduction puts $R = I$ at the top when A is reduced to R_0 with rank n:

$$\text{Full column rank } r = n \quad R_0 = \begin{bmatrix} I \\ 0 \end{bmatrix} = \begin{bmatrix} n \text{ by } n \text{ identity matrix} \\ m - n \text{ rows of zeros} \end{bmatrix}$$

See that in this case the matrix has the following properties:

> Every matrix A with **full column rank** $(r = n)$ has all these properties:
>
> 1.   All columns of A are pivot columns (**independent**). No free variables.
> 2.   The nullspace $N(A)$ contains only the zero vector $x = 0$.
> 3.   If $Ax = b$ has a solution (it might not) then it has only *one solution*.

With full column rank, $Ax = b$ will have *one solution or no solution.* (think of a mapping from n dimensional space into m dimensional space where $m \geq n$, there aren't enough vectors in n space to encompass all of m space, so there may be no solution for a particular vector in m space; or see that the columns only span a n dimensional hyperplane in a higher m dimensional space—any m dimensional vector not on that hyperplane has no solution)

Full row rank

The other case is full row rank—now $Ax = b$ has *one or infinitely many solutions.* In this case A must be *short and wide* ($m \leq n$); the matrix has full row rank if $r = m$, where every row has a pivot.

(If $m < n$, then a nullspace consisting of more than just the zero vector exists and there will be multiple solutions to $Ax = b$.) See that a matrix like this has the following properties:

> Every matrix A with *full row rank* $(r=m)$ has all these properties:
>
> 1.   All rows have pivots, and R_0 has no zero rows: $R_0 = R$.
> 2. $Ax = b$ has a solution for every right side b.
> 3.   The column space of A is the whole space $\mathbf{R}^m$.
> 4.   If $m < n$ the equation $Ax = b$ is **underdetermined** (many solutions).

(next page)

Cont.

The four possibilities for linear equations depend on the rank r

$r = m$	and	$r = n$	Square and invertible	$Ax = b$	has 1 solution
$r = m$	and	$r < n$	Short and wide	$Ax = b$	has ∞ solutions
$r < m$	and	$r = n$	Tall and thin	$Ax = b$	has 0 or 1 solution
$r < m$	and	$r < n$	Not full rank	$Ax = b$	has 0 or ∞ solutions

If the matrix A is square and invertible, it indicates a mapping from $m = n = r$ space into that same space; the basis specified by A spans the whole of r space and there is only one linear combination of that basis that solves for $Ax = b$ (since A has linearly independent columns and therefore a trivial nullspace).

If the matrix is not full rank, then the columns span a hyperplane in the space equal to the row length, meaning some $Ax = b$ may not have a solution, and if some b does lie within that hyperplane there will be infinite solutions to it (since the columns are not independent and therefore a nontrivial nullspace exists).

Their reduced row echelon form will fall into the following categories:

Four types for R_0	$\begin{bmatrix} I \end{bmatrix}$	$\begin{bmatrix} I & F \end{bmatrix}$	$\begin{bmatrix} I \\ 0 \end{bmatrix}$	$\begin{bmatrix} I & F \\ 0 & 0 \end{bmatrix}$
Their ranks	$r = m = n$	$r = m < n$	$r = n < m$	$r < m, r < n$

Cases 1 and 2 have full row rank, case 3 has full column rank but not row rank, case 4 is not full rank. See that in the last two cases, when $Ax = b$ is reduced to $R_0 x = d$, d must end in $m - r$ zeros for the equation to be solvable. F refers to the top part of the dependent columns.

3.5 Intuition for four subspaces

We have

Four Fundamental Subspaces	**Dimensions**
1. The *row space* is $\mathbf{C}(A^{\mathrm{T}})$, a subspace of $\mathbf{R}^n$.	r
2. The *column space* is $\mathbf{C}(A)$, a subspace of $\mathbf{R}^m$.	r
3. The *nullspace* is $\mathbf{N}(A)$, a subspace of $\mathbf{R}^n$.	$n - r$
4. The *left nullspace* is $\mathbf{N}(A^{\mathrm{T}})$, a subspace of $\mathbf{R}^m$.	$m - r$

Column space of reduced form not the same as original matrix
Note that although the reduced row echelon form provides the pivot positions
to determine the row and column rank of a matrix, while the *rows* of the rref
form span the same row space as the original unreduced matrix, the columns
of the rref form cannot act as substitutes for the original column space, instead
only providing information on dimensionality and on which original columns act
as basis vectors for the column space. That is

$$\boldsymbol{C(A)} \neq \boldsymbol{C(R_0)} \quad \text{but} \quad \boldsymbol{C(A^T)} = \boldsymbol{C(R_0^T)}$$

(none of the row operations in elimination change the row space, but they do
change the column space)

Nullspace dimension is $n - r$
The intuition for the dimension of $\boldsymbol{N}(A)$ being $n - r$ is clear from elimination,
where each dependent column provides a new basis vector for the nullspace (we
can find a basis by substituting one free variable as 1 and the rest zero, repeating
for all free variables), so the number of basis vectors equals the number of
dependent columns equals total columns minus independent columns—so $n - r$.

Left nullspace dimensionality
We know the dimensions for $\boldsymbol{A}$ is the same as that of $\boldsymbol{A}^T$. Transposing $\boldsymbol{A}$
gives us m columns, of which we know r are independent. So there are $m - r$
dependent columns which each provide a basis vector for the nullspace.

3.6 $A = CR$ and Block elimination

The earlier notes on the rref form introduced it as a simple way to express the entire matrix in terms of its dependent rows, where for a matrix A, with independent components W and dependent components H, reduction to rref looks like:

$$A = \begin{bmatrix} W & H \end{bmatrix} \implies W^{-1}A = W^{-1}\begin{bmatrix} W & H \end{bmatrix} = \begin{bmatrix} I & W^{-1}H \end{bmatrix}$$

See that we can recover the dependent components of H with $W^{-1}H$ by multiplying it by the independent columns W, so

$$A = \underbrace{W}_{C}\underbrace{\begin{bmatrix} I & W^{-1}H \end{bmatrix}}_{R}$$

where C means the same thing as W, that is, the independent columns of A. See that W is gauranteed to be square since row and column rank are equal.

Block elimination

The above doesn't show how the zero rows in R_0 (if they exist) are redundant. We can develop a better idea of elimination if we consider working with blocks of the original A. This is called block elimination; consider reducing a matrix A with rank r to rref using the following three steps:

Step 1: Exchange columns of A using P_C and exchange rows of A using P_R to put the r independent columns first and r independent rows first. This looks like

$$P_R A P_C = \begin{bmatrix} W & H \\ J & K \end{bmatrix}$$

$\begin{bmatrix} W \\ J \end{bmatrix}$ has full column rank and $\begin{bmatrix} W & H \end{bmatrix}$ has full row rank. See that W is a square matrix with full rank r and is therefore invertible.

Step 2: Multiply the top rows by W^{-1}:

$$\begin{bmatrix} W & H \\ J & K \end{bmatrix} \rightarrow \begin{bmatrix} I & W^{-1}H \\ J & K \end{bmatrix}$$

Step 3: Subtract $J\begin{bmatrix} I & W^{-1}H \end{bmatrix}$ from the $m - r$ rows $\begin{bmatrix} J & K \end{bmatrix}$ to produce $\begin{bmatrix} 0 & 0 \end{bmatrix}$:

$$\begin{bmatrix} I & W^{-1}H \\ J & K \end{bmatrix} \rightarrow \begin{bmatrix} I & W^{-1}H \\ 0 & 0 \end{bmatrix}$$

To understand why $JW^{-1}H = K$, we know that the first r rows $\begin{bmatrix} I & W^{-1}H \end{bmatrix}$ are linearly independent, and since A has rank r, the lower rows $\begin{bmatrix} J & K \end{bmatrix}$ must be combinations of the upper rows. These combinations must be given by J to get the first r columns correct: $JI = J$. Then J times $W^{-1}H$ must equal K to make the last columns correct.

(next page)

Cont.

We have block elimination as the following transformations:

$$P_R A P_C = \begin{bmatrix} W & H \\ J & K \end{bmatrix} \rightarrow \begin{bmatrix} I & W^{-1}H \\ J & K \end{bmatrix} \rightarrow \begin{bmatrix} I & W^{-1}H \\ 0 & 0 \end{bmatrix} = R_0$$

We can, in a manner similar to the steps taken, factor out parts of A as follows to acquire the reduced row echelon form; for step 2:

$$P_R A P_C = \begin{bmatrix} W & H \\ J & K \end{bmatrix} = \begin{bmatrix} W & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & W^{-1}H \\ J & K \end{bmatrix}$$

For step 3:

$$\begin{bmatrix} W & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & W^{-1}H \\ J & K \end{bmatrix} = \begin{bmatrix} W & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ J & 0 \end{bmatrix} \begin{bmatrix} I & W^{-1}H \\ 0 & 0 \end{bmatrix}$$

The result is

$$P_R A P_C = \begin{bmatrix} W & 0 \\ J & 0 \end{bmatrix} \begin{bmatrix} I & W^{-1}H \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} W \\ J \end{bmatrix} \begin{bmatrix} I & W^{-1}H \end{bmatrix}$$

See that this is just the $A = CR$ factorisation, but this time showing that the zero rows are redundant rather than just using a reduced form where zero rows don't exist. Another way of writing this result is

$$\text{The conclusion is that } P_R A P_C = \begin{bmatrix} W \\ J \end{bmatrix} W^{-1} \begin{bmatrix} W & H \end{bmatrix} = CW^{-1}B$$

Chapter 4

Orthogonality

4.1 Orthogonal subspaces

Recall that two vectors $\boldsymbol{v}$ and $\boldsymbol{w}$ are orthogonal if $\boldsymbol{v}^T\boldsymbol{w} = 0$. To say that two subspaces are orthogonal means that every vector in one space is orthogonal to every vector in the other space.

We can make the claim that for any matrix $\boldsymbol{A}$, *the nullspace of $\boldsymbol{A}$ is orthogonal to the row space of $\boldsymbol{A}$*. To see this just consider $\boldsymbol{Ax} = \boldsymbol{0}$:

$$\boldsymbol{Ax} = \begin{bmatrix} \textbf{row 1 of } \boldsymbol{A} \\ \vdots \\ \textbf{row } \boldsymbol{m} \textbf{ of } \boldsymbol{A} \end{bmatrix} \begin{bmatrix} \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \\ \vdots \\ \boldsymbol{0} \end{bmatrix} \qquad \begin{array}{l} \longleftarrow \quad \textbf{(row 1)} \cdot \boldsymbol{x} \textbf{ is zero} \\ \\ \longleftarrow \quad \textbf{(row } \boldsymbol{m}\textbf{)} \cdot \boldsymbol{x} \textbf{ is zero} \end{array}$$

Every row has a zero dot product with $\boldsymbol{x}$. Then every combination of the rows is perpendicular to $\boldsymbol{x}$. That is, the whole row space $\boldsymbol{C}(\boldsymbol{A}^T)$ is orthogonal to the nullspace $\boldsymbol{N}(\boldsymbol{A})$ in n dimensional space (since $\boldsymbol{A}^T$ has n rows). Another way to show this is

$$\textbf{\textit{x} in nullspace orthogonal to } \boldsymbol{A}^{\textbf{T}}\boldsymbol{y} \textbf{ in row space} \quad \boldsymbol{x}^{\textbf{T}}(\boldsymbol{A}^{\textbf{T}}\boldsymbol{y}) = (\boldsymbol{Ax})^{\textbf{T}}\boldsymbol{y} = \boldsymbol{0}^{\textbf{T}}\boldsymbol{y} = \boldsymbol{0}.$$

See that we can analagously reason that the *the column space $\boldsymbol{C}(\boldsymbol{A})$ and the left nullspace $\boldsymbol{N}(\boldsymbol{A}^T)$ are perpendicular inside m dimensional space.*
(next page)

Cont.
See that the only common vector between two orthogonal subspaces would be the zero vector (we can't sum the columns of a matrix to produce a vector orthogonal to all the columns). There is a very important restriction on the dimension of any two orthogonal subspaces:

> If V and W are orthogonal subspaces in $\mathbf{R}^n$ then $\dim V + \dim W \leq n$.

For instance, the row space of a matrix is a subspace of dimension r in n space, and its orthogonal complement, by construction, will have dimensionality $n - r$.

4.1.1 Orthogonal complements

When two orthogonal subspaces account for the whole space, they are called *orthogonal complements*. The orthogonal complement of V is written as $V^{\perp}$. The row space and the nullspace, as well as the column space and left nullspace, are instances of orthogonal complements:

Orthogonal complements	Row space and nullspace	$r + (n - r) = n$
	Column space and left nullspace	$r + (m - r) = m$

4.1.2 Intuition for $x = x_{\text{row}} + x_{\text{null}}$

See that because the row space and the nullspace combined span the entire n space, we can say that any vector in $\mathbb{R}^n$ can be expressed as a sum of vectors from both subspaces. That is, any vector x in $\mathbb{R}^n$ is the sum $x = x_{\text{row}} + x_{\text{null}}$ of its row space component and its nullspace component. Any vector y in $\mathbb{R}^m$ is the sum $y = y_{\text{col}} + y_{\text{null}}$ of its column space component and its left nullspace component from $N(A^T)$:

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4.1.3 A is invertible from the row space to the column space

Consider again the illustration from the previous page:

Every vector in Ax is in the column space; that is obvious. Every x comes from $\mathbb{R}^n$ space, which is made up of the the row space $C(A^T)$ and its orthogonal complement, the nullspace $N(A)$. In that context, every candidate x either comes from the nullspace, which would map to 0, or the row space, which would then map to some b in the column space—every b in the column space can be found by some Ax with x from the row space.

We can also go on to say that *every vector b in the column space comes from exactly one vector x_r in the row space.* Proof: If $Ax_r = Ax'_r$, the difference $x_r - x'_r$ is in the nullspace (since $A(x_r - x'_r) = 0$); however, should x_r and x'_r come from the row space, then $x_r - x'_r$ would also have to be in the row space. The only way for a vector to be in both the nullspace and the row space would be if it were the zero vector; so $x_r - x'_r = 0$ and $x_r = x'_r$.

