Graphs with singular adjacency matrix

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Jiaotong University Shanghai, April 2019

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SINGULAR GRAPHS

Let $\Gamma$ be a graph with adjacency matrix $A$. Then $\Gamma$ is singular if $A$ is a singular matrix. Alternatively, the graph is singular if its spectrum contains the eigenvalue 0. All graphs in this talk are finite, undirected, without loops and without multiple edges.

Singular graphs are significant in applied mathematics, physics and chemistry, and combinatorics and group theory.

We begin with a general discussion of singularity and applications. In some cases the singularity problem can be solved for graphs with 'large' automorphism group.

This includes certain Cayley graphs where the character theory of automorphism groups can be used to decide singularity.
Number of singular graphs on \( n \) vertices:

Invertible Adjacency Matrix, Unlabelled Graphs, A109717
\[0, 1, 1, 4, 9, 57, 354, 5795, 141494, 7866527, 728952205\]

Singular Adjacency Matrix, Unlabelled Graphs, A133206
\[1, 1, 3, 7, 25, 99, 690, 6551, 133174, 4138641, 290045659\]

Some Reasons for Singularity: (1) Isolated vertices;

(2) **High average degree** forces dependent columns;

(3) **Unequal parts** for bipartite graphs: Here \( V = V' \cup V'' \) and accordingly \( A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \) is a blocked matrix. It has rank \( \leq 2 \min\{|V'|, |V''|\} \leq |V| \). Hence \( \Gamma \) is **singular if** \( |V'| \neq |V''| \).

(4) **No recursions known** for frequency of non-singular graphs
PROGRAMME

1 Random Graphs $\Gamma(n,p)$
2 Applications in Mechanics
3 Incidence Structures and Incidence Graphs
4 Cayley Graphs
5 Singular Graphs and Finite Simple Groups
6 Some Ideas about Proofs
1: Random Graphs $\Gamma(n, p)$

**Probabilistic Graph Theory:** Let $0 < p < 1$. Then the graph $\Gamma$ on $n$ vertices is an **Erdős-Rényi $\Gamma(n, p)$ random graph** if for every pair of vertices of $\Gamma$ probability to be linked by an edge is $p$. What happens in the random case?

**Theorem 1.1** (Costello, Vu, 2008) Let $c > 1$ be a constant and suppose that $c \ln(n)/n < p < 1/2$. Then a $\Gamma(n, p)$ random graph is **almost surely non-singular**.

Let $0 < \epsilon < 1$ and suppose that $p < (1 - \epsilon) \ln(n)/n$. Then a $\Gamma(n, p)$ random graph is **almost surely singular**.

(Kahn, Komlós, Szemerédi, 1995; Tao, Vu 2006, 2007; )
Discrete Mechanics: Let $S$ be a system of nodes and links for which 'energy' is defined in some way. Classically it is known that its Laplacian operator involves the spectrum of an underlying graph $\Gamma = \Gamma(S)$.

![Graph of a hydro-carbon molecule](image)

The graph $\Gamma(S)$ (on 12 vertices) underlying this hydro-carbon molecule has eigenvalues $\pm 1 \pm \sqrt{2}$, $\frac{1}{2}(\pm 1 \pm \sqrt{5})$ and $\frac{1}{2}(\pm 1 \pm \sqrt{5})$. So, non-singular.
It is confirmed experimentally that singular graphs $\Gamma = \Gamma(S)$ give rise to **unstable or non-existing molecules, and so to explosive chemicals!**

For instance, an $n$-cycle with $n$ divisible by 4 is singular. (Indeed, 4 or 8-cycles for molecules are very rare in chemistry ?!)


A sense of such instability is captured in the following balance condition:

**Theorem 2.1** (A Sultan Tarimshawy, 2018) Let $\Gamma$ be a graph with vertex set $V$, without isolated vertices. Then $\Gamma$ is singular if and only if there are non-empty disjoint subsets $X, Y \subseteq V$ and a function $f: X \cup Y \rightarrow \{1, 2, 3, \ldots\}$ such that

$$\sum_{v \sim x \in X} f(x) = \sum_{v \sim y \in Y} f(y)$$

for all $v \in V$. (Here $v \sim x$ means that $v$ is adjacent to $y$ in $\Gamma$.)

**Proof:** Consider a vector $x$ with $Ax = 0$. \(\square\)
3: Incidence Structures and Incidence Graphs

Let $P$ and $B$ be sets, and let $I \subseteq P \times B$. Then $S := (P, B; I)$ is an **incidence structure** with point set $P$ and block set $B$. Here $p$ is **incident** with $b$ iff $(p, b \in I)$. Incidence structures are the **basic objects of geometry**, going back to Euclid.

The structure defines a bi-partite **incidence graph** $\Gamma(S)$ on $V = P \cup B$ where $v \sim b$ iff $v$ is incident with $b$. Its incidence matrix is

\[
A = \begin{pmatrix}
0 & I \\
I^T & 0
\end{pmatrix}
\]

if we interpret $I \subseteq P \times B$ as a $(0, 1)$-matrix. Clearly $\text{rank}(A) \leq 2 \min\{|P|, |B|\}$.

