DSC 140B Representation Learning

Lecture 05 | Part 1

**Change of Basis Matrices** 

# **Changing Basis**

Suppose 
$$\vec{x} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1 \hat{e}^{(1)} + a_2 \hat{e}^{(2)}$$
.

- $\hat{u}^{(1)}$  and  $\hat{u}^{(2)}$  form a new, **orthonormal** basis  $\mathcal{U}$ .
- What is  $[\vec{x}]_{\mathcal{U}}$ ?

Final term That is, what are  $b_1$  and  $b_2$  in  $\vec{x} = b_1 \hat{u}^{(1)} + b_2 \hat{u}^{(2)}$ .



# **Change of Basis**

Suppose  $\hat{u}^{(1)}$  and  $\hat{u}^{(2)}$  are our new, **orthonormal** basis vectors.

We know 
$$\vec{x} = x_1 \hat{e}^{(1)} + x_2 \hat{e}^{(2)}$$

• We want to write  $\vec{x} = b_1 \hat{u}^{(1)} + b_2 \hat{u}^{(2)}$ 

Solution

$$b_1 = \vec{x} \cdot \hat{u}^{(1)}$$
  $b_2 = \vec{x} \cdot \hat{u}^{(2)}$ 

### **Change of Basis Matrix**

Changing basis is a linear transformation

$$\vec{f}(\vec{x}) = (\vec{x} \cdot \hat{u}^{(1)})\hat{u}^{(1)} + (\vec{x} \cdot \hat{u}^{(2)})\hat{u}^{(2)} = \begin{pmatrix} \vec{x} \cdot \hat{u}^{(1)} \\ \vec{x} \cdot \hat{u}^{(2)} \end{pmatrix}_{\mathcal{U}}$$

We can represent it with a matrix

$$\begin{pmatrix}\uparrow&\uparrow\\f(\hat{e}^{(1)})&f(\hat{e}^{(2)})\\\downarrow&\downarrow\end{pmatrix}$$

$$\begin{aligned} \mathbf{Example} \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \begin{pmatrix} \hat{\mathbf{e}}^{(1)} \cdot \hat{\mathbf{u}}^{(2)} \\ \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(2)} \\ \hat{\mathbf{u}}^{(2)} &= (-1/2, \sqrt{3}/2)^{\mathsf{T}} \\ \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \\ \mathbf{f}(\hat{\mathbf{e}}^{(2)}) &= \\ A &= \begin{pmatrix} \sqrt{3}/2 & 1/2 \\ -1/2 & \sqrt{3}/2 \\ -1/2 & \sqrt{3}/2 \\ \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \\ A &= \begin{pmatrix} \sqrt{3}/2 & 1/2 \\ -1/2 & \sqrt{3}/2 \\ -1/2 & \sqrt{3}/2 \\ \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \\ \mathbf{f}(\hat{\mathbf{e}}^{(2)}) &= \begin{pmatrix} \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(1)} \\ \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(2)} \\ \hat{\mathbf{e}}^{(2)} &= \begin{pmatrix} \sqrt{3}/2 \\ \sqrt{3}/2 \\ \sqrt{3}/2 \\ \sqrt{3}/2 \\ \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \\ \mathbf{f}(\hat{\mathbf{e}}^{(2)}) &= \begin{pmatrix} \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(1)} \\ \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(2)} \\ \frac{1}{\sqrt{3}/2} \\ \sqrt{3}/2 \\ \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \\ \mathbf{f}(\hat{\mathbf{e}}^{(2)}) &= \begin{pmatrix} \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(2)} \\ \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(2)} \\ \frac{1}{\sqrt{3}/2} \\ \frac{1}{\sqrt{3}/2} \\ \mathbf{f}(\hat{\mathbf{e}}^{(1)}) &= \\ \mathbf{f}(\hat{\mathbf{e}}^{(2)}) &= \begin{pmatrix} \hat{\mathbf{e}}^{(2)} \cdot \hat{\mathbf{u}}^{(2)} \\ \frac{1}{\sqrt{3}/2} \\$$

#### Observation

The new basis vectors become the rows of the matrix.



### **Change of Basis Matrix**

• Let  $\hat{u}^{(1)}, \dots, \hat{u}^{(d)}$  form an orthonormal basis  $\mathcal{U}$ .

