LECTURE 1

Determinants

Next year, you will study molecular orbital theory: an area of chemistry which relies on solving simultaneous linear equations. You'll have seen these at school, for the case of two unknowns, x and y:

$$ax + by = c$$
$$dx + ey = f.$$

The general case of n equations with n unknowns can be solved using *determinants*. We'll see how this happens in the next lecture: today, we'll focus on introducing the idea of a determinant and its properties.

Notice the word 'can' rather than 'should'. We'll see later that there are more efficient methods than by using determinants. However, it is pedagogically useful to introduce the determinant method first.

Definition of a determinant

A determinant is a *number*, calculated from an $n \times n$ 'grid' of numbers using a rule. The rule is called the *cofactor expansion* (or 'Laplace expansion') of the determinant.

The cofactor expansion goes as follows:

1. A 1×1 determinant is just the number itself.
2. An $n \times n$ determinant can be written in terms of $(n-1)\times(n-1)$ determinants by the following procedure:
   (a) Pick any row or any column.
   (b) Write down the numbers along that row or down that column.
   (c) Multiply each number by the $(n-1) \times (n-1)$ determinant obtained by 'crossing out' the row and column that the number lies in.
   (d) Multiply each term by either $+1$ or -1, according to the checkerboard rule:

$$\begin{matrix} + & - & + & \cdots \\ - & + & - & \cdots \\ + & - & + & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{matrix}$$

   (e) Add the terms and then use cofactor expansion on the smaller determinants you have generated above.

We denote the determinant by vertical lines either side of the grid of numbers.

For those who have studied matrices already: *note that a determinant is* **not** *a matrix!* We will come to matrices in due course.

Example 1. Evaluate the determinant

$$D = \begin{vmatrix} 1 & 2 \\ 3 & 4 \end{vmatrix}$$

We have a 2×2 determinant, so we cannot apply step 1 yet. So, following step 2(a), let's pick the first row. We write down its numbers:

$$1 \qquad\qquad\qquad 2$$

Then, following step 2(b), we obtain 1×1 determinants by crossing out rows and columns of D. For the '1' term, we cross out row 1 and column 1:

$$\begin{vmatrix} \cancel{1} & \cancel{2} \\ \cancel{3} & 4 \end{vmatrix} \qquad \to \qquad \begin{vmatrix} 4 \end{vmatrix}$$

For the '2' term we cross out row 1 and column 2:

$$\begin{vmatrix} \cancel{1} & \cancel{2} \\ 3 & \cancel{4} \end{vmatrix} \qquad \to \qquad \begin{vmatrix} 3 \end{vmatrix}$$

Then, continuing with step 2(b), we multiply the numbers 1 and 2 by these determinants to get

$$1 \times \begin{vmatrix} 4 \end{vmatrix} \qquad\qquad\qquad 2 \times \begin{vmatrix} 3 \end{vmatrix}$$

Now we proceed to step 2(c). We'll draw a checkerboard (always with a '+' in the top-left corner) next to the original determinant D:

$$\begin{vmatrix} 1 & 2 \\ 3 & 4 \end{vmatrix} \qquad \begin{matrix} + & - \\ - & + \end{matrix}$$

This tells us that the '1' term should be multiplied by $+1$, and the '2' term should be multiplied by -1:

$$1 \times (+1) \times \begin{vmatrix} 4 \end{vmatrix} \qquad\qquad\qquad 2 \times (-1) \times \begin{vmatrix} 3 \end{vmatrix}$$

Then we use step 2(d) to say that

$$\begin{aligned} D &= 1 \times (+1) \times \begin{vmatrix} 4 \end{vmatrix} \qquad + \qquad 2 \times (-1) \times \begin{vmatrix} 3 \end{vmatrix} \\ &= 1 \times \begin{vmatrix} 4 \end{vmatrix} - 2 \times \begin{vmatrix} 3 \end{vmatrix}, \end{aligned}$$

and we're then told to apply the cofactor expansion method again. Fortunately, we now have 1×1 determinants, which step 1 tells us can be replaced by the number inside, so

$$\begin{aligned} D &= 1 \times 4 - 2 \times 3 \\ &= -2. \end{aligned}$$

In practice, most people will just remember that a 2×2 determinant will evaluate as

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

instead of working through the cofactor expansion. But for 3×3 determinants and higher, it would be very difficult to remember the general result.

