



10-301/10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Principal Component Analysis (PCA)

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Lecture 24
Apr. 12, 2023

Reminders

- **Homework 8: Reinforcement Learning**
 - **Out: Mon, Apr. 10**
 - **Due: Fri, Apr. 21 at 11:59pm**

Playing Atari games with Deep RL



Source: https://www.youtube.com/watch?v=V1eYniJoRnk&t=2s&ab_channel=TwoMinutePapers

DIMENSIONALITY REDUCTION

High Dimension Data

Examples of high dimensional data:

- High resolution images (millions of pixels)



High Dimension Data

Examples of high dimensional data:

- Multilingual News Stories
(vocabulary of hundreds of thousands of words)



High Dimension Data

Examples of high dimensional data:

- Brain Imaging Data (100s of MBs per scan)

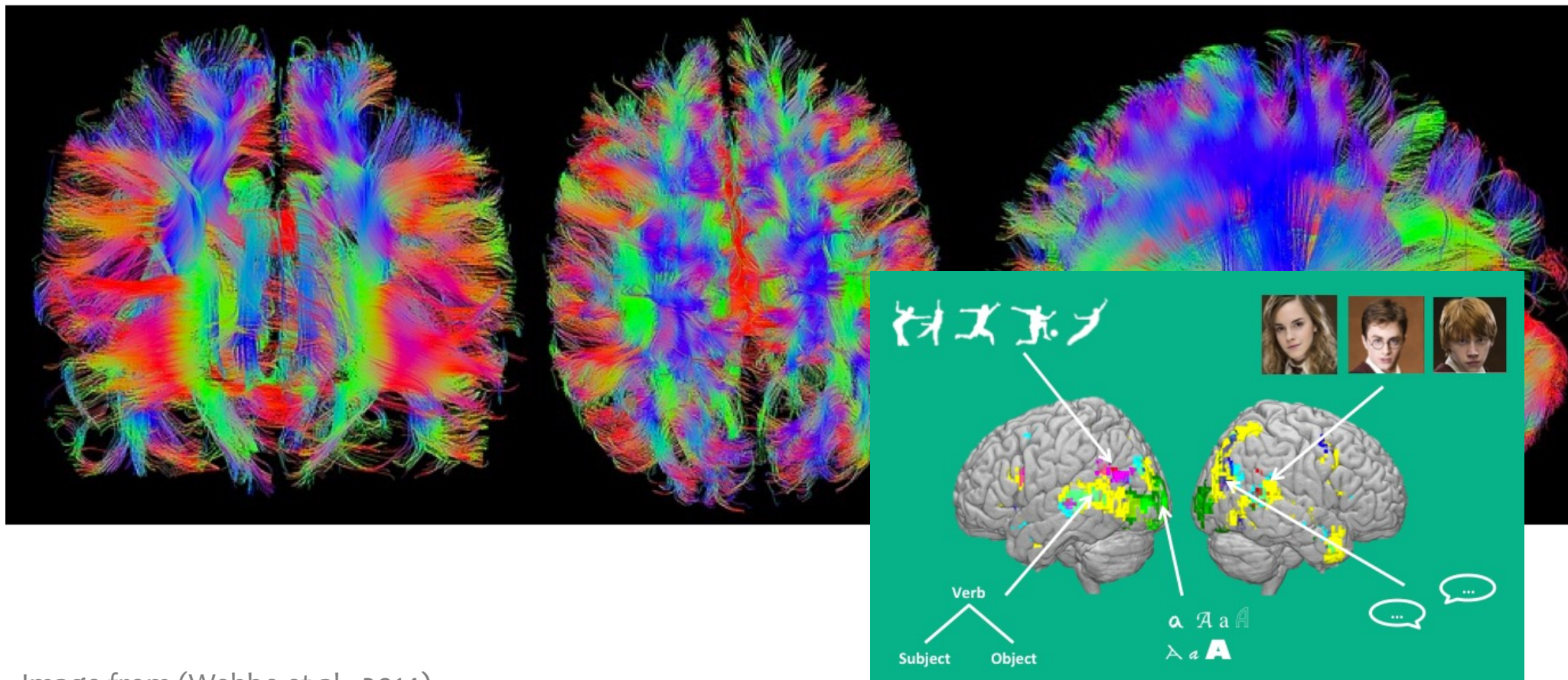


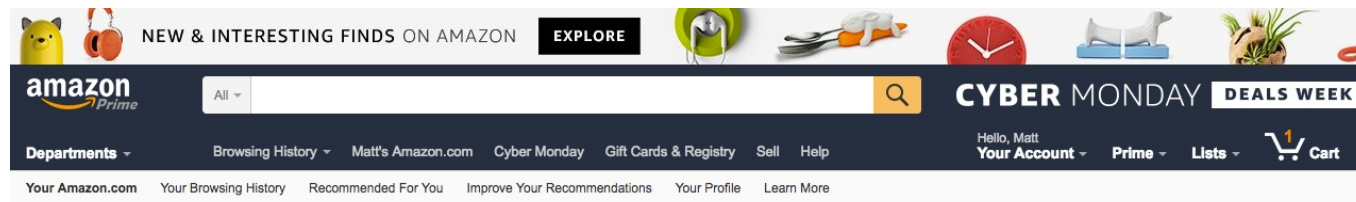
Image from (Wehbe et al., 2014)

Image from <https://pixabay.com/en/brain-mrt-magnetic-resonance-imaging-1728449/>

High Dimension Data

Examples of high dimensional data:

– Customer Purchase Data



You could be seeing useful stuff here!
Sign in to get your order status, balances and rewards.

Sign In

Recommended for you, Matt



Grocery

14 ITEMS



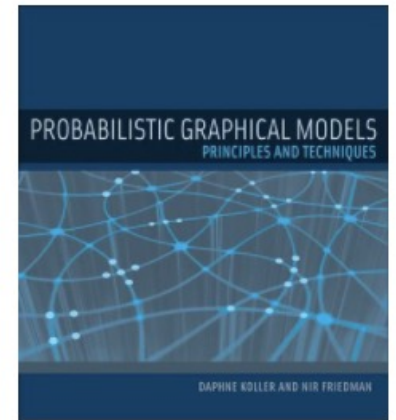
Pets

6 ITEMS



Baby Products

5 ITEMS



Engineering Books

86 ITEMS

Learning Representations

Dimensionality Reduction Algorithms:

Powerful (often unsupervised) learning techniques for extracting hidden (potentially lower dimensional) structure from high dimensional datasets.

