DSC 190

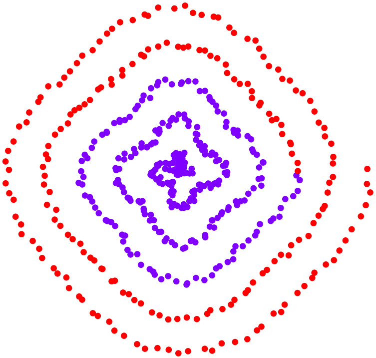
Machine Learning: Representations

Lecture 10 | Part 1

Nonlinear Dimensionality Reduction

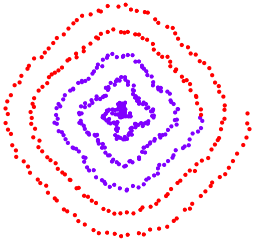
Scenario

- 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?

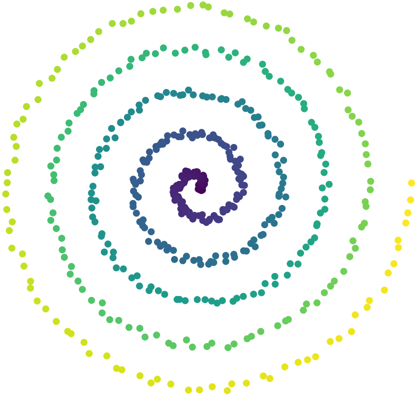
- PCA simply “rotates” the data.
- No amount of rotation will “unroll” the spiral.
- We need a fundamentally different approach that works for non-linear patterns.

Today

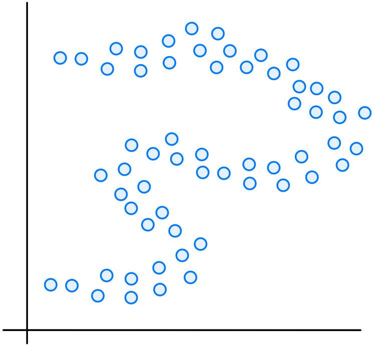
- Non-linear dimensionality reduction via **spectral embeddings**.

Rethinking Dimensionality

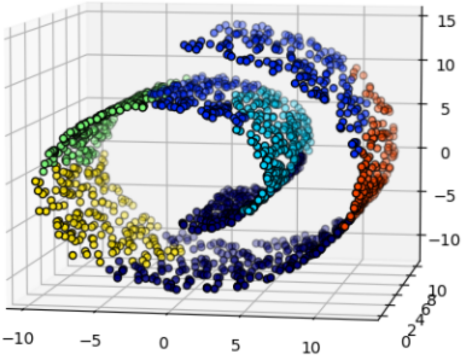
- Each point is an (x, y) coordinate in two dimensional space
- But the structure is one-dimensional
- Could (roughly) locate point using one number: distance from end.



Rethinking Dimensionality



Rethinking Dimensionality

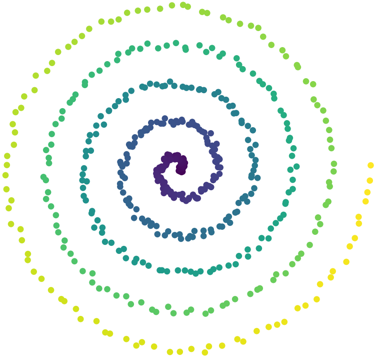


Rethinking Dimensionality

- Informally: data expressed with d dimensions, but its *really* confined to k-dimensional region
- This region is called a **manifold**
- d is the **ambient** dimension
- k is the **intrinsic** dimension

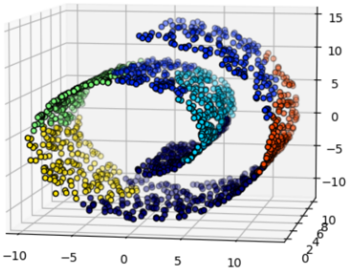
Example

- Ambient dimension: 2
- Intrinsic dimension: 1



Example

- Ambient dimension: 3
- Intrinsic dimension: 2



Example

- Ambient dimension:
- Intrinsic dimension:

Manifold Learning

- **Given**: data in high dimensions
- **Recover**: the low-dimensional manifold

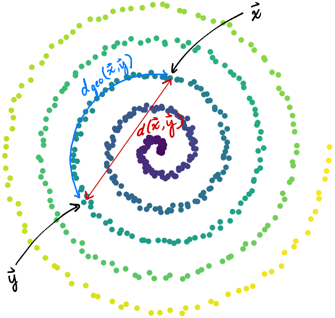
Types of Manifolds

- Manifolds can be linear
  - E.g., linear subpaces – hyperplanes
  - Learned by PCA

