Permutation Groups Associated to a Complete Invariant for Graphs

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Graphs and Digraphs

A *digraph* is a pair $\Gamma = (V, E)$, where V is the set of *vertices* (or *nodes*), and is the set of edges $E \subseteq V \times V$.
(A digraph just a relation E on V.)

The *reverse edge* to $e = (x, y) \in E$ is $\bar{e} = (y, x)$
An *(undirected) graph* is a vertex set V and set of undirected edges (pairs of nodes $\{x, y\}$). To a graph $\Gamma = (V, E)$ we associate a directed graph $\Gamma' = (V, E')$ with edges $(x, y) \in E'$ if $\{x, y\}$ is an edge of Γ.

Clearly, digraphs closed under reversing edges are "the same" as (un)directed graphs. (Digraphs closed under reverse are just symmetric relations on their node set V.) We identify (undirected) graphs with directed graphs closed under reversing edges.
*(Undirected) graphs are a full subcategory of digraphs.

Spectrum of Graph

Algebraic graph theory considers finite (di)graphs without self-loops. That is, $(v, v) \notin E$.

The *adjacency matrix* $A = A(\Gamma)$ of $\Gamma = (V, E)$ is a matrix of 0's and 1's with $A_{x,y} = 1$ iff $(x, y) \in E$.

The multiset of eigenvalues of A is called the *spectrum* of A.

Theorem. The spectrum of graphs and digraphs is invariant for isomorphic (di)graphs.

Proof: Any graph isomorphic to Γ has adjacency matrix obtained from $A(\Gamma)$ by permuting its rows and columns. This does not change the determinant of $A - \lambda I$, so the characteristic polynomial and spectrum is fixed. □

Co-spectral Graphs

The spectrum is a very useful too for analysis of graphs and networks. The spectrum determines many properties of the graph....

But there exist so-called *co-spectral graphs*, i.e. non-isomorphic graphs with the same spectrum, e.g. $K_{1,4}$ and $C_4 \sqcup K_1$.

That is, spectrum is not a *complete invariant* for graphs or digraphs.

(And the proportion of cospectral graphs grows with size of V ... E.g., it is eventually more than the number of regular graphs...)

Elementary Collapsings of Directed Edges

Let $\Gamma = (V, E)$ be a digraph (without self-loops).

To each edge $e = (x, y)$ of Γ we associate an *elementary collapsing* function $T_{x,y}$ (or T_e) on the set of nodes V:

$T_e : V \to V$ is defined by

$$T_e(x) = y \text{ and } T_e(v) = v \text{ for } v \in V \setminus \{x\}.$$

We say a mapping $f : V \to V$ has *defect k* if $|f(V)| = |V| - k$.

T_e is an idempotent mapping of *defect 1*. That is, its image has cardinality $|V| - 1$. Permutations have defect 0.

Semigroup of Flows on a Graph

Now define the *transformation semigroup* of a digraph Γ to be the collection of transformations of V generated by the T_e $(e \in E)$. That is,

$$S(\Gamma) = \langle T_{x,y} \in V^V \mid (x, y) \text{ is an edge of } \Gamma \rangle.$$

This is also called the *semigroup of flows* on Γ.

Theorem. $S(\Gamma)$ is an invariant for graphs and for digraphs.

Proof: Isomorphic (di)graphs obviously have isomorphic semigroups of flows. □

Complete Invariance for Graphs

Main Theorem (Nehaniv-Rhodes).

1. There exist non-isomorphic digraphs with the same flow semigroup.
2. $S(\Gamma)$ is a complete algebraic invariant for undirected graphs.

Elementary Collapsings in the Flow Semigroup

Lemma.
If $T_{x,y} = T_{x_1,y_1} \cdots T_{x_k,y_k}$, then $T_{x,y}$ or $T_{y,x}$ appears among the T_{x_i,y_i}. In fact, it appears as T_{x_1,y_1}.

Corollary. If $T_{x,y} \in S(\Gamma)$ then either $e = (x, y)$ or $\bar{e} = (y, x)$ is an edge of Γ.

This shows we can recover the undirected edges of Γ from its flow semigroup.
This proves (2) of the Main Theorem, i.e. $S(\Gamma)$ is a complete invariant for graphs.

Reversing Edges in Directed Cycles.

