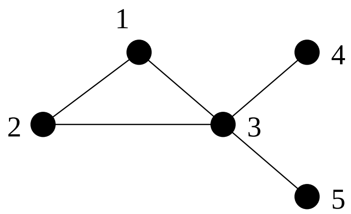
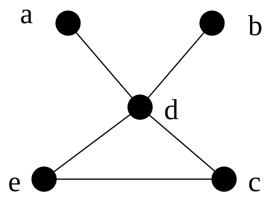
COMPUTING ISOMORPHISM

In this chapter, we will look at graph isomorphism (and automorphism), includying algorithms using invariants and certificates. We will also see isomorphism of other structures.

Graph Isomorphism

Example 1:

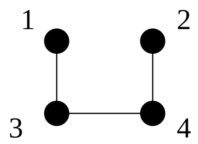


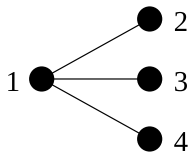


G_1 and G_2 are **isomorphic**, since there is a bijection $f : V_1 \to V_2$ that preserve edges:

$$\begin{array}{ccc} 1 & \to & c \\ 2 & \to & e \\ 3 & \to & d \\ 4 & \to & a \\ 5 & \to & b \end{array}$$

Example 2:





G_3 and G_4 are not isomorphic. Any bijection would not preserve edges since G_3 has no vertex of degree 3, while G_4 does (the degree sequence of a graph is invariant (in sorted order) under isomorphism).

Definition. Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are *isomorphic* if there is a bijection $f : V_1 \to V_2$ such that

$$\{f(x), f(y)\} \in E_2 \iff \{x, y\} \in E_1.$$

The mapping f is said to be an *isomorphism* between G_1 and G_2.

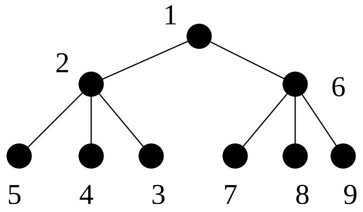
If f is an isomorphism from G to itself, it is called an *automorphism*. The set of all automorphisms of a graph is a permutation group (which is a group under the "composition of permutations" operation). See chapter 6 for more on permutation groups.

The problem of determining if two graphs are isomorphic is in general difficult, but most researchers believe it is not NP-complete.

Some special cases can be solved in polynomial time, such as: graphs with maximum degree bounded by a constant and trees.

Invariants

Let $DS = [deg(v_1), deg(v_2), \ldots, deg(v_n)]$ be the degree sequence of a graph. And let $SDS = [d_1, d_2, \ldots, d_n]$ be its degree sequence in sorted order.



$$DS = [2, 4, 1, 1, 1, 4, 1, 1, 1]$$
$$SDS = [1, 1, 1, 1, 1, 1, 2, 4, 4]$$

SDS is the same for all graphs that are isomorphic to G. So, SDS is *invariant* (under isomorphism).

DEFINITION. Let $\mathcal{F}$ be a family of graphs. An *invariant* on $\mathcal{F}$ is a function ϕ with domain $\mathcal{F}$ such that $\phi(G_1) = \phi(G_2)$ if G_1 is isomorphic to G_2.

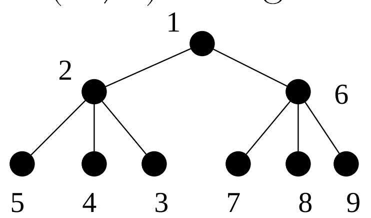
If $\phi(G_1) \neq \phi(G_2)$ we can conclude G_1 and G_2 are not isomorphic. If $\phi(G_1) = \phi(G_2)$, we still need to check whether they are isomorphic.

Definition. Let $\mathcal{F}$ be a family of graphs on the vertex set V. Let $D : \mathcal{F} \times V \to \{0, 1, \ldots, k\}$. Then, the *partition of* V *induced by* D is

$$B = [B[0], B[1], \ldots, B[k]]$$

where $B[i] = \{v \in V : D(G, v) = i\}$.
If $\phi_D(G) = [|B[0]|, |B[1]|, \ldots, |B[k]|]$ is an invariant, then we say that D is an invariant inducing function.

Example:
$D(G, u) =$ degree of vertex u in graph G.