So A maps every row space component to a specific column space component; see that there is an r by r invertible matrix hiding inside A if we throw away the two nullspaces. A *is invertible from the row space to the column space.*

4.2 $A^T A$ is invertible only if A has linearly independent columns

$A^T A$ is a square matrix (n by n). We prove the above by showing that $A^T A$ *has the same nullspace as* A; so that when the columns of A are linearly independent, and its nullspace only contains the zero vector, then $A^T A$, with this same nullspace, is also invertible.

First we show that a vector in the nullspace of A is also in that of $A^T A$. Let A be any matrix; if x is in the nullspace, then $Ax = 0$. Multiplying by A^T gives $A^T A x = 0$, so x is also in the nullspace of $A^T A$.

Now the other way, we show that a vector in the nullspace of $A^T A$ is in that of A. Starting with $A^T A x = 0$, multiplying by x^T:

$$(x^T) A^T A x = 0 \quad \text{or} \quad (Ax)^T (Ax) = 0 \quad \text{or} \quad \|Ax\|^2 = 0.$$

So if $A^T A x = 0$ then Ax has length 0, so $Ax = 0$.

Every vector x in one nullspace is in the other nullspace, so if $A^T A$ has dependent columns then so does A, and if $A^T A$ has independent columns then so does A:

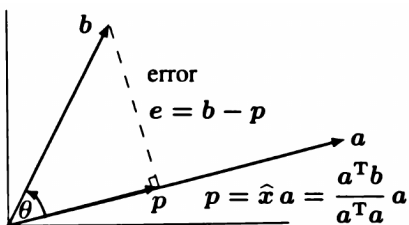**When A has independent columns, $A^T A$ is square, symmetric, and invertible.**

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4.3 Projections

4.3.1 Projection onto a line

We want to project any b onto the column space of any m by n matrix A. This entails finding the point p on that subspace that is closest to our arbitrary point b. We start with a line.

Considering a one dimensional subspace (a line) with basis $a = (a_1, \ldots, a_m)$. Along that line, we want the point p closest to $b = (b_1, \ldots, b_m)$; the key to projection is orthogonality: *the line from b to p, that is $b - p$, is perpendicular to the vector a.*

We know that the projection p will be some multiple of a; call it $p = \hat{x}a$ (so here $\hat{x}$ denotes a constant)—computing this number $\hat{x}$ will give us the vector p. We can call the perpendicular line $b - p$ the 'error' $e = b - \hat{x}a$, and use the fact that it is perpendicular to a to derive $\hat{x}$:

$$\text{Projecting } b \text{ onto } a \text{ with error } e = b - \hat{x}a$$
$$a \cdot (b - \hat{x}a) = 0 \quad \text{or} \quad a \cdot b - \hat{x}a \cdot a = 0 \qquad \hat{x} = \frac{a \cdot b}{a \cdot a} = \frac{a^\mathsf{T} b}{a^\mathsf{T} a}.$$

With that we can compute the projection $p = \hat{x}a$:

The projection of b onto the line through a is the vector $p = \hat{x}a = \dfrac{a^\mathsf{T} b}{a^\mathsf{T} a} a$.

Special case 1 : If $b = a$ then $\hat{x} = 1$. The projection of a onto a is itself. $Pa = a$.

Special case 2 : If b is perpendicular to a then $a^\mathsf{T} b = 0$. The projection is $p = 0$.

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Projection matrix

We had the projection of $\boldsymbol{b}$ onto the line through $\boldsymbol{a}$ as the vector $\boldsymbol{p}$ given by

$$\boldsymbol{p} = \hat{x}\boldsymbol{a} = \frac{\boldsymbol{a}^T \boldsymbol{b}}{\boldsymbol{a}^T \boldsymbol{a}}\boldsymbol{a}$$

Now comes the *projection matrix*, where we want a matrix $\boldsymbol{P}$ that can be applied to the arbitrary point $\boldsymbol{b}$ to get the desired projection $\boldsymbol{p}$, so $\boldsymbol{Pb} = \boldsymbol{p}$. This can found easily; since $\hat{x}$ is a constant, we can rearrange the above equation:

Projection matrix P $\boldsymbol{p} = \boldsymbol{a}\hat{\boldsymbol{x}} = \boldsymbol{a}\dfrac{\boldsymbol{a}^T\boldsymbol{b}}{\boldsymbol{a}^T\boldsymbol{a}} = \boldsymbol{Pb}$ *when the matrix is* $\boldsymbol{P} = \dfrac{\boldsymbol{a}\boldsymbol{a}^T}{\boldsymbol{a}^T\boldsymbol{a}}.$

The projection matrix $\boldsymbol{P}$ is a m by m rank one matrix. Notice that the line through $\boldsymbol{a}$, the subspace we are projecting onto, is the column space of $\boldsymbol{P}$.

4.3.2   Projection onto a subspace

Now we project onto a n-dimensional subspace of $\mathbb{R}^m$. We start with n vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ in $\mathbb{R}^m$, *assume that they are linearly independent.*

We want to find a projection of $\boldsymbol{b}$ onto the subspace spanned by these vectors, that is, *the combination $\boldsymbol{p} = \hat{x}_1\boldsymbol{a}_1 + \cdots + \hat{x}_n\boldsymbol{a}_n$ closest to a given vector $\boldsymbol{b}$.* See that this can be written as $\boldsymbol{A}\hat{\boldsymbol{x}}$, where $\hat{\boldsymbol{x}} = (\hat{x}_1, \ldots, \hat{x}_n)$.

As before, the idea here is that the error vector $\boldsymbol{e} = \boldsymbol{b} - \boldsymbol{p} = \boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}}$ is perpendicular to the subspace we are projecting onto. Every basis vector is perpendicular to this error vector, so

$$\begin{array}{l} \boldsymbol{a}_1^T(\boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}}) = 0 \\ \qquad \vdots \\ \boldsymbol{a}_n^T(\boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}}) = 0 \end{array} \quad \text{or} \quad \begin{bmatrix} - \boldsymbol{a}_1^T - \\ \vdots \\ - \boldsymbol{a}_n^T - \end{bmatrix}\begin{bmatrix} \boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}} \end{bmatrix} = \begin{bmatrix} 0 \end{bmatrix} \quad \text{or} \quad A^T A\hat{\boldsymbol{x}} = A^T \boldsymbol{b}.$$

We have

$$\boldsymbol{A}^T(\boldsymbol{b} - \boldsymbol{A}\hat{x}) = \boldsymbol{0} \implies \boldsymbol{A}^T \boldsymbol{A}\hat{x} = \boldsymbol{A}^T \boldsymbol{b}$$

(next page)

Cont.

We had the projection of b onto the column space of A as $p = A\hat{x}$. We showed that

$$A^T(b - A\hat{x}) = 0 \implies A^T A\hat{x} = A^T b$$

With this we can derive the projection matrix:

The combination $p = \hat{x}_1 a_1 + \cdots + \hat{x}_n a_n = A\hat{x}$ that is closest to b comes from $\hat{x}$:

$$\text{Find } \hat{x}\ (n \times 1) \quad A^T(b - A\hat{x}) = 0 \quad \text{or} \quad A^T A\hat{x} = A^T b. \tag{5}$$

This symmetric matrix $A^T A$ is n by n. It is invertible if the a's are independent. The solution is $\hat{x} = (A^T A)^{-1} A^T b$. The *projection* of b onto the subspace is p:

$$\text{Find } p\ (m \times 1) \qquad p = A\hat{x} = A(A^T A)^{-1} A^T b. \tag{6}$$

The *projection matrix* P is multiplying b in (6). It has four A's:

$$\text{Find } P\ (m \times m) \qquad P = A(A^T A)^{-1} A^T. \tag{7}$$

Again see that this only works if $A^T A$ is invertible, which is only when the column vectors of A are independent. See that the final projection matrix formula is analagous to the formula derived in the one dimensional case.

The subspace we are projecting onto is the the column space of A, that is, $C(A)$. See that the error $e = b - A\hat{x}$ *belongs to the perpendicular subspace* $N(A^T)$ (since $A^T(b - A\hat{x}) = 0$).

A note on the projection matrix

The matrix $P = A(A^T A)^{-1} A^T$ is deceptive. One might try to split $(A^T A)^{-1}$ into A^{-1} times $(A^T)^{-1}$ and find that the entire formula reduces to I.

This is wrong because *the matrix A is rectangular and therefore has no inverse.* We cannot split $(A^T A)^{-1}$ into A^{-1} times $(A^T)^{-1}$ because there is no A^{-1} in the first place.

■ REVIEW OF THE KEY IDEAS ■

1. The projection of b onto the line through a is $p = a\hat{x} = a(a^T b / a^T a)$.

2. The rank one projection matrix $P = aa^T / a^T a$ multiplies b to produce p.

3. Projecting b onto a subspace leaves $e = b - p$ perpendicular to the subspace.

4. When A has full rank n, the equation $A^T A\hat{x} = A^T b$ leads to $\hat{x}$ and $p = A\hat{x}$.

5. The projection matrix $P = A(A^T A)^{-1} A^T$ has $P^T = P$ and $P^2 = P$ and $Pb = p$.

4.4   Projection matrices are symmetrical

Given a projection matrix $\boldsymbol{P}$, we can decompose any vectors $\boldsymbol{v}$ and $\boldsymbol{w}$ into

$$\boldsymbol{v} = \boldsymbol{v}_p + \boldsymbol{v}_n$$
$$\boldsymbol{w} = \boldsymbol{w}_p + \boldsymbol{w}_n$$

With the p subscript indicating the component of the vector in the subspace of $\boldsymbol{P}$, and the n subscript the component outside (normal to) the subspace of $\boldsymbol{P}$. (the sum of the projection and its orthogonal 'error' make up the original vector before projecion)

The projection of a vector lies in a subspace. The dot produc of anything in this subspace with anything orthogonal to this subspace is zero. So see that

$$\begin{aligned}
(\boldsymbol{Pv}) \cdot \boldsymbol{w} &= \boldsymbol{v}_p \cdot \boldsymbol{w} \\
&= \boldsymbol{v}_p \cdot (\boldsymbol{w}_p + \boldsymbol{w}_n) \\
&= \boldsymbol{v}_p \cdot \boldsymbol{w}_p + \boldsymbol{v}_p \cdot \boldsymbol{w}_n \\
&= \boldsymbol{v}_p \cdot \boldsymbol{w}_p
\end{aligned}$$

and similarly

$$\begin{aligned}
\boldsymbol{v} \cdot (\boldsymbol{Pw}) &= \boldsymbol{v} \cdot \boldsymbol{w}_p \\
&= (\boldsymbol{v}_p + \boldsymbol{v}_n) \cdot \boldsymbol{w}_p \\
&= \boldsymbol{v}_p \cdot \boldsymbol{w}_p + \boldsymbol{v}_n \cdot \boldsymbol{w}_p \\
&= \boldsymbol{v}_p \cdot \boldsymbol{w}_p
\end{aligned}$$

As such we can conclude that

$$(\boldsymbol{Pv}) \cdot \boldsymbol{w} = \boldsymbol{v} \cdot (\boldsymbol{Pw})$$

and using the definition of the dot product:

$$(\boldsymbol{Pv})^T \boldsymbol{w} = \boldsymbol{v}^T \cdot (\boldsymbol{Pv})$$
$$\boldsymbol{v}^T \boldsymbol{P}^T \boldsymbol{w} = \boldsymbol{v}^T \boldsymbol{P} \boldsymbol{w}$$

so

$$\boldsymbol{P}^T = \boldsymbol{P}$$

4.5 Least Squares Approximations

Illustrative example

Consider trying to find the closest line to three points $(0,6), (1,0), (2,0)$. No straight line $b = C + Dt$ goes through those three points; we want two numbers C and D that satisfy a system of three equations (this leads us to a 3 by 2 matrix):

$t = 0$ The first point is on the line $b = C + Dt$ if $C + D \cdot 0 = 6$

$t = 1$ The second point is on the line $b = C + Dt$ if $C + D \cdot 1 = 0$

$t = 2$ The third point is on the line $b = C + Dt$ if $C + D \cdot 2 = 0.$

(This is essentially sampling a straight line at the three time points and comparing it to the desired data points at those times) This 3 by 2 system has *no solution*: $b = (6, 0, 0)$ is not a combination of the columns $(1, 1, 1)$ and $(0, 1, 2)$ (of the matrix A):

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{bmatrix} \quad x = \begin{bmatrix} C \\ D \end{bmatrix} \quad b = \begin{bmatrix} 6 \\ 0 \\ 0 \end{bmatrix} \quad Ax = b \text{ is } not \text{ solvable.}$$

The idea here is to choose a vector of parameters x that makes $e = b - Ax$ as small as possible—so finding a point in the column space of A that is *closest to* b—see that this is just the projection. So the best x, which we denote as $\hat{x}$, is found by $A^T A \hat{x} = A^T b$, where the projection p of b onto the column space of A is denoted by $p = A\hat{x}$:

$$Ax = b = p + e \text{ is impossible} \qquad A\hat{x} = p \text{ is solvable} \qquad \hat{x} \text{ is } (A^T A)^{-1} A^T b.$$

See that the solution to $A\hat{x} = p$ results in the least possible squared error:

Squared error for any x $\|Ax - b\|^2 = \|Ax - p\|^2 + \|e\|^2.$

Since any x other than $\hat{x}$ would lead to $||Ax - p||^2 > 0$. (This expression comes from the pythagorean theorem, where the vector from some point Ax to point b, that is $Ax - b$, whose length we want to minimise, is the hypotenuse, while the the error $e = b - p$, perpendicular to the vector $Ax - p$, are the opposite and adjacent sides respectively)

By choosing $x = \hat{x}$, we leave the smallest possible error $e = (e_1, e_2, e_3)$ that we can't reduce, while reducing $Ax - p$ to zero. There is some ambiguity in the idea of 'smallest', but here it means that we minimise the *squared length of* $Ax - b$:

The least squares solution $\hat{x}$ makes $E = \|Ax - b\|^2$ as small as possible.

