Colouring the Cube

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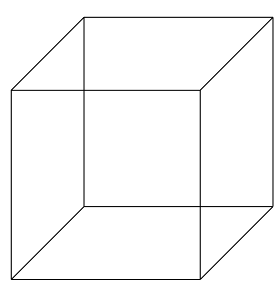
1 Cubes

The n-cube Q_n is the graph whose vertex set consists of all the 2^n binary n-tuples, and where two vertices are adjacent if the corresponding n-tuples differ in exactly one coordinate position.

The graphs Q_3 and Q_4 are sometimes known as the *cube* and the *hypercube* respectively, and some authors call the entire sequence of graphs *hypercubes*.

There are a number of other descriptions of these graphs, with the vertices being variously described as binary numbers from 0 to $2^n - 1$ or vectors in $GF(2)^n$ or subsets of an n-set or the elements of the elementary abelian group Z_2^n, to mention a few.

Here is a nice picture of the 3-cube:



2 Automorphisms

We can easily identify a number of automorphisms of the cube Q_n. Any permutation of the coordinate positions does not alter the number of positions in which two n-tuples differ, and so there are $n!$ automorphisms of this type.

Example 1 *The permutation* $(1, 2, 3) \in \mathrm{Sym}(3)$ *acts as follows on the vertices of* Q_3

Vertex	$\rightarrow$	*Vertex*
000		000
001		100
010		001
011		101
100		010
101		110
110		011
111		111

These $n!$ automorphisms all fix the vertices 0^n and 1^n. In addition to this, the mapping ρ_i ($i = 1, \ldots, n$) which interchanges $0 \leftrightarrow 1$ in the i'th coordinate position of every n-tuple is also an automorphism. These automorphisms clearly do not have any fixed points, and are independent of each other, so between them they generate 2^n different automorphisms.

It is not too difficult to prove that there are no automorphisms other than those arising as combinations of these two types.

Theorem 1 *The automorphism group of the n-cube has order*

$$2^n \cdot n!$$

and each automorphism is the combination of a permutation of the coordinates together with the interchange of 0s and 1s in some coordinate positions.

The symmetric group Sym(n) is generated by the two permutations

$$a = (1, 2) \qquad b = (1, 2, \ldots, n)$$

and so the automorphism group of the cube can be generated by $n + 2$ permutations.

Question 1 *Write a GAP function* `cubeGroup(n)` *that returns the automorphism group of the n-cube as a permutation group on the set $\{1, \ldots, 2^n\}$.*

This will require numbering the vertices of the n-cube as $\{1, 2, \ldots, 2^n\}$ and then computing how each of the $n+2$ automorphisms described above permutes the vertices. The "natural" numbering of the vertices of the n-cube is obtained by just taking each n-tuple to be the binary representation of an integer, but this results in a numbering using $\{0, 1, \ldots, 2^n - 1\}$. However it is easy to add and subtract 1 and so the most logical numbering system is to have the number i represent the n-tuple that is the binary representation of $i - 1$.

Thus for Q_3 we have

i	3-tuple
1	000
2	001
3	010
4	011
5	100
6	101
7	110
8	111

Now let σ be one of the automorphisms of the n-cube described above. Then for each $i \in \{1, \ldots, 2^n\}$ we we can calculate the image $i\sigma$ by performing the following steps:

- Find the vertex (as an n-tuple) by calculating the binary representation of $i - 1$.
- Apply σ to the n-tuple; this may involve permuting the coordinates or exchanging 0s with 1s.
- Convert the mapped n-tuple back from binary and add 1.

Then given a list

$$[1\sigma, 2\sigma, \ldots, 2^n\sigma]$$

of the images of every point, use GAP's `PermList` to transform from image notation to GAP's normal permutation notation.

Repeat this for all $n+2$ automorphisms that generate $\mathrm{Aut}(Q_n)$ and return the group generated by this collection of permutations.

Check that `cubeGroup(3)` returns

```
Group([ (3,5)(4,6), (2,5,3)(4,6,7), (1,5)(2,6)(3,7)(4,8),
  (1,3)(2,4)(5,7)(6,8), (1,2)(3,4)(5,6)(7,8) ])
```

and that the group has order 48.

3 Cycle Index

Question 2 *Write a GAP function* `cycleIndex(G)` *to calculate the cycle index of any (smallish) group.*

Start by using GAP's `ConjugacyClasses` function to calculate the conjugacy classes of G.