Examples:

PCA, Kernel PCA, ICA, CCA, t-SNE, Autoencoders, Matrix Factorization

Useful for:

- Visualization
- More efficient use of resources (e.g., time, memory, communication)
- Statistical: fewer dimensions → better generalization
- Noise removal (improving data quality)

Shortcut Example

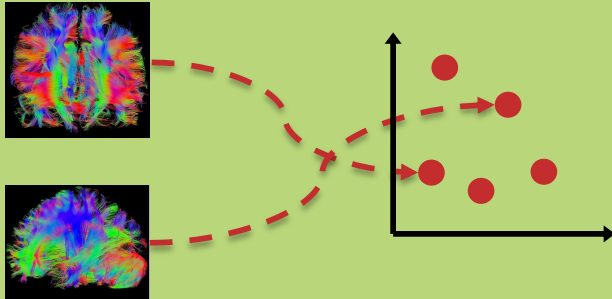


Shortcut Example



This section in one slide...

1. Dimensionality reduction:



2. Random Projection:

① Randomly sample matrix $V \in \mathbb{R}^{K \times M}$
② Project down: $\vec{U}^{(i)} = V \vec{X}^{(i)}$

3. Definition of PCA:

Choose the matrix V that either...

1. minimizes reconstruction error
2. consists of the K eigenvectors with largest eigenvalue

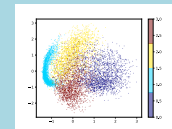
The above are equivalent definitions.

4. Algorithm for PCA:

The option we'll focus on:

Run Singular Value Decomposition (SVD) to obtain all the eigenvectors. Keep just the top- K to form V . Play some tricks to keep things efficient.

5. An Example



DIMENSIONALITY REDUCTION BY RANDOM PROJECTION

Random Projection

Example: 2D to 1D

Goal: project from M -dimensions down to K -dimensions

Data:

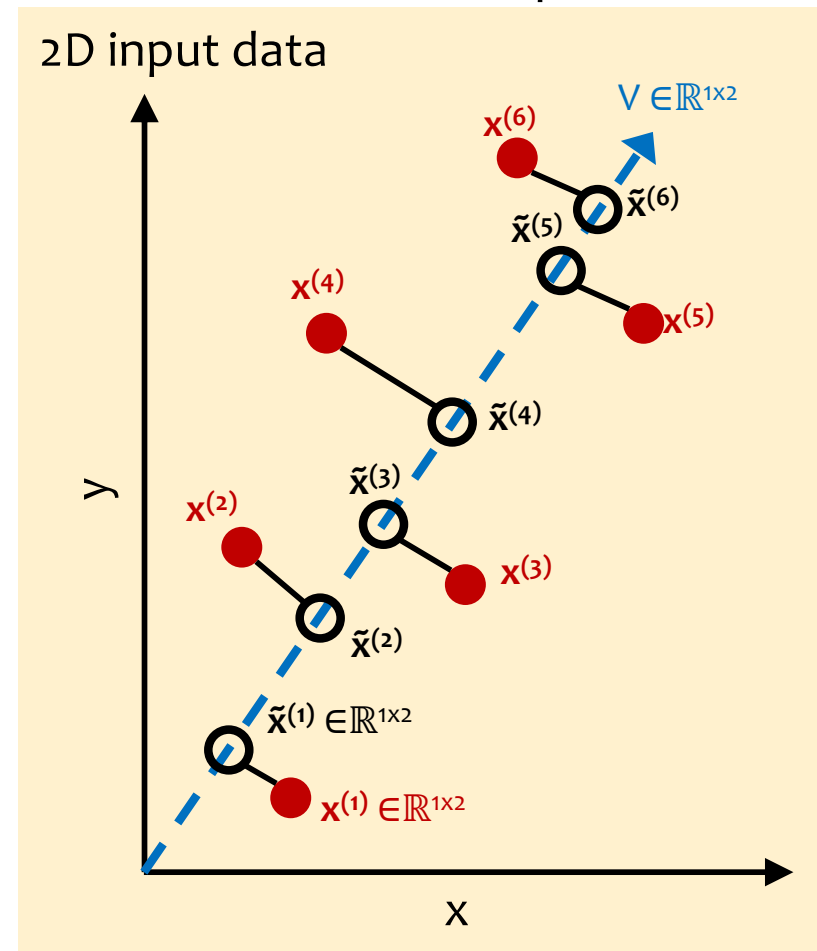
$$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N \text{ where } \mathbf{x}^{(i)} \in \mathbb{R}^M$$

Algorithm:

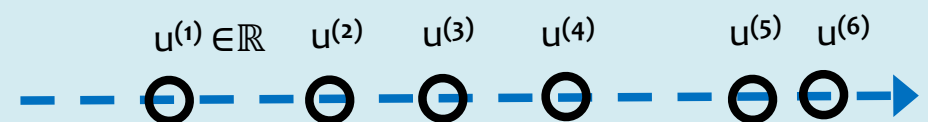
1. Randomly sample matrix: $\mathbf{V} \in \mathbb{R}^{K \times M}$
 $V_{km} \sim \text{Gaussian}(0, 1)$

2. Project down: $\underbrace{\mathbf{u}^{(i)}}_{K \times 1} = \underbrace{\mathbf{V}}_{K \times M} \underbrace{\mathbf{x}^{(i)}}_{M \times 1}$

3. Project up: $\underbrace{\tilde{\mathbf{x}}^{(i)}}_{M \times 1} = \underbrace{\mathbf{V}^T}_{M \times K} \underbrace{\mathbf{u}^{(i)}}_{K \times 1} = \mathbf{V}^T (\mathbf{V} \mathbf{x}^{(i)})$



