DSC 140B
Representation Learning

Lecture 14 | Part 1

Embedding Similarities

Similar Netflix Users

- Suppose you are a data scientist at Netflix
- You're given an $n \times n$ **similarity matrix** W of users
  - entry (i, j) tells you how *similar* user i and user j are
  - 1 means "very similar", 0 means "not at all"
- Goal: visualize to find patterns

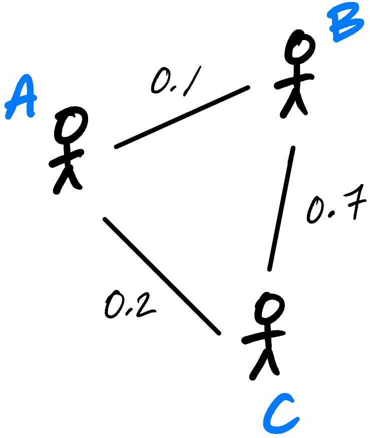
Idea

- We like scatter plots. Can we make one?
- Users are **not** vectors / points!
- They are nodes in a **similarity graph**

Similarity Graphs

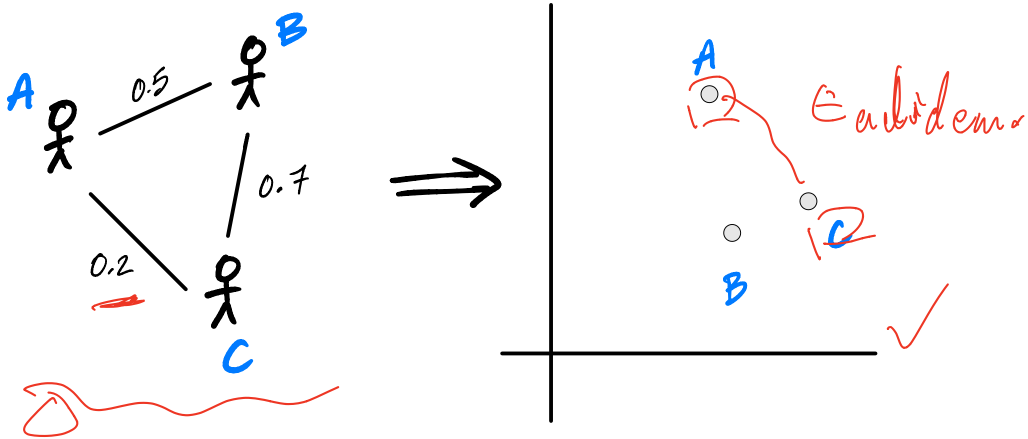
- Similarity matrices can be thought of as weighted graphs, and *vice versa*.

$$\begin{array}{c|c} & \begin{array}{ccc} A & B & C \end{array} \\ \begin{array}{c} A \\ B \\ C \end{array} & \begin{pmatrix} 1 & 0.1 & 0.2 \\ 0.1 & 1 & 0.7 \\ 0.2 & 0.7 & 1 \end{pmatrix} \end{array}$$



Goal

- **Embed** nodes of a similarity graph as points.
- Similar nodes should map to nearby points.



Today

- We will design a graph embedding approach:
  - **Spectral embeddings** via **Laplacian eigenmaps**

More Formally

- **Given**:
  - A **similarity graph** with n nodes
  - a number of dimensions, k

- **Compute**: an **embedding** of the n points into $\mathbb{R}^k$ so that similar objects are placed nearby

To Start

- **Given**:
  - A **similarity graph** with n nodes

$k=1$

- **Compute**: an **embedding** of the n points into $\mathbb{R}^1$ so that similar objects are placed nearby

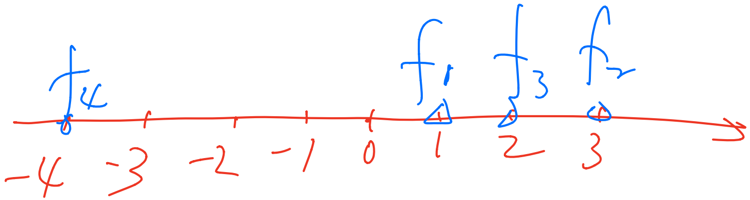
Vectors as Embeddings into $\mathbb{R}^1$

- Suppose we have n nodes (objects) to embed
- Assume they are numbered 1, 2, ..., n
- Let $f_1, f_2, \ldots, f_n \in \mathbb{R}$ be the embeddings
- We can pack them all into a vector: $\vec{f}$.
- Goal: find a good set of embeddings, $\vec{f}$.

