DSC 140B
Representation Learning

Lecture 10 | Part 1

Covariance Matrices

Variance

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

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

- 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

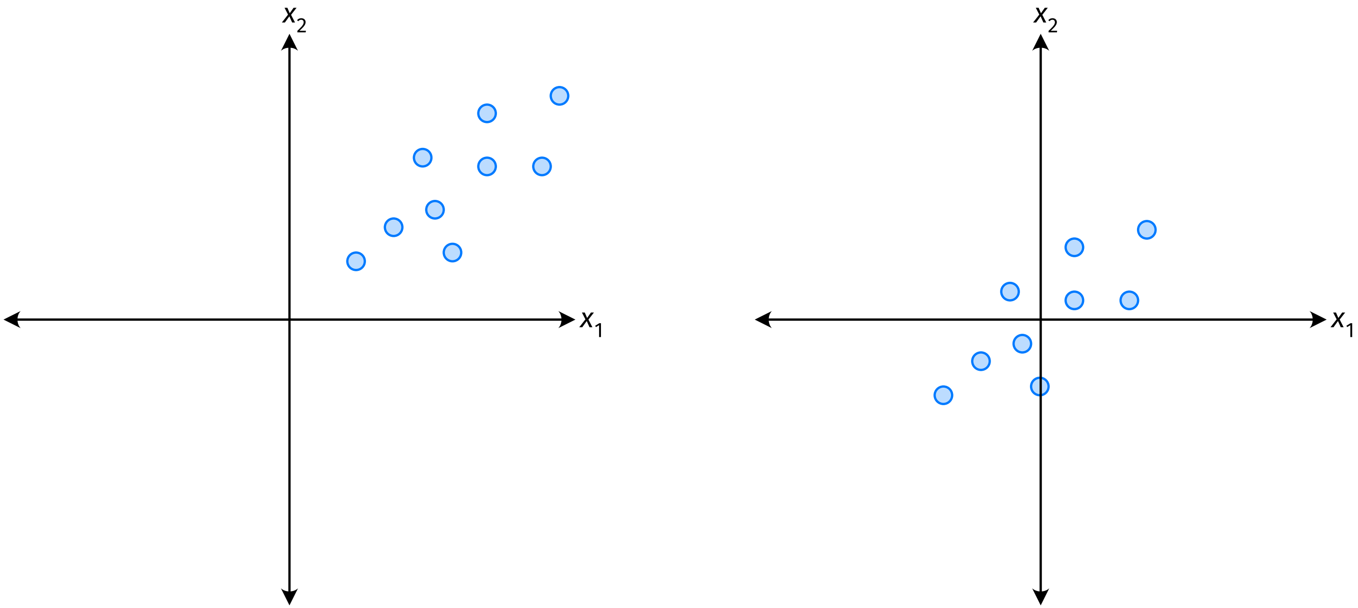
- Features which share information if they *vary together*.
  - A.k.a., they “co-vary”
- Positive association: when one is above average, so is the other
- Negative association: when one is above average, the other is below average

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[1].

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

  - 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*.

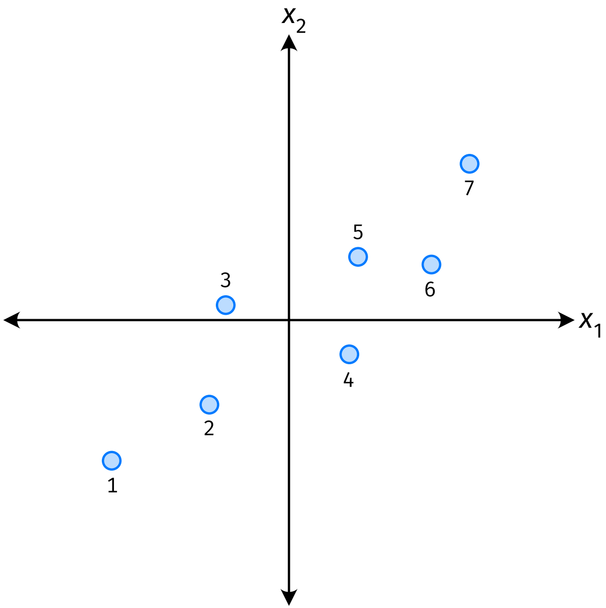
---

[1]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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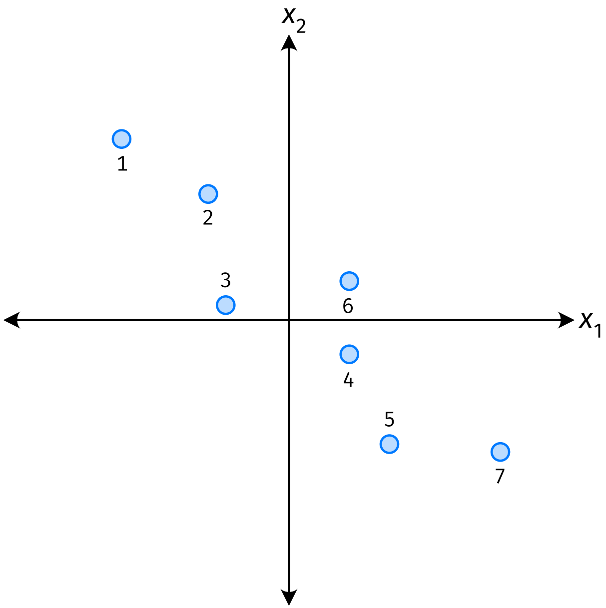

Quantifying Covariance

- Assume the data are **centered**.

