Isospectral Graph Reductions

Leonid Bunimovich

Outline

1. Graphs Reductions
   - Networks and Graphs
   - Definitions
   - Graph Reductions
   - Main Results
2. Eigenvalue Estimation
   - Gershgorin's Theorem
   - Brauer's Theorem
   - Brualdi's Theorem
3. Summary and Implications
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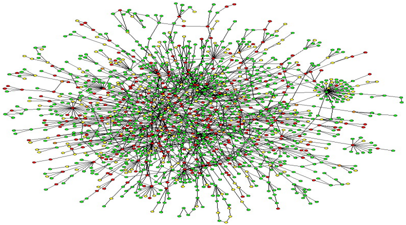
Network Structure

Typical real networks are defined by some large graph with complicated structure [2,8,11].

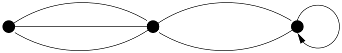


E.coli metabolic network

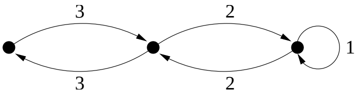
Question: To what extent can this structure be simplified/reduced while maintaining some characteristic of the network?

The collection of graphs $\mathbb{G}$

The graph of a network may or may not be directed, weighted, have multiple edges or loops.



Each such graph can be considered a weighted, directed graph without multiple edges possibly with loops.



Let $\mathbb{G}$ be the collection of all such graphs.

The collection of graphs $\mathbb{G}$

Definition

A graph $G \in \mathbb{G}$ is triple $G = (V, E, \omega)$ where V is its vertices, E its edges, and $\omega : E \to \mathbb{W}$ where $\mathbb{W}$ is the set of *edge weights*.

An important characteristic of a network/graph is the spectrum of its weighted adjacency matrix [1,3,10].

Weighted Adjacency Matrix

Definition

If $G = (V, E, \omega)$ where $V = \{v_1, \dots, v_n\}$ and e_{ij} is the edge from v_i to v_j the *weighted adjacency matrix* $M(G) = M(G, \lambda)$ of G is

$$M(G,\lambda)_{ij} = \begin{cases} \omega(e_{ij}) \text{ if } e_{ij} \in E \\ 0, \ \text{otherwise} \end{cases}.$$

Question: How can the number of vertices in a graph be reduced while maintaining the eigenvalues, including multiplicities, of its adjacency matrix?

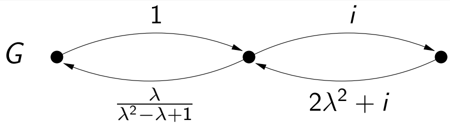
Spectrum of a Graph $G \in \mathbb{G}$

Definition

Let $\mathbb{C}[\lambda]$ be the polynomials in the variable λ with complex coefficients. Define $\mathbb{W}$ to be the rational functions of the form p/q where $p, q \in \mathbb{C}[\lambda]$ such that p and q have no common factors.

Definition

For $G \in \mathbb{G}$ let $\sigma(G)$ denote the *spectrum* of G or the set $\{\lambda \in \mathbb{C} | \det(M(G,\lambda) - \lambda I) = 0\}$ including multiplicities.



$$\sigma(G) = \{1, \pm\sqrt{(1-2i)/5}\}$$

Structural Sets

Definition

For $G = (V, E, \omega)$ the nonempty vertex set $S \subseteq V$ is a *structural set* of G if each nontrivial cycle of G contains a vertex of S. We denote by $st(G)$ the set of all structural sets of G.

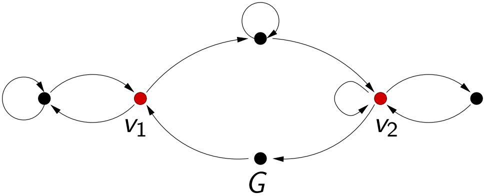


Figure: $S = \{v_1, v_2\}$ a structural set of G

Structural Sets

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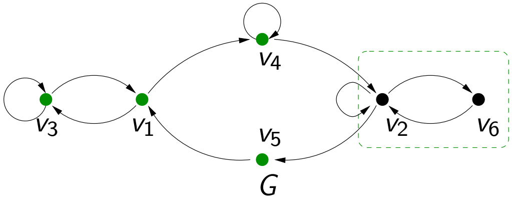


Figure: $T = \{v_1, v_3, v_4, v_5\}$ **not** a structural set of G

Branches

Definition

For $G = (V, E)$ with $S = \{v_1, \ldots, v_m\} \in st(G)$ let $\mathcal{B}_{ij}(G, S)$ be the set of paths or cycles from v_i to v_j having no interior vertices in S. Furthermore, let $\mathcal{B}_S(G) = \bigcup_{1 \leq i,j \leq m} \mathcal{B}_{ij}(G, S)$ be the *branches* of G with respect to S.