- Can also be non-linear (locally linear)
  - Example: the spiral data
  - Learned by **Laplacian eigenmaps**, among others

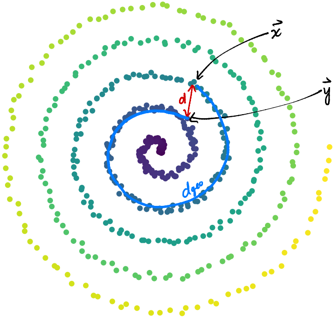
Euclidean vs. Geodesic Distances

- **Euclidean distance**: the “straight-line” distance
- **Geodesic distance**: the distance along the manifold



Euclidean vs. Geodesic Distances

- **Euclidean distance**: the “straight-line” distance
- **Geodesic distance**: the distance along the manifold



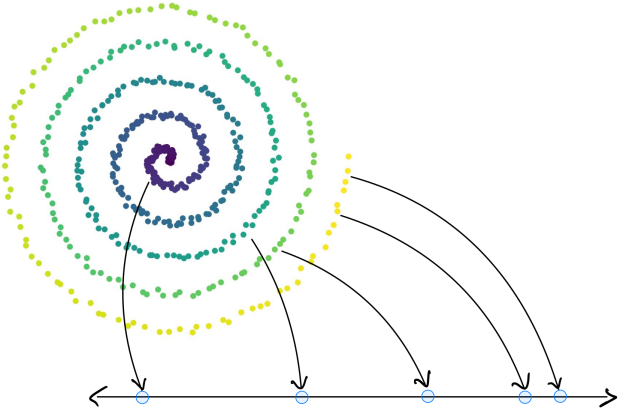
Euclidean vs. Geodesic Distances

- If data is close to a linear manifold, geodesic ≈ Euclidean
- Otherwise, can be very different

Non-Linear Dimensionality Reduction

- **Goal**: Map points in $\mathbb{R}^d$ to $\mathbb{R}^k$
- **Such that**: if $\vec{x}$ and $\vec{y}$ are close in **geodesic** distance in $\mathbb{R}^d$, they are close in **Euclidean** distance in $\mathbb{R}^k$

Embeddings



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Machine Learning: Representations

Lecture 10 | Part 2

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

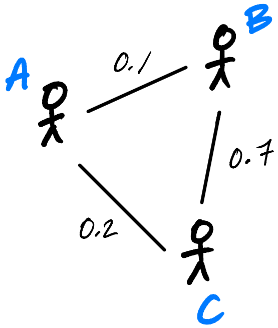
Idea

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

Similarity Graphs

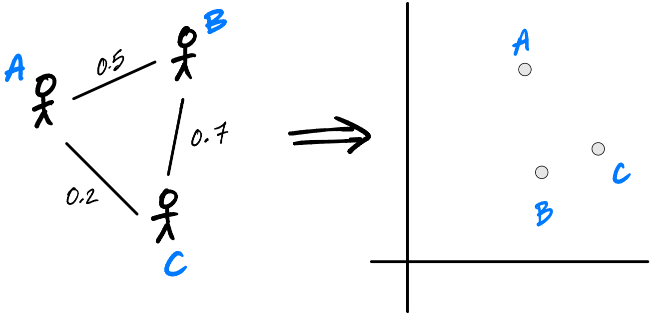
- Similarity matrices can be thought of as weighted graphs, and *vice versa*.

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



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

- **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

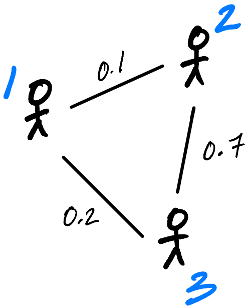
$\vec{f} = (1, 3, 2, -4)^T$

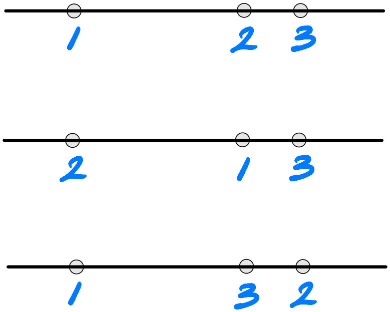
An Optimization Problem

- 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 $\vec{f} = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T$.

- This is a "**trivial**" solution. Again, not useful.