The matrix U whose rows are the new basis vectors is the change of basis matrix from the standard basis to U:

$$U = \begin{pmatrix} \leftarrow \hat{u}^{(1)} \rightarrow \\ \leftarrow \hat{u}^{(2)} \rightarrow \\ \vdots \\ \leftarrow \hat{u}^{(d)} \rightarrow \end{pmatrix}$$

#### **Change of Basis Matrix**

▶ If U is the change of basis matrix,  $[\vec{x}]_{\mathcal{U}} = U\vec{x}$ 

• To go *back* to the standard basis, use  $U^T$ :

 $\vec{x} = U^T [\vec{x}]_{\mathcal{U}}$ 

 $U \Rightarrow = [ \Rightarrow ]_{\mu}$  $\mathcal{U}^{\mathsf{T}}[\vec{\mathbf{x}}] = \vec{\mathbf{x}}$ 



Representation Learning

Lecture 05 | Part 2

Diagonalization

#### **Matrices of a Transformation**

• Let  $\vec{f} : \mathbb{R}^d \to \mathbb{R}^d$  be a linear transformation

► The matrix representing  $\vec{f}$  wrt the **standard basis** is:  $A = \begin{pmatrix} \uparrow & \uparrow & \uparrow & \uparrow \\ [\vec{f}(\hat{e}^{(1)})] \in \vec{f}(\hat{e}^{(2)}) & \cdots & \vec{f}(\hat{e}^{(d)}) \\ \downarrow & \downarrow & \downarrow & \downarrow \end{pmatrix}$ 

#### **Matrices of a Transformation**

▶ If we use a different basis  $U = \{\hat{u}^{(1)}, ..., \hat{u}^{(d)}\}$ , the matrix representing  $\vec{f}$  is:

$$A_{\mathcal{U}} = \begin{pmatrix} \uparrow & \uparrow & \uparrow \\ [\vec{f}(\hat{u}^{(1)})]_{\mathcal{U}} & [\vec{f}(\hat{u}^{(2)})]_{\mathcal{U}} & \cdots & [\vec{f}(\hat{u}^{(d)})]_{\mathcal{U}} \\ \downarrow & \downarrow & \downarrow & \downarrow \end{pmatrix}$$

► If  $\vec{y} = A\vec{x}$ , then  $[\vec{y}]_{\mathcal{U}} = A_{\mathcal{U}}[\vec{x}]_{\mathcal{U}}$ 

### **Diagonal Matrices**

- Diagonal matrices are very nice / easy to work with.
- Suppose A is a matrix. Is there a basis U where A<sub>U</sub> is diagonal?
- > Yes! *If* A is symmetric.

# The Spectral Theorem<sup>1</sup>

Theorem: Let A be an n × n symmetric matrix. Then there exist n eigenvectors of A which are all mutually orthogonal.

<sup>1</sup>for symmetric matrices

# Eigendecomposition

- ▶ If A is a symmetric matrix, we can pick d of its eigenvectors  $\hat{u}^{(1)}, ..., \hat{u}^{(d)}$  to form an orthonormal basis.
- Any vector x can be written in terms of this eigenbasis.
- This is called its eigendecomposition:

$$\vec{x} = b_1 \hat{u}^{(1)} + b_2 \hat{u}^{(2)} + \dots + b_d \hat{u}^{(d)}$$

# Matrix in the Eigenbasis

- Claim: the matrix of a linear transformation *f*, written in a basis of its eigenvectors, is a diagonal matrix.
- The entries along the diagonal will be the eigenvalues.

Why?

$$A_{\mathcal{U}} = \begin{pmatrix} \uparrow & \uparrow & \uparrow & \uparrow \\ [\vec{f}(\hat{u}^{(1)})]_{\mathcal{U}} & [\vec{f}(\hat{u}^{(2)})]_{\mathcal{U}} & \cdots & [\vec{f}(\hat{u}^{(d)})]_{\mathcal{U}} \\ \downarrow & \downarrow & \downarrow & \downarrow \end{pmatrix}$$

$$\vec{f}(\hat{u}^{(1)}) = \lambda_1 \hat{u}^{(1)}, \text{ so } [\vec{f}(\hat{u}^{(1)})]_{\mathcal{U}} = (\lambda_1, 0, \dots, 0)^T.$$

$$\vec{f}(\hat{u}^{(2)}) = \lambda_2 \hat{u}^{(2)}, \text{ so } [\vec{f}(\hat{u}^{(2)})]_{\mathcal{U}} = (0, \lambda_2, \dots, 0)^T.$$

$$\cdots \qquad A_{\mathcal{U}} \sim \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \\ 0 & 0 & \lambda_4 \\ 0 &$$

# **Matrix Multiplication**

We have seen that matrix multiplication evaluates a linear transformation.