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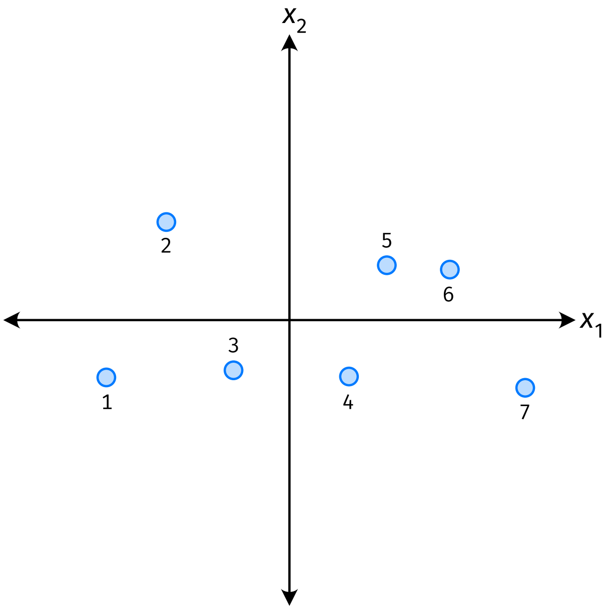

Quantifying Covariance

- 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 $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)} \in \mathbb{R}^d$.
- 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)[2]

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

[2] Or use `np.cov`

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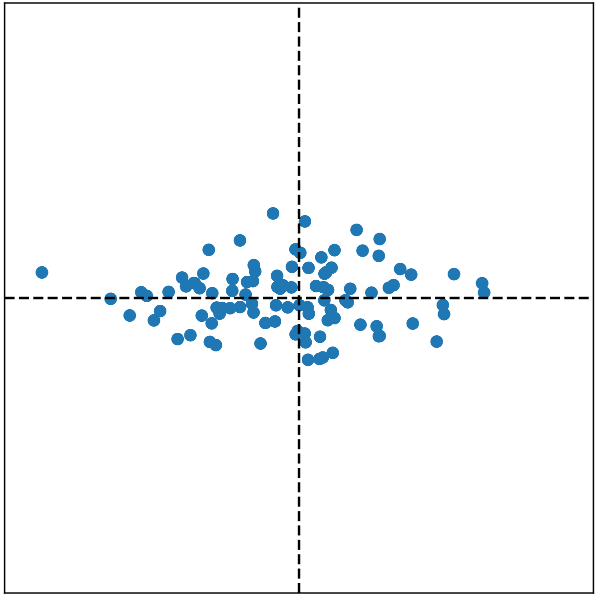
Lecture 10 | Part 2

Visualizing Covariance Matrices

Visualizing Covariance Matrices

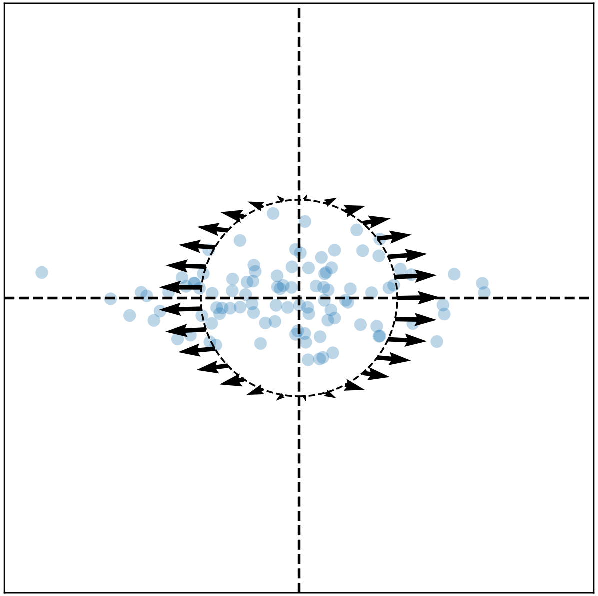
- Covariance matrices are symmetric.
- They have axes of symmetry (eigenvectors and eigenvalues).
- What are they?