Example 2. Evaluate $D = \begin{vmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{vmatrix}$

We'll use cofactor expansion along the first row (and will do it quicker this time). The numbers in the first row are 1, 0, and -1. The corresponding 2×2 determinants are, respectively:

$$\begin{vmatrix} \cancel{1} & \cancel{0} & \cancel{-1} \\ \cancel{0} & 1 & 0 \\ \cancel{-1} & 0 & 1 \end{vmatrix} \quad \rightarrow \quad \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}$$

$$\begin{vmatrix} \cancel{1} & \cancel{0} & \cancel{-1} \\ 0 & \cancel{1} & 0 \\ -1 & \cancel{0} & 1 \end{vmatrix} \quad \rightarrow \quad \begin{vmatrix} 0 & 0 \\ -1 & 1 \end{vmatrix}$$

$$\begin{vmatrix} \cancel{1} & \cancel{0} & \cancel{-1} \\ 0 & 1 & \cancel{0} \\ -1 & 0 & \cancel{1} \end{vmatrix} \quad \rightarrow \quad \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}$$

These smaller determinants are called the *minors* of the elements whose rows and columns were crossed out.

The sign factors for expanding along the top row are $+$, $-$, $+$ according to the checkerboard rule. So putting this all together,

$$D = 1 \times (+1) \times \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} + 0 \times (-1) \times \begin{vmatrix} 0 & 0 \\ -1 & 1 \end{vmatrix} + (-1) \times (+1) \times \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}$$

$$= \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} - \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}$$

The product of the sign factor and corresponding minor is called the *cofactor* of the element from which they were obtained.

So we can summarise the cofactor expansion as: pick a row/column, then sum the products of each element and its cofactor.

Then we can use cofactor expansion again, or just remember the formula for a 2×2 determinant, to get

$$D = [1 \times 1 - 0 \times 0] - [0 \times 0 - 1 \times (-1)] = 0$$

The 'magic' of the cofactor expansion

You may have noticed that step 2(a) of the cofactor expansion says 'pick *any* row or column'. This is because **the cofactor expansion gives the same result, whichever row or column you expand along!**.

I'm afraid I won't even attempt to show you the proof of this remarkable result, as it is quite tricky. But let's check that it holds for the example above.

If you want to read about this yourself, I'd suggest viewing the cofactor expansion as a *result* that can be derived from an alternative definition (Leibniz's formula, which involves permutations). It is then easier to show that all cofactor expansions are equal.

Example 3. Evaluate $D = \begin{vmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{vmatrix}$ by expanding down column 2.

The numbers in column 2 are 0, 1, 0. If we're awake, we'll realise that the terms in the cofactor expansion involving the zeros will not contribute to the final answer, because they will contain factors of 0. So we only need to worry about the middle term. Its minor is

$$\begin{vmatrix} 1 & \cancel{0} & -1 \\ \cancel{0} & \cancel{1} & \cancel{0} \\ -1 & \cancel{0} & 1 \end{vmatrix} \qquad \to \qquad \begin{vmatrix} 1 & -1 \\ -1 & 1 \end{vmatrix}$$

Now we need the checkerboard:

$$\begin{vmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{vmatrix} \qquad \qquad \begin{matrix} + & - & + \\ - & + & - \\ + & - & + \end{matrix}$$

Clearly the middle term, when expanding down column 2, picks up a factor of $(+1)$. So

$$\begin{aligned} D &= 1 \times (+1) \times \begin{vmatrix} 1 & -1 \\ -1 & 1 \end{vmatrix} \\ &= 1 \times 1 - (-1) \times (-1) \\ &= 0, \text{ as before.} \end{aligned}$$

Notice that it is much quicker to do the cofactor expansion along a row or column that contains lots of zeros!

The cofactor expansion leads to several important rules of determinants. I won't prove them rigorously, but I'll try to justify where each comes from.

Transposing rows and columns

Determinants are unchanged by *transposing* rows and columns. For a 3×3 determinant, this means that

$$\begin{vmatrix} r & u & x \\ s & v & y \\ t & w & z \end{vmatrix} = \begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} \qquad \text{'transpose' property} \qquad (1.1)$$

More generally, this property holds for any sized determinant.

