Learning Paradigms

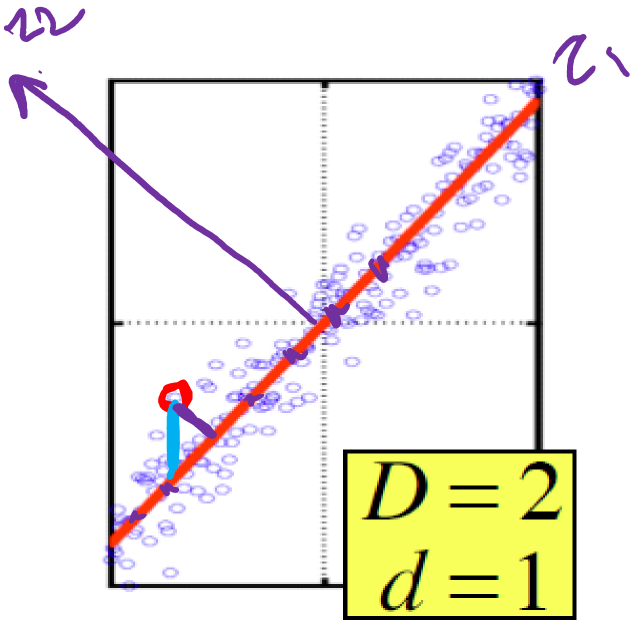
Paradigm	Data
Supervised	$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$ $\quad \mathbf{x} \sim p^*(\cdot)$ and $y = c^*(\cdot)$
$\hookrightarrow$ Regression	$y^{(i)} \in \mathbb{R}$
$\hookrightarrow$ Classification	$y^{(i)} \in \{1, \ldots, K\}$
$\hookrightarrow$ Binary classification	$y^{(i)} \in \{+1, -1\}$
$\hookrightarrow$ Structured Prediction	$\mathbf{y}^{(i)}$ is a vector
Unsupervised	$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ $\quad \mathbf{x} \sim p^*(\cdot)$
$\hookrightarrow$ Clustering	predict $\{z^{(i)}\}_{i=1}^N$ where $z^{(i)} \in \{1, \ldots, K\}$
$\hookrightarrow$ Dimensionality Reduction	convert each $\mathbf{x}^{(i)} \in \mathbb{R}^M$ to $\mathbf{u}^{(i)} \in \mathbb{R}^K$ with $K << M$
Semi-supervised	$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N_1} \cup \{\mathbf{x}^{(j)}\}_{j=1}^{N_2}$
Online	$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), (\mathbf{x}^{(3)}, y^{(3)}), \ldots\}$
Active Learning	$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N$ and can query $y^{(i)} = c^*(\cdot)$ at a cost
Imitation Learning	$\mathcal{D} = \{(s^{(1)}, a^{(1)}), (s^{(2)}, a^{(2)}), \ldots\}$
Reinforcement Learning	$\mathcal{D} = \{(s^{(1)}, a^{(1)}, r^{(1)}), (s^{(2)}, a^{(2)}, r^{(2)}), \ldots\}$

