Expedition in Data and Harmonic Analysis on Graphs

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Wikipedia graph

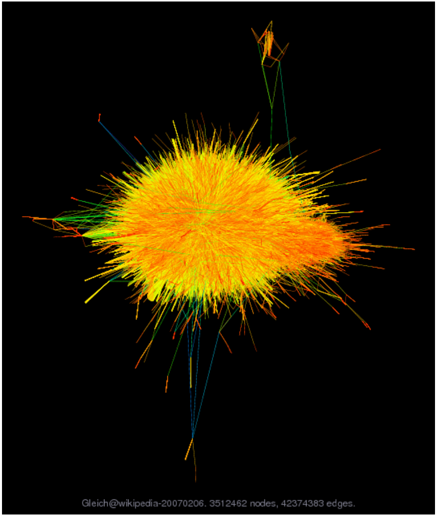

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Image Source: Sparse Matrix collection, http://www.cise.ufl.edu/research/sparse/matrices/Gleich/index.html

Facebook graph

Image Source: Facebook, https://www.facebook.com/note.php?note_id=469716398919

Outline

Graph Preliminaries and the Laplacian

Graph Time-Frequency operators

Support of eigenvectors

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Graph Time-Frequency operators

Support of eigenvectors

Graph Preliminaries

- Denote a graph by $G = G(V, E)$.
- Vertex set $V = \{x_i\}_{i=1}^N$. $|V| = N < \infty$.
- Edge set, E:

$$E = \{(x, y) : x, y \in V \text{ and } x \sim y\}.$$

- A graph is *connected* if for any $x, y \in V$ there exists a path (sequence of adjacent edges) from x to y.
- We consider functions on a graph defined on the vertex set, V.

$$f : V \to \mathbb{C}$$

- Since $|V| = N < \infty$, can view f as a vector in $\mathbb{C}^N$

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Graph Laplacian Matrix

Definition

The pointwise formulation for the *graph Laplacian* acting on $f : V \to \mathbb{R}$ is

$$Lf(x) = \sum_{y \sim x} f(x) - f(y).$$

- For a finite graph, the Laplacian can be represented as a matrix.
- D denotes the diagonal $N \times N$ *degree matrix*, $D = \mathrm{diag}(d_x)$.
- A denotes the $N \times N$ *adjacency matrix*,

$$A(i,j) = \begin{cases} 1, & \text{if } x_i \sim x_j \\ 0, & \text{otherwise.} \end{cases}$$

- Then the graph Laplacian matrix can be written as

$$L = D - A.$$

Spectrum of the Laplacian

- L is symmetric and positive semidefinite.
- By the spectral theorem, L has real eigenvalues

$$\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{N-1}$$

  and real-valued orthonormal eigenvectors $\{\varphi_k\}_{k=0}^{N-1}$.
- Fact: If G is connected then $\lambda_0 = 0$, $\varphi_0 = 1/\sqrt{N}$, and $\lambda_k > 0$ for all $k \in \{1, ..., N-1\}$.
- In general the multiplicity of eigenvalue 0 gives the number of connected components of the graph.
- The spectrum of the Laplacian is fixed but one's choice of eigenvectors can vary. We assume that the choice of eigenvectors is fixed.

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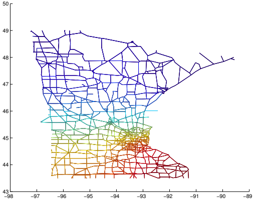
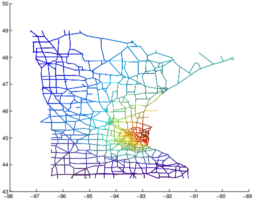
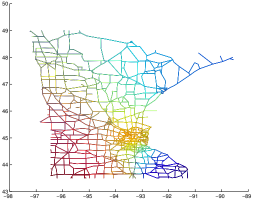
Data Sets - Minnesota Road Network



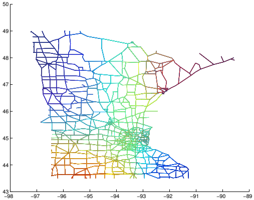
(a) φ_1



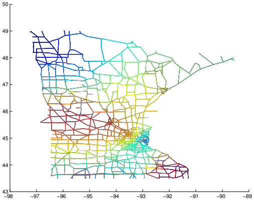
(b) φ_2



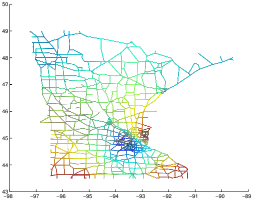
(c) φ_3



(d) φ_4



(e) φ_5



(f) φ_6

Figure : Eigenfunctions corresponding to the first six nonzero eigenvalues. Minnesota road graph (2640 vertices, 3302 edges)

