Chemicals and Necklaces

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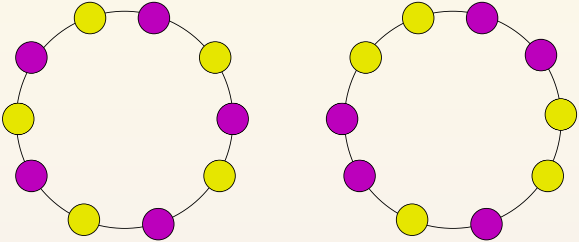


Inequivalent Colourings

Often we would like to know how many *different* colourings of objects exist.

Necklaces

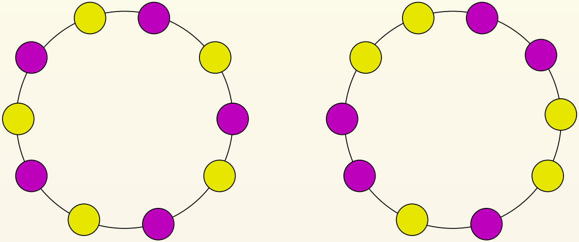
Consider a necklace with n beads.

Question: In how many ways can we colour the beads in two colours and obtain essentially different colourings?

Different colourings

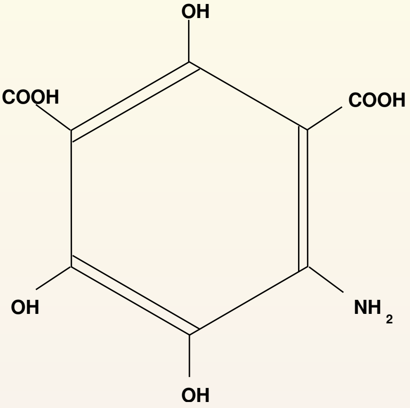
Two colourings are *inequivalent* if one cannot be obtained from the other by rotations or reflections.

Two inequivalent Colourings



Chemical Formulas

How many different chemicals exist with a benzene molecule in the centre and two radicals OH and 4 radicals COOH attached to the carbon atoms?



Symmetry Group

The symmetries of a necklace with n beads are the elements of D_{2n}.

Different Colourings

Consider an object (e.g. n-gon) with a known symmetry group G.

Definition:
Two colourings of an object are *equivalent* if there is an element $g \in G$ which maps one to the other.

Abstracting again

We now describe the object we consider by a set Ω of points.

For example, a necklace with n beads can be represented by $\Omega = \{1, \ldots, n\}$.

A graph with n vertices can also be represented by $\Omega = \{1, \ldots, n\}$.

Notation

From now on suppose G is a permutation group on $\Omega = \{1, \ldots, n\}$.

Fixed Points

For $g \in G$ we define

$$\mathrm{Fix}_\Omega(g) := \{a \in \Omega \mid a^g = a\}.$$

Thus $\mathrm{Fix}_\Omega(g)$ consists of all points not moved by g.

Orbit-Counting Lemma

Theorem [Frobenius (1887)]
The number of orbits of G on Ω is

$$\frac{1}{|G|}\sum_{g\in G}|\mathrm{Fix}_{\Omega}(g)|.$$

Remarks

The Orbit-Counting Lemma is often known as Burnside's Lemma, even though Burnside was not the first to prove this lemma.

We present the proof as it shows how many theorems in Combinatorics are proved by counting the same thing in two different ways.