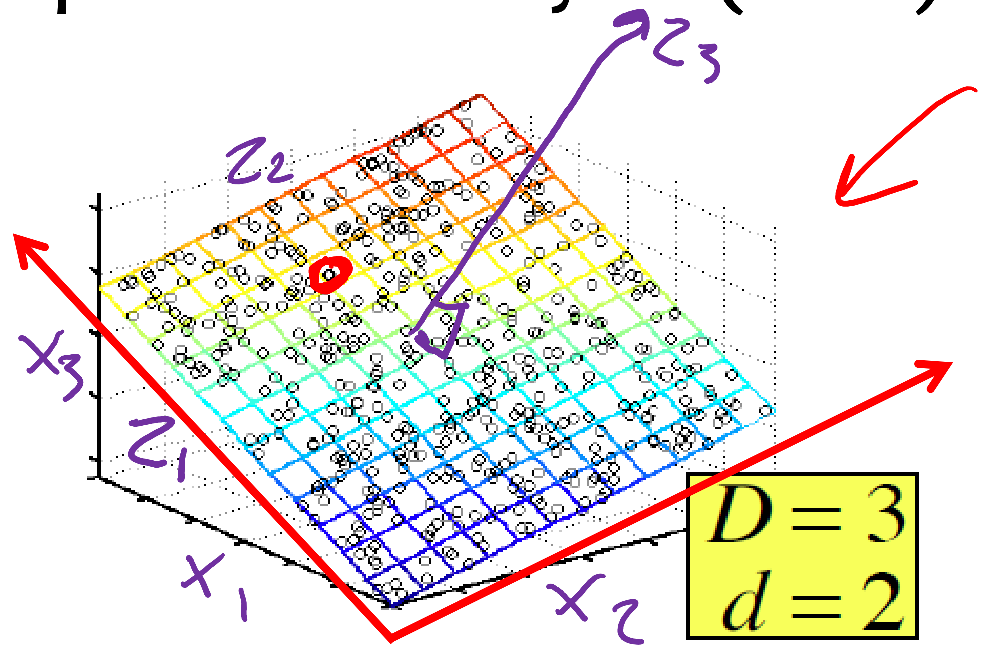
PCA Outline

- **Dimensionality Reduction**
  - High-dimensional data
  - Learning (low dimensional) representations
- **Principal Component Analysis (PCA)**
  - Examples: 2D and 3D
  - Data for PCA
  - PCA Definition
  - Objective functions for PCA
  - PCA, Eigenvectors, and Eigenvalues
  - Algorithms for finding Eigenvectors / Eigenvalues
- **PCA Examples**
  - Image Compression
  - MRI Image Reconstruction

DIMENSIONALITY REDUCTION

Principal Component Analysis (PCA)





In case where data lies on or near a low d-dimensional linear subspace, axes of this subspace are an effective representation of the data.

Identifying the axes is known as Principal Components Analysis, and can be obtained by using classic matrix computation tools (Eigen or Singular Value Decomposition).

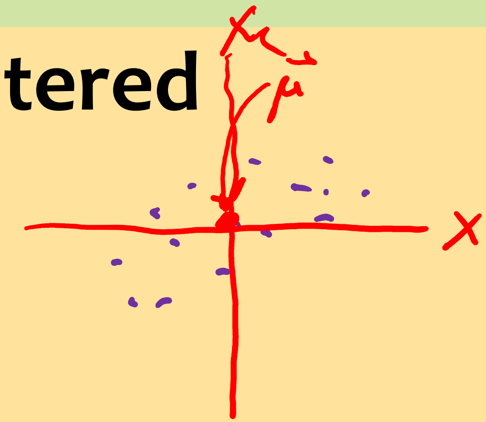
Data for PCA

$$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^{N}$$

$$\mathbf{X} = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ (\mathbf{x}^{(2)})^T \\ \vdots \\ (\mathbf{x}^{(N)})^T \end{bmatrix}$$

We assume the data is **centered**

$$\vec{\mu} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}^{(i)} = \mathbf{0}$$



Q: What if your data is **not** centered?

A: Subtract off the sample mean

Slide from Matt Gormley

Sample Covariance Matrix

The sample covariance matrix is given by:

$$\Sigma_{jk} = \frac{1}{N} \sum_{i=1}^{N} (x_j^{(i)} \cancel{- \mu_j})(x_k^{(i)} \cancel{- \mu_k})$$

Since the data matrix is centered, we rewrite as:

$$\mathbf{\Sigma} = \frac{1}{N} \mathbf{X}^T \mathbf{X}$$

$$\mathbf{X} = \begin{bmatrix} \left(\mathbf{x}^{(1)}\right)^T \\ \left(\mathbf{x}^{(2)}\right)^T \\ \vdots \\ \left(\mathbf{x}^{(N)}\right)^T \end{bmatrix}$$