1D projection onto the real line



Random Projection

Goal: project from M -dimensions down to K -dimensions

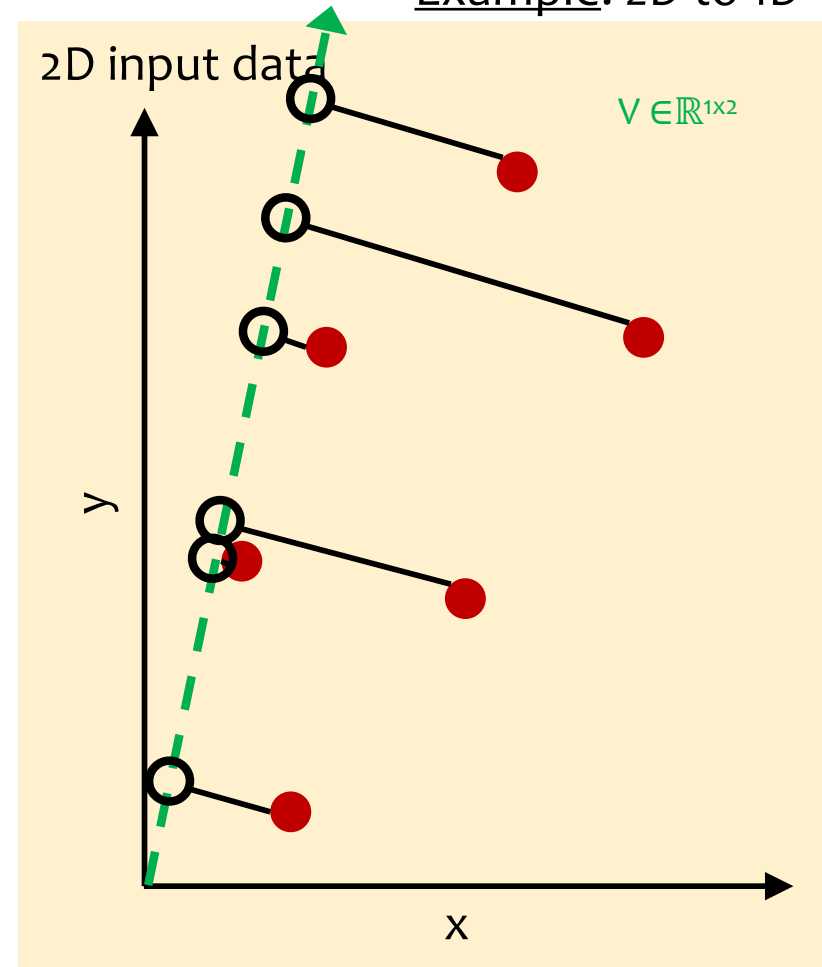
Data:

$$\mathcal{D} = \{\mathbf{x}^{(i)}\}_{i=1}^N \text{ where } \mathbf{x}^{(i)} \in \mathbb{R}^M$$

Algorithm:

1. Randomly sample matrix: $\mathbf{V} \in \mathbb{R}^{K \times M}$
 $V_{km} \sim \text{Gaussian}(0, 1)$
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Example: 2D to 1D



Problem: a random projection might give us a poor low dimensional representation of the data

Johnson-Lindenstrauss Lemma

Q: But how could we ever hope to preserve any useful information by randomly projecting into a low-dimensional space?

A: Even random projection enjoys some surprisingly impressive properties. In fact, a standard of the J-L lemma starts by assuming we have a random linear projection obtained by sampling each matrix entry from a $\text{Gaussian}(0,1)$.



An Elementary Proof of a Theorem of Johnson and Lindenstrauss

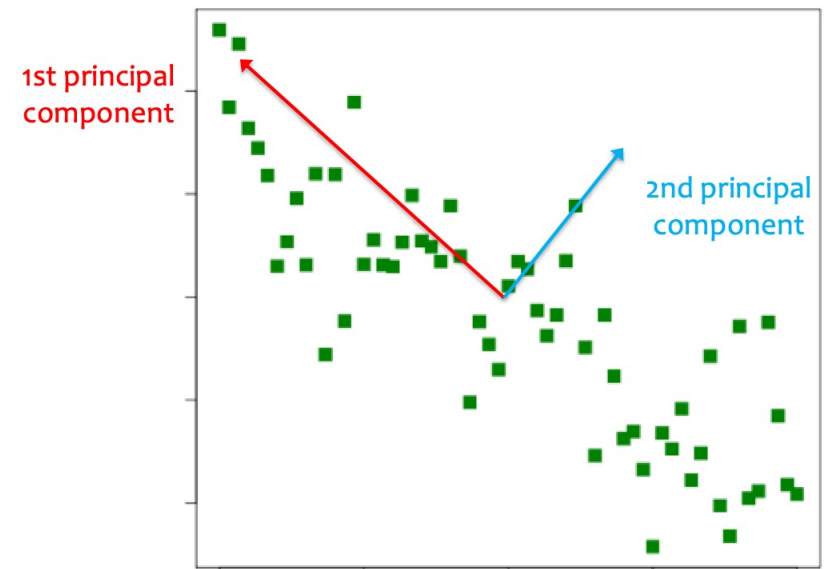
Sanjoy Dasgupta,¹ Anupam Gupta²

ABSTRACT: A result of Johnson and Lindenstrauss [13] shows that a set of n points in high dimensional Euclidean space can be mapped into an $O(\log n/\epsilon^2)$ -dimensional Euclidean space such that the distance between any two points changes by only a factor of $(1 \pm \epsilon)$. In this note, we prove this theorem using elementary probabilistic techniques. © 2003 Wiley Periodicals, Inc. Random Struct. Alg., 22: 60–65, 2002

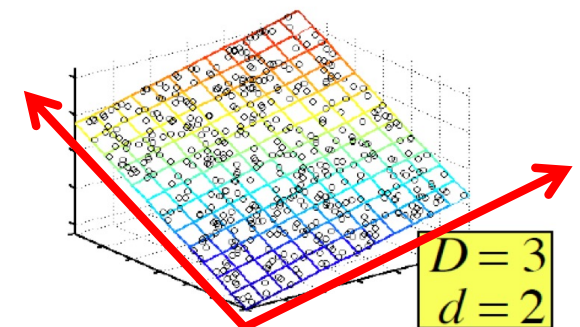
DEFINITION OF PRINCIPAL COMPONENT ANALYSIS (PCA)

Principal Component Analysis (PCA)

- **Assumption:** the data lies on a low K -dimensional linear subspace
- **Goal:** identify the axes of that subspace, and project each point onto hyperplane
- **Algorithm:** find the K eigenvectors with largest eigenvalue using classic matrix decomposition tools



PCA Example: 2D Gaussian Data



Data for PCA

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

$$\mathbf{x}^{(i)} \in \mathbb{R}^M$$

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

We assume the data is **centered**,
i.e. the **sample mean** is zero

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

Q: What if
your data is
not centered?

A: Subtract off the sample mean

$$\tilde{\mathbf{x}}^{(i)} = \mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}, \forall i$$

Background: Sample Variance

Suppose we have a sequence of random samples $\{x^{(1)}, \dots, x^{(N)}\}$ from a random variable X .

The (biased) **sample variance** $\hat{\sigma}^2$ is given by:

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{i=1}^N (x^{(i)} - \hat{\mu})^2$$

where $\hat{\mu}$ is the sample mean.