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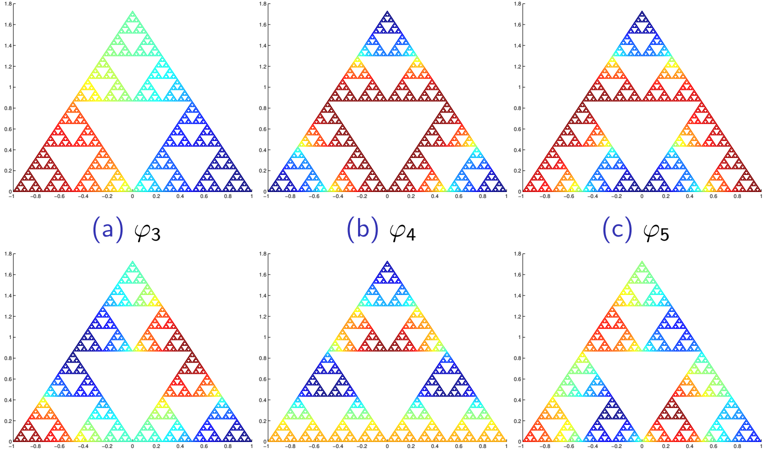
Data Sets - Sierpinski gasket graph approximation



(a) φ_3 (b) φ_4 (c) φ_5

(d) φ_6 (e) φ_7 (f) φ_8

Figure : Eigenfunctions corresponding to the first six nonzero eigenvalues. Level-8 graph approximation to Sierpinski gasket (9843 vertices)

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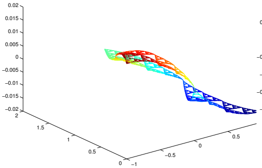
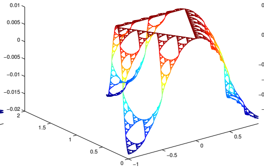
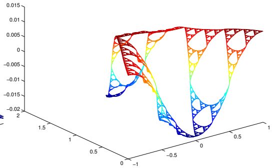


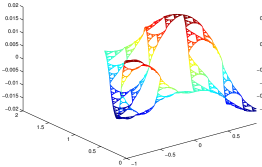
(a) φ_3



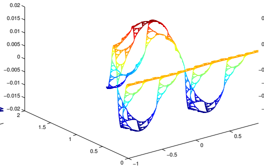
(b) φ_4



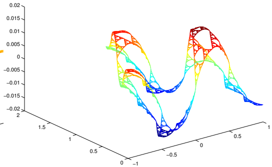
(c) φ_5



(d) φ_6



(e) φ_7



(f) φ_8

Figure : Eigenfunctions corresponding to the first six nonzero eigenvalues. Level-8 graph approximation to Sierpinski gasket (9843 vertices)

Outline

Graph Fourier Transform

Shuman, D.I., Ricaud, B., and Vandergheynst, P., "Vertex-frequency analysis on graphs", Applied and Computational Harmonic Analysis, 2016, vol. 40(2), pp.260-291.

- The Fourier transform on $\mathbb{R}$ is given by

$$\hat{f}(\xi) = \int_{\mathbb{R}} f(t) e^{-2\pi i \xi t}\, dt = \langle f, e^{2\pi i \xi t} \rangle.$$

  This is precisely the inner product of f with an eigenfunction of the Laplace operator.