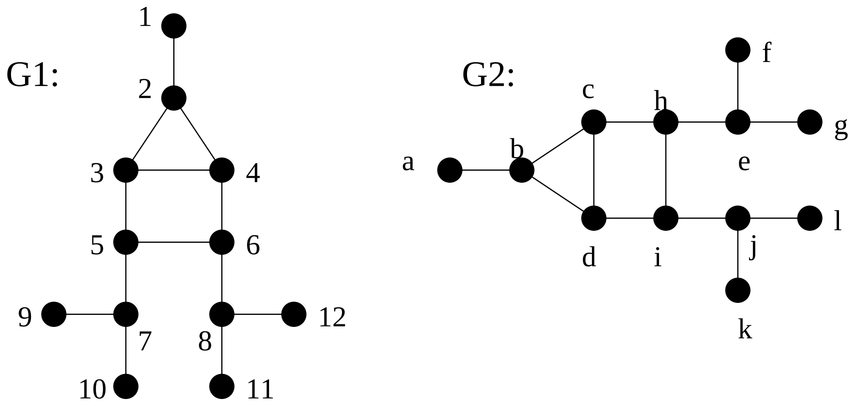


Ordered partition induced by D:

$$B = [\emptyset, \{3, 4, 5, 7, 8, 9\}, \{1\}, \emptyset, \{2, 6\}, \emptyset, \emptyset, \emptyset, \emptyset]$$

$$\phi_D(G) = [0, 6, 1, 0, 2, 0, 0, 0, 0]$$

$\phi_D(G)$ is an invariant for $\mathcal{F} =$ family of all graphs on V.
So, D is an invariant inducing function.



Initial partition:
$X_0(G_1) = [\{1, 2, \ldots, 12\}]$ $X_0(G_2) = [\{a, b, \ldots, l\}]$

1st invariant inducing function:
$D_1(G, v) = \#$ of neighbours for each degree

$D_1(G_1, 1) = [0010 \cdots 0]$	$D_1(G_2, a) = [0010 \cdots 0]$
$D_1(G_1, 2) = [1020 \cdots 0]$	$D_1(G_2, b) = [1020 \cdots 0]$
$D_1(G_1, 3) = [0030 \cdots 0]$	$D_1(G_2, c) = [0030 \cdots 0]$
$D_1(G_1, 4) = [0030 \cdots 0]$	$D_1(G_2, d) = [0030 \cdots 0]$
$D_1(G_1, 5) = [0030 \cdots 0]$	$D_1(G_2, e) = [2010 \cdots 0]$
$D_1(G_1, 6) = [0030 \cdots 0]$	$D_1(G_2, f) = [0010 \cdots 0]$
$D_1(G_1, 7) = [2010 \cdots 0]$	$D_1(G_2, g) = [0010 \cdots 0]$
$D_1(G_1, 8) = [2010 \cdots 0]$	$D_1(G_2, h) = [0030 \cdots 0]$
$D_1(G_1, 9) = [0010 \cdots 0]$	$D_1(G_2, i) = [0030 \cdots 0]$
$D_1(G_1, 10) = [0010 \cdots 0]$	$D_1(G_2, j) = [2010 \cdots 0]$
$D_1(G_1, 11) = [0010 \cdots 0]$	$D_1(G_2, k) = [0010 \cdots 0]$
$D_1(G_1, 12) = [0010 \cdots 0]$	$D_1(G_2, l) = [0010 \cdots 0]$

partition refinement of X_0 induced by D_1:
$X_1(G_1) = [\{1, 9, 10, 11, 12\}, \{2\}, \{3, 4, 5, 6\}, \{7, 8\}]$
$X_1(G_2) = [\{a, f, g, k, l\}, \{b\}, \{c, d, h, i\}, \{e, f\}]$

$X_1(G_1) = [\{1, 9, 10, 11, 12\}, \{2\}, \{3, 4, 5, 6\}, \{7, 8\}]$
$X_1(G_2) = [\{a, f, g, k, l\}, \{b\}, \{c, d, h, i\}, \{e, j\}]$

2nd invariant inducing function:
$D_2(G, v) = \#$ of triangles in G passing through v.

