DSC 190

Machine Learning: Representations

Lecture 9 | Part 1

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

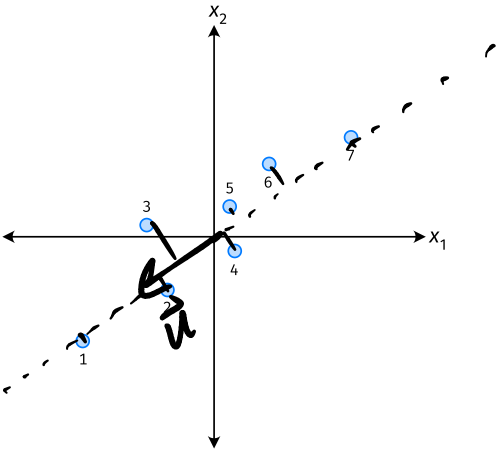
- Let $\vec{u}$ be a unit vector.

- $z^{(i)} = \vec{x}^{(i)} \cdot \vec{u}$ is the new feature for $\vec{x}^{(i)}$.

- The variance of the new features is:

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

Example



Note

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

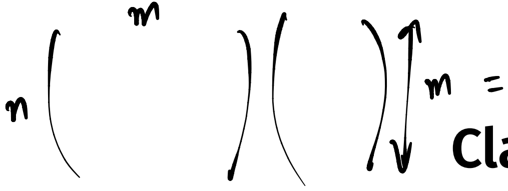
$$\begin{aligned}\text{Var}(z) &= \frac{1}{n}\sum_{i=1}^{n}(z^{(i)})^2 \\ &= \frac{1}{n}\sum_{i=1}^{n}\left(\vec{x}^{(i)} \cdot \vec{u}\right)^2\end{aligned}$$

Goal

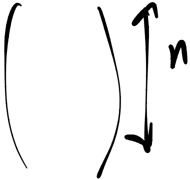
- The variance of a data set in the direction of $\vec{u}$ is:

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

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

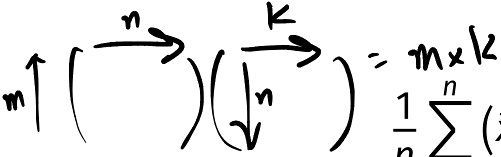


Claim



$g(\vec{u})$

Covariance mtx of $\vec{x}^{(1)}, \vec{x}^{(2)}, \ldots$



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

C is $d \times d$

$\vec{u}$ is $d \times 1$

$C\vec{u}$ is $d \times 1$

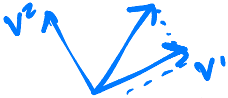
$\vec{u}^T$ is $1 \times d$

$\vec{u}^T(C\vec{u})$ is $(1 \times d) \times (d \times 1)$ is 1×1

Our Goal (Again)

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

Claim



Assume C is symmetric.

- To maximize $\vec{u}^T C \vec{u}$ over unit vectors, choose $\vec{u}$ to be the top eigenvector of C.
- Proof: Let $\hat{v}^{(1)}$ & $\hat{v}^{(2)}$ be orthogonal eigvecs of C, say λ_1 & λ_2 are their eigvalues.

$Cv^{(1)} = \lambda_1 \hat{v}^{(1)}$

Any unit vector $\vec{u}$ can be written

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

Then

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

$$= u_1 \lambda_1 \hat{v}^{(1)} + u_2 \lambda_2 \hat{v}^{(2)}$$

Claim

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

- Proof: $\vec{u}^T C \vec{u} = \vec{u}^T \left(u_1 \lambda_1 \hat{v}^{(1)} + u_2 \lambda_2 \hat{v}^{(2)} \right)$

$$= \left(u_1 \hat{v}^{(1)T} + u_2 \hat{v}^{(2)T} \right)\left(u_1 \lambda_1 \hat{v}^{(1)} + u_2 \lambda_2 \hat{v}^{(2)} \right)$$

