

# DSC 140B

*Representation Learning*

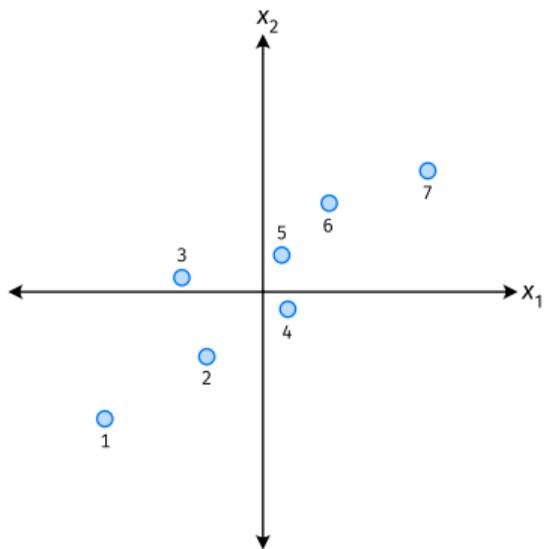
Lecture 06 | Part 1

**Dimensionality Reduction**

# Last Time: Dimensionality Reduction

- ▶ **Given:** data points  $\vec{x}^{(1)}, \dots, \vec{x}^{(n)} \in \mathbb{R}^d$
- ▶ **Goal:** create a new, lower-dimensional data set without losing too much useful information
- ▶ For now, focus on reducing to just one dimension.

# Example



- ▶ Each point is a phone.
- ▶  $\vec{x} = (\text{width}, \text{weight})^T$ .
- ▶ Can we reduce  $\vec{x}$  to a single feature,  $z$ , without losing too much information?

# The Idea from Last Time

- ▶ Our new feature should be a “mixture” of the old features:

$$\begin{aligned}z &= u_1 \times \text{width} + u_2 \times \text{weight} \\ &= u_1 X_1 + u_2 X_2 \\ &= \vec{u} \cdot \vec{X}\end{aligned}$$

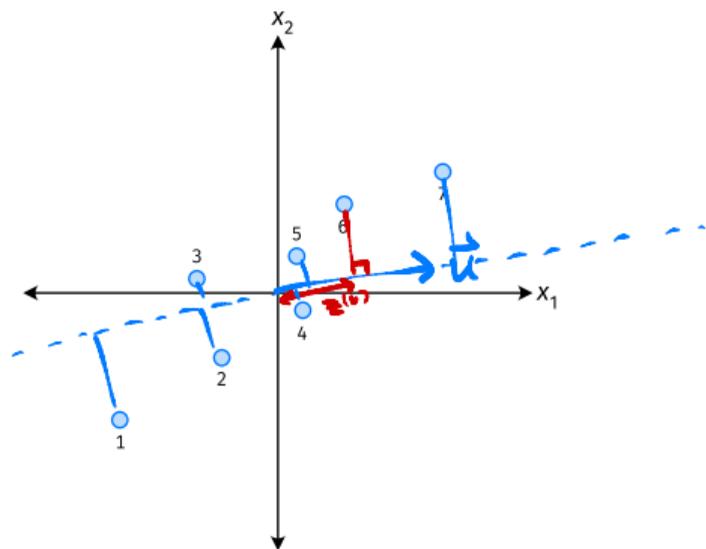
~~$$|u_1| + |u_2| = 1$$~~

- ▶ We get to choose  $\vec{u} = (u_1, u_2)^T$ .

- ▶ Constraint:  $\|\vec{u}\| = 1$ .

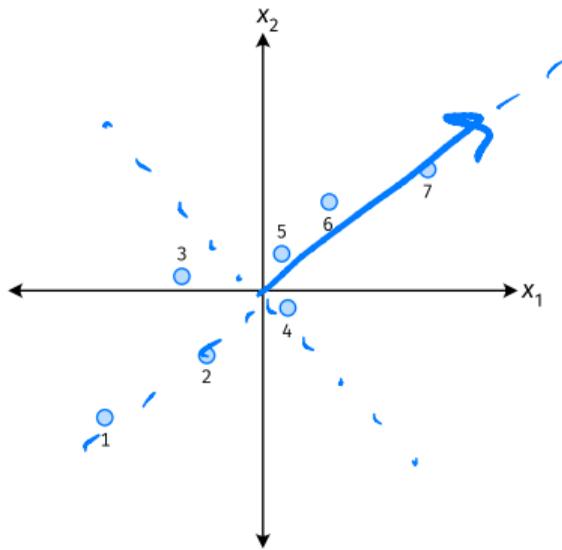
$$u_1^2 + u_2^2 = 1$$

# Geometrically



- ▶  $\vec{u}$  defines a direction in  $\mathbb{R}^2$ .
- ▶  $z$  is the projection of  $\vec{x}$  onto that direction.
- ▶ Which direction should we pick?
  - ▶ Concluded: direction of max variance.

# Another View



- ▶ Our data came to us in the standard basis.
- ▶ If we could pick a better basis, what would be our first basis vector?

# Our Algorithm (Informally)

- ▶ **Given:** data points  $\vec{x}^{(1)}, \dots, \vec{x}^{(n)} \in \mathbb{R}^d$
- ▶ Pick  $\vec{u}$  to be the direction of “max variance”
- ▶ Create a new feature,  $z$ , for each point:

$$z^{(i)} = \vec{x}^{(i)} \cdot \vec{u}$$

# PCA

- ▶ This algorithm is called **Principal Component Analysis**, or **PCA**.
- ▶ The direction of maximum variance is called the **principal component**.

## Exercise

Suppose the direction of maximum variance in a data set is

$$\vec{u} = (1/\sqrt{2}, -1/\sqrt{2})^T$$

Let  $\vec{x}^{(1)} = (3, -2)^T$  and  $\vec{x}^{(2)} = (1, 4)^T$ .

What are  $z^{(1)}$  and  $z^{(2)}$ ?

A)  ~~$z^{(1)} = \frac{1}{\sqrt{2}}, z^{(2)} = \frac{3}{\sqrt{2}}$~~

B)  $z^{(1)} = \frac{5}{\sqrt{2}}, z^{(2)} = \frac{3}{\sqrt{2}}$

C)  $z^{(1)} = \frac{5}{\sqrt{2}}, z^{(2)} = \frac{-3}{\sqrt{2}}$

Live Q&A

$$\begin{aligned} z^{(1)} &= \vec{x}^{(1)} \cdot \vec{u} \\ &= \begin{pmatrix} 3 \\ -2 \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \frac{3}{\sqrt{2}} + \frac{2}{\sqrt{2}} \\ &= \frac{5}{\sqrt{2}} \end{aligned}$$

## Exercise

Suppose the direction of maximum variance in a data set is

$$\vec{u} = (1/\sqrt{2}, -1/\sqrt{2})^T$$

Let  $\vec{x}^{(1)} = (3, -2)^T$  and  $\vec{x}^{(2)} = (1, 4)^T$ .

What are  $z^{(1)}$  and  $z^{(2)}$ ?

A)  $z^{(1)} = \frac{1}{\sqrt{2}}, \quad z^{(2)} = \frac{-3}{\sqrt{2}}$

B)  $z^{(1)} = \frac{5}{\sqrt{2}}, \quad z^{(2)} = \frac{3}{\sqrt{2}}$

C)  $z^{(1)} = \frac{5}{\sqrt{2}}, \quad z^{(2)} = \frac{-3}{\sqrt{2}}$

$$\begin{aligned} z^{(2)} &= \vec{x}^{(2)} \cdot \vec{u} \\ &= \begin{pmatrix} 1 \\ 4 \end{pmatrix} \cdot \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}} - \frac{4}{\sqrt{2}} \\ &= \frac{-3}{\sqrt{2}} \end{aligned}$$

# Problem

- ▶ How do we compute the “direction of maximum variance”?

# DSC 140B

*Representation Learning*

Lecture 06 | Part 2

**Covariance Matrices**

# Variance

- ▶ We know how to compute the variance of a set of numbers  $X = \{x^{(1)}, \dots, x^{(n)}\}$ :

$$\text{Var}(X) = \frac{1}{n} \sum_{i=1}^n (x^{(i)} - \mu)^2$$

- ▶ The variance measures the “spread” of the data

# Generalizing Variance

- ▶ If we have two features,  $x_1$  and  $x_2$ , we can compute the variance of each as usual:

$$\text{Var}(x_1) = \frac{1}{n} \sum_{i=1}^n (\vec{x}_1^{(i)} - \mu_1)^2$$

*← feature 1 for phone i*

$$\text{Var}(x_2) = \frac{1}{n} \sum_{i=1}^n (\vec{x}_2^{(i)} - \mu_2)^2$$

- ▶ Can also measure how  $x_1$  and  $x_2$  “vary together”.

# Measuring Similar Information

- ▶ Features which share information if they *vary together*.
  - ▶ A.k.a., they “co-vary”
- ▶ Positive association: when one is above average, so is the other
- ▶ Negative association: when one is above average, the other is below average

# Examples

- ▶ Positive: temperature and ice cream cones sold.
- ▶ Positive: temperature and shark attacks.
- ▶ Negative: temperature and coats sold.

# Quantifying Co-Variance

- ▶ One approach is as follows:

$$\text{Cov}(x_i, x_j) = \frac{1}{n} \sum_{k=1}^n (\vec{X}_i^{(k)} - \mu_i)(\vec{X}_j^{(k)} - \mu_j)$$

- ▶ For each data point, multiply the value of feature  $i$  and feature  $j$ , then average these products.
- ▶ This is the **covariance** of features  $i$  and  $j$ .

weight of  
k<sup>th</sup> phone

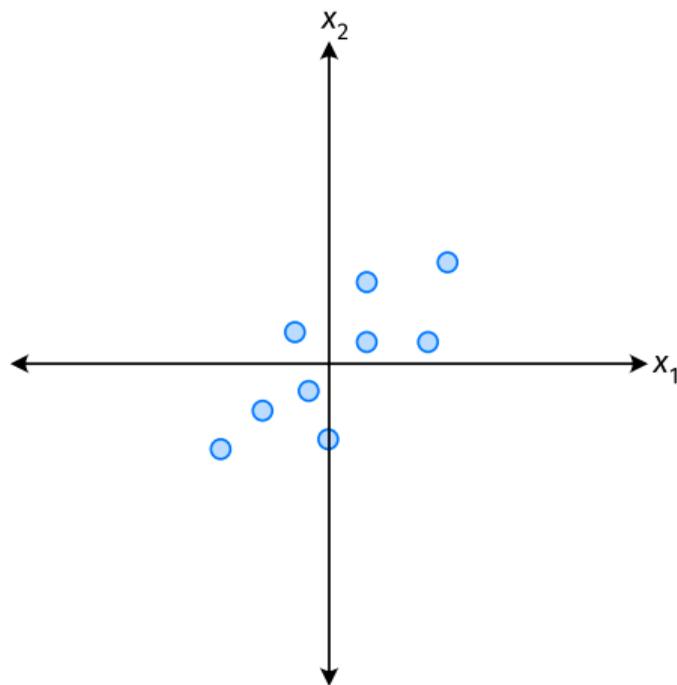
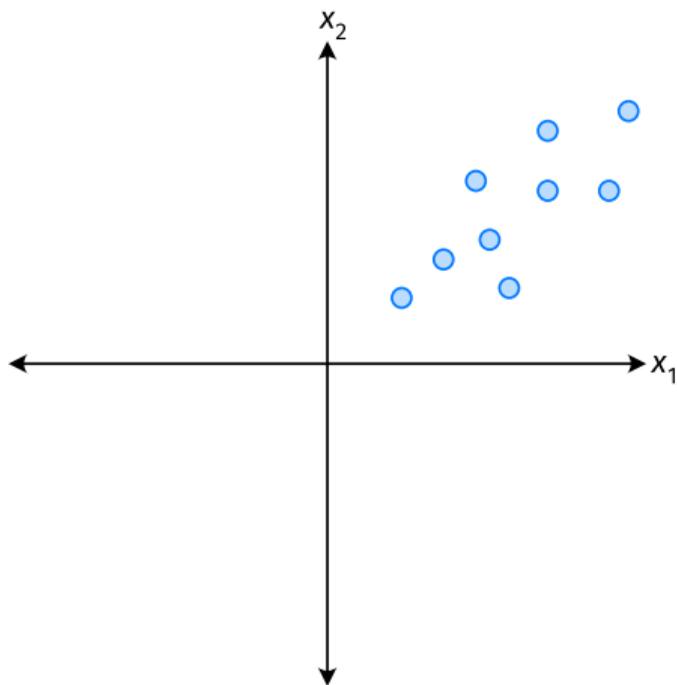
width of k<sup>th</sup>  
phone

mean weight

mean  
width

# Centering

- ▶ We often **center** the data.



# Centering

- ▶ Compute the mean of each feature:

$$\mu_j = \frac{1}{n} \sum_1^n \vec{x}_j^{(i)}$$

- ▶ Define new centered data:

$$\begin{pmatrix} \vec{x}_1^{(i)} \\ \vec{x}_2^{(i)} \\ \vdots \\ \vec{x}_d^{(i)} \end{pmatrix} \mapsto \begin{pmatrix} \vec{x}_1^{(i)} - \mu_1 \\ \vec{x}_2^{(i)} - \mu_2 \\ \vdots \\ \vec{x}_d^{(i)} - \mu_d \end{pmatrix}$$

# Centering (Equivalently)

- ▶ Compute the mean of all data points:

$$\vec{\mu} = \frac{1}{n} \sum_1^n \vec{x}^{(i)}$$

- ▶ Define new centered data:

$$\vec{x}^{(i)} \mapsto \vec{x}^{(i)} - \vec{\mu}$$

## Exercise

Center the data set:

$$\vec{x}^{(1)} = (1, 2, 3)^T - (0, 1, 2) \mapsto (1, 1, 1)^T$$

$$\vec{x}^{(2)} = (-1, -1, 0)^T$$

$$\vec{x}^{(3)} = (0, 2, 3)^T$$

$$\vec{\mu} = (0, 1, 2)^T$$

## Covariance (Again)

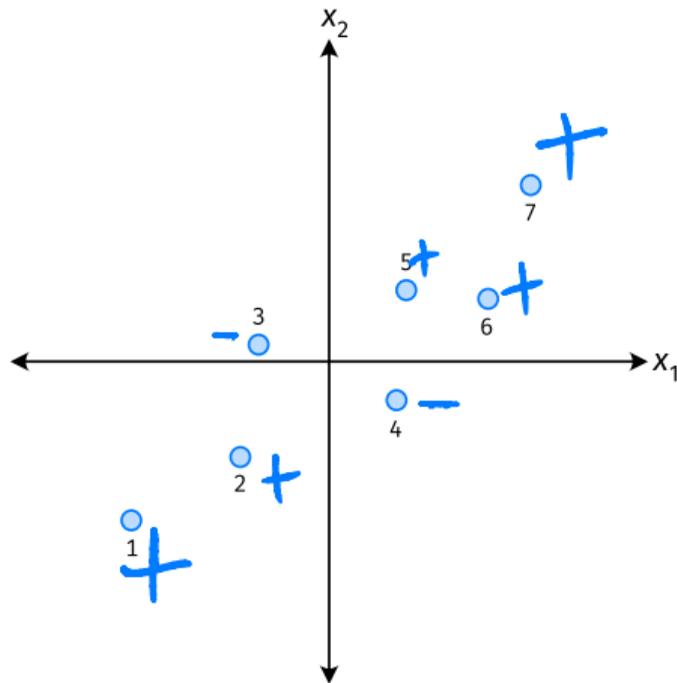
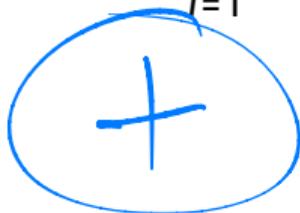
- ▶ If the data are **centered**, covariance is:

$$\text{Cov}(x_i, x_j) = \frac{1}{n} \sum_{k=1}^n \vec{x}_i^{(k)} \vec{x}_j^{(k)}$$

# Quantifying Covariance

- ▶ Assume the data are **centered**.

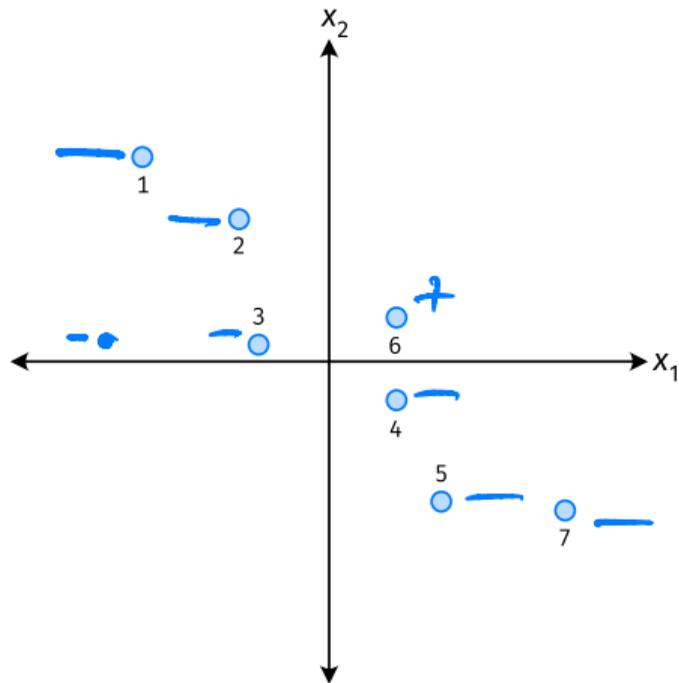
$$\text{Covariance} = \frac{1}{7} \sum_{i=1}^7 \vec{X}_1^{(i)} \times \vec{X}_2^{(i)}$$



# Quantifying Covariance

- ▶ Assume the data are **centered**.

$$\text{Covariance} = \frac{1}{7} \sum_{i=1}^7 \vec{X}_1^{(i)} \times \vec{X}_2^{(i)}$$

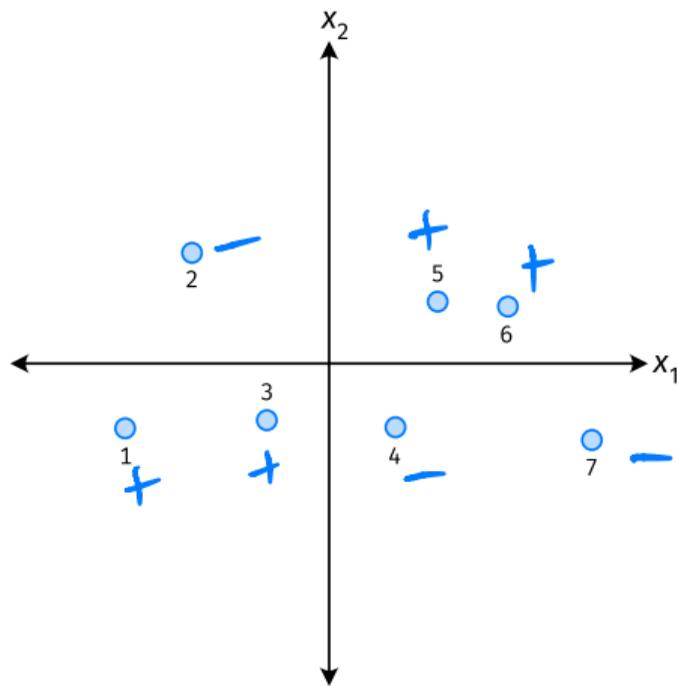


# Quantifying Covariance

- ▶ Assume the data are **centered**.

$$\text{Covariance} = \frac{1}{7} \sum_{i=1}^7 \vec{X}_1^{(i)} \times \vec{X}_2^{(i)}$$

$\approx 0$



# Quantifying Covariance

- ▶ The **covariance** quantifies extent to which two variables “vary together”.
- ▶ Assume we have centered the data.
- ▶ The **sample covariance** of feature  $i$  and  $j$  is:

$$\sigma_{ij} = \frac{1}{n} \sum_{k=1}^n \vec{x}_i^{(k)} \vec{x}_j^{(k)}$$

## Exercise

True or False:  $\sigma_{ij} = \sigma_{ji}$ ?

$$\sigma_{ij} = \frac{1}{n} \sum_{k=1}^n \vec{X}_i^{(k)} \vec{X}_j^{(k)}$$

# Covariance Matrices

- ▶ Given data  $\vec{x}^{(1)}, \dots, \vec{x}^{(n)} \in \mathbb{R}^d$ .

$$\begin{aligned}\sigma_{ii} &= \frac{1}{n} \sum_k \vec{x}_i^{(k)} \vec{x}_i^{(k)} \\ &= \frac{1}{n} \sum_k (\vec{x}_i^{(k)})^2\end{aligned}$$

- ▶ The **sample covariance matrix**  $C$  is the  $d \times d$  matrix whose  $ij$  entry is defined to be  $\sigma_{ij}$ .

$$\sigma_{ij} = \frac{1}{n} \sum_{k=1}^n \vec{x}_i^{(k)} \vec{x}_j^{(k)}$$

\* Assuming we have centered!

# Observations

- ▶ Diagonal entries of  $C$  are the variances.
- ▶ The matrix is **symmetric!**

## Note

- ▶ Sometimes you'll see the sample covariance defined with  $1/(n - 1)$  instead of  $1/n$ :

$$\sigma_{ij} = \frac{1}{n - 1} \sum_{k=1}^n \vec{X}_i^{(k)} \vec{X}_j^{(k)}$$

- ▶ This is an **unbiased** estimator of the population covariance.
- ▶ Our definition is the **maximum likelihood** estimator.
- ▶ In practice, it doesn't matter:  $1/(n - 1) \approx 1/n$ .
- ▶ For consistency, in this class use  $1/n$ .

## Exercise

Which of the following could be the covariance matrix for the data shown below?

Var  $x_1$

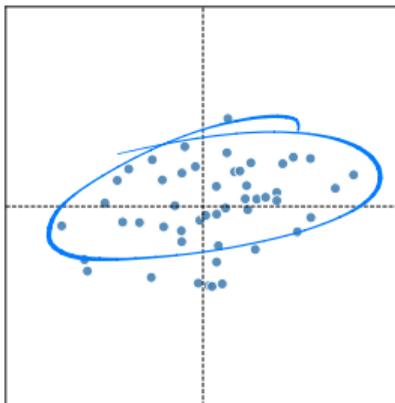
A)  $\begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix}$

Var  $x_2$

~~B)  $\begin{pmatrix} 4 & -2 \\ -2 & 2 \end{pmatrix}$~~

C)  $\begin{pmatrix} 2 & 2 \\ 2 & 4 \end{pmatrix}$

~~D)  $\begin{pmatrix} 4 & 0 \\ 0 & 2 \end{pmatrix}$~~



# Computing Covariance

- ▶ There is a “trick” for computing sample covariance matrices.
- ▶ Step 1: make  $n \times d$  data matrix,  $X$
- ▶ Step 2: make  $Z$  by centering columns of  $X$
- ▶ Step 3:  $C = \frac{1}{n}Z^T Z$

## Computing Covariance (in code)<sup>1</sup>

```
»» mu = X.mean(axis=0)
»» Z = X - mu
»» C = 1 / len(X) * Z.T @ Z
```

---

<sup>1</sup>Or use `np.cov`

# Meaning of the Covariance Matrix

- ▶ On the one hand,  $C$  is just a table of numbers.
- ▶ But remember: every matrix represents a linear transformation.
- ▶ What linear transformation does  $C$  represent?

# Meaning of the Covariance Matrix

- ▶ Suppose  $\vec{u}$  is a unit vector listing our “mixture coefficients”:

$$z = u_1x_1 + u_2x_2 + \dots + u_dx_d$$

- ▶  $C\vec{u}$  computes the covariances of the new feature  $z$  with each of the original features,  $x_1, \dots, x_d$ :

$$C\vec{u} = (\text{Cov}(z, x_1), \text{Cov}(z, x_2), \dots, \text{Cov}(z, x_d))^T$$

- ▶ We'd like each to be large.
  - ▶ Then, the new feature would be highly correlated with the original features.

# Intuition

- ▶  $\|C\vec{u}\|$  is large when the new feature  $z = \vec{u} \cdot \vec{x}$  is **highly correlated** with the original features.

# Intuition

- ▶  $\|C\vec{u}\|$  is large when the new feature  $z = \vec{u} \cdot \vec{x}$  is **highly correlated** with the original features.
- ▶ That is, when  $z$  contains a lot of the same information.

# Intuition

- ▶  $\|C\vec{u}\|$  is large when the new feature  $z = \vec{u} \cdot \vec{x}$  is **highly correlated** with the original features.
- ▶ That is, when  $z$  contains a lot of the same information.
- ▶ To maximize this correlation, we want to find  $\vec{u}$  which maximizes  $\|C\vec{u}\|$ .

# DSC 140B

## Representation Learning

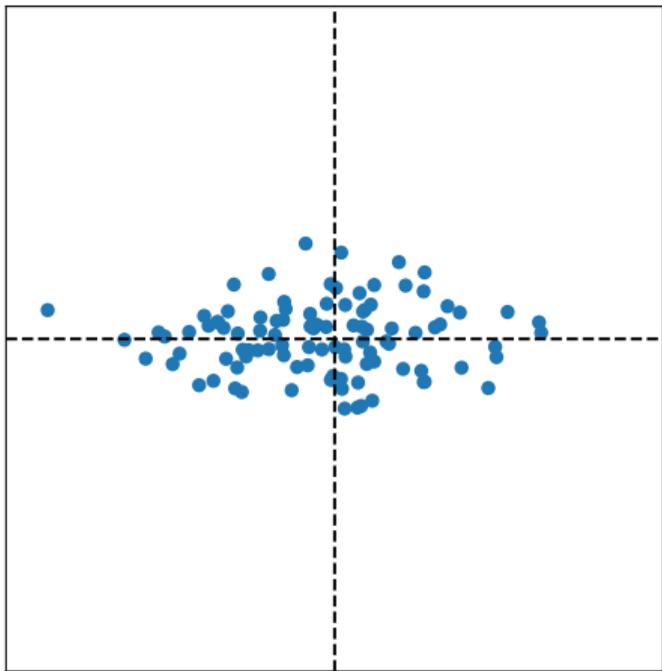
Lecture 06 | Part 3

**Visualizing Covariance Matrices**

# Visualizing Covariance Matrices

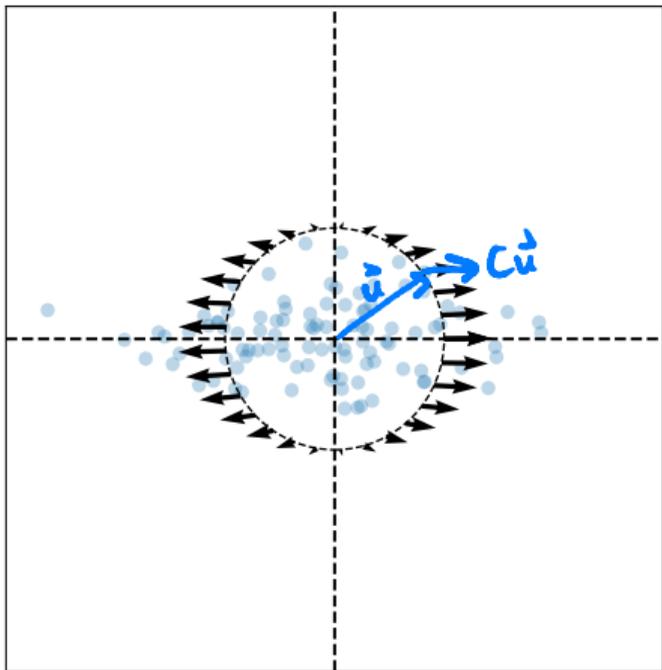
- ▶ Covariance matrices are symmetric.
- ▶ They have axes of symmetry (eigenvectors and eigenvalues).
- ▶ What are they?

# Visualizing Covariance Matrices



$$C \approx \begin{pmatrix} 4 & 0 \\ 0 & 2 \end{pmatrix}$$

# Visualizing Covariance Matrices

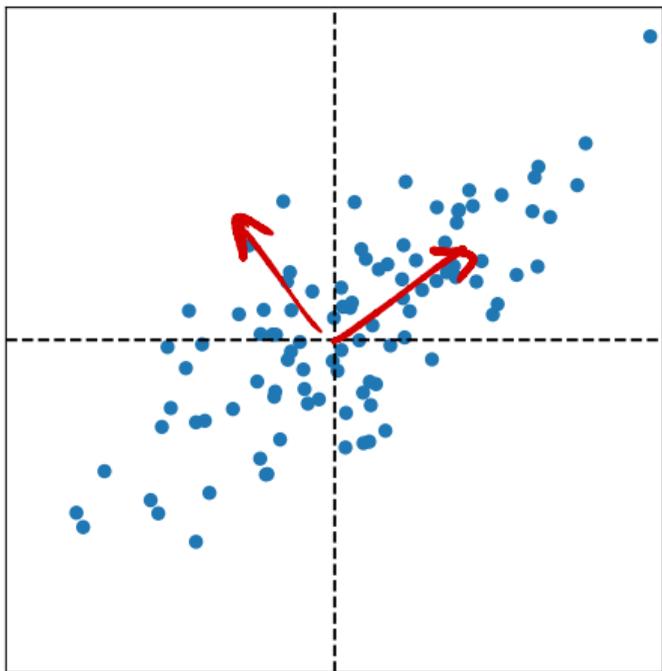


Eigenvectors:

$$\vec{u}^{(1)} \approx (1, 0)^T$$

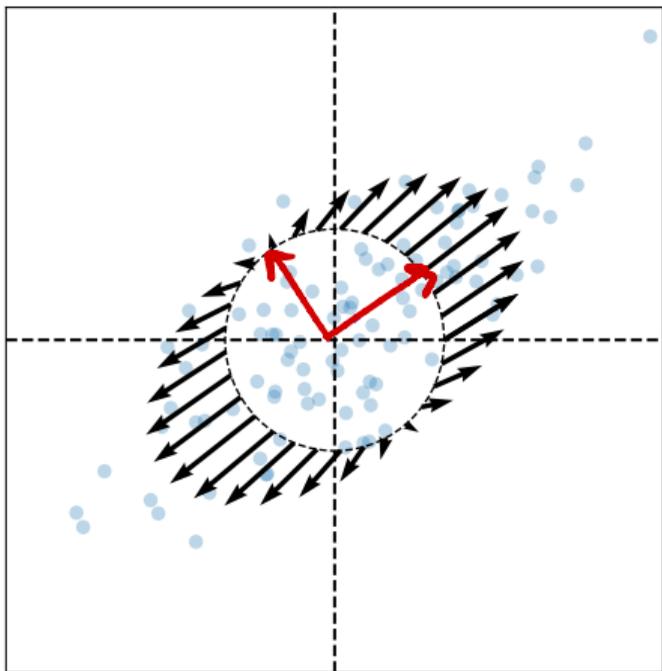
$$\vec{u}^{(2)} \approx (0, 1)^T$$

# Visualizing Covariance Matrices



$$C \approx \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$$

# Visualizing Covariance Matrices



Eigenvectors:

$$\vec{u}^{(1)} \approx (1, 1)^T$$

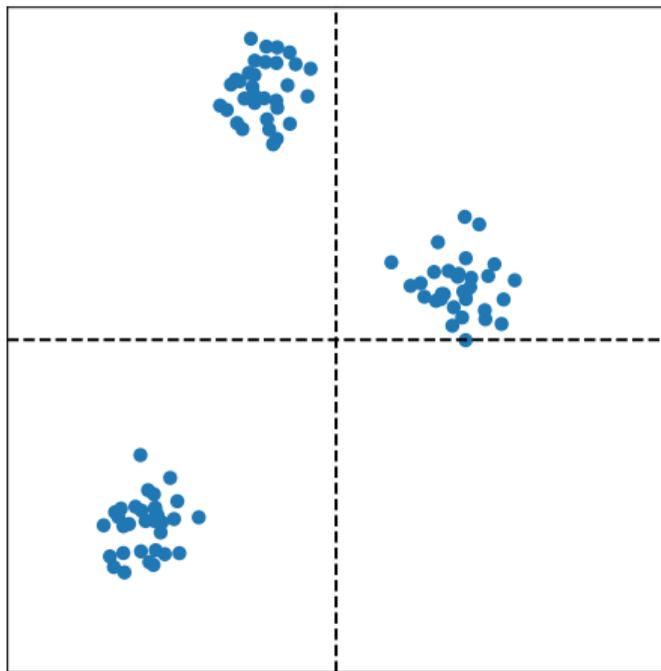
$$\vec{u}^{(2)} \approx (-1, 1)^T$$

# Observations

- ▶ The **eigenvectors** of the covariance matrix describe the data's "principal directions"
  - ▶  $C$  tells us something about data's shape.
- ▶ The **top eigenvector** points in the direction of "maximum variance".
- ▶ The **top eigenvalue** is proportional to the variance in this direction.

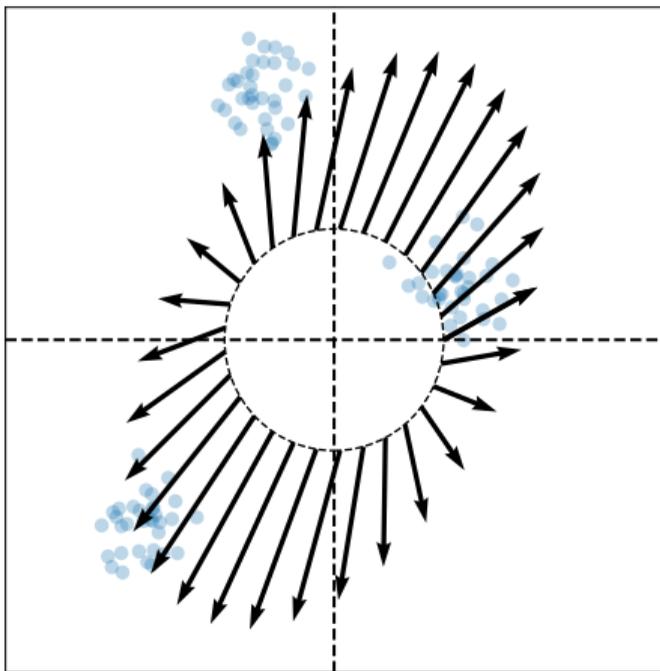
# Caution

- ▶ The data doesn't always look like this.
- ▶ We can always compute covariance matrices.
- ▶ They just may not describe the data's shape very well.



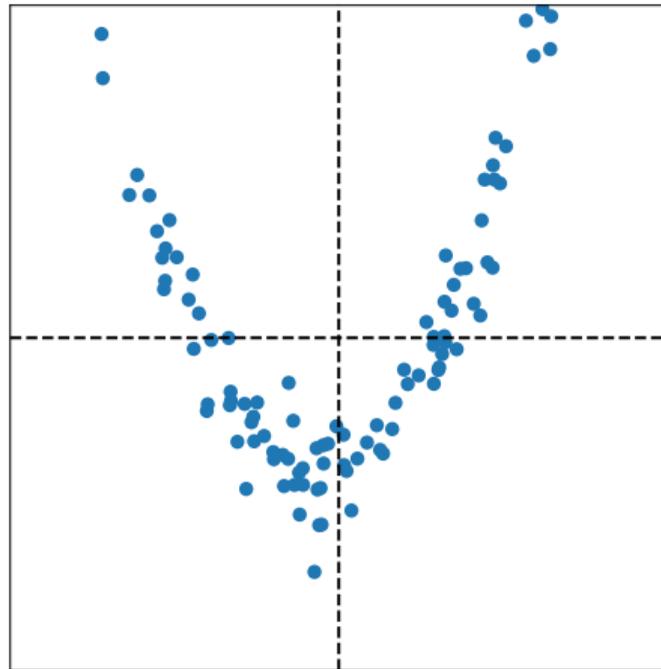
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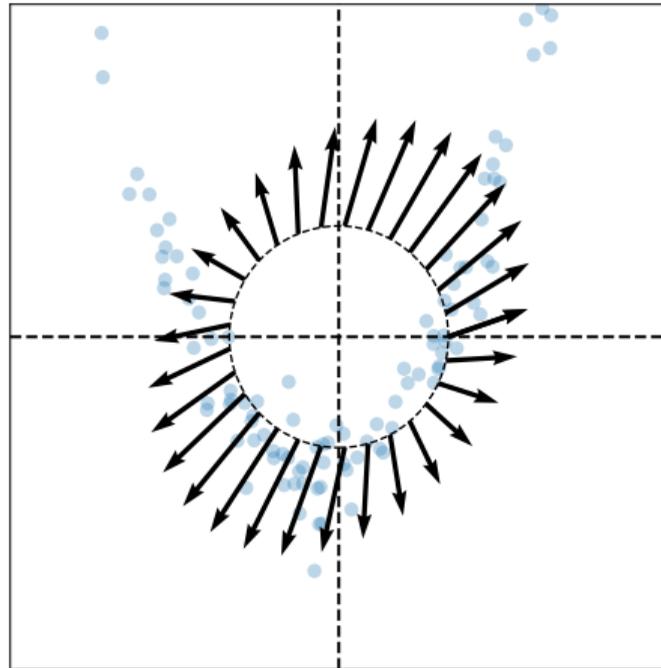
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# DSC 140B

## Representation Learning

Lecture 06 | Part 4

**PCA, More Formally**

# The Story (So Far)

- ▶ We want to create a single new feature,  $z$ .
- ▶ Our idea:  $z = \vec{x} \cdot \vec{u}$ ; choose  $\vec{u}$  to point in the “direction of maximum variance”.
- ▶ Intuition: the top eigenvector of the covariance matrix points in direction of maximum variance.

## More Formally...

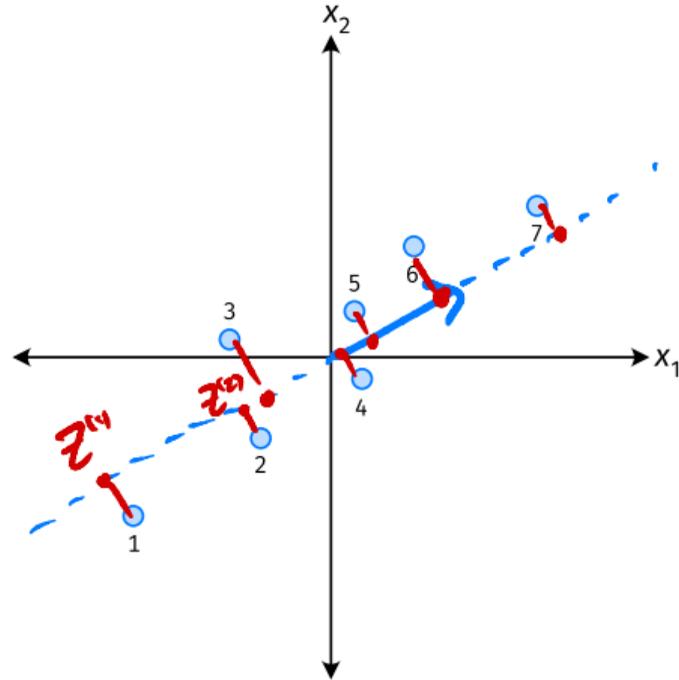
- ▶ We haven't actually defined "direction of maximum variance"
- ▶ Let's derive PCA more formally.

# Variance in a Direction

- ▶ Let  $\vec{u}$  be a unit vector.
- ▶  $z^{(i)} = \vec{x}^{(i)} \cdot \vec{u}$  is the new feature for  $\vec{x}^{(i)}$ .
- ▶ The **variance in the direction of  $\vec{u}$**  is defined to be the variance of the new features:

$$\begin{aligned}\text{Var}(z) &= \frac{1}{n} \sum_{i=1}^n (z^{(i)} - \mu_z)^2 \\ &= \frac{1}{n} \sum_{i=1}^n (\vec{x}^{(i)} \cdot \vec{u} - \mu_z)^2\end{aligned}$$

# Example



## Note

- ▶ If the data are centered, then  $\mu_z = 0$  and the variance of the new features is:

$$\begin{aligned}\text{Var}(z) &= \frac{1}{n} \sum_{i=1}^n (z^{(i)})^2 \\ &= \frac{1}{n} \sum_{i=1}^n (\vec{x}^{(i)} \cdot \vec{u})^2\end{aligned}$$

# Goal

- ▶ The variance of a data set in the direction of  $\vec{u}$  is:

$$g(\vec{u}) = \frac{1}{n} \sum_{i=1}^n (\vec{x}^{(i)} \cdot \vec{u})^2$$

- ▶ Our goal: Find a unit vector  $\vec{u}$  which maximizes  $g$ .

# Claim

$$\frac{1}{n} \sum_{i=1}^n (\vec{x}^{(i)} \cdot \vec{u})^2 = \vec{u}^T C \vec{u}$$

- ▶ Proven on this week's homework.

## Our Goal (Again)

- ▶ Find a unit vector  $\vec{u}$  which maximizes  $\vec{u}^T C \vec{u}$ .

# Recall

- ▶ When  $C$  is symmetric, the unit vector which maximizes the quadratic form  $\vec{u}^T C \vec{u}$  is the eigenvector of  $C$  with the largest eigenvalue.
- ▶ **Solution:** the direction of maximum variance is the top eigenvector of the covariance matrix.

# PCA (for a single new feature)

► **Given:** data points  $\vec{x}^{(1)}, \dots, \vec{x}^{(n)} \in \mathbb{R}^d$

1. Compute the covariance matrix,  $C$ .
2. Compute the top<sup>2</sup> eigenvector  $\vec{u}$ , of  $C$ .
3. For  $i \in \{1, \dots, n\}$ , create new feature:

$$z^{(i)} = \vec{u} \cdot \vec{x}^{(i)}$$

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<sup>2</sup>All eigenvalues are positive. Why?

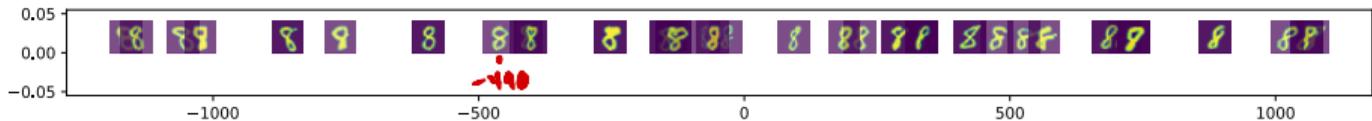
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## A Parting Example

- ▶ 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



# DSC 140B

## Representation Learning

Lecture 06 | Part 5

**Dimensionality Reduction with  $d \geq 2$**

## So far: PCA

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

# 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  $\mathbb{R}^d \rightarrow \mathbb{R}^1$

# 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



## 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  $\vec{u}^{(1)} = (u_1^{(1)}, u_2^{(1)}, \dots, u_d^{(1)})^T$ .

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

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



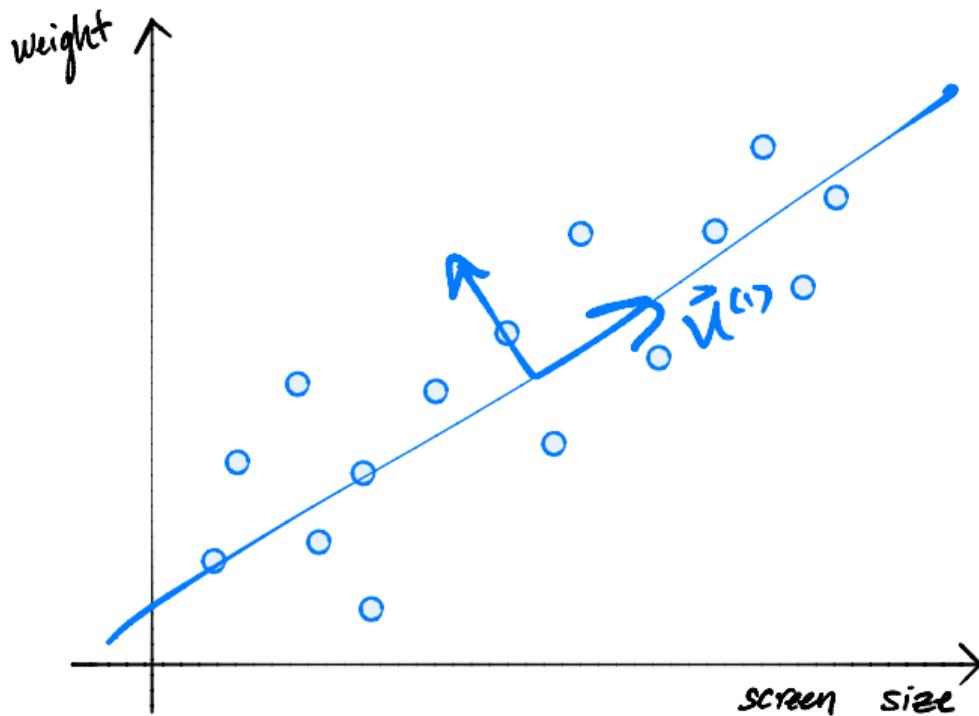
## A Second Feature

- ▶ Make same assumption for second feature:

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

- ▶ 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



# 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.

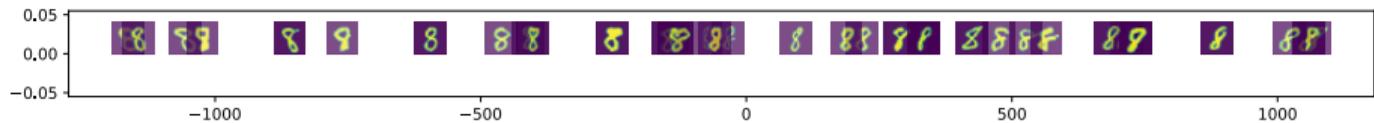
# PCA: Two Components

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

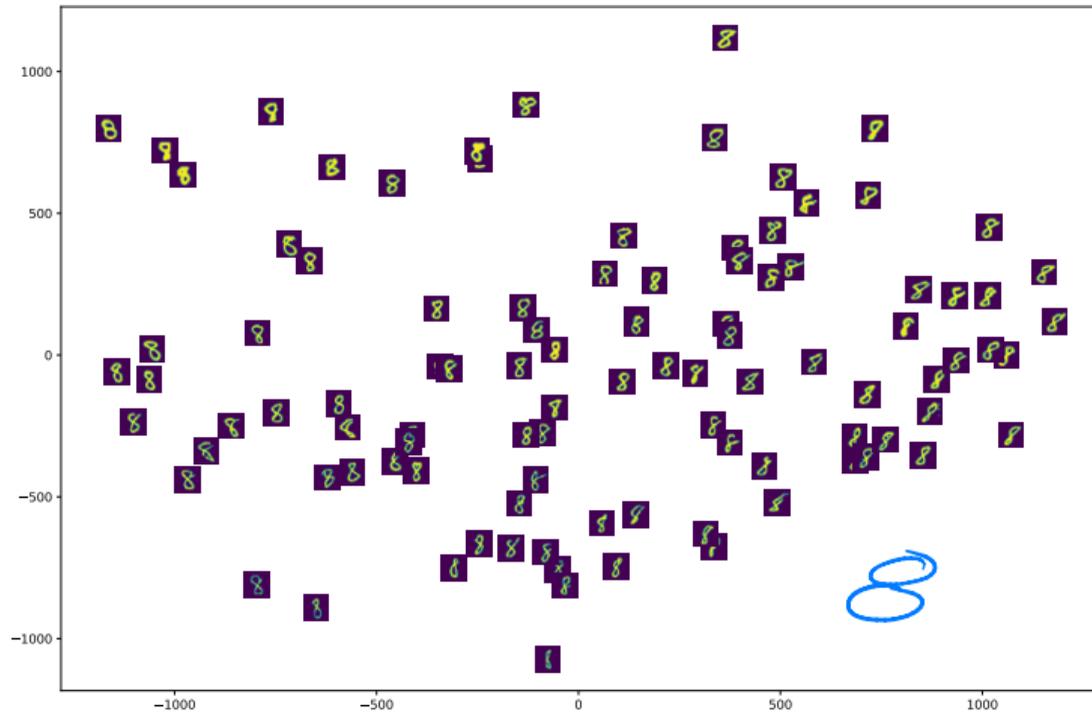
$$z_1 = \vec{x} \cdot \vec{u}^{(1)}$$

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

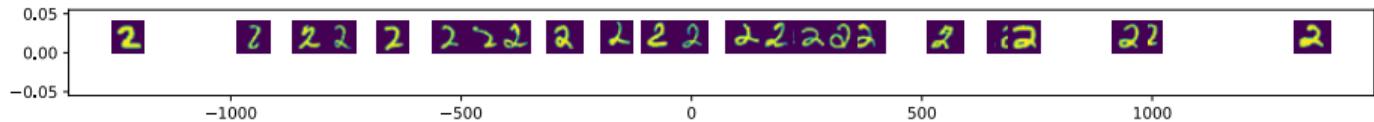
# Example



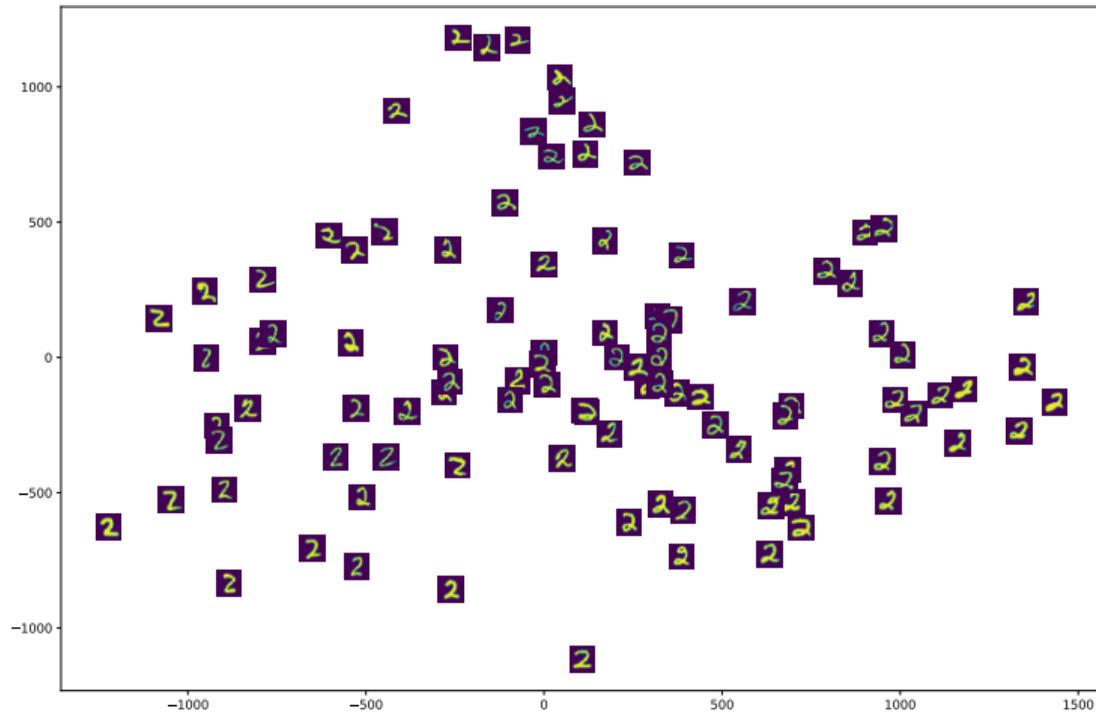
# Example



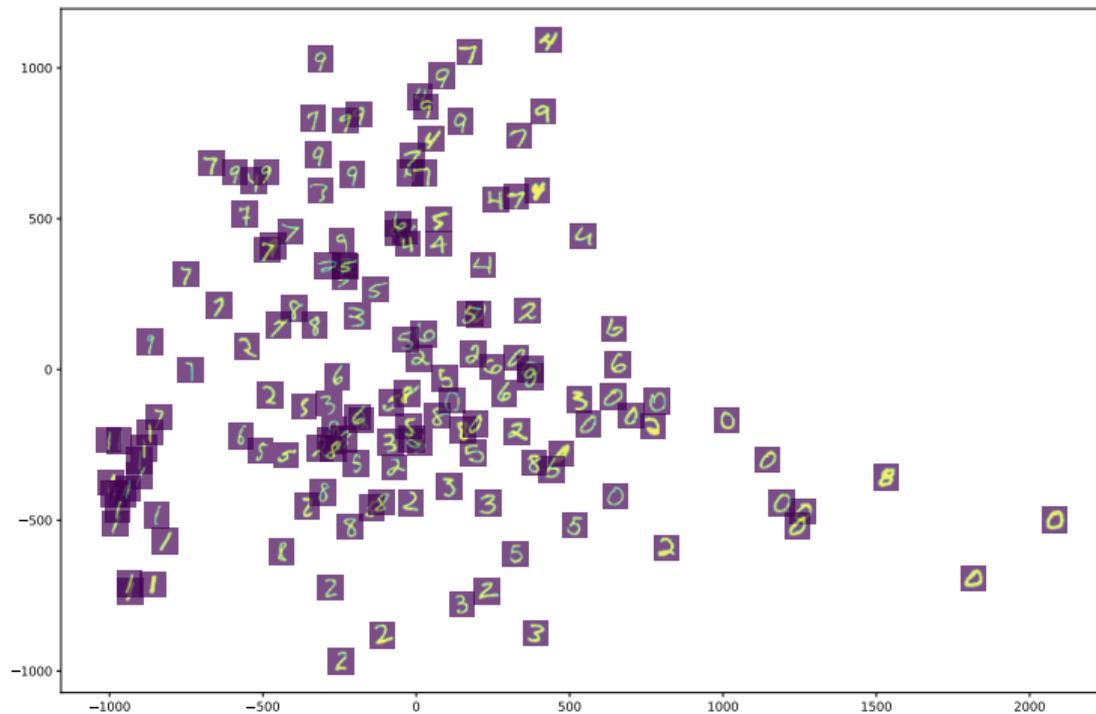
# Example



# Example



# Example



# PCA: $k$ Components

- ▶ Given data  $\{\vec{x}^{(1)}, \dots, \vec{x}^{(n)}\} \in \mathbb{R}^d$ , 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  $\vec{x} \in \mathbb{R}^d$ , its new representation in  $\mathbb{R}^k$  is  $\vec{z} = (z_1, z_2, \dots, z_k)^T$ , where:

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

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

$$\vdots$$

$$z_k = \vec{x} \cdot \vec{u}^{(k)}$$

# 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:  $Z = XU$

# DSC 140B

*Representation Learning*

Lecture 06 | Part 6

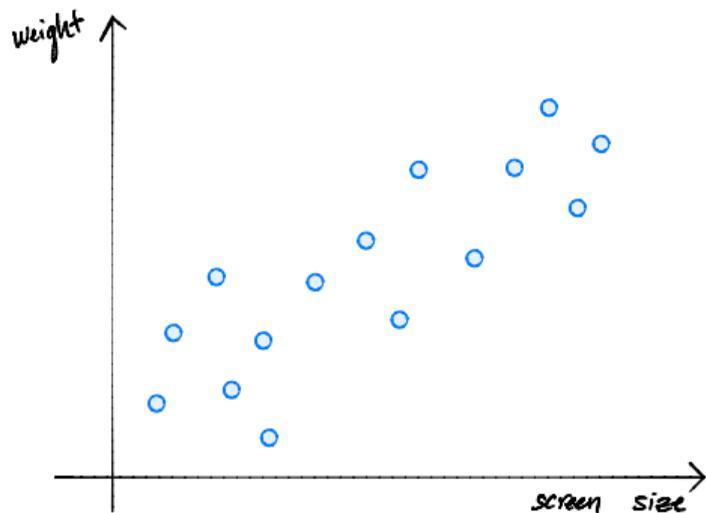
**Reconstructions**

# Reconstructing Points

- ▶ PCA helps us reduce dimensionality from  $\mathbb{R}^d \rightarrow \mathbb{R}^k$
- ▶ 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  $\vec{x}$ ,  $\vec{z} = (z_1, \dots, z_k) \in \mathbb{R}^k$
- ▶ And top  $k$  eigenvectors,  $\vec{u}^{(1)}, \dots, \vec{u}^{(k)}$
- ▶ The **reconstruction** of  $\vec{x}$  is

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

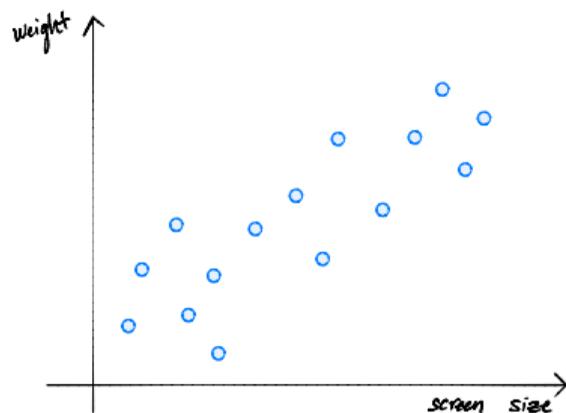
# Reconstruction Error

- ▶ 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:

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



# DSC 140B

## Representation Learning

Lecture 06 | Part 7

**Interpreting PCA**

# Three Interpretations

- ▶ What is PCA doing?
- ▶ Three interpretations:
  1. Maximizing 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

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

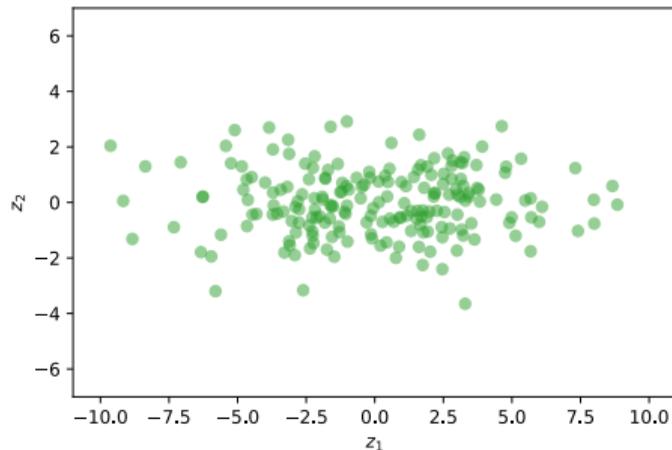
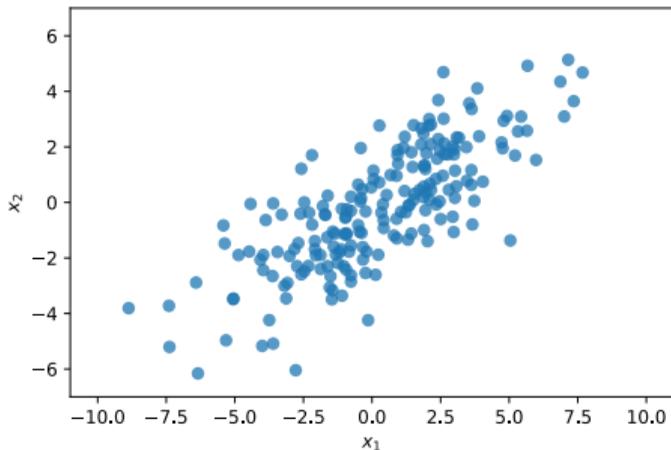
- ▶ Goal: minimize total reconstruction error.
- ▶ Claim: Choosing  $U$  to be top eigenvectors of  $C$  minimizes reconstruction error among all choices of orthonormal  $U$

## 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.

# DSC 140B

## Representation Learning

Lecture 06 | Part 8

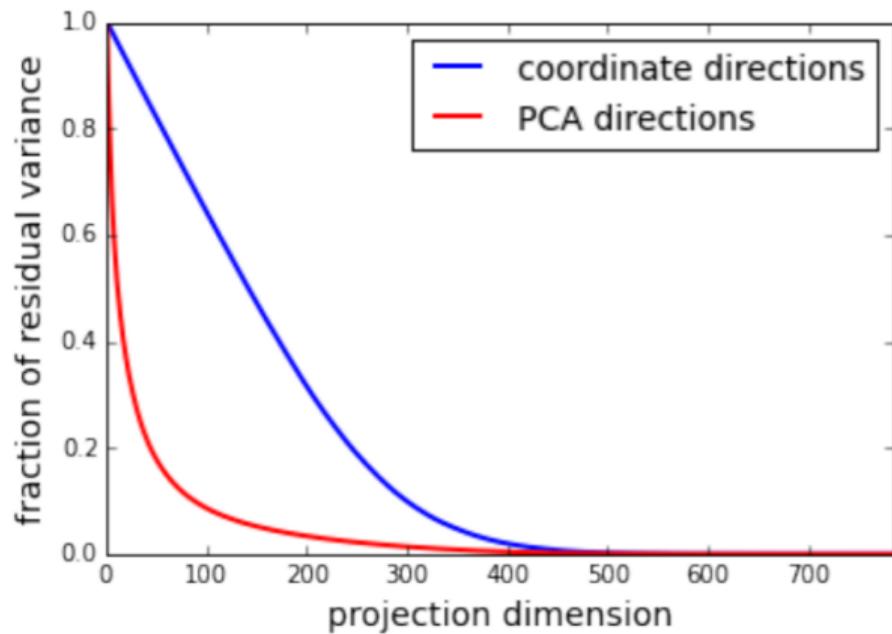
**PCA in Practice**

# 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.



# Caution

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