The justification is as follows. For a 1×1 determinant, it is obviously true because the determinant contains only one number. And it is easy to prove for a 2×2:

$$\begin{vmatrix} w & y \\ x & z \end{vmatrix} = wz - yx = wz - xy = \begin{vmatrix} w & x \\ y & z \end{vmatrix}.$$

For the 3×3 above, we can justify the result by expanding the LHS of (1.1) down the first column:

$$\begin{vmatrix} r & u & x \\ s & v & y \\ t & w & z \end{vmatrix} = r\begin{vmatrix} v & y \\ w & z \end{vmatrix} - s\begin{vmatrix} u & x \\ w & z \end{vmatrix} + t\begin{vmatrix} u & x \\ v & y \end{vmatrix};$$

and the RHS along the first row:

$$\begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} = r\begin{vmatrix} v & w \\ y & z \end{vmatrix} - s\begin{vmatrix} u & w \\ x & z \end{vmatrix} + t\begin{vmatrix} u & v \\ x & y \end{vmatrix}$$

The right-hand sides of the two preceding equations are the same, because we have already shown that a 2×2 determinant is unaffected by transposing rows and columns.

By extending this approach, a little thought should convince you that any $n\times n$ determinant is unchanged by transposing rows and columns.

Crucially, it means that any property we prove below for the rows of a determinant will also hold for columns, because transposing rows to columns does not change the determinant.

Multilinear property

Consider the determinant

$$\begin{vmatrix} au+bv & w \\ ax+by & z \end{vmatrix}$$

Expanding down the first column, we get

$$\begin{vmatrix} au+bv & w \\ ax+by & z \end{vmatrix} = (au+bv)\times(+1)\times\begin{vmatrix} z \end{vmatrix} + (ax+by)\times(-1)\times\begin{vmatrix} w \end{vmatrix}$$

We can collect up the a and b terms of the RHS separately:

$$\begin{vmatrix} au+bv & w \\ ax+by & z \end{vmatrix} = a\left\{u\times(+1)\times\begin{vmatrix} z \end{vmatrix} + x\times(-1)\times\begin{vmatrix} w \end{vmatrix}\right\} + b\left\{v\times(+1)\times\begin{vmatrix} z \end{vmatrix} + y\times(-1)\times\begin{vmatrix} w \end{vmatrix}\right\}$$

Then, each of the terms in curly brackets can be rewritten as a determinant, to get

$$\begin{vmatrix} au+bv & w \\ ax+by & z \end{vmatrix} = a\begin{vmatrix} u & w \\ x & z \end{vmatrix} + b\begin{vmatrix} v & w \\ y & z \end{vmatrix}. \qquad \text{multilinear property} \tag{1.2}$$

With a little thought, it can be seen that this generalizes to any $n\times n$ determinant. And, by the magic of the cofactor expansion, it works along any row or any column.

There are three special cases that are worth pointing out. First, a and b can obviously be 1:

$$\begin{vmatrix} u+v & w \\ x+y & z \end{vmatrix} = \begin{vmatrix} u & w \\ x & z \end{vmatrix} + \begin{vmatrix} v & w \\ y & z \end{vmatrix}. \tag{1.3}$$

Notice that this says we can add two determinants if they differ *only* in one row or one column. Generally, we **cannot** add two determinants elementwise!

The second special case is if $b = 0$, which gives

$$\begin{vmatrix} au & w \\ ax & z \end{vmatrix} = a \begin{vmatrix} u & w \\ x & z \end{vmatrix} \qquad \text{'common factor' property} \tag{1.4}$$

A common factor can be taken out of any row or column.

The third special case is $a = b = 0$. Then we have

$$\begin{vmatrix} 0 & w \\ 0 & z \end{vmatrix} = 0 \qquad \text{'zero row/column' property} \tag{1.5}$$

A determinant with a full row or column of zeros is identically zero.

Determinants with two equal rows or columns are zero

A 2×2 determinant is obviously zero if its rows or columns are the same:

$$\begin{vmatrix} u & v \\ u & v \end{vmatrix} = uv - vu = 0.$$

Let's now consider this 3×3 determinant, expanding it along the top row.

$$\begin{vmatrix} u & v & w \\ x & y & z \\ x & y & z \end{vmatrix} = u \begin{vmatrix} y & z \\ y & z \end{vmatrix} - v \begin{vmatrix} x & z \\ x & z \end{vmatrix} + w \begin{vmatrix} x & y \\ x & y \end{vmatrix}.$$

Each of the 2×2 determinants is zero, so

$$\begin{vmatrix} u & v & w \\ x & y & z \\ x & y & z \end{vmatrix} = 0.$$

A moment's thought will convince you that this argument can be generalized to any $n \times n$ determinant. If two rows are the same, do successive cofactor expansions along all the other rows until you're left with 2×2 determinants made up from the original identical rows. Those will all be zero. Hence we have a general rule:

$$\begin{vmatrix} u & v & w \\ x & y & z \\ x & y & z \end{vmatrix} = 0. \qquad \text{'equal rows/columns' property.} \qquad (1.6)$$

Any determinant with two equal rows or columns is zero.

