CS-E4075 - Special Course in Machine Learning, Data Science and Artificial Intelligence D: Signed graphs: spectral theory and applications

Spectral graph drawing

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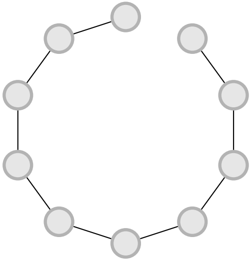
Aalto University 2021

Graph visualization

Consider a path graph P_{10} with adjacency matrix A.
We want to plot it on the real line.



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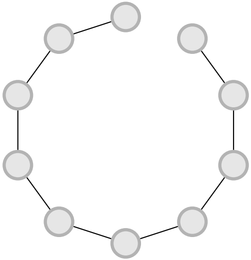

We would like connected vertices to be "close" to each other. So we will seek to assign a real number x_i to vertex i so as to minimize

$$\sum_{i,j} A_{ij}(x_i - x_j)^2.$$

Graph visualization

We want to find a vector x that minimizes

$$\sum_{i,j} A_{ij}(x_i - x_j)^2.$$

First, observe that

$$\sum_{i,j} A_{ij}(x_i - x_j)^2 = 2x^T Lx.$$

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- To avoid $x_i = 0$ for all i, we impose $\sum_i x^2 = x^T x = \|x\|_2^2 = 1$.

Graph visualization

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- To avoid $x_i = x_j$ for all i, j, we impose $\sum_i x_i = x^T 1 = 0$.

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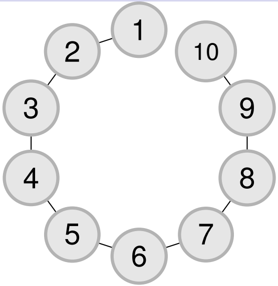
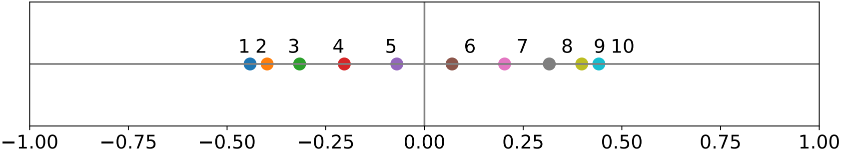
So we are looking for the eigenvector associated to the smallest non-zero eigenvalue of L.

Graph visualization

Result:

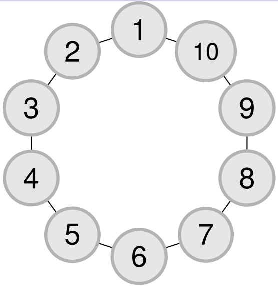




Spectrum: $(0, 0.098, 0.382, 0.824, 1.382, 2, 2.618, 3.176, 3.618, 3.902)$

Graph visualization

Let us now consider a cycle graph C_{10}.



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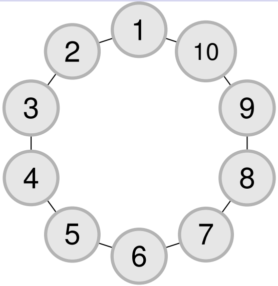

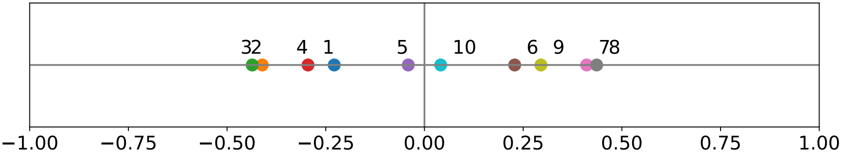

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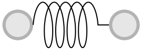
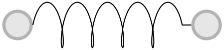
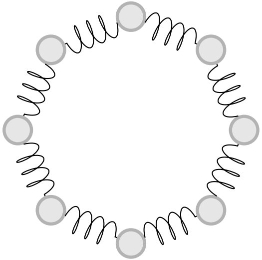
Graph visualization

Let us add a second dimension.

We will consider a physical metaphor: spring network. We seek energy minimization.

Low energy: 

High energy: 



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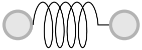
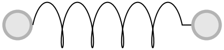
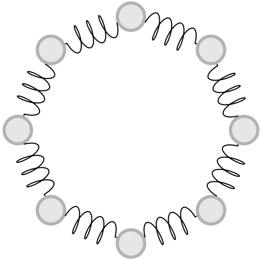
Low energy: 

High energy: 



We assign x_i, y_i coordinates to vertex i.