Projections

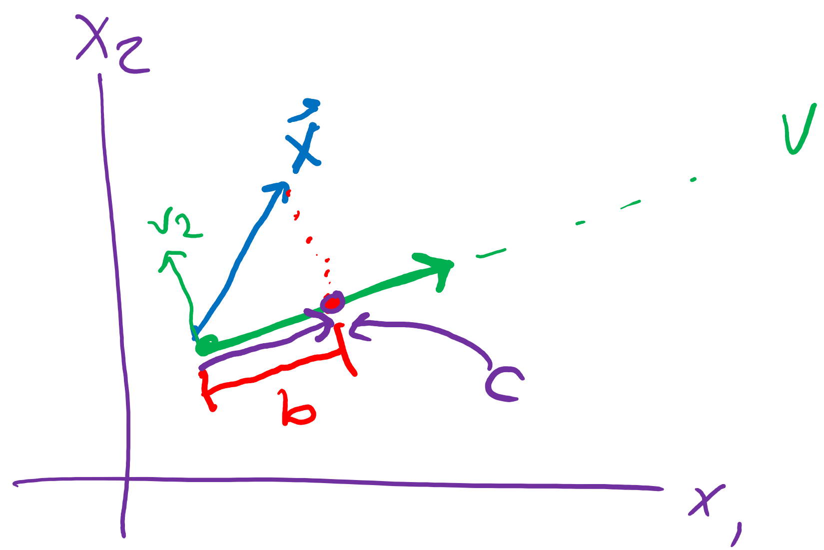
Quiz: What is the projection of point $\boldsymbol{x}$ onto vector $\boldsymbol{v}$, assuming that $\|v\|_2 = 1$?

A. ~~$\boldsymbol{v}\boldsymbol{x}$~~

B. $\boldsymbol{v}^T\boldsymbol{x}$ = b

C. $(\boldsymbol{v}^T\boldsymbol{x})\boldsymbol{v}$ = c

D. $\boldsymbol{v}^T\boldsymbol{x}\,\boldsymbol{x}^T\boldsymbol{v}$



Principal Component Analysis (PCA)

Whiteboard

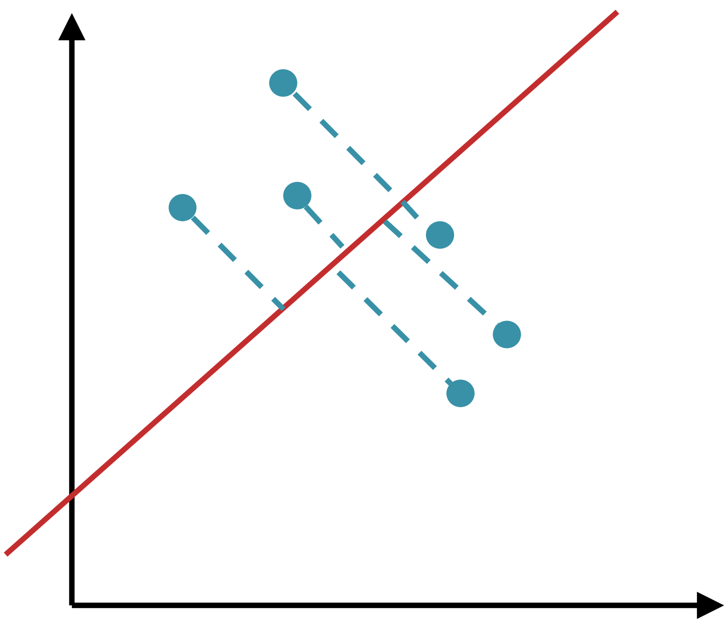
- PCA Sketch
- Objective functions for PCA

