10-301/601: Introduction to Machine Learning Lecture 25: Dimensionality Reduction

Matt Gormley & Henry Chai

11/25/24

Front Matter

- Announcements
  - HW8 released 11/17, due 11/25 (today!) at 11:59 PM
    - Please be mindful of your grace day usage (see the course syllabus for the policy)
  - HW9 released 11/25 (today!), due 12/5 at 11:59 PM
    - You are not expected to work on HW9 over Thanksgiving break
      - Relatedly, there are no OH over break
    - **You may only take at most 2 grace days on HW9**
    - Recitation for HW9 on Monday, 12/2 (after break)

Recall: K-means Algorithm

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}\right)\right\}_{n=1}^{N}, K$

1. Initialize cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$
2. While NOT CONVERGED
   a. Assign each data point to the cluster with the nearest cluster center:
   $$z^{(n)} = \underset{k}{\operatorname{argmin}} \left\|\boldsymbol{x}^{(n)} - \boldsymbol{\mu}_k\right\|_2$$
   b. Recompute the cluster centers:
   $$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n\,:z^{(n)}=k} \boldsymbol{x}^{(n)}$$
   where N_k is the number of data points in cluster k

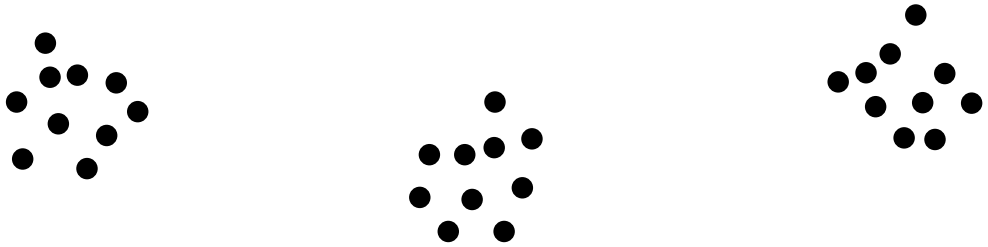
- Output: cluster centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$ and cluster assignments $z^{(1)}, \ldots, z^{(N)}$

Setting K

- Idea: choose the value of K that minimizes the objective function

Initializing K-means: Lloyd's Method

- Randomly choose K data points to be the initial cluster centers



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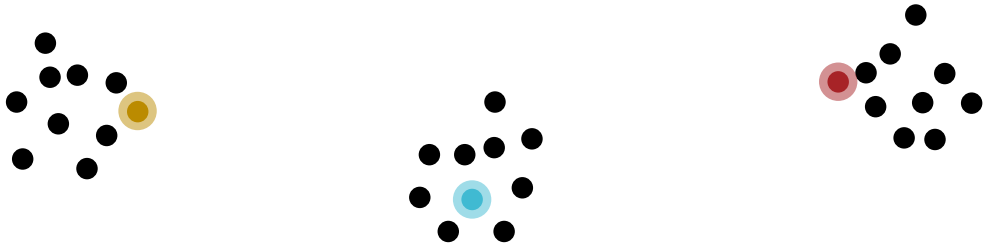

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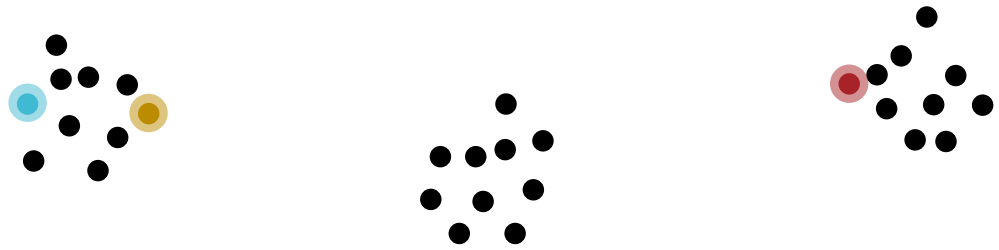

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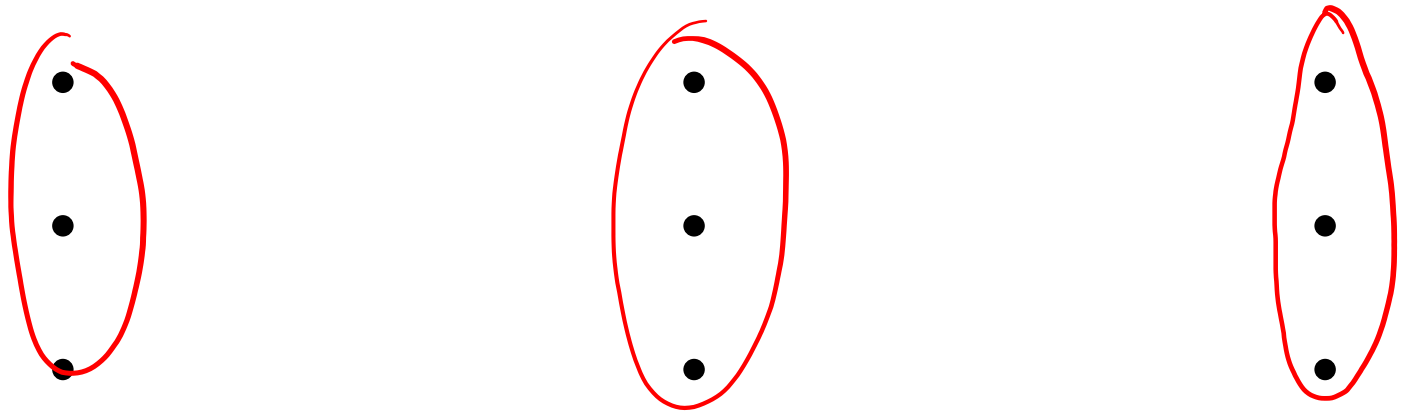