Sample Covariance Matrix

The **sample covariance matrix** $\Sigma \in \mathbb{R}^{M \times M}$ is given by:

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

Since the data matrix is centered, we rewrite as:

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

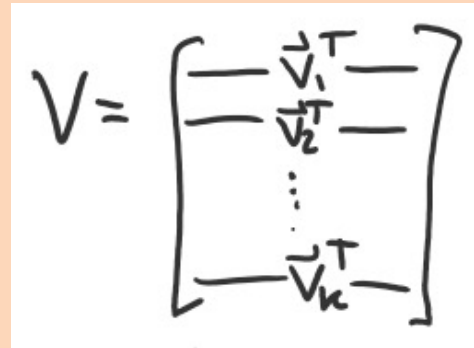
$$\mathbf{X} = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ (\mathbf{x}^{(2)})^T \\ \vdots \\ (\mathbf{x}^{(N)})^T \end{bmatrix}$$

Principal Component Analysis (PCA)

Linear Projection:

Given $K \times M$ matrix $\mathbf{V}$, and $M \times 1$ vector $\mathbf{x}^{(i)}$ we obtain the $K \times 1$ projection $\mathbf{u}^{(i)}$ by:

$$\mathbf{u}^{(i)} = \mathbf{V} \mathbf{x}^{(i)}$$



A handwritten diagram of a matrix V enclosed in large square brackets. Inside the brackets, there are four rows. The first row contains a horizontal line followed by $\vec{v}_1^T$ followed by another horizontal line. The second row contains a horizontal line followed by $\vec{v}_2^T$ followed by another horizontal line. The third row contains a vertical ellipsis. The fourth row contains a horizontal line followed by $\vec{v}_k^T$ followed by another horizontal line.

Definition of PCA:

PCA repeatedly chooses a next vector $\mathbf{v}_j$ that **minimizes the reconstruction error** s.t. $\mathbf{v}_j$ is orthogonal to $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{j-1}$.

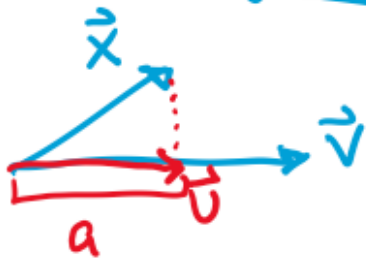
Vector $\mathbf{v}_j$ is called the **jth principal component**.

Notice: Two vectors $\mathbf{a}$ and $\mathbf{b}$ are **orthogonal** if $\mathbf{a}^T \mathbf{b} = 0$.

→ the K -dimensions in PCA are uncorrelated

Vector Projection

Recall: Projection



length of projection of $\vec{x}$ onto $\vec{v}$

$$a = \frac{\vec{v}^T \vec{x}}{\|\vec{v}\|_2} \quad \begin{array}{l} \text{if } \|\vec{v}\|_2 = 1 \\ \text{otherwise} \end{array}$$

projection of $\vec{x}$ onto $\vec{v}$

$$\vec{u} = a \vec{v} = \frac{(\vec{v}^T \vec{x})}{\|\vec{v}\|_2^2} \vec{v} \quad \begin{array}{l} \text{if } \|\vec{v}\|_2 = 1 \\ \text{otherwise} \end{array}$$

Principal Component Analysis (PCA)

Whiteboard

- Objective functions for PCA

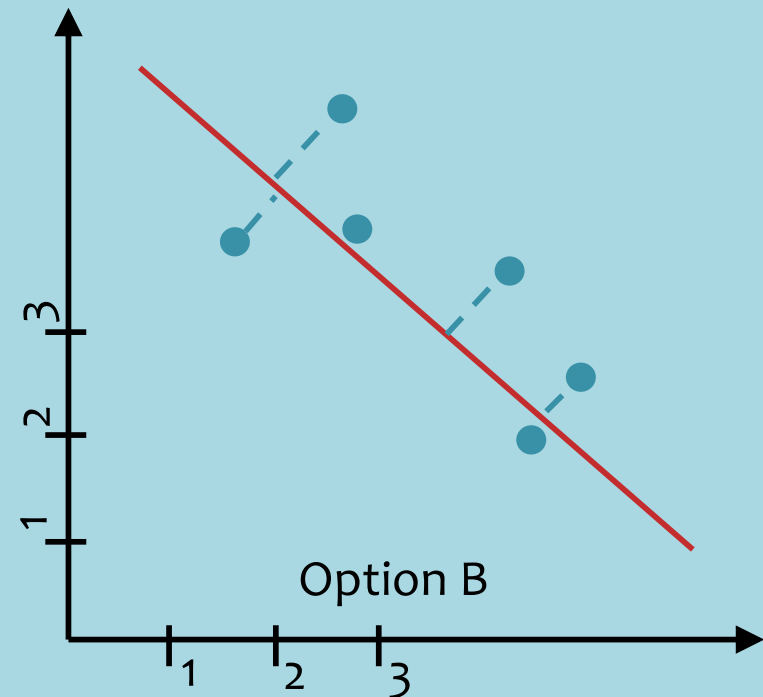
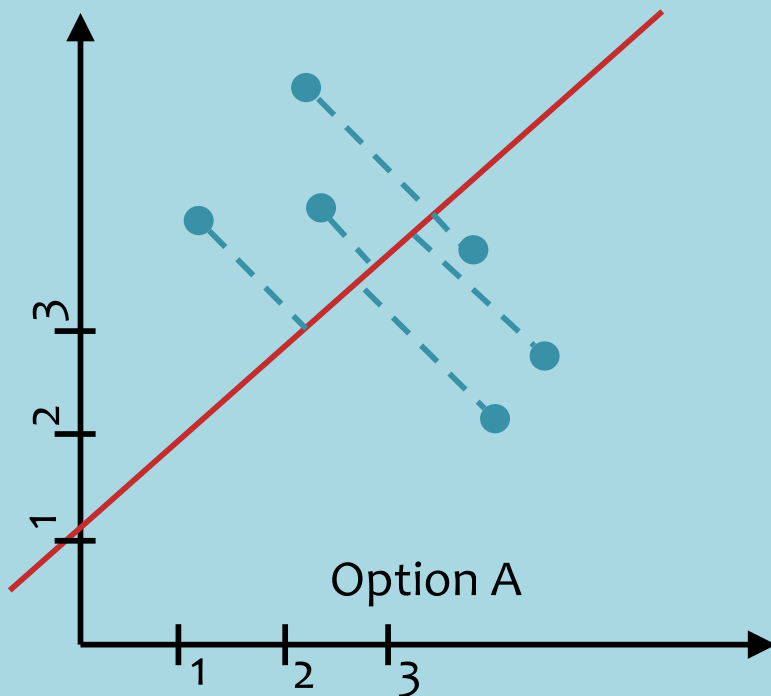
Projection Example

Question:

Below are two plots of the same dataset D. Consider the two projections shown.