Maximizing the Variance

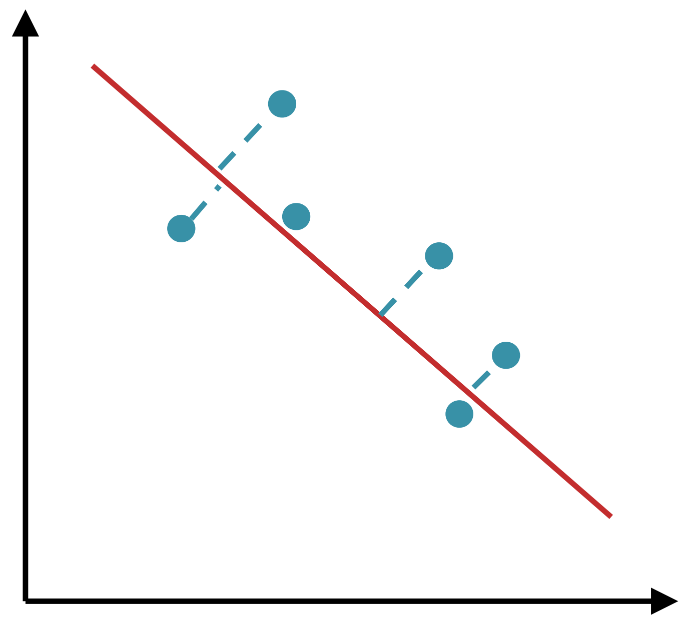
Quiz: Consider the two projections below

2. Which maximizes the variance?
3. Which minimizes the reconstruction error?

Option A



Option B 2) 3)



PCA

Equivalence of Maximizing Variance and Minimizing Reconstruction Error

Claim: Minimizing the reconstruction error is equivalent to maximizing the variance.

Proof: First, note that:

$$||\mathbf{x}^{(i)} - (\mathbf{v}^T\mathbf{x}^{(i)})\mathbf{v}||^2 = ||\mathbf{x}^{(i)}||^2 - (\mathbf{v}^T\mathbf{x}^{(i)})^2 \tag{1}$$

since $\mathbf{v}^T\mathbf{v} = ||\mathbf{v}||^2 = 1$.

Substituting into the minimization problem, and removing the extraneous terms, we obtain the maximization problem.

$$\mathbf{v}^* = \underset{\mathbf{v}:||\mathbf{v}||^2=1}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N} ||\mathbf{x}^{(i)} - (\mathbf{v}^T\mathbf{x}^{(i)})\mathbf{v}||^2 \tag{2}$$

$$= \underset{\mathbf{v}:||\mathbf{v}||^2=1}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N} ||\mathbf{x}^{(i)}||^2 - (\mathbf{v}^T\mathbf{x}^{(i)})^2 \tag{3}$$

$$= \underset{\mathbf{v}:||\mathbf{v}||^2=1}{\operatorname{argmax}} \frac{1}{N}\sum_{i=1}^{N} (\mathbf{v}^T\mathbf{x}^{(i)})^2 \tag{4}$$

(5)

PCA: the First Principal Component

To find the first principal component, we wish to solve the following constrained optimization problem (variance minimization).

$$\mathbf{v}_1 = \operatorname*{argmax}_{\mathbf{v}:||\mathbf{v}||^2=1} \mathbf{v}^T \mathbf{\Sigma} \mathbf{v} \tag{1}$$

So we turn to the method of Lagrange multipliers. The Lagrangian is:

$$\mathcal{L}(\mathbf{v}, \lambda) = \mathbf{v}^T \mathbf{\Sigma} \mathbf{v} - \lambda(\mathbf{v}^T \mathbf{v} - 1) \tag{2}$$

Taking the derivative of the Lagrangian and setting to zero gives:

$$\frac{d}{d\mathbf{v}} \left(\mathbf{v}^T \mathbf{\Sigma} \mathbf{v} - \lambda(\mathbf{v}^T \mathbf{v} - 1) \right) = 0 \tag{3}$$

$$\mathbf{\Sigma} \mathbf{v} - \lambda \mathbf{v} = 0 \tag{4}$$

$$\mathbf{\Sigma} \mathbf{v} = \lambda \mathbf{v} \tag{5}$$

Recall: For a square matrix $\mathbf{A}$, the vector $\mathbf{v}$ is an **eigenvector** iff there exists **eigenvalue** λ such that:

$$\mathbf{A} \mathbf{v} = \lambda \mathbf{v} \tag{6}$$

SVD for PCA

For any arbitrary matrix $\mathbf{A}$, SVD gives a decomposition:

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T \tag{1}$$

where $\mathbf{\Lambda}$ is a diagonal matrix, and $\mathbf{U}$ and $\mathbf{V}$ are orthogonal matrices.