For (1) of the Main Theorem : Let Δ be the directed n-cycle with n nodes and edges $(1,2)$, .. $(n-1,n)$, and $(n,1)$. Observe that $W = T_{n,1}T_{n-1,n}T_{n-2,n-1}\ldots T_{1,2}$ maps i to $i+1$ unless $i=n$ which it maps to 2 (like 1). Thus, $W = (2,3,\ldots n-1,n)T_{1,2}$. So W^{n-1} is the identity on $V \setminus \{1\}$ but sends 1 to n. That is,

$$W^{(n-1)} = T_{1,n}.$$

So if we add the reverse edge $(1,n)$ to Δ then $S(\Delta)$ is unchanged. This proves (1).

It follows that

Theorem. For any directed cycle in a digraph, we may add the reverse of any edge in the cycle without changing the flow semigroup.

Caveat

NB: It is the transformation semigroup that is the complete invariant for graphs, not just the semigroup. For instance, given any graph Γ , the graph $\Gamma \sqcup K_1$ with a new, isolated node has an isomorphic semigroup to $S(\Gamma)$. Their transformation semigroups are not isomorphic, since one acts on $|V|$ points and the other on $|V| + 1$ points.

Induced Subgraphs

Theorem If Γ' is a subgraph of Γ, then $S(\Gamma')$ is a sub-transformation semigroup of $S(\Gamma)$.

Cf. Interlacing theorem for the spectrum of graphs.

For biochemical reactions, transitions are modelled as products of commuting elementary collapsings, $f = \prod T_{a,b}$, where $T_{x,y}$ and $T_{y,z}$ do not both occur among the $T_{a,b}$ for any x,, y, and z. Notice that these are idempotents. Any transformation semigroup generated by these is obviously a sub-transformation semigroup of the flow semigroup of the underlying digraph.

Permutator Groups

If $e^2 = e$ is an idempotent $S(\Gamma)$. Let $X_e = V \cdot e = \{v \cdot e \,|, \, v \in V\}$ be its image. Let G_e be the (unique) maximal subgroup of $S(\Gamma)$ containing e.

Then (X_e, G_e) is the (faithful) *permutator group* of subset X_e and consists of defect k maps on the vertices, where $k = |V| - |X_e|$.

Theorem. The defect k permutator groups (up to isomorphism) are invariants for digraphs.

Finding the Defect k Permutator Groups

The Defect k Digraph of Digraph Γ. Let D_k be the digraph with nodes $V \cdot f = f(K)$ with $f^2 = f \in S(\Gamma)$ having defect k (for $1 \leq k \leq |V| - 2$). Then e in Γ is a edge from X to Y in D_k if and only $X \cdot T_e = Y$. That is, T_e maps the elements of X one-to-one onto Y.

Proposition (Rhodes).
The permutator group G_e is generated by all directed cycles in D_k starting at X_e.

Constructing $S(\Gamma)$ from the Defect k Groups

Theorem Let Γ be a digraph with n nodes. Then $S(\Gamma)$ divides a cascade of $H_{n-2} \wr \cdots \wr H_1$, where H_i is a direct product or (partial) coproduct of defect i groups with constant maps adjoined.
(One needs permutator groups in H_k per strongly connected component of the D_k.)
Proof: Apply the holonomy decomposition theorem to $S(\Gamma)$ □

Remark. If Γ is connected at most one defect k group occurs at each level.

Corollary Krohn-Rhodes complexity of $S(\Gamma)$ is at most $|V| - 2$ for $|V|$ node (di)graphs.

Defect k Groups in Particular Graphs

What do these decompositions look like for particular graphs?

If the graph is a nontrivial simple closed walk with n nodes then C_{n-1} occurs as a permutation group of defect 1 in $S(\Gamma)$ (as a subtransformation semigroup). Moreover, C_{n-k} occurs as a permutation group of defect k in $S(\Gamma)$ acting on successively smaller state sets for $k = 1, 2, ..., n-2$.

If the closed walk is crossed by an edge, then the alternating group A_{n-1} or the symmetric group S_{n-1} occurs at defect 1, and S_{n-k} occurs too in subgroup permutation groups of $S(\Gamma)$ acting on successively smaller state sets for $k = 2, ..., n-2$.

Surprise: $K_{1,n}$ is a tree, an acyclic graph, but $S(K_{1,n})$ has nontrivial subgroups, although not of defect 1, corresponding to 'swap' operations using temporary storage for defect 2 for $n \geq 3$.

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