We will quantify the energy as

$$\sum_{i,j} A_{ij} \left((x_i - x_j)^2 + (y_i - y_j)^2 \right) .$$

Graph visualization

$$\sum_{i,j} A_{ij} \left((x_i - x_j)^2 + (y_i - y_j)^2 \right) = 2x^T Lx + 2y^T Ly.$$

We impose

- $x^T y = 0,$
- $x^T 1 = y^T 1 = 0,$
- $\|x\| = \|y\| = 1.$

Graph visualization

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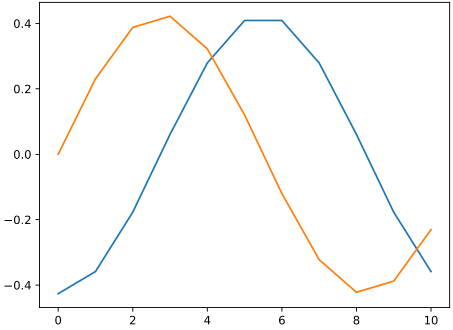
We impose

- $x^T y = 0$,
- $x^T 1 = y^T 1 = 0$,
- $\|x\| = \|y\| = 1$.

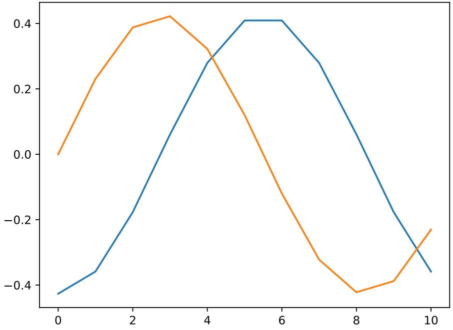
x and y are the eigenvectors corresponding to the smallest non-zero eigenvalues.

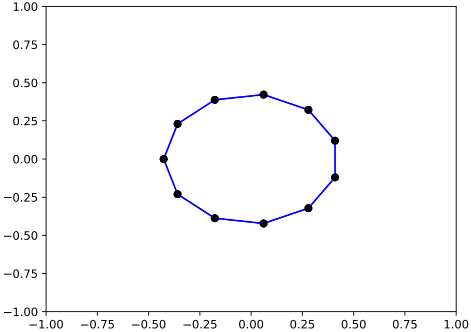
Graph visualization



Eigenvectors.

Graph visualization





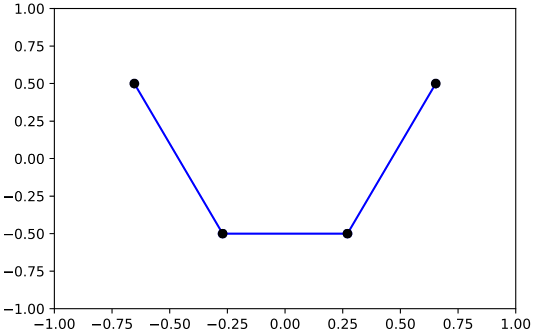
Eigenvectors.

Graph visualization

What if we plot the path in 2D?

Path graph P_n: $E = \{(1,2),(2,3),\ldots,(n-2,n-1),(n-1,n)\}$.

n=4



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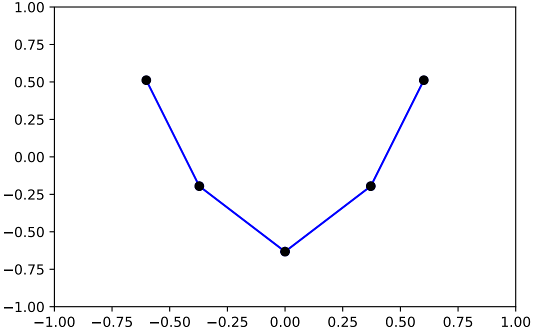
n=5



Graph visualization

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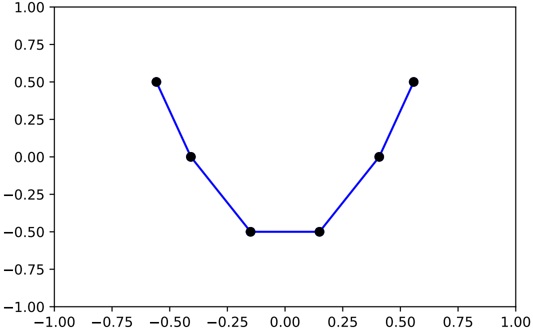
n=6



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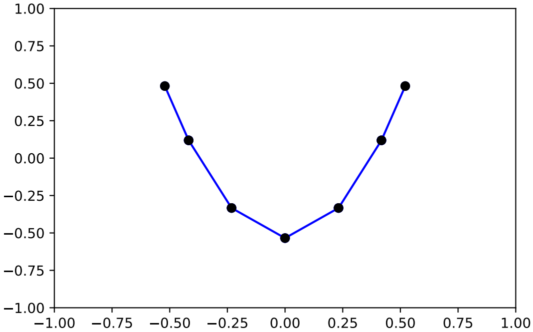
n=7