(next page)

Cont.
By taking $x = \hat{x}$, where $A\hat{x}$ corresponds to the projection of b onto the column space of A, we have the x that minimises the squared error $||Ax - b||^2$:

errors = vertical distances to line   errors $e = (1, -2, 1) = b - p$
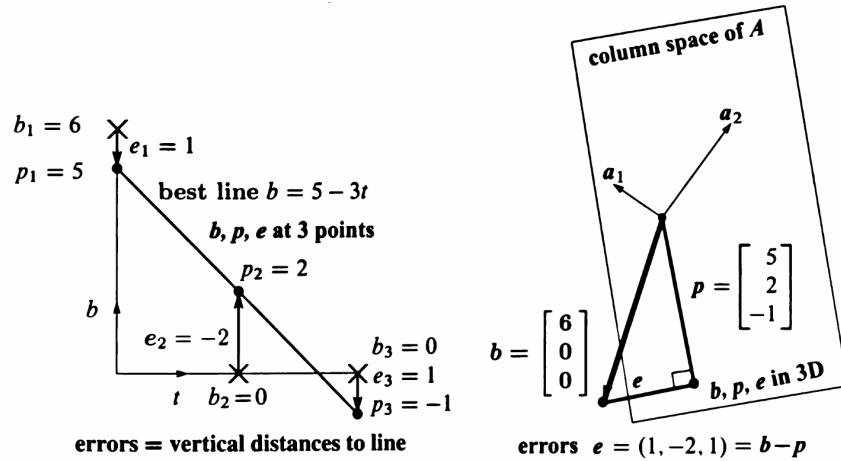
Figure 4.6: **Best line and projection: Two pictures, same problem.** The line has heights $p = (5, 2, -1)$ with errors $e = (1, -2, 1)$. The equations $A^{\mathrm{T}}A\hat{x} = A^{\mathrm{T}}b$ give $\hat{x} = (5, -3)$. Same answer! The best line is $b = 5 - 3t$ and the closest point is $p = 5a_1 - 3a_2$.

Projection allows us to minimise squared error.

Intuition from calculus
Consider minimising the squared error by calculus. The total squared error of the system, with parameters C and D, is

$$E = ||Ax - b||^2 = (C + D \cdot 0 - 6)^2 + (C + D \cdot 1)^2 + (C + D \cdot 2)^2.$$

We take the partial derivative with respect to each parameter and set them to 0:

$$\partial E / \partial C = 2(C + D \cdot 0 - 6) \quad + 2(C + D \cdot 1) \quad + 2(C + D \cdot 2) \quad = 0$$

$$\partial E / \partial D = 2(C + D \cdot 0 - 6)(0) + 2(C + D \cdot 1)(1) + 2(C + D \cdot 2)(2) = 0.$$

Simplifying leaves us with the system

The C derivative is zero: $3C + 3D = 6$
The D derivative is zero: $3C + 5D = 0$ **This matrix** $\begin{bmatrix} 3 & 3 \\ 3 & 5 \end{bmatrix}$ **is** $A^{\mathrm{T}}A$

This system is exactly $A^T A\hat{x} = A^T b$, where optimisation leads us to the exact same system we derived by projection:

$$\boxed{\textit{The partial derivatives of } \ ||Ax - b||^2 \ \textit{ are zero when } A^{\mathrm{T}}A\hat{x} = A^{\mathrm{T}}b.}$$

(next page)

The big picture for least squares

The intuition for the four subspaces can be applied here. Given some b that isn't in the column space of A, we can split it into the sum of its projection p in the column space and the minimum error e in the orthogonal subspace; that is, we have $b = p + e$:
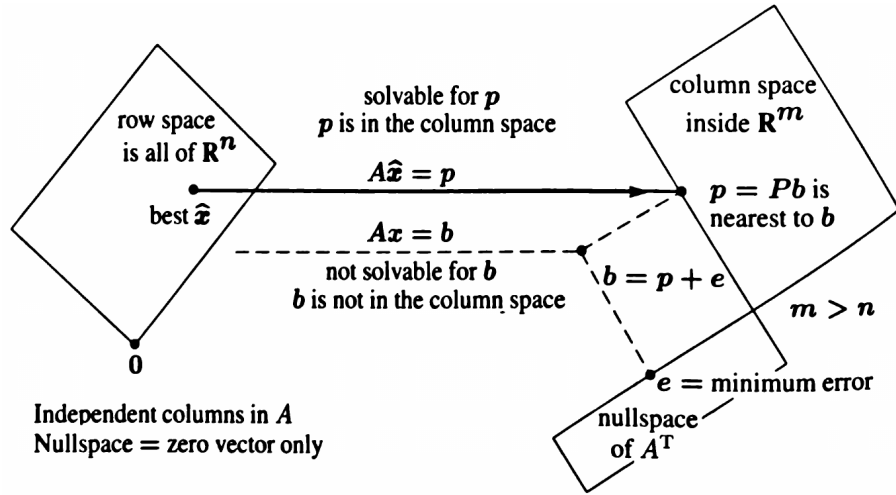
Figure 4.7: The projection $p = A\widehat{x}$ is closest to b, so $\widehat{x}$ minimizes $E = \|b - Ax\|^2$.

As discussed earlier, see that the row space has a solution for any vector in the column space of A, meaning that it contains $\hat{x}$. Also notice that since we construct A as having full column rank, its nullspace will just be the zero vector. (next page)

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4.5.1 Fitting a straight line

Fitting a line is the clearest application of least squares. It starts with $m > 2$ points $b_1, \ldots, b_m$, at times $t_1, \ldots, t_m$. The best fit line $C + D\boldsymbol{t}$ misses the point by vertical distances $e_1, \ldots, e_m$. The least squares line minimises $E = e_1^2 + \cdots + e_m^2$ (note that this is not the minimum error as in the previous pages).

A line goes through all m points when we can exactly solve $A\boldsymbol{x} = \boldsymbol{b}$; generally this isn't possible so we want a best fit. Two unknowns C and D determine a line, so A only has $n = 2$ columns. To fit m points, we are trying to solve m equations:

$$
A\boldsymbol{x} = \boldsymbol{b} \quad \text{is} \qquad
\begin{aligned}
C + Dt_1 &= b_1 \\
C + Dt_2 &= b_2 \\
&\vdots \\
C + Dt_m &= b_m
\end{aligned}
\qquad \text{with} \qquad
A = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix}.
$$

The column space is so thin that $\boldsymbol{b}$ is almost certainly outside of it (if $\boldsymbol{b}$ happens to lie in the column space then $\boldsymbol{b} = \boldsymbol{p}$ and the errors are $\boldsymbol{e} = \boldsymbol{0}$). The parameters $\hat{\boldsymbol{x}}$ for the line that minimises the squared error $||A\boldsymbol{x} - \boldsymbol{b}||^2$ is found by the projection:

The closest line $C + Dt$ has heights $p_1, \ldots, p_m$ with errors $e_1, \ldots, e_m$.

Solve $A^{\mathsf{T}} A \hat{\boldsymbol{x}} = A^{\mathsf{T}} \boldsymbol{b}$ for $\hat{\boldsymbol{x}} = (C, D)$. The errors are $e_i = b_i - C - Dt_i$.

See that the matrix $A^T A$ looks like

Dot-product matrix $\quad A^{\mathsf{T}} A = \begin{bmatrix} 1 & \cdots & 1 \\ t_1 & \cdots & t_m \end{bmatrix} \begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_m \end{bmatrix} = \begin{bmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix}.$

and $A^T \boldsymbol{b}$,

$$
A^{\mathsf{T}} \boldsymbol{b} = \begin{bmatrix} 1 & \cdots & 1 \\ t_1 & \cdots & t_m \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix} = \begin{bmatrix} \sum b_i \\ \sum t_i b_i \end{bmatrix}.
$$

The line $C + D\boldsymbol{t}$ minimises the error $\boldsymbol{E}(x) = e_1^2 + \cdots + e_m^2 = ||A\boldsymbol{x} - \boldsymbol{b}||^2$ when $A^T A \hat{\boldsymbol{x}} = A^T \boldsymbol{b}$:

$$
A^{\mathsf{T}} A \hat{\boldsymbol{x}} = A^{\mathsf{T}} \boldsymbol{b} \qquad \begin{bmatrix} m & \sum t_i \\ \sum t_i & \sum t_i^2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum b_i \\ \sum t_i b_i \end{bmatrix}.
$$

$$
\boldsymbol{E}(\boldsymbol{x}) = ||A\boldsymbol{x} - \boldsymbol{b}||^2 = (C + Dt_1 - b_1)^2 + \cdots + (C + Dt_m - b_m)^2.
$$

4.6 Orthonormal Bases

The vectors $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ are *orthogonal* when their dot products $\boldsymbol{q}_1 \cdots \boldsymbol{q}_j$ are zero—$\boldsymbol{q}_i^T \boldsymbol{q}_j = 0$ whenever $i \neq j$. By *dividing each vector by its length*, the vectors become orthogonal *unit vectors*—their lengths are all 1—in this case the basis is called *orthonormal*:

DEFINITION The n vectors $\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n$ are ***orthonormal*** if

$$\boldsymbol{q}_i^T \boldsymbol{q}_j = \begin{cases} 0 & \text{when } i \neq j \quad (\textbf{\textit{orthogonal}} \text{ vectors}) \\ 1 & \text{when } i = j \quad (\textbf{\textit{unit}} \text{ vectors: } \|\boldsymbol{q}_i\| = 1) \end{cases}$$

A matrix Q with orthonormal columns has $Q^T Q = I$. Typically $m > n$.

The matrix $\boldsymbol{Q}$ is easy to work with because $\boldsymbol{Q}^T \boldsymbol{Q} = \boldsymbol{I}$ (since each column is orthonormal):

$$\boldsymbol{Q}^T \boldsymbol{Q} = \begin{bmatrix} - \boldsymbol{q}_1^T - \\ - \boldsymbol{q}_2^T - \\ - \boldsymbol{q}_n^T - \end{bmatrix} \begin{bmatrix} | & | & & | \\ \boldsymbol{q}_1 & \boldsymbol{q}_2 & & \boldsymbol{q}_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = \boldsymbol{I}$$

On the diagonal the unit vectors give $\boldsymbol{q}_i^T \boldsymbol{q}_i = \|\boldsymbol{q}_i\|^2 = 1$. Note an important implication:

When Q is square, $Q^T Q = I$ means that $Q^T = Q^{-1}$: transpose $=$ inverse.

Note that generally if $m \neq n$ then $\boldsymbol{Q}\boldsymbol{Q}^T \neq \boldsymbol{I}$; although $\boldsymbol{Q}^T \boldsymbol{Q} = \boldsymbol{I}$ even when $\boldsymbol{Q}$ is rectangular, $\boldsymbol{Q}^T$ here is only a 1-sided inverse from the left. Only for square matrices do we also have $\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}$ (from the definition of the inverse of square matrices as covered earlier).

(The matrix must have full column rank since if its columns were to be orthonormal; so we have $m \geq n$. A mapping by $\boldsymbol{Q}$ in the case where $m > n$ is invertible since it has full column rank, but the transpose (size nxm) doesn't have full column rank and therefore a specific mapping $\boldsymbol{Q}^T \boldsymbol{x} = \boldsymbol{b}$ would have infinite solutions—a $\boldsymbol{x}$ cannot be exactly recovered given a $\boldsymbol{Q}^T$ and $\boldsymbol{b}$. As such only applying $\boldsymbol{Q}$ first works.)

If we have a *square* $\boldsymbol{Q}$ with orthonormal columns, its transpose is its inverse from both sides; and as such also has orthonormal columns—both the rows and columns of $\boldsymbol{Q}$ are orthonormal. A square matrix with orthonormal columns is called an *orthogonal matrix*.

Also see that if the columns are only orthogonal and not orthonormal, their dot products still give a diagonal matrix.
(next page)

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4.6.1 Multiplication by any orthogonal matrix preserves length and angle

Length is preserved during multiplication with an orthogonal matrix:

Proof $\|Qx\|^2$ equals $\|x\|^2$ because $(Qx)^{\mathrm{T}}(Qx) \;=\; x^{\mathrm{T}}Q^{\mathrm{T}}Qx \;=\; x^{\mathrm{T}}Ix \;=\; x^{\mathrm{T}}x$.

If Q has orthonormal columns $(Q^{\mathrm{T}}Q = I)$, it leaves lengths unchanged :

$$\text{Same length for } Qx \qquad \|Qx\| = \|x\| \text{ for every vector } x. \qquad (3)$$

The dot product, and therefore the angle, is also preserved:

$$\boldsymbol{Q \text{ also preserves dot products}:} \ (Qx)^{\mathrm{T}}(Qy) = x^{\mathrm{T}}Q^{\mathrm{T}}Qy = x^{\mathrm{T}}y.$$

4.6.2 Projections using orthonormal bases

Using orthonormal bases for projection greatly simplifies computation. For projections onto subspaces, all formulas involve $A^T A$; suppose the basis vectors are orthonormal, then $A^T A$ simplifies to $Q^T Q = I$. Our projection becomes

$$\widehat{x} = Q^{\mathrm{T}}b \quad \text{and} \quad p = Q\widehat{x} \quad \text{and} \quad P = QQ^{\mathrm{T}}. \qquad (4)$$

The least squares solution of $Qx = b$ is $\widehat{x} = Q^{\mathrm{T}}b$. The projection matrix is QQ^{T}.

See that no inversion is required—this is the point of an orthonormal basis—the best $\hat{x} = Q^T b$ is just dot products of $q_1, \ldots, q_n$ with b:

$$
\begin{array}{l}
\textbf{\textit{Projection}} \\
\textbf{\textit{onto q's}}
\end{array}
\qquad
p \;=\;
\begin{bmatrix} | & & | \\ q_1 & \cdots & q_n \\ | & & | \end{bmatrix}
\begin{bmatrix} q_1^{\mathrm{T}}b \\ \vdots \\ q_n^{\mathrm{T}}b \end{bmatrix}
\;=\;
q_1(q_1^{\mathrm{T}}b) + \cdots + q_n(q_n^{\mathrm{T}}b).
$$

Also see that when Q is square (so an orthonormal basis spanning the entire space), $\hat{x} = Q^T b$ leads to $p = Q\hat{x} = QQ^T b = Ib = b$. The projection of b onto the basis that spans the entire space is b itself. (See that $QQ^T = I$ only works for square matrices)

4.7 Gram-Schmidt Process

Given three *independent vectors* a, b, c, we intend to construct three *orthogonal* vectors A, B, C. Then, by dividing A, B, C by their lengths, we can produce three orthonormal vectors $q_1 = A/\|A\|$, $q_2 = B/\|B\|$, $q_3 = C/\|C\|$.

