Complex Networks 2022

Node Vector Distances: Methods and Applications

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IT UNIVERSITY OF COPENHAGEN

Download the Material

https://github.com/mikk-c/complexnetworks22-tutorial

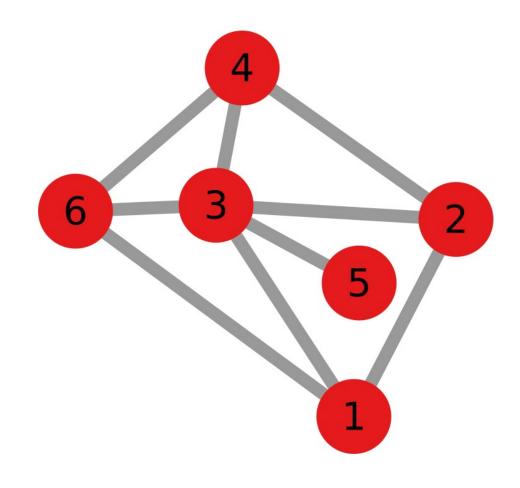
Readings

- The Atlas for the Aspiring Network Scientist
 - Chapter 40
 - https://www.networkatlas.eu/
- The node vector distance problem in complex networks, ACM Computing Surveys (CSUR) 53 (6), 1-27



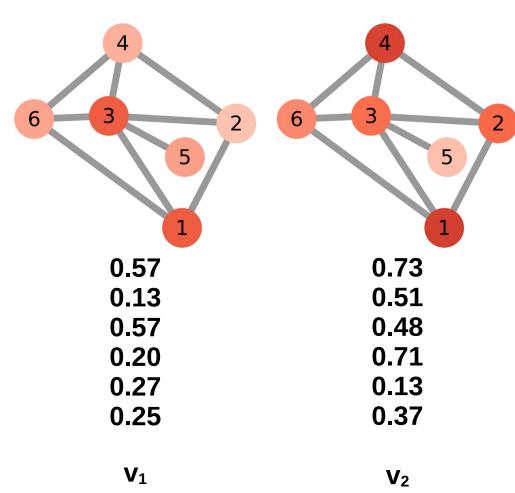
NVD: What?