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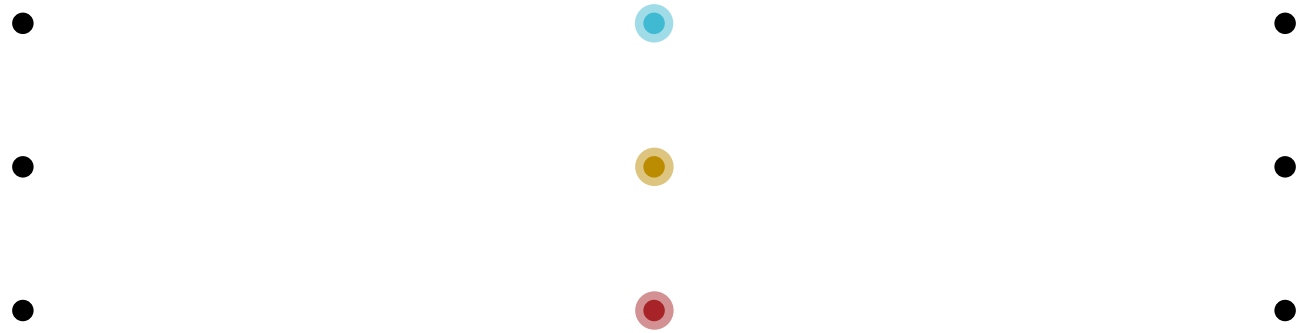

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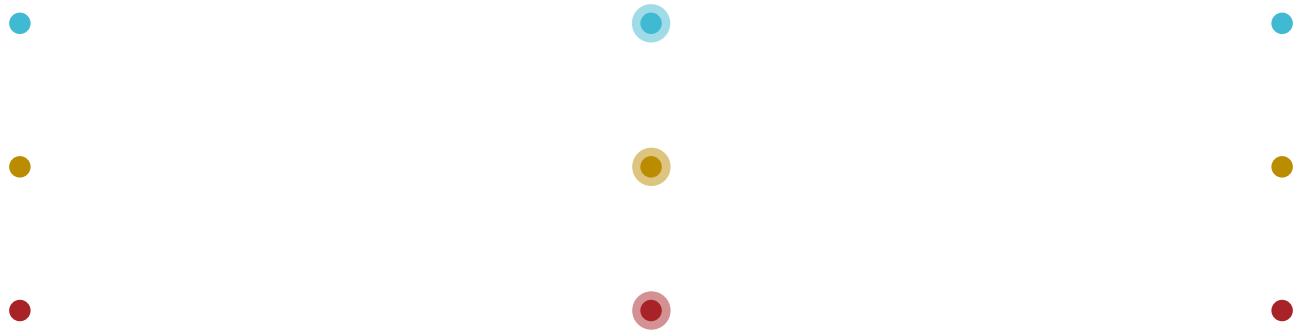
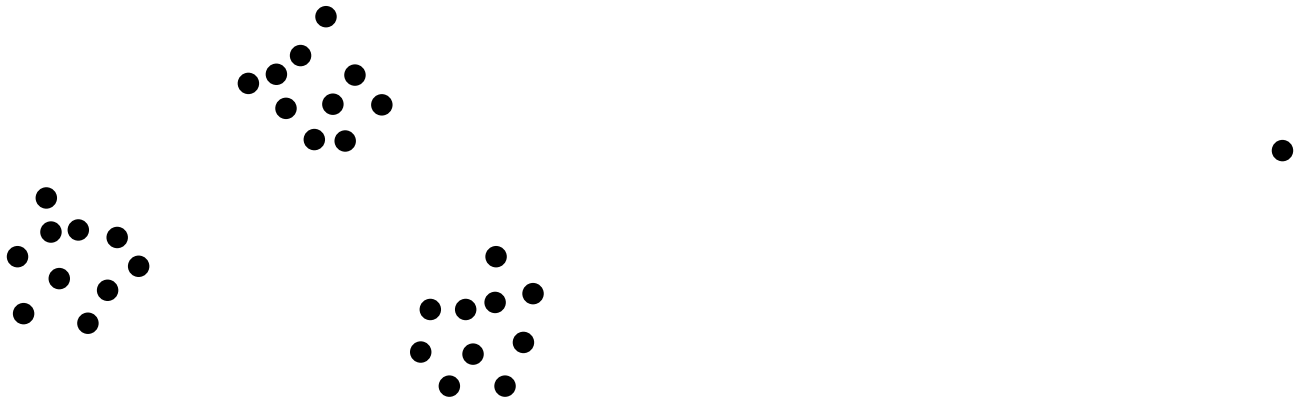


- Lloyd's method converges to a local minimum and that local minimum can be arbitrarily bad (relative to the optimal clusters)
- Intuition: want initial cluster centers to be far apart from one another

Initializing K-means: Furthest Point

1. Choose the first cluster center randomly from the data points
2. For each other data point $\boldsymbol{x}$, compute $D(\boldsymbol{x})$, the distance between $\boldsymbol{x}$ and the closest cluster center to $\boldsymbol{x}$
3. Select the data point with the largest $D(\boldsymbol{x})$ as the next cluster center
4. Repeat 2 and 3 $K - 1$ times



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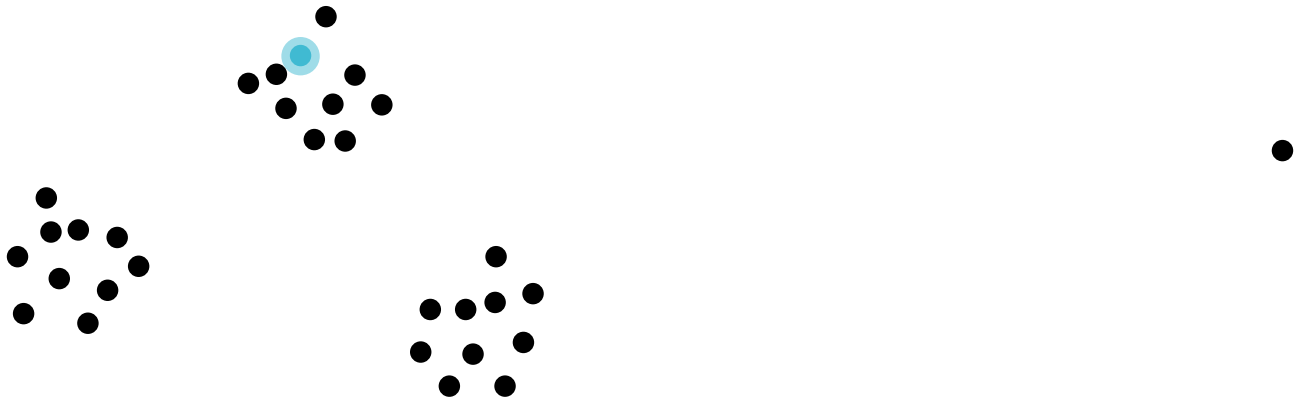