Example

$$\vec{f} = (1, 3, 2, -4)^T$$

x_1



$\vec{x}$

An Optimization Problem

- We'll turn it into an optimization problem:

- **Step 1:** Design a cost function quantifying how good a particular embedding $\vec{f}$ is

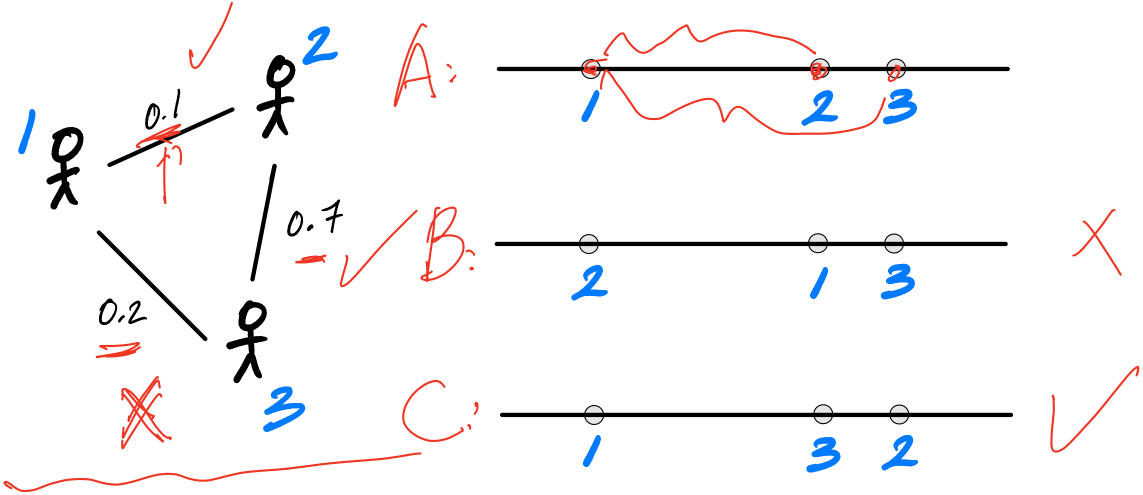
  loss

- **Step 2:** Minimize the cost

PCA : $\max_{\vec{u}} \vec{u}^T C \vec{u}$ $\quad \|\vec{u}\| = 1$

Example

- Which is the best embedding?



Cost Function for Embeddings

- Idea: cost is low if similar points are close

$|f_i - f_j|$

- Here is one approach:

$$\text{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2$$

squared Euclidean distance

- where w_{ij} is the weight between i and j.

Interpreting the Cost

$$\text{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2$$

$i \quad j \quad w_{ij}$

- If $w_{ij} \approx 0$, that pair can be placed very far apart without increasing cost
- If $w_{ij} \approx 1$, the pair should be placed close together in order to have small cost.

Exercise

Do you see a problem with the cost function?

$$\mathrm{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 \qquad = 0$$

Hint: what embedding $\vec{f}$ minimizes it?

$\vec{f} = (0, 0, 0, \ldots, 0)$

Problem

- The cost is **always** minimized by taking $\vec{f} = 0$.
- This is a "**trivial**" solution. Not useful.
- **Fix:** require $\|\vec{f}\| = 1$
  - Really, any number would work. 1 is convenient.

Exercise

Do you see **another** problem with the cost function, even if we require $\vec{f}$ to be a unit vector?

$$\text{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \underbrace{(f_i - f_j)^2}_{=0}$$

$\|\vec{f}\| = 1$

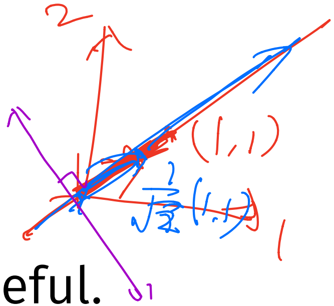
Hint: what other choice of $\vec{f}$ will **always** make this zero?

$\vec{f} = \frac{1}{\sqrt{n}}(1, 1, 1, \ldots, 1)$

Problem

$\|\vec{f}\| = 1$ ✓

- The cost is **always** minimized by taking $\vec{f} = \frac{1}{\sqrt{n}}(1, 1, \dots, 1)^T$.



- This is a "**trivial**" solution. Again, not useful.
- **Fix**: require $\vec{f}$ to be orthogonal to $(1, 1, \dots, 1)^T$.
  - Written: $\vec{f} \perp (1, 1, \dots, 1)^T$
  - Ensures that solution is not close to trivial solution
  - Might seem strange, but it will work!