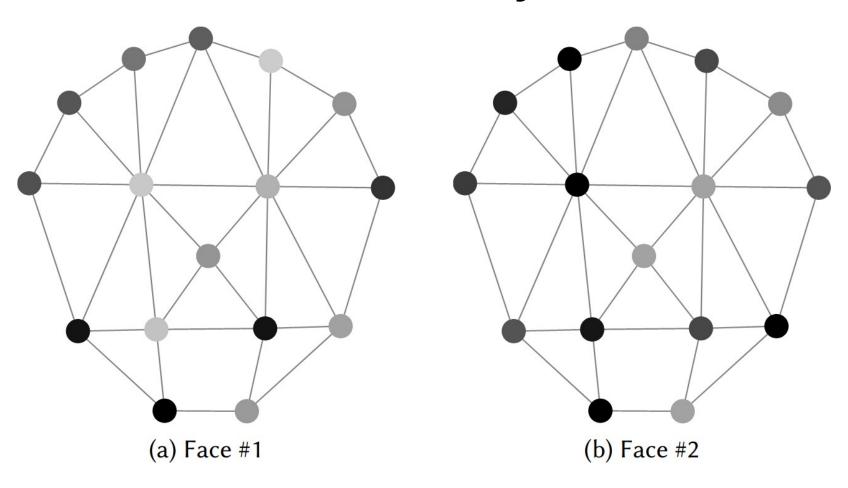
A graph G

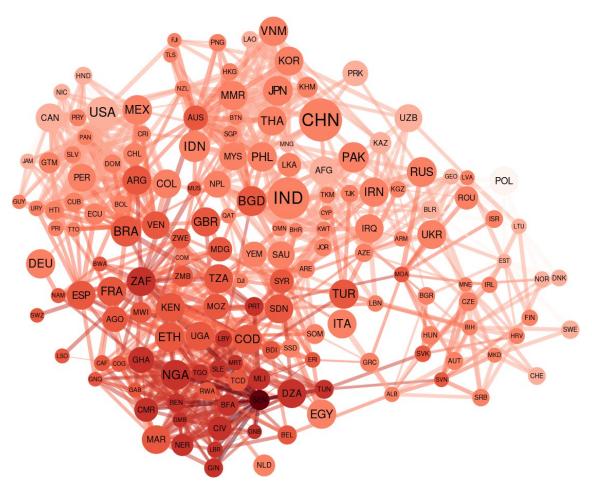


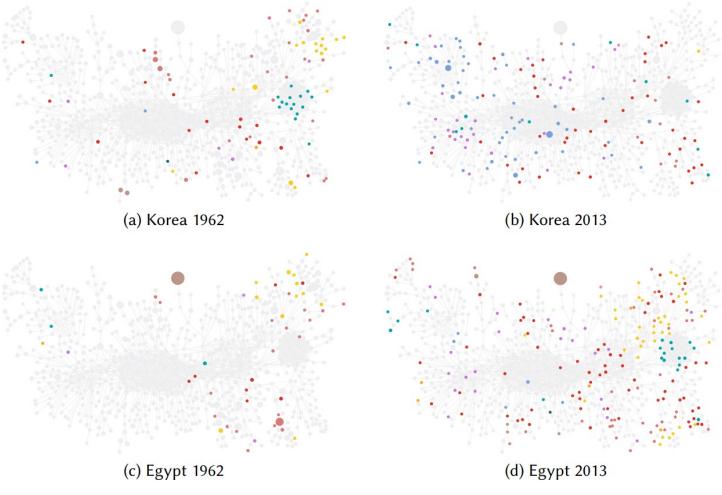
NVD: What?

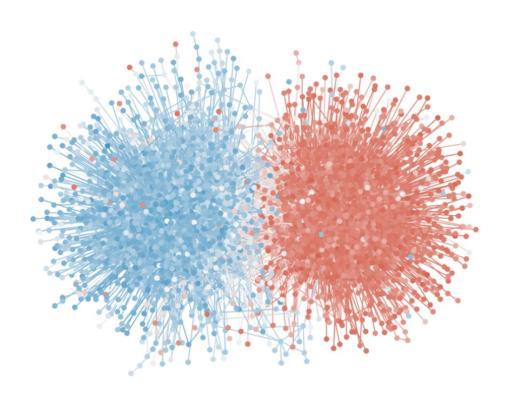
- A graph G
- Two vectors v₁ and v₂
 - One value per node
- How far is v_1 from v_2 ?

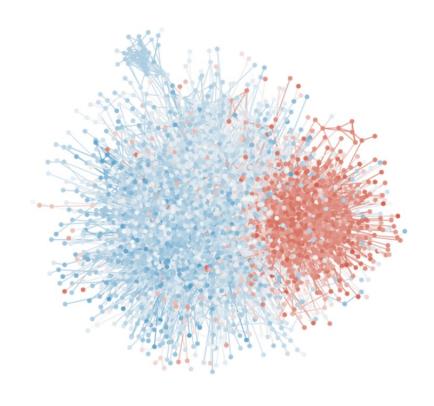












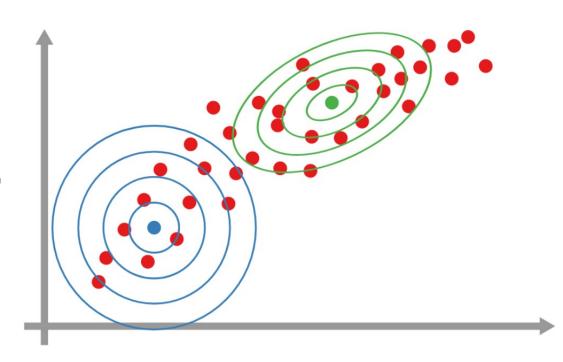
Re-Cap on Distances

Euclidean "straight line"