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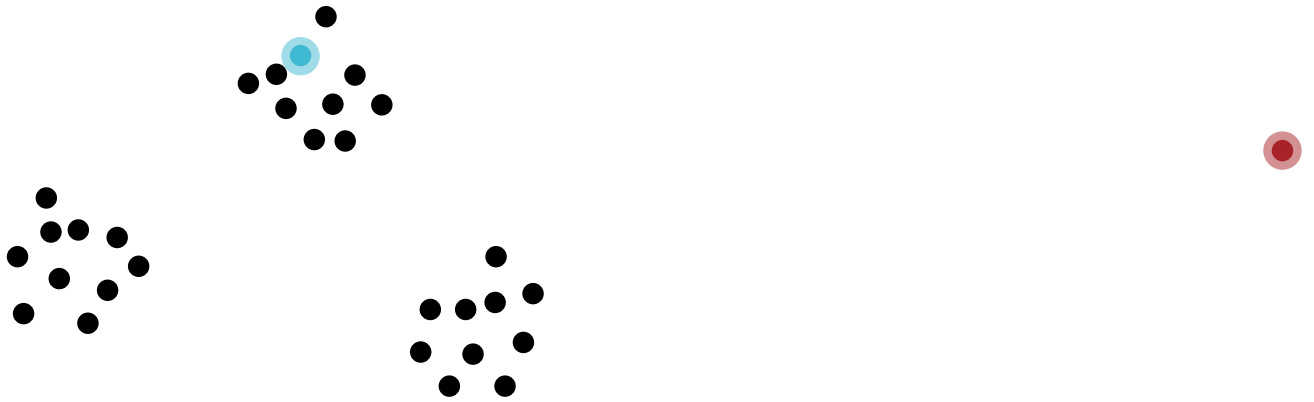

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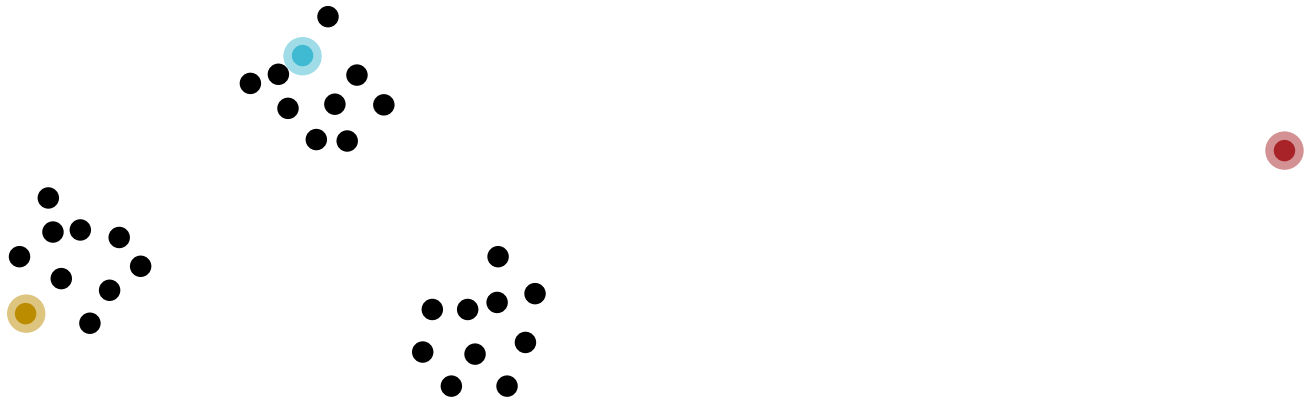

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3. Select the data point with the largest $D(\boldsymbol{x})$ as the next cluster center
4. Repeat 2 and 3 $K - 1$ times

- Works great in the case of well-clustered data!
- Can struggle with outliers...

Initializing K-means: K-means++

1. Choose the first cluster center randomly from the data points
2. For each other data point $\boldsymbol{x}$, compute $D(\boldsymbol{x})$, the distance between $\boldsymbol{x}$ and the closest cluster center to $\boldsymbol{x}$
3. *Sample* the next cluster center with probability proportional to $D(\boldsymbol{x})^2$
4. Repeat 2 and 3 $K-1$ times

i	$D(x^{(i)})$	$D(x^{(i)})^2$	Probability of Being Selected
1	4	16	$16/123$
2	7	49	$49/123$
⋮	⋮	⋮	⋮
N	1	1	$1/123$
Total		123	$123/123 = 1$

Initializing K-means: K-means++

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3. *Sample* the next cluster center with probability proportional to $D(\boldsymbol{x})^2$
4. Repeat 2 and 3 $K-1$ times

- K-means++ achieves a $O(\log K)$ approximation to the optimal clustering in expectation!
- All initialization methods can benefit from multiple random restarts