- Analogously, we define the *graph Fourier transform* of a function, $f : V \to \mathbb{R}$, as

$$\hat{f}(\lambda_k) = \langle f, \varphi_k \rangle = \sum_{n=1}^{N} f(n) \varphi_k^*(n).$$

Graph Modulation and Graph Convolution

- Motivated by modulation in $\mathbb{R}$, $M_k = e^{2\pi ikx}f(x)$ we define *graph modulation* by

$$M_k f = \varphi_k f.$$

- Motivated by the identity in $\mathbb{R}$, $\widehat{f * g}(\xi) = \hat{f}(\xi)\hat{g}(\xi)$, we define *graph convolution* by

$$f * g = (\hat{f}\hat{g})^{\vee}$$

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Nice Properties

- Parseval's Identity: $\langle f, g \rangle = \langle \hat{f}, \hat{g} \rangle$
- Plancherel's Identity: $\|f\| = \left\|\hat{f}\right\|$
- Commutativity, associativity, and distributivity of graph convolution:

$$f * g = g * f,$$

$$(f * g) * h = f * (g * h),$$

$$f * (g + h) = f * g + f * h$$

Graph Translation

- Translation by vector u in $\mathbb{R}$ can be viewed as convolution with δ_u.

$$T_u f(x) = f(x-u) = f * \delta u$$

- δ_u has Fourier transform $\hat{\delta}_u(\xi) = e^{-2\pi i \xi u} = \overline{\varphi_\xi(u)}$

Definition

For $f : V \to \mathbb{R}$ the *graph translation operator*, T_i, is defined as

$$T_i f = (\hat{f}\widehat{\Phi_i})^\vee,$$

where Φ_i is the vector

$$\Phi_i = [\varphi_0(i), \varphi_1(i), \cdots, \varphi_{N-1}(i)]^\top.$$

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Not nice properties of graph translation

- T_i is generally not isometric. $\|T_i f\|_{\ell^2} \neq \|f\|_{\ell^2}$.
- The graph translation operators do not form a group like in the classical Euclidean setting.

$$T_i T_j \neq T_{i+j}$$

Theorem

Graph translation is a semigroup, i.e., $T_i T_j = T_{i \bullet j}$ for some semigroup operator $\bullet : \{1, ..., N\} \times \{1, ..., N\} \to \{1, ..., N\}$, only if the eigenvector matrix $\Phi = (1/\sqrt{N})H$, where H is a Hadamard matrix.

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Invertibility of Translation operator T_i

- T_i need not be injective.

Theorem

The graph translation operator T_i is invertible if and only if $\varphi_k(i) \neq 0$ for all $k = 1, ..., N-1$.
Furthermore, the nullspace of T_i has a basis equal to those eigenvectors that vanish on the ith vertex.

This theorem stresses the importance of characterizing vertices in which eigenvectors of the Laplacian vanish.

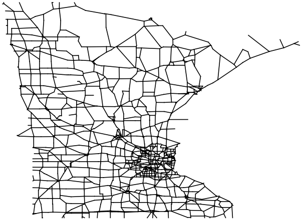
Outline

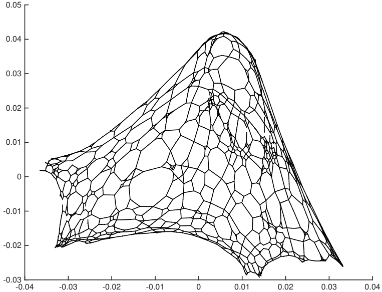
The Fiedler vector: φ_1

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{N-1}$$

- The first nonzero eigenvalue, λ_1, is called the *algebraic connectivity*.
- The eigenvector φ_1 corresponding to λ_1 is called the *Fiedler vector*.
- The Fiedler vector is of great importance in nonlinear dimension reduction techniques, image segmentation, and graph drawing.

Spectral graph drawing





Hall, K. "An *r*-dimensional quadratic placement algorithm", Management science, 1970, vol 17(3), pp. 219–229.

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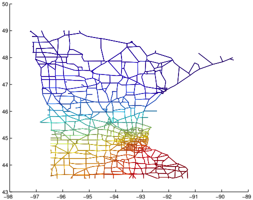
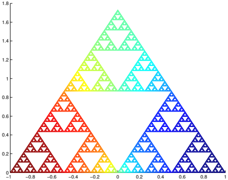
Characteristic vertices

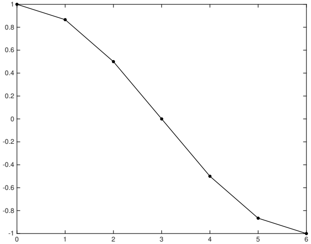
- For a Fiedler eigenvector φ_1, decompose the vertieces into disjoint subsets
$$V = V_+ \cup V_- \cup V_0.$$
- V_+ is the set of vertices $x \in V$ where $\varphi_1(x) > 0$.
- V_- is the set of vertices $x \in V$ where $\varphi_1(x) < 0$.
- V_0 is the set of vertices $x \in V$ where $\varphi_1(x) = 0$.
  V_0 is known as nodal set, or *characteristic vertices*.
- We wish to describe the size and structure of V_0.