**Many problems in combinatorics** are concerned with the case $\text{rank}(A) = 2 \min\{|P|, |B|\}$. Such structures are said to have **maximum rank**.
For incidence graphs singularity is too crude. Instead we should look at **spectrum** of the incidence graph, and the **nullity** of the incidence matrix.

**Example:** Let \( \mathbb{D} := (P, B; I) \) be a 2-design. Then we determine numbers \( \mu_1 > \mu_2 > 0 \) from the parameters of \( \mathbb{D} \). This is easy, see next page. The spectrum of \( \mathbb{D} \) then is

\[
\pm \sqrt{\mu_1} \binom{1}{1}, \pm \sqrt{\mu_2} \left( |P| - 1 \right), \ 0 \left( |B| - |P| \right),
\]

the exponents are the multiplicities. We see that \( \mathbb{D} = (P, B; I) \) has **maximum rank**. Further, it is **singular** iff \( |B| > |V| \).

To confirm this, compute

\[
A^2 = \left( \begin{array}{c|c} 0 & I \\ \hline I^T & 0 \end{array} \right)^2 = \left( \begin{array}{c|c} I \cdot I^T & 0 \\ \hline 0 & I^T \cdot I \end{array} \right)
\]
For a 2-design we have

\[ I \cdot I^T = \begin{pmatrix} r & \lambda & \ldots & \lambda \\ \lambda & r & \ldots & \lambda \\ \vdots & \vdots & \ddots & \vdots \\ \lambda & \lambda & \ldots & r \end{pmatrix} \]

and so we get the spectrum of \( I \cdot I^T \). For the remainder use the

**Lemma 3.1** For a real matrix \( X \), the non-zero part of \( \text{spec}(XX^T) \) is the same as the non-zero part of \( \text{spec}(X^TX) \).

Let \( (\mathcal{P},<) \) be a **ranked partially ordered set**. (Say, all subspaces of a finite vector space, ordered by inclusion.)

For \( t < k \) let \( \mathcal{P}_{t,k} \) be the induced incidence structure between elements of rank \( t \) and rank \( k \), and let \( \Gamma(\mathcal{P}_{t,k}) \) be the corresponding incidence graph.
The spectrum of $\Gamma(\mathcal{P}_{t,k})$ is known in many cases, including the Boolean Lattice and finite projective spaces. In these examples $\mathcal{P}_{t,k}$ has maximum rank for all $t \leq k$.

With B Summers (2017) we have studied the face poset of the $n$-dimensional hyperoctahedron, closely related to the Boolean algebra. We show that for certain parameter pairs $(t, k)$ the incidence structure $\mathcal{P}_{t,k}$ does not have maximum rank.

When does $\mathcal{P}_{t,k}$ have of maximum rank for your favourite poset? In general this question will remain difficult. It is linked to many deep problems in mathematics.
4: Cayley Graphs

Let $G$ be a finite group with identity element 1. Let $H$ be a subset of $G$. Then $H$ is a connecting set for $G$ if:

(i) 1 does not belong to $H$,
(ii) $H^{-1} := \{h^{-1} | h \in H\} = H$ and
(iii) $H$ generates $G$.

Define the graph $\Gamma = \text{Cay}(G,H)$ on the vertex set $V = G$ by calling two vertices $u,v \in G$ adjacent if there is some $h$ in $H$ with $hu = v$, using multiplication in $G$. **Note:** By the first condition $\Gamma$ has no loops, by the second conditions all edges are undirected, by the last condition $\Gamma$ is connected.

- Xiaogang Liu, Sanming Zhou, Eigenvalues of Cayley Graphs, arXiv Jan 2019
Cayley graph on \( G \) with connecting set \( H \). For group theory and representation theory is useful to change notation slightly:

\[ V = G, \text{ the elements of the group } G \]

\[ \mathbb{R}^n, \mathbb{C}^n \leftrightarrow \mathbb{C}V = \{ \text{all formal sums } f = \sum_{v \in V} f_v v \text{ with } f_v \in \mathbb{C} \} \]

\[ A \leftrightarrow \alpha : \mathbb{C}V \rightarrow \mathbb{C}V, \text{ the adjacency map, defined by } \]

\[ \alpha(v) := \sum_{h \in H} h^{-1}v \in \mathbb{C}V \text{ for all vertices } v \in V. \] (1)

**Notice, (1):** \( u \) is a neighbour of \( v \), by definition, if and only if \( hu = v \) for some \( h \in H \), so \( u = h^{-1}v \);

**Notice also (2):** for \( g \in G \), the map \( v \mapsto vg \) (right multiplication) is an automorphism, since \( hu = v \) implies \((hu)g = vg\).
5: Singular $\text{Cay}(G, H)$ for simple groups

Given a group $G$, do there exist connecting sets $H$ so that $\text{Cay}(G, H)$ is singular?