v	$D_2(G_1, v)$
1	0
2	1
3	1
4	1
5	0
6	0
7	0
8	0
9	0
10	0
11	0
12	0

v	$D_2(G_2, v)$
a	0
b	1
c	1
d	1
e	0
f	0
g	0
h	0
i	0
j	0
k	0
l	0

partition refinement of X_1 induced by D_2:

$X_2(G_1) = [\{1, 9, 10, 11, 12\}, \{2\}, \{3, 4\}, \{5, 6\}, \{7, 8\}]$
$X_2(G_2) = [\{a, f, g, k, l\}, \{b\}, \{c, d\}, \{h, i\}, \{e, j\}]$

G_1 and G_2 are still compatible.

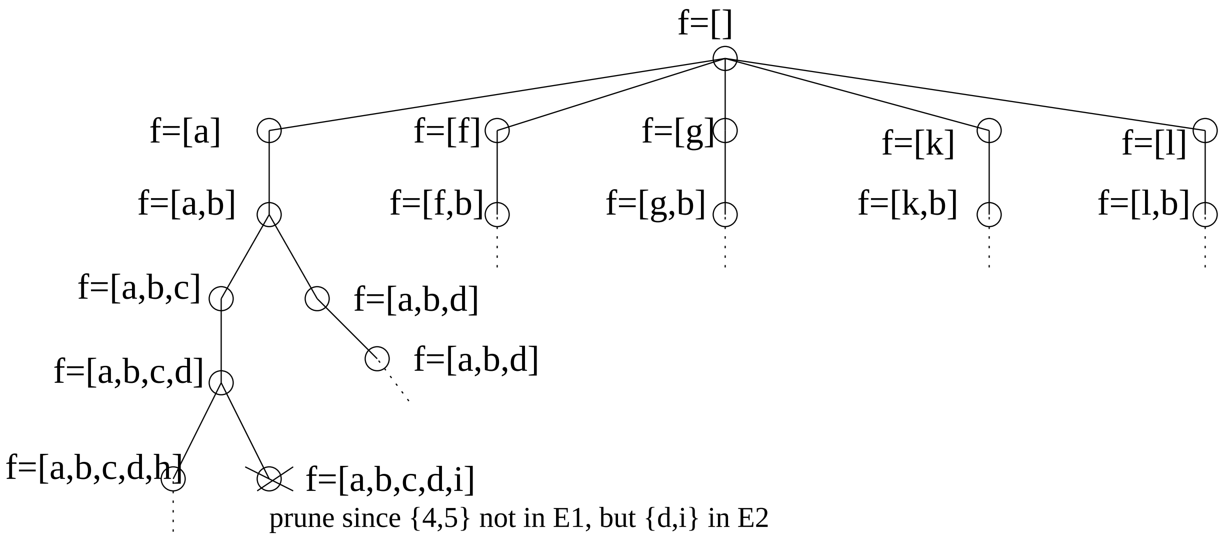
$X_2(G_1) = [\{1,9,10,11,12\},\{2\},\{3,4\},\{5,6\},\{7,8\}]$
$X_2(G_2) = [\{a,f,g,k,l\},\{b\},\{c,d\},\{h,i\},\{e,f\}]$

We only need to check bijections between the following sets:

$$\begin{array}{rcl} \{1,9,10,11,12\} & \leftrightarrow & \{a,f,g,k,l\} \\ \{2\} & \leftrightarrow & \{b\} \\ \{3,4\} & \leftrightarrow & \{c,d\} \\ \{5,6\} & \leftrightarrow & \{h,i\} \\ \{7,8\} & \leftrightarrow & \{e,f\} \end{array}$$

# of bijections to test: $5! \times 1! \times 2! \times 2! \times 2! = 960$.
Without partition refinement, we would have to test 12! bijections!