Support of Fiedler vector

It is perhaps a misconception that the Fiedler vector must have (near) full support.







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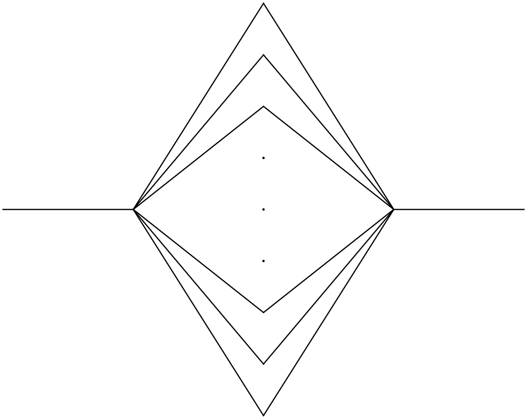
Arbitrarily many characteristic verties possible

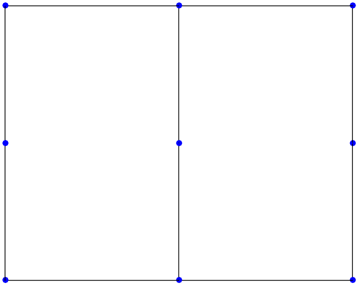
It was shown in 1998 that the set V_0 may be arbitrarily large.

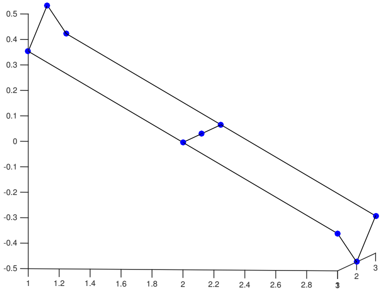
Bapart, R. and Pati, S. "Algebraic connectivity and the characteristic set of a graph", Linear and Multilinear Algebra, 1998, vol. 45(2-3), pp. 247–273.



Arbitrarily large and connected V_0

We can show that the family of generalized ladders can have an arbitrarily large characteristic set that is also connected.





Can there exist a vertex $x \in V_0$ with 3 or more neighbors also in V_0?

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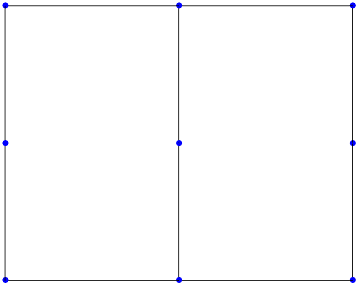

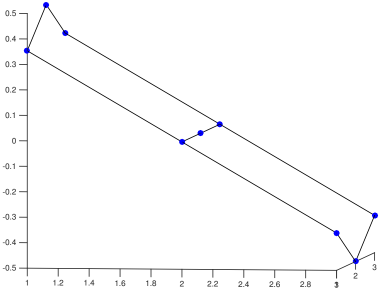

Can there exist a vertex $x \in V_0$ with 3 or more neighbors also in V_0?

Graph balls

Definition

A *graph ball* centered at vertex $x \in V$ with radius r is defined as

$$B_r(x) = \{y \in V : d(x, y) \leq r\}.$$

Question

Restate the orginal question as

Can there exist a graph ball $B_1(x) \subseteq V_0$ with $|B_1(x)| \geq 4$?

Answer:

- Yes, it is possible in general.
- The result is not possible for planar graphs

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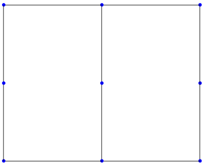
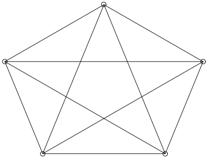
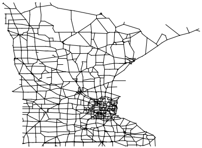
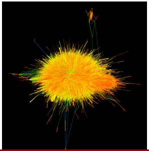
Planar graphs

Definition

A *planar graph* is a graph whose vertices and edges can be embedded in $\mathbb{R}^2$ with edges intersection only at vertices.