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

Answer:



PCA Objective Functions

What is the first principal component $\mathbf{v}_1$ chosen by PCA?

Option 1: The vector that *minimizes* the **reconstruction error**

$$\mathbf{v}_1 = \underset{\mathbf{v}: \|\mathbf{v}\|^2=1}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}^{(i)} - (\mathbf{v}^T \mathbf{x}^{(i)}) \mathbf{v}\|^2$$

Option 2: The vector that *maximizes* the **variance**

$$\mathbf{v}_1 = \underset{\mathbf{v}: \|\mathbf{v}\|^2=1}{\operatorname{argmax}} \frac{1}{N} \sum_{i=1}^N (\mathbf{v}^T \mathbf{x}^{(i)})^2$$

Equivalence of Maximizing Variance and Minimizing Reconstruction Error

PCA

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

Proof: First, note that:

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

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.

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

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

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

PCA Objective Functions

What is the first principal component $\mathbf{v}_1$ chosen by PCA?

Option 1: The vector that *minimizes* the **reconstruction error**

$$\mathbf{v}_1 = \operatorname{argmin}_{\mathbf{v}: \|\mathbf{v}\|^2=1} \frac{1}{N} \sum_{i=1}^N \|\mathbf{x}^{(i)} - (\mathbf{v}^T \mathbf{x}^{(i)}) \mathbf{v}\|^2$$

Question: Why can't we just use gradient descent to find the principal components?

Option 2: The vector that *maximizes* the **variance**

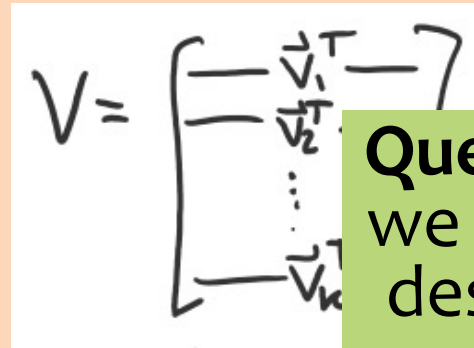
$$\mathbf{v}_1 = \operatorname{argmax}_{\mathbf{v}: \|\mathbf{v}\|^2=1} \frac{1}{N} \sum_{i=1}^N (\mathbf{v}^T \mathbf{x}^{(i)})^2$$

Principal Component Analysis (PCA)

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$$\mathbf{u}^{(i)} = \mathbf{V} \mathbf{x}^{(i)}$$



A handwritten diagram showing a matrix V enclosed in large square brackets. Inside the brackets, there are several rows, each starting with a horizontal line followed by a vertical vector arrow pointing upwards, labeled $\vec{v}_1^T$, $\vec{v}_2^T$, and $\vec{v}_k^T$. Ellipses between $\vec{v}_2^T$ and $\vec{v}_k^T$ indicate intermediate rows.

Question: Why can't we just use gradient descent to find the principal components?

Definition of PCA:

PCA repeatedly chooses a next vector $\mathbf{v}_j$ that **minimizes the reconstruction error** s.t. $\mathbf{v}_j$ is orthogonal to $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{j-1}$.

Vector $\mathbf{v}_j$ is called the **jth principal component**.

Notice: Two vectors $\mathbf{a}$ and $\mathbf{b}$ are **orthogonal** if $\mathbf{a}^T \mathbf{b} = 0$.

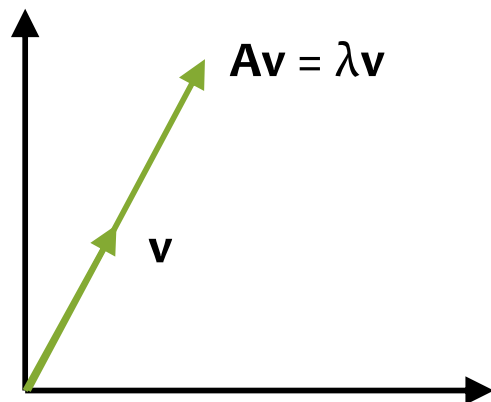
→ the K -dimensions in PCA are uncorrelated

Background:

Eigenvectors & Eigenvalues

For a square matrix **A** ($n \times n$ matrix), the vector **v** ($n \times 1$ matrix) is an **eigenvector** iff there exists **eigenvalue** λ (scalar) such that:

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



The linear transformation **A** is only stretching vector **v**.

That is, $\lambda\mathbf{v}$ is a *scalar multiple* of **v**.

Background:

Eigenvectors & Eigenvalues

Fact #1: The eigenvectors of a **symmetric matrix** are **orthogonal** to each other.

Fact #2: The **covariance matrix Σ** is **symmetric**.

The First Principal Component

PCA

Claim: The vector that maximizes the variances is the eigenvector of Σ with largest eigenvalue.

Proof Sketch: To find the first principal component, we wish to solve the following constrained optimization problem (variance maximization).

$$\mathbf{v}_1 = \operatorname{argmax}_{\mathbf{v}: \|\mathbf{v}\|^2=1} \mathbf{v}^T \Sigma \mathbf{v} \quad (1)$$

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

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

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

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

$$\Sigma \mathbf{v} - \lambda \mathbf{v} = 0 \quad (4)$$

$$\Sigma \mathbf{v} = \lambda \mathbf{v} \quad (5)$$

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

$$\mathbf{A} \mathbf{v} = \lambda \mathbf{v} \quad (6)$$

Rewriting the objective of the maximization shows that not only will the optimal vector $\mathbf{v}_1$ be an eigenvector, it will be one with maximal eigenvalue.

$$\mathbf{v}^T \Sigma \mathbf{v} = \mathbf{v}^T \lambda \mathbf{v} \quad (7)$$

$$= \lambda \mathbf{v}^T \mathbf{v} \quad (8)$$

$$= \lambda \|\mathbf{v}\|^2 \quad (9)$$

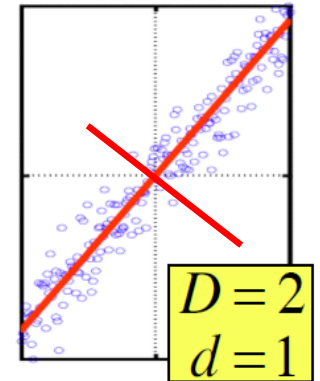
$$= \lambda \quad (10)$$

Principal Component Analysis (PCA)

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

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

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



Eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \dots$

- The 1st PC $\mathbf{v}_1$ is the the eigenvector of the sample covariance matrix $X X^T$ associated with the largest eigenvalue
- The 2nd PC $\mathbf{v}_2$ is the the eigenvector of the sample covariance matrix $X X^T$ associated with the second largest eigenvalue
- And so on ...