We say that $H$ is **G-invariant** if $gH = Hg$ for all $g \in G$. For instance, if $G$ is a simple group then any $G$-invariant subset generates $G$, so satisfies (iii) of the connecting set definition.

A **representation** of $G$ is a homomorphism $\rho : G \rightarrow \text{GL}(W)$ for some vector space $W \neq \{0\}$ over $\mathbb{C}$.

It is **irreducible** if the only subspace $U$ of $W$ that is left invariant under all $\rho(g)$, for $g \in G$, is $U = \{0\}$.

The **character** of $\rho$ is the function $\chi : G \rightarrow \mathbb{C}$ given by $\chi(g) = \text{trace}(\rho(g))$. It is **irreducible** if the representation $\rho$ irreducible.
We have the following results on singular Cayley graphs (recall, graphs for which 0 is an eigenvalue) when the connecting set is $G$-invariant:

**Theorem 5.1 (P Zieschang 1988, JS & A Zaleskii 2019)**

Let $G$ be a group with $G$-invariant connecting set $H$. Then $\text{Cay}(G, H)$ is singular if and only if $G$ has an irreducible character $\chi$ with

$$\sum_{h \in H} \chi(h) = 0.$$ 

In particular, if $H = \{g^{-1}hg \mid g \in G\}$ for some $h \in G$ then $\text{Cay}(G, H)$ is singular if and only if $G$ has an irreducible character $\chi$ such that $\chi(h) = 0$.

**Comments:** 1. For instance, if $\chi(h) = 0$ for all $h \in H$, then $\text{Cay}(G, H)$ is singular. (The character $\chi$ **vanishes** on $H$.)
2. By Burnside’s theorem on character zeros every irreducible character $\chi$ of degree $> 1$ vanishes for some $h \in G$.

**Theorem 5.2 (JS & A Zaleskii 2019)** Let $G$ be a non-abelian group. Then there exists a singular Cayley graph on $G$ for some suitable connecting set $H$.

**Comment 3:** If the character table for $G$ is known explicitly (say, for all sporadic simple groups $G$) then one can determine all singular Cayley graphs $(G, M \cup M^{-1})$ for $G$-invariant $M$.

**Theorem 5.3 (JS & AZ)** Let $p > 3$ be a prime. Let $G$ be a non-abelian simple group and $M \subset G \setminus \{1\}$ a $G$-invariant subset so that all elements in $M$ have order divisible by $p$. Then $\text{Cay}(G, M \cup M^{-1})$ is singular. This remains true for $p = 2, 3$ unless $G$ is an alternating group or a sporadic simple group.
**Comment 4:** The exceptions occur for alternating groups $A_n$ with $n = 7, 11, 13$, possibly other $n$ as well.

**Theorem 5.4 (JS & AZ)** Let $G = A_n$ with $n \geq 4$ and let $M \subset G$ be any set of non-real elements. Then there exists an irreducible character of $G$ that vanishes on all elements of $M$. Furthermore, $H = M \cup M^{-1}$ is a connecting set and $\text{Cay}(G, H)$ is singular.
6: Proofs

The first comment applies to any graph $\Gamma$. Its adjacency matrix gives rise to a linear map

$$A: \mathbb{R}^n \to \mathbb{R}^n.$$ 

As $A$ is symmetric all eigenvalues are real. Let the distinct eigenvalues be $\mu_1, \ldots, \mu_s$. Then $\mathbb{R}^n$ decomposes into eigenspaces for $A$,

$$\mathbb{R}^n = E_1 \oplus E_2 \oplus \cdots \oplus E_s$$

where $E_i$ is the eigenspace of $\mu_i$, for $1 \leq i \leq s$.

With Fenjin Liu we are working to improve this fundamental statement. We suggest that one should replace $\mathbb{R}$ of $\mathbb{C}$ by the splitting field of the characteristic polynomial of $G$. Only this will reveal the action of the Galois group on these spaces.
The next comment is that any automorphism $g$ of $G$ gives a linear map $g : \mathbb{C}V \rightarrow \mathbb{C}V$ which preserves eigenspaces. That is, $g(E_i) = E_i$ for all $1 \leq i \leq s$. We therefore have a fundamental fact:

**The automorphism group of $\Gamma$ decomposes each eigenspace of $\Gamma$ into a sum of irreducible modules for this group.**

This becomes particularly useful when the graph has a 'large' automorphism group. The presentation theory of groups is very highly developed!

For Cayley graphs $\text{Cay}(G, H)$ we are certainly in this fortunate situation: The kernel of $A$ is a sum of irreducible modules of $G$. 
For Cayley graphs $\text{Cay}(G, H)$ with $G$-invariant connecting set $H$ the theorem of Zieschang is the right starting point and the key to the results in our paper.

However, if $H$ is not $G$-invariant then no results seem to be available currently. This leads to many open questions:

1. Characterize the spectrum and nullity of Cayley graphs when the connecting set $H$ which is not $G$-invariant.

2. Extend these results to vertex-transitive graphs.

Thank You!