Suppose we obtain an SVD of our data matrix $\mathbf{X}$, so that:

$$\mathbf{X} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T \tag{1}$$

Now consider what happens when we rewrite $\mathbf{\Sigma} = \frac{1}{N}\mathbf{X}^T\mathbf{X}$ terms of this SVD.

$$\begin{aligned}
\mathbf{\Sigma} &= \frac{1}{N}\mathbf{X}^T\mathbf{X} && (2)\\
&= \frac{1}{N}(\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T)^T(\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T) && (3)\\
&= \frac{1}{N}(\mathbf{V}\mathbf{\Lambda}^T\mathbf{U}^T)(\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T) && (4)\\
&= \frac{1}{N}\mathbf{V}\mathbf{\Lambda}^T\mathbf{\Lambda}\mathbf{V}^T && (5)\\
&= \frac{1}{N}\mathbf{V}(\mathbf{\Lambda})^2\mathbf{V}^T && (6)
\end{aligned}$$

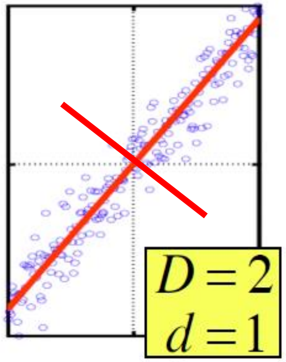
Above we used the fact that $\mathbf{U}^T\mathbf{U} = \mathbf{I}$ since $\mathbf{U}$ is orthogonal by definition.

We find that $(\mathbf{\Lambda})^2$ is a diagonal matrix whose entries are $\Lambda_{ii} = \lambda_i^2$ the squares of the eigenvalues of the SVD of $\mathbf{X}$. Further, both $\mathbf{X}$ and $\mathbf{X}^T\mathbf{X}$ share the same eigenvectors in their SVD.

Thus, we can run SVD on $\mathbf{X}$ without ever instantiating the large $\mathbf{X}^T\mathbf{X}$ to obtain the necessary principal components more efficiently.

Principal Component Analysis (PCA)

Principal Component Analysis (PCA)



$(\mathrm{X}^{\mathrm{T}}\mathrm{X})\mathrm{v} = \lambda \mathrm{v}$, so v (the first PC) is the eigenvector of sample correlation/covariance matrix $X^T X$

Sample variance of projection $\mathrm{v}^T X^T X\, \mathrm{v} = \lambda \mathrm{v}^T \mathrm{v} = \lambda$

Thus, the eigenvalue λ denotes the amount of variability captured along that dimension (aka amount of energy along that dimension).

Eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots$

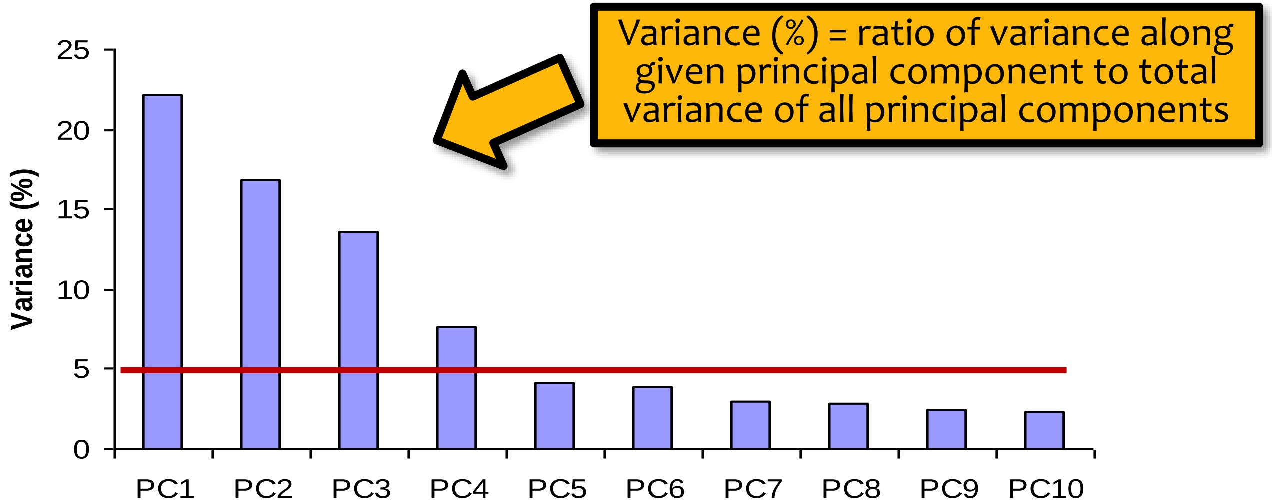
- The 1st PC v_1 is the the eigenvector of the sample covariance matrix $X^T X$ associated with the largest eigenvalue
- The 2nd PC v_2 is the the eigenvector of the sample covariance matrix $X^T X$ associated with the second largest eigenvalue
- And so on …