Backtracking algorithm to find all isomorphisms



Algorithm $\textsc{Iso}(\mathcal{I}, G_1, G_2)$ (global n, W, X, Y)

procedure $\textsc{GetPartitions}()$

$X[0] \leftarrow V(G_1)$; $Y[0] \leftarrow V(G_2)$; $N \leftarrow 1$;
for each $D \in \mathcal{I}$ do
  for $i \leftarrow 0$ to $N-1$ do
    Partition $X[i]$ into sets $X_1[i], X_2[i], \ldots, X_{m_i}[i]$,
      where $x, x' \in X_j[i] \iff D(x) = D(x')$
    Partition $Y[i]$ into sets $Y_1[i], Y_2[i], \ldots, Y_{n_i}[i]$,
      where $y, y' \in Y_j[i] \iff D(y) = D(y')$
    if $m_i \neq n_i$ then exit; (G_1 and G_2 are not isomorphic)
    Order $Y_1[i], Y_2[i], \ldots, Y_{m_i}[i]$ so that for all j
      $D(x) = D(y)$ whenever $x \in X_j[i]$ and $y \in Y_j[i]$
    if ordering is not possible then exit; (not isomorphic)
  Order the partitions so that:
    $|X[i]| = |Y[i]| \leq |X[i+1]| = |Y[i+1]|$ for all i
  $N \leftarrow N + m - 1$;
return (N);

procedure $\textsc{FindIsomorphism}(l)$

if $l = n$ then output (f);
$j \leftarrow W[l]$;
for each $y \in Y[j]$ do
  $OK \leftarrow true$;
  for $u \leftarrow 0$ to $l-1$ do
    if $(\{u, l\} \in E(G_1)$ and $\{f[u], y\} \notin E(G_2))$ or
      $(\{u, l\} \notin E(G_1)$ and $\{f[u], y\} \in E(G_2))$ then $OK \leftarrow false$;
  if OK then $f[l] \leftarrow y$; $\textsc{FindIsomorphism}(l+1)$;

main $N \leftarrow \textsc{GetPartitions}()$;
for $i \leftarrow 0$ to N do for each $x \in X[i]$ do $W[x] \leftarrow i$;
$\textsc{FindIsomorphism}(0)$;

Computing Certificates

DEFINITION. A *certificate* $Cert()$ for a family $\mathcal{F}$ of graphs is a function such that for $G_1, G_2 \in \mathcal{F}$, we have

$$Cert(G_1) = Cert(G_2) \iff G_1 \text{ and } G_2 \text{ are isomorphic}$$

Certificates for Trees

We will compute certificates in polynomial time for the family of **trees**. Consequently, graph isomorphism for trees can be solved in polynomial time.
Algorithm to compute certificates for a tree:

1. Label all vertices with string 01.
2. While there are more than 2 vertices in G:
   for each non-leaft x of G do
   2.1. Let Y be the set of labels of the leaves adjacent to x and the label of x with initial 0 and trailing 1 deleted from x;
   2.2. Replace the label of x with the concatenation of the labels in Y, sorted in increasing lexicographic order, with a 0 prepended and a 1 appended.
   2.3. Remove all leaves adjacent to x.
3. If there is only one vertex x left, report x's label as the certificate.
4. If there are 2 vertices x and y left, concatenate x and y in increasing lexicographic order, and report it as the certificate.

Here, see slides with Examples 7.2,7.3,7.4,7.5 from the textbook.

Certificates for general graphs

Let $G = (V, E)$. Consider all permutations $\pi : V \to V$.
Each Π determines an adjacenc matrix:

$$A_\pi[u, v] \;=\; 1,\ \text{if } \{\pi(u), \pi(v)\} \in E \\ 0,\ \text{otherwise.}$$

Example: $G = (V = \{1, 2, 3\}, E = \{\{1, 2\}, \{1, 3\}\})$.

π :	A_π :	Num_π	π :	A_π :	Num_π
$[1, 2, 3]$	$\begin{bmatrix} - & 1 & 1 \\ - & - & 0 \\ - & - & - \end{bmatrix}$	110	$[1, 3, 2]$	$\begin{bmatrix} - & 1 & 1 \\ - & - & 0 \\ - & - & - \end{bmatrix}$	110
$[2, 1, 3]$	$\begin{bmatrix} - & 1 & 0 \\ - & - & 1 \\ - & - & - \end{bmatrix}$	101	$[2, 3, 1]$	$\begin{bmatrix} - & 0 & 1 \\ - & - & 1 \\ - & - & - \end{bmatrix}$	011
$[3, 1, 2]$	$\begin{bmatrix} - & 1 & 0 \\ - & - & 1 \\ - & - & - \end{bmatrix}$	101	$[3, 2, 1]$	$\begin{bmatrix} - & 0 & 1 \\ - & - & 1 \\ - & - & - \end{bmatrix}$	011

We could define the certificate to be

$$Cert(G) = min\{Num_\pi(G) : \pi \in Sym(V)\}.$$

$Cert(G)$ is difficult to compute. $Cert(G)$ has as many leading 0's as possible. So, k is as large as possible, where k is the number of all-zero columns above the diagonal. So, vertices $\{1, 2, \ldots, k\}$ form a maximum independent set in G (or equivalently a maximum clique in the complement graph $\overline{G}$).