In the standard basis:

$$\vec{f}(\vec{x}) = A\vec{x}$$

In another basis:

$$[\vec{f}(\vec{x})]_{\mathcal{U}} = A_{\mathcal{U}}[\vec{x}]_{\mathcal{U}}$$

# Diagonalization Ar

Another way to compute  $\vec{f}(x)$ , starting with  $\vec{x}$  in the standard basis:

L

1. Change basis to the eigenbasis with U.  $[\overleftarrow{s}]_{\mu}$ 

2 Apply 
$$\vec{f}$$
 in the eigenbasis with the diagonal  
 $A_{\mathcal{U}}$ .  $A_{\mathcal{U}}[\vec{x}]_{\mathcal{U}} = (f(\vec{x}))_{\mathcal{U}}$ 

**3.** Go back to the standard basis with  $U^{T}$ .

► That is, 
$$A\vec{x} = U^T A_U U \vec{x}$$
. It follows that  $A = U^T A_U U$ .

# Spectral Theorem (Again)

- Theorem: Let A be an n × n symmetric matrix. Then there exists an orthogonal matrix U and a diagonal matrix A such that A = U<sup>T</sup>AU.
- The rows of U are the eigenvectors of A, and the entries of Λ are its eigenvalues.

U is said to diagonalize A.

DSC 140B Representation Learning

Lecture 05 | Part 3

**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





- 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 R<sup>d</sup> to R<sup>1</sup>
- 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<sub>1</sub>: screen width
  - $\triangleright$   $x_2$ : phone weight
- Both measure a phone's "size".
- Instead of representing a phone with both x<sub>1</sub> and x<sub>2</sub>, 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.

$$z = u_1 x_1 + u_2 x_2 \qquad \vec{u} = (u_1, u_2)$$
$$= \vec{u} \cdot \vec{x} \qquad \vec{y} = (x_1, x_2)$$

u<sub>1</sub>,..., u<sub>2</sub> are the mixture coefficients; we can choose them.

#### $1000 \times 12000 \times 7$ $1 \times 12 \times 7$ 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  $\|\vec{u}\| = 1$  $\|\vec{u}\| = \sqrt{u_1^2 + u_2^2}$
# $z = \overline{x} \cdot \overline{u} = \|\overline{x}\| \|\overline{y}\| \cos \Theta$ 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
  - $\triangleright$   $x_2$ : phone thickness
- We'll create single new feature, z, from x₁ and x₂.
   Assume z = u₁x₁ + u₂x₂ = x · u
   Interpretation: z is a measure of a phone's size
- How should we choose  $\vec{u} = (u_1, u_2)^T$ ?



ū=(1,0)

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

#### Example



- $\blacktriangleright$  *\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: u
   should point in direction of "max variance".

## Example



- Phone "size" varies most along a diagonal direction.
- Along direction of "max variance", phones are well-separated.
- Idea: *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 *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

$$\vec{x}^{(1)} = (3, -2)^7$$
  
 $\vec{x}^{(2)} = (1, 4)^7$ 

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

#### Problem

How do we compute the "direction of maximum variance"?

Representation Learning

Lecture 05 | Part 4

**Covariance Matrices** 

#### Variance

We know how to compute the variance of a set of numbers X = {x<sup>(1)</sup>, ..., x<sup>(n)</sup>}:

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

The variance measures the "spread" of the data

## **Generalizing Variance**

If we have two features, x<sub>1</sub> and x<sub>2</sub>, we can compute the variance of each as usual:

$$Var(x_1) = \frac{1}{n} \sum_{i=1}^{n} (\vec{x}_1^{(i)} - \mu_1)^2$$
$$Var(x_2) = \frac{1}{n} \sum_{i=1}^{n} (\vec{x}_2^{(i)} - \mu_2)^2$$

• 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:

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

• One approach is as follows<sup>2</sup>.

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

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*.

<sup>2</sup>Assuming centered data



Covariance = 
$$\frac{1}{7} \sum_{i=1}^{7} \vec{x}_{1}^{(i)} \times \vec{x}_{2}^{(i)}$$



Assume the data are centered.

Covariance = 
$$\frac{1}{7} \sum_{i=1}^{7} \vec{x}_{1}^{(i)} \times \vec{x}_{2}^{(i)}$$





Covariance = 
$$\frac{1}{7} \sum_{i=1}^{7} \vec{x}_{1}^{(i)} \times \vec{x}_{2}^{(i)}$$



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

The sample covariance matrix C is the d × d matrix whose ij entry is defined to be σ<sub>ii</sub>.

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

#### 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 × 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>3</sup>

<sup>3</sup>Or use np.cov

DSC 140B Representation Learning

#### Lecture 05 | Part 5

#### **Visualizing Covariance Matrices**

Covariance matrices are symmetric.

They have axes of symmetry (eigenvectors and eigenvalues).

▶ What are they?



C ≈ (



Eigenvectors:

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



C ≈ (



Eigenvectors:

 $\vec{u}^{(1)} \approx \vec{u}^{(2)} \approx$
#### **Visualizing Covariance Matrices**



C ≈ (

### **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.

- 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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