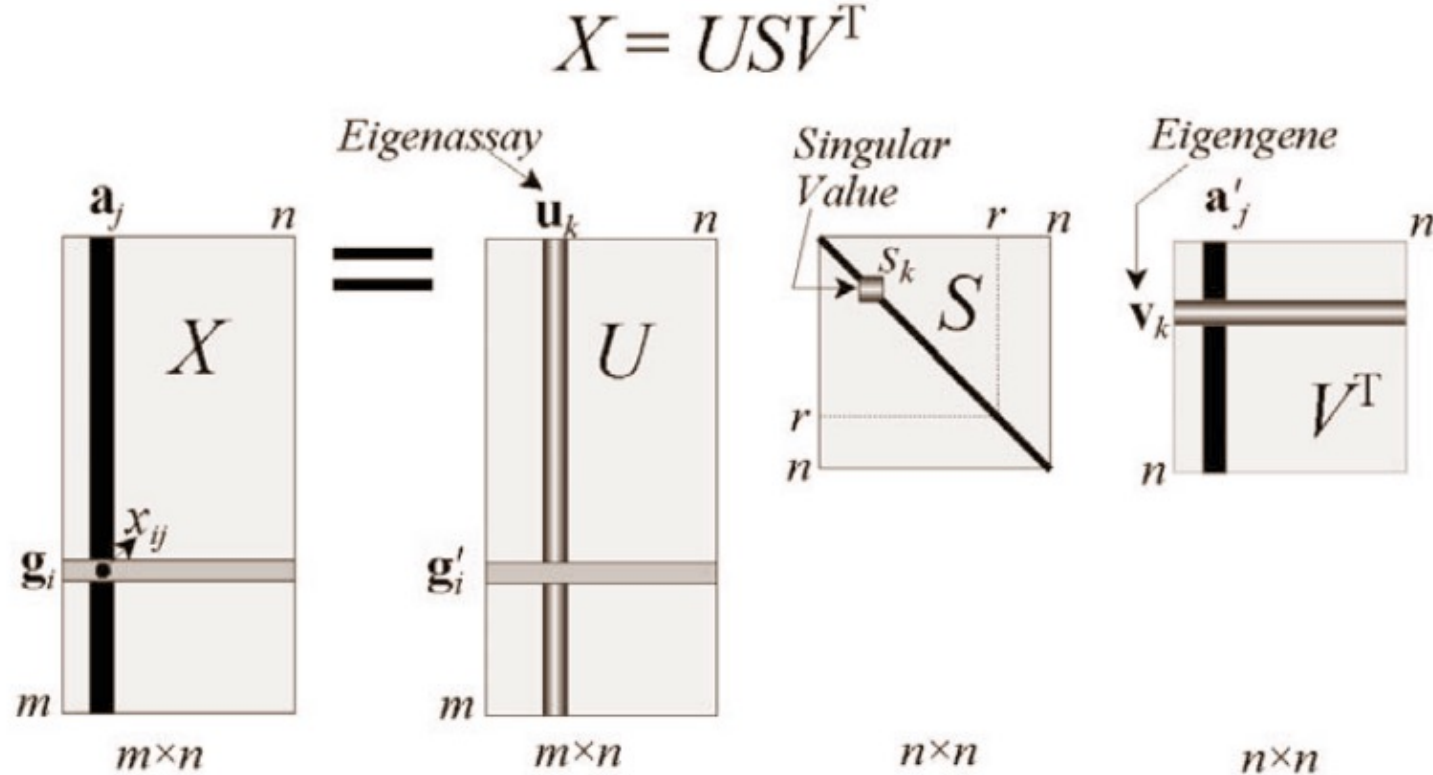
ALGORITHMS FOR PCA

Algorithms for PCA

How do we find principal components (i.e. eigenvectors)?

- Power iteration (aka. Von Mises iteration)
 - finds **each** principal component **one at a time** in order
- Singular Value Decomposition (SVD)
 - finds **all** the principal components **at once**
 - two options:
 - Option A: run SVD on $X^T X$
 - Option B: run SVD on X
(not obvious why Option B should work...)
- Stochastic Methods (approximate)
 - **very efficient** for high dimensional datasets with lots of points

SVD



Data X , one row per data point

US gives coordinates of rows of X in the space of principle components

S is diagonal, $S_k > S_{k+1}$, S_k^2 is k th largest eigenvalue

Rows of V^T are unit length eigenvectors of $X^T X$

If cols of X have zero mean, then $X^T X = c \Sigma$ and eigenvects are the Principle Components

Singular Value Decomposition

To generate principle components:

- Subtract mean $\bar{x} = \frac{1}{N} \sum_{n=1}^N x^n$ from each data point, to create zero-centered data
- Create matrix X with one row vector per (zero centered) data point
- Solve SVD: $X = USV^T$
- Output Principle components: columns of V (= rows of V^T)
 - Eigenvectors in V are sorted from largest to smallest eigenvalues
 - S is diagonal, with s_k^2 giving eigenvalue for k th eigenvector

Singular Value Decomposition

To project a point (column vector x) into PC coordinates:

$$V^T x$$

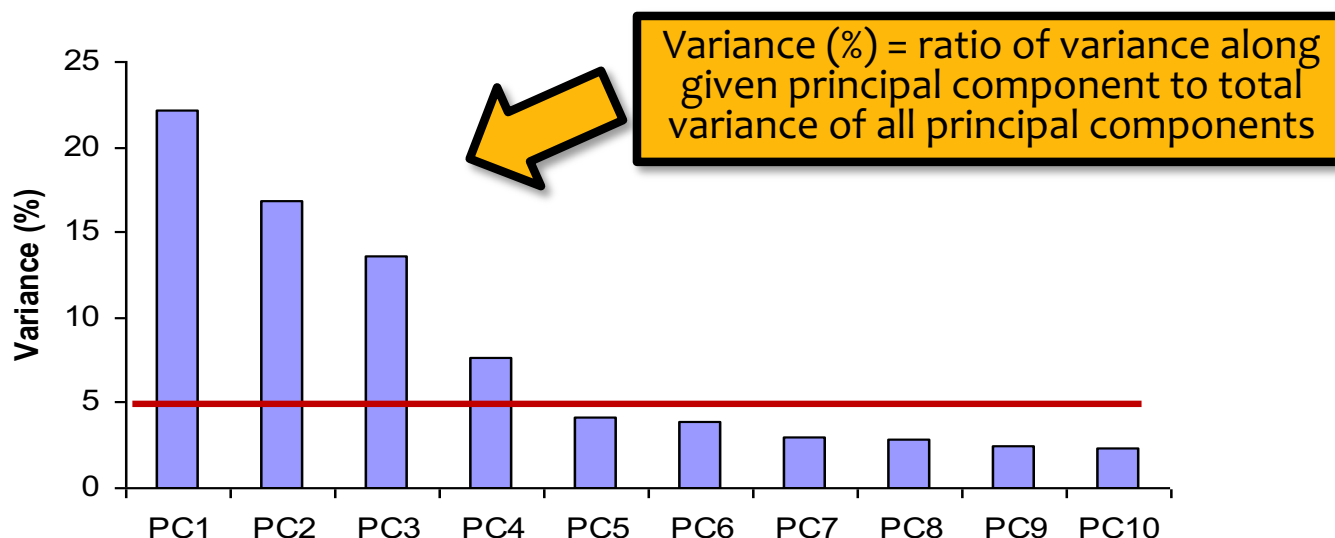
If x_i is i^{th} row of data matrix X , then

- $(i^{\text{th}} \text{ row of } US) = V^T x_i^T$
- $(US)^T = V^T X^T$

To project a column vector x to M dim Principle Components subspace, take just the first M coordinates of $V^T x$

How Many PCs?

- For M original dimensions, sample covariance matrix is $M \times M$, and has up to M eigenvectors. So M principal components (PCs).
- Where does dimensionality reduction come from?
Can ignore the components of lesser significance.



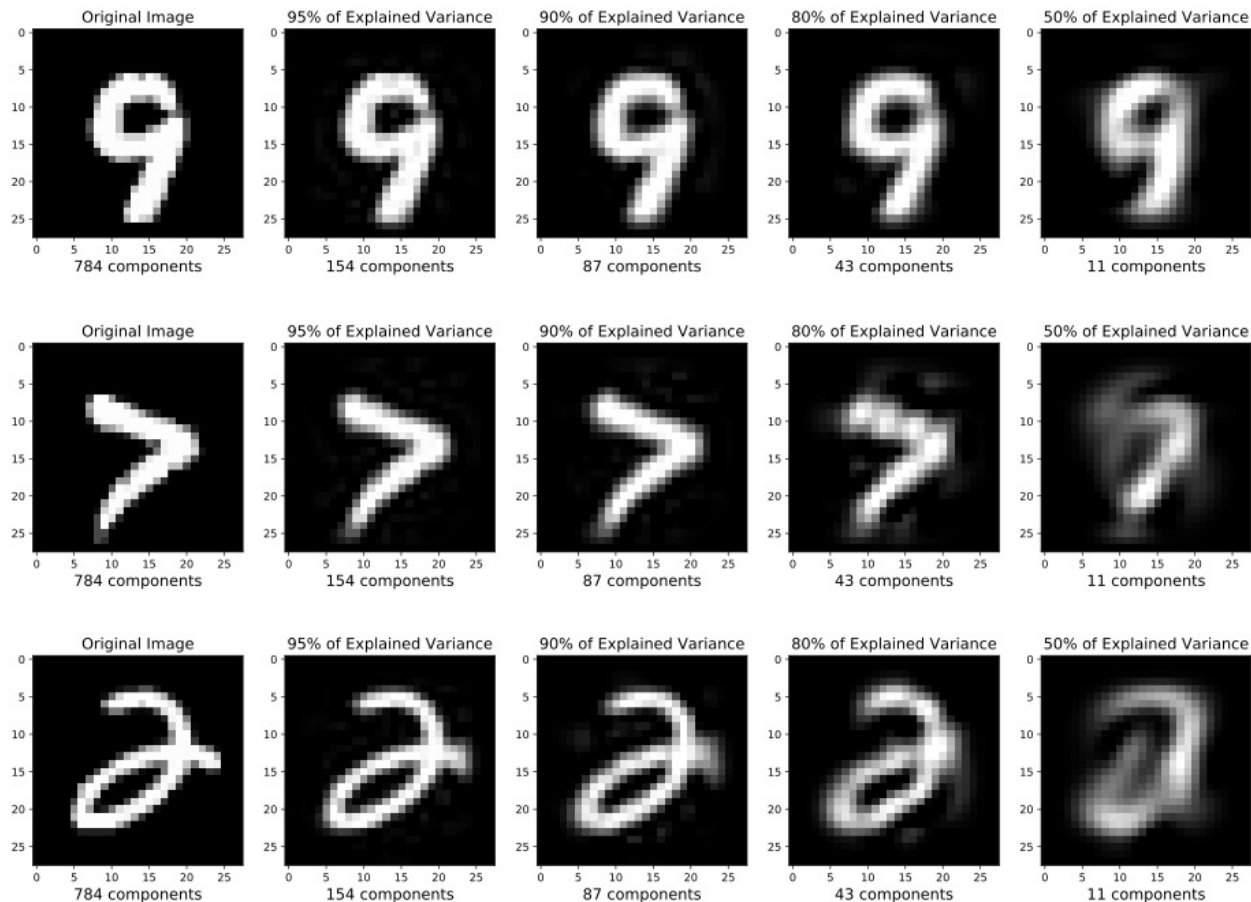
- You do lose some information, but if the eigenvalues are small, you don't lose much
 - M dimensions in original data
 - calculate M eigenvectors and eigenvalues
 - choose only the first D eigenvectors, based on their eigenvalues
 - final data set has only D dimensions

PCA EXAMPLES

Projecting MNIST digits

Task Setting:

1. Take each 28x28 image of a digit (i.e. a vector $\mathbf{x}^{(i)}$ of length 784) and project it down to K components (i.e. a vector $\mathbf{u}^{(i)}$)
2. Report percent of variance explained for K components
3. Then project back up to 28x28 image (i.e. a vector $\tilde{\mathbf{x}}^{(i)}$ of length 784) to visualize how much information was preserved