Proof

see e.g. J. Gallian, Contemporary Abstract Algebra

Count Pairs: (a, g) with $a^g = a$ in two different ways. Let N denote their number

Method I: Given g

$|\mathrm{Fix}_\Omega(g)|$ elements $a \in \Omega$ such that $a^g = a$. So

$$N = \sum_{g \in G} |\mathrm{Fix}_\Omega(g)|.$$

Proof

see e.g. J. Gallian, Contemporary Abstract Algebra

Count Pairs: (a, g) with $a^g = a$ in two different ways. Let N denote their number

Method II: Given a

$|\mathrm{Stab}_G(a)|$ elements $g \in G$ such that $a^g = a$. So

$$N = \sum_{a \in \Omega} |\mathrm{Stab}_G(a)|.$$

Proof

see e.g. J. Gallian, Contemporary Abstract Algebra

Count Pairs: (a, g) with $a^g = a$ in two different ways. Let N denote their number

Rewrite Stbilisers:

Suppose G has r orbits on Ω:

$$\mathrm{orb}_G(b_1), \ldots, \mathrm{orb}_G(b_r)$$

For all $a \in \mathrm{orb}_G(b_i)$ we have

$$|\mathrm{Stab}_G(a)| = |\mathrm{Stab}_G(b_i)|.$$

Proof

see e.g. J. Gallian, Contemporary Abstract Algebra
Count Pairs: (a, g) with $a^g = a$ in two different ways. Let N denote their number

Rewrite Stbilisers:
Hence

$$
\begin{aligned}
N &= \sum_{i=1}^{r} |\mathrm{orb}_G(b_i)||\mathrm{Stab}_G(b_i)| \\
&= \sum_{i=1}^{r} |G| = r|G|.
\end{aligned}
$$

Proof

see e.g. J. Gallian, Contemporary Abstract Algebra

Count Pairs: (a, g) with $a^g = a$ in two different ways. Let N denote their number

Equating:

$$\sum_{g \in G} |\mathrm{Fix}_\Omega(g)| = N = r|G|.$$

Hence

$$r = \frac{1}{|G|} \sum_{g \in G} |\mathrm{Fix}_\Omega(g)|.$$

Applying the Orbit-Counting Lemma

Consider the set of all n-gons coloured in c colours.

- The equivalent n-gons are orbits under G.
- Count the non-equivalent n-gons by counting number of orbits.
- G acts on *all* n-gons.
- There are c^n such n-gons.

Is there a quicker way?

Can we look at the group G again to find a better way?

Cycle Structure

If g has α_i cycles of length i we say g has *cycle structure*

$$1^{\alpha_1} 2^{\alpha_2} \cdots n^{\alpha_n}.$$

Cycle Number

$$\zeta(g) = \alpha_1 + \alpha_2 + \cdots + \alpha_n$$

denote the number of cycles of g.

…

and now we can prove the following, which is a special case of a more general theorem by G. Pólya.

Pólya counting

Theorem

Let G be a permutation group on $\Omega = \{1, \ldots, n\}$. Then the number of inequivalent colourings of Ω with c colours is

$$\frac{1}{|G|} \sum_{g \in G} c^{\zeta(g)}.$$

Proof

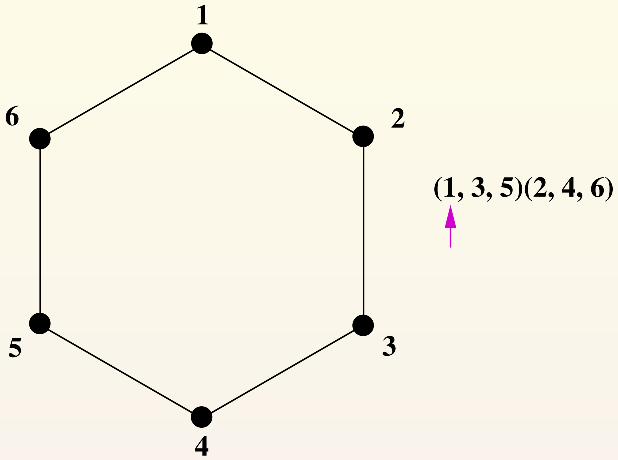
Let X be the set of all colourings of Ω. Thus $|X| = c^n$.