Begin by choosing $A = a$ (we make all other vectors orthogonal to this). The next vector B must be perpendicular to A; we *start with b and subtract its projection along A*. This leaves the perpendicular part, which is the orthogonal vector B:

First Gram-Schmidt step
B is perpendicular to A

$$B = b - \frac{A^{\mathrm{T}}b}{A^{\mathrm{T}}A}A.$$

We use the one dimensional projection of b onto a to produce a vector orthogonal to a; then we use it as our next basis vector.

The third direction starts with c. We can say that c is not a comination of A and B because c is not a combination of a and b (see that B is just a combination of b and $A = a$ since $\hat{x}$ in the one dimensional case is just a constant). It is also unlikely that c is already perpendicular to A and B; the idea here is that we subtract off its components in those two directions to get a perpendicular direction C:

Next Gram-Schmidt step
C is perpendicular to A and B

$$C = c - \frac{A^{\mathrm{T}}c}{A^{\mathrm{T}}A}A - \frac{B^{\mathrm{T}}c}{B^{\mathrm{T}}B}B.$$

This is the entire idea behind the Gram-Schmidt process; *Subtract from every vector its projections in the directions already set*, repeating for each new basis vector. At the end, or immediately when each one is found, dividing the orthogonal vectors A, B, C, D by their lengths leaves us with *orthonormal* results q_i
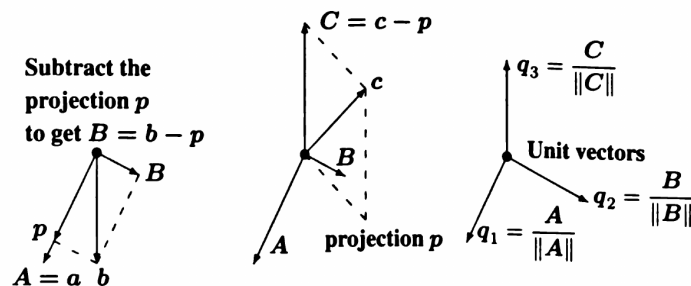

Figure 4.10: First project b onto the line through a and find the orthogonal $B = b - p$. Then project c to p on the AB plane and find $C = c - p$. Divide by $\|A\|, \|B\|, \|C\|$.

4.8 $A = QR$ factorisation

Using the Gram-Schmidt process we can derive an orthonormal matrix $\boldsymbol{Q}$ with columns $\boldsymbol{q}_1, \boldsymbol{q}_2$, and $\boldsymbol{q}_3$ from a matrix $\boldsymbol{A}$ with columns $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$. The vectors $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$ come from linear combinations of $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$ and vice versa. As such there must be a third matrix that maps $\boldsymbol{Q}$ to $\boldsymbol{A}$.

Matrix $\boldsymbol{A}$ has independent columns, and so any mapping using its column space has a one to one mapping; a mapping to $\boldsymbol{Q}$ in the same dimension suggests a *square invertible matrix* applied to the right of $\boldsymbol{A}$, lets call it $\boldsymbol{R}^{-1}$; so $\boldsymbol{AR}^{-1} = \boldsymbol{Q}$ (the linear combinations of the columns of $\boldsymbol{A}$ to produce $\boldsymbol{Q}$ must themselves be linearly independent). This square invertible matrix has an inverse $\boldsymbol{R}$, which when applied to the right of this equation, gives us

$$\boldsymbol{AR}^{-1}\boldsymbol{R} = \boldsymbol{A} = \boldsymbol{QR}$$

so we can say that there is some $\boldsymbol{R}$ connecting the orthonormal $\boldsymbol{Q}$ back to $\boldsymbol{A}$.

To find this $\boldsymbol{R}$, we simply multiply the entire expression by $\boldsymbol{Q}^T$:

$$\boldsymbol{Q}^T \boldsymbol{A} = \boldsymbol{Q}^T \boldsymbol{QR} = \boldsymbol{R}$$

So we have $\boldsymbol{R} = \boldsymbol{Q}^T \boldsymbol{A}$:

$$\boldsymbol{R} = \begin{bmatrix} \boldsymbol{q}_1^T \\ \boldsymbol{q}_2^T \\ \boldsymbol{q}_3^T \end{bmatrix} \begin{bmatrix} \boldsymbol{a} & \boldsymbol{b} & \boldsymbol{c} \end{bmatrix} = \begin{bmatrix} \boldsymbol{q}_1^T \boldsymbol{a} & \boldsymbol{q}_1^T \boldsymbol{b} & \boldsymbol{q}_1^T \boldsymbol{c} \\ \boldsymbol{q}_2^T \boldsymbol{a} & \boldsymbol{q}_2^T \boldsymbol{b} & \boldsymbol{q}_2^T \boldsymbol{c} \\ \boldsymbol{q}_3^T \boldsymbol{a} & \boldsymbol{q}_3^T \boldsymbol{b} & \boldsymbol{q}_3^T \boldsymbol{c} \end{bmatrix}$$

This can be simplified. We know that

- The vectors $\boldsymbol{a}$ and $\boldsymbol{A}$ and $\boldsymbol{q}_1$ are all along a single line

- The vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{q}_1$, $\boldsymbol{q}_2$ are all in the same plane

- The vectors $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ and $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$ and $\boldsymbol{q}_1$, $\boldsymbol{q}_2$, $\boldsymbol{q}_3$ are all in the same 3 dimensional subspace

The point here is that q_2 is orthogonal to that entire first line, and q_3 is orthogonal to that entire second plane. Looking back at $\boldsymbol{R}$, see that $\boldsymbol{q}_2^T \boldsymbol{a} = 0$ by orthogonality, as well as $\boldsymbol{q}_3^T \boldsymbol{a}$ and $\boldsymbol{q}_3^T \boldsymbol{b}$. Our simplified matrix looks like

$$\begin{bmatrix} \boldsymbol{a} & \boldsymbol{b} & \boldsymbol{c} \end{bmatrix} = \begin{bmatrix} \boldsymbol{q}_1 & \boldsymbol{q}_2 & \boldsymbol{q}_3 \end{bmatrix} \begin{bmatrix} \boldsymbol{q}_1^T \boldsymbol{a} & \boldsymbol{q}_1^T \boldsymbol{b} & \boldsymbol{q}_1^T \boldsymbol{c} \\ & \boldsymbol{q}_2^T \boldsymbol{b} & \boldsymbol{q}_2^T \boldsymbol{c} \\ & & \boldsymbol{q}_3^T \boldsymbol{c} \end{bmatrix} \quad \text{or} \quad \boldsymbol{A} = \boldsymbol{QR}.$$

(next page)

Cont.
We had

$$
\begin{bmatrix} a & b & c \end{bmatrix} = \begin{bmatrix} q_1 & q_2 & q_3 \end{bmatrix} \begin{bmatrix} q_1^\mathsf{T} a & q_1^\mathsf{T} b & q_1^\mathsf{T} c \\ & q_2^\mathsf{T} b & q_2^\mathsf{T} c \\ & & q_3^\mathsf{T} c \end{bmatrix} \quad \text{or} \quad A = QR.
$$

Intuitively, at every step $a_1, \ldots, a_k$ are combinations of $q_1, \ldots, q_k$, and so column i of R, which specifies a_i as a combination of the columns of Q, will only have nonzero entries in the rows corresponding to the columns of Q that contribute to that a_i.

See that this leads to R being *triangular*—any a_j only depends on the q_i where $i < j$—so all the entries below the jth row in R will be zero.

> **(Gram-Schmidt)** From independent vectors $a_1, \ldots, a_n$, Gram-Schmidt constructs orthonormal vectors $q_1, \ldots, q_n$. The matrices with these columns satisfy $A = QR$. Then $R = Q^\mathsf{T} A$ *is upper triangular* because later q's are orthogonal to earlier a's.

In the context of Least Squares
See that using our factorisation:

$$
A^T A = (QR)^T QR = R^T Q^T QR = R^T R
$$

the least squares formula
$$
A^T A \hat{x} = A^T b
$$

simplifies to

$$
R^T R \hat{x} = (QR)^T b
$$
$$
R^T R \hat{x} = R^T Q^T b
$$
$$
R \hat{x} = Q^T b \quad \text{or} \quad \hat{x} = R^{-1} Q^T b
$$

(R is invertible since it has full column rank. It has full row rank too so R^T also has full column rank and is invertible (justifying the last step))

This allows us to solve for the least squares solution $\hat{x}$ using back substitution (which is very fast). The real cost is the computation for Gram-Schmidt, which is needed to construct the orthogonal Q and the triangular $R = Q^T A$.
(next page)

An algorithm

Here is an algorithm for the Gram-Schmidt process:

```
for j = 1:n                         % modified Gram-Schmidt in n loops
    v = A(:, j);                    % v begins as column j of the original A
    for i = 1:j−1                   % columns q₁ to q_{j−1} are already settled in Q
        R(i, j) = Q(:, i)' * v;     % compute R_ij = qᵢᵀaⱼ which is qᵢᵀv
        v = v − R(i, j)*Q(:, i);    % subtract the projection (qᵢᵀv)qᵢ
    end                             % v is now perpendicular to all of q₁,…,q_{j−1}
    R(j, j) = norm(v);              % the diagonal entries R_jj in R are lengths
    Q(:, j) = v/R(j, j);            % divide v by its length to get the next qⱼ
end                                 % for j = 1 : n produces all of the qⱼ
```

Which essentially executes

$$r_{kj} = \sum_{i=1}^{m} q_{ik} v_{ij} \ \text{ and } \ v_{ij} = v_{ij} - q_{ik} r_{kj} \ \text{ and } \ r_{jj} = \left(\sum_{i=1}^{m} v_{ij}^2 \right)^{1/2} \ \text{ and } \ q_{ij} = \frac{v_{ij}}{r_{jj}}.$$

Where r denotes entries of $\boldsymbol{R}$ and $\boldsymbol{v}$ a column in the original $\boldsymbol{A}$.

The diagonal entries of $\boldsymbol{R}$ are just the norms of the unnormalised projections in the Gram-schmidt process. For instance

$$\boldsymbol{q}_2^T \boldsymbol{b} = \boldsymbol{q}_2 \cdot \boldsymbol{b} = \cos(\theta)||\boldsymbol{q}_2|| \, ||\boldsymbol{b}|| = \cos(\theta)||\boldsymbol{b}|| = ||\boldsymbol{B}||$$

θ, the angle between $\boldsymbol{b}$ and its projection $\boldsymbol{q}_2$, is the same angle between $\boldsymbol{b}$ and its unnormalised projection $\boldsymbol{B}$.

4.9   Pseudoinverses

Left Inverse
Consider a 'tall and thin' matrix $\boldsymbol{A}$, where $m > n$ with rank $r = n$. A matrix like this only has a *left sided* inverse (consider that $\boldsymbol{x}^T\boldsymbol{A}$ would produce a matrix whose rows are combinations of linearly dependent rows—this cannot be 'undone' to recover $\boldsymbol{x}^T$ given a result. On the other hand $\boldsymbol{A}\boldsymbol{x}$ can be 'undone' since this way the mapping $\boldsymbol{A}$ is unique to each $\boldsymbol{x}$.)

In this case $\boldsymbol{A}$ has independent columns, so $\boldsymbol{A}^T\boldsymbol{A}$ (nxn) is invertible, and

$$(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{A} = \boldsymbol{I}$$

We say that

$$\boldsymbol{A}_{\text{left}}^{-1} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T$$

is the *left inverse* of $\boldsymbol{A}$ (there may be other left inverses), where $\boldsymbol{A}_{\text{left}}^{-1}\boldsymbol{A} = \boldsymbol{I}$.

Right inverse
In another case consider if $\boldsymbol{A}$ were 'short and fat', where $m < n$ with rank $r = m$. A matrix like this only has a right sided inverse. $\boldsymbol{A}$ has independent rows, so now $\boldsymbol{A}\boldsymbol{A}^T$ is invertible and

$$\boldsymbol{A}\boldsymbol{A}^T(\boldsymbol{A}\boldsymbol{A}^T)^{-1} = \boldsymbol{I}$$

A nice *right inverse* is therefore:

$$\boldsymbol{A}_{\text{right}}^{-1} = \boldsymbol{A}^T(\boldsymbol{A}\boldsymbol{A}^T)^{-1}$$

where $\boldsymbol{A}\boldsymbol{A}_{\text{right}}^{-1} = \boldsymbol{I}$.

Left and right inverses as projections
If $\boldsymbol{A}$ has full column rank and $\boldsymbol{A}_{\text{left}}^{-1} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T$, applying the left inverse on the right leads us to

$$\boldsymbol{A}\boldsymbol{A}_{\text{left}}^{-1} = \boldsymbol{A}(\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T = \boldsymbol{P}$$

Is just a matrix which projects $\mathbb{R}^m$ onto the *column space* of $\boldsymbol{A}$.

Similarly, if $\boldsymbol{A}$ has full row rank then

$$\boldsymbol{A}_{\text{right}}^{-1}\boldsymbol{A} = \boldsymbol{A}^T(\boldsymbol{A}\boldsymbol{A}^T)^{-1}\boldsymbol{A} = \boldsymbol{P}$$

Is just a matrix that projects $\mathbb{R}^n$ onto the *row space* of $\boldsymbol{A}$.
(next page)

Intuition for the pseudoinverse

The remaining case to consider is a matrix $\boldsymbol{A}$ for which $r < n$ and $r < m$. The vector $\boldsymbol{Ax}$ is always in the column space of $\boldsymbol{A}$; recall that the correspondence between vectors $\boldsymbol{x}$ in the (r dimensional) row space and vectors $\boldsymbol{Ax}$ in the (r dimensional) column space is one-to-one—meaning that if $\boldsymbol{x} \neq \boldsymbol{y}$ are vectors in the row space of $\boldsymbol{A}$ then $\boldsymbol{Ax} \neq \boldsymbol{Ay}$ in the column space of $\boldsymbol{A}$—we can show this.