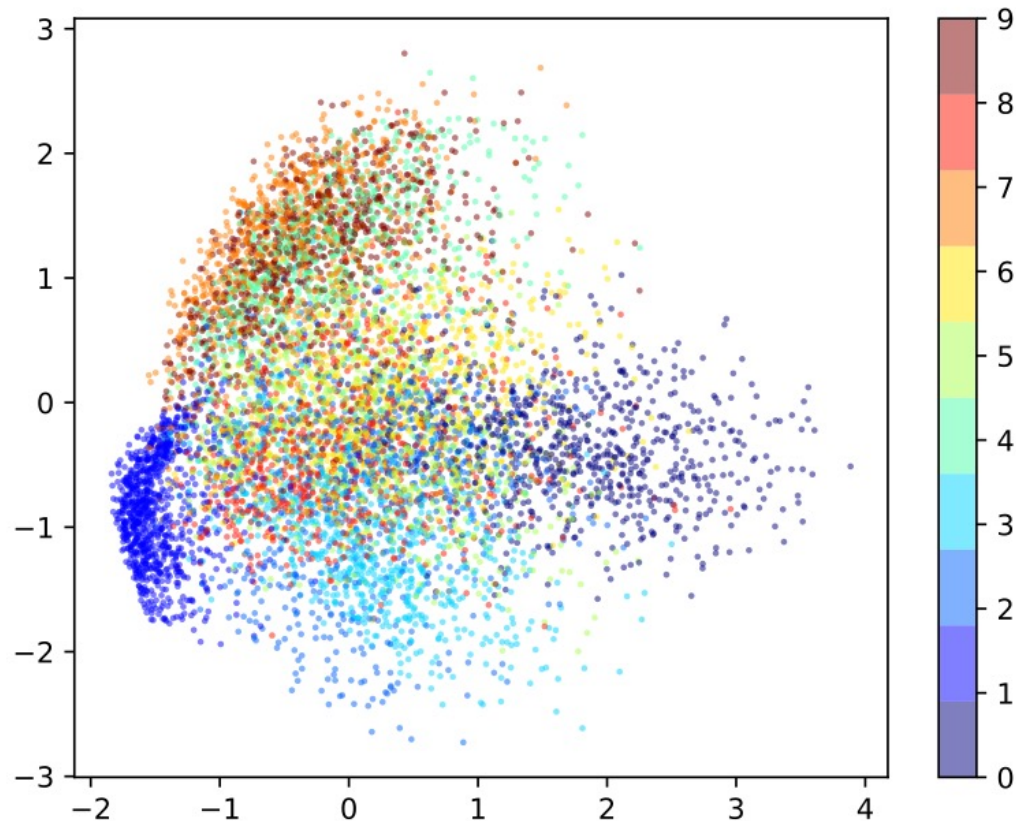
Takeaway:
Using fewer principal components K leads to higher reconstruction error.

But even a small number (say 43) still preserves a lot of information about the original image.

Projecting MNIST digits

Task Setting:

1. Take each 28x28 image of a digit (i.e. a vector $\mathbf{x}^{(i)}$ of length 784) and project it down to $K=2$ components (i.e. a vector $\mathbf{u}^{(i)}$)
2. Plot the 2 dimensional points $\mathbf{u}^{(i)}$ and label with the (unknown to PCA) label $y^{(i)}$ as the color
3. Here we look at all ten digits 0 - 9

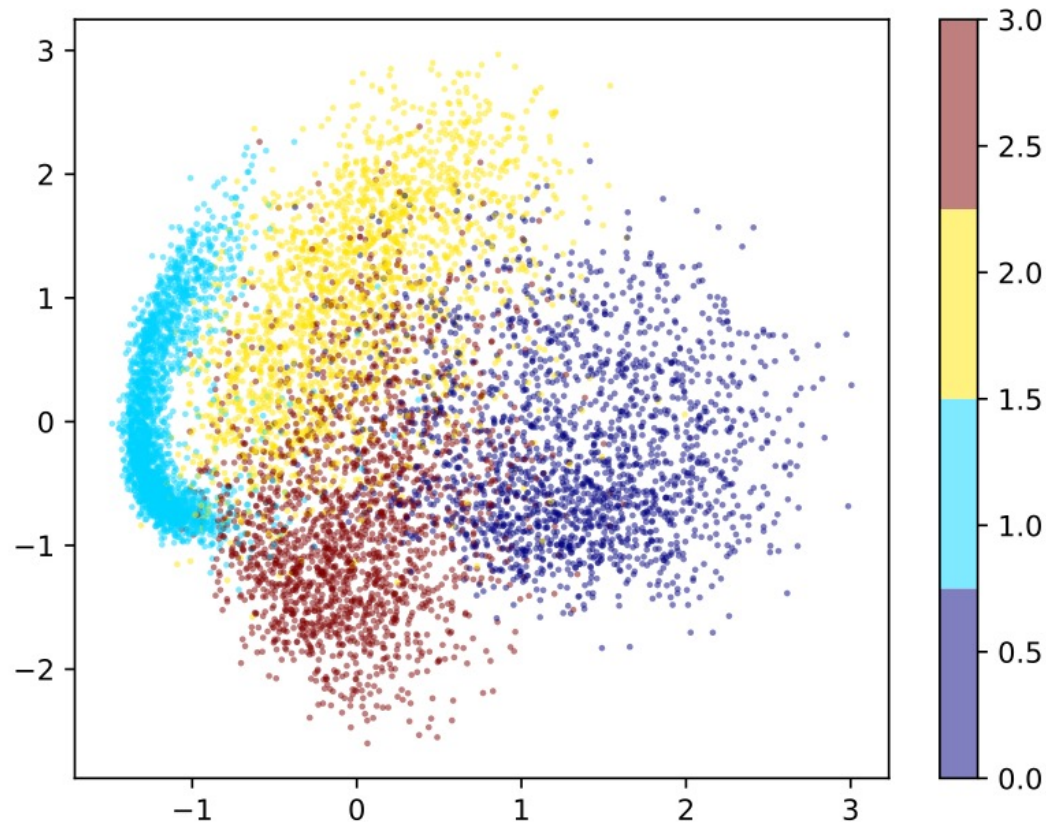


Takeaway:
Even with a tiny number of principal components $K=2$, PCA learns a representation that captures the *latent* information about the type of digit

Projecting MNIST digits

Task Setting:

1. Take each 28x28 image of a digit (i.e. a vector $\mathbf{x}^{(i)}$ of length 784) and project it down to $K=2$ components (i.e. a vector $\mathbf{u}^{(i)}$)
2. Plot the 2 dimensional points $\mathbf{u}^{(i)}$ and label with the (unknown to PCA) label $y^{(i)}$ as the color
3. Here we look at just four digits 0, 1, 2, 3



Takeaway:
Even with a tiny number of principal components $K=2$, PCA learns a representation that captures the *latent* information about the type of digit

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