There are some immediate consequences that follow, by combining this result with the multilinear property. Consider the following determinant, which is zero because the first two columns are equal.

$$0 = \begin{vmatrix} r+s & r+s & t \\ u+v & u+v & w \\ x+y & x+y & z \end{vmatrix}$$

Using the multilinear property,

$$\begin{aligned} 0 &= \begin{vmatrix} r+s & r+s & t \\ u+v & u+v & w \\ x+y & x+y & z \end{vmatrix} \\ &= \begin{vmatrix} r & r+s & t \\ u & u+v & w \\ x & x+y & z \end{vmatrix} + \begin{vmatrix} s & r+s & t \\ v & u+v & w \\ y & x+y & z \end{vmatrix} \\ &= \begin{vmatrix} r & r & t \\ u & u & w \\ x & x & z \end{vmatrix} + \begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} + \begin{vmatrix} s & r & t \\ v & u & w \\ y & x & z \end{vmatrix} + \begin{vmatrix} s & s & t \\ v & v & w \\ y & y & z \end{vmatrix} \end{aligned}$$

The first and fourth terms are both zero, because they each have two identical columns. Hence

$$0 = \begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} + \begin{vmatrix} s & r & t \\ v & u & w \\ y & x & z \end{vmatrix}$$

which rearranges to

$$\begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} = - \begin{vmatrix} s & r & t \\ v & u & w \\ y & x & z \end{vmatrix} \qquad \text{'swapping rows or columns' property} \qquad (1.7)$$

A determinant changes sign if two of its rows, or two of its columns, are swapped. (This rule is very important for quantum mechanics.)

A further corollary of the 'equal columns' property follows in a couple of lines. Use the multilinear property on the following:

$$\begin{vmatrix} r+as & s & t \\ u+av & v & w \\ x+ay & y & z \end{vmatrix} = \begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} + a \begin{vmatrix} s & s & t \\ v & v & w \\ y & y & z \end{vmatrix}$$

The second determinant on the RHS is zero because it has two identical columns. So, turning the equation around, we have

$$\begin{vmatrix} r & s & t \\ u & v & w \\ x & y & z \end{vmatrix} = \begin{vmatrix} r+as & s & t \\ u+av & v & w \\ x+ay & y & z \end{vmatrix} \quad \text{`add a multiple of a row/column' property} \tag{1.8}$$

Obviously a can be -1, i.e. subtracting one row/column from another does not change a determinant.

In words, a determinant is unchanged by adding a constant multiple of any row to another row (or column to another column).

Finally, perhaps the *most important* thing to remember about determinants follows by a similar argument. Consider the following and use the multilinear property:

$$\begin{vmatrix} as+bt & s & t \\ av+bw & v & w \\ ay+bz & y & z \end{vmatrix} = a\begin{vmatrix} s & s & t \\ v & v & w \\ y & y & z \end{vmatrix} + b\begin{vmatrix} t & s & t \\ w & v & w \\ z & y & z \end{vmatrix}.$$

Both determinants on the RHS have two equal columns, so they are zero. Hence

$$\begin{vmatrix} as+bt & s & t \\ av+bw & v & w \\ ay+bz & y & z \end{vmatrix} = 0 \qquad \text{`linear dependence' property.} \tag{1.9}$$

Again, it is easy to see how this argument can be generalised to the $n \times n$ case. All it requires is that one column is a *linear combination* of the other columns.

In words: *a determinant is zero if its columns are* **linearly dependent**.

Hence, by transposing, a determinant is zero if its *rows* are linearly dependent.

Taken together, these implications show that linear dependence of rows implies linear dependence of columns, and vice versa.

Moreover, the implications work the other way round. *If* a determinant is zero, its columns are linearly dependent *and* its rows are linearly dependent. This is easiest to justify using a geometrical argument, when we relate determinants to vectors in a lecture or two's time.