The New Optimization Problem

- **Given**: an $n \times n$ similarity matrix W
- **Compute**: embedding vector $\vec{f}$ minimizing

$$\text{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2$$

subject to $\|\vec{f}\| = 1$ and $\vec{f} \perp (1, 1, \ldots, 1)^T$

How?

- This looks difficult.
- Let's write it in matrix form.
- We'll see that it is actually (hopefully) familiar.

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The Graph Laplacian

The Problem

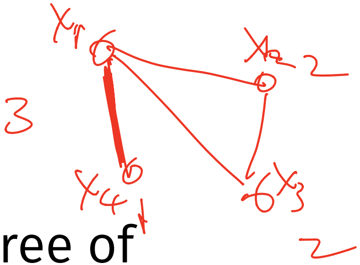
- **Compute**: embedding vector $\vec{f}$ minimizing

$$\text{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2$$

subject to $\|\vec{f}\| = 1$ and $\vec{f} \perp (1, 1, \ldots, 1)^T$

- Now: write the cost function as a matrix expression.

The Degree Matrix



- Recall: in an unweighted graph, the degree of node i equals number of neighbors.

- Equivalently (where A is the adjacency matrix):

$$\text{degree}(i) = \sum_{j=1}^{n} A_{ij}$$

$$A = \begin{array}{cccc} 1 & 2 & 3 & 4 \\ \end{array}$$
$$\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ - & - & - & \end{bmatrix}$$

- Since $A_{ij} = 1$ only if j is a neighbor of i

The Degree Matrix

- In a weighted graph, define **degree** of node i similarly:

$$\text{degree}(i) = \sum_{j=1}^{n} w_{ij}$$

- That is, it is the total weight of all neighbors.

The Degree Matrix

- The **degree matrix** D of a weighted graph is the diagonal matrix where entry (i, i) is given by:

$$d_{ii} = \text{degree}(i)$$
$$= \sum_{j=1}^{n} w_{ij}$$

$$\begin{bmatrix} d_{11} & & & 0 \\ & d_{22} & & \\ & & \ddots & \\ 0 & & & d_{nn} \end{bmatrix}$$

The Graph Laplacian

- Define $L = D - W$
  - D is the degree matrix
  - W is the similarity matrix (weighted adjacency)
- L is called the **Graph Laplacian** matrix.
- It is a very useful object

Very Important Fact

- Claim:

$w_{ij} f_i^2 + w_{ij} f_j^2 - 2 w_{ij} f_i f_j$

$$\text{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 = \vec{f}^T L \vec{f}$$

$\vec{f}^T (D - W) \vec{f}$

- Proof: expand both sides [1]

$\vec{f}^T D \vec{f} - \vec{f}^T W \vec{f}$

[1] Note that there was originally a $\frac{1}{2}$ in front of $\vec{f}^T L \vec{f}$, but this was not correct as written. See Problem 06 in the Midterm 02 practice for a longer explanation.

Proof

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Solving the Optimization Problem

A New Formulation

- **Given**: an $n \times n$ similarity matrix W

- **Compute**: embedding vector $\vec{f}$ **minimizing**

$$\text{Cost}(\vec{f}) = \vec{f}^T L \vec{f}$$

subject to $\|\vec{f}\| = 1$ and $\vec{f} \perp (1, 1, \dots, 1)^T$

- This might sound familiar...

Recall: PCA

- **Given**: a $d \times d$ covariance matrix C
- **Find**: vector $\vec{u}$ **maximizing** the variance in the direction of $\vec{u}$:
$$\vec{u}^T C \vec{u}$$
subject to $\|\vec{u}\| = 1$.
- **Solution**: take $\vec{u}$ = top eigenvector of C

A New Formulation

- Forget about orthogonality constraint for now.
- **Compute**: embedding vector $\vec{f}$ **minimizing**

Symmetric $L = D - W$

$$\text{Cost}(\vec{f}) = \vec{f}^T L \vec{f}$$

subject to $\|\vec{f}\| = 1$.

- **Solution**: the *bottom* eigenvector of L.
  - That is, eigenvector with smallest eigenvalue.

Claim

- The bottom eigenvector is $\vec{f} = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T$
- It has associated eigenvalue of 0.
- That is, $L\vec{f} = 0\vec{f} = \vec{0}$

Spectral[2] Theorem

Theorem
If A is a symmetric matrix, eigenvectors of A with distinct eigenvalues are orthogonal to one another.