Visualizing Covariance Matrices



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

Visualizing Covariance Matrices

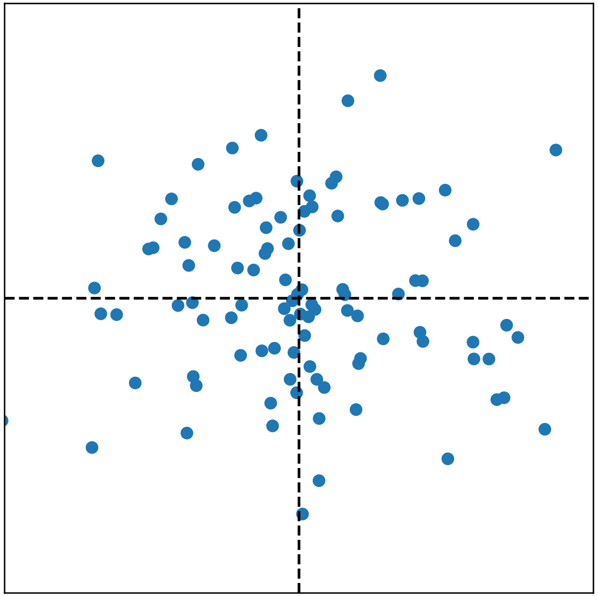


Eigenvectors:

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

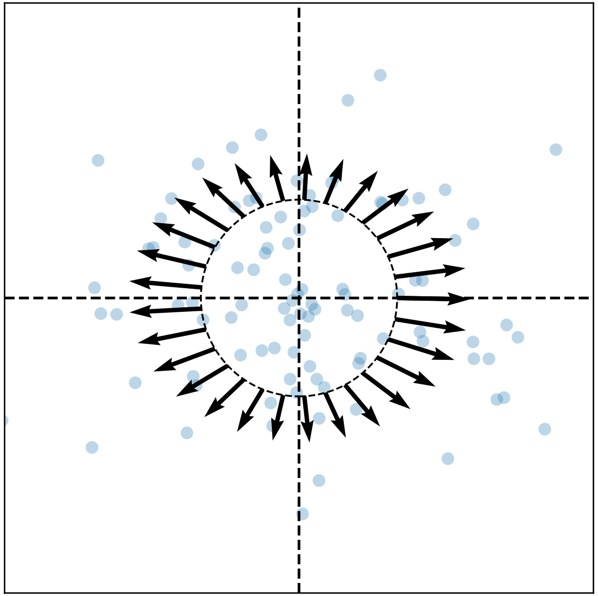
$\vec{u}^{(2)} \approx$

Visualizing Covariance Matrices



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

Visualizing Covariance Matrices



Eigenvectors:

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

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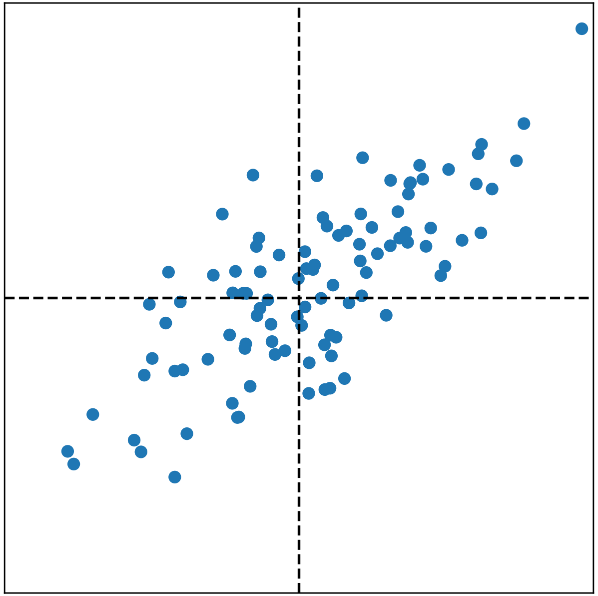
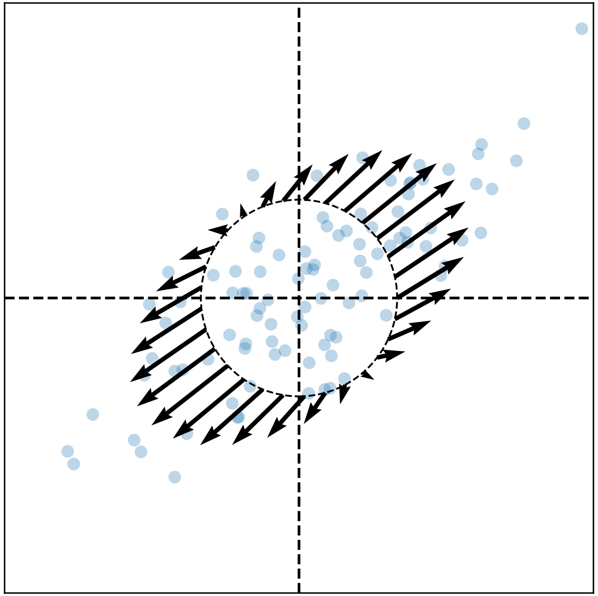
Visualizing Covariance Matrices



