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

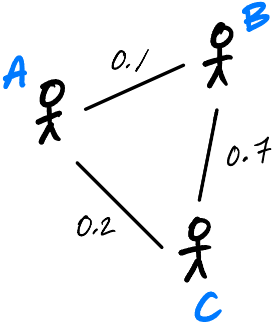
Idea

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

Similarity Graphs

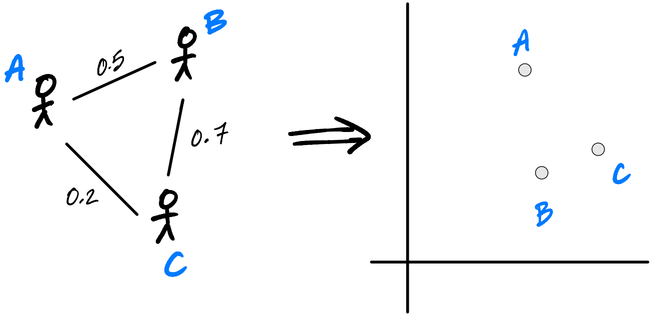
- Similarity matrices can be thought of as weighted graphs, and *vice versa*.

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



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

- **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

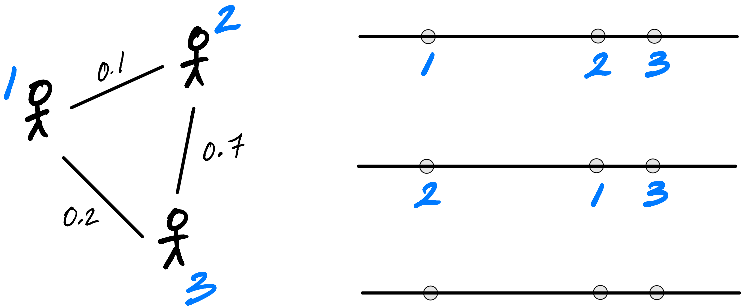
$\vec{f} = (1, 3, 2, -4)^T$

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

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 14 | 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 $\vec{f} \perp (1, 1, \ldots, 1)^T$

- 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):

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

- 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:

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

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

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Lecture 14 | Part 3

Solving the Optimization Problem

A New Formulation

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

$$\text{Cost}(\vec{f}) = \frac{1}{2}\vec{f}^T L \vec{f}$$

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

- 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**

$$\text{Cost}(\vec{f}) = \frac{1}{2}\vec{f}^T L \vec{f}$$

  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[1] Theorem

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

[1]"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**

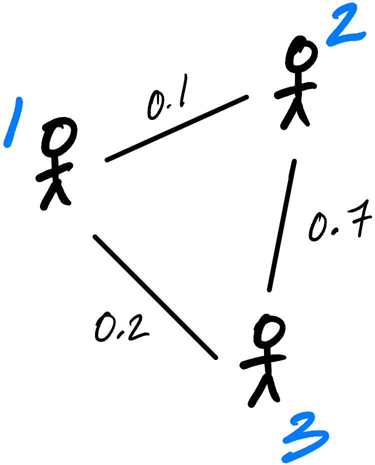
$$\mathrm{Cost}(\vec{f}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 = \frac{1}{2} \vec{f}^T L \vec{f}$$

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

Spectral Embeddings: Solution

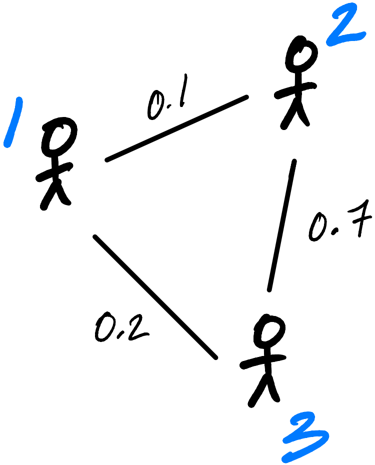
- Form the **graph Laplacian** matrix, $L = D - W$
- Choose $\vec{f}$ be an eigenvector of L with smallest eigenvalue > 0
- This is the embedding!