[2]"Spectral" not in the sense of specters (ghosts), but because the eigenvalues of a transformation form the "spectrum"

The Fix

- Remember: we wanted $\vec{f}$ to be orthogonal to $\frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T$.
  - i.e., should be orthogonal to bottom eigenvector of L.
- Fix: take $\vec{f}$ to the be eigenvector of L with with smallest eigenvalue $\neq 0$.
- Will be $\perp \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T$ by the **spectral theorem**.

Spectral Embeddings: Problem

- **Given**: similarity graph with n nodes
- **Compute**: an **embedding** of the n points into $\mathbb{R}^1$ so that similar objects are placed nearby
- **Formally**: find embedding vector $\vec{f}$ **minimizing**

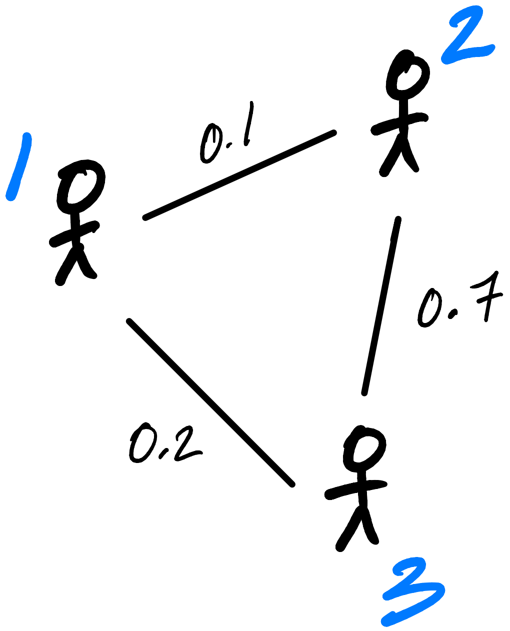
$$\mathrm{Cost}(\vec{f}) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 = \vec{f}^T L \vec{f}$$

subject to $\|\vec{f}\| = 1$ and $\vec{f} \perp (1, 1, \dots, 1)^T$

Spectral Embeddings: Solution

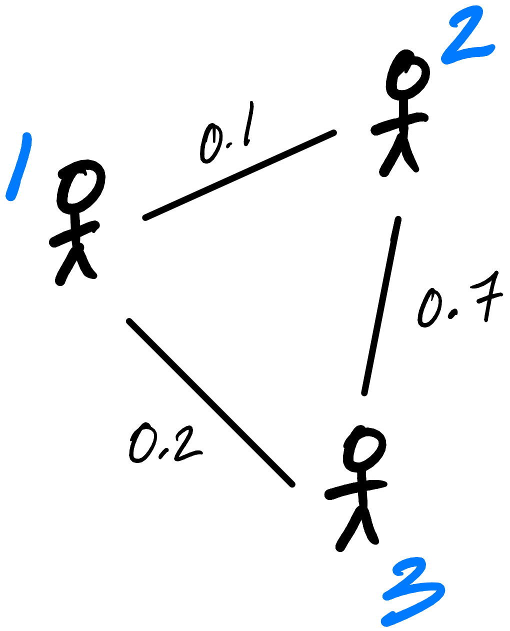
- Form the **graph Laplacian** matrix, $L = D - W$
- Choose $\vec{f}$ be an eigenvector of L with smallest eigenvalue > 0
- This is the embedding!

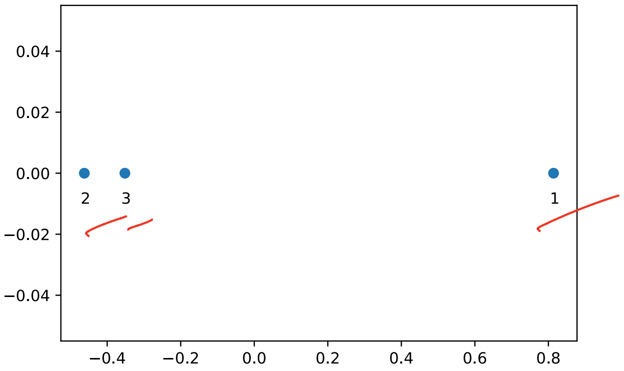
Example




```
W = np.array([
    [1, 0.1, 0.2],
    [0.1, 1, 0.7],
    [0.2, 0.7, 1]
])

D = np.diag(W.sum(axis=1))
L = D - W

vals, vecs = np.linalg.eigh(L)

f = vecs[:,1]
```