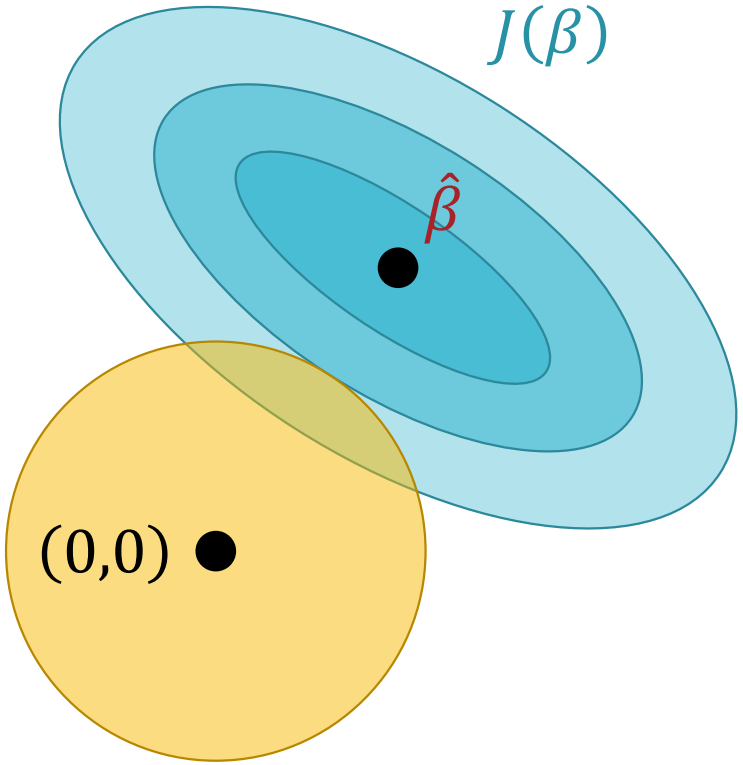
K-means Learning Objectives

You should be able to…

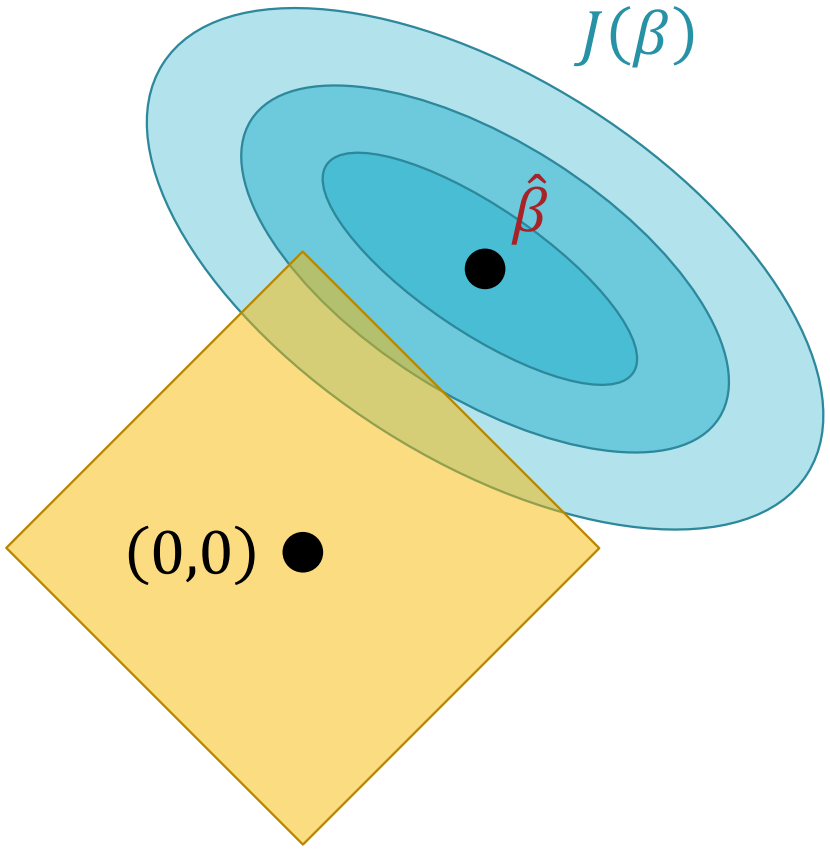
- Distinguish between coordinate descent and block coordinate descent
- Define an objective function that gives rise to a "good" clustering
- Apply block coordinate descent to an objective function preferring each point to be close to its nearest objective function to obtain the K-Means algorithm
- Implement the K-Means algorithm
- Connect the nonconvexity of the K-Means objective function with the (possibly) poor performance of random initialization

Dimensionality Reduction

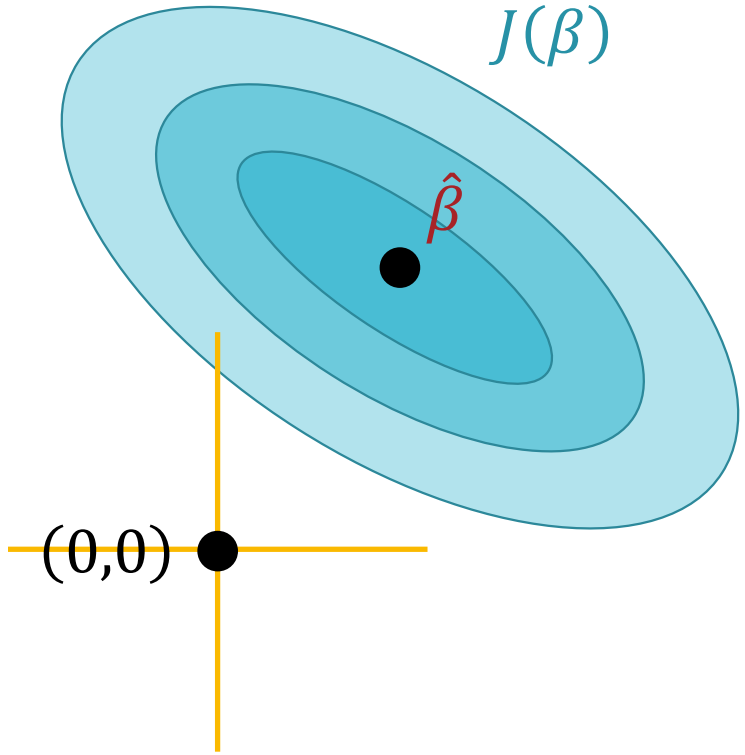
- Goal: given some unlabeled data set, learn a latent (typically lower-dimensional) representation
- Use cases:
  - Reducing computational cost (runtime, storage, etc…)
  - Improving generalization
  - Visualizing data
- Applications:
  - word embeddings
  - image/video/audio
  - ratings on social media platforms