Slide from Nina Balcan

How Many PCs?

- For M original dimensions, sample covariance matrix is MxM, and has up to M eigenvectors. So M PCs.
- Where does dimensionality reduction come from?

  Can *ignore the components of lesser significance*.

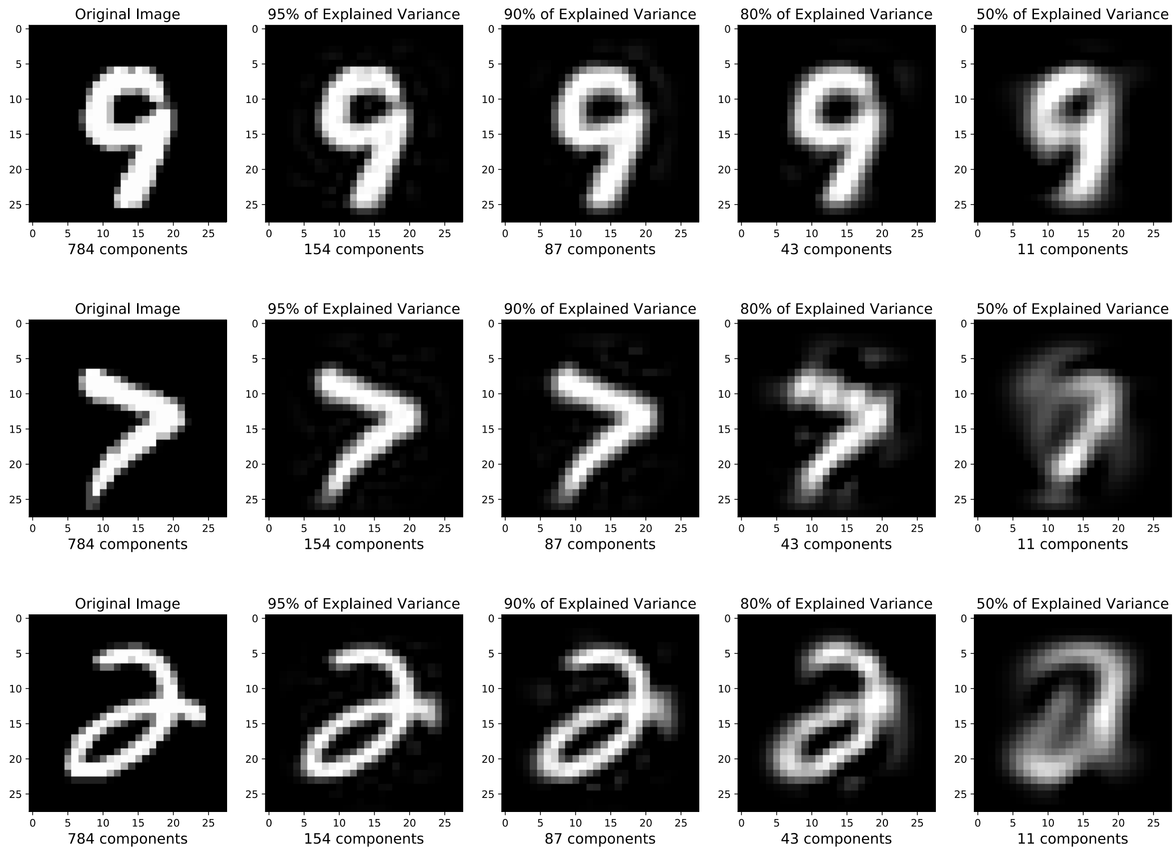


- You do lose some information, but if the eigenvalues are small, you don't lose much
  - M dimensions in original data
  - calculate M eigenvectors and eigenvalues