Example





Embedding into $\mathbb{R}^k$

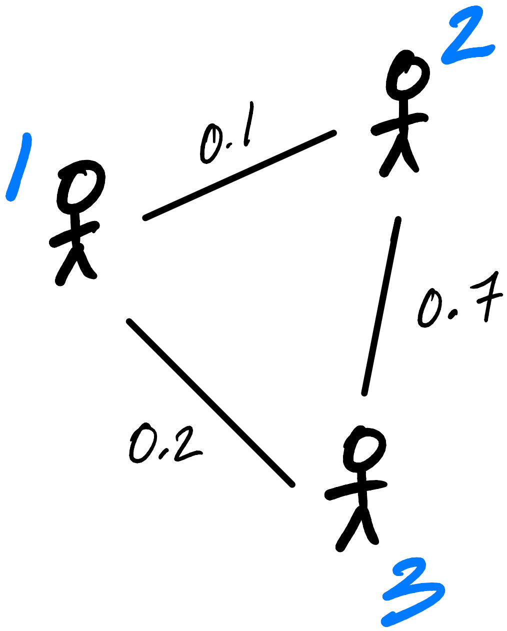
- This embeds nodes into $\mathbb{R}^1$.
- What about embedding into $\mathbb{R}^k$?
- Natural extension: find bottom k eigenvectors with eigenvalues > 0

New Coordinates

- With k eigenvectors $\vec{f}^{(1)}, \vec{f}^{(2)}, \ldots, \vec{f}^{(k)}$, each node is mapped to a point in $\mathbb{R}^k$.

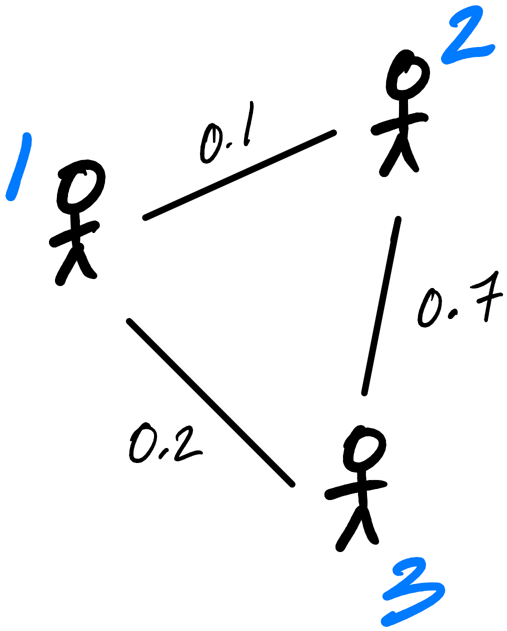
- Consider node i.
  - First new coordinate is $\vec{f}_i^{(1)}$.
  - Second new coordinate is $\vec{f}_i^{(2)}$.
  - Third new coordinate is $\vec{f}_i^{(3)}$.
  - $\vdots$

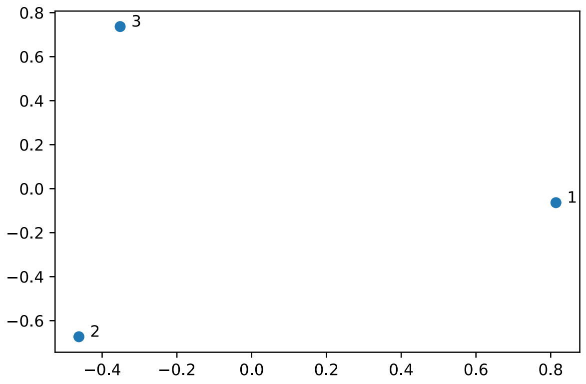
Example




```
W = np.array([
      [1, 0.1, 0.2],
      [0.1, 1, 0.7],
      [0.2, 0.7, 1]
])

D = np.diag(W.sum(axis=1))
L = D - W

vals, vecs = np.linalg.eigh(L)

# take two eigenvectors
# to map to R^2
f = vecs[:,1:3]
```

Example





Laplacian Eigenmaps

- This approach is part of the method of "**Laplacian eigenmaps**"
- Introduced by Mikhail Belkin[3] and Partha Niyogi
- It is a type of **spectral embedding**

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[3] Now at HDSI

A Practical Issue

- The Laplacian is often **normalized**:

$$L_{\text{norm}} = D^{-1/2} L D^{-1/2}$$

  where $D^{-1/2}$ is the diagonal matrix whose ith diagonal entry is $1/\sqrt{d_{ii}}$.

- Proceed by finding the eigenvectors of L_{norm}.

In Summary

- We can **embed** a similarity graph's nodes into $\mathbb{R}^k$ using the eigenvectors of the graph Laplacian
- Yet another instance where eigenvectors are solution to optimization problem
- Next time: using this for dimensionality reduction