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

$$= u_1^2 \lambda_1 + u_2^2 \lambda_2$$

Claim

- To maximize $\vec{u}^T C \vec{u}$ over unit vectors, choose $\vec{u}$ to be the top eigenvector of C.
- Proof: $\hat{u}^T C \hat{u} = u_1^2 \lambda_1 + u_2^2 \lambda_2$

For $\hat{u}$ to be a unit vector, $u_1^2 + u_2^2 = 1$

To maximize, set $u_1 = 1$, $u_2 = 0$

So $\vec{u} = u_1 \hat{v}^{(1)} + u_2 \hat{v}^{(2)} = \hat{v}^{(1)}$ maximizes $\vec{u}^T C \vec{u}$ s.t. $\|\vec{u}\| = 1$.

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:

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

$\vec{u}^T C \vec{u}$ is largest

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Lecture 9 | Part 2

Dimensionality Reduction with d ≥ 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.

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

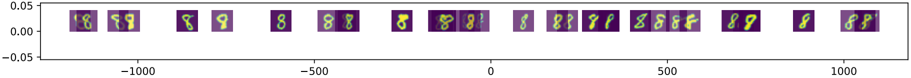
A Single Principal Component

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

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

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

A Second Feature

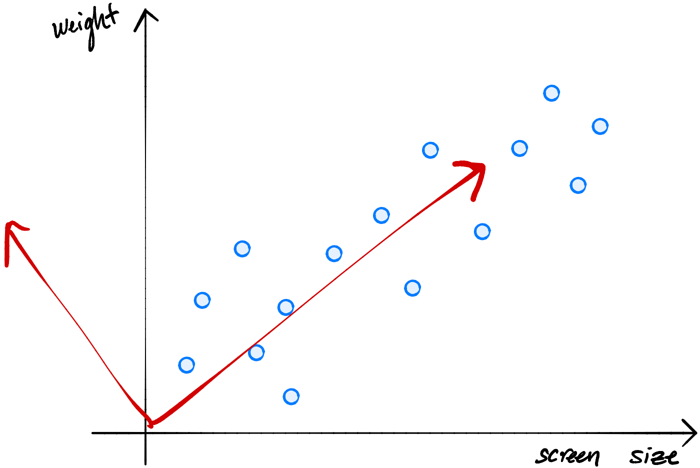
- Make same assumption for second feature:

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

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

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

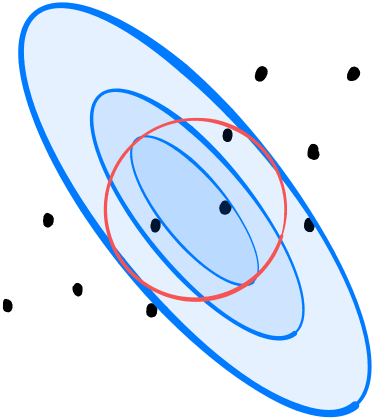
A Second Feature



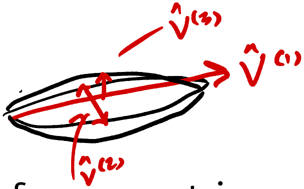
A Second Feature

C

$Cu = \lambda u$



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

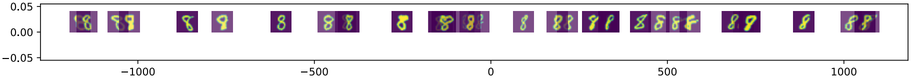
- Given a covariance matrix C.
- The principal component $\vec{u}^{(1)}$ is the top eigenvector of C.
  - Points in the direction of maximum variance.
- The *second* principal component $\vec{u}^{(2)}$ is the *second* eigenvector of C.
  - Out of all vectors orthogonal to the principal component, points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

