

# DSC 140B

*Representation Learning*

Lecture 06 | Part 1

**Dimensionality Reduction**

# High Dimensional Data

- ▶ Data is often high dimensional (many features)
- ▶ Example: Netflix user
  - ▶ Number of movies watched
  - ▶ Number of movies saved
  - ▶ Total time watched
  - ▶ Number of logins
  - ▶ Days since signup
  - ▶ Average rating for comedy
  - ▶ Average rating for drama
  - ▶ ⋮

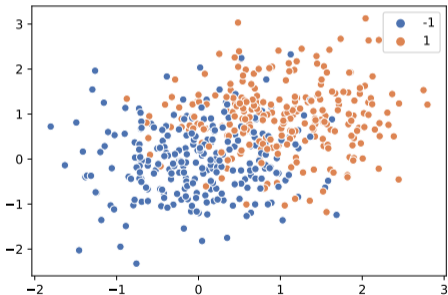
# High Dimensional Data

- ▶ More features can give us more information
- ▶ But it can also cause problems
- ▶ **Today:** how do we reduce dimensionality without losing too much information?

# More Features, More Problems

- ▶ Difficulties with high dimensional data:
  1. Requires more compute time / space
  2. Hard to visualize / explore
  3. The “curse of dimensionality”: it’s harder to learn

# Experiment



- ▶ On this data, low 80% train/test accuracy
- ▶ Add 400 features of pure noise, re-train
- ▶ Now: 100% train accuracy, **58%** test accuracy
- ▶ **Overfitting!**

# Task: Dimensionality Reduction

- ▶ We'd often like to **reduce** the dimensionality to improve performance, or to visualize.
- ▶ We will typically lose information
- ▶ Want to minimize the loss of useful information

# Redundancy

- ▶ Two (or more) features may share the same information.
- ▶ Intuition: we may not need all of them.

# Today

- ▶ Today we'll think about reducing dimensionality from  $\mathbb{R}^d$  to  $\mathbb{R}^1$
- ▶ Next time we'll go from  $\mathbb{R}^d$  to  $\mathbb{R}^{d'}$ , with  $d' \leq d$



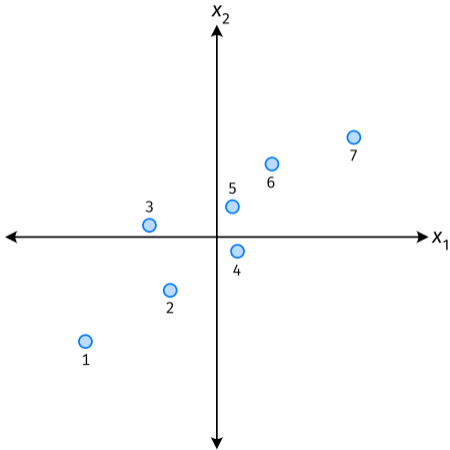
# Today's Example

- ▶ Let's say we represent a phone with two features:
  - ▶  $x_1$ : screen width
  - ▶  $x_2$ : phone weight
- ▶ Both measure a phone's "size".
- ▶ Instead of representing a phone with both  $x_1$  and  $x_2$ , can we just use a single number,  $z$ ?
  - ▶ Reduce dimensionality from 2 to 1.

# First Approach: Remove Features

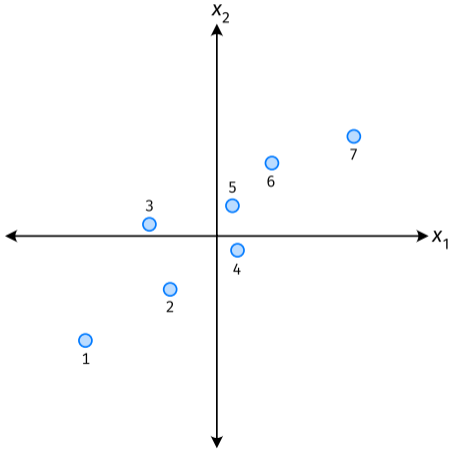
- ▶ Screen width and weight share information.
- ▶ **Idea:** keep one feature, remove the other.
- ▶ That is, set new feature  $z = x_1$  (or  $z = x_2$ ).

# Removing Features



- ▶ Say we set  $z^{(i)} = \vec{x}_1^{(i)}$  for each phone,  $i$ .
- ▶ Observe:  $z^{(4)} > z^{(5)}$ .
- ▶ Is phone 4 really “larger” than phone 5?