Proving that if $\boldsymbol{x} \neq \boldsymbol{y}$ then $\boldsymbol{Ax} \neq \boldsymbol{Ay}$: Suppose that the statement is false, then we can find $\boldsymbol{x} \neq \boldsymbol{y}$ in the row space of $\boldsymbol{A}$ for which $\boldsymbol{Ax} = \boldsymbol{Ay}$. But then $\boldsymbol{A}(\boldsymbol{x} - \boldsymbol{y}) = \boldsymbol{0}$ and $\boldsymbol{x} - \boldsymbol{y}$ is in the nullspace of $\boldsymbol{A}$; however since the row space is closed under linear combinations (including subtraction), $\boldsymbol{x} - \boldsymbol{y}$ is also in the row space of $\boldsymbol{A}$. The only vector in both the nullspace and row space is the zero vector, so $\boldsymbol{x} - \boldsymbol{y} = \boldsymbol{0}$, and the two vectors must be equal.

We can therefore conclude that the mapping $\boldsymbol{x} \mapsto \boldsymbol{Ax}$ from the row space to the column space is *invertible*. The inverse of this operation is called the *pseudoinverse*.

Chapter 5

Determinants

5.1 Properties of determinants

We can derive a number of ideas given the following three properties of determinants:

1. **The n by n identity matrix has $\det I = 1$.**

2. **Exchanging two rows of A reverses $\det A$ to $-\det A$.**

3. **If row 1 of A is a combination $cv + dw$, then add 2 determinants :**

$$
\det \begin{bmatrix} cv + dw \\ \text{row } 2 \\ \cdot \cdot \\ \text{row } n \end{bmatrix} = c \det \begin{bmatrix} v \\ \text{row } 2 \\ \cdot \cdot \\ \text{row } n \end{bmatrix} + d \det \begin{bmatrix} w \\ \text{row } 2 \\ \cdot \cdot \\ \text{row } n \end{bmatrix}
$$

For a nice geometric way to think of the determinant, consider a unit cube in N dimensional space: the set of N vectors of length 1 with coordinates 0 or 1 in each spot. The determinant of the linear transformation (matrix) T is the *signed volume of the region after applying T to the unit cube.*

If we apply the identity to the unit cube, we get back the unit cube, with volume 1 (the first property). If we stretch the cube by a constant factor in one direction only, the new volume is that constant; if we stack two blocks together aligned on the same direction, their combined volume is the sum of their volumes—showing that the signed volume is linear in each coordinate (property 3).
(next page)

Cont.—linearity in all rows separately

The third property essentially states that the determinant is linear with respect to row 1; then property 2 leads us further: $\det(\boldsymbol{A})$ is linear *to every row separately*:

$$
\det \begin{bmatrix} \text{row 1} \\ c\boldsymbol{v} + d\boldsymbol{w} \\ \ldots \\ \text{row } n \end{bmatrix} = -\det \begin{bmatrix} c\boldsymbol{v} + d\boldsymbol{w} \\ \text{row 1} \\ \ldots \\ \text{row } n \end{bmatrix}
$$

$$
= -c \det \begin{bmatrix} \boldsymbol{v} \\ \text{row 1} \\ \ldots \\ \text{row } n \end{bmatrix} - d \det \begin{bmatrix} \boldsymbol{w} \\ \text{row 1} \\ \ldots \\ \text{row } n \end{bmatrix}
$$

$$
= c \det \begin{bmatrix} \text{row 1} \\ \boldsymbol{v} \\ \ldots \\ \text{row } n \end{bmatrix} + d \det \begin{bmatrix} \text{row 1} \\ \boldsymbol{w} \\ \ldots \\ \text{row } n \end{bmatrix}
$$

5.1.1 If $\boldsymbol{A}$ has two equal rows, its determinant is 0; row operations don't change the determinant

Consider property 2; if $\boldsymbol{A}$ were to have two equal rows, exchanging them would have no effect on $\boldsymbol{A}$. Then $\det(\boldsymbol{A}) = -\det(\boldsymbol{A})$, and $\det(\boldsymbol{A})$ must be zero.

Now consider this with property 3, and see that *subtracting d times row i from row j leaves det($\boldsymbol{A}$) unchanged*:

$$
\det \begin{bmatrix} \text{row 1} \\ \text{row 2} - d\,\text{row 1} \\ \ldots \\ \text{row } n \end{bmatrix} = \det \begin{bmatrix} \text{row 1} \\ \text{row 2} \\ \ldots \\ \text{row } n \end{bmatrix} - d \det \begin{bmatrix} \text{row 1} \\ \text{row 1} \\ \ldots \\ \text{row } n \end{bmatrix} = \det \begin{bmatrix} \text{row 1} \\ \text{row 2} \\ \ldots \\ \text{row } n \end{bmatrix}
$$

See that this means that the elimination steps (excluding row exchanges) *does not change the determinant*, and elimination (without row exchanges) is the way to simplify the determinant of a matrix.

5.1.2   Upper triangular and diagonal matrices, Transpose

Finally, see that given any *upper triangular matrix*, row exchanges are not required and upward elimination will reduce the matrix to its diagonal. As such, given an upper triangular matrix, we can just immediately multiply the diagonal entries to find the determinant:

Triangular matrix
Diagonal matrix

$$\det \begin{bmatrix} a & b & c \\ & q & r \\ & & z \end{bmatrix} = \det \begin{bmatrix} a & & \\ & q & \\ & & z \end{bmatrix} = aqz$$

Now see that transposing an invertible matrix won't change the diagonals, and if the matrix is invertible its transposed form is guaranteed to have an upper triangular form (taking into account row exchanges). So by row reductions we can obtain the same diagonal matrix as if we had performed elimination on the orignal matrix:

$$\det(\boldsymbol{A}) = \det(\text{rref form}) = \det(\boldsymbol{A}^T)$$

and so we can conclude that transposing a matrix $\boldsymbol{A}$ doesn't change the determinant:

Transpose the matrix $\qquad \det(\boldsymbol{A}^{\mathbf{T}}) = \det(\boldsymbol{A})$

5.1.3 $\det(\boldsymbol{AB}) = (\det \boldsymbol{A})(\det \boldsymbol{B})$

For a singular matrix $\boldsymbol{A}$, recall that it can be reduced to an identity matrix by elimination matrices (all of which are invertible); then by using the inverse (which is just the reverse of each row operation) of each elimination matrix, we can express $\boldsymbol{A}$ as

$$\boldsymbol{A} = \boldsymbol{E}_k \boldsymbol{E}_{k-1} \cdots \boldsymbol{E}_1$$

These matrices are also called *elementary row matrices*, which are just identity matrices on which exactly *one elementary row operation has been performed*. These elementary row operations are the same as those executed during elimination—scaling a row, adding a scaled row to another row, and exchanging rows.

We can write

$$\det(\boldsymbol{AB}) = \det(\boldsymbol{E}_k \boldsymbol{E}_{k-1} \cdots \boldsymbol{E}_1 \boldsymbol{B})$$

See that any elementary row operation just scales the determinant by a constant. Scaling a single row scales the entire determinant by that constant, exchanging rows negates the determinant, and adding (or subtracting) a scaled row to (or from) another row doesn't change the determinant. As such,

$$\det(\boldsymbol{E}_k \boldsymbol{E}_{k-1} \cdots \boldsymbol{E}_1 \boldsymbol{B}) = c_k c_{k-1} \cdots c_1 \det(\boldsymbol{B}) = \alpha \det(\boldsymbol{B})$$

where c denotes the constants multiplied to the determinant as a result of the row operations.
(next page)

Cont.

We had

$$\det(\boldsymbol{AB}) = \det(\boldsymbol{E}_k\boldsymbol{E}_{k-1}\cdots\boldsymbol{E}_1\boldsymbol{B}) = c_kc_{k-1}\cdots c_1\det(\boldsymbol{B}) = \alpha\det(\boldsymbol{B})$$

Then by setting $\boldsymbol{B}$ to $\boldsymbol{I}$:

$$\det(\boldsymbol{AI}) = \det(\boldsymbol{E}_k\boldsymbol{E}_{k-1}\cdots\boldsymbol{E}_1\boldsymbol{I}) = c_kc_{k-1}\cdots c_1\det(\boldsymbol{I}) = \alpha\det(\boldsymbol{I})$$
$$\det(\boldsymbol{A}) = \alpha$$

and

$$\det(\boldsymbol{AB}) = \det(\boldsymbol{A})\det(\boldsymbol{B})$$

5.1.4 Orthogonal matrices have determinant 1 or -1

We know that
$$\det(\boldsymbol{A}) = \det(\boldsymbol{A}^T)$$

and that
$$\det(\boldsymbol{AB}) = \det(\boldsymbol{A})\det(\boldsymbol{B})$$

Given an orthogonal matrix $\boldsymbol{Q}$, we know

$$\boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{I}$$

so
$$\det(\boldsymbol{Q}^T\boldsymbol{Q}) = \det(\boldsymbol{Q}^T)\det(\boldsymbol{Q}) = \det(\boldsymbol{I}) = 1$$

and since the determinant doesn't change under transposition:

$$(\det(\boldsymbol{Q}))^2 = 1$$

and $\det(\boldsymbol{Q})$ is ± 1.

5.1.5 Matrix factorisations and permutation matrix

Recall the matrix factorisation $\boldsymbol{A} = \boldsymbol{LU}$. $\boldsymbol{L}$ is invertible with 1s along the main diagonal, $\boldsymbol{U}$ is upper triangular. In this case

$$\det\boldsymbol{A} = (\det\boldsymbol{L})(\det\boldsymbol{U}) = \det\boldsymbol{U}$$

Where the determinant can be found by just multiplying down the diagonal.

Similarly, we could have $\boldsymbol{PA} = \boldsymbol{LU}$ due to row exchanges being required before elimination. We know that the permutation matrix $\boldsymbol{P}$ is just the identity with row exchanges applied to it, and so we just have to factor in $\det\boldsymbol{P}$, which will be equal to 1 or -1 depending on how many row exchanges occur.

Elimination, followed by multiplying down the diagonal, is how determinants are computed by virtually all computer systems for linear algebra.

5.2 Intuition for determinant formula

Consider a 3 by 3 determinant of the following matrix

$$\det \begin{bmatrix} a & b & c \\ p & q & r \\ x & y & z \end{bmatrix}$$

By linearity,

$$\det \begin{bmatrix} a & b & c \\ p & q & r \\ x & y & z \end{bmatrix} = \det \begin{bmatrix} a & 0 & 0 \\ p & q & r \\ x & y & z \end{bmatrix} + \det \begin{bmatrix} 0 & b & 0 \\ p & q & r \\ x & y & z \end{bmatrix} + \det \begin{bmatrix} 0 & 0 & c \\ p & q & r \\ x & y & z \end{bmatrix}$$

Looking closer at the first matrix on the right side, again by linearity,

$$\det \begin{bmatrix} a & 0 & 0 \\ p & q & r \\ x & y & z \end{bmatrix} = \det \begin{bmatrix} a & 0 & 0 \\ p & 0 & 0 \\ x & y & z \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & q & 0 \\ x & y & z \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & r \\ x & y & z \end{bmatrix}$$

$$= \det \begin{bmatrix} a & 0 & 0 \\ p & 0 & 0 \\ x & 0 & 0 \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ p & 0 & 0 \\ 0 & y & 0 \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ p & 0 & 0 \\ 0 & 0 & z \end{bmatrix} +$$

$$\det \begin{bmatrix} a & 0 & 0 \\ 0 & q & 0 \\ x & 0 & 0 \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & q & 0 \\ 0 & y & 0 \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & z \end{bmatrix} +$$

$$\det \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & r \\ x & 0 & 0 \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & r \\ 0 & y & 0 \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & r \\ 0 & 0 & z \end{bmatrix}$$

Looking at that final equality, see that the matrices containing a zero column are immediately noninvertible and have determinant 0. This leaves us with the simplification

$$\det \begin{bmatrix} a & 0 & 0 \\ p & q & r \\ x & y & z \end{bmatrix} = \det \begin{bmatrix} a & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & z \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & r \\ 0 & y & 0 \end{bmatrix}$$

The other two matrices on the right side of that first equation can be expanded in a similar manner,

$$\det \begin{bmatrix} 0 & b & 0 \\ p & q & r \\ x & y & z \end{bmatrix} = \det \begin{bmatrix} 0 & b & 0 \\ p & 0 & 0 \\ 0 & 0 & z \end{bmatrix} + \det \begin{bmatrix} 0 & b & 0 \\ 0 & 0 & r \\ x & 0 & 0 \end{bmatrix}$$

$$\det \begin{bmatrix} 0 & 0 & c \\ p & q & r \\ x & y & z \end{bmatrix} = \det \begin{bmatrix} 0 & 0 & c \\ 0 & q & 0 \\ x & 0 & 0 \end{bmatrix} + \det \begin{bmatrix} 0 & 0 & c \\ p & 0 & 0 \\ 0 & y & 0 \end{bmatrix}$$

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Cont.