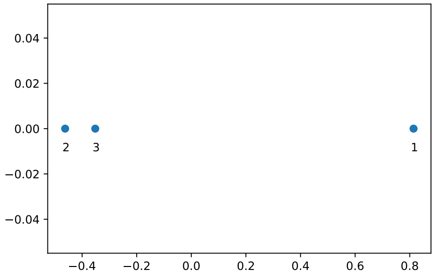
Example




```
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 $\mathbb{R}^k$

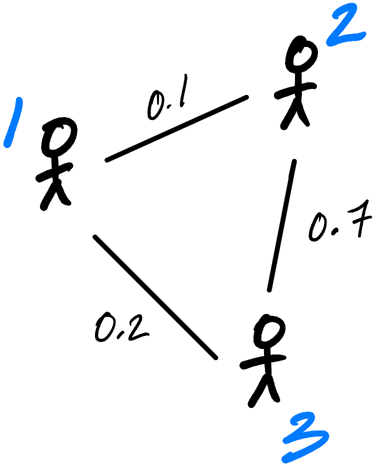
- This embeds nodes into $\mathbb{R}^1$.
- What about embedding into $\mathbb{R}^k$?
- Natural extension: find bottom k eigenvectors with eigenvalues > 0

New Coordinates

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

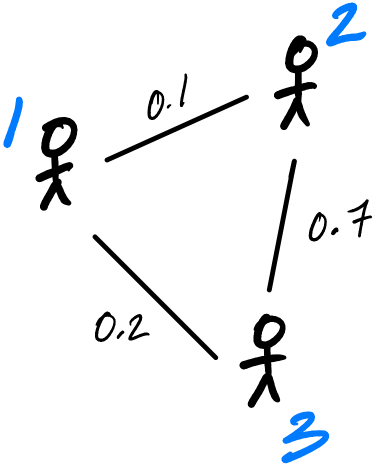
- Consider node i.
  - First new coordinate is $\vec{f}_i^{(1)}$.
  - Second new coordinate is $\vec{f}_i^{(2)}$.
  - Third new coordinate is $\vec{f}_i^{(3)}$.
  - $\vdots$

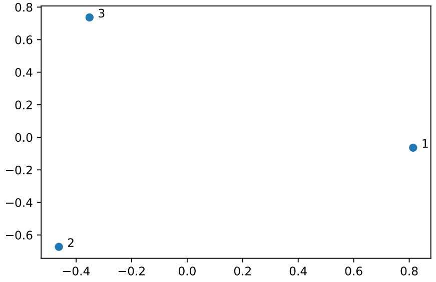
Example




```
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[2] and Partha Niyogi
- It is a type of **spectral embedding**

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[2] 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

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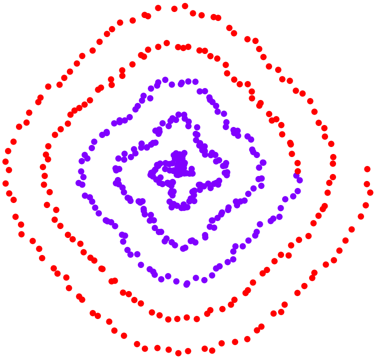
Lecture 14 | Part 4

Nonlinear Dimensionality Reduction

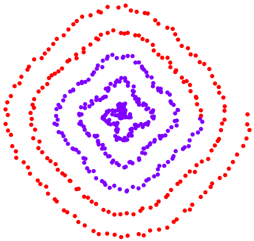
Scenario

- You want to train a classifier on this data.
- It would be easier if we could “unroll” the spiral.
- Data seems to be one-dimensional, even though in two dimensions.
- Dimensionality reduction?



PCA?

- Does PCA work here?
- Try projecting onto one principal component.



No

PCA?

- PCA simply “rotates” the data.
- No amount of rotation will “unroll” the spiral.
- We need a fundamentally different approach that works for non-linear patterns.