$$\sqrt{(p-q)^T I(p-q)}$$

 Mahalanobis "bendy" space

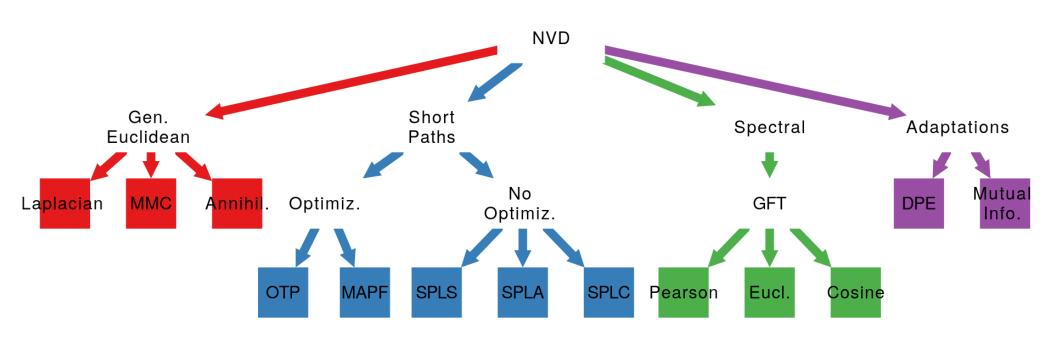
$$\sqrt{(p-q)^T \operatorname{cov}(p,q)^{-1}(p-q)}$$



Euclidean vs Network

Same Euclidean distances, different network distances The network "bends" the space, like in Mahalanobis

Current Methods



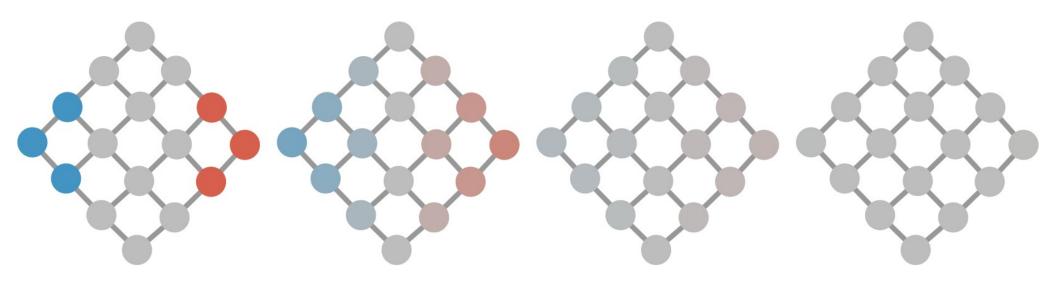
Tutorial Part #1

- Objectives:
 - Refresher on vector distances
 - Understand I/O of library
 - Set up the data

```
nvd_session01.ipynb
1 + % □ □ ▶ ■ C → Code
    [54]: import numpy as np
          import pandas as pd
          import networkx as nx
          from scipy.linalg import inv
          from scipy.stats import pearsonr
          from scipy.spatial import distance
          import network distance as nd # From: https://www.michelecoscia.com/wp-content/uploads/2021/04/network distance.zip
   [21]: vector df = pd.read csv("../data/obama nodevectors.csv")
          vector df
            0 347971482 0.429952 0.032242
            1 181692013 -0.391304 -0.135905
            2 1433227584 0.812500 0.770574
           3 394166747 0.770833 0.363461
               20728008 -0.413043 -0.162574
          220 549600704 0.666667 0.227302
          221 21773704 0.666667 0.301933
               14662354 0.479167 0.276551
               14979330 -0.391304 -0.137066
          224 522718572 -0.413043 -0.071466
         225 rows × 3 columns
   [22]: v1_dict = vector_df.set_index("node").to_dict()["X"]
          v2_dict = vector_df.set_index("node").to_dict()["Y"]
          nodes = sorted(list(set(v1_dict.keys()) | set(v2_dict.keys())))
          v1_array = np.array([v1_dict[node] if node in v1_dict else 0 for node in nodes])
          v2 array = nn array([v2 dict[node] if node in v2 dict else A for node in nodes])
```

Generalized Euclideans

Heat Diffusion



- Imagine each node as a thermometer
- Connected to other thermometers to pass heat
- If we know the heat h at time t
- What would be the heat at t + 1?

$$\frac{\partial h}{\partial t} = -Lh$$
Laplacian

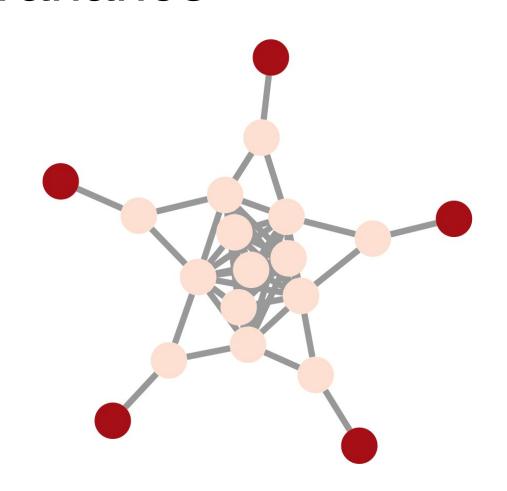
Generalized Euclidean: Laplacian

- L tells us how easy it is to pass heat between nodes
- Which is via random walks
- Thus its inverse gives a sense of distance

