Canonical form of positive definite matrix

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I. The automorphism and isomorphism problems

The graph isomorphism problem

- We consider vertex colored graphs G on n vertices with each vertex $i \in \{1, \ldots, n\}$ having a color $c_G(i)$.
- Suppose that we have a graph G on n vertices $\{1, \ldots, n\}$, we want to compute its automorphism group $Aut(G)$.
  g is formed of all elements in $Sym(n)$ such that

$$\{g(i), g(j)\} \in E(G) \text{ if and only if } \{i, j\} \in E(G)$$

  and $c(g(i)) = c(i)$ for $1 \leq i \leq n$.
- Suppose that G_1 and G_2 are two graphs on n vertices $\{1, \ldots, n\}$, we want to test if G_1 and G_2 are isomorphic, i.e. if there is $g \in Sym(n)$ such that

$$\{g(i), g(j)\} \in E(G_2) \text{ if and only if } \{i, j\} \in E(G_1)$$

  and $c_{G_2}(g(i)) = c_{G_1}(i)$.

Complexity: Theoretical and Practical

Theoretical

- The theoretical complexity of the Graph isomorphism problem was unknown for a long time.
- Then in 2015 following happened
  - László Babai, *Graph Isomorphism in Quasipolynomial Time*, arXiv:1512.03547

  that is running time is $\exp((\log n)^{O(1)})$.

Practical

- Since the 70s we have very efficient graph isomorphism programs.
- They can compute the automorphisms of graphs with thousands of vertices.
- Some hard graphs from Projective planes with about 100 vertices can be problematic.

The program nauty

- The program nauty by Brendan McKay solves the graph isomorphism and the automorphism problems.

  http://cs.anu.edu.au/people/bdm/nauty/

- nauty is extremely efficient in doing those computations.
- nauty can deal with directed graph but this is not recommended.
- nauty can deal with vertex colors.
- nauty iterates over all $n!$ permutation but it prunes the search tree so as to obtain a fast running time.
- nauty has exponential runtime in worst case.
- There are alternatives such as bliss or traces with the same performance features.

II. Vertex colored graph reductions

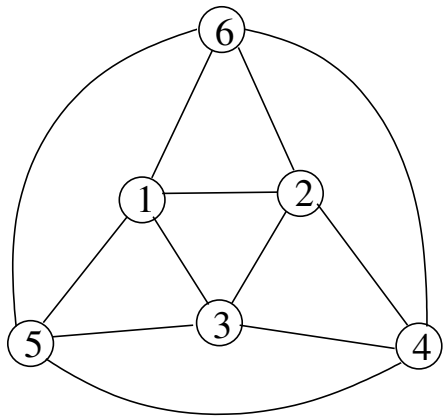
The reduction to a graph

Why focus on graph?

- We have many other combinatorial problems:
  - subset of vertex-set of a graph,
  - set system,
  - edge weighted graph,
  - plane graph,
  - partially ordered set, etc.
- If M is a "combinatorial structure", then we have to define a graph $G(M)$, such that:
  - If M_1 and M_2 are two "combinatorial structure", then M_1 and M_2 are isomorphic if and only if $G(M_1)$ and $G(M_2)$ are isomorphic.
  - If M is a "combinatorial structure", then $Aut(M)$ is isomorphic to $Aut(G(M))$.

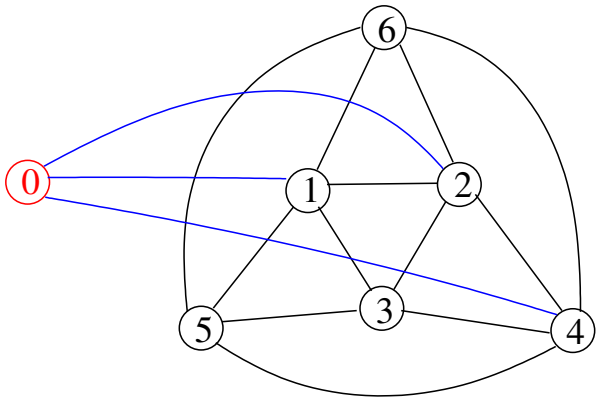
Subset of vertex-set of a graph

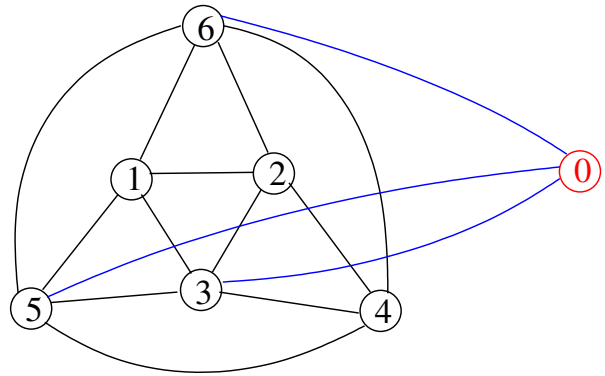
- Suppose that we have a graph G, two subsets S_1, S_2 of G, we want to know if there is an automorphism ϕ of G such that $\phi(S_1) = S_2$.