# Removing Features



- ▶ Say we set  $z^{(i)} = \vec{x}_2^{(i)}$  for each phone,  $i$ .
- ▶ Observe:  $z^{(3)} > z^{(4)}$ .
- ▶ Is phone 3 really “larger” than phone 4?

# Better Approach: Mixtures of Features

- ▶ **Idea:**  $z$  should be a combination of  $x_1$  and  $x_2$ .
- ▶ One approach: linear combination.

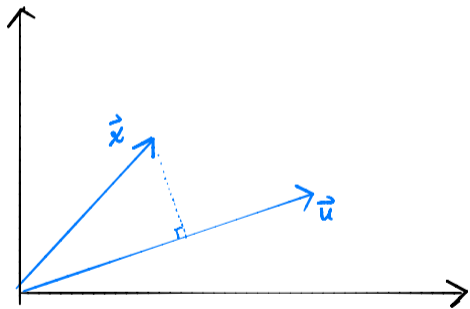
$$\begin{aligned}z &= u_1 x_1 + u_2 x_2 \\ &= \vec{u} \cdot \vec{x}\end{aligned}$$

- ▶  $u_1, \dots, u_2$  are the mixture coefficients; we can choose them.

# Normalization

- ▶ Mixture coefficients generalize proportions.
- ▶ We could assume, e.g.,  $|u_1| + |u_2| = 1$ .
- ▶ But it makes the math easier if we assume  $u_1^2 + u_2^2 = 1$ .
- ▶ Equivalently, if  $\vec{u} = (u_1, u_2)^T$ , assume  $\|\vec{u}\| = 1$

# Geometric Interpretation



- ▶  $z$  measures how much of  $\vec{x}$  is in the direction of  $\vec{u}$
- ▶ If  $\vec{u} = (1, 0)^T$ , then  $z = x_1$
- ▶ If  $\vec{u} = (0, 1)^T$ , then  $z = x_2$

# Choosing $\vec{u}$

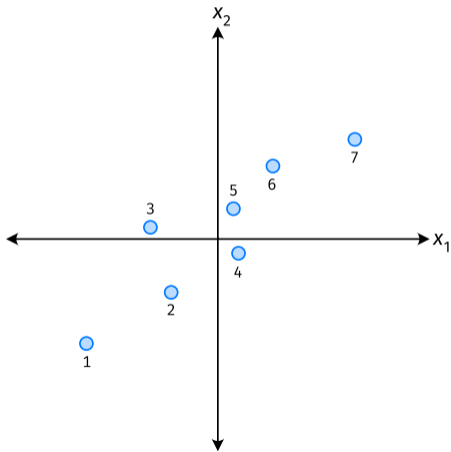
- ▶ Suppose we have only two features:
  - ▶  $x_1$ : screen size
  - ▶  $x_2$ : phone thickness
- ▶ We'll create single new feature,  $z$ , from  $x_1$  and  $x_2$ .
  - ▶ Assume  $z = u_1x_1 + u_2x_2 = \vec{x} \cdot \vec{u}$
  - ▶ Interpretation:  $z$  is a measure of a phone's size
- ▶ How should we choose  $\vec{u} = (u_1, u_2)^T$ ?



# Visualization

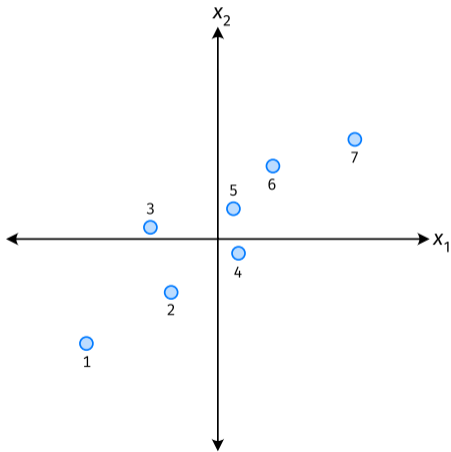
[http://dsc140b.com/static/vis/pca-max\\_variance/](http://dsc140b.com/static/vis/pca-max_variance/)

# Example



- ▶  $\vec{u}$  defines a direction
- ▶  $\vec{z}^{(i)} = \vec{x}^{(i)} \cdot \vec{u}$  measures position of  $\vec{x}$  along this direction

# Example



- ▶ Phone “size” varies most along a diagonal direction.
- ▶ Along direction of “max variance”, phones are well-separated.
- ▶ **Idea:**  $\vec{u}$  should point in direction of “max variance”.