The number C of inequivalent colourings is equal to the number of orbits of G on X. Hence by the previous theorem

$$C = \frac{1}{|G|} \sum_{g \in G} |\mathrm{Fix}_X(g)|.$$

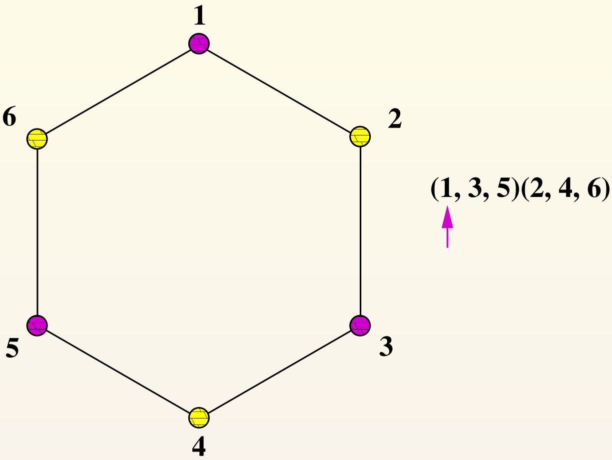
Proof

Let X be the set of all colourings of Ω.
Thus $|X| = c^n$.



Proof

Let X be the set of all colourings of Ω.
Thus $|X| = c^n$.



Proof

Let X be the set of all colourings of Ω. Thus $|X| = c^n$.

Now pick a colouring $x \in X$ which is fixed by g, so $x^g = x$. Hence if $(i_1, \ldots, i_k)$ is a cycle of g and $i_1 \in \Omega$ has colour red, say, then so must $i_2, i_3, \ldots, i_k$ and thus all elements in a cycle of g have same colour.

Proof

Let X be the set of all colourings of Ω. Thus $|X| = c^n$.

If g has t cycles, then there are c^t colourings which agree in each cycle of g: One element in each cycle can be coloured any way we want, the others have same colour.

Proof

Let X be the set of all colourings of Ω. Thus $|X| = c^n$.

$t = \alpha_1 + \cdots + \alpha_n = \zeta(g)$ and so

$$|\mathrm{Fix}_X(g)| = c^t = c^{\zeta(g)}.$$

$$C = \frac{1}{|G|} \sum_{g \in G} |\mathrm{Fix}_X(g)| = \frac{1}{|G|} \sum_{g \in G} c^{\zeta(g)}.$$

□

Conjugacy Class

Let $a \in G$. Then $cl(a) = \{g^{-1}ag \mid g \in G\}$ is the *conjugacy class* of a in G.

It consists of all conjugates a.

Conjugacy Classes

The elements of G can be divided into conjugacy classes.

Example

$$\begin{aligned} D_{12} = \{ & (), (2,6)(3,5), (1,2)(3,6)(4,5), \\ & (1,2,3,4,5,6), (1,3)(4,6), \\ & (1,3,5)(2,4,6), (1,4)(2,3)(5,6), \\ & (1,4)(2,5)(3,6), (1,5)(2,4), \\ & (1,5,3)(2,6,4), (1,6,5,4,3,2), \\ & (1,6)(2,5)(3,4)\} \end{aligned}$$

Conjugacy Classes of D_{12}

$$\{()\}, \quad \{(2,6)(3,5),(1,3)(4,6),(1,5)(2,4)\}$$
$$\{(1,2)(3,6)(4,5),(1,4)(2,3)(5,6),$$
$$(1,6)(2,5)(3,4)\}$$
$$\{(1,2,3,4,5,6),(1,6,5,4,3,2)\}$$
$$\{(1,3,5)(2,4,6),(1,5,3)(2,6,4)\}$$
$$\{(1,4)(2,5)(3,6)\}$$

Geometric Interpretation

The elements in each conjugacy class are

- rotations by angles of equal magnitude,
- reflections along the same axes.