Planar graphs	Nonplanar graphs
	
	

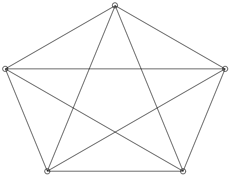
Characterizing Planar Graphs

Definition

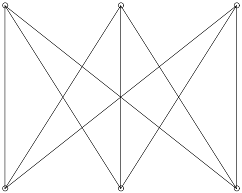
Contracting an edge (u, v) entials deleting edge e and identifying u and v as the same vertex. A graph H, formed by a contraction of G, is known as a *minor* of G.

Theorem (Wagner's Theorem)

G is a planar graph if and only if it does not contain a K_5 or $K_{3,3}$ as a minor.



K_5



$K_{3,3}$

Main Theorem

Theorem

Let $G(V, E)$ be a planar graph with Fiedler vector φ_1. Then V_0 contains no balls of radius 1 with more than 3 vertices.

Strategy: Proof by contradiction.
Suppose V_0 contains such a ball and demonstrate that the graph G will contain one of the forbidden minors.

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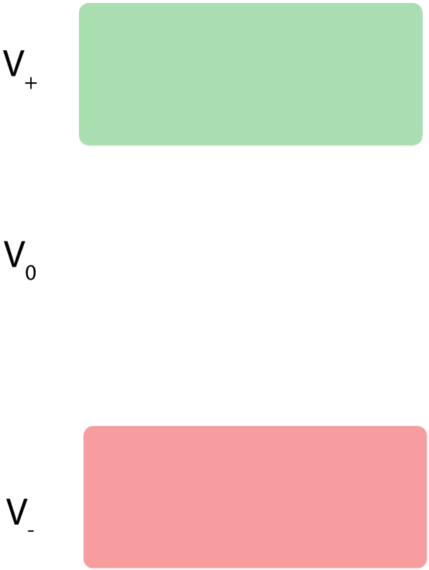
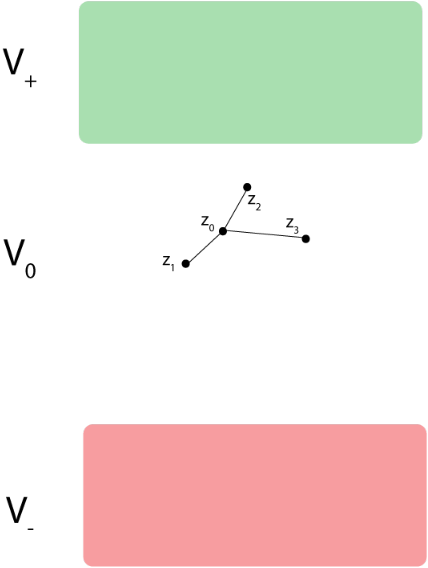
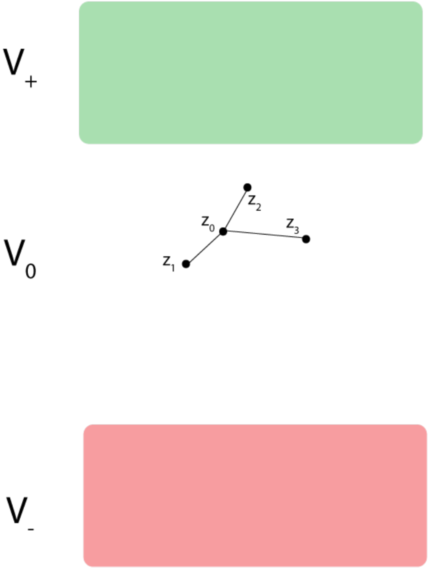