Ridge or $L2$

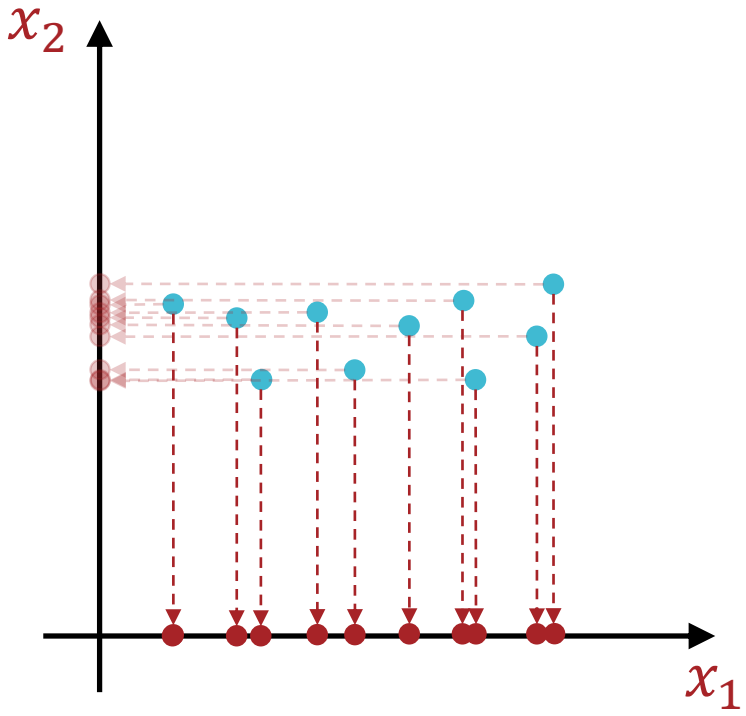


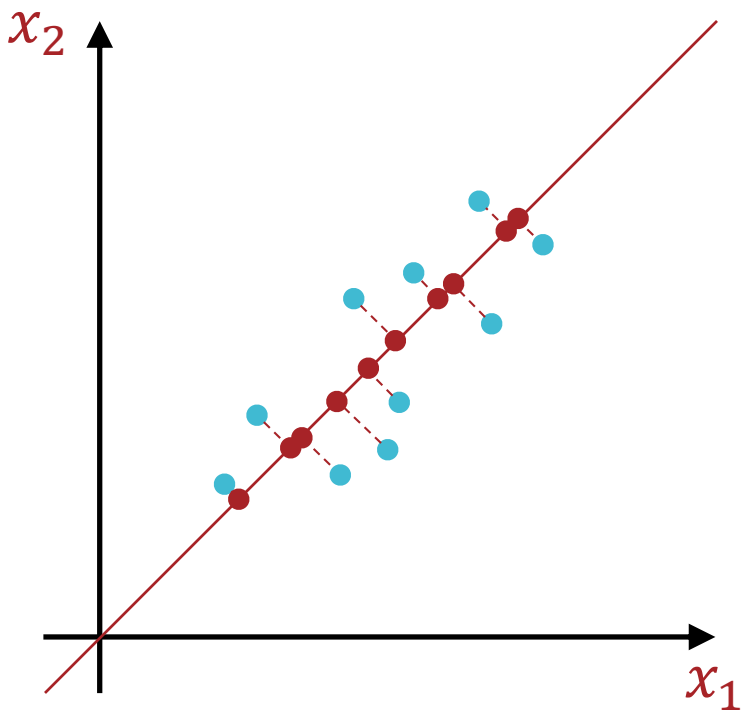
Lasso or $L1$



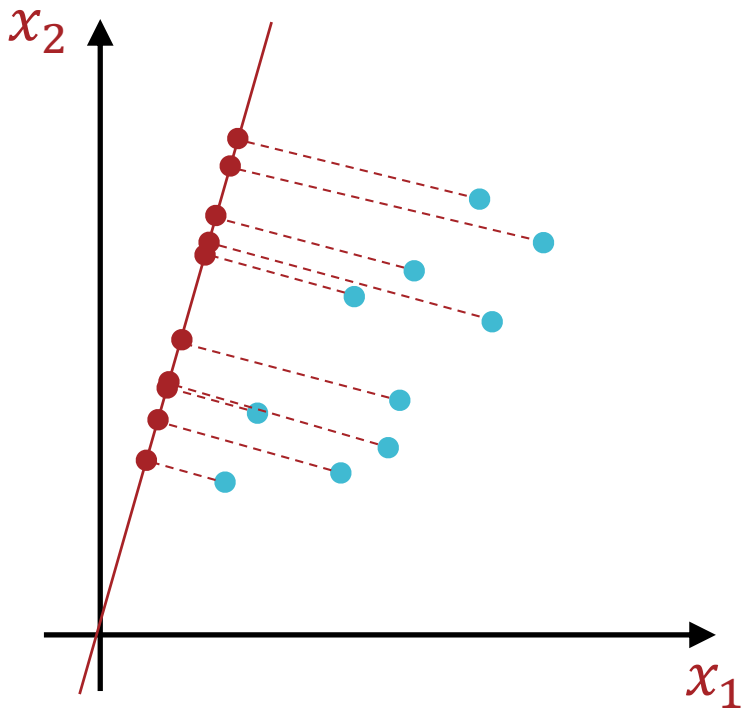
$L0$

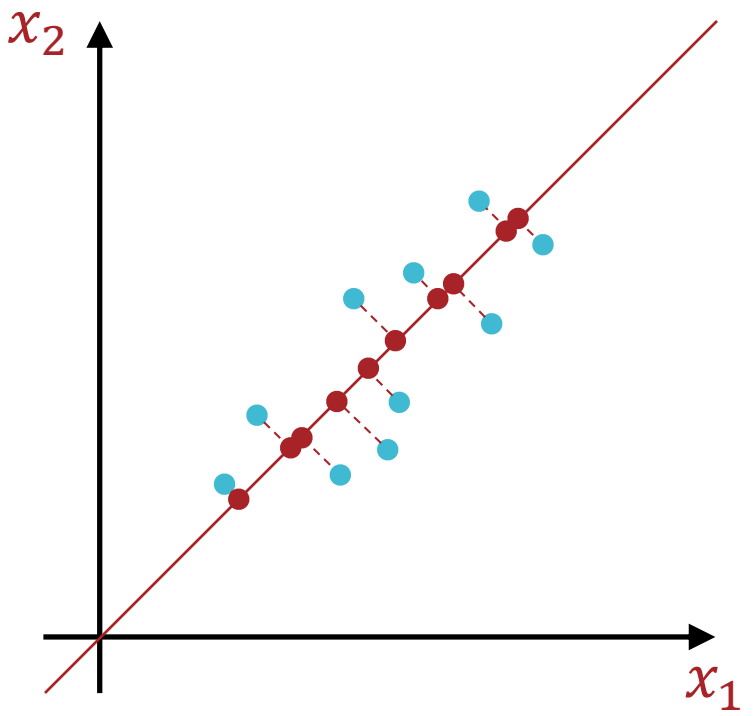
Recall: $L1$ (or $L0$) Regularization



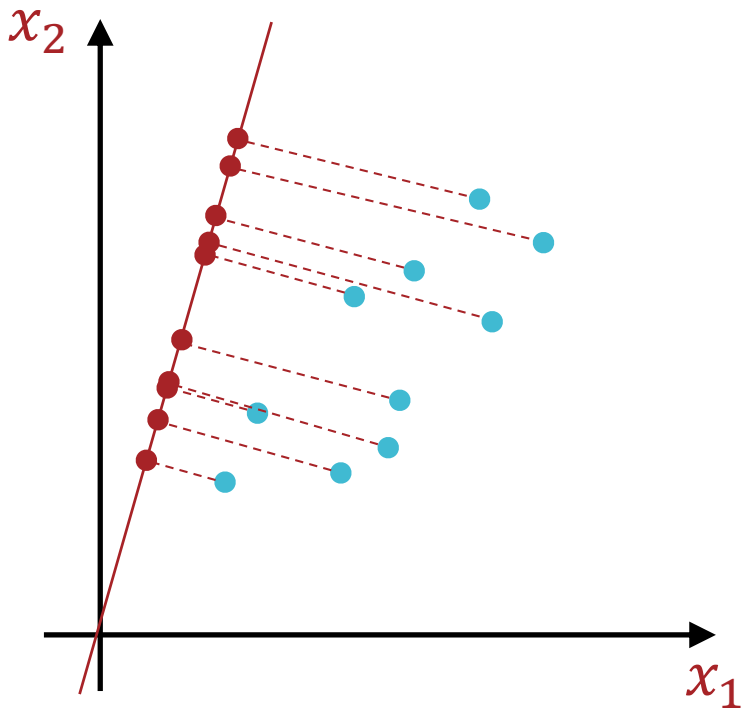


Feature Elimination

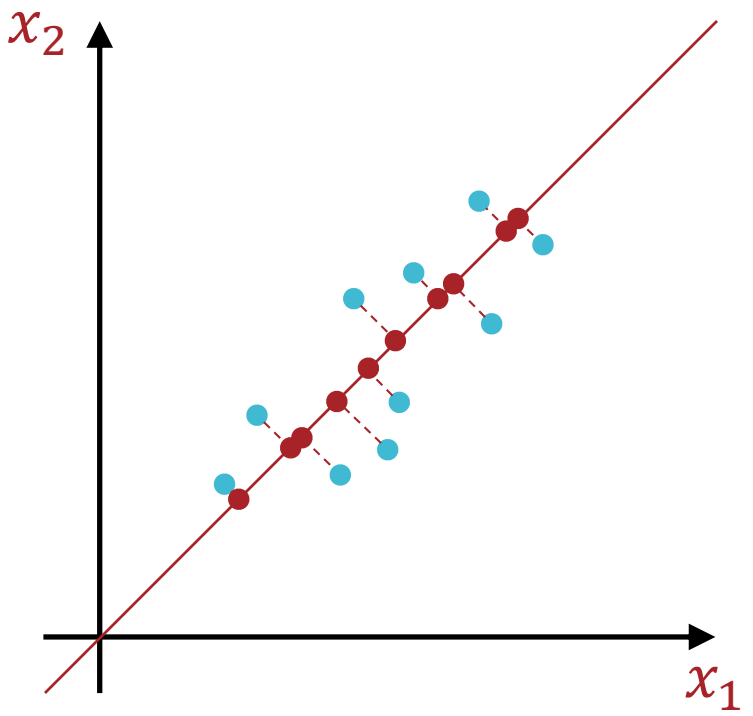




Feature Reduction



Option A



Option B (TOXIC)

Option C

Which projection do you prefer (Q1) and why (Q2)?

Background: Sample Variance and Covariance

- Given a collection of N 1-dimensional samples $\left[x^{(1)}, x^{(2)}, \ldots, x^{(N)}\right]$ from some random variable, the **sample variance** is

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

- Given a collection of N D-dimensional samples $\left[\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(N)}\right]$ from some random variable, the **sample covariance** between dimension j and k is

$$\Sigma_{jk} = \frac{1}{N}\sum_{i=1}^{N}\left(x_j^{(i)} - \hat{\mu}_j\right)\left(x_k^{(i)} - \hat{\mu}_k\right) \text{ where } \hat{\mu}_d = \frac{1}{N}\sum_{n=1}^{N} x_d^{(n)}$$

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- Given a collection of N D-dimensional samples $\left[\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \ldots, \boldsymbol{x}^{(N)}\right]$ from some random variable, the **sample covariance matrix** is

$$\Sigma = \frac{1}{N}X^T X \text{ where } X = \begin{bmatrix} (\boldsymbol{x}^{(1)} - \boldsymbol{\mu})^T \\ (\boldsymbol{x}^{(2)} - \boldsymbol{\mu})^T \\ \vdots \\ (\boldsymbol{x}^{(N)} - \boldsymbol{\mu})^T \end{bmatrix}$$

Centering the Data

- To be consistent, we will constrain principal components to be *orthogonal unit vectors* that begin at the origin