Computing Conjugacy Classes in GAP

```
gap> grp :=
DihedralGroup(IsPermGroup,12);
gap>cc := ConjugacyClasses(grp);
[ ()^G, (2,6)(3,5)^G,
(1,2)(3,6)(4,5)^G,
(1,2,3,4,5,6)^G,
(1,3,5)(2,4,6)^G,
(1,4)(2,5)(3,6)^G ]
```

Computing Conjugacy Classes in GAP

```
gap> List( cc , i->Elements(i) );
[ [ () ], [ (2,6)(3,5), (1,3)(4,6),
(1,5)(2,4) ],
[ (1,2)(3,6)(4,5), (1,4)(2,3)(5,6),
(1,6)(2,5)(3,4) ],
[ (1,2,3,4,5,6), (1,6,5,4,3,2) ],
[ (1,3,5)(2,4,6), (1,5,3)(2,6,4) ],
[ (1,4)(2,5)(3,6) ]]
```

Conjugacy Class Representatives

We say $S = \{a_1, \ldots, a_k\}$ is a set of *representatives* of the conjugacy classes of G if exactly one element of each class is contained in S.

Conjugacy Class Representatives in GAP

```
gap> List(cc,i->Representative(i));
[ (), (2,6)(3,5), (1,2)(3,6)(4,5),
(1,2,3,4,5,6), (1,3,5)(2,4,6),
(1,4)(2,5)(3,6) ]
```

Centralisers

Let $a \in G$. Then $C_G(a) = \{g \in G \mid g^{-1}ag = a\}$ is the *Centraliser* of a in G.

It consists of all elements which conjugate a to itself.

Centralisers and Conjugacy Classes

Theorem

Let $a \in G$. Then

$$|cl(a)| = [G : C_G(a)] = \frac{|G|}{|C_G(a)|}.$$

Thus the number of elements conjugate in G to a is equal to the number of cosets of $C_G(a)$ in G.

Centralisers and Conjugacy Classes

Theorem
Let $a \in G$. Then

$$|cl(a)| = [G : C_G(a)] = \frac{|G|}{|C_G(a)|}.$$

This follows by the Orbit-Stabiliser Theorem thinking of G as a group of permutations of the set $\Omega = G$, where $g \in G$ maps a to $g^{-1}ag$.

Centralisers and Conjugacy Classes

Theorem
Let $a \in G$. Then

$$|cl(a)| = [G : C_G(a)] = \frac{|G|}{|C_G(a)|}.$$

We say G *acts* on $\Omega = G$ via conjugation.

Pólya counting

Recall the counting theorem:

Theorem

Let G be a permutation group on $\Omega = \{1, \ldots, n\}$. Then the number of inequivalent colourings of Ω with c colours is

$$\frac{1}{|G|} \sum_{g \in G} c^{\zeta(g)}.$$

Using Centralisers

We do not wish to loop over all elements of G. Instead suppose $S = \{a_1, \ldots, a_k\}$ is a set of *representatives* of the conjugacy classes of G.

Using Centralisers

If g is in the same conjugacy class as a then g and a have the same cycle structure.

Hence $\zeta(g) = \zeta(a)$.

Using Centralisers

Look at the representatives and count $c^{\zeta(a_i)}$ as often as $|cl(a_i)|$.

Using Centralisers

$$\begin{aligned}\frac{1}{|G|}\sum_{g\in G} c^{\zeta(g)} &= \frac{1}{|G|}\sum_{i=1}^{k} |cl(a_i)|c^{\zeta(a_i)} \\ &= \frac{1}{|G|}\sum_{i=1}^{k} |G : C_G(a_i)|c^{\zeta(a_i)} \\ &= \frac{1}{|G|}\sum_{i=1}^{k} \frac{|G|}{|C_G(a_i)|}c^{\zeta(a_i)} \\ &= \sum_{i=1}^{k} \frac{1}{|C_G(a_i)|}c^{\zeta(a_i)}.\end{aligned}$$

Pólya counting with Centralisers

Theorem

Let G be a permutation group on $\Omega = \{1, \dots, n\}$ and $S = \{a_1, \dots, a_k\}$ is a set of *representatives* of the conjugacy classes of G.

Then the number of inequivalent colourings of Ω with c colours is

$$\sum_{i=1}^{k} \frac{1}{|C_G(a_i)|} c^{\zeta(a_i)}.$$