V_+
V_0
V_-

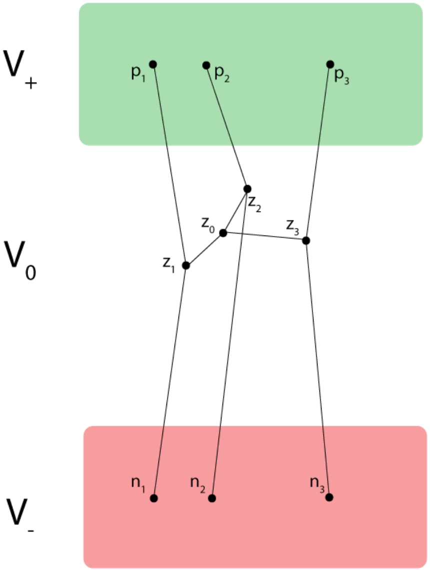

V_+
z_2
z_0
z_3
V_0
z_1
V_-

Lemma

Every vertex $x \in V_0$ either has

1. *all neighbors in V_0 or*
2. *at least one neighbor in V_+ and one in V_-.*


V_+
z_2
z_0
z_3
V_0
z_1
V_-

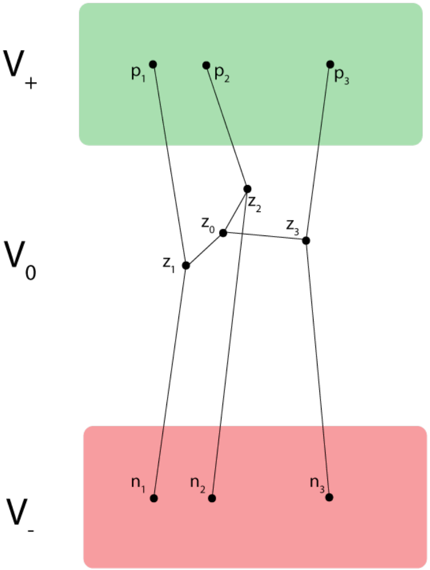


V+
p1
p2
p3
z2
z0
z3
V0
z1
n1
n2
n3
V-

Lemma: Connectedness of V_+ and V_-

1975: Miroslav Fiedler proves $V_+ \cup V_0$ forms a connected subgraph.

Fiedler, M. "A property of eigenvectors of nonnegative symmetric matrices and its applications to graph theory.", Czechoslovak Mathematical Journal, 1975, vol. 25(4), pp. 619–633


V_+
p_1
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V_-
n_1
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n_3

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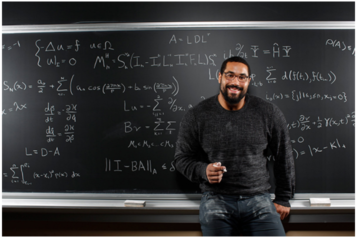


2014: John Urschell proves that V_+ forms a connected subgraph.

Urschel, J.C., Zikatanov, L.T., "Spectral bisection of graphs and connectedness", 2014, Linear Algebra and its Applications, vol.449, pp.1–

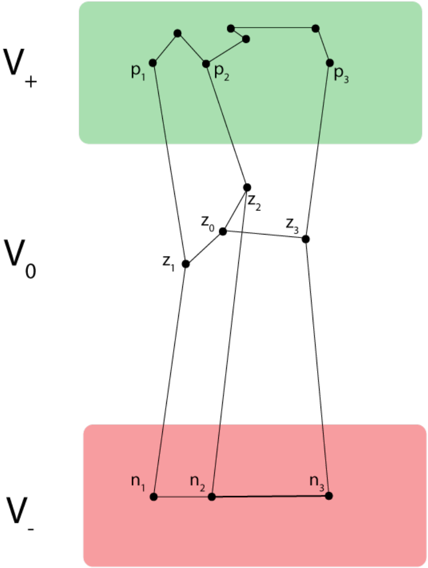
Lemma: Connectedness of V_+ and V_-

1975: Miroslav Fiedler proves $V_+ \cup V_0$ forms a connected subgraph.

Fiedler, M. "A property of eigenvectors of nonnegative symmetric matrices and its applications to graph theory.", Czechoslovak Mathematical Journal, 1975, vol. 25(4), pp. 619–633

2014: John Urschell proves that V_+ forms a connected subgraph.

Urschel, J.C., Zikatanov, L.T., "Spectral bisection of graphs and connectedness", 2014, Linear Algebra and its Applications, vol.449, pp.1–16