Then for each class, determine its cycle structure — GAP has a function called `CycleStructurePerm` but you must read the documentation *carefully* because it returns its data in an odd way. Given the cycle structure, it is easy to calculate the contribution that the conjugacy class makes to the cycle index.

For example, the permutation

$$(1, 2, 3)(4, 5)(6, 7)$$

has 1 cycle of length 3 and 2 cycles of length 2. Therefore its contribution to the cycle index of a group is

$$X_3^1 X_2^2.$$

You will need to use GAP's somewhat clunky mechanism for manipulating the indeterminates, using `Indeterminate(Rationals,1)`, `Indeterminate(Rationals,2)` and so on for X_1, X_2.

Each element in the conjugacy class makes the same contribution, and so it is best to calculate the term associated with the conjugacy class representative and then multiply it by the number of group elements in that conjugacy class. Look up and use `Representative` and `Size` for this purpose.

Make sure that `cycleIndex(cubeGroup(3))` returns the value:

```
1/6*x_2*x_6+1/4*x_4^2+1/6*x_1^2*x_3^2+13/48*x_2^4+1/8*x_1^4*x_2^2+1/48*x_1^8
```

GAP uses `x_1`, `x_2` and so on for `Indeterminate(Rationals,1)`, `Indeterminate(Rationals,2)` etc, but be warned that this is only a cosmetic touch to make the output readable, and you cannot actually *use* `x_1` yourself to refer to this indeterminate.

4 Vertex colourings

By the one-variable version of Pólya's enumeration theorem, the number of inequivalent ways to colour the vertices of the cube with k colours is given by

$$Z_{\mathrm{Aut}(Q_n)}(k, k, \ldots, k).$$

If we specialize to $k = 2$, then this gives us the number of inequivalent 2-colourings of the cube, or the number of *boolean functions* on n variables.

In order to calculate this number in GAP, use the function `Value` which takes three arguments — a polynomial, a list of indeterminates and a list of values. It substitutes the values for the indeterminates and returns the result (which may be a polynomial with fewer indeterminates or a completely evaluated value). If we had used `zg3` for the cycle index of $\mathrm{Aut}(Q_3)$ then the GAP code might be something like

```
gap>  Value(zg3,[Indeterminate(Rationals,1), Indeterminate(Rationals,2),
> Indeterminate(Rationals,3), Indeterminate(Rationals,4),
> Indeterminate(Rationals,6)], [2,2,2,2,2]);
22
gap>
```

If we repeat this for the next few cubes, we discover that the number of inequivalent boolean functions grows rapidly,

n	Equivalence classes
2	6
3	22
4	402
5	1228158
6	400507806843728

This sequence is `A000616` in the OEIS.

Yet another interpretation of a subset of an n-cube is that it consists of the points of a 0/1-*polytope* in n-dimensional space. There are many interesting problems about these polytopes, with one of the major researchers in the area being Günter Ziegler of TU Berlin.

4.1 The special substitution $1 + x$

The multivariate version of Pólya's Enumeration Theorem shows that we can count the number of equivalence classes of a given "weight" by subsituting the appropriate values into the cycle index. For example, when 2-colouring the cube, we could set the weights to be b (for black) and w (for white) and then substitute

$$\begin{array}{ccc} X_1 & \leftarrow & b+w \\ X_2 & \leftarrow & b^2+w^2 \\ \vdots & \vdots & \vdots \\ X_i & \leftarrow & b^i+w^i \\ \vdots & \vdots & \vdots \end{array}$$

in order to count the number of 2-colourings with given numbers of black vertices and white vertices.

However when we are viewing a 2-colouring as representing a *subset* of the vertices of the cube, it is more natural to consider the 2 colours as representing "in" and "out" and we are usually only interested in counting the number of vertices that are "in".

We can achieve this by using the special weight set $\{1, x\}$ where 1 represents "out" and x represents "in". Then by substituting

$$\begin{array}{ccc} X_1 & \leftarrow & 1+x \\ X_2 & \leftarrow & 1+x^2 \\ \vdots & \vdots & \vdots \\ X_i & \leftarrow & 1+x^i \\ \vdots & \vdots & \vdots \end{array}$$

into the cycle index, we get a polynomial in x where the coefficient of x^i is the number of equivalence classes of i-element subsets.

If we do this for $Z_{\mathrm{Aut}(Q_3)}$ then the resulting polynomial is

$$1 + x + 3x^2 + 3x^3 + 6x^4 + 3x^5 + 3x^6 + x^7 + x^8.$$

This tells us, among other things, that there are 3 inequivalent ways of selecting a subset of size 2 from the vertices of the 3-cube and 6 inequivalent ways of selecting a subset of size 4.