  - choose only the first D eigenvectors, based on their eigenvalues
  - final data set has only D dimensions

PCA EXAMPLES

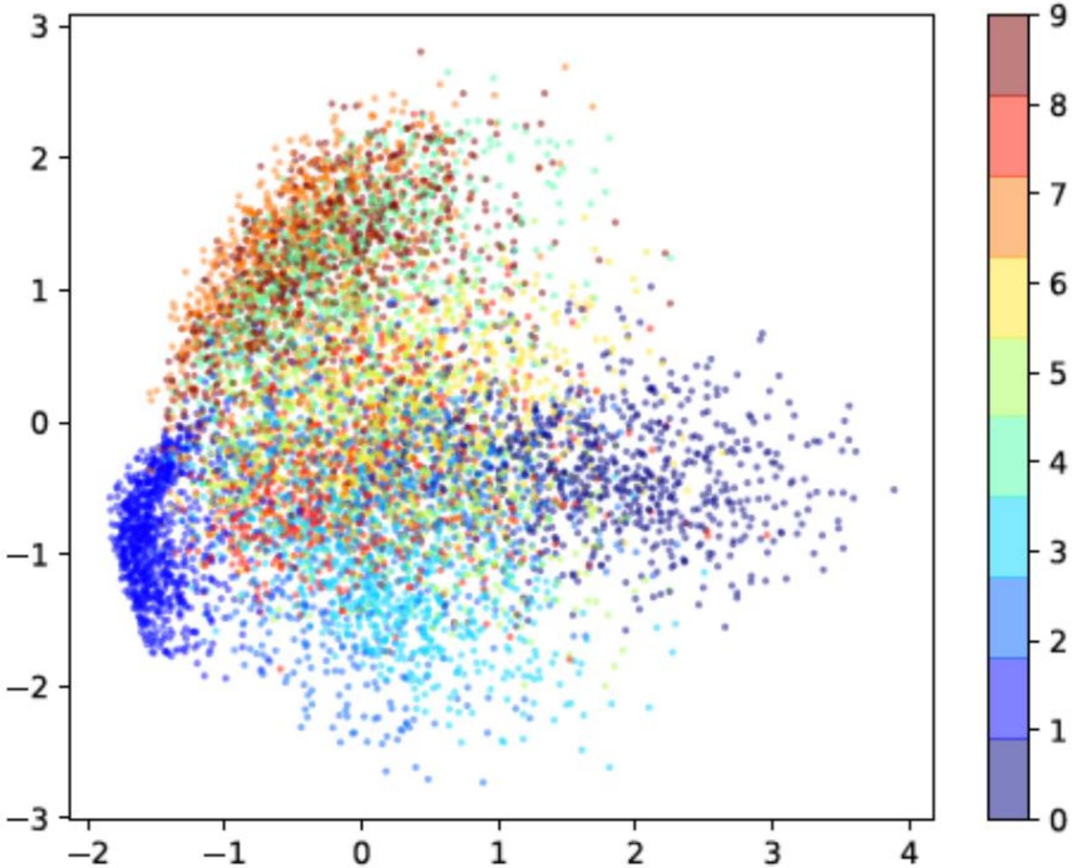
Projecting MNIST digits

Task Setting:
1. Take 28x28 images of digits and project them down to K components
2. Report percent of variance explained for K components
3. Then project back up to 28x28 image to visualize how much information was preserved