$$S_1 = \{1, 2, 4\}$$
$$S_2 = \{3, 5, 6\}$$

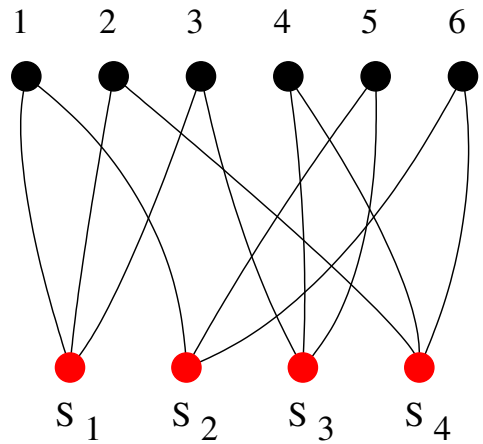
- The method is to define two graphs associated to it:





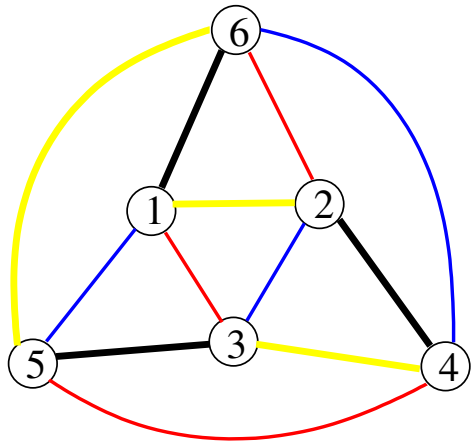
Set systems

- Suppose we have some subsets $S_1, \ldots, S_r$ of $\{1, \ldots, n\}$. We want to find the permutations of $\{1, \ldots, n\}$, which permutes the S_i.
- We define a graph with $n + r$ vertices j and S_i with j adjacent to S_i if and only if $j \in S_i$
- Example $\mathcal{S} = \{\{1, 2, 3\}, \{1, 5, 6\}, \{3, 4, 5\}, \{2, 4, 6\}\}$:



Edge colored graphs

- G is a graph with vertex-set $(v_i)_{1 \leq i \leq N}$, edges are colored with k colors $C_1, \ldots, C_k$:

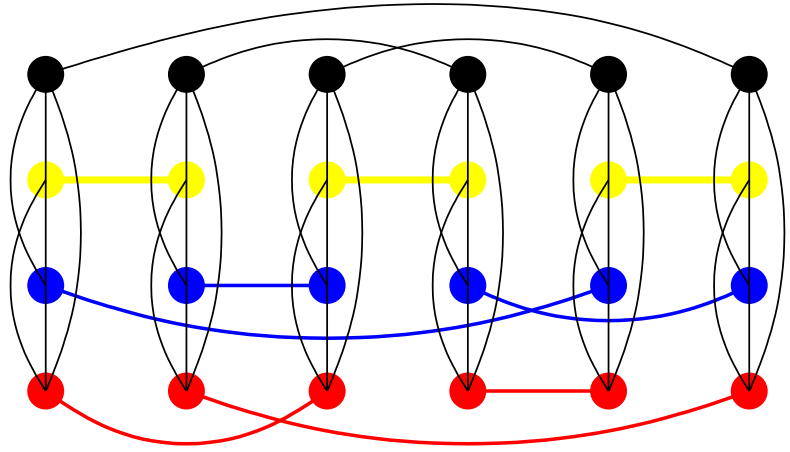


- We want to find automorphisms preserving the graph and the edge colors.
- We form the graph with vertex-set (v_i, C_j) and
  - edges between (v_i, C_j) and $(v_i, C_{j'})$
  - edges between (v_i, C_j) and $(v_{i'}, C_j)$ if there is an edge between v_i and $v_{i'}$ of color C_j

  We get a graph with kN vertices.