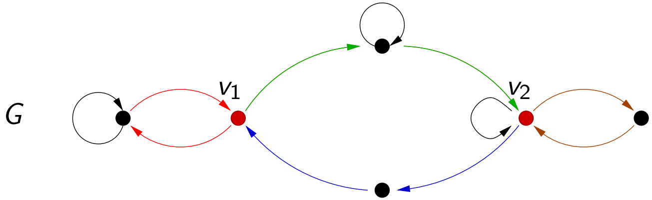


Figure: Branches of $\mathcal{B}_S(G)$ each colored either red, brown, green, or blue.

Branch Products

Definition

Let $G = (V, E, \omega)$ and $\beta \in \mathcal{B}_S(G)$. If $\beta = v_1, \dots, v_m$, $m > 2$ and $\omega_{ij} = \omega(e_{ij})$ then

$$\mathcal{P}_\omega(\beta) = \frac{\prod_{i=1}^{m-1} \omega_{i,i+1}}{\prod_{i=2}^{m-1}(\lambda - \omega_{ii})}$$

is the *branch product* of β. If $m = 2$ then $\mathcal{P}_\omega(\beta) = \omega_{12}$.

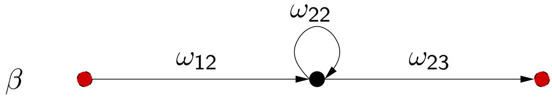


Figure: $\mathcal{P}_\omega(\beta) = \frac{\omega_{12}\omega_{23}}{\lambda - \omega_{22}}$.

Reductions of $G \in \mathbb{G}$

Definition

For $G = (V, E, \omega)$ with structural set $S = \{v_1 \ldots, v_m\}$ let $\mathcal{R}_S(G) = (S, \mathcal{E}, \mu)$ where $e_{ij} \in \mathcal{E}$ if $\mathcal{B}_{ij}(G, S) \neq \emptyset$ and

$$\mu(e_{ij}) = \sum_{\beta \in \mathcal{B}_{ij}(G,S)} \mathcal{P}_\omega(\beta), \quad 1 \leq i, j \leq m.$$

We call $\mathcal{R}_S(G)$ the *isospectral reduction* of G over S.

Note: $\mathcal{R}_S(G) \in \mathbb{G}$ for all $S \in st(G)$.

Reduction Example

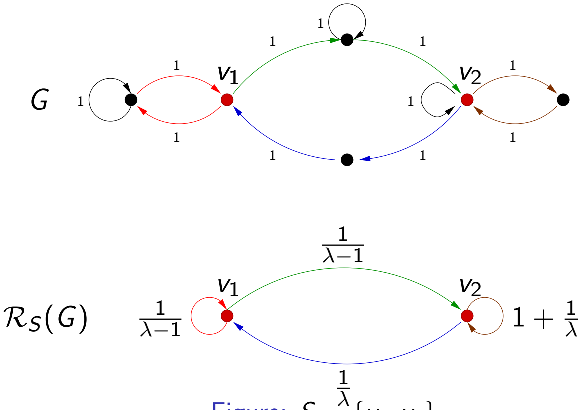


Figure: $S = \{v_1, v_2\}$

Alternate Reduction

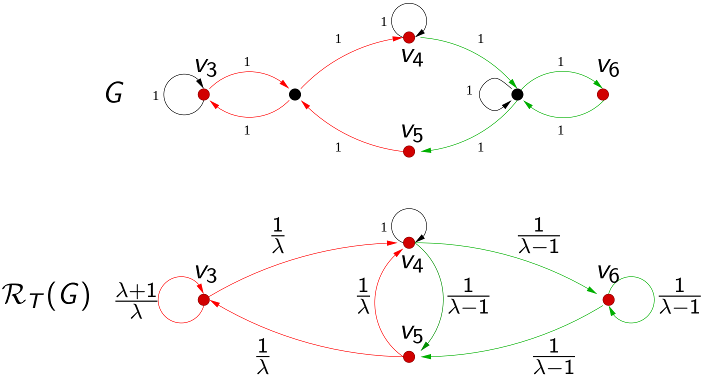


Figure: $T = \{v_3, v_4, v_5, v_6\}$

Difference in Spectrum

Question: How are $\sigma(G)$ and $\sigma(\mathcal{R}_S(G))$ related?