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

Visualizing Covariance Matrices



Eigenvectors:

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

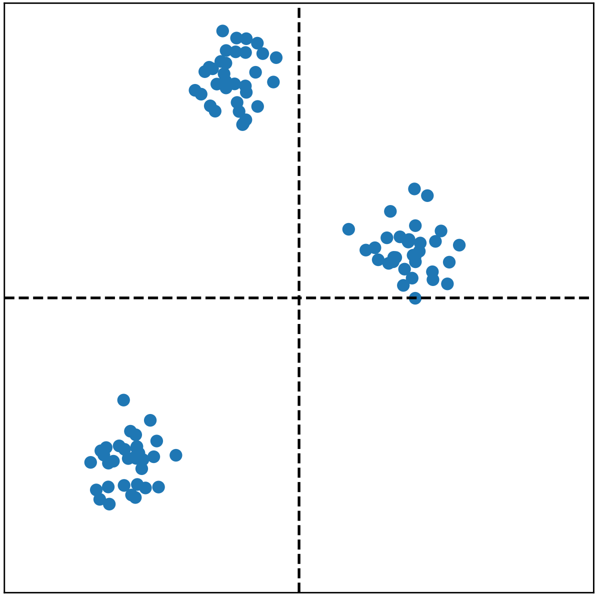
$\vec{u}^{(2)} \approx$

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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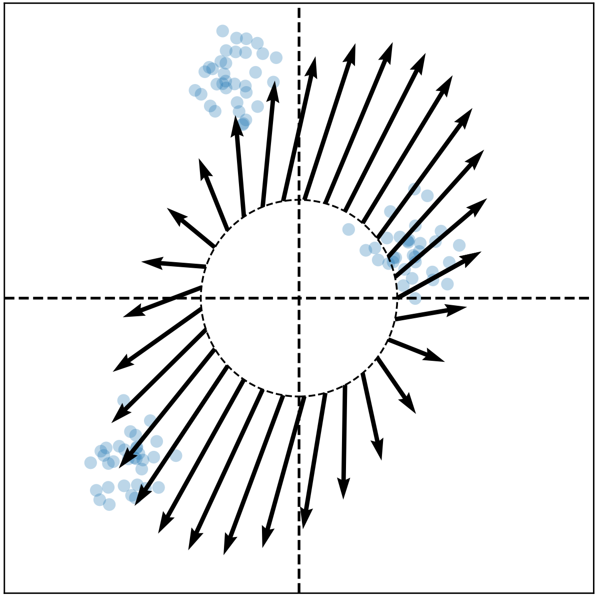

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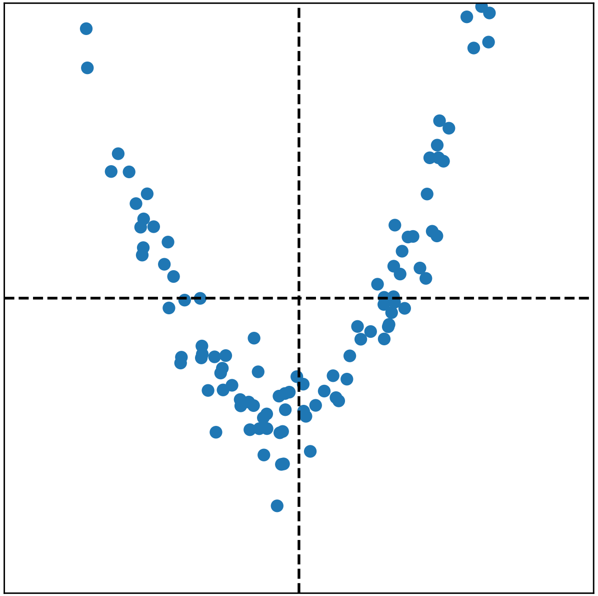

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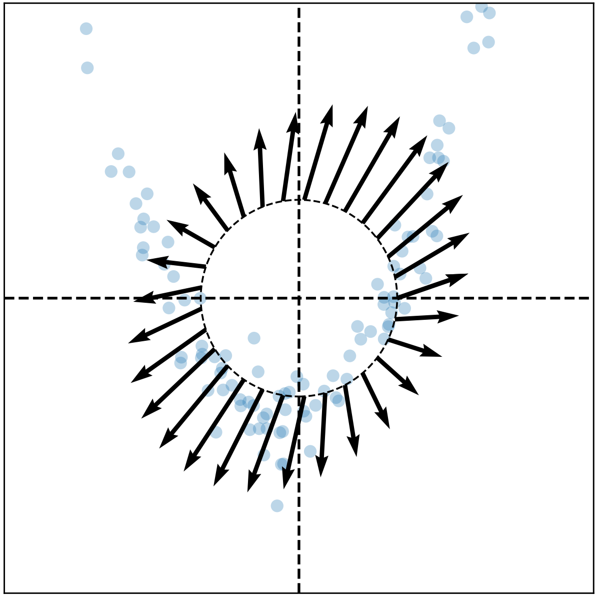