Edge colored graphs

- The picture obtained is:

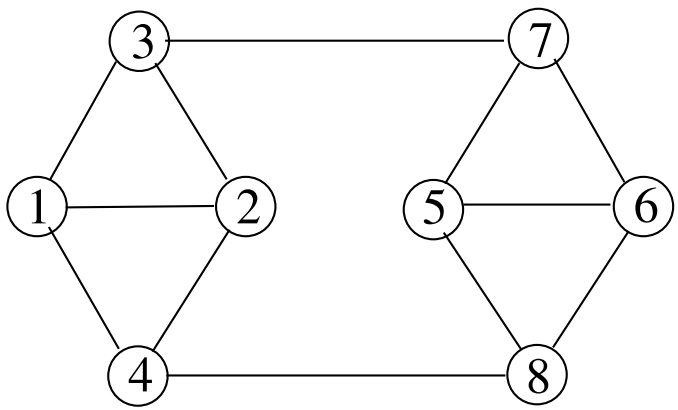


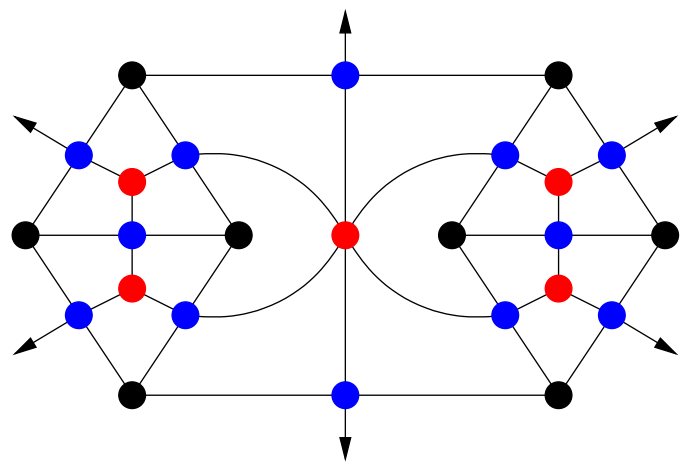
- Actually, one can do better, if the binary expression of j is $b_1 \dots b_r$ with $b_i = 0$ or 1 then we form the graph with vertex-set (v_i, l), $1 \leq l \leq r$ and
  - edges between (v_i, l) and (v_i, l')
  - edges between (v_i, l) and $(v_{i'}, l)$ if the binary number b_l of the expression of C_j is 1.

  This makes a graph with $\lceil \log_2(k) \rceil N$ vertices.

Plane graphs

- If G is a simple 3-connected plane graph then the skeleton determine the embedding, we can forget the faces.
- If G has multiple edge and/or is not 3-connected we consider the graph formed by its vertices, edges and faces with adjacency given by incidence





- This idea extends to partially ordered sets, face lattices, etc.

III. Canonical forms

Canonical form

- One possible canonical form of a graph is obtained by taking the lexicographic minimum of all possible adjacency matrix of a given graph.
- Partition backtrack algorithms provide a way to get a canonical form of a given graph. This will varies from program to program and with option chosen.
- Suppose that one has N different graphs from which we want to select the non-isomorphic ones:
  - If one do isomorphism tests then at worst we have $\frac{N(N-1)}{2}$ tests.
  - If one computes canonical forms, then we have N canonical form computation and then string equality tests.

  This is a key to many computer enumeration goals.
- The runtime of canonical form computation is about the same as computing the automorphism group.

IV. Positive definite form

Problem setting

- For given $n \geq 2$ define $S^n_{>0}$ the set of positive definite quadratic forms.
- The group $\mathrm{GL}_n(\mathbb{Z})$ acts on $S^n_{>0}$ by

$$(P, A) \to PAP^T$$

  Quadratic forms are used in lattice theory for covering, packing, etc.
- For $x \in \mathbb{R}^n$ define $A[x] = xAx^T$
- There is a canonical form via the Minkowski reduction theory but it is hard to compute.
- A canonical form function is just as useful in this field of computational mathematics.
- There is an existing program (AUTO/ISOM) by Plesken & Souvignier for computing the stabilizer and isomorphism.