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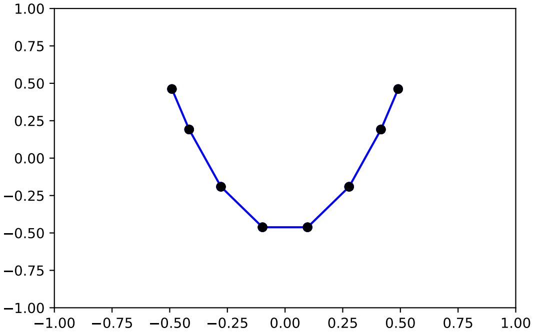
n=8



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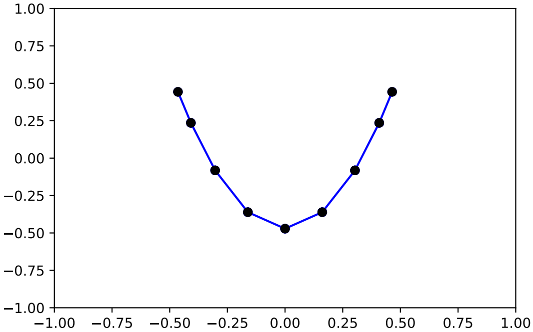
n=9



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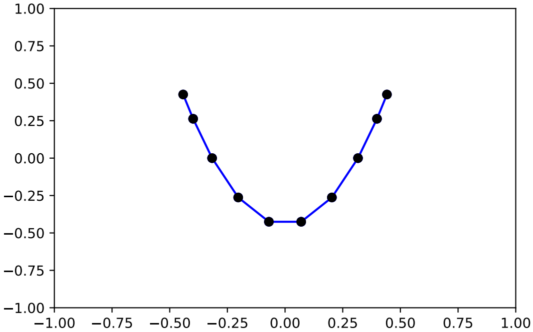
n=10



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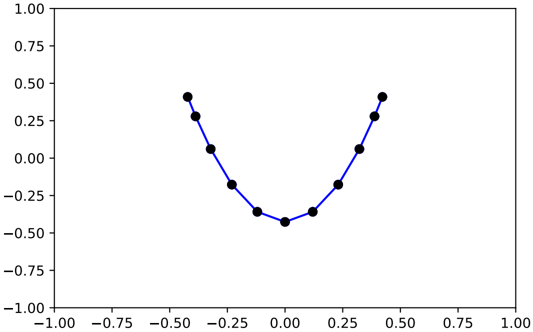
n=11



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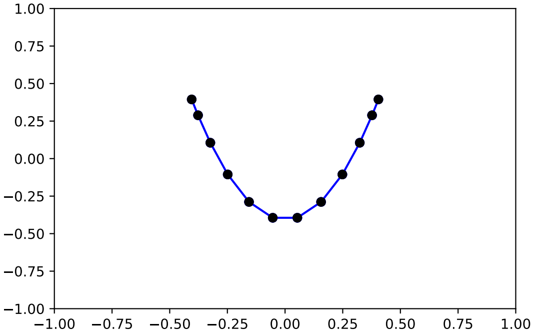
n=12



Graph visualization

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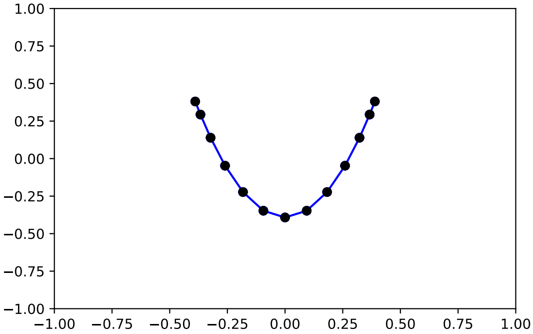
Path graph P_n: $E = \{(1, 2), (2, 3), \ldots, (n-2, n-1), (n-1, n)\}$.

n=13



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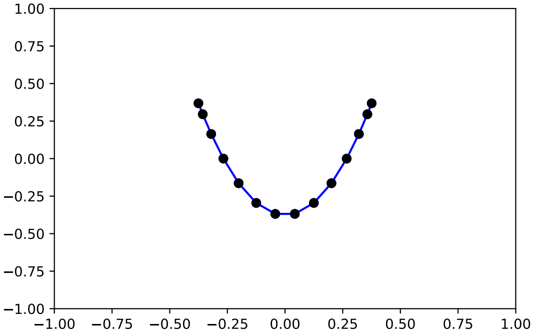
n=14