- **Fix**: require $\vec{f}$ to be orthogonal to $(1, 1, \ldots, 1)^T$.
  - Written: $\vec{f} \perp (1, 1, \ldots, 1)^T$
  - 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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Machine Learning: Representations

Lecture 10 | Part 3

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

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Machine Learning: Representations

Lecture 10 | Part 4

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 $\frac{1}{\sqrt{n}}(1, 1, \dots, 1)^T$.
  - 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 $\perp \frac{1}{\sqrt{n}}(1, 1, \dots, 1)^T$ 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**

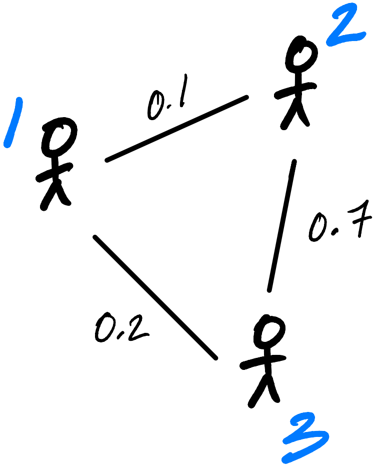
$$\mathrm{Cost}(\vec{f}) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(f_i - f_j)^2 = \frac{1}{2}\vec{f}^T L \vec{f}$$

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

Spectral Embeddings: Solution

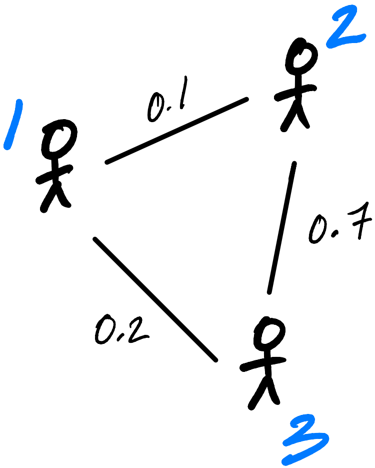
- Form the **graph Laplacian** matrix, $L = D - W$
- Choose $\vec{f}$ be an eigenvector of L with smallest eigenvalue > 0
- This is the embedding!

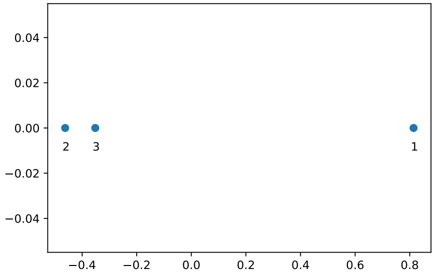
Example




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

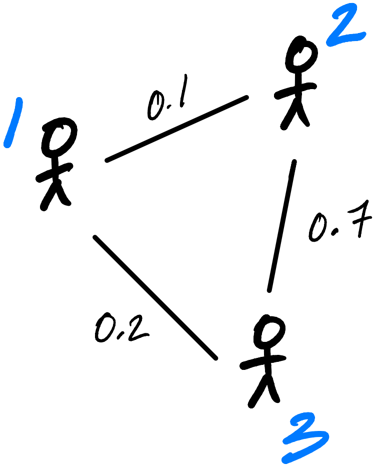
- This embeds nodes into $\mathbb{R}^1$.
- What about embedding into $\mathbb{R}^k$?
- Natural extension: find bottom k eigenvectors with eigenvalues > 0

New Coordinates

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

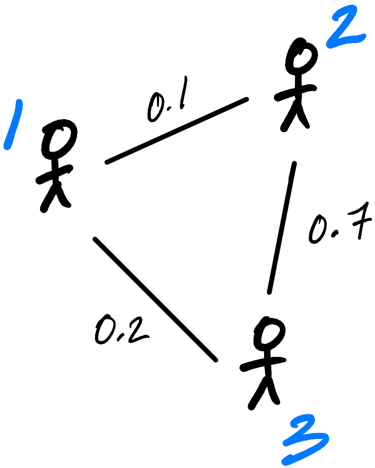
- Consider node i.
  - First new coordinate is $\vec{f}_i^{(1)}$.
  - Second new coordinate is $\vec{f}_i^{(2)}$.
  - Third new coordinate is $\vec{f}_i^{(3)}$.
  - $\vdots$

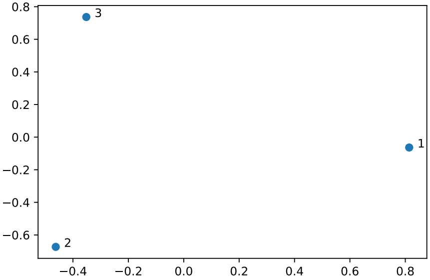
Example




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

[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