As per our reasoning, we can write the determinant of a 3 by 3 matrix as

$$\det \begin{bmatrix} a & b & c \\ p & q & r \\ x & y & z \end{bmatrix} = \det \begin{bmatrix} a & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & z \end{bmatrix} + \det \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & r \\ 0 & y & 0 \end{bmatrix} +$$

$$\det \begin{bmatrix} 0 & b & 0 \\ p & 0 & 0 \\ 0 & 0 & z \end{bmatrix} + \det \begin{bmatrix} 0 & b & 0 \\ 0 & 0 & r \\ x & 0 & 0 \end{bmatrix} +$$

$$\det \begin{bmatrix} 0 & 0 & c \\ 0 & q & 0 \\ x & 0 & 0 \end{bmatrix} + \det \begin{bmatrix} 0 & 0 & c \\ p & 0 & 0 \\ 0 & y & 0 \end{bmatrix}$$

This is the sum of the determinants of the following matrices

$$\begin{bmatrix} a & & \\ & q & \\ & & z \end{bmatrix} \begin{bmatrix} & b & \\ p & & \\ & & z \end{bmatrix} \begin{bmatrix} & b & \\ & & r \\ x & & \end{bmatrix} \begin{bmatrix} & & c \\ & q & \\ x & & \end{bmatrix} \begin{bmatrix} & & c \\ p & & \\ & y & \end{bmatrix} \begin{bmatrix} a & & \\ & & r \\ & y & \end{bmatrix}$$

See that this is as if we had taken all the possible row permutations of a 3 by 3 identity, and then for each permutation, we replace the ones with the numbers at those same positions from the matrix of interest. Then we sum up their determinants.

So how do we compute the determinants? Starting with the identity matrix ($\det(\boldsymbol{A})$=1), exchanging two rows negates the determinant to -1, exchanging again puts it back to 1 and so on. See that there are six ways to permute the rows of the 3 by 3 identity, each with determinants alternating between 1 and -1:

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

$$\det = +1 \qquad -1 \qquad +1 \qquad -1 \qquad +1 \qquad -1$$

Multiplying a row by a constant multiplies the determinant by that constant. So supposing the three rows are a, b, c and p, q, r and x, y, z,

$$\begin{bmatrix} a & & \\ & q & \\ & & z \end{bmatrix} \begin{bmatrix} & b & \\ p & & \\ & & z \end{bmatrix} \begin{bmatrix} & b & \\ & & r \\ x & & \end{bmatrix} \begin{bmatrix} & & c \\ & q & \\ x & & \end{bmatrix} \begin{bmatrix} & & c \\ p & & \\ & y & \end{bmatrix} \begin{bmatrix} a & & \\ & & r \\ & y & \end{bmatrix}$$

$$\det = +aqz \qquad -bpz \qquad +brx \qquad -cqx \qquad +cpy \qquad -ary$$

Summing up all the individual determinants gives the final desired determinant. See that the 'checkerboard' pattern of negating the determinant in the laplace expansion just comes from row exchanges.

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Link to recursive computation

Consider the 4 by 4 determinant

$$\det \begin{bmatrix} A & 0 & 0 & 0 \\ 0 & a & b & c \\ 0 & p & q & r \\ 0 & x & y & z \end{bmatrix}$$

and see that by linearity, this just evaluates to

$$A \det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & a & b & c \\ 0 & p & q & r \\ 0 & x & y & z \end{bmatrix} = A \left(\det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & a & 0 & 0 \\ 0 & 0 & q & 0 \\ 0 & 0 & 0 & z \end{bmatrix} + \det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & p & 0 & 0 \\ 0 & 0 & 0 & z \end{bmatrix} + \right.$$

$$\left. \det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & r \\ 0 & x & 0 & 0 \end{bmatrix} + \det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c \\ 0 & 0 & q & 0 \\ 0 & x & 0 & 0 \end{bmatrix} + \cdots \right)$$

$$= A \det \begin{bmatrix} a & b & c \\ p & q & r \\ x & y & z \end{bmatrix}$$

and so from a general 4 by 4 matrix, (now using different alphabets for the entries so don't confuse this with the earlier notation)

$$\det \begin{bmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} = \det \begin{bmatrix} a & 0 & 0 & 0 \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} + \det \begin{bmatrix} 0 & b & 0 & 0 \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix}$$

$$+ \det \begin{bmatrix} 0 & 0 & c & 0 \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} + \det \begin{bmatrix} 0 & 0 & 0 & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix}$$

considering the first right hand side matrix, see that by linearity

$$\det \begin{bmatrix} a & 0 & 0 & 0 \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} = \det \underbrace{\begin{bmatrix} a & 0 & 0 & 0 \\ e & 0 & 0 & 0 \\ i & j & k & l \\ m & n & o & p \end{bmatrix}}_{=0} + \det \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix}$$

where the first matrix on the right hand side is clearly noninvertible and therefore has determinant 0.

(next page)

Cont.
Continuing

$$\det \begin{bmatrix} a & 0 & 0 & 0 \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} = \det \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix}$$

$$= \det \underbrace{\begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ i & 0 & 0 & 0 \\ m & n & o & p \end{bmatrix}}_{=0} + \det \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ 0 & j & k & l \\ m & n & o & p \end{bmatrix}$$

$$= \det \underbrace{\begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ 0 & j & k & l \\ m & 0 & 0 & 0 \end{bmatrix}}_{=0} + \det \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ 0 & j & k & l \\ 0 & n & o & p \end{bmatrix}$$

and using our previous idea,

$$\det \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & f & g & h \\ 0 & j & k & l \\ 0 & n & o & p \end{bmatrix} = a \det \begin{bmatrix} f & g & h \\ j & k & l \\ n & o & p \end{bmatrix}$$

deriving the formula for the laplace expansion from here is fairly straightforward. It is just a matter of applying this reasoning to the other matrices while taking into account the negation caused by required row exchanges. We eventually get

$$\det \begin{bmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{bmatrix} = a \det \begin{bmatrix} f & g & h \\ j & k & l \\ n & o & p \end{bmatrix} - b \det \begin{bmatrix} e & g & h \\ i & k & l \\ m & o & p \end{bmatrix} +$$

$$c \det \begin{bmatrix} e & f & h \\ i & j & l \\ m & n & p \end{bmatrix} - d \det \begin{bmatrix} e & f & g \\ i & j & k \\ m & n & o \end{bmatrix}$$

which is the usual 'formula' used when computing matrices by hand.

5.3 Cofactors, Adjugate, and Inverse

The laplace expansion allows us to reduce a n by n determinant to a sum of scaled $(n-1)$ by $(n-1)$ determinants. The *cofactors* in a laplace transform are essentially these smaller determinants, but with alternanting negation to account for row exchanges:

For the i, j cofactor C_{ij}, **remove row i and column j from the matrix** A.

C_{ij} equals $(-1)^{i+j}$ times the determinant of the remaining matrix (size $n-1$).

The cofactor formula along row i is $\det A = a_{i1}C_{i1} + \cdots + a_{in}C_{in}$

So given a 3 by 3 matrix A

$$A = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

Taking the cofactor for every entry in the matrix, we can construct a cofactor matrix C as

$$C = \begin{bmatrix} \det \begin{bmatrix} e & f \\ h & i \end{bmatrix} & -\det \begin{bmatrix} d & f \\ g & i \end{bmatrix} & \det \begin{bmatrix} d & e \\ g & h \end{bmatrix} \\ -\det \begin{bmatrix} b & c \\ h & i \end{bmatrix} & \det \begin{bmatrix} a & c \\ g & i \end{bmatrix} & -\det \begin{bmatrix} a & b \\ g & h \end{bmatrix} \\ \det \begin{bmatrix} b & c \\ e & f \end{bmatrix} & -\det \begin{bmatrix} a & c \\ d & f \end{bmatrix} & \det \begin{bmatrix} a & b \\ d & e \end{bmatrix} \end{bmatrix}$$

We define C^T as the *adjugate matrix*:

$$C^T = \begin{bmatrix} \det \begin{bmatrix} e & f \\ h & i \end{bmatrix} & -\det \begin{bmatrix} b & c \\ h & i \end{bmatrix} & \det \begin{bmatrix} b & c \\ e & f \end{bmatrix} \\ -\det \begin{bmatrix} d & f \\ g & i \end{bmatrix} & \det \begin{bmatrix} a & c \\ g & i \end{bmatrix} & -\det \begin{bmatrix} a & c \\ d & f \end{bmatrix} \\ \det \begin{bmatrix} d & e \\ g & h \end{bmatrix} & -\det \begin{bmatrix} a & b \\ g & h \end{bmatrix} & \det \begin{bmatrix} a & b \\ d & e \end{bmatrix} \end{bmatrix}$$

(next page)

Cont.

We had

$$\boldsymbol{A} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix}$$

and

$$\boldsymbol{C}^T = \begin{bmatrix} \det\begin{bmatrix} e & f \\ h & i \end{bmatrix} & -\det\begin{bmatrix} b & c \\ h & i \end{bmatrix} & \det\begin{bmatrix} b & c \\ e & f \end{bmatrix} \\ -\det\begin{bmatrix} d & f \\ g & i \end{bmatrix} & \det\begin{bmatrix} a & c \\ g & i \end{bmatrix} & -\det\begin{bmatrix} a & c \\ d & f \end{bmatrix} \\ \det\begin{bmatrix} d & e \\ g & h \end{bmatrix} & -\det\begin{bmatrix} a & b \\ g & h \end{bmatrix} & \det\begin{bmatrix} a & b \\ d & e \end{bmatrix} \end{bmatrix}$$

Now consider the expression $\boldsymbol{AC}^T$. See that computing the *diagonal* of the result is the same as taking the laplace expansion along each row of $\boldsymbol{A}$:

$$\boldsymbol{AC}^T = \begin{bmatrix} \det(\boldsymbol{A}) & \cdots & \cdots \\ \cdots & \det(\boldsymbol{A}) & \cdots \\ \cdots & \cdots & \det(\boldsymbol{A}) \end{bmatrix}$$

This expression has a unique property—every entry on the off diagonal is 0. This is because computing those entries would be equivalent to the *laplace expansion for the determinant of a matrix with two linearly dependent or identical rows.* For instance consider the $(1, 2)$ of $\boldsymbol{AC}^T$:

$$(\boldsymbol{AC}^T)_{1,2} = -a\det\begin{bmatrix} b & c \\ h & i \end{bmatrix} + b\det\begin{bmatrix} a & c \\ g & i \end{bmatrix} - c\det\begin{bmatrix} a & b \\ g & h \end{bmatrix}$$

See that this is the same as taking the determinant of

$$\begin{bmatrix} -a & -b & -c \\ a & b & c \\ g & h & i \end{bmatrix}$$

Which is zero because two rows are linearly dependent. This property can be seen in any of the off-diagonal entries. Our final result is

$$\boldsymbol{AC}^T = \begin{bmatrix} \det(\boldsymbol{A}) & 0 & 0 \\ 0 & \det(\boldsymbol{A}) & 0 \\ 0 & 0 & \det(\boldsymbol{A}) \end{bmatrix}$$

This pattern can be extrapolated to higher order matrices. We have the formula

$$\boldsymbol{AC}^T = (\det(\boldsymbol{A}))\boldsymbol{I}$$

This gives us a nice formula for the inverse matrix $\boldsymbol{A}^{-1}$:

$$\boldsymbol{A}^{-1} = \frac{1}{\det(\boldsymbol{A})}\boldsymbol{C}^T$$

See that, as expected, the determinant of an invertible matrix cannot be zero.

5.4 Cramer's Rule to solve $Ax = b$

Cramer's rule allows us to procedurally find the components x_i, of the solution vector in $Ax = b$. The idea here is to construct a matrix starting with I; by replacing the first column of I by x, *this triangular matrix M_1 has a determinant equal to x_1*:

$$\det \begin{bmatrix} x_1 & 0 & 0 \\ x_2 & 1 & 0 \\ x_3 & 0 & 1 \end{bmatrix} = x_1$$

(consider eliminating downward using row operations then taking the product down the diagonal). By multiplying by A, *the first column of the result becomes Ax which is b*; the other columns are copied from A. We denote this final matrix by B_1:

Key idea

$AM_1 = B_1$

$$\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} \begin{bmatrix} x_1 & 0 & 0 \\ x_2 & 1 & 0 \\ x_3 & 0 & 1 \end{bmatrix} = \begin{bmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{bmatrix} = B_1.$$

See that if we had the determinants of B_1 and A, we can obtain x_1:

Product rule $\boxed{(\det A)(x_1) = \det B_1 \quad \text{or} \quad x_1 = \det B_1/\det A.}$

This allowed us to obtain the first component of x. To obtain the other components we apply the same principle again; to find x_2 and B_2, we replace the *second column* of I with x:

Same idea

$AM_2 = B_2$

$$\begin{bmatrix} a_1 & a_2 & a_3 \end{bmatrix} \begin{bmatrix} 1 & x_1 & 0 \\ 0 & x_2 & 0 \\ 0 & x_3 & 1 \end{bmatrix} = \begin{bmatrix} a_1 & b & a_3 \end{bmatrix} = B_2.$$

and take determinants to get

$$(\det A)(x_2) = \det B_2 \implies x_2 = \frac{\det B_2}{\det A}$$

CRAMER's RULE If det A is not zero, $Ax = b$ is solved by determinants:

$$x_1 = \frac{\det B_1}{\det A} \qquad x_2 = \frac{\det B_2}{\det A} \qquad \dots \qquad x_n = \frac{\det B_n}{\det A}$$

The matrix B_j has the jth column of A replaced by the vector b.

To solve an n by n system, Cramer's rule evaluates $n + 1$ determinants (of A and n different B_i). Computing each determinant would involve $n!$ terms (row permutations of n by n I)—totalling $(n + 1)!$ terms. This is a very inefficient method for solving equations (although it does give an explicit formula).