Theorem: (Bunimovich, Webb [6])

For $G = (V, E, \omega)$ and $S \in st(G)$

$$det\big(M(\mathcal{R}_S(G)) - \lambda I\big) = \frac{det\big(M(G) - \lambda I\big)}{\prod_{v_i \in \bar{S}}(\omega_{ii} - \lambda)}$$

where $\bar{S}$ is the complement of S in V.

The $\mathcal{N}_S^{\pm}$ Sets

Definition

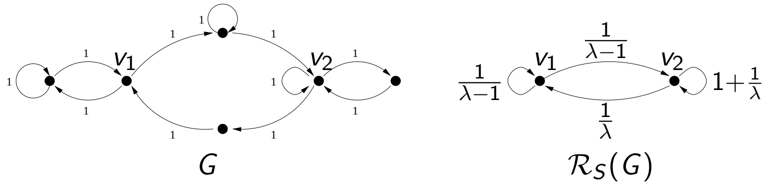
For $G = (V, E, \omega)$, $S \in st(G)$, and $S(\lambda) = \prod_{v_i \in \bar{S}}(\omega_{ii} - \lambda)$ let
(i) $\mathcal{N}_S^- = \{\lambda \in \mathbb{C} : S(\lambda) = 0\}$ and
(ii) $\mathcal{N}_S^+ = \{\lambda \in \mathbb{C} : S(\lambda) \text{ is undefined}\}$
where both sets include multiplicities.

Corollary: (Bunimovich, Webb)

Let $G \in \mathbb{G}$ with $S \in st(G)$. Then

$$\sigma(\mathcal{R}_S(G)) = \left(\sigma(G) \setminus \mathcal{N}_S^-\right) \cup \mathcal{N}_S^+.$$

Main Result (Example)



$$\sigma(G) = \{2, -1, 1, 1, 0, 0\}$$

$S(\lambda) = \lambda^2(1-\lambda)^2$ implying $\mathcal{N}_S^- = \{1, 1, 0, 0\}$, and $\mathcal{N}_S^+ = \emptyset$.

Hence, $\sigma(\mathcal{R}_S(G)) = \{2, -1\}$.

Sequential Reductions

As $\mathcal{R}_S(G) \in \mathbb{G}$ it may possible to further reduce $\mathcal{R}_S(G) \in \mathbb{G}$.

Question: To what extent is the structure of a graph preserved under different sequential reductions?

Commutativity of Sequential Reductions

Definition

Let $\mathcal{R}(G;S_1,\dots,S_m)$ be the graph G reduced first over S_1, then S_2 and so on up to the vertex set S_m. If this can be done we say $S_1,\dots,S_m$ *induces a sequence of reductions* on G.

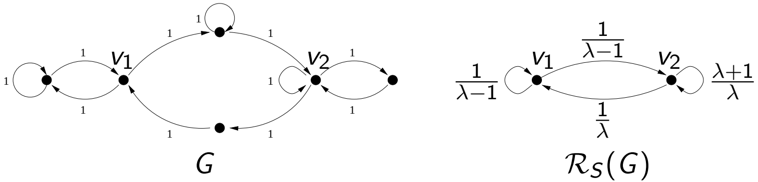
Theorem: Commutativity of Reductions (Bunimovich, Webb [7])

For $G \in \mathbb{G}$ suppose the sequences $S_1,\dots,S_m$ and $T_1,\dots,T_n$ both induce a sequence of reductions on G. If $S_m = T_n$ then $\mathcal{R}(G;S_1,\dots,S_m) = \mathcal{R}(G;T_1,\dots,T_n)$.