PCA: Two Components

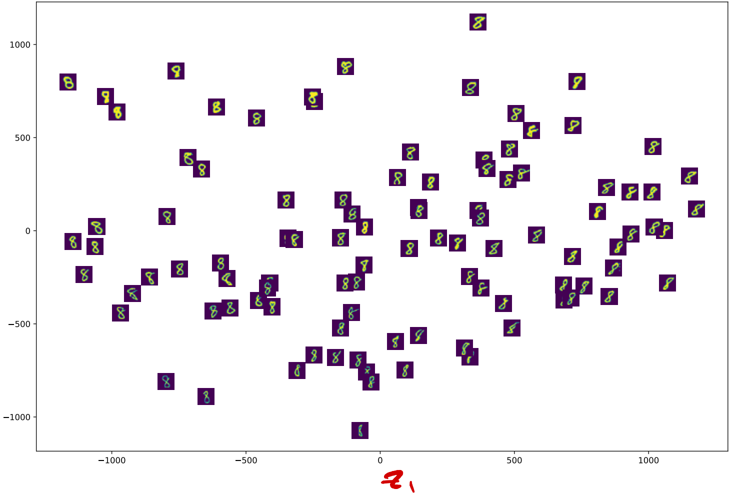
- Given data $\{\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}\} \in \mathbb{R}^d$.
- Compute covariance matrix C, top two eigenvectors $\vec{u}^{(1)}$ and $\vec{u}^{(2)}$.
- For any vector $\vec{x} \in \mathbb{R}$, its new representation in $\mathbb{R}^2$ is $\vec{z} = (z_1, z_2)^T$, where:

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

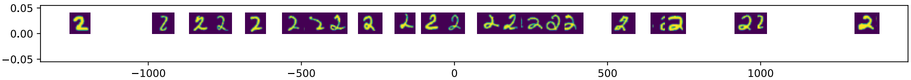
Example



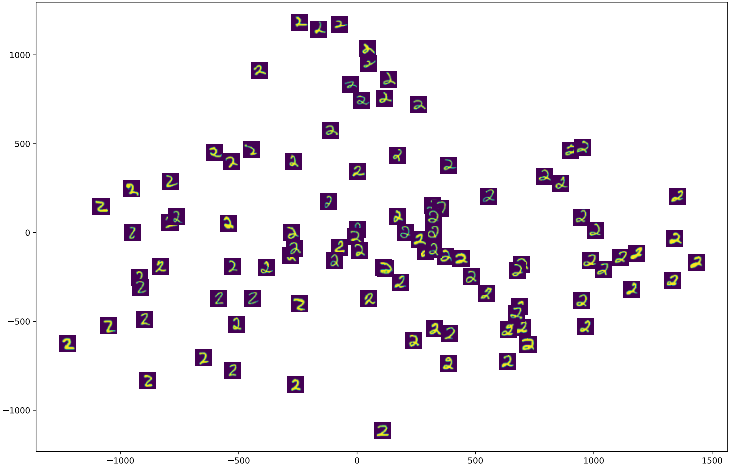
Example



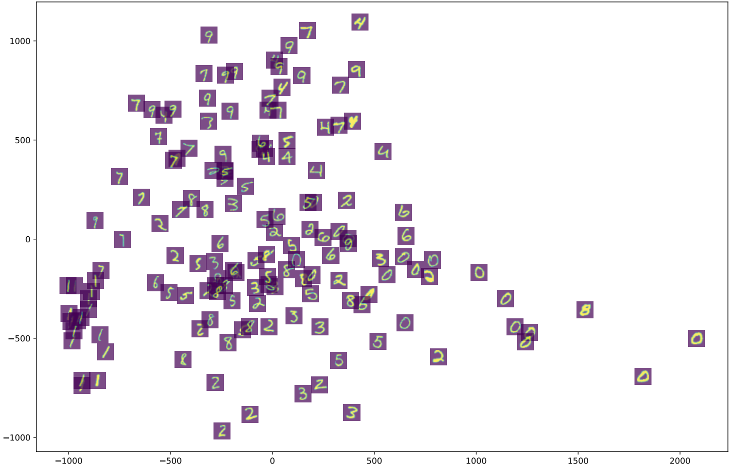
Example



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 $\vec{u}^{(1)}$, $\vec{u}^{(2)}$, ..., $\vec{u}^{(k)}$.