$$\sqrt{(p-q)^T L^{-1}(p-q)}$$

Network Variance

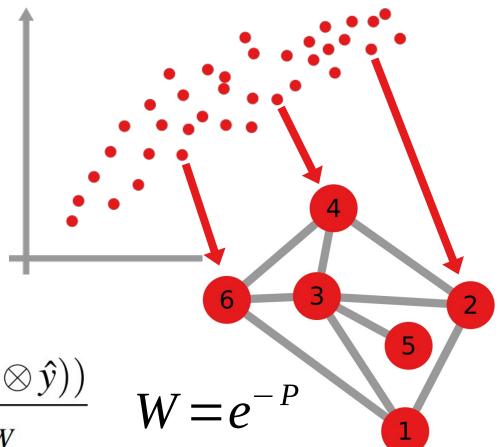
- Not only about distances!
- Vector v: how spread out is on the network?
- Same as variance, now network variance



Network Correlation

- How are two variables related?
- Pearson works in a flat space
- What if we have a network?
- E.g. correlation between age and sharing activity in a social network

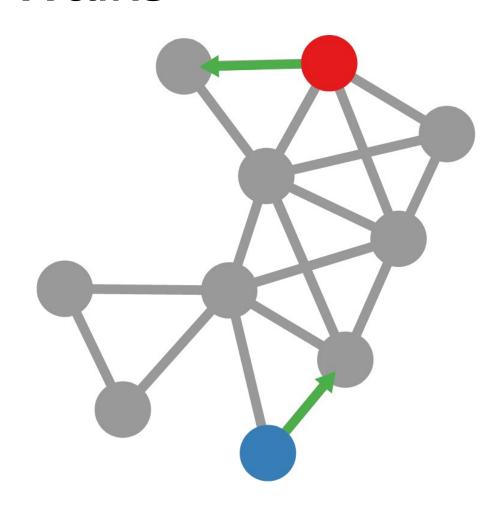
$$\rho_{x,y,G} = \frac{\operatorname{sum}(W \times (\hat{x} \otimes \hat{y}))}{\sigma_{x,W} \sigma_{y,W}}$$



Random Walks

- If we move randomly, we expect bump into each other
- The later we do so from what we expected, the farther we were
- Z-scores!

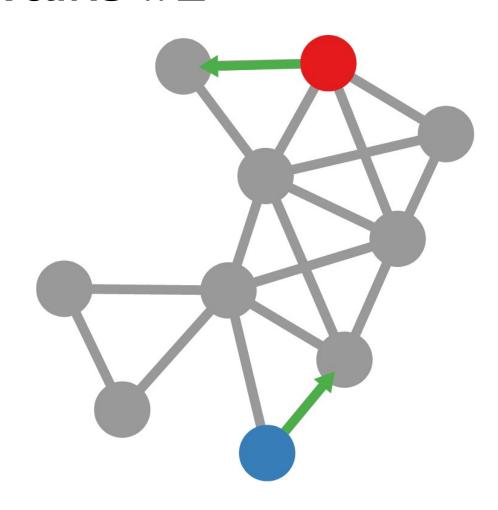
$$\sqrt{(p-q)^T Z^{-1}(p-q)}$$



Random Walks #2

- A^k: p of going from v₁
 to v₂ in k steps (RW)
- For which k would our vectors completely overlap each other?

$$\sqrt{(p-q)^T\sum_{k=0}^{\infty}A^k(p-q)}$$



Tutorial Part #2

Objectives:

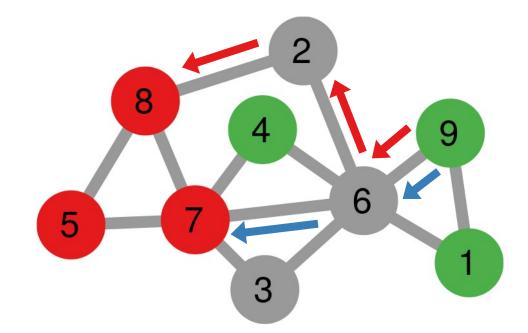
- Build an intuition of the measure with a simple toy experiment
- Calculate Euclidean, variance, and correlation on a network
- Calculate alternative Euclideans

```
1 + % □ □ ▶ ■ C → Code
    [16]: import numpy as np
          import pandas as pd
          import networkx as nx
          import network distance as nd
          import matplotlib.pyplot as plt
          from scipy.stats import pearsonr
          from scipy.spatial import distance
         warnings.simplefilter(action = "ignore", category = FutureWarning)
          for l in range(2, 101):
             G = nx.path_graph(l) # Creating longer and longer path graphs: 0-0-0-0-0
                                  # In the first vector, the leftmost node in the path graph has value 1, everything else has
                                  # In the second vector, the rightmost node in the path graph has value 1, everything else ha
              df.append((l, nd.ge(v1, v2, G)))
         df = pd.DataFrame(data = df, columns = ("l", "ge"))
         df = df.set_index("l")
         df.plot()
         plt.show()
    [20]: vector df = pd.read csv("../data/obama nodevectors.csv")
```

Shortest Path Distances

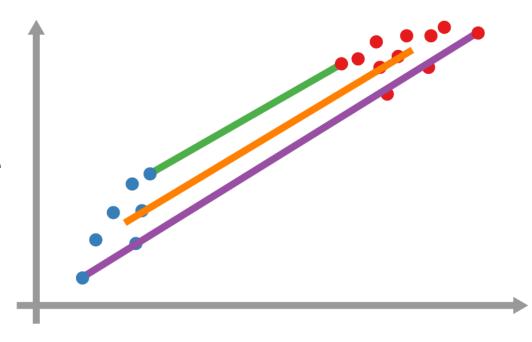
NVD Seems Easy

- Just calculate shortest paths!
- But then: which ones do we choose?



Non-Optimized

- Single linkage
 - Always pick the shortest available
- Complete Linkage
 - Always pick the longest available
- Average Linkage
 - Pick them all and weigh the alternatives



Non-Optimized

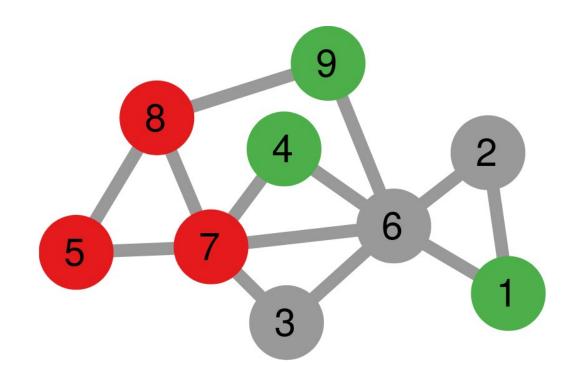
Single Linkage

$$-1+1+3$$

Complete Linkage

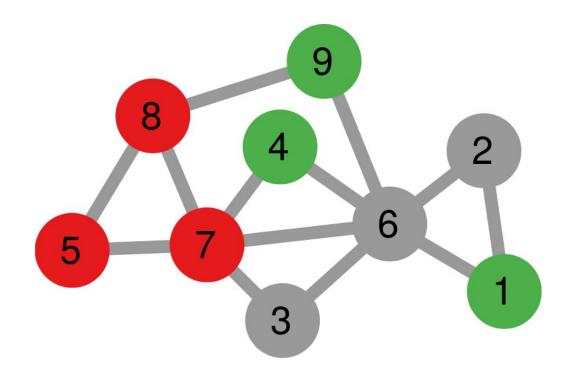
$$-3+2+2$$

- Average Linkage
 - 18/3



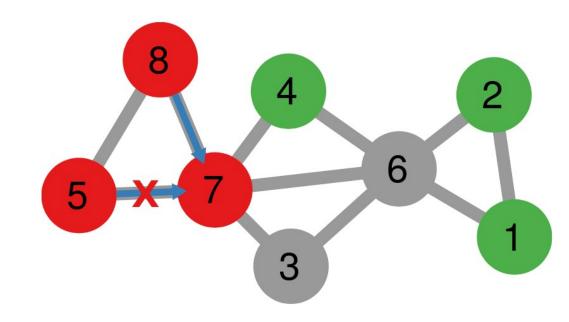
Earth Mover Distance

- Find the best set of paths
- Minimize the cost
- Similar to single linkage



Multi Agent Path Finding

- Similar to EMD
- With constraints
- Nodes & edges have capacity limits
- E.g. cannot use the same link at the same time



