

DSC 140B

Representation Learning

Lecture 08 | Part 1

Diagonalization

Matrices of a Transformation

- ▶ Let $\vec{f} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be a linear transformation
- ▶ The matrix representing \vec{f} wrt the **standard basis** is:

$$A = \begin{pmatrix} \uparrow & \uparrow & \uparrow & \uparrow \\ \vec{f}(\hat{e}^{(1)}) & \vec{f}(\hat{e}^{(2)}) & \dots & \vec{f}(\hat{e}^{(d)}) \\ \downarrow & \downarrow & \downarrow & \downarrow \end{pmatrix}$$

Matrices of a Transformation

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

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

- ▶ 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 \mathcal{U} where $A_{\mathcal{U}}$ is diagonal?
- ▶ Yes! *If* A is symmetric.

The Spectral Theorem¹

- ▶ **Theorem:** Let A be an $n \times n$ *symmetric* matrix. Then there exist n eigenvectors of A which are all mutually orthogonal.

¹for symmetric matrices

Eigendecomposition

- ▶ If A is a symmetric matrix, we can pick d of its eigenvectors $\hat{u}^{(1)}, \dots, \hat{u}^{(d)}$ to form an orthonormal basis.
- ▶ Any vector \vec{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 \vec{f} , written in a basis of its eigenvectors, is a **diagonal** matrix.
- ▶ The entries along the diagonal will be the **eigenvalues**.

Why?

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

- ▶ $\vec{f}(\hat{u}^{(1)}) = \lambda_1 \hat{u}^{(1)}$, so $[\vec{f}(\hat{u}^{(1)})]_{\mathcal{U}} = (\lambda_1, 0, \dots, 0)^T$.
- ▶ $\vec{f}(\hat{u}^{(2)}) = \lambda_2 \hat{u}^{(2)}$, so $[\vec{f}(\hat{u}^{(2)})]_{\mathcal{U}} = (0, \lambda_2, \dots, 0)^T$.
- ▶ ...

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

- ▶ Another way to compute $\vec{f}(x)$, starting with \vec{x} in the standard basis:
 1. Change basis to the eigenbasis with U .
 2. Apply \vec{f} in the eigenbasis with the diagonal $A_{\mathcal{U}}$.
 3. Go *back* to the standard basis with U^T .
- ▶ That is, $A\vec{x} = U^T A_{\mathcal{U}} U\vec{x}$. It follows that $A = U^T A_{\mathcal{U}} U$.

Spectral Theorem (Again)

- ▶ **Theorem:** Let A be an $n \times n$ *symmetric* matrix. Then there exists an orthogonal matrix U and a diagonal matrix Λ such that $A = U^T \Lambda U$.
- ▶ The *rows* of U are the eigenvectors of A , and the entries of Λ are its eigenvalues.
- ▶ U is said to **diagonalize** A .