Today

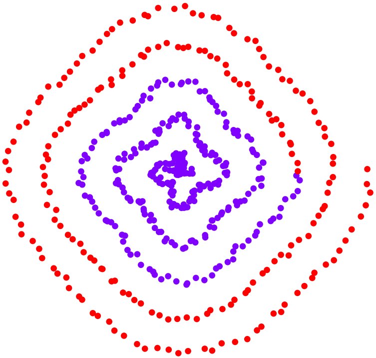
- Non-linear dimensionality reduction via **spectral embeddings**.

Last Time: Spectral Embeddings

- **Given**: a similarity graph with n nodes, number of dimensions k.
- **Embed**: each node as a point in $\mathbb{R}^k$ such that similar nodes are mapped to nearby points
- **Solution**: *bottom k* non-constant eigenvectors of graph Laplacian

Idea

- Build a similarity graph from points.
- Points *near the spiral* should be similar.
- Embed the similarity graph into $\mathbb{R}^1$



Today

- 1) How do we build a graph from a set of points?
- 2) Dimensionality reduction with Laplacian eigenmaps

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Lecture 14 | Part 5

From Points to Graphs

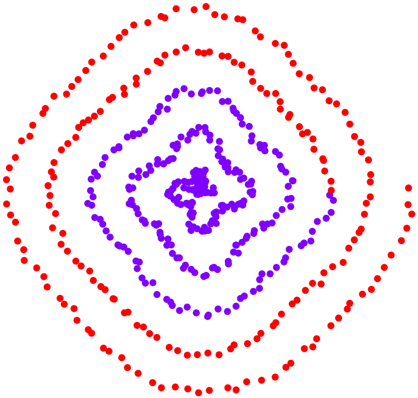
Dimensionality Reduction

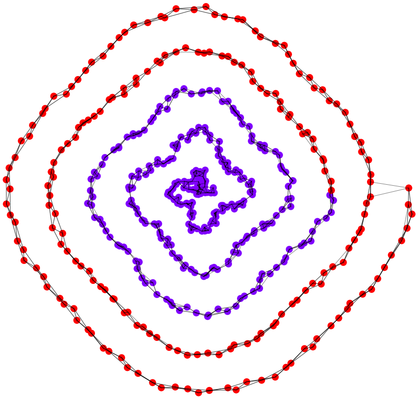
- **Given**: n points in $\mathbb{R}^d$, number of dimensions $k \leq d$
- **Map**: each point $\vec{x}$ to new representation $\vec{z} \in \mathbb{R}^k$

Idea

- Build a similarity graph from points in $\mathbb{R}^2$
- Use approach from last lecture to embed into $\mathbb{R}^k$
- But how do we represent a set of points as a similarity graph?

Why graphs?





Three Approaches

- 1) Epsilon neighbors graph
- 2) *k*-Nearest neighbor graph
- 3) fully connected graph with similarity function

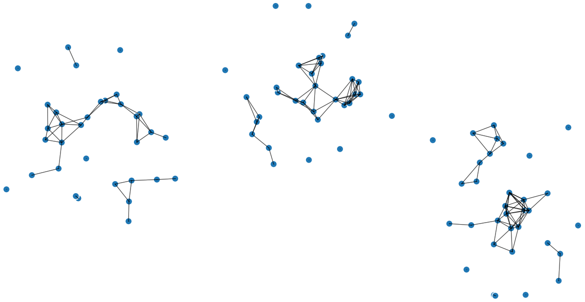
Epsilon Neighbors Graph

- Input: vectors $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}$, a number ε
- Create a graph with one node i per point $\vec{x}^{(i)}$
- Add edge between nodes i and j if $\|\vec{x}^{(i)} - \vec{x}^{(j)}\| \leq \varepsilon$
- Result: **unweighted** graph

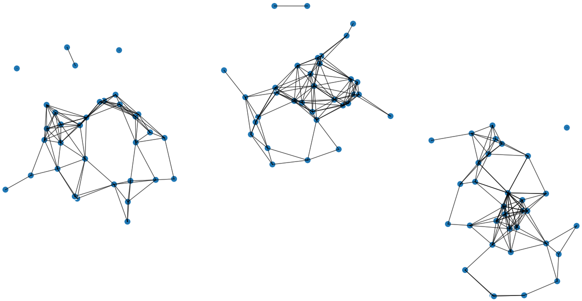
Exercise

What will the graph look like when ε is small? What about when it is large?