# 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

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

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

## 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:

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

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

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

# Measuring Similar Information

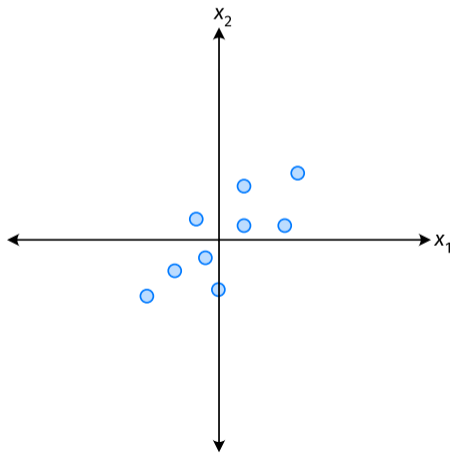
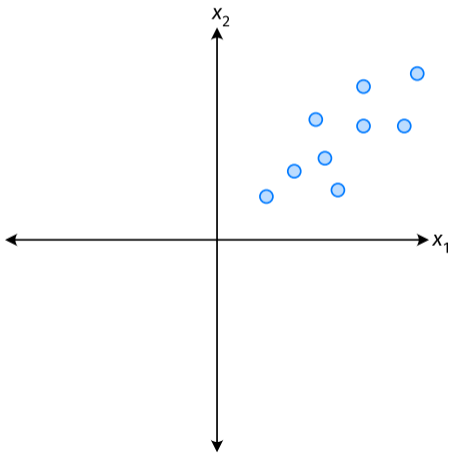
- ▶ Features which share information if they *vary together*.
  - ▶ A.k.a., they “co-vary”
- ▶ Positive association: when one is above average, so is the other
- ▶ Negative association: when one is above average, the other is below average

# Examples

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

# Centering

- First, it will be useful to **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:

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

# Centering (Equivalently)

- ▶ Compute the mean of all data points:

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

- ▶ Define new centered data:

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

## Exercise

Center the data set:

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

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

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



# Quantifying Co-Variance

- ▶ One approach is as follows<sup>1</sup>.

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

- ▶ 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  $j$ .

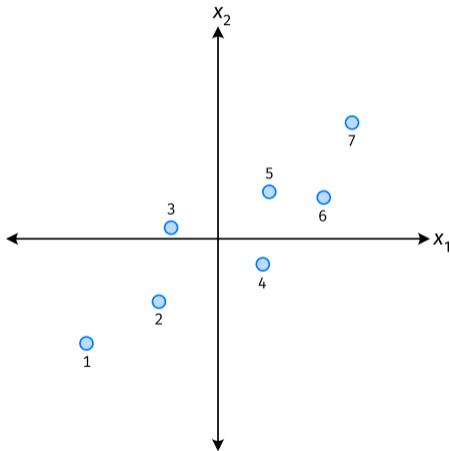
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<sup>1</sup>Assuming centered data

# Quantifying Covariance

- ▶ Assume the data are **centered**.

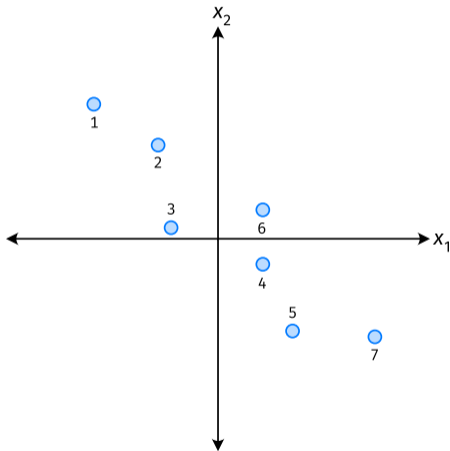
$$\text{Covariance} = \frac{1}{7} \sum_{i=1}^7 \vec{X}_1^{(i)} \times \vec{X}_2^{(i)}$$



# Quantifying Covariance

- ▶ Assume the data are **centered**.

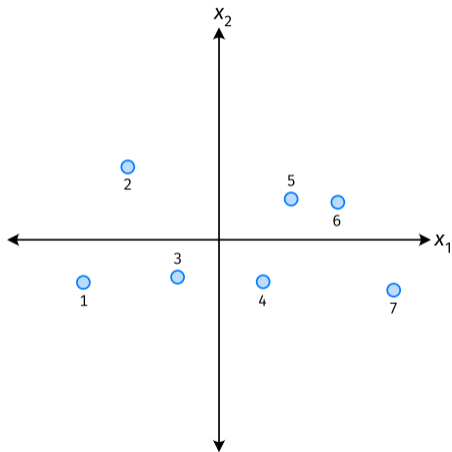
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# Quantifying Covariance

- ▶ 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

- ▶ 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  $\vec{x}^{(1)}, \dots, \vec{x}^{(n)} \in \mathbb{R}^d$ .
- ▶ The **sample covariance matrix**  $C$  is the  $d \times d$  matrix whose  $ij$  entry is defined to be  $\sigma_{ij}$ .