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Representation Learning

Lecture 08 | Part 2

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
 - ▶ ⋮

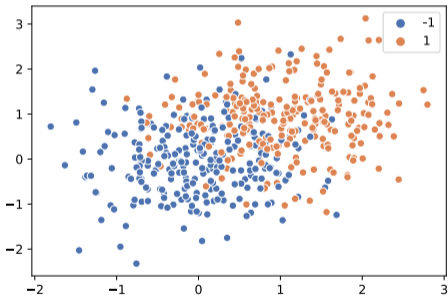
High Dimensional Data

- ▶ 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 $d' \leq d$

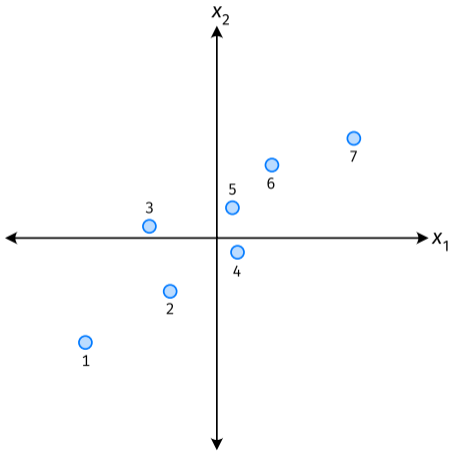
Today's Example

- ▶ 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

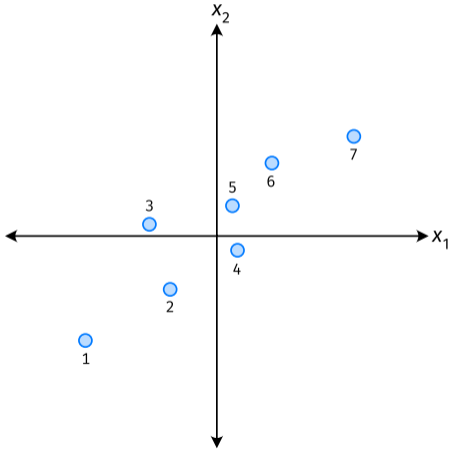
- ▶ Screen width and weight share information.
- ▶ **Idea:** keep one feature, remove the other.
- ▶ That is, set new feature $z = x_1$ (or $z = x_2$).

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.

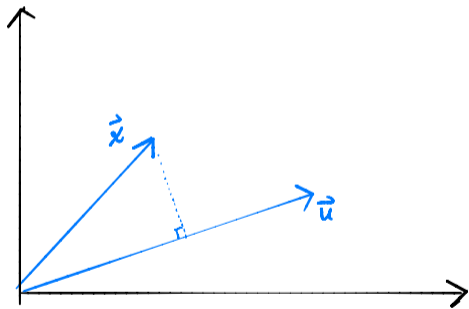
$$\begin{aligned}z &= u_1 x_1 + u_2 x_2 \\ &= \vec{u} \cdot \vec{x}\end{aligned}$$

- ▶ 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 $z = x_2$

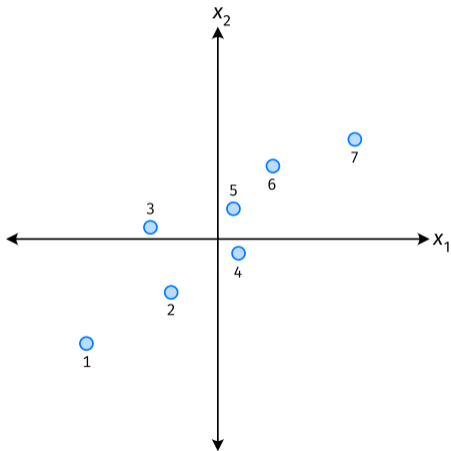
Choosing \vec{u}

- ▶ 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

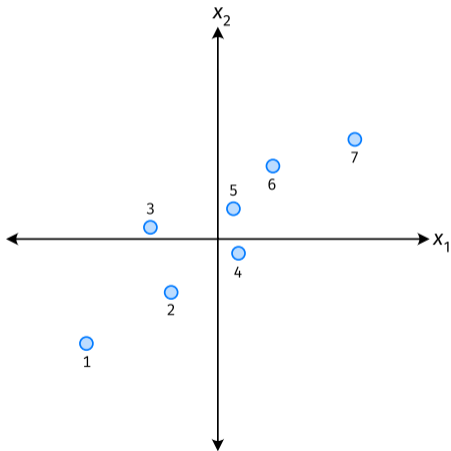
http://dsc140b.com/static/vis/pca-max_variance/

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”?

