DSC 140B
Representation Learning

Lecture 13 | 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

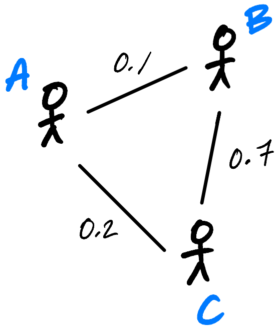
Idea

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

Similarity Graphs

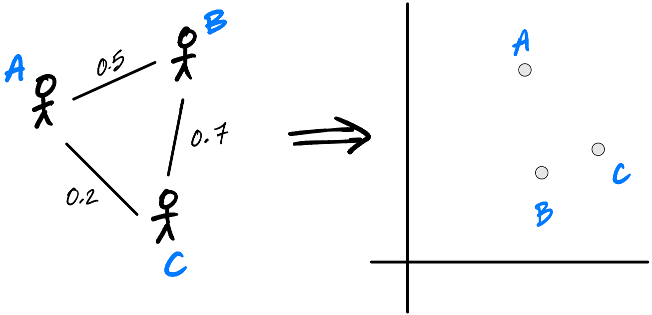
- Similarity matrices can be thought of as weighted graphs, and *vice versa*.

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



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

- **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

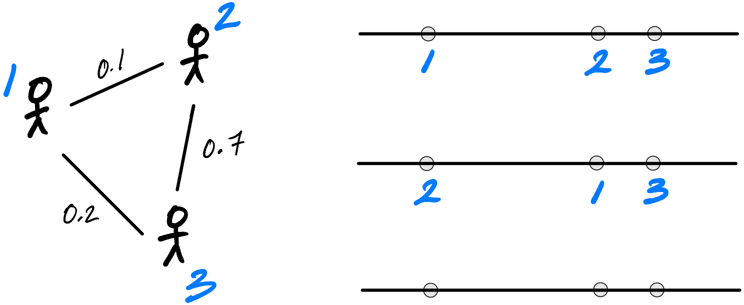
$\vec{f} = (1, 3, 2, -4)^T$

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
- **Step 2**: Minimize the cost

Example

- Which is the best embedding?



Cost Function for Embeddings

- Idea: cost is low if similar points are close
- Here is one approach:

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

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

Interpreting the Cost

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

- 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?

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

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

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?

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

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

Problem

- 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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Lecture 13 | Part 2

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 $\vec{f} \perp (1, 1, \dots, 1)^T$

- 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):

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

- 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:

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

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:

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

- Proof: expand both sides

Proof