So, computing $Cert(G)$ as defined before is NP-hard.

However, it is believed that determining if $G_1 \sim G_2$ (G_1 isomorph to G_2) is not NP-complete.

So, it is possible that the approach of computing $Cert(G)$ to solve the graph isomorphism problem is more work than necessary.
So, instead, we will define the certificate as follows:

$$Cert(G) = min\{Num_\pi(G) : \pi \in \Pi_G\},$$

where Π_G is a set of permutations determined by the structure of G but not by any particular ordering of V.

Discrete and equitable partitions

Definitions.
A partition B is a **discrete partition** if $|B[j]| = 1$ for all j, $0 \leq j \leq k$.
It is a **unit partition** if $|B| = 1$.

Let $G = (V, E)$ be a graph and $N_G(u) = \{x \in V : \{u, x\} \in E\}$.
A partition B is an **equitable partition** with respect to the graph G if for all i and j

$$|N_G(u) \cap B[j]| = |N_G(v) \cap B[j]|$$

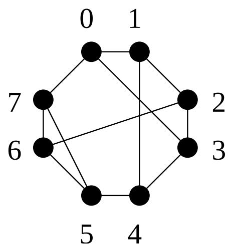
for all $u, v \in B[i]$.

Given B an ordered equitable partition with k parts, we can define M_B to be a $k \times k$ matrix where
$M_B[i, j] = |N(G(v) \cap B[j]|$ where $v \in B[i]$.

Since B is equitable any choice of v produces the same result.

Also define $Num(B)$ = sequence of $k(k-1)/2$ elements above diagonal written column by column.

Example:



$B = [\{0\}, \{2,4\}, \{5,6\}, \{7\}, \{1,3\}]$ is an equitable partition with respect to the graph above.

$$M_B = \begin{bmatrix} 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 1 & 0 & 2 \\ 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 2 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 \end{bmatrix}$$

and $Num(B) = [0,0,1,1,0,1,2,3,0,0]$.

If B is a **discrete** partition then B corresponds to a permutation $\pi : B[i] = \{\pi[i]\}$, in which case

$$Num(B) = Num_{\pi}(G),$$

adjusting so that $Num(B)$ is interpreted as the sequence of bits of a binary number.

Partition Refinement

Definition. An ordered partition B is a *refinement* of the ordered partition A if

1. every block $B[i]$ of B is contained in some block $A[j]$ of A; and
2. if $u \in A[i_1]$ and $v \in A[j_1]$ with $i_1 \leq j_1$, then $u \in B[i_2]$ and $v \in B[j_2]$ with $i_2 \leq j_2$.

The definition basically says that B must refine A and preserve its order.
Example:
$A = [\{0,3\},\{1,2,4,5,6\}]$
$B = [\{0,3\},\{1,5,6\},\{2,4\}]$ is a refinement of A,
but $B' = [\{1,5,6\},\{2,4\},\{0,3\}]$ is not a refinement of A because blocks are out of order with respect to A.
Let A be an ordered partition and T be any block of A. Define a function $D_T : V \rightarrow \{0,1,\ldots,n-1\}$:

$$D_T(v) = |N_G(v) \cap T|$$

This function can be used to refine A.

1. Set B equal to A.
2. Let $\mathcal{S}$ be a list containing the blocks of B.
3. While ($\mathcal{S} \neq \emptyset$) do
4. remove a block T from the list $\mathcal{S}$
5. for each block $B[i]$ of B do
6. for each h, set $L[h] = \{v \in B[i] : D_T(v) = h\}$
7. if there is more than pne non-empty block in L then
8. replace $B[i]$ with he non-empty blocks in L in order of the index h, $h = 0, 1, \ldots, n-1$.
9. add the non-empty blocks in L to the end of the list $\mathcal{S}$

Notes: in step 4 we ignore blocks of $\mathcal{S}$ if the block has already been partitioned in B.
The procedure will produce an equitable partition.
The ordering at step 8 is chosen in order to make $Num(B)$ smaller.