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Representation Learning

Lecture 10 | Part 3

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

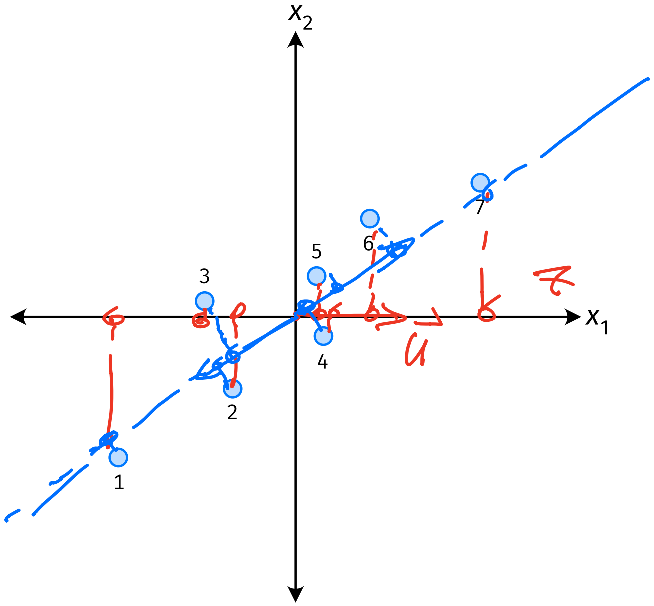
- Let $\vec{u}$ be a unit vector.
- $z^{(i)} = \vec{x}^{(i)} \cdot \vec{u}$ is the new feature for $\vec{x}^{(i)}$.
- The variance of the new features is:

$$\text{Var}(z) = \frac{1}{n}\sum_{i=1}^{n}(z^{(i)} - \mu_z)^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}\left(\vec{x}^{(i)} \cdot \vec{u} - \mu_z\right)^2$$

$z^{(i)} \in \mathbb{R}$

Example



Note

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

$$\text{Var}(z) = \frac{1}{n}\sum_{i=1}^{n}(z^{(i)})^2$$

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

Goal

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

$$\max_{\vec{u}} \; g(\vec{u}) = \frac{1}{n}\sum_{i=1}^{n}\left(\vec{x}^{(i)} \cdot \vec{u}\right)^2 \qquad \text{s.t. } \|\vec{u}\| = 1$$

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

Claim

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

Our Goal (Again)

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

Claim

$\max_{\vec{u}} \|C\vec{u}\|$ s.t. $\|\vec{u}\| = 1$

$\max_{\vec{u}} \vec{u}^T C \vec{u}$ s.t. $\|\vec{u}\| = 1$

s.t. $u_1^2 + u_2^2 = 1$

C: symmetric matrix

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

$d=2$

$\vec{v}^{(1)}, \vec{v}^{(2)}$: eigenvec of C. orthonormal

$\lambda_1 > \lambda_2$: eigen value

$$\vec{u} = u_1 \vec{v}^{(1)} + u_2 \vec{v}^{(2)}$$

$$C\vec{u} = C\cdot(u_1 \vec{v}^{(1)} + u_2 \vec{v}^{(2)}) = u_1 C \vec{v}^{(1)} + u_2 C \vec{v}^{(2)} = u_1 \lambda_1 \vec{v}^{(1)} + u_2 \lambda_2 \vec{v}^{(2)}$$

$$(u_1 \vec{v}^{(1)} + u_2 \vec{v}^{(2)})^T (u_1 \lambda_1 \vec{v}^{(1)} + u_2 \lambda_2 \vec{v}^{(2)}) = u_1^2 \lambda_1 \underbrace{\vec{v}^{(1)} \cdot \vec{v}^{(1)}}_{=1} + u_1 u_2 \lambda_2 \underbrace{\vec{v}^{(1)} \cdot \vec{v}^{(2)}}_{0} + u_1 u_2 \lambda_1 \underbrace{\vec{v}^{(2)} \cdot \vec{v}^{(1)}}_{0} + u_2^2 \lambda_2 \underbrace{\vec{v}^{(2)} \cdot \vec{v}^{(2)}}_{1}$$

$$\vec{u}^T C \vec{u} = u_1^2 \lambda_1 + u_2^2 \lambda_2$$

$$\begin{cases} u_1 = 1 \\ u_2 = 0 \end{cases}$$

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:

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

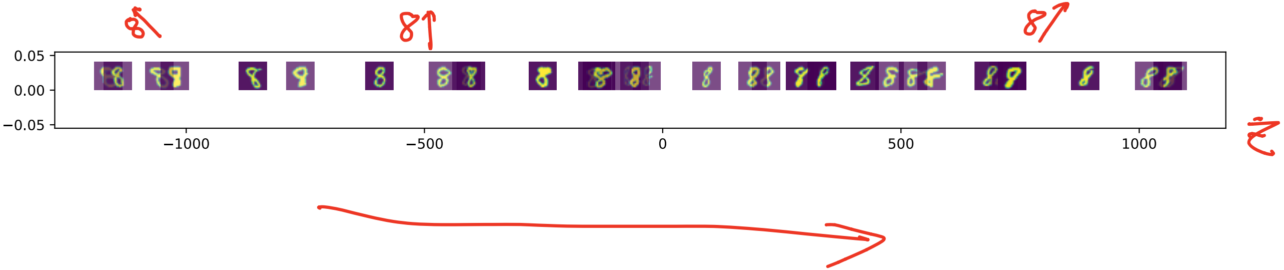
0, 1, 2, ..., 9   10 classes

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

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

Example



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Representation Learning

Lecture 10 | Part 4

Dimensionality Reduction with $d \geq 2$

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, $\vec{z}^{(i)} = (z_1^{(i)}, \ldots, z_k^{(i)})$.

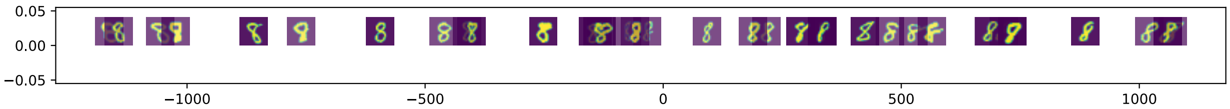
A Single Principal Component

- 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 $\mathbb{R}^{784} \to \mathbb{R}^1$ loses a lot of information

- What about mapping from $\mathbb{R}^{784} \to \mathbb{R}^2$? $\mathbb{R}^k$?

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:

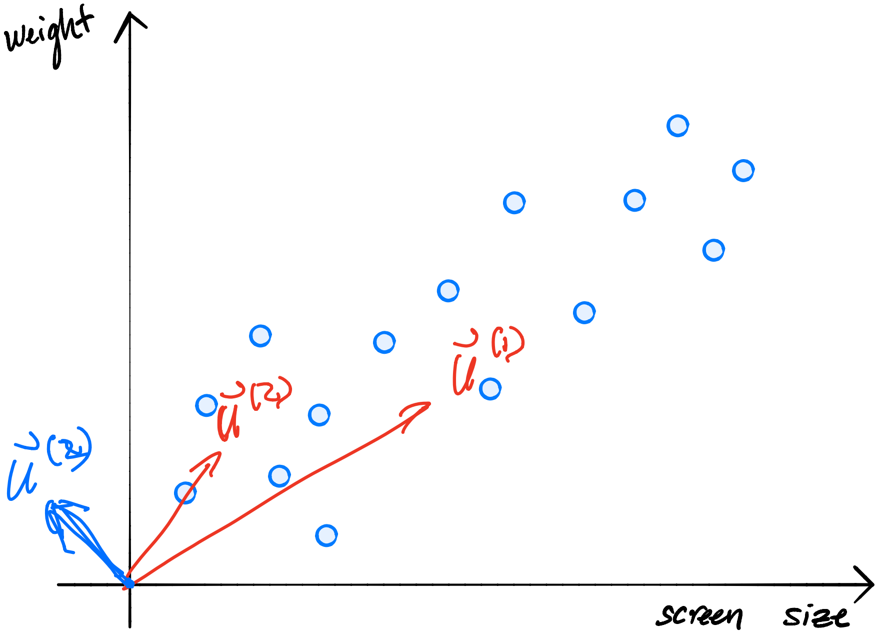
$$z_2 = \vec{u}^{(2)} \cdot \vec{x} = u_1^{(2)} x_1 + \ldots + u_d^{(2)} x_d$$

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

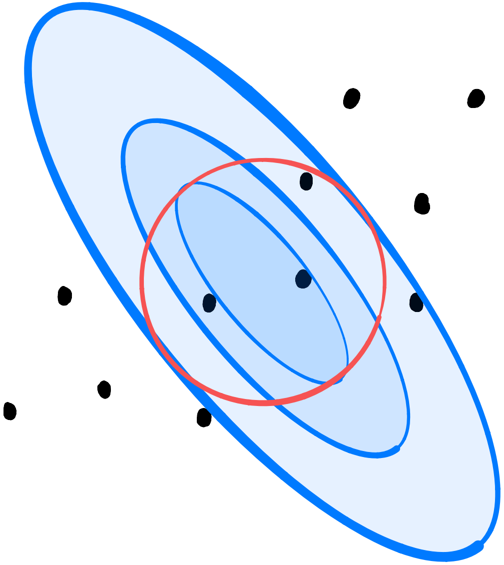
- We should choose $\vec{u}^{(2)}$ to be **orthogonal** to $\vec{u}^{(1)}$.
  - ① No "redundancy".