The Weight Set $\mathbb{W}_\pi$

Definition

Let $\mathbb{W}_\pi = \{\omega \in \mathbb{W} : \omega = \frac{p}{q},\ deg(p) \leq deg(q)\}$ and $\mathbb{G}_\pi \subset \mathbb{G}$ be the graphs with weights in $\mathbb{W}_\pi$.

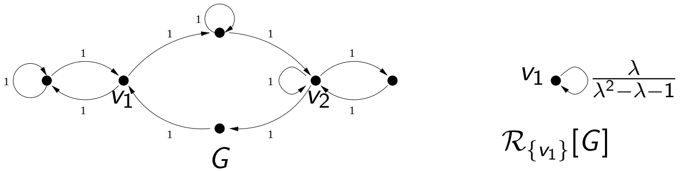


Both $G, \mathcal{R}_S(G) \in \mathbb{G}_\pi$.

Existence and Uniqueness of Sequential Reductions

Theorem: Existence and Uniqueness (Bunimovich, Webb [7])

Let $G = (V, E, \omega)$ be in $\mathbb{G}_\pi$. Then for any nonempty set $\mathcal{V} \subseteq V$ there is a sequence of reductions that reduces G to the unique graph $\mathcal{R}_\mathcal{V}[G] = (\mathcal{V}, \mathcal{E}, \mu)$.



Remark

Any graph G where $M(G) \in \mathbb{C}^{n\times n}$ is a graph in the set $\mathbb{G}_\pi$.

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Gershgorin Theorem

If $A \in \mathbb{C}^{n \times n}$ let $r_i(A) = \sum_{j=1,\ j \neq i}^{n} |A_{ij}|, \quad 1 \leq i \leq n.$

Theorem: (Gershgorin [9,12])

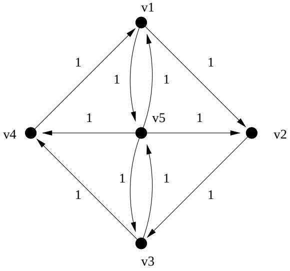
Let A be an $n \times n$ matrix with complex entries. Then all eigenvalues of A are located in the set

$$\Gamma(A) = \bigcup_{i=1}^{n} \{z \in \mathbb{C} : |z - A_{ii}| \leq r_i(A)\}.$$

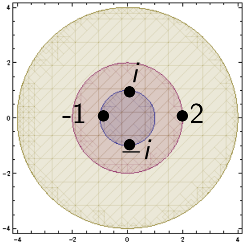
Gershgorin Theorem (Example)

Consider the graph $\mathcal{G}$ with adjacency matrix:

$$M(\mathcal{G}) = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix}.$$



$\mathcal{G}$



$\Gamma\big(M(\mathcal{G})\big)$

Polynomial Extension

Let $\mathbb{G}^n$ be the graphs in $\mathbb{G}$ with n vertices.

Definition

If $G \in \mathbb{G}^n$ and $M_G(\lambda)ij = p_{ij}/q_{ij}$ let $L(G)_i = \prod_{j=1}^{n} q_{ij}$ for $1 \leq i \leq n$. We call the graph $\bar{G}$ with adjacency matrix

$$M(\bar{G})_{ij} = \begin{cases} L(G)_i M(G)_{ij} & i \neq j \\ L(G)_i \big(M(G)_{ij} - L(G)_i \lambda\big) + \lambda & i = j \end{cases}$$

the polynomial extension of G.

Example: $M(G) = \begin{bmatrix} 1/\lambda & 1 \\ (\lambda+1)/\lambda & 1/\lambda^2 \end{bmatrix}, \quad M(\bar{G}) = \begin{bmatrix} -\lambda^2+\lambda+1 & \lambda \\ \lambda^3+\lambda^2 & \lambda^4+2\lambda \end{bmatrix}$

$\mathcal{BW}_\Gamma$ Regions

For $G \in \mathbb{G}^n$ let $r(G)_i = \sum_{j=1, j\neq i}^{n} |M(G)_{ij}|$ for $1 \leq i \leq n$.