Tutorial Part #3

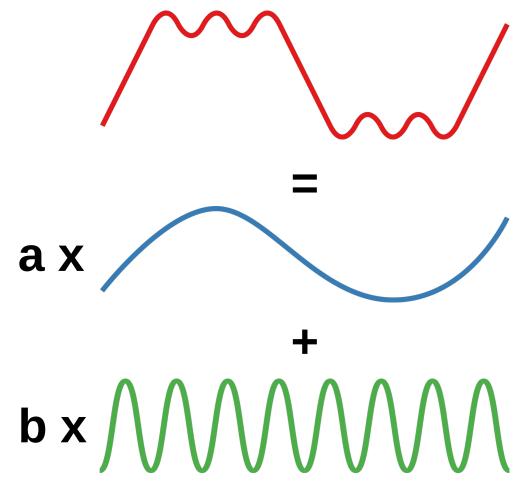
- Objectives:
 - Experiment with different linkage criteria
 - Use optimal EMD solution
 - (Skipping ahead) Test spectral distance

```
nvd_session02.ipynb
                                                1 + % □ □ 1 • • Code
    [15]: import pandas as pd
          import networkx as nx
         import network distance as nd
         import matplotlib.pyplot as plt
         warnings.simplefilter(action = "ignore", category = FutureWarning)
   [10]: vector_df = pd.read_csv("../data/obama_nodevectors.csv")
          vector_df["X"] -= vector_df["X"].min()
          vector_df["Y"] -= vector_df["Y"].min()
         v1_dict = vector_df.set_index("node").to_dict()["X"]
         v2_dict = vector_df.set_index("node").to_dict()["Y"]
         G = nx.read_edgelist("../data/obama_edgelist.csv", delimiter = ",", nodetype = int)
          Single linkage: {nd.spl(v1_dict, v2_dict, G, linkage = "single")};
          Average linkage: {nd.spl(v1 dict, v2 dict, G, linkage = "avg")};
         Complete linkage: {nd.spl(v1_dict, v2_dict, G, linkage = "complete")}.
         Single linkage: 0.19261940695605487;
         Average linkage: 2.492817629483678;
         Complete linkage: 3.344816651914214
   [13]: print(f"""
         EMD: {nd.emd(v1_dict, v2_dict, G)}.
         EMD: 0.17431584907100547
         GFT Euclidean: {nd.gft(v1_dict, v2_dict, G, linkage = "euclidean")};
         GFT Cosine: {nd.gft(v1_dict, v2_dict, G, linkage = "cosine")};
         GFT Pearson: {nd.gft(v1_dict, v2_dict, G, linkage = "pearson")}.
```

Spectral Methods

Graph Fourier Transform

 FT: decompose any signal into its component frequencies

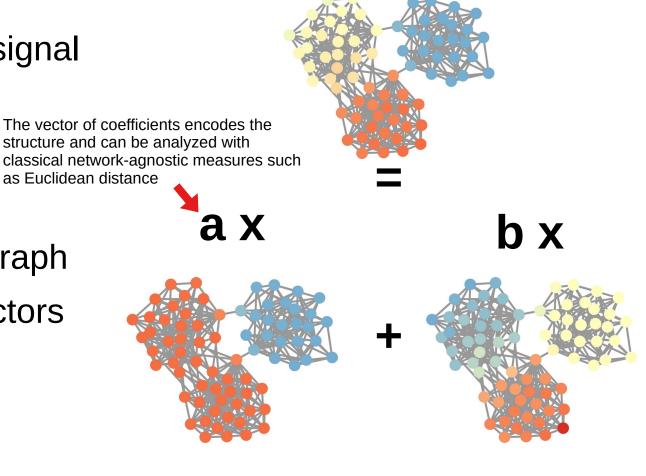


Graph Fourier Transform

FT: decompose any signal into its component frequencies

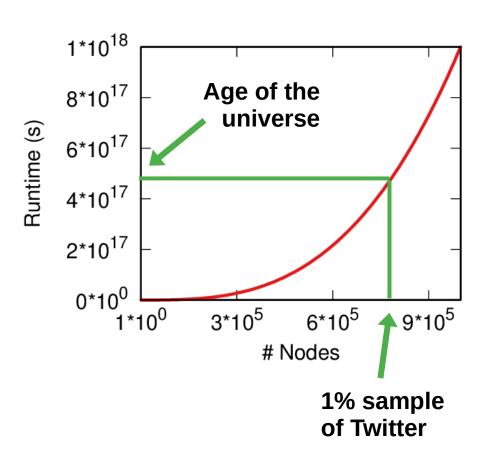
GFT: same, but the as Euclidence
 components are the
 eigenvectors of the graph