Projecting MNIST digits

Task Setting:
1. Take 28x28 images of digits and project them down to 2 components
2. Plot the 2 dimensional points



Projecting MNIST digits

Task Setting:

1. Take 28x28 images of digits and project them down to 2 components
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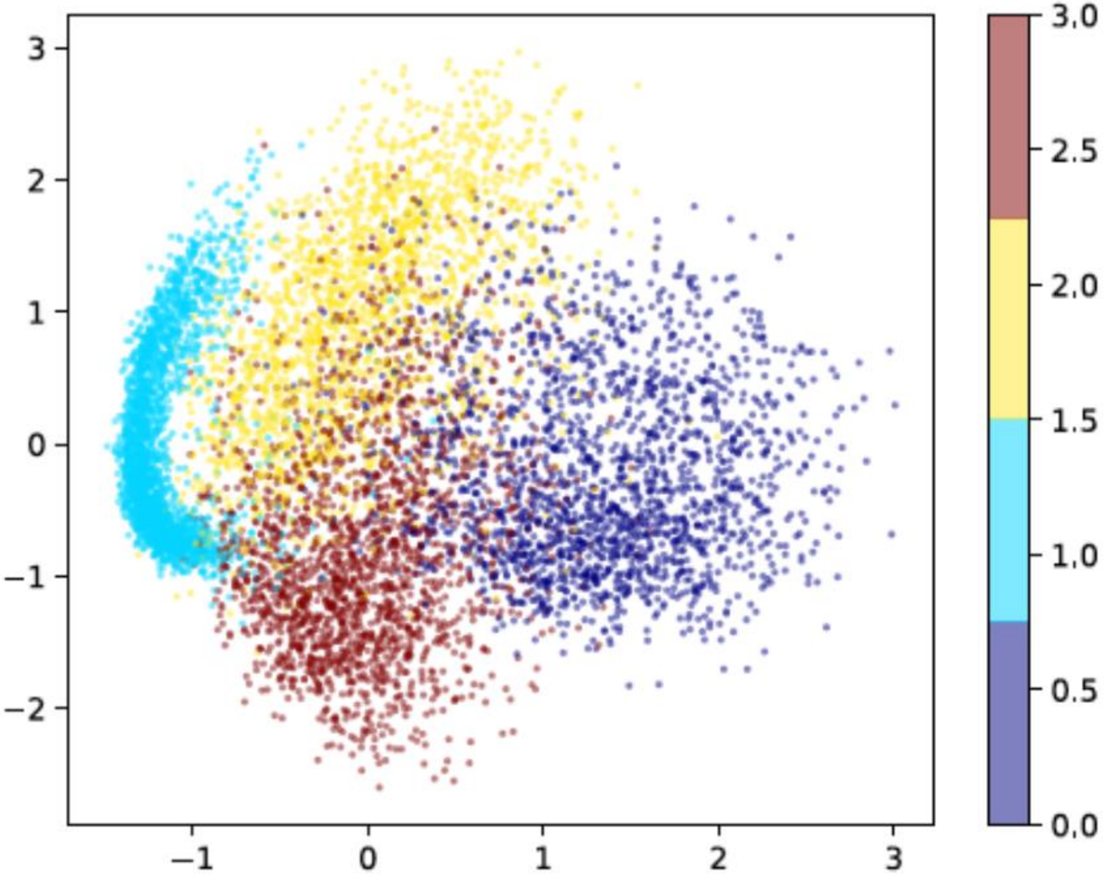

Learning Objectives

Dimensionality Reduction / PCA

You should be able to…

1. Define the sample mean, sample variance, and sample covariance of a vector-valued dataset
2. Identify examples of high dimensional data and common use cases for dimensionality reduction
3. Draw the principal components of a given toy dataset
4. Establish the equivalence of minimization of reconstruction error with maximization of variance
5. Given a set of principal components, project from high to low dimensional space and do the reverse to produce a reconstruction
6. Explain the connection between PCA, eigenvectors, eigenvalues, and covariance matrix
7. Use common methods in linear algebra to obtain the principal components