Theorem (Bunimovich, Webb [6])

For $G \in \mathbb{G}^n$, $\sigma(G)$ is contained in the Gershgorin-type region given by

$$\mathcal{BW}_\Gamma(G) = \bigcup_{i=1}^{n} \{\lambda \in \mathbb{C} : |\lambda - M(\bar{G})_{ii}| \leq r(\bar{G})_i\}.$$

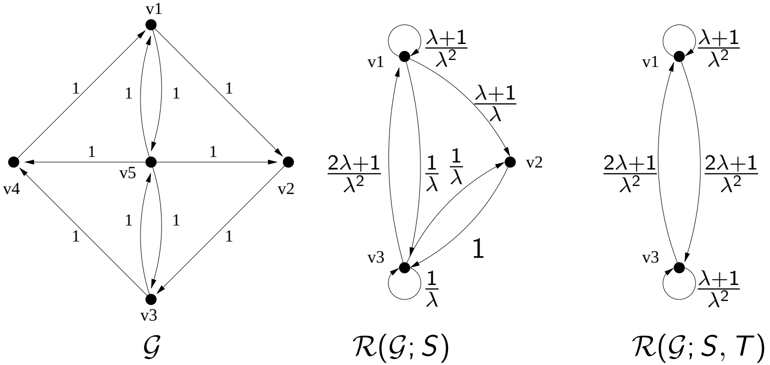
$\mathcal{BW}_\Gamma$ Regions

Question: How do graph reductions effect Gershgorin-type regions?

Theorem: Improved Gershgorin Regions (Bunimovich, Webb [6])

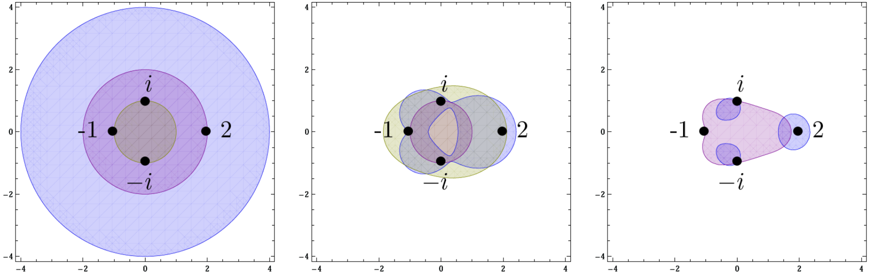
Let $G = (V, E, \omega)$ where $\mathcal{V}$ is any nonempty subset of V. If $G \in \mathbb{G}_\pi$ then $\mathcal{BW}_\Gamma(\mathcal{R}_\mathcal{V}[G]) \subseteq \mathcal{BW}_\Gamma(G)$.

Example: $BW_\Gamma(\mathcal{R}_S(G)) \subseteq \mathcal{BW}_\Gamma(G)$



$$S = \{v_1, v_2, v_3\},\ T = \{v_1, v_2\}$$

Example: $BW_\Gamma(\mathcal{R}_S(G)) \subseteq \mathcal{BW}_\Gamma(G)$



$\mathcal{BW}_\Gamma(\mathcal{G}) = \Gamma(M(\mathcal{G}))$ $\mathcal{BW}_\Gamma(\mathcal{R}(\mathcal{G}; S))$ $\mathcal{BW}_\Gamma(\mathcal{R}(\mathcal{G}; S, T))$

Figure: $\sigma(\mathcal{G}) = \{-1, -1, 2, -i, i\}$.

Brauer's Ovals of Cassini $\mathcal{K}$

Theorem: (Brauer [4,12])

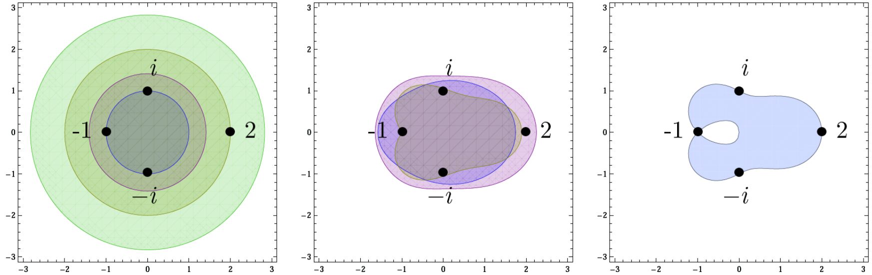
Let $A \in \mathbb{C}^{n\times n}$ where $n \geq 2$. Then all eigenvalues of A are in

$$\mathcal{K}(A) = \bigcup_{\substack{1\leq i,j\leq n \\ i\neq j}} \{z \in \mathbb{C} : |z - A_{ii}||z - A_{jj}| \leq r_i(A)r_j(A)\}.$$

Also, $\mathcal{K}(A) \subseteq \Gamma(A)$.