Example 4. Using the properties shown above, factorise $D = \begin{vmatrix} x & x^2 & yz \\ y & y^2 & zx \\ z & z^2 & xy \end{vmatrix}$.

The first (and only) rule of answering such questions is: **do not use cofactor expansion until you have a row/column with only one non-zero element**. Otherwise it will be very difficult to factorise afterwards!

To start, we subtract row 1 from row 2, and then from row 3, using (1.8).

$$D = \begin{vmatrix} x & x^2 & yz \\ y-x & y^2-x^2 & zx-yz \\ z & z^2 & xy \end{vmatrix} = \begin{vmatrix} x & x^2 & yz \\ y-x & y^2-x^2 & zx-yz \\ z-x & z^2-x^2 & xy-yz \end{vmatrix}.$$

Then, notice that row 2 has a common factor of $(y-x)$, and row 3 has a common factor of $(z-x)$. We take these out, to get

$$D = (y-x)(z-x)\begin{vmatrix} x & x^2 & yz \\ 1 & y+x & -z \\ 1 & z+x & -y \end{vmatrix}.$$

I spot that subtracting x lots of column 1 from column 2 will simplify it further

$$D = (y-x)(z-x)\begin{vmatrix} x & 0 & yz \\ 1 & y & -z \\ 1 & z & -y \end{vmatrix},$$

and then I subtract row 3 from row 2 to get

$$D = (y-x)(z-x)\begin{vmatrix} x & 0 & yz \\ 0 & y-z & y-z \\ 1 & z & -y \end{vmatrix}.$$

This has another common factor to take out of the middle row:

$$D = (y-x)(z-x)(y-z)\begin{vmatrix} x & 0 & yz \\ 0 & 1 & 1 \\ 1 & z & -y \end{vmatrix}$$

Another zero can be generated in row 2 by subtracting column 2 from column 3:

$$D = (y-x)(z-x)(y-z)\begin{vmatrix} x & 0 & yz \\ 0 & 1 & 0 \\ 1 & z & -y-z \end{vmatrix}.$$

Then we can expand along row 2, to end up with

$$\begin{aligned} D &= (y-x)(z-x)(y-z)(-xy-yz-zx) \\ &= (x-y)(y-z)(z-x)(xy+yz+zx). \end{aligned}$$

Example 5. Using the properties of determinants, solve

$$\begin{vmatrix} x & 1 & 0 & 1 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 1 & 0 & 1 & x \end{vmatrix} = 0.$$

This is important for chemistry: it gives the energies of the π molecular orbitals of cyclobutadiene within so-called 'Hückel theory'. You'll study this next year.

There is a useful trick here. Notice that all the rows contain the same four elements, just in different orders. So, if we add column 2 (C2) to C1, then add C3 to C1, then add C4 to C1, we get the same thing all the way down column 1.

$$\begin{vmatrix} x+2 & 1 & 0 & 1 \\ x+2 & x & 1 & 0 \\ x+2 & 1 & x & 1 \\ x+2 & 0 & 1 & x \end{vmatrix} = 0.$$

So there is a factor of $(x + 2)$ that can be taken out of column 1, to get

$$(x+2)\begin{vmatrix} 1 & 1 & 0 & 1 \\ 1 & x & 1 & 0 \\ 1 & 1 & x & 1 \\ 1 & 0 & 1 & x \end{vmatrix} = 0.$$

Now, notice that we can create a lot of zeros in column 1 by subtracting R1 from R2, then from R3, and then from R4:

$$(x+2)\begin{vmatrix} 1 & 1 & 0 & 1 \\ 0 & x-1 & 1 & -1 \\ 0 & 0 & x & 0 \\ 0 & -1 & 1 & x-1 \end{vmatrix} = 0.$$

We can then expand down column 1 to get

$$(x+2)\begin{vmatrix} x-1 & 1 & -1 \\ 0 & x & 0 \\ -1 & 1 & x-1 \end{vmatrix} = 0,$$

and then expand across row 2 to get

$$x(x+2)\begin{vmatrix} x-1 & -1 \\ -1 & x-1 \end{vmatrix} = 0.$$

Expanding this 2×2 determinant leads to

$$x(x+2)\left[(x-1)^2 - 1\right] = 0,$$

which simplifies to

$$x^2(x+2)(x-2) = 0.$$

Hence, $x = 2$, $x = 0$ (repeated root), or $x = -2$.