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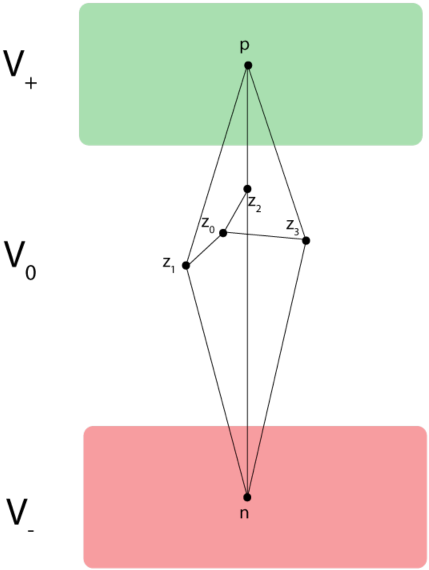
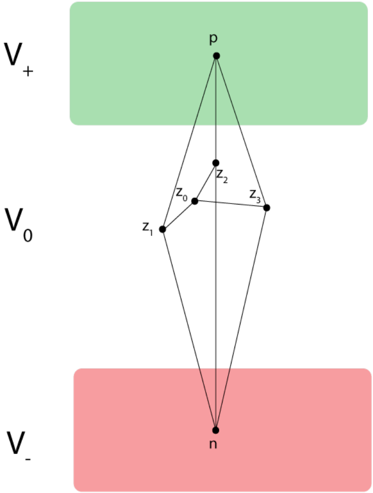
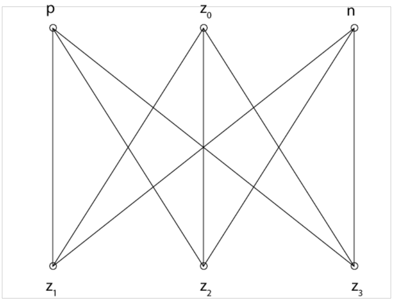

V+
V0
V-
p
z2
z0
z3
z1
n





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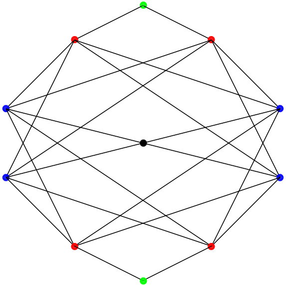
Nonplanar graphs with large balls contained in V_0

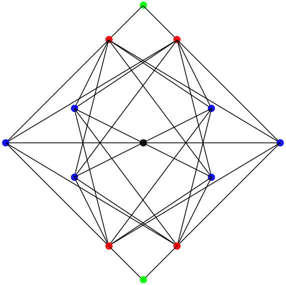
- For $N \geq 3$, we construct a family of graphs called the barren graph, Barr(N), with $|V| = N + 7$.
- Barr(N) has characteristic set V_0 that is a graph ball of radius 1 and $|V_0| = N + 1$.
- Let $\{V_i\}_{i=1}^{6}$ denote distinct vertex sets with given cardinalities $\{|V_i|\}_{i=1}^{6} = \{N, 1, 2, 2, 1, 1\}$. Barr($N$) is the following graph sum of the 5 complete bipartite graphs

$$\mathrm{Barr}(N) = K(V_1, V_2) + K(V_1, V_3) + K(V_1, V_4) + K(V_3, V_5) + K(V_4, V_6).$$

Barren graphs



Barr(4)



Barr(6)

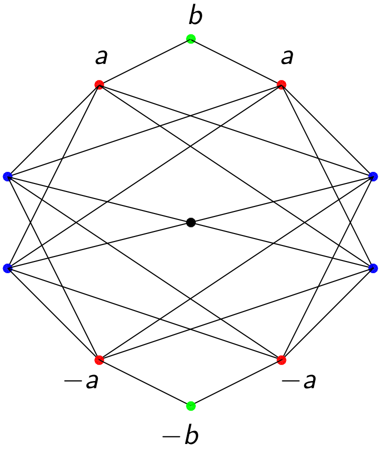
Spectrum of Barren graph

λ_k	value
λ_0	0
λ_1	$\frac{1}{2}\left(N+3-\sqrt{N^2-2N+9}\right)$
λ_2	y_1
$\lambda_3 = \cdots = \lambda_{N+1}$	5
λ_{N+2}	y_2
$\lambda_{N+3} = \lambda_{N+4}$	$N+1$
λ_{N+5}	$\frac{1}{2}\left(N+3+\sqrt{N^2-2N+9}\right)$
λ_{N+6}	y_3

y_1, y_2, and y_3 are the roots of the polynomial

$$\lambda^3 + (-2N-8)\lambda^2 + (N^2+10N+15)\lambda + (-2N^2-14N)$$

Fiedler vector of the barren graph



$$\begin{cases} 4a^2 + 2b^2 & = & 1 & (\|\varphi\| = 1) \\ 2(b - a) & = & \lambda b & (green) \\ Na + (a - b) & = & \lambda a & (red) \end{cases}$$

Thank You