- Preprocess data to be centered around the origin:

1. $\boldsymbol{\mu} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}^{(n)}$
2. $\tilde{\boldsymbol{x}}^{(n)} = \boldsymbol{x}^{(n)} - \boldsymbol{\mu}\ \forall\ n$
3. $X = \begin{bmatrix} \tilde{\boldsymbol{x}}^{(1)^T} \\ \tilde{\boldsymbol{x}}^{(2)^T} \\ \vdots \\ \tilde{\boldsymbol{x}}^{(N)^T} \end{bmatrix}$

Reconstruction Error

- The projection of $\tilde{\boldsymbol{x}}^{(n)}$ onto a vector $\boldsymbol{v}$ is

$$\boldsymbol{z}^{(n)} = \left(\frac{\boldsymbol{v}^T \tilde{\boldsymbol{x}}^{(n)}}{\|\boldsymbol{v}\|_2}\right) \frac{\boldsymbol{v}}{\|\boldsymbol{v}\|_2}$$

Length of projection

Direction of projection

$(a-b)^T = a^T - b^T$

Reconstruction Error

- The projection of $\tilde{\boldsymbol{x}}^{(n)}$ onto a unit vector $\boldsymbol{v}$ is

$$\boldsymbol{z}^{(n)} = \left(\boldsymbol{v}^T \tilde{\boldsymbol{x}}^{(n)}\right)\boldsymbol{v}$$

$$\hat{\boldsymbol{v}} = \underset{\boldsymbol{v}:\|\boldsymbol{v}\|_2^2=1}{\operatorname{argmin}} \sum_{n=1}^{N} \left\| \tilde{\boldsymbol{x}}^{(n)} - \left(\boldsymbol{v}^T \tilde{\boldsymbol{x}}^{(n)}\right)\boldsymbol{v} \right\|_2^2$$

$$\left(\tilde{x}^{(n)} - (v^T \tilde{x}^{(n)})v\right)^T \left(\tilde{x}^{(n)} - (v^T \tilde{x}^{(n)})v\right)$$

$$= \tilde{x}^{(n)T}\tilde{x}^{(n)} - 2(v^T \tilde{x}^{(n)})\, v^T \tilde{x}^{(n)} + (v^T \tilde{x}^{(n)})^2 \underbrace{v^T v}_{=1}$$

$$= \tilde{x}^{(n)T}\tilde{x}^{(n)} - (v^T \tilde{x}^{(n)})^2$$

Minimizing the Reconstruction Error

$$\hat{\boldsymbol{v}} = \underset{\boldsymbol{v}:\|\boldsymbol{v}\|_2^2=1}{\operatorname{argmin}} \sum_{n=1}^{N} \left\| \tilde{\boldsymbol{x}}^{(n)} - \left(\boldsymbol{v}^T \tilde{\boldsymbol{x}}^{(n)}\right)\boldsymbol{v} \right\|_2^2$$