- For any vector $\vec{x} \in \mathbb{R}^d$, its new representation in $\mathbb{R}^k$ is $\vec{z} = (z_1, z_2, \ldots z_k)^T$, 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 9 | Part 3

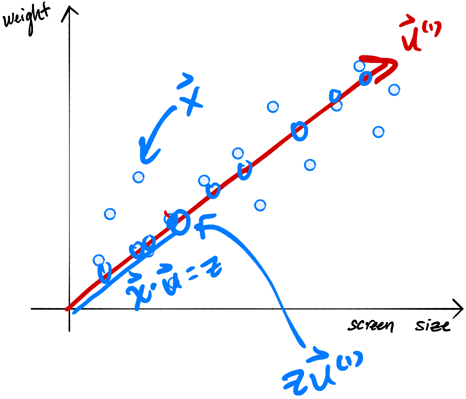
Reconstructions

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

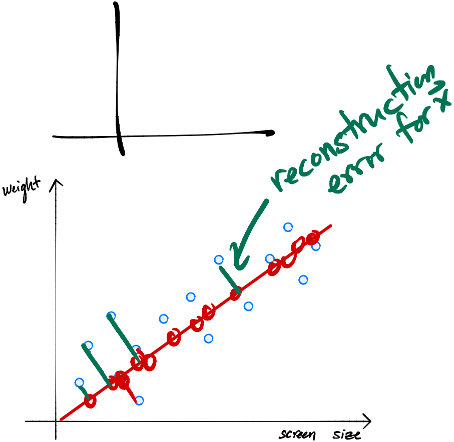
- The reconstruction *approximates* the original point, $\vec{x}$.

- The **reconstruction error** for a single point, $\vec{x}$:

$$\|\vec{x} - U\vec{z}\|^2$$

- Total reconstruction error:

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



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Machine Learning: Representations

Lecture 9 | Part 4

Interpreting PCA

Three Interpretations

- What is PCA doing?

- Three interpretations:
    1. Mazimizing 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.

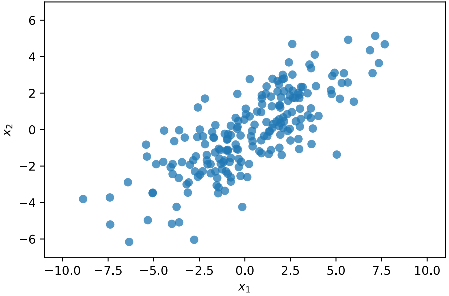
- Claim: Choosing U to be top eigenvectors of C minimizes reconstruction error among all choices of orthonormal U

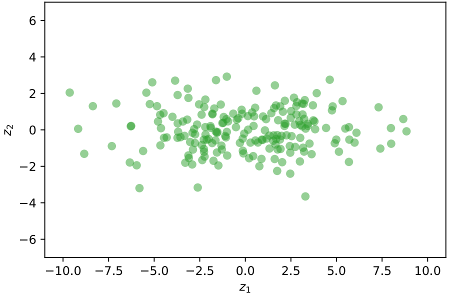
Main Idea

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

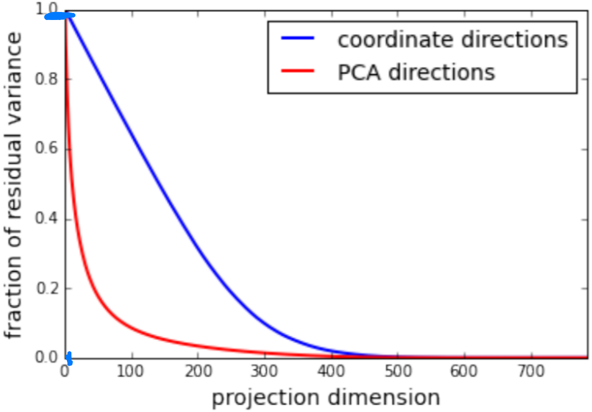
vectors are the principal directions (eigenvectors of the covariance matrix). PCA changes the basis to this natural basis.

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.



coordinate directions
PCA directions
fraction of residual variance
projection dimension
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
600
700

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Machine Learning: Representations

Lecture 9 | Part 5

Demos