If we let $b(n, k)$ be the number of equivalence classes of k-subsets of the n-cube, then these numbers can be arranged in a triangle:

$$\begin{array}{ccccccccc} & & & b(0,0) & b(0,1) & & & & \\ & & & b(1,0) & b(1,1) & b(1,2) & & & \\ & & b(2,0) & b(2,1) & b(2,2) & b(2,3) & b(2,4) & & \\ b(3,0) & b(3,1) & b(3,2) & b(3,3) & b(3,4) & b(3,5) & b(3,6) & b(3,7) & b(3,8) \end{array}$$

(Notice that the 0-cube is a single vertex!)

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5 Edge colourings

Now let's consider colouring the *edges* of the n-cube, and counting the equivalence classes of colourings using PET. Again we will consider two colourings to be equivalent if there is some automorphism of the cube that maps one to the other.

This means that we need to determine how the automorphisms of the cube permute the *set of edges* of the cube. Now each edge of the cube is determined by its two endvertices and so it follows that for $g \in \mathrm{Aut}(Q_n)$ and $\{u, v\} \in E(Q_n)$, we have

$$\{u, v\}g = \{ug, vg\}.$$

It would be relatively straightforward to determine directly how each of the $n + 2$ automorphisms that generate $\mathrm{Aut}(Q_n)$ act on the set of edges, but it is even easier to use GAP's functions for this task.

First we need a list of all the edges of the cube, and as $\mathrm{Aut}(Q_n)$ is *transitive* on the set of edges, we can get GAP to compute this for us using the function `Orbit`.

```
gap> G := cubeGroup(3);
Group([ (3,5)(4,6), (2,5,3)(4,6,7), (1,5)(2,6)(3,7)(4,8),
  (1,3)(2,4)(5,7)(6,8), (1,2)(3,4)(5,6)(7,8) ])
gap> edges := Orbit(G,[1,2],OnSets);
[ [ 1, 2 ], [ 1, 5 ], [ 5, 6 ], [ 3, 4 ], [ 1, 3 ], [ 3, 7 ], [ 2, 6 ],
  [ 7, 8 ], [ 5, 7 ], [ 2, 4 ], [ 4, 8 ], [ 6, 8 ] ]
```

This command computes the orbit of the edge $\{1, 2\}$ (that is, the edge joining 000 to 001) under the action of the group g. Notice that we need to tell the `Orbit` function that we want to view $[1, 2]$ as an *unordered set* of 2 vertices by specifying that the action should be "on sets" (`OnSets`). The reason for this is that when we are talking about edges, we want to view `[1,2]` as being the same as `[2,1]`.

Now we can ask GAP to tell us how g permutes these 12 edges — this is called the *action of g on edges.*

```
gap> G_on_edges := Action(G,edges,OnSets);
Group([ (2,5)(3,4)(6,9)(7,10)(11,12), (1,2,5)(3,6,10)(4,7,9)(8,11,12),
  (1,3)(4,8)(5,9)(10,12), (1,4)(2,6)(3,8)(7,11), (2,7)(5,10)(6,11)(9,12) ])
gap>
```

This command is asking GAP to tell us how G permutes the elements of the list `edges`. Again we have to specify that we want it to treat these elements as unordered 2-sets. The response is a permutation group of degree 12 — GAP has given the 12 edges numbers from 1 to 12 and has calculated how each element of g permutes these 12 elements, giving us exactly the group that we want.

We can check that this is doing what we want by working through in detail the situation for the first generator of `G`, namely

$$(3, 5)(4, 6)$$

This permutes the edges of Q_3 as follows:

Number	Edge	Edge Image	Number
1	[1, 2]	[1, 2]	1
2	[1, 5]	[1, 3]	5
3	[5, 6]	[3, 4]	4
4	[3, 4]	[5, 6]	3
5	[1, 3]	[1, 5]	2
6	[3, 7]	[5, 7]	9
7	[2, 6]	[2, 4]	10
8	[7, 8]	[7, 8]	8
9	[5, 7]	[3, 7]	6
10	[2, 4]	[2, 6]	7
11	[4, 8]	[6, 8]	12
12	[6, 8]	[4, 8]	11

Therefore as a permutation on edges, this permutation is

$$(2, 5)(3, 4)(6, 9)(7, 10)(11, 12)$$

which is indeed the first generator of `G_on_edges`.

Now, we can calculate the cycle index of this group, and hence use PET to answer questions about edge colourings of the n-cubes.