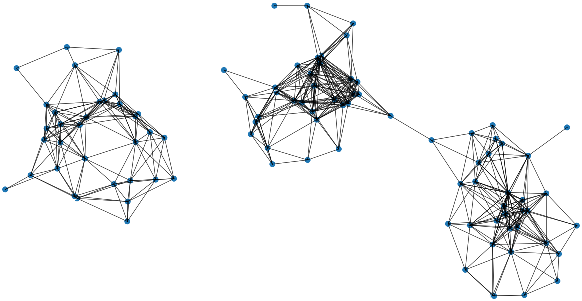
Epsilon Neighbors Graph



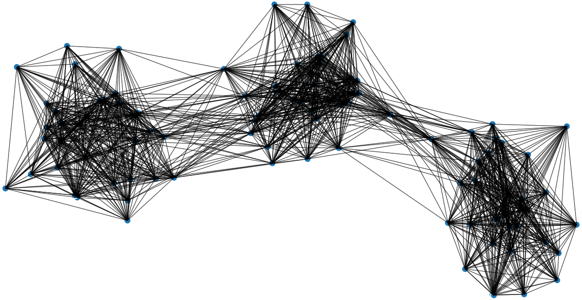
Epsilon Neighbors Graph



Epsilon Neighbors Graph



Epsilon Neighbors Graph



Note

- We’ve drawn these graphs by placing nodes at the same position as the point they represent
- But a graph’s nodes can be drawn in any way

Epsilon Neighbors: Pseudocode

```
# assume the data is in X
n = len(X)
adj = np.zeros_like(X)
for i in range(n):
    for j in range(n):
        if distance(X[i], X[j]) <= epsilon:
            adj[i, j] = 1
```

Picking ε

- If ε is too small, graph is underconnected
- If ε is too large, graph is overconnected
- If you cannot visualize, just try and see

With scikit-learn

```
import sklearn.neighbors
adj = sklearn.neighbors.radius_neighbors_graph(
        X,
        radius=...
    )
```

k-Neighbors Graph

- Input: vectors $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}$, a number k
- Create a graph with one node i per point $\vec{x}^{(i)}$
- Add edge between each node i and its k closest neighbors
- Result: **unweighted** graph

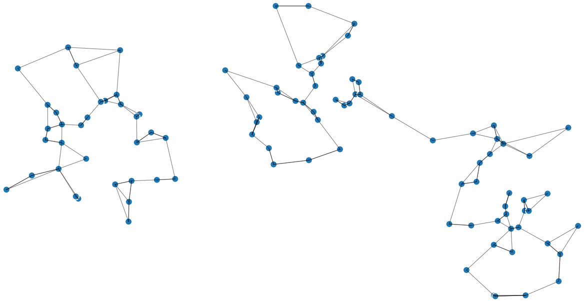
k-Neighbors: Pseudocode

```
# assume the data is in X
n = len(X)
adj = np.zeros_like(X)
for i in range(n):
    for j in k_closest_neighbors(X, i):
        adj[i, j] = 1
```

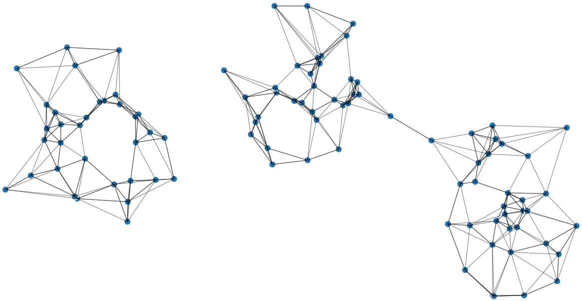
Exercise

Is it possible for a k-neighbors graph to be disconected?