5.4.1 Inverse formula from Cramer's rule

Consider using Cramer's rule to solve for A^{-1}. For the 2 by 2 case, A^{-1} has two columns; denoting them by x and y, we solve

$$AA^{-1} = A \begin{bmatrix} x & y \end{bmatrix} = I$$

solving each column at a time,

$$Ax = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad Ay = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Given $|A|$ and the other required determinants

$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} 1 & b \\ 0 & d \end{vmatrix} \quad \begin{vmatrix} a & 1 \\ c & 0 \end{vmatrix} \quad \begin{vmatrix} 0 & b \\ 1 & d \end{vmatrix} \quad \begin{vmatrix} a & 0 \\ c & 1 \end{vmatrix}$$

with that we compute the components as

$$x_1 = \frac{d}{|A|}, \; x_2 = \frac{-c}{|A|}, \; y_1 = \frac{-b}{|A|}, \; y_2 = \frac{a}{|A|} \; \text{and} \; A^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

When using Cramer's rule to solve $AA^{-1} = I$, *the determinant of each B_j is a cofactor of A*. Consider the 3 by 3 case; we want the inverse of

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

solving for the first *column* of A^{-1} requires the determinants

Determinants of B's are Cofactors of A
$$\begin{vmatrix} 1 & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & a_{32} & a_{33} \end{vmatrix} \quad \begin{vmatrix} a_{11} & 1 & a_{13} \\ a_{21} & 0 & a_{23} \\ a_{31} & 0 & a_{33} \end{vmatrix} \quad \begin{vmatrix} a_{11} & a_{12} & 1 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & 0 \end{vmatrix}$$

see that these determinants are the same as those on the first *row* of the cofactor matrix (transposing and eliminating downward using row operations, then transposing back gives the exact cofactor). As such we have

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FORMULA FOR A^{-1} $\qquad (A^{-1})_{ij} = \dfrac{C_{ji}}{\det A} \qquad A^{-1} = \dfrac{C^T}{\det A}$

Which leaves us with the inverse matrix formula as derived earlier.

5.5   Sign of a permutation and determinants

Notation
We introduce the concept of a sign/signature of a permutation of a set of natural numbers. Consider a set of the first n natural numbers

$$1, 2, \ldots, n$$

We will denote a permuation by

$$\pi(1), \ldots, \pi(n)$$

where $\pi(1)$ is the first element of the permutation, $\pi(2)$ is the second, and so on. For instance, a possible permutation of the first 4 natural numbers is 2,1,4,3; its elements can be denoted as

$$\pi(1) = 2, \quad \pi(2) = 1, \quad \pi(3) = 4, \quad \pi(4) = 3$$

Inversions
Two elements of a permutation $\pi(i)$ and $\pi(j)$ is said to be an inversion if and only if

$$i < j \quad \text{but} \quad \pi(i) > \pi(j)$$

in other words, two elements are an inversion if their natural order is inverted. For instance, the permutation 4,1,3,2 has the inversions

$$(4, 1), \quad (4, 3), \quad (4, 2), \quad (3, 2)$$

Parity of a permutation
A permutation is said to be *even* if and only if the total number of inversions it contains is even. Otherwise it is said to be *odd*.

In the previous example, the permutation 4,1,3,2 has 4 inversions. As such it is *even*.

Definition of sign
The sign of a permutation π, denoted by $\mathrm{sgn}(\pi)$ is a function defined as follows:

$$\mathrm{sgn}(\pi) = \begin{cases} 1 & \text{if } \pi \text{ is even} \\ -1 & \text{if } \pi \text{ is odd} \end{cases}$$

For instance, the permutation $\pi = \langle 4, 1, 3, 2 \rangle$ was even. Therefore $\mathrm{sgn}(\pi) = 1$. (next page)

Transpositions
The operation of *interchanging any two distinct elements of a permutation* is called a *transposition*.

For instance, considering the following permutation of the first five natural numbers:
$$4, 3, 2, 1, 5$$

The operation of interchanging its second and fourth element so as to obtain the new permuation
$$4, 1, 2, 3, 5$$

is a transposition. Note the effect of transpositions on parity:

- If a permuation is odd, a transposition makes it even.

- If a permutation is even, a transposition makes it odd.

Intuitively, a transposition either adds or removes an inversion. Either way it makes an odd number of inversions even or an even number of inversions odd.

Definition of determinant
Let $\boldsymbol{A}$ be a K x K matrix. Let P be the set of all possible permutations of the first K natural numbers.

The determinant of $\boldsymbol{A}$, denoted by $\det(\boldsymbol{A})$ or $|\boldsymbol{A}|$, is

$$\det = \sum_{\pi \in P} \text{sgn}(\pi) \prod_{k=1}^{K} A_{k,\pi(k)}$$

See how this formally describes the intuitive idea of the determinant as a discussed before. The product

$$\prod_{k=1}^{K} A_{k,\pi(k)}$$

is over K entries of $\boldsymbol{A}$. For each row $k = 1, \ldots, K$, we choose the entry located in column $\pi(k)$; there is exactly one chosen entry $A_{k,\pi(k)}$ in each column and row. The sign handles the negation (the row exchanges), and we sum over the set P of all possible permuations π.

5.6 Determinants of block-triangular matrices and matrices with identity blocks

A block matrix is of the form

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

where

- A and B have the same number of rows;

- C and D have the same number of rows;

- A and C have the same number of columns;

- B and D have the same number of columns.

An important fact about block matrices is that their multiplication can be carried out as per standard matrix multiplication

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}\begin{bmatrix} E & F \\ G & H \end{bmatrix} = \begin{bmatrix} AE+BG & AF+BH \\ CE+DG & CF+DH \end{bmatrix}$$

With the only caveat being that the shape of the blocks must be conformable (for instance the columns of A and the rows of E must coincide.

Determinant of block-diagonal matrix with identity blocks The first result concerns block matrices of the form

$$\boldsymbol{\Gamma} = \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix} \quad \text{or} \quad \boldsymbol{\Gamma} = \begin{bmatrix} I & 0 \\ 0 & A \end{bmatrix}$$

Where I denotes the identity and A a square matrix. Block matrices whose off-diagonal blocks are all zero are called block-diagonal.

We can show that, given one of the above forms,

$$\det(\boldsymbol{\Gamma}) = \det(\boldsymbol{A})$$

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Cont.

We can show that,

$$\det\left(\begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix}\right) = \det(A) = \det\left(\begin{bmatrix} I & 0 \\ 0 & A \end{bmatrix}\right)$$

First consider the case where

$$\Gamma = \begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix}$$

Suppose A is KxK and I is 1x1. Then Γ is $(K+1)$x$(K+1)$. We use the definition of the determinant:

$$\det(\Gamma) = \sum_{\pi \in P} \mathrm{sgn}(\pi) \prod_{k=1}^{K+1} \Gamma_{k,\pi(k)}$$

$$= \sum_{\pi \in P} \mathrm{sgn}(\pi) \Gamma_{K,\pi(K+1)} \prod_{k=1}^{K} \Gamma_{k,\pi(k)}$$

where P is the set of all permutations of the first $K+1$ natural numbers. See that the term $\Gamma_{K,\pi(K+1)}$ is only equal to 1 when $\pi(K+1) = K+1$ (since that row is zero everywhere except on the $(K+1)$th entry).

Also notice that the sign of the permutations would then only depend on $\pi(1), \ldots, \pi(K)$ (because $\pi(K+1) = K+1$ does not determine any inversion). As such we have

$$\det(\Gamma) = \sum_{\pi \in Q} \mathrm{sgn}(\pi) \prod_{k=1}^{K} \Gamma_{k,\pi(k)}$$

$$= \sum_{\pi \in Q} \mathrm{sgn}(\pi) \prod_{k=1}^{K} A_{k,\pi(k)}$$

$$= \det(A)$$

where Q is the set of permutations of the first K natural numbers.
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Cont.

The result for the case in which I is not 1x1 is proved recursively. For instance if I is 2x2, we have

$$\det\left(\begin{bmatrix} A & 0 \\ 0 & I \end{bmatrix}\right)$$

$$= \det\left(\begin{bmatrix} \begin{bmatrix} A & 0 \\ 0 & 1 \end{bmatrix} & 0 \\ 0 & 1 \end{bmatrix}\right)$$

$$= \det\left(\begin{bmatrix} A & 0 \\ 0 & 1 \end{bmatrix}\right) = \det(A)$$

and analagously for larger dimensions. The proof for the other case:

$$\Gamma = \begin{bmatrix} I & 0 \\ 0 & A \end{bmatrix}$$

Is similar to the one just proved.

Block-upper-triangular matrix

An block-upper-triangular matrix is of the form

$$\Gamma = \begin{bmatrix} A & B \\ 0 & D \end{bmatrix}$$

We can show that

$$\det(\Gamma) = \det(A)\det(D)$$

Suppose that A is KxK, D is LxL, B is KxL and 0 is LxK. Using subscripts to denote shape, we can factor the matrix as

$$\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix}\begin{bmatrix} I_K & B \\ 0_{LK} & I_L \end{bmatrix}\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}$$

$$= \begin{bmatrix} I_K I_K + 0_{KL}0_{LK} & I_K B + 0_{KL}I_L \\ 0_{LK}I_K + D0_{LK} & 0_{LK}B + DI_L \end{bmatrix}\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}$$

$$= \begin{bmatrix} I_K & B \\ 0_{LK} & D \end{bmatrix}\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}$$

$$= \begin{bmatrix} I_K A + B0_{LK} & I_K 0_{KL} + BI_L \\ 0_{LK}A + D0_{LK} & 0_{LK}0_{KL} + DI_L \end{bmatrix}$$

$$= \begin{bmatrix} A & B \\ 0 & D \end{bmatrix}$$

Cont.
Thus,

$$
\det(\Gamma)
$$

$$
= \det\left(\begin{bmatrix} A & B \\ 0 & D \end{bmatrix}\right)
$$

$$
= \det\left(\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix}\begin{bmatrix} I_K & B \\ 0_{LK} & I_L \end{bmatrix}\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}\right)
$$

$$
= \det\left(\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix}\right)\det\left(\begin{bmatrix} I_K & B \\ 0_{LK} & I_L \end{bmatrix}\right)\det\left(\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}\right)
$$

$$
= \det(D)\det\left(\begin{bmatrix} I_K & B \\ 0_{LK} & I_L \end{bmatrix}\right)\det(A)
$$

$$
= \det(A)\det(D)
$$

In the last step we have

$$
\det\left(\begin{bmatrix} I_K & B \\ 0_{LK} & I_L \end{bmatrix}\right) = 1
$$

(the determinant is just the product of pivots since we can eliminate upward without changing the determinant) The other two determinants come from the earlier derived determinants of matrices with identity blocks.

Block-lower-triangular matrix
A block-lower-triangular matrix is of the form

$$
\Gamma = \begin{bmatrix} A & 0 \\ C & D \end{bmatrix}
$$

Again we can show that

$$
\det(\boldsymbol{\Gamma}) = \det(\boldsymbol{A})\det(\boldsymbol{D})
$$

Cont.

Suppose that A is KxK, D is LxL, C is LxK and 0 is KxL. Using subscripts to denote shape, we can factor the matrix as

$$
\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}
\begin{bmatrix} I_K & 0_{KL} \\ C & I_L \end{bmatrix}
\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix}
$$

$$
= \begin{bmatrix} AI_K + 0_{KL}C & A0_{KL} + 0_{KL}I_L \\ 0_{LK}I_K + I_LC & 0_{LK}0_{KL} + I_LI_L \end{bmatrix}
\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix}
$$

$$
= \begin{bmatrix} A & 0_{KL} \\ C & I_L \end{bmatrix}
\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix}
$$

$$
= \begin{bmatrix} AI_K + 0_{KL}0_{LK} & A0_{KL} + 0_{KL}D \\ CI_K + I_L0_{KL} & C0_{KL} + I_LD \end{bmatrix}
$$

$$
= \begin{bmatrix} A & 0 \\ C & D \end{bmatrix}
$$

Then, similar to the previous proof,

$$\det(\Gamma)$$

$$
= \det\left(\begin{bmatrix} A & 0 \\ C & D \end{bmatrix} \right)
$$

$$
= \det\left(\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix}
\begin{bmatrix} I_K & 0_{KL} \\ C & I_L \end{bmatrix}
\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix} \right)
$$

$$
= \det\left(\begin{bmatrix} A & 0_{KL} \\ 0_{LK} & I_L \end{bmatrix} \right)
\det\left(\begin{bmatrix} I_K & 0_{KL} \\ C & I_L \end{bmatrix} \right)
\det\left(\begin{bmatrix} I_K & 0_{KL} \\ 0_{LK} & D \end{bmatrix} \right)
$$

$$
= \det(A)\det(I_L)\det(I_K)\det(D)
$$

$$
= \det(A)\det(D)
$$

Chapter 6

Eigenvalues and Eigenvectors

6.1 Computation

x is an eigenvector if
$$Ax = \lambda x$$

We have
$$Ax - \lambda Ix = 0$$
$$(Ax - \lambda I)x = 0$$

The matrix $(A - \lambda I)$ times the eigenvector x is the zero vector. *the eigenvectors make up the nullspace of $A - \lambda I$.*

First we find the eigenvalues. If $(A - \lambda I)x = 0$ has a nonzero solution, then $(A - \lambda I)$ is *not invertible*—the determinant of $(A - \lambda I)$ must be zero. This gives us a means to find the eigenvalues:

Eigenvalues   The number λ is an eigenvalue of A if and only if $A - \lambda I$ is singular.

     Equation for the n eigenvalues of A $\boxed{\det(A - \lambda I) = 0.}$ (5)

An n by n $(A - \lambda I)$ has $A_{ii} - \lambda$ down the main diagonal. This means that the *characterstic polynomial* $\det(A - \lambda I)$ has a degree of n—the determinant, after expansion into a polynomial, has n solutions λ_1 to λ_n—and A has n eigenvalues:

    An n by n matrix has n eigenvalues (repeated λ's are possible !) Each λ leads to x :

    For each eigenvalue λ solve $(A - \lambda I)x = 0$ or $Ax = \lambda x$ to find an eigenvector x.

(next page)

Cont.

After obtaining the eigenvalues, we can find the eigenvectors by substituting the eigenvalues back into

$$(\boldsymbol{A} - \lambda \boldsymbol{I})\boldsymbol{x} = \boldsymbol{0}$$

and solve for $\boldsymbol{x}$.

Invertibility

Consider again the intial equation

$$\boldsymbol{Ax} = \lambda \boldsymbol{x}$$

If $\boldsymbol{A}$ were singular, it has a nontrivial nullspace and 0 is an eigenvalue, with the eigenvectors for $\lambda = 0$ filling the nullspace.

If $\boldsymbol{A}$ were invertible, zero cannot be an eigenvalue. (the nullspace is just the zero vector, so any eigenvector cannot have a zero eigenvalue)

Summary To solve the eigenvalue problem for an n by n matrix, follow these steps:

1. ***Compute the determinant of*** $A - \lambda I$. With λ subtracted along the diagonal, this determinant starts with λ^n or $-\lambda^n$. It is a polynomial in λ of degree n.