② keep as much info of data as possible

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

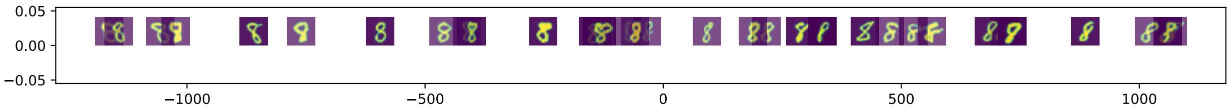
- Given a covariance matrix C.
- The principal component $\vec{u}^{(1)}$ is the top eigenvector of C.
  - Points in the direction of maximum variance.
- The *second* principal component $\vec{u}^{(2)}$ is the *second* eigenvector of C.
  - Out of all vectors orthogonal to the principal component, points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

PCA: Two Components

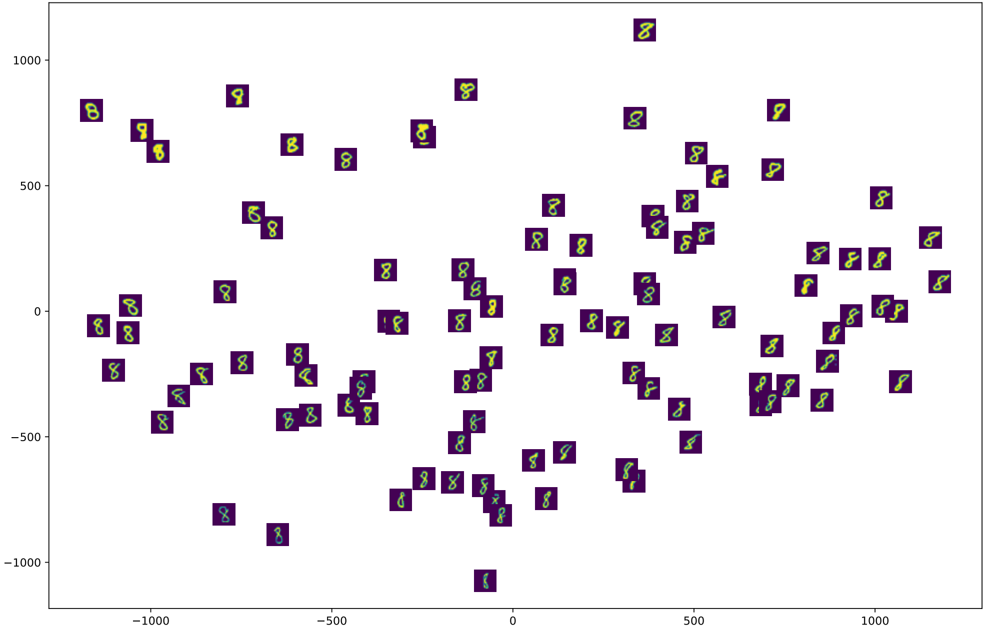
- Given data $\{\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}\} \in \mathbb{R}^d$.
- Compute covariance matrix C, top two eigenvectors $\vec{u}^{(1)}$ and $\vec{u}^{(2)}$.
- For any vector $\vec{x} \in \mathbb{R}$, its new representation in $\mathbb{R}^2$ is $\vec{z} = (z_1, z_2)^T$, where:

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

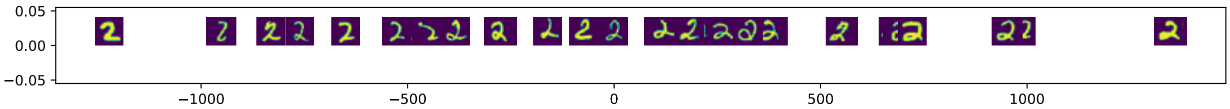
Example



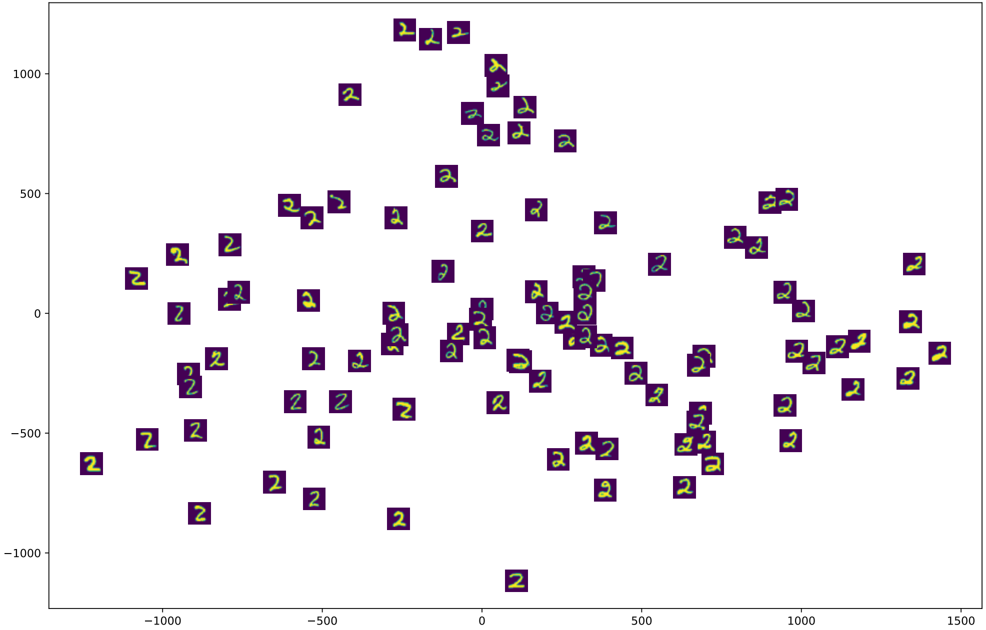
Example



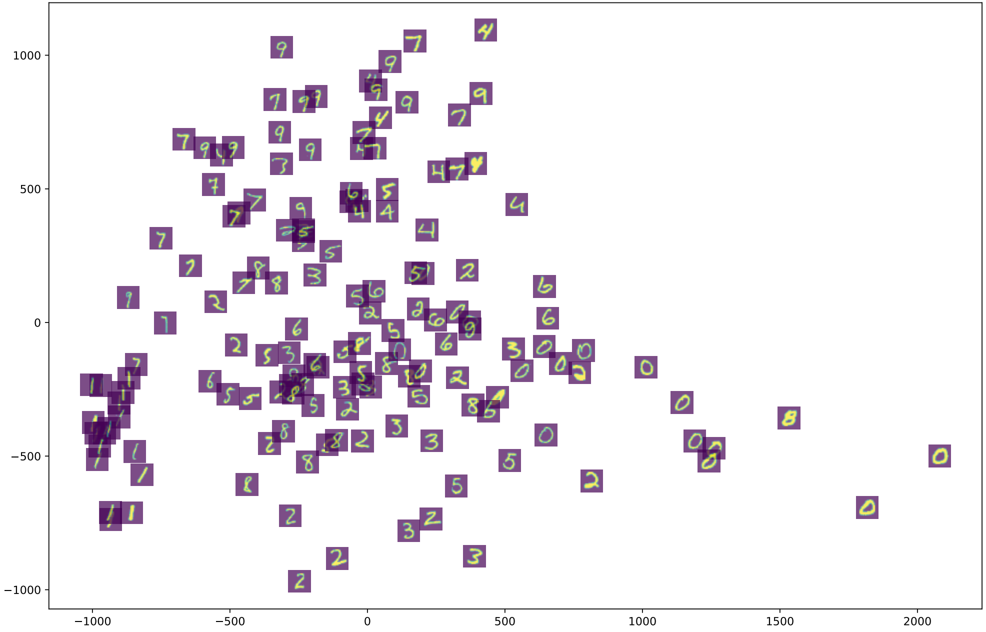
Example



Example



Example



PCA: k Components

- Given data $\{\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}\} \in \mathbb{R}^d$, number of components k.

- Compute covariance matrix C, top $k \leq d$ eigenvectors $\vec{u}^{(1)}$, $\vec{u}^{(2)}, \ldots, \vec{u}^{(k)}$.

- 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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Lecture 10 | Part 5

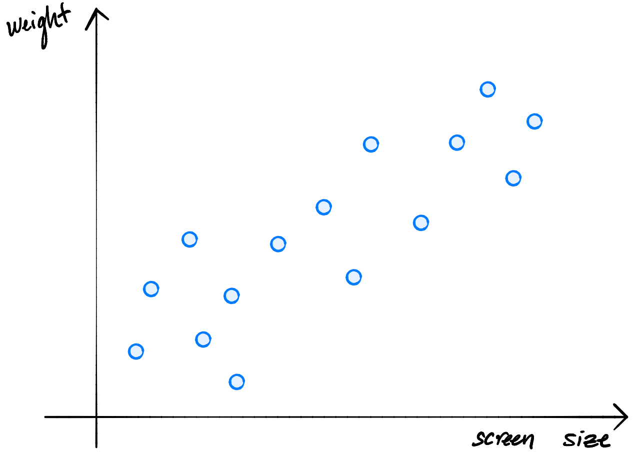
Reconstructions

Reconstructing Points

- PCA helps us reduce dimensionality from $\mathbb{R}^d \to R^k$
- 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:

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