Using shortest vectors

- For $A \in S^n_{>0}$ and $\lambda > 0$ define

$$\mathrm{Min}_\lambda(A) = \{x \in \mathbb{Z}^n \text{ s.t.} A[x] \leq \lambda\}$$

- Define

$$Span(A) = \{\text{smallest } \lambda \text{ s.t. } \mathrm{Min}_\lambda(A) \ \mathbb{Z}\text{-spans } \mathbb{Z}^n\}$$

- For $A \in S^n_{>0}$ define the edge weighted graph $G(A)$ over $Span(A)$ with edge weight $w(v, v') = v' A v^T$.
- The edge weighted graph can be converted into a vertex colored graph $G_2(A)$.
- The vertices of $G(A)$ correspond to disjoint sets of vertices in $G_2(A)$.
- Thus we can order the sets of vertices in $G_2(A)$ by $\min(S) < \min(S')$.
- And so we have a canonical ordering of the vectors $Span(A)$.

Canonical spanning set

- Given a family of vector $(v_i)_{1 \le i \le N}$ we want to find a $\mathbb{Z}$-basis $\mathcal{B}$ of it.
- We want a function $Basis(\mathcal{V})$ such that $Basis(\mathcal{V}P) = Basis(\mathcal{V})P$ for $P \in \mathrm{GL}_n(\mathbb{Z})$.
- We start with $\mathcal{B} = \emptyset$ and add vectors one by one starting from v_1, ending with v_N.
  - If v_i is $\mathbb{R}$-linearly independent from $\mathcal{B}$ then we insert it into $\mathcal{B}$.
  - If v_i is belongs to the $\mathbb{Z}$-span of $\mathcal{B}$ then we do nothing.
  - If v_i does not belong to the $\mathbb{Z}$-span of $\mathcal{B}$ and is $\mathbb{R}$-linearly independent then take $\beta > 0$ the smallest integer such that

$$\beta v_i = \sum_{v \in \mathcal{B}} \alpha_v v \text{ with } \alpha_v \in \mathbb{Z}$$

    The α and α_v are uniquely determined and invariant under linear transformation.
    We then extract a $\mathbb{Z}$-basis from this and change $\mathcal{B}$ accordingly.
- $Span(A)$ spans $\mathbb{Z}^n$ so $P = (Basis(Span(A)))^{-1} \in \mathrm{GL}_n(\mathbb{Z})$.
- The canonical form is then PAP^T.

Extension 1: Symplectic group

- We are interested in the group $G = \mathrm{Sp}(2n, \mathbb{Z})$ defined as

$$G = \left\{ M \in \mathrm{GL}_{2n}(\mathbb{Z}) \text{ s.t. } MJM^T = J \right\} \text{ with } J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$$

- So, for a positive definite matrix $A \in S^{2n}_{>0}(\mathbb{R})$ we take the canonical form in $\mathrm{GL}_{2n}(\mathbb{Z})$ and the matrix $P = (Basis(Span(A)))^{-1}$.
- We take $B = PJP^T$ which is a priori different from J.
- The matrix B is integral antisymmetric. We can find a matrix $U \in \mathrm{GL}_{2n}(\mathbb{Z})$ such that $B = UJU^T$ [Hint: Do operations on rows and column at the same time].
- We have $W = U^{-1}P \in \mathrm{Sp}(2n, \mathbb{Z})$ and the canonical form is

$$WAW^T$$

Extension 2: Finite index subgroups of $\mathrm{GL}_n(\mathbb{Z})$

- The approach for the symplectic group can be considered to other subgroups G of $\mathrm{GL}_n(\mathbb{Z})$.
- Since G is of finite index we have a coset decomposition

$$\mathrm{GL}_n(\mathbb{Z}) = \cup_{i=1}^{m} g_i G$$

- Consider a positive definite form $A \in S^n_{>0}$ and take the canonical form PAP^T.
- The element P corresponds to one coset $g_{i_0} G$. The canonical form is then

$$(g_{i_0}^{-1} P) A (g_{i_0}^{-1} P)^T$$

- The problem is that this is not a practical algorithm right now:
  - The coset representatives g_i have to be chosen
  - It is difficult to find which coset the element belongs to.

Other extensions?

- Another aspect is that we would like to use vector sets that are not necessarily $\mathbb{Z}$-basis. This would require a canonical form for group action on sets.
- It is not likely to obtain an uniform description for finite index subgroups of $\mathrm{GL}_n(\mathbb{Z})$. But what special finite index subgroups could be doable?
  For subgroups G of $\mathrm{GL}_n(\mathbb{Z})$ preserving a finite list of n-dimensional lattices $L_1, \ldots, L_m$ we have generalization of stabilizer/isomorphy formalism.
- Number rings are also important.
  For number rings which are Euclidean, e.g. Gaussian integers we could have further generalization.

THANK YOU