2. ***Find the roots of this polynomial***, by solving $\det(A - \lambda I) = 0$. The n roots are the n eigenvalues of A. They make $A - \lambda I$ singular.

3. For each eigenvalue λ, ***solve*** $(A - \lambda I)\boldsymbol{x} = 0$ ***to find an eigenvector*** $\boldsymbol{x}$.

6.2 Eigenvalues, Determinant, and Trace

Note that if we perform row operations on $\boldsymbol{A}$, the eigenvalues usually change. However, the determinant and trace of a matrix still harbour useful properties.

The determinant of $\boldsymbol{A}$ is the product of its eigenvalues
We can show that
$$\det(\boldsymbol{A}) = \lambda_1\lambda_2\cdots\lambda_n$$

Supposing that $\lambda_1,\ldots,\lambda_n$ are the eigenvalues of $\boldsymbol{A}$, then the λ are also the roots of the characteristic polynomial:

$$
\begin{aligned}
\det(\boldsymbol{A} - \lambda\boldsymbol{I}) = p(\lambda) &= (-1)^n(\lambda - \lambda_1)(\lambda - \lambda_2)\cdots(\lambda - \lambda_n) \\
&= (-1)(\lambda - \lambda_1)(-1)(\lambda - \lambda_2)\cdots(-1)(\lambda - \lambda_n) \\
&= (\lambda_1 - \lambda)(\lambda_2 - \lambda)\cdots(\lambda_n - \lambda)
\end{aligned}
$$

The leading coefficient $(-1)^n$ can be obtained by considering the contribution of the main diagonal to the determinant (the main diagonal is the only permutation that contributes to the coefficient of λ^n). Setting λ to zero gives us our desired result.

The trace of $\boldsymbol{A}$ is the sum of its eigenvalues
Look again at the characteristic polynomial. See that it can be rewritten as

$$p(\lambda) = (-1)^n(\lambda^n - (\lambda_1 + \cdots + \lambda_n)\lambda^{n-1} + \cdots)$$

Looking at the determinant of interest $\det(\boldsymbol{A} - \lambda\boldsymbol{I})$, see that, in a similar manner to the previous part, the main diagonal is the only permutation that contributes to the λ^{n-1} coefficient in the result. Consider the laplace expansion along a row i, we see that any term involving an off diagonal element $[\boldsymbol{A} - \lambda\boldsymbol{I}]_{ij}$ eliminates $a_{ii} - \lambda$ and $a_{jj} - \lambda$ from the main diagonal (also see that any permutation with an off diagonal entry (most of them) would have to be missing at least two elements on the main diagonal).

Therefore the coefficient for λ^{n-1} comes solely from the main diagonal:

$$(a_{11} - \lambda)(a_{22} - \lambda)\cdots(a_{nn} - \lambda) = \cdots + (-1)^{n-1}(a_{11} + \cdots + a_{nn})\lambda^{n-1} + \cdots$$

Comparing coefficients with our characteristic polynomial we get the result

$$a_{11} + \cdots + a_{nn} = \operatorname{tr}(\boldsymbol{A}) = \lambda_1 + \cdots + \lambda_n$$

In short

> *The product $(\lambda_1)\cdots(\lambda_n)$ of the n eigenvalues equals the determinant of A*
> *$\lambda_1 + \lambda_2 + \cdots + \lambda_n$ equals the sum of the n diagonal entries $=$ (trace of A)*

6.3 Commuting matrices share eigenvectors

Say we have two matrices that commute:

$$AB = BA$$

Starting from $Ax = \lambda x$, we have

$$ABx = BAx = B\lambda x = \lambda Bx$$

So x and Bx are both eigenvectors of A with the same eigenvalue.

If we make a further assumption that the eigenvalues of A are distinct—the eigenspaces of A are one dimensional—then Bx must also be a multiple of x, making x also an eigenvector of B.

6.4 AB and BA have the same eigenvalues

If v is an eigenvector of AB with some nonzero eigenvalue λ, then $Bv \neq 0$ and

$$\lambda Bv = B(ABv) = (BA)Bv$$

so Bv is an eigenvector for BA with the same eigenvalue.

For the case of a zero eigenvalue, if 0 is an eigenvalue of AB, then the matrix is noninvertible and

$$0 = \det(AB) = \det(A)\det(B) = \det(BA)$$

so 0 will also be an eigenvalue of BA.

6.5   Diagonalisation

Suppose the n by n matrix $\boldsymbol{A}$ has $\boldsymbol{n}$ linearly independent eigenvectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$. Placing those $\boldsymbol{x}_i$ into the columns of an invertible *eigenvector matrix* $\boldsymbol{X}$, then $\boldsymbol{X}^{-1}\boldsymbol{A}\boldsymbol{X}$ is the diagonal *eigenvalue matrix* $\boldsymbol{\Lambda}$:

Eigenvector matrix X
Eigenvalue matrix Λ

$$X^{-1}AX = \Lambda = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}.$$

To understand this, see that $\boldsymbol{A}\boldsymbol{X} = \boldsymbol{X}\boldsymbol{\Lambda}$:

A times X

$$AX = A \begin{bmatrix} \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_n \end{bmatrix} = \begin{bmatrix} \lambda_1\boldsymbol{x}_1 & \cdots & \lambda_n\boldsymbol{x}_n \end{bmatrix}.$$

X times Λ

$$\begin{bmatrix} \lambda_1\boldsymbol{x}_1 & \cdots & \lambda_n\boldsymbol{x}_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_n \end{bmatrix}\begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} = X\Lambda.$$

Assuming that n by n $\boldsymbol{X}$ consists of n linearly independent eigenvectors, it then has an inverse, and so

$$\boxed{AX = X\Lambda \quad \text{is} \quad X^{-1}AX = \Lambda \quad \text{or} \quad A = X\Lambda X^{-1}.}$$

One benefit of diagonalisation is that it becomes easy to compute matrix powers, $\boldsymbol{A}^k$:

$$A^k = (X\Lambda X^{-1})(X\Lambda X^{-1})\ldots(X\Lambda X^{-1}) = X\Lambda^k X^{-1}.$$

(next page)

Diagonalisability

We have a condition that guarantees diagonalisability: *Eigenvectors for n different λ's are independent*—if the eigenvectors are distinct then we can diagonalise $\boldsymbol{A}$:

> **Independent $\boldsymbol{x}$ from different λ** Eigenvectors that correspond to distinct (all different) eigenvalues are linearly independent. An n by n matrix that has n different eigenvalues (**no repeated λ's**) must be diagonalizable.

Proof: Suppose $c_1\boldsymbol{x}_1 + c_2\boldsymbol{x}_2 = \boldsymbol{0}$ (suppose two eigenvectors with different eigenvalues are dependent) Multiply the entire expression by $\boldsymbol{A}$:

$$\boldsymbol{A}(c_1\boldsymbol{x}_1 + c_2\boldsymbol{x}_2) = c_1\lambda_1\boldsymbol{x}_1 + c_2\lambda_2\boldsymbol{x}_2 = \boldsymbol{0}$$

now consider the first expression multiplied by λ_2

$$\lambda_2(c_1\boldsymbol{x}_1 + c_2\boldsymbol{x}_2) = c_1\lambda_2\boldsymbol{x}_1 + c_2\lambda_2\boldsymbol{x}_2 = \boldsymbol{0}$$

subtracting the two expressions gives us

$$c_1\lambda_1\boldsymbol{x}_1 - c_1\lambda_2\boldsymbol{x}_1 = (\lambda_1 - \lambda_2)c_1\boldsymbol{x}_1 = \boldsymbol{0}$$

Since $\lambda_1 \neq \lambda_2$ and $\boldsymbol{x}_1 \neq \boldsymbol{0}$, we must have $c_1 = 0$. See that we can repeat the same process but multiply by λ_1 instead to show that we must also have $c_2 = 0$. Only the combination with $c_1 = c_2 = 0$ gives $c_1\boldsymbol{x}_1 + c_2\boldsymbol{x}_2 = \boldsymbol{0}$—the eigenvectors $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ must be independent.

Generalising to n eigenvectors: Suppose that

$$c_1\boldsymbol{x}_1 + \cdots + c_n\boldsymbol{x}_n = \boldsymbol{0}$$

First multiply by $\boldsymbol{A}$:

$$c_1\lambda_1\boldsymbol{x}_1 + \cdots + c_n\lambda_n\boldsymbol{x}_n = \boldsymbol{0}$$

then multiply that same first expression by λ_n:

$$c_1\lambda_n\boldsymbol{x}_1 + \cdots + c_n\lambda_n\boldsymbol{x}_n = \boldsymbol{0}$$

and subtract the two expressions to get

$$(\lambda_1 - \lambda_n)c_1\boldsymbol{x}_1 + \cdots + c_n(\lambda_n - \lambda_n)\boldsymbol{x}_n$$
$$=(\lambda_1 - \lambda_n)c_1\boldsymbol{x}_1 + \cdots + c_{n-1}(\lambda_{n-1} - \lambda_n)\boldsymbol{x}_{n-1} = \boldsymbol{0}$$

Now take the result and multiply by $\boldsymbol{A}$ again. Subtract that same expression, but now multiplied by λ_{n-1}:

$$(\lambda_1 - \lambda_n)(\lambda_1 - \lambda_{n-1})c_1\boldsymbol{x}_1 + \cdots + c_{n-1}(\lambda_{n-1} - \lambda_n)(\lambda_{n-1} - \lambda_{n-1})\boldsymbol{x}_{n-1} = \boldsymbol{0}$$

repeating this process, we eventually end up with

$$(\lambda_1 - \lambda_n)(\lambda_1 - \lambda_{n-1})\cdots(\lambda_1 - \lambda_2)c_1\boldsymbol{x}_1 = \boldsymbol{0}$$

Cont.
We have
$$(\lambda_1 - \lambda_n)(\lambda_1 - \lambda_{n-1})\cdots(\lambda_1 - \lambda_2)c_1\boldsymbol{x}_1 = \boldsymbol{0}$$

Forcing $c_1 = 0$. We can repeat this same process to show that every $c_i = 0$; when the λ are different, $c_1\boldsymbol{x}_1 + \ldots + c_n\boldsymbol{x}_n = \boldsymbol{0}$ only when $c_i = 0$, the eigenvectors are independent.

Repeated eigenvalues don't imply non-diagonalisability
Distinct eigenvalues guarantee diagonalisability, however this does not mean that repeated eigenvalues implies non-diagonalisability—if all the eigenvalues of a matrix are distinct, then the matrix is automatically diagonalisable, but there are plenty of cases where a matrix is diagonalisable, but has repeated eigenvalues.

6.6

Appendix A

Misc. topics

A.1 Taylor series, Difference approximations

Taylor series
Recall the idea of the taylor series, where $f(x)$ near some point $x = x_0$ can be approximated as

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \cdots$$

See that this comes from approximating $f(x)$ as a polynomial

$$y(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + a_3(x - x_0)^3 + \cdots$$

where we have $a_0 = y(x_0)$; now consider differentiating:

$$y'(x) = a_1 + 2a_2(x - x_0) + 3a_3(x - x_0)^2 + \cdots$$
$$y''(x) = 2a_2 + (3)(2)a_3(x - x_0) + (4)(3)a_4(x - x_0)^2 \cdots$$
$$y^{(n)}(x) = n!\, a_n + ((n + 1) \cdot (n - 1) \cdots 3 \cdot 2)a_{n+1}(x - x_0) + \cdots$$

so we have
$$a_1 = y'(x_0), \quad a_2 = \frac{y''(x_0)}{2!}, \ \cdots, a_n = \frac{y^{(n)}(x_0)}{n!}$$

where substituting into our initial approximation gives us

$$y(x) \approx y(x_0) + y'(x_0)(x - x_0) + \frac{y''(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{y^{(n)}(x_0)}{n!}(x - x_0)^n + \cdots$$

(next page)

Cont.
We had

$$y(x) \approx y(x_0) + y'(x_0)(x - x_0) + \frac{y''(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{y^{(n)}(x_0)}{n!}(x - x_0)^n + \cdots$$

substituting $x - x_0 = h$ gives us

$$y(x_0 + h) \approx y(x_0) + y'(x_0)(h) + \frac{y''(x_0)}{2!}(h)^2 + \cdots + \frac{y^{(n)}(x_0)}{n!}(h)^n + \cdots$$

Which can be rewritten as

$$y(x + h) \approx y(x) + hy'(x) + \frac{1}{2!}h^2 y''(x) + \cdots + \frac{1}{n!}h^n y^{(n)}(x) + \cdots$$

Difference formulas
Considering the first few terms of the taylor series approximation, we have

$$y(x + h) - y(x) \approx hy'(x) + \frac{1}{2}h^2 y''(x)$$

$$y(x - h) - y(x) \approx -hy'(x) + \frac{1}{2}h^2 y''(x)$$

This allows us to have an approximation to dy/dx:

$$\boxed{\textbf{Centered difference} \qquad \frac{\boldsymbol{y(x + h) - y(x - h)}}{\boldsymbol{2h}} \approx \frac{\boldsymbol{dy}}{\boldsymbol{dx}}}$$

and also to the second derivative

$$\boxed{\textbf{Second difference} \qquad \frac{\boldsymbol{y(x + h) - 2y(x) + y(x - h)}}{\boldsymbol{h^2}} \approx \frac{\boldsymbol{d^2 y}}{\boldsymbol{dx^2}}}$$

The individual formulas also yield approximations:

$$\boxed{\begin{array}{lll} \textbf{Forward difference} & \dfrac{\boldsymbol{dy}}{\boldsymbol{dx}} = \dfrac{\boldsymbol{y(x + h) - y(x)}}{\boldsymbol{h}} + \boldsymbol{O(h)} \text{ error} \\[3mm] \textbf{Backward difference} & \dfrac{\boldsymbol{dy}}{\boldsymbol{dx}} = \dfrac{\boldsymbol{y(x) - y(x - h)}}{\boldsymbol{h}} + \boldsymbol{O(h)} \text{ error} \end{array}}$$