The following slides should be inserted here:

- Slide with a copy of `Algorithm 7.5:  Refine`, for partition refinement (page 256).
- Slide with copy of example 7.8 (pages 258-261).
- Slides with a copy of `Algorithm 7.8:Cert1` (as well as, `Algorithm 7.7:Canon1` and `Algorithm 7.6:Compare` for computing certificates for general graphs.

Pruning with Automorphisms

Let $G = (V, E)$ and $\pi \in Sym(V)$, a permutation on V.

Recall that π is an automorphism of G if it is an isomorphism from G to itself.

Let A be the adjacency matrix of G and
let A_π the the adjacency matrix of G with respect to a permutation π, that is, $A_\pi[i, j] = A[\pi[i], \pi[j]]$, for all i, j.
Then, π is an automorphism of G if and only if $A_\pi = A$.

THEOREM. If $Num_{\pi_1}(G) = Num_\mu(G)$ then
$\pi_2 = \pi_1\mu^{-1}$ is an automorphism of G.

PROOF.

$$\begin{aligned}
A_{\pi_2}[i, j] &= A_{\pi_1\mu^{-1}}[i, j] \\
&= A[\pi_1\mu^{-1}[i], \pi_1\mu^{-1}[j]] \\
&= A_{\pi_1}[\mu^{-1}[i], \mu^{-1}[j]] \\
&= A_\mu[\mu^{-1}[i], \mu^{-1}[j]] \\
&= A[\mu\mu^{-1}[i], \mu\mu^{-1}[j]] \\
&= A[i, j].
\end{aligned}$$

How to prune with automorphisms?

1. When algortihm `Compare` returns "equal", we record one more automorphism.
2. When branching on the backtracking tree, use known automorphisms for further pruning.

   Example:
   Node N_0: `1|3|567|024`
   Children:
   N_1: `1|3|5|67|024`
   N_2: `1|3|6|57|024`
   N_3: `1|3|7|56|024`
   If $g_1 = (24)(56)$ and $g_2 = (04)(57)$ are automorphisms, then
   prune N_2, since $g_1(N_1) = N_2$ and
   prune N_3, since $g_2(N_1) = N_3$.

What do we need to compute efficiently in order to prune with automorphisms?

- Store/update information on the automorphisms found so far: if $g_1, g_2, \ldots, g_k$ have been found, store the subgroup S of $Aut(G)$ generated by $g_1, g_2, \ldots, g_k$.
- Quickly determine if partitions
  $R = q_0|q_1|\cdots|q_{l-1}|u|Q[l] - u|\cdots|$ and
  $R' = q_0|q_1|\cdots|q_{l-1}|u'|Q[l] - u'|\cdots|$ are equivalent, that is, determine if there exists $g \in S$ such that $g(R) = R'$.

We need some definitions and results found in Chapter 5.

A *group* is a set G wuth operation $*$ such that 1) there exists an identity $I \in G$ such that $g * I = g$ for all $g \in G$, and 2) for all $g \in G$ there exists an inverse $g^{-1} \in G$ such that $g^{-1} * g = I$.

A subgroup S of G is a subset $S \subseteq G$ that is a group.

THEOREM. (Lagrange) Let G be a finite group. If H is a subgroup of G then

1. G can be written as $G = g_1 H \cup g_2 H \cup \ldots \cup g_r H$ for some $g_1, g_2, \ldots, g_r \in G$ (where the unions are disjoint)
2. $|H|$ divides $|G|$.

We say that $T = \{g_1, g_2, \ldots, g_r\}$ is a *system of left coset representatives* of a *left transversal* of H in G.

THEOREM. $Sym(X)$, the set of all permutations on X, is a group under the operation of *composition of functions*.

THEOREM. $Aut(G)$, the set of automorphisms of a graph G, is a group under the operation of *composition of functions*.