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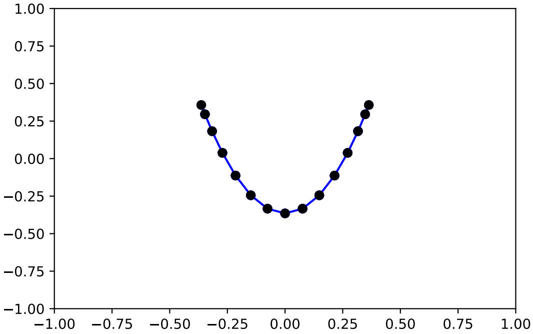
n=15



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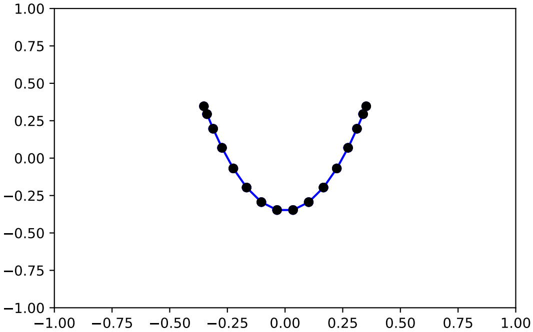
n=16



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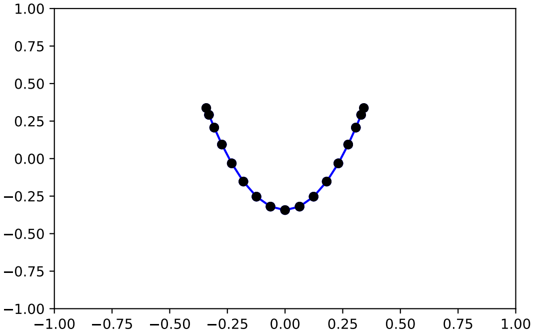

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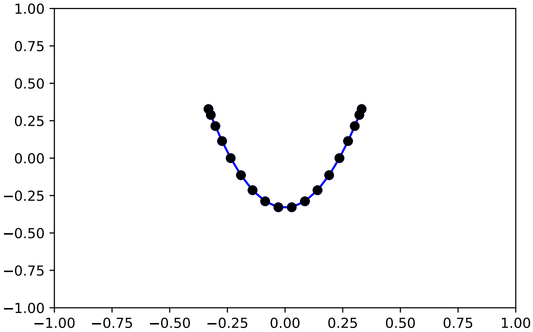
n=18



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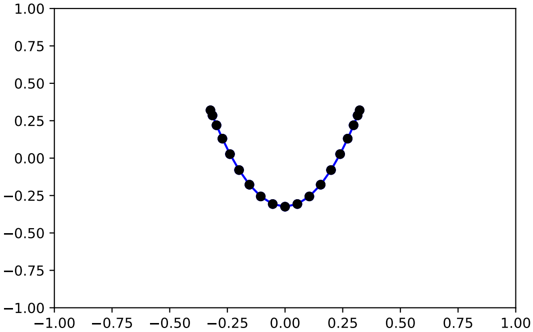
n=19



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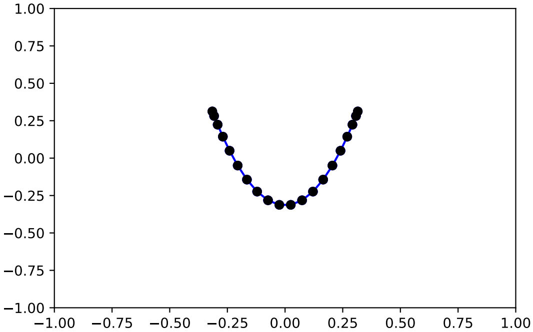
n=20



Graph visualization

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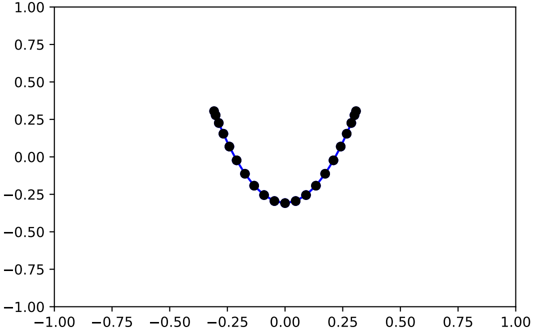
n=21



