# DSC 140B

## Representation Learning

Lecture 11 | Part 1

**Dimensionality Reduction with d ≥ 2**

# So far: PCA

- **Given**: data $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)} \in \mathbb{R}^d$
- **Map**: each data point $\vec{x}^{(i)}$ to a single feature, $z_i$.
  - Idea: maximize the variance of the new feature
- **PCA**: Let $z_i = \vec{x}^{(i)} \cdot \vec{u}$, where $\vec{u}$ is top eigenvector of covariance matrix, $C$.

# Now: More PCA

- **Given**: data $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)} \in \mathbb{R}^d$
- **Map**: each data point $\vec{x}^{(i)}$ to $k$ new features, $\vec{z}^{(i)} = (z_1^{(i)}, \ldots, z_k^{(i)})$.

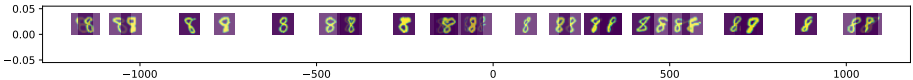
# A Single Principal Component

- Recall: the **principal component** is the top eigenvector $\vec{u}$ of the covariance matrix, $C$
- It is a unit vector in $\mathbb{R}^d$
- Make a new feature $z \in \mathbb{R}$ for point $\vec{x} \in \mathbb{R}^d$ by computing $z = \vec{x} \cdot \vec{u}$
- This is dimensionality reduction from $\mathbb{R}^d \to \mathbb{R}^1$

# Example

- MNIST: 60,000 images in 784 dimensions
- Principal component: $\vec{u} \in \mathbb{R}^{784}$
- We can project an image in $\mathbb{R}^{784}$ onto $\vec{u}$ to get a single number representing the image

# Example



# Another Feature?

- Clearly, mapping from $\mathbb{R}^{784} \rightarrow \mathbb{R}^1$ loses a lot of information
- What about mapping from $\mathbb{R}^{784} \rightarrow \mathbb{R}^2$? $\mathbb{R}^k$?

# A Second Feature

- Our first feature is a mixture of features, with weights given by unit vector $\vec{u}^{(1)} = (u_1^{(1)}, u_2^{(1)}, \ldots, u_d^{(1)})^T$.

$$z_1 = \vec{u}^{(1)} \cdot \vec{x} = u_1^{(1)} x_1 + \ldots + u_d^{(1)} x_d$$

- To maximize variance, choose $\vec{u}^{(1)}$ to be top eigenvector of $C$.

# A Second Feature

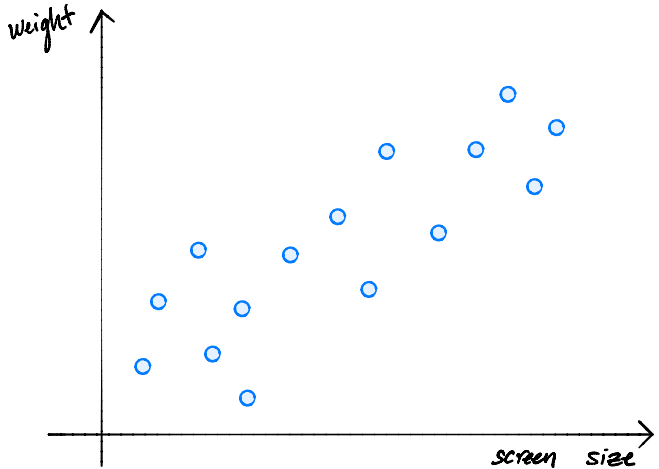
- Make same assumption for second feature:

$$z_2 = \vec{u}^{(2)} \cdot \vec{x} = u_1^{(2)} x_1 + \ldots + u_d^{(2)} x_d$$

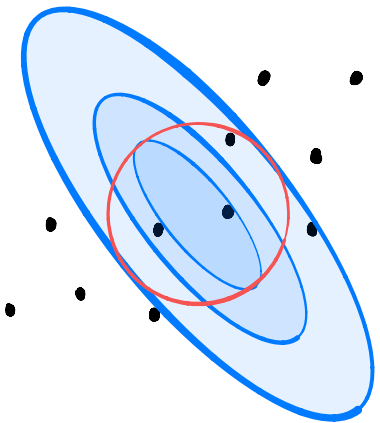
- How do we choose $\vec{u}^{(2)}$?

- We should choose $\vec{u}^{(2)}$ to be **orthogonal** to $\vec{u}^{(1)}$.
  - No “redundancy”.

# A Second Feature



# A Second Feature



# Intuition

- Claim: if $\vec{u}$ and $\vec{v}$ are eigenvectors of a symmetric matrix with distinct eigenvalues, they are orthogonal.
- We should choose $\vec{u}^{(2)}$ to be an **eigenvector** of the covariance matrix, $C$.
- The second eigenvector of $C$ is called the **second principal component**.

# A Second Principal Component

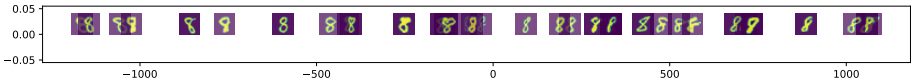
- Given a covariance matrix $C$.
- The principal component $\vec{u}^{(1)}$ is the top eigenvector of $C$.
  - Points in the direction of maximum variance.
- The *second* principal component $\vec{u}^{(2)}$ is the *second* eigenvector of $C$.
  - Out of all vectors orthogonal to the principal component, points in the direction of max variance.

# PCA: Two Components

- Given data $\{\vec{x}^{(1)}, ..., \vec{x}^{(n)}\} \in \mathbb{R}^d$.
- Compute covariance matrix $C$, top two eigenvectors $\vec{u}^{(1)}$ and $\vec{u}^{(2)}$.
- For any vector $\vec{x} \in \mathbb{R}$, its new representation in $\mathbb{R}^2$ is $\vec{z} = (z_1, z_2)^T$, where:

$$z_1 = \vec{x} \cdot \vec{u}^{(1)}$$
$$z_2 = \vec{x} \cdot \vec{u}^{(2)}$$

# Example



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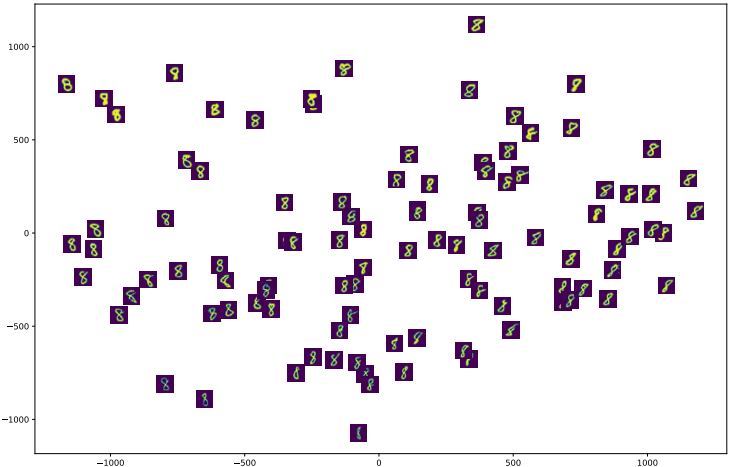
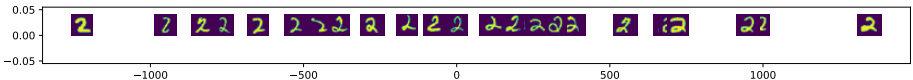


# Example



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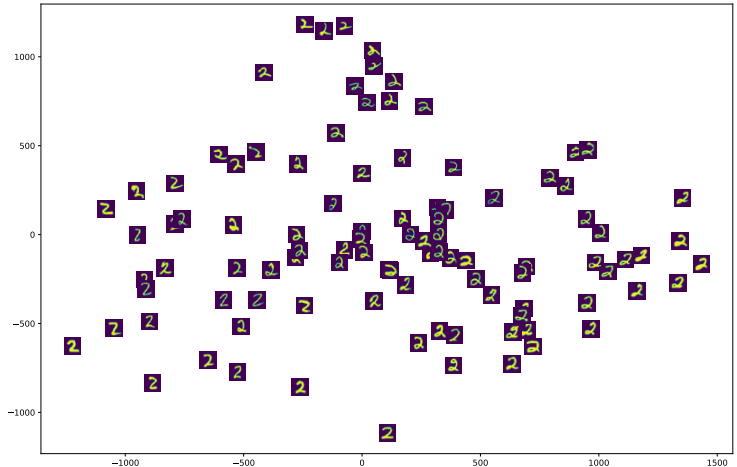
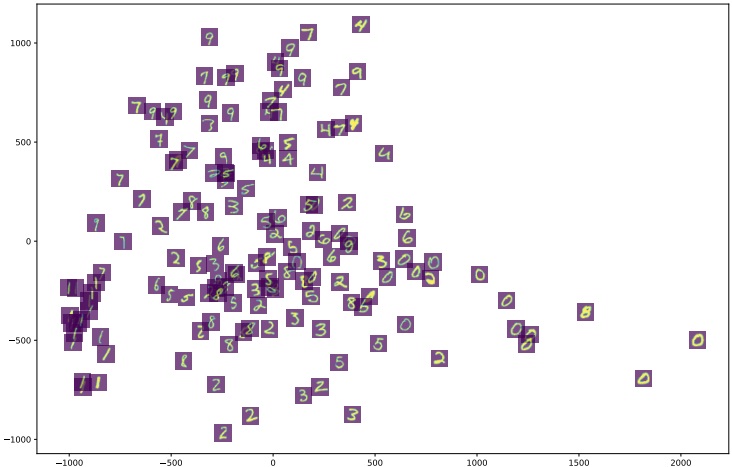


# Example



# PCA: $k$ Components

- Given data $\{\vec{x}^{(1)}, ..., \vec{x}^{(n)}\} \in \mathbb{R}^d$, number of components $k$.
- Compute covariance matrix $C$, top $k \leq d$ eigenvectors $\vec{u}^{(1)}$, $\vec{u}^{(2)}$, ..., $\vec{u}^{(k)}$.
- For any vector $\vec{x} \in \mathbb{R}$, its new representation in $\mathbb{R}^k$ is $\vec{z} = (z_1, z_2, \ldots z_k)^T$, where:

$$\begin{aligned} z_1 &= \vec{x} \cdot \vec{u}^{(1)} \\ z_2 &= \vec{x} \cdot \vec{u}^{(2)} \\ &\vdots \\ z_k &= \vec{x} \cdot \vec{u}^{(k)} \end{aligned}$$

# Matrix Formulation

- Let $X$ be the **data matrix** ($n$ rows, $d$ columns)
- Let $U$ be matrix of the $k$ eigenvectors as columns ($d$ rows, $k$ columns)
- The new representation: $Z = XU$

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## Representation Learning

Lecture 11 | Part 2

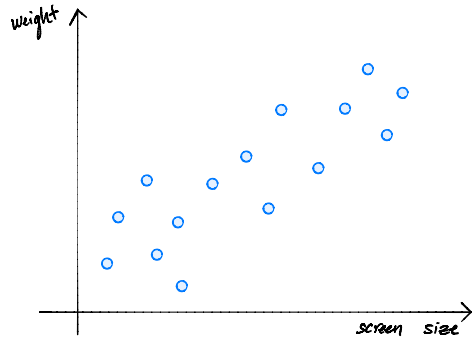
**Reconstructions**

# Reconstructing Points

- PCA helps us reduce dimensionality from $\mathbb{R}^d \rightarrow R^k$
- Suppose we have the “new” representation in $\mathbb{R}^k$.
- Can we “go back” to $\mathbb{R}^d$?
- And why would we want to?

# Back to $\mathbb{R}^d$

- Suppose new representation of $\vec{x}$ is $z$.
- $z = \vec{x} \cdot \vec{u}^{(1)}$
- Idea: $\vec{x} \approx z\vec{u}^{(1)}$



# Reconstructions

- Given a "new" representation of $\vec{x}$, $\vec{z} = (z_1, \ldots, z_k) \in \mathbb{R}^k$
- And top $k$ eigenvectors, $\vec{u}^{(1)}, \ldots, \vec{u}^{(k)}$
- The **reconstruction** of $\vec{x}$ is

$$z_1 \vec{u}^{(1)} + z_2 \vec{u}^{(2)} + \ldots + z_k \vec{u}^{(k)} = U\vec{z}$$

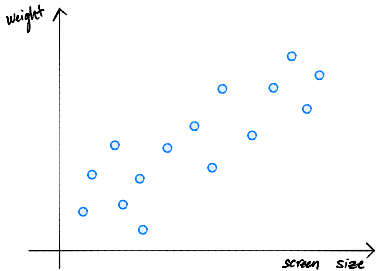
# Reconstruction Error

- The reconstruction *approximates* the original point, $\vec{x}$.
- The **reconstruction error** for a single point, $\vec{x}$:

$$\|\vec{x} - U\vec{z}\|^2$$

- Total reconstruction error:

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



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## Representation Learning

Lecture 11 | Part 3

**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.

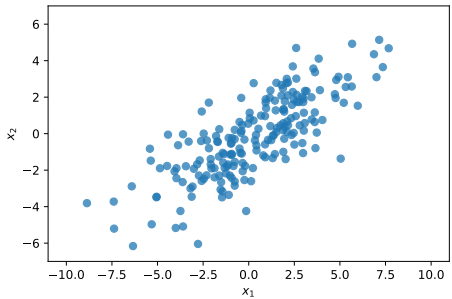
- Claim: Choosing $U$ to be top eigenvectors of $C$ minimizes reconstruction error among all choices of orthonormal $U$

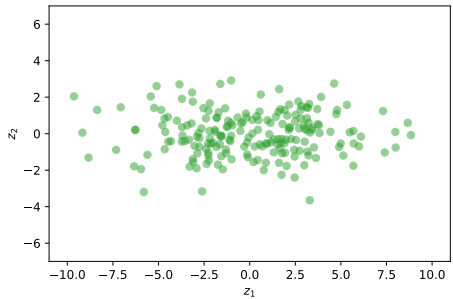
## Main Idea

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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## Representation Learning

Lecture 11 | Part 4

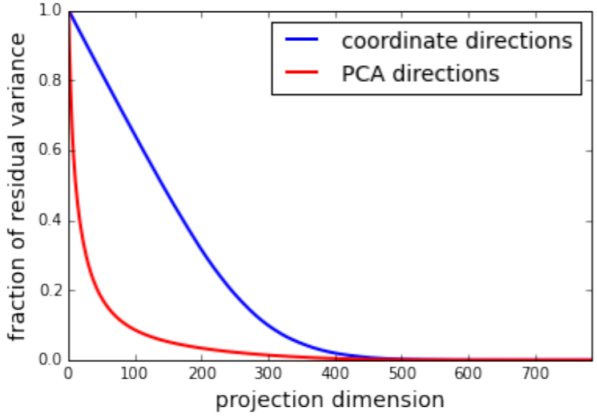
**PCA in Practice**

# 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!