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Representation Learning

Lecture 08 | Part 3

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

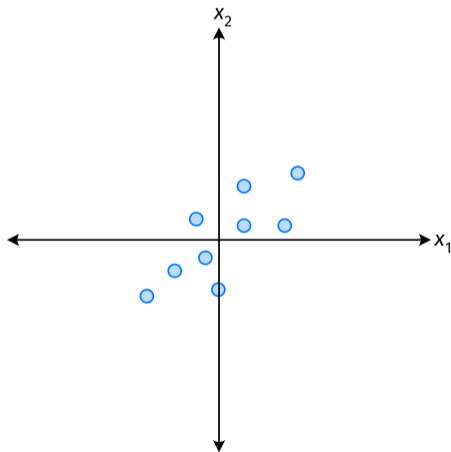
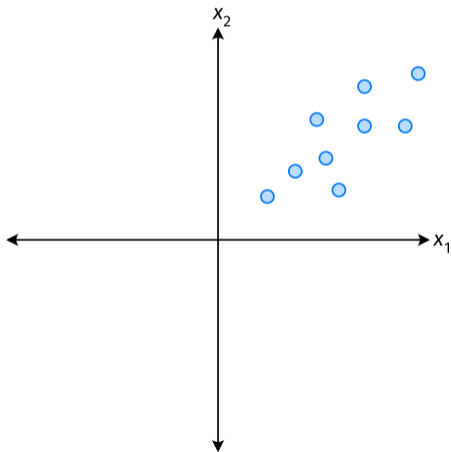
- ▶ Features which share information if they *vary together*.
 - ▶ A.k.a., they “co-vary”
- ▶ Positive association: when one is above average, so is the other
- ▶ Negative association: when one is above average, the other is below average

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 follows².

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

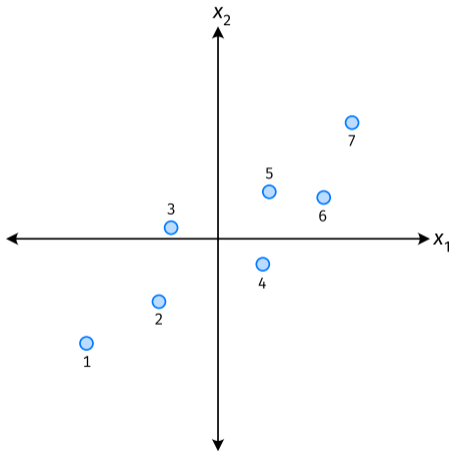
- ▶ For each data point, multiply the value of feature i and feature j , then average these products.
- ▶ This is the **covariance** of features i and j .

²Assuming centered data

Quantifying Covariance

- ▶ Assume the data are **centered**.

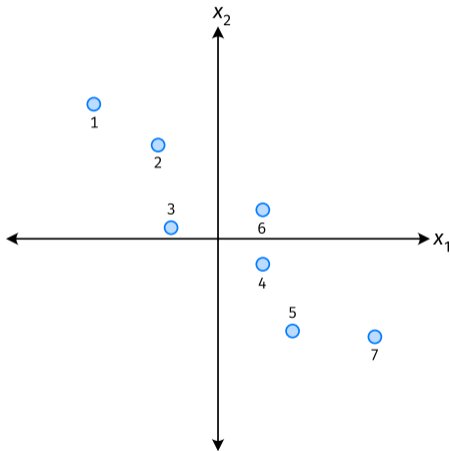
$$\text{Covariance} = \frac{1}{7} \sum_{i=1}^7 \vec{X}_1^{(i)} \times \vec{X}_2^{(i)}$$



Quantifying Covariance

- ▶ Assume the data are **centered**.

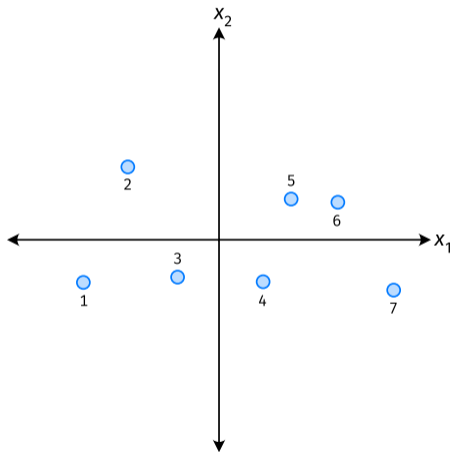
$$\text{Covariance} = \frac{1}{7} \sum_{i=1}^7 \vec{X}_1^{(i)} \times \vec{X}_2^{(i)}$$



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

- ▶ 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 σ_{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)³

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

³Or use `np.cov`