Graph visualization

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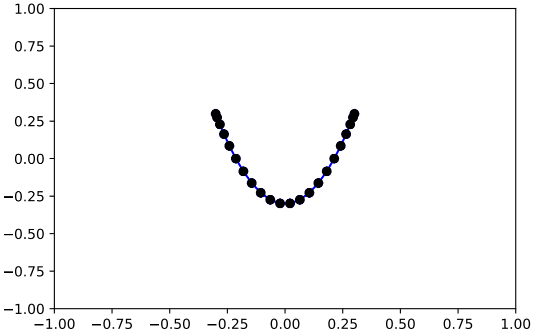
n=22



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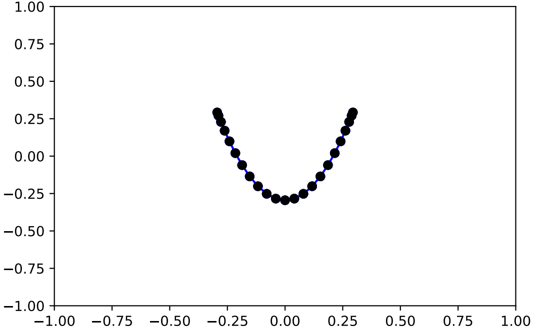

Graph visualization

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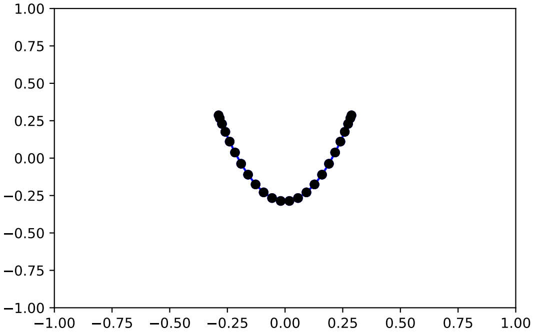
n=24



Graph visualization

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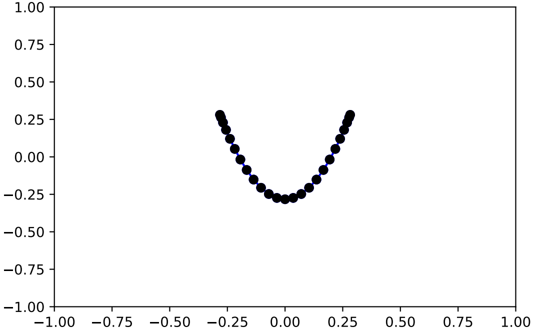
n=25

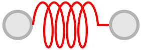


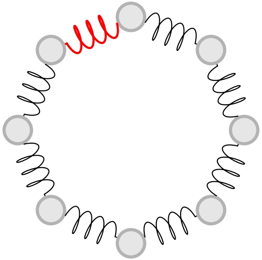
Signed graphs

Graph visualization

For negative edges we consider repulsive springs.

Low energy: 

High energy: 



Graph visualization

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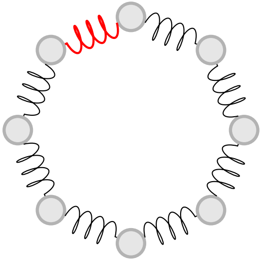

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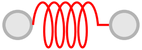
High energy: 

We assign x_i, y_i coordinates to vertex i.
Earlier we wanted

$$x^T L x + y^T L y$$

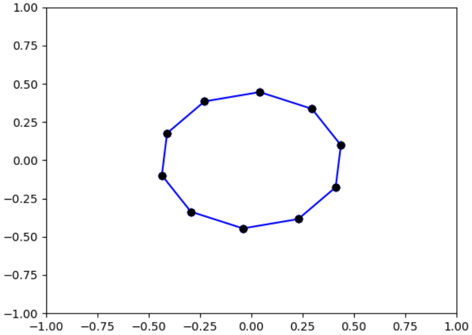
to be minimal.

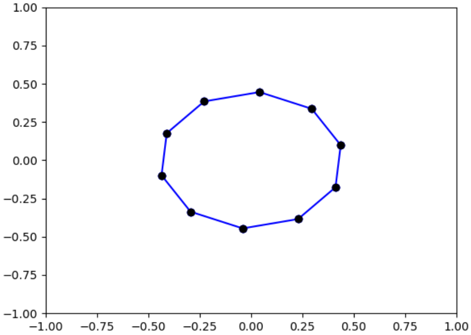
In the case of the signed Laplacian,

$$x^T L x = \sum_{i,j} |A_{ij}|(x_i - sgn(i,j) x_j)^2,$$

where $sgn(i,j) = A_{ij}/|A_{ij}|$ if $A_{ij} \neq 0$.

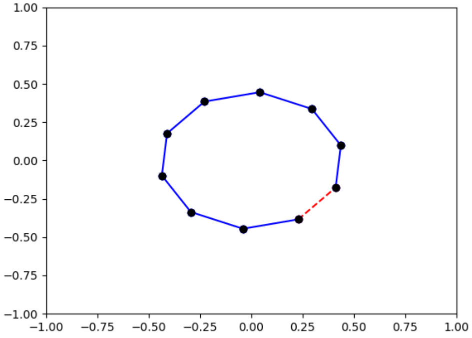
Graph visualization

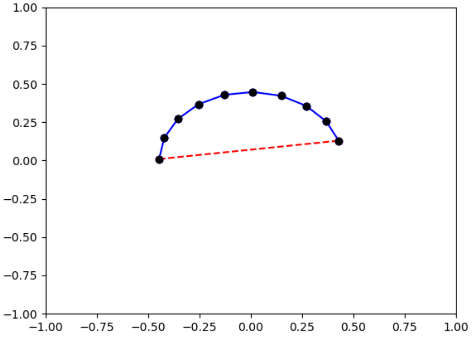




Spectrum: (0, 0.382, 0.382, 1.382, 1.382, 2.618, 2.618, 3.618, 3.618, 4)

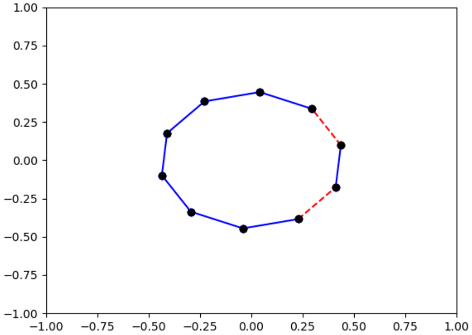
Graph visualization

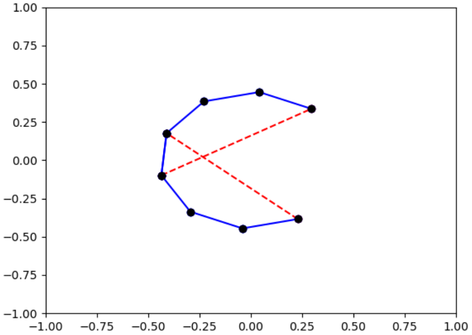




Spectrum: (0.098, 0.098, 0.824, 0.824, 2, 2, 3.176, 3.176, 3.902, 3.902)

Graph visualization





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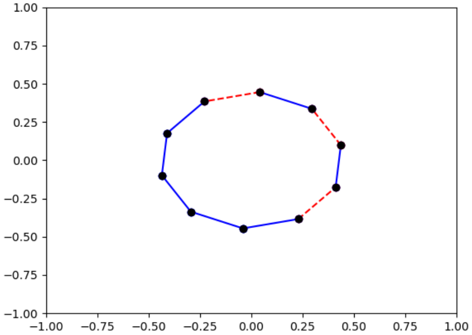
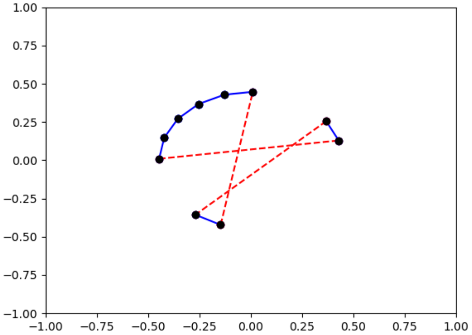
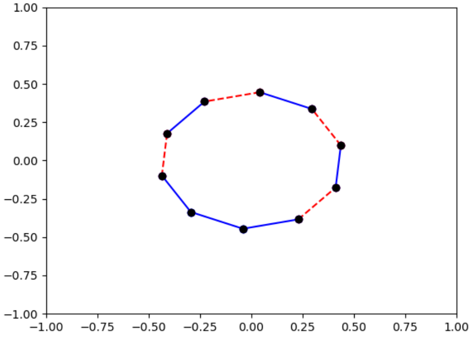
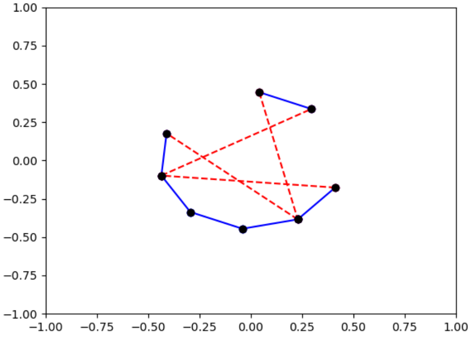




Spectrum: (0.098, 0.098, 0.824, 0.824, 2, 2, 3.176, 3.176, 3.902, 3.902)

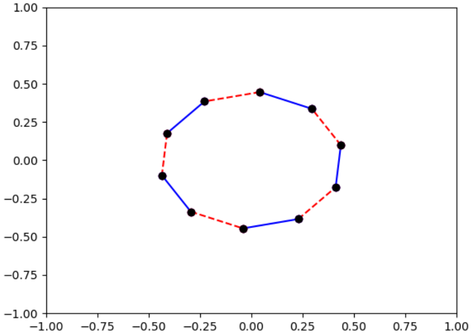
Graph visualization

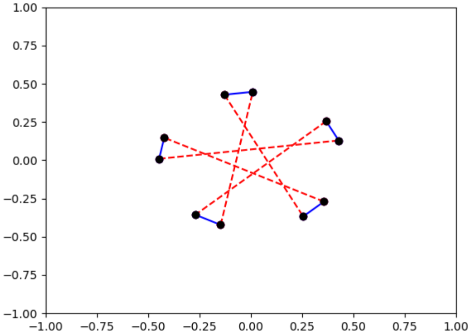




Spectrum: (0, 0.382, 0.382, 1.382, 1.382, 2.618, 2.618, 3.618, 3.618, 4)

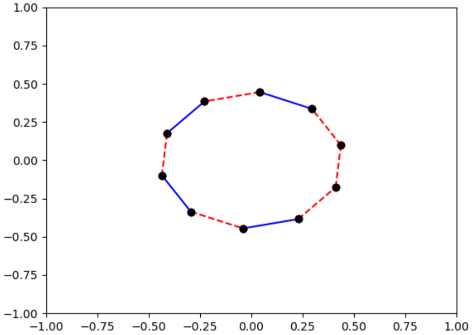
Graph visualization

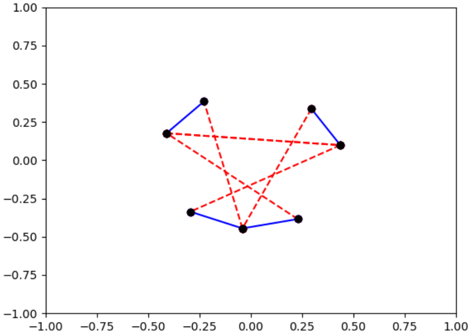




Spectrum: (0.098, 0.098, 0.824, 0.824, 2, 2, 3.176, 3.176, 3.902, 3.902)

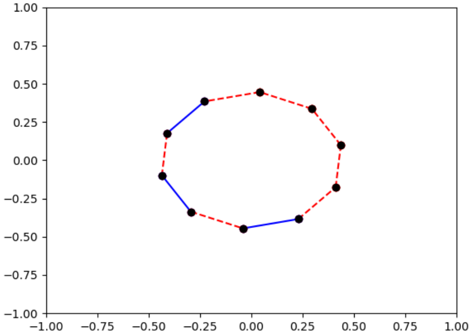
Graph visualization

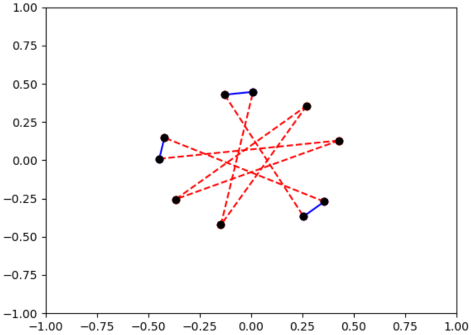




Spectrum: (0, 0.382, 0.382, 1.382, 1.382, 2.618, 2.618, 3.618, 3.618, 4)

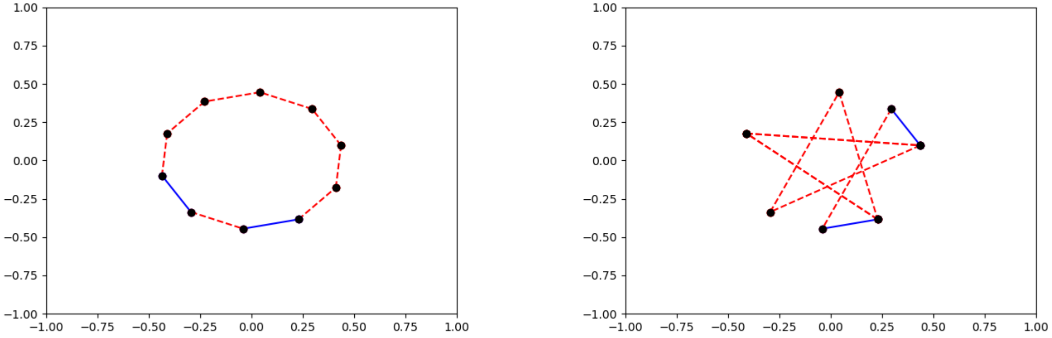
Graph visualization





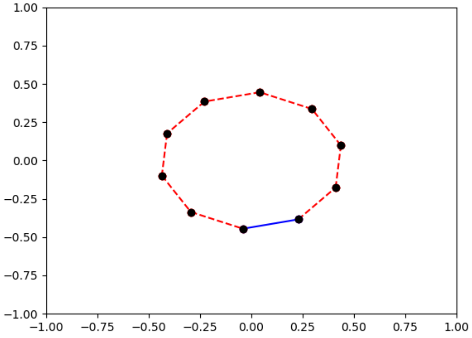
Spectrum: (0.098, 0.098, 0.824, 0.824, 2, 2, 3.176, 3.176, 3.902, 3.902)

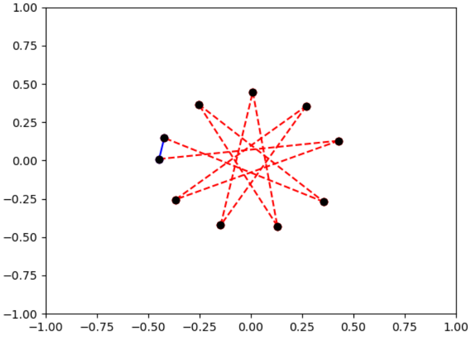
Graph visualization



Spectrum: (0, 0.382, 0.382, 1.382, 1.382, 2.618, 2.618, 3.618, 3.618, 4)

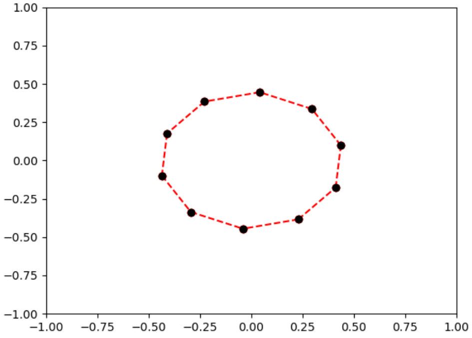
Graph visualization

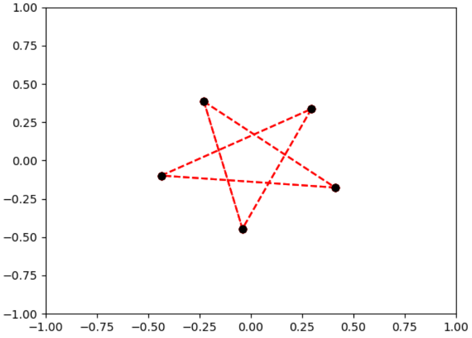




Spectrum: (0.098, 0.098, 0.824, 0.824, 2, 2, 3.176, 3.176, 3.902, 3.902)

Graph visualization





Spectrum: (0, 0.382, 0.382, 1.382, 1.382, 2.618, 2.618, 3.618, 3.618, 4)

Graph visualization

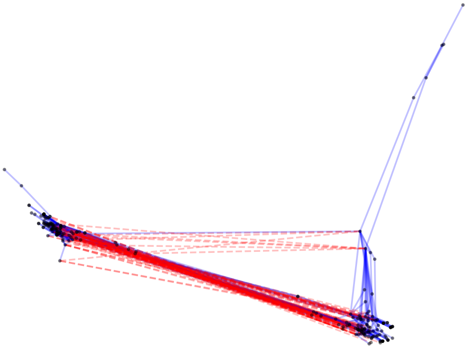
Real example.

Congress data set: positive and negative mentions between members of the US Congress.

Graph visualization

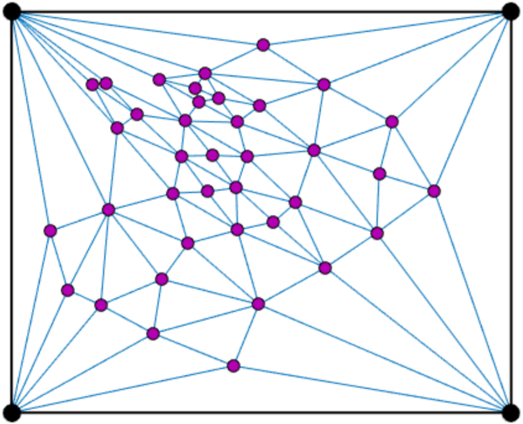
Real example.

Congress data set: positive and negative mentions between members of the US Congress.



Graph visualization

Tutte embedding.



If a graph is 3-connected, its Tutte embedding is planar.

Take-aways from this lecture:

- Graph drawing as energy minimization using eigenvectors.
- Physical metaphor: spring network.
- Signed edges as repulsive springs.