$$= \underset{v:\|v\|_2^2=1}{\operatorname{argmin}} \sum_{n=1}^{N} \tilde{x}^{(n)T}\tilde{x}^{(n)} - \left(v^T\tilde{x}^{(n)}\right)^2$$

$$= \underset{v:\|v\|_2^2=1}{\operatorname{argmax}} \frac{1}{N}\sum_{n=1}^{N}\left(v^T\tilde{x}^{(n)}\right)^2 \quad \leftarrow \text{is equivalent to maximizing the variance of the projections}$$

$$= \underset{v:\|v\|_2^2=1}{\operatorname{argmax}} \sum_{n=1}^{N}\left(v^T\tilde{x}^{(n)}\right)\left(\tilde{x}^{(n)T}v\right)$$

$$= \underset{v:\|v\|_2^2=1}{\operatorname{argmax}} \; v^T\left(\sum_{n=1}^{N}\tilde{x}^{(n)}\tilde{x}^{(n)T}\right)v$$

$$X^TX$$

Maximizing the Variance

$$\hat{\boldsymbol{v}} = \underset{\boldsymbol{v}:\|\boldsymbol{v}\|_2^2=1}{\operatorname{argmax}} \boldsymbol{v}^T (X^T X)\boldsymbol{v}$$

$\star$ $L(v) = v^T X^T X v - \lambda(v^T v - 1)$

$$\frac{\partial L}{\partial v} = 2X^T X v - 2\lambda v$$

$$\Rightarrow 2X^T X \hat{v} - 2\lambda \hat{v} = 0$$

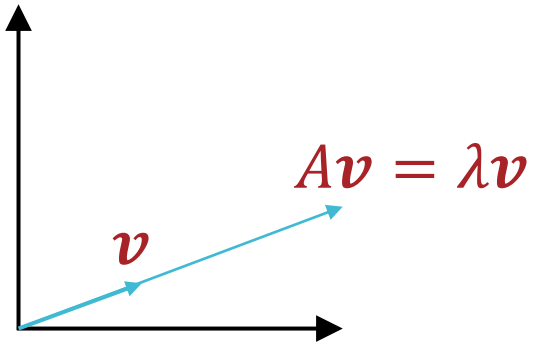
$$\Rightarrow X^T X \hat{v} = \lambda \hat{v}$$

$\hat{v}$ is an eigenvector for the matrix $X^T X$ w/ eigenvalue λ

Background: Eigenvectors & Eigenvalues

- Given a square matrix $A \in \mathbb{R}^{N \times N}$, a vector $\boldsymbol{v} \in \mathbb{R}^{N \times 1}$ is an **eigenvector** of A iff there exists some scalar λ such that

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



Intuition: A scales or stretches $\boldsymbol{v}$ but does not rotate it

- Key property: the eigenvectors of symmetric matrices (e.g., the covariance matrix of a data set) are orthogonal!

Maximizing the Variance

$$\hat{\boldsymbol{v}} = \underset{\boldsymbol{v}:\|\boldsymbol{v}\|_2^2=1}{\operatorname{argmax}} \boldsymbol{v}^T (X^T X)\boldsymbol{v}$$

$$\mathcal{L}(\boldsymbol{v}, \lambda) = \boldsymbol{v}^T (X^T X)\boldsymbol{v} - \lambda(\|\boldsymbol{v}\|_2^2 - 1)$$
$$= \boldsymbol{v}^T (X^T X)\boldsymbol{v} - \lambda(\boldsymbol{v}^T \boldsymbol{v} - 1)$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{v}} = 2(X^T X)\boldsymbol{v} - 2\lambda \boldsymbol{v}$$

$$\rightarrow (X^T X)\hat{\boldsymbol{v}} - \lambda\hat{\boldsymbol{v}} = 0 \rightarrow (X^T X)\hat{\boldsymbol{v}} = \lambda\hat{\boldsymbol{v}}$$

- $\hat{\boldsymbol{v}}$ is an eigenvector of $X^T X$ and λ is the corresponding eigenvalue!
- But which one?