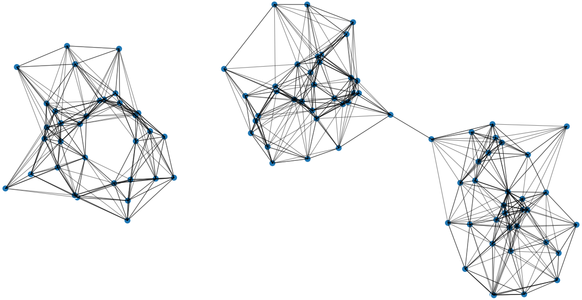
k-Neighbors Graph



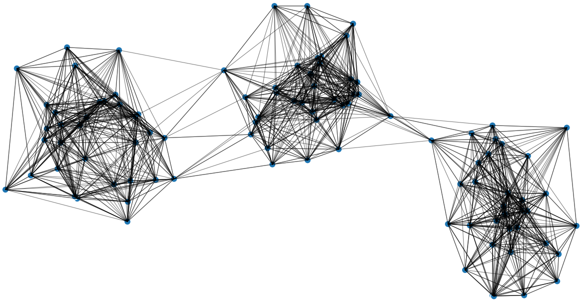
k-Neighbors Graph



k-Neighbors Graph



k-Neighbors Graph



With scikit-learn

```
import sklearn.neighbors
adj = sklearn.neighbors.kneighbors_graph(
        X,
        n_neighbors=...
    )
```

Fully Connected Graph

- Input: vectors $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}$, a similarity function h
- Create a graph with one node i per point $\vec{x}^{(i)}$
- Add edge between every pair of nodes. Assign weight of $h(\vec{x}^{(i)}, \vec{x}^{(j)})$
- Result: **weighted** graph

Gaussian Similarity

- A common similarity function: Gaussian
- Must choose σ appropriately

$$h(\vec{x}, \vec{y}) = e^{-\|\vec{x}-\vec{y}\|^2/\sigma^2}$$

Fully Connected: Pseudocode

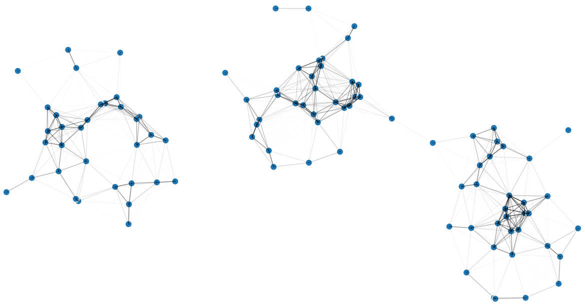
```
def h(x, y):
    dist = np.linalg.norm(x, y)
    return np.exp(-dist**2 / sigma**2)

# assume the data is in X
n = len(X)
w = np.ones_like(X)
for i in range(n):
    for j in range(n):
        w[i, j] = h(X[i], X[j])
```

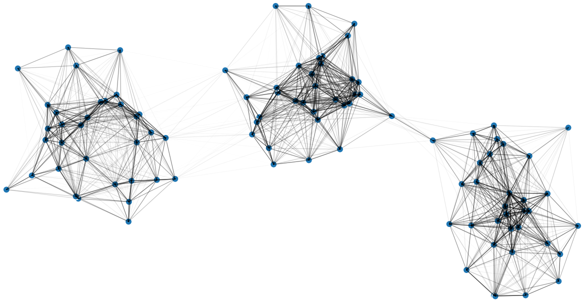
With SciPy

```
distances = scipy.spatial.distance_matrix(X, X)
w = np.exp(-distances**2 / sigma**2)
```

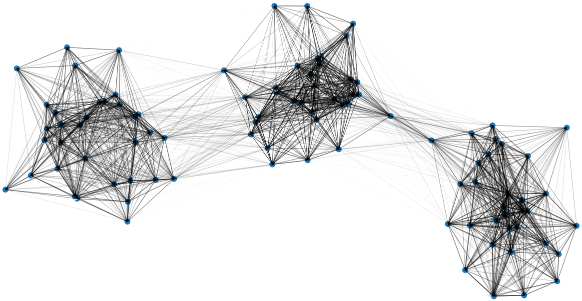
Gaussian Similarity



Gaussian Similarity



Gaussian Similarity



Gaussian Similarity