This theorem can likewise be extended to $G \in \mathbb{G}$ by defining the analogous region $\mathcal{BW}_{\mathcal{K}}(G)$. Moreover, these regions also decrease in size as G is reduced (Theorem: Bunimovich, Webb [6]).

Example: $BW_{\mathcal{K}}(\mathcal{R}_S(G)) \subseteq \mathcal{BW}_{\mathcal{K}}(G)$



$\mathcal{BW}_{\mathcal{K}}(\mathcal{G}) = \mathcal{K}(M(\mathcal{G}))$ $\mathcal{BW}_{\mathcal{K}}(\mathcal{R}(\mathcal{G}; S))$ $\mathcal{BW}_{\mathcal{K}}(\mathcal{R}(\mathcal{G}; S, T))$

Figure: $\sigma(\mathcal{G}) = \{-1, -1, 2, -i, i\}$.

Varga's Extension of Brualdi's Theorem [5]

Theorem: (Varga [12])

Let $A \in \mathbb{C}^{n\times n}$ have one strongly connected component. Then the eigenvalues of A are contained in the set

$$B(A) = \bigcup_{\gamma \in C(A)} \{z \in \mathbb{C} : \prod_{v_i \in \gamma} |z - A_{ii}| \leq \prod_{v_i \in \gamma} \tilde{r}_i(A)\}.$$

Also, $B(A) \subseteq \mathcal{K}(A)$.

This theorem can also be extended to $G \in \mathbb{G}_\pi$ by defining the analogous region $\mathcal{BW}_B(G)$. However, it is not always the case that $\mathcal{BW}_B(\mathcal{R}_S(G)) \subseteq \mathcal{BW}_B(G)$.

Sufficient Condition

Theorem: Improved Brualdi Regions (Bunimovich,Webb [6])

Let $G = (V, E, \omega)$ where $G \in \mathbb{G}_\pi$ and V contains at least two vertices. If $v \in V$ such that both $\mathcal{A}(v, G) = \emptyset$ and $C(v, G) = \mathcal{S}(v, G)$ then $\mathcal{BW}_B(\mathcal{R}_{V \setminus v}(G)) \subseteq \mathcal{BW}_B(G)$.

Here the set $\mathcal{A}(v, G)$ is the set of cycles in G adjacent to v and the condition $C(v, G) = \mathcal{S}(v, G)$ means that every cycle through v has a specific but easily described graph structure.

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Summary and Implications: Isospectral Graph Reductions

- The class of graphs which can be isospectrally reduced is very general.
- It is possible to consider different isospectral reductions of the same graph, as well as sequences of such reductions.
- If $\mathcal{V}$ is any nonempty subset of the vertices of $G \in \mathbb{G}_\pi$ then there is a unique reduction of G over $\mathcal{V}$. That is, it is possible to (uniquely) simplify the structure of G to whatever degree is desired.
- It is possible to establish new relations between topologies of graphs e.g. if two graphs have similar reductions.

Summary and Implications: Isospectral Graph Reductions

- The process of reducing a graph can be done knowing only the local structure of the graph.
- The techniques applied in graph reductions can be used for optimal design, in the sense of structural simplicity of dynamical networks with prescribed dynamical properties ranging from synchronizability to chaoticity.
- It is possible to reduce a graph over specific weight sets.

Summary and Implications: Eigenvalue Estimates

- Gershgorin and Brauer-type estimates of $\sigma(G)$ improve as the graph G is reduced.
- Brualdi-type estimates of $\sigma(G)$ can be improved by reducing over specific types of structural sets.
- This process can be used to improve eigenvalue estimates to any desired degree.
- Graph reductions decrease the number of subregions needed to compute the Gershgorin, Brauer, and Brualdi-type regions simplifying the computational procedure.
- Applications include, estimating the spectrum of the Laplacian matrix of a graph and estimating the spectral radius of a given matrix.

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