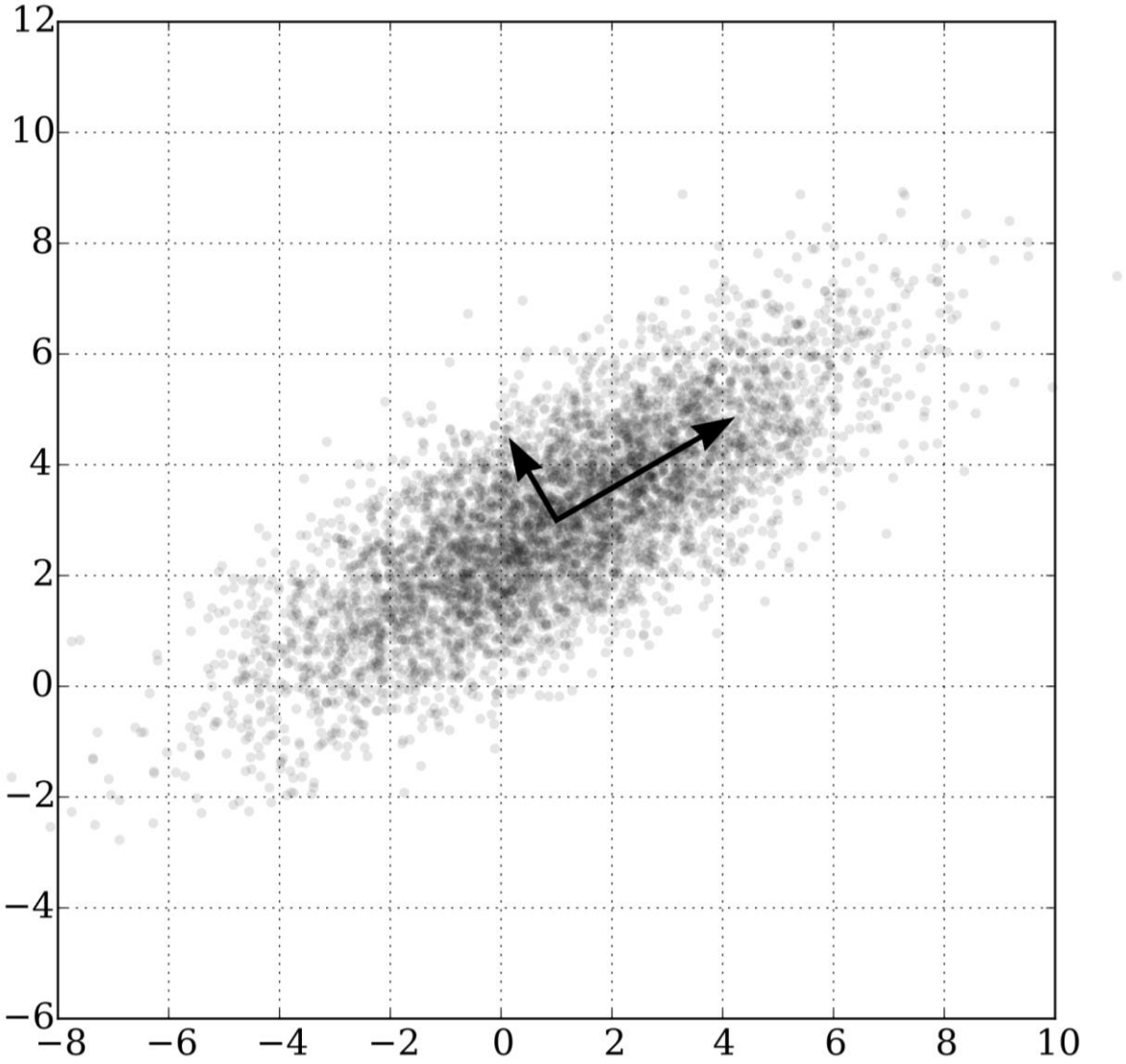
Maximizing the Variance

$$\hat{\boldsymbol{v}} = \underset{\boldsymbol{v}:\|\boldsymbol{v}\|_2^2=1}{\operatorname{argmax}} \boldsymbol{v}^T (X^T X)\boldsymbol{v}$$

$$(X^T X)\hat{\boldsymbol{v}} = \lambda\hat{\boldsymbol{v}} \rightarrow \hat{\boldsymbol{v}}^T (X^T X)\hat{\boldsymbol{v}} = \lambda\hat{\boldsymbol{v}}^T\hat{\boldsymbol{v}} = \lambda$$

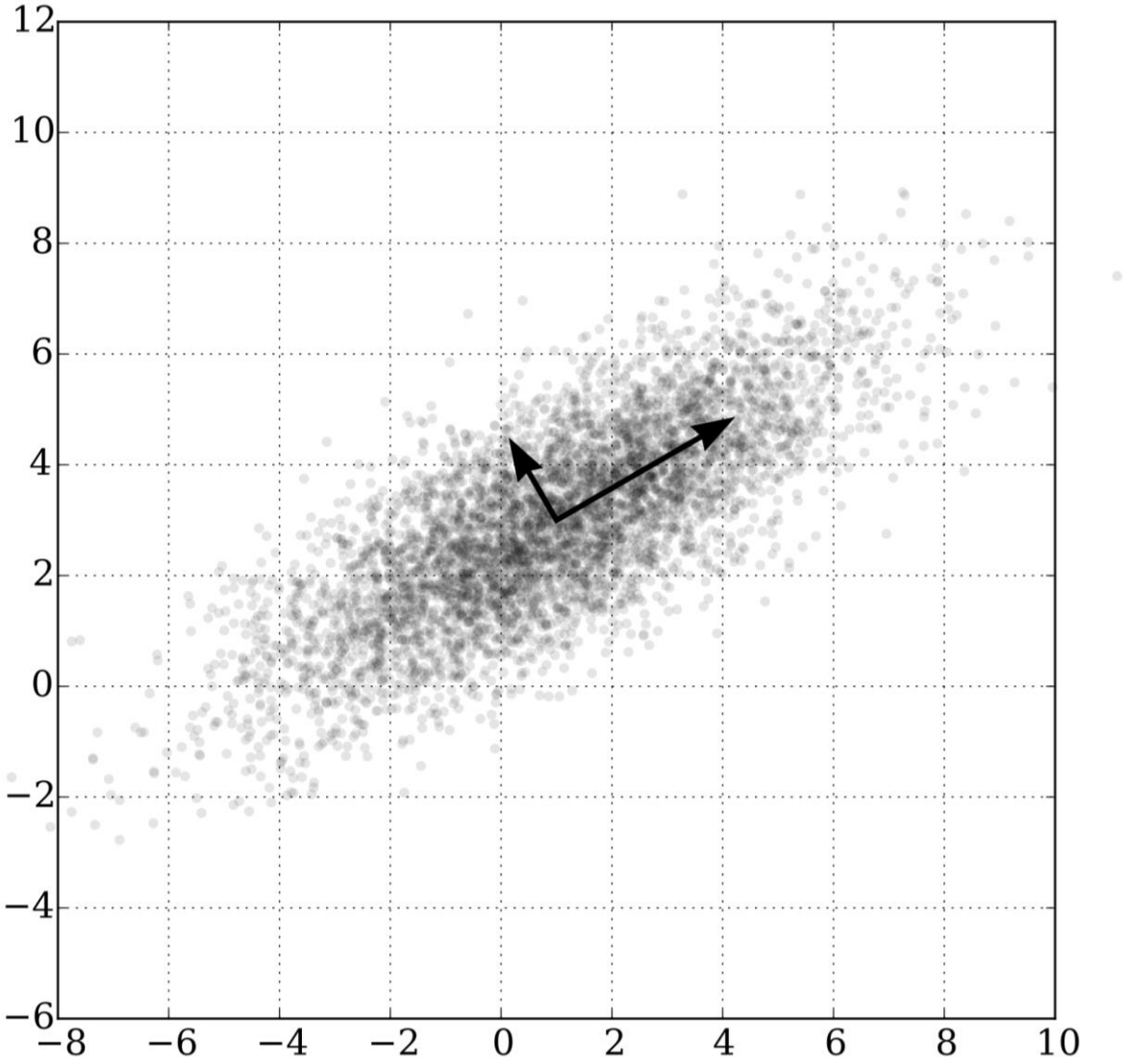
- The first principal component is the eigenvector $\hat{\boldsymbol{v}}_1$ that corresponds to the largest eigenvalue λ_1
- The second principal component is the eigenvector $\hat{\boldsymbol{v}}_2$ that corresponds to the second largest eigenvalue λ_2
  - $\hat{\boldsymbol{v}}_1$ and $\hat