 Remember: eigenvectors encode structure



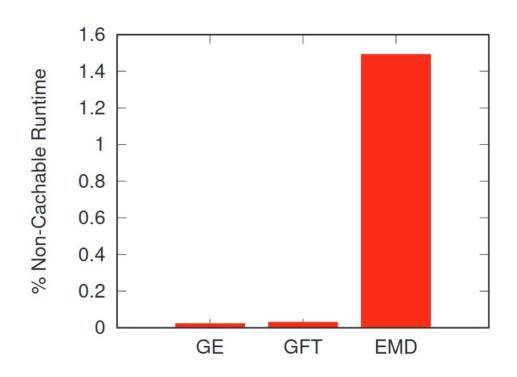
Computational Efficiency

- Expensive steps can be $O(|V|^3)...$
 - Pseudoinverse for GE
 - Shortest paths
 - Eigenvectors of Laplacian

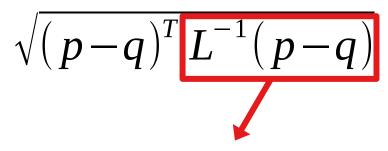


Some Tricks

- Expensive part needs to be done once per network
- You can re-use it for all node vector pairs you have
- E.g. disease spreading on an unchanging social network



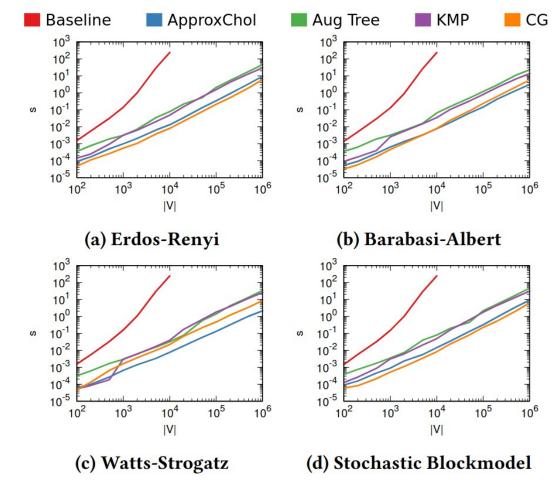
Laplacian Solvers



This part can be calculated efficiently

Without pseudo-inverting the Laplacian!

With Laplacian solvers (in Julia)



Tutorial Parts #4 & #5

- Objectives:
 - Testing runtimes
 - Experimenting with Laplacian solvers
 - Trying out some application scenarios

```
nvd_session04.ipynb
     [1]: using Graphs, SimpleWeightedGraphs
          include("NetworkDistance.jl");
     [7]: runtimes baseline = Dict{Int64, Float64}();
          runtime solver = Dict{Int64, Float64}();
     [5]: for n in [100, 200, 500, 1000, 2000, 5000]
              for r in 0:1
                  G = adjacency_matrix(SimpleWeightedGraph(erdos_renyi(n, n * 2)));
                  s = rand(Float64, n);
                  t = rand(Float64, n);
                  trial = @timed NetworkDistance.ge(G, s - t, "base");
                     runtimes_baseline[n] = trial.time;
          end
          runtimes_baseline
     [5]: Dict{Int64, Float64} with 6 entries:
            200 => 0.00569799
            500 => 0.0333335
            2000 => 1.10601
            5000 => 28.627
            1000 => 0.155771
            100 => 0.00148311
     [8]: for n in [100, 200, 500, 1000, 2000, 5000]
              for r in 0:1
                  G = adjacency_matrix(SimpleWeightedGraph(erdos_renyi(n, n * 2)));
                  s = rand(Float64, n);
                  t = rand(Float64, n);
                  trial = @timed NetworkDistance.ge(G, s - t, "approxchol");
                      runtime_solver[n] = trial.time;
          runtime_solver
         Dict{Int64 Float64} with 6 entries
```