Schreier-Syms representation of a permutation group

Let G be a permutation group on $X = \{0, 1, \ldots, n-1\}$, and let

$$\begin{aligned} G_0 &= \{g \in G : g(0) = 0\} \\ G_1 &= \{g \in G_0 : g(1) = 1\} \\ G_2 &= \{g \in G_1 : g(2) = 2\} \\ &\vdots \\ G_{n-1} &= \{g \in G_{n-2} : g(n-1) = n-1\} = I \end{aligned}$$

$G \supseteq G_0 \supseteq G_1 \supseteq G_2 \cdots \supseteq G_{n-1} = I$ are subgroups.

For all $i \in \{0, 1, 2, \ldots, n-1\}$ (taking $G_{-1} = G$),
let $orb(i) = \{g(i) : g \in G_{i-1}\} = \{x_{i,1}, x_{i,2}, \ldots, x_{i,n_i}\}$ and
$U_i = \{h_{i,1}, h_{i,2}, \ldots, h_{i,n_i}\}$ such that $h_{i,j}(i) = x_{i,j}$.

Theorem. U_i is a left transversal of G_i in G_{i-1}.

The data structure: $[U_0, U_1, \ldots, U_{n-1}]$ is called the Schreier-Syms representation of the group G.

Any $g \in G$ can be uniquely written as
$g = h_{0,i_0} * h_{1,i_1} * \cdots * h_{n-1,i_{n-1}}$.

The following algorithms from Chapter 5 are going to be used when pruning with automorphisms:

PROCEDURE ENTER($n, g, [U_0, U_1, \ldots, U_{n-1}]$)
INPUT: n, PERMUTATION g, AND $[U_0, U_1, \ldots, U_{n-1}]$, THE SCHREIER-SYMS REPRESENTATION OF G.
OUTPUT: $[U'_0, U'_1, \ldots, U'_{n-1}]$, THE SCHREIER-SYMS REPRESENTATION OF G', THE GROUP GENERATED BY G AND g.

Changing the base: modify the Schreier-Syms representation to work on a base permutation β.
Redefine $G_i = \{g \in G_{i-1} : g(\beta(i)) = \beta(i)\}$.
$[\beta, [U_0, U_1, \ldots, U_{n-1}]]$ is the (modified) Schreier-Syms representation.

PROCEDURE CHANGEBASE(n, $[\beta, [U_0, U_1, \ldots, U_{n-1}]]$, β')
INPUT: n, $[\beta, [U_0, U_1, \ldots, U_{n-1}]]$, NEW BASIS β'
OUPUT: $[\beta', [U'_0, U'_1, \ldots, U'_{n-1}]]$

The following slides should be inserted here:

- Slides with a copy of `Algorithm 7.10:Cert2` (as well as, `Algorithm 7.9:Canon2`) for computing certificates for general graphs with pruning with automorsphisms (pages 271,272).
- Slide with Figure 7.3, illustrating the algorithm (page 270).

Using known automorphisms

If we know some or all automorphisms of G we can input the Schreier-Syms representation of the group generated by these automorphisms to the algorithm **Canon2**.

For the previous example, if we input $Aut(G)$, the backtracking tree would have only 10 nodes instead of 16 (se page 273).

Isomorphisms of set systems

We can check for set system isomorphisms via graph isomorphisms.
Let $(V, \mathcal{B})$ be a set system.
Define a bipartite graph $G_{V,\mathcal{B}}$ with vertex set $V \cup \mathcal{B}$ and with an edge connecting $x \in V$ to $B \in \mathcal{B}$ if and only if $x \in B$.
This is usually called the point-block incidence graph.

Then, $(V_1, \mathcal{B}_1) \sim (V_2, \mathcal{B}_2)$ if and only if $G_{V_1,\mathcal{B}_1} \sim G_{V_2,\mathcal{B}_2}$ with respect to initial partitions $P_1 = [V_1, \mathcal{B}_1]$ and $P_2 = [V_2, \mathcal{B}_2]$, respectively.

We can extract the automorphism group of $(V, \mathcal{B})$ from the automorphism group of $G_{V,\mathcal{B}}$.
The automorphism group of $(V, \mathcal{B})$ is the automorphism group of $G_{V,\mathcal{B}}$ restricted to V.