DSC 140B
Representation Learning

Lecture 12 | Part 1

Interpreting PCA

Three Interpretations

- What is PCA doing?
- Three interpretations:
    1. Mazimizing variance
    2. Finding the best reconstruction
    3. Decorrelation

Recall: Matrix Formulation

- Given data matrix X.
- Compute new data matrix $Z = XU$.
- PCA: choose U to be matrix of eigenvectors of C.
- For now: suppose U can be anything – but columns should be orthonormal
  - Orthonormal = “not redundant”

View #1: Maximizing Variance

- This was the view we used to derive PCA

- Define the **total variance** to be the sum of the variances of each column of Z.

- Claim: Choosing U to be top eigenvectors of C maximizes the total variance among all choices of orthonormal U.

Main Idea

PCA maximizes the total variance of the new data. I.e., chooses the most "interesting" new features which are not redundant.

View #2: Minimizing Reconstruction Error

- Recall: total reconstruction error

$$\sum_{i=1}^{n} \|\vec{x}^{(i)} - U\vec{z}^{(i)}\|^2$$

- Goal: minimize total reconstruction error.

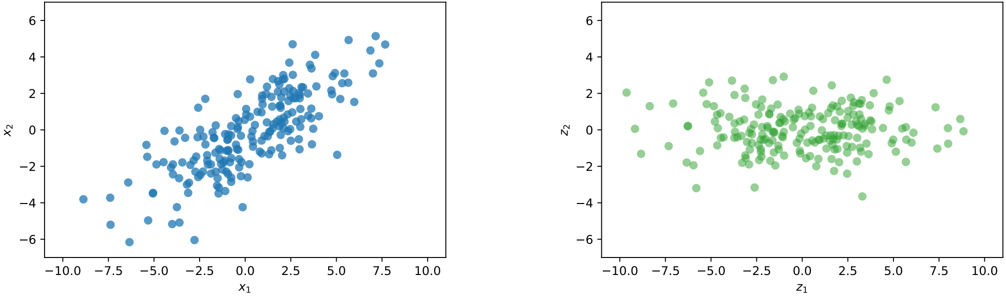
- Claim: Choosing U to be top eigenvectors of C minimizes reconstruction error among all choices of orthonormal U

Main Idea

PCA minimizes the reconstruction error. It is the "best" projection of points onto a linear subspace of dimensionality k. When $k = d$, the reconstruction error is zero.

View #3: Decorrelation

- PCA has the effect of “decorrelating” the features.



Main Idea

PCA learns a new representation by rotating the data into a basis where the features are uncorrelated (not redundant). That is: the natural basis

vectors are the principal directions (eigenvectors of the covariance matrix). PCA changes the basis to this natural basis.

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Lecture 12 | Part 2

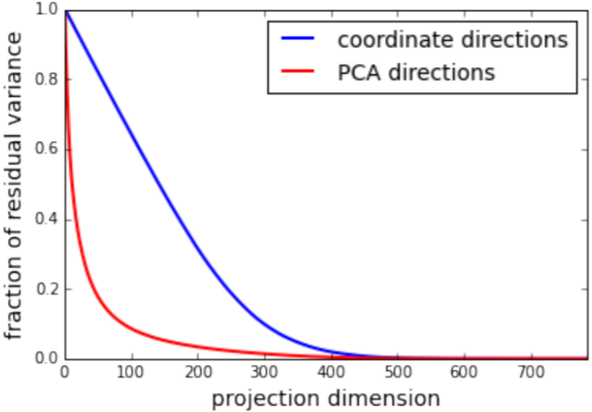
PCA in Practice

PCA in Practice

- PCA is often used in **preprocessing** before classifier is trained, etc.
- Must choose number of dimensions, k.
- One way: cross-validation.
- Another way: the elbow method.

Total Variance

- The **total variance** is the sum of the eigenvalues of the covariance matrix.
- Or, alternatively, sum of variances in each orthogonal basis direction.



coordinate directions
PCA directions
fraction of residual variance
projection dimension
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
600
700

Caution

- PCA's assumption: variance is interesting
- PCA is totally unsupervised
- The direction most meaningful for classification may not have large variance!

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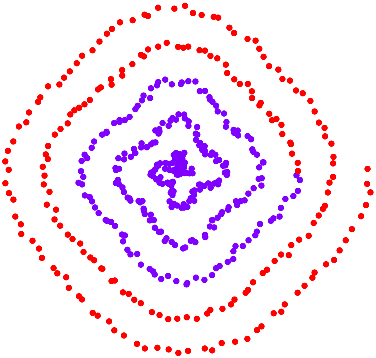
Lecture 12 | Part 3

Nonlinear Dimensionality Reduction

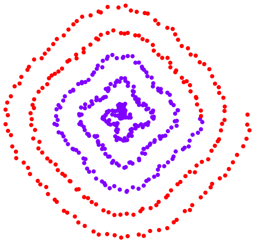
Scenario

- 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?

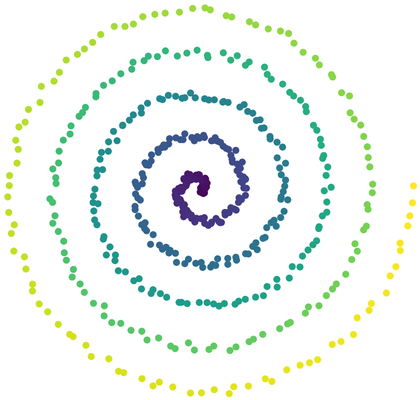
- PCA simply “rotates” the data.
- No amount of rotation will “unroll” the spiral.
- We need a fundamentally different approach that works for non-linear patterns.

Today

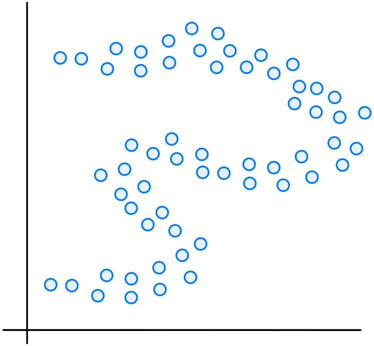
- Non-linear dimensionality reduction via **spectral embeddings**.

Rethinking Dimensionality

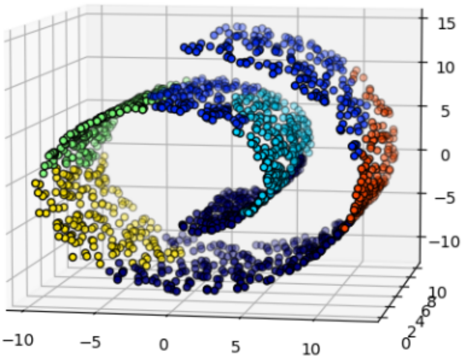
- Each point is an (x, y) coordinate in two dimensional space
- But the structure is one-dimensional
- Could (roughly) locate point using one number: distance from end.



Rethinking Dimensionality



Rethinking Dimensionality

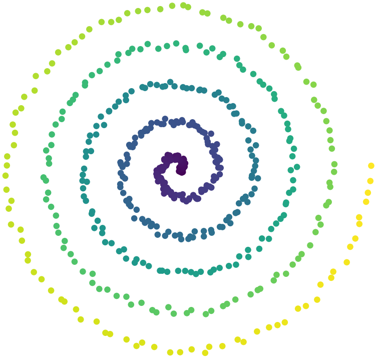


Rethinking Dimensionality

- 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

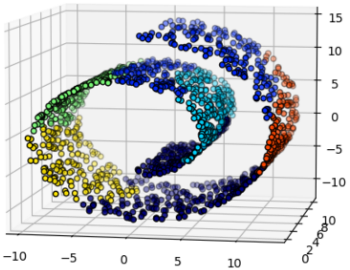
Example

- 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

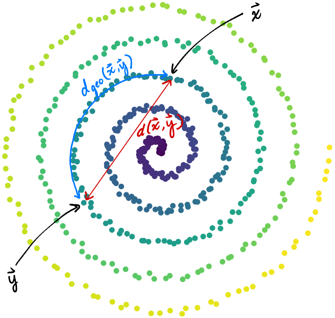
Types of Manifolds

- 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

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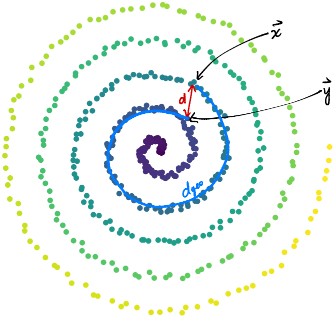


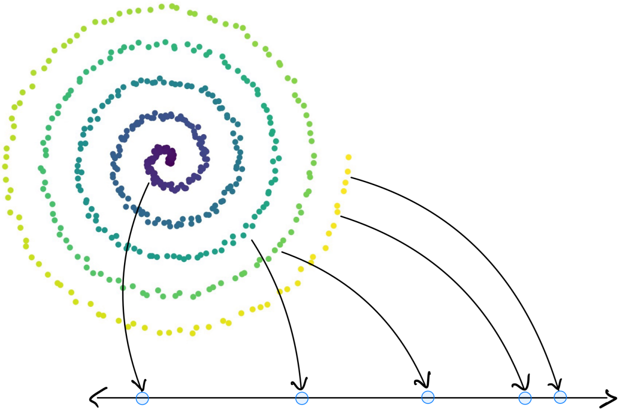
Euclidean vs. Geodesic Distances

- 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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Lecture 12 | Part 4

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

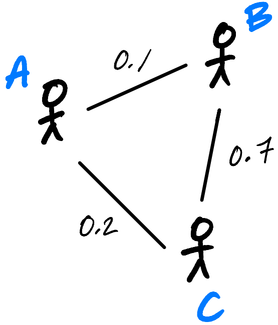
Idea

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

Similarity Graphs

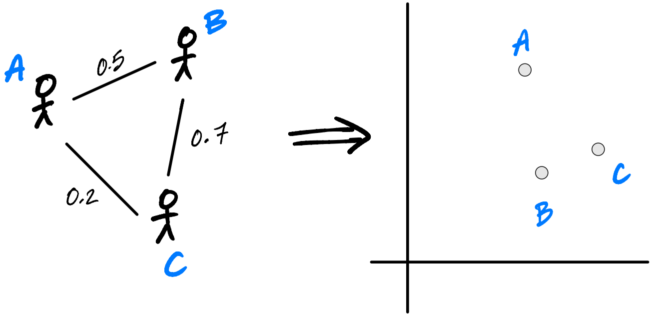
- Similarity matrices can be thought of as weighted graphs, and *vice versa*.

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



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

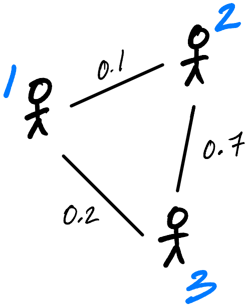
$\vec{f} = (1, 3, 2, -4)^T$

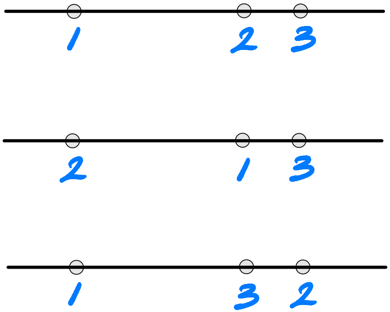
An Optimization Problem

- 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

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

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.