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

# Observations

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



# Note

- ▶ Sometimes you'll see the sample covariance defined as:

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

Note the  $1/(n-1)$

- ▶ 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  $1/n$ .

# 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>2</sup>

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

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<sup>2</sup>Or use `np.cov`

# DSC 140B

## Representation Learning

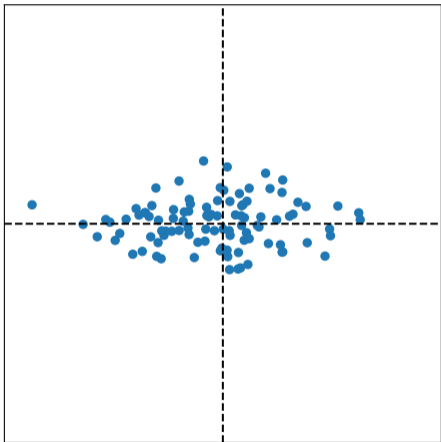
Lecture 06 | Part 3

**Visualizing Covariance Matrices**

# Visualizing Covariance Matrices

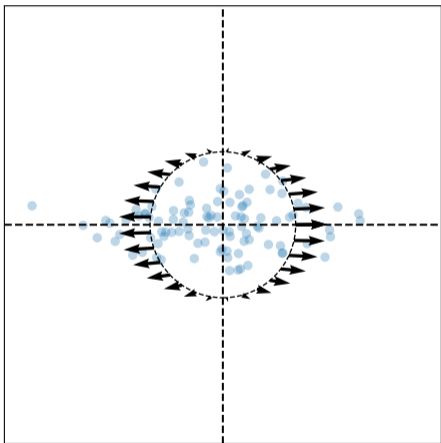
- ▶ Covariance matrices are symmetric.
- ▶ They have axes of symmetry (eigenvectors and eigenvalues).
- ▶ What are they?

# Visualizing Covariance Matrices



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

# Visualizing Covariance Matrices

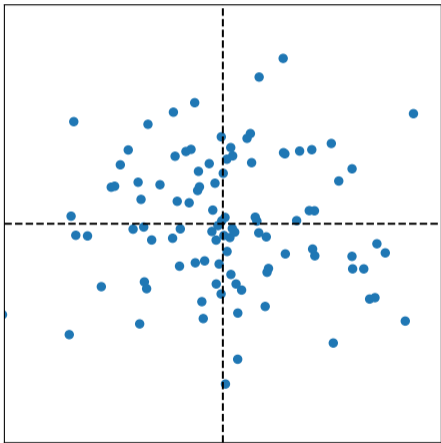


Eigenvectors:

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

$$\vec{u}^{(2)} \approx$$

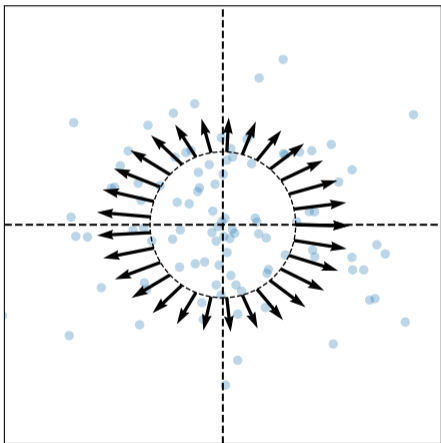
# Visualizing Covariance Matrices



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# Visualizing Covariance Matrices

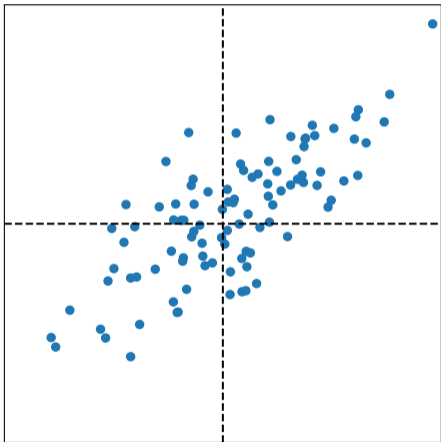


Eigenvectors:

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

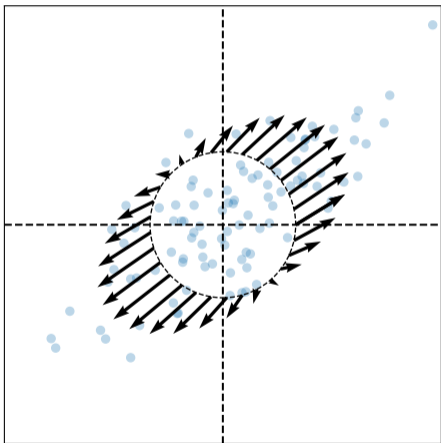
$$\vec{u}^{(2)} \approx$$

# Visualizing Covariance Matrices



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

# Visualizing Covariance Matrices



Eigenvectors:

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

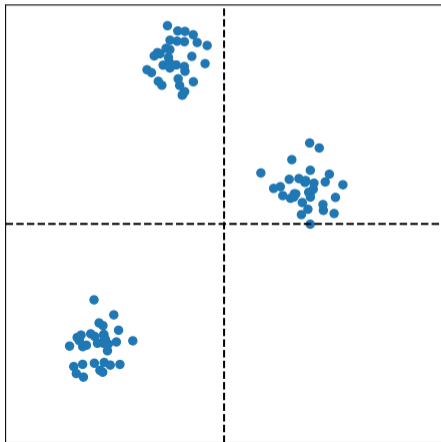
$$\vec{u}^{(2)} \approx$$

# Intuitions

- ▶ 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.

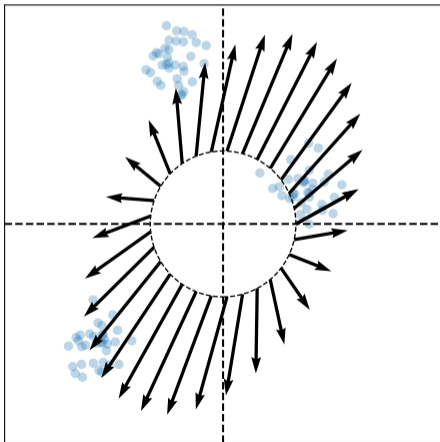
# Caution

- ▶ 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.



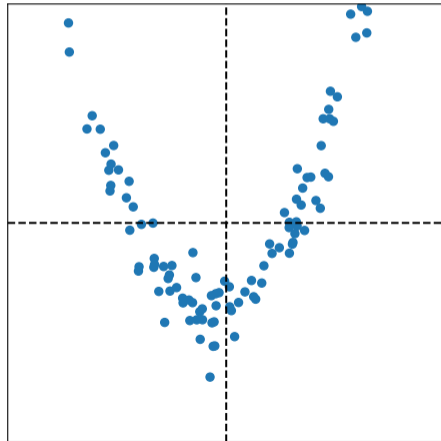
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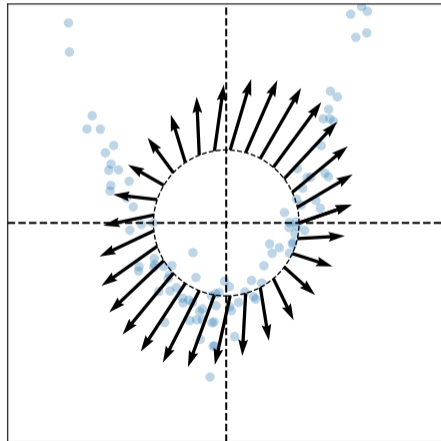
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# DSC 140B

## 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...

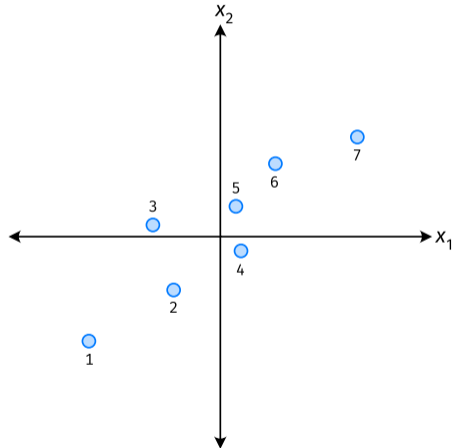
- ▶ We haven't actually defined "direction of maximum variance"
- ▶ Let's derive PCA more formally.

# 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 of the new features is:

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

# 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

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



## Our Goal (Again)

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

# Claim

- ▶ To maximize  $\vec{u}^T C \vec{u}$  over unit vectors, choose  $\vec{u}$  to be the top eigenvector of  $C$ .
- ▶ Proof:

# 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 eigenvector  $\vec{u}$ , of  $C$ .
  3. For  $i \in \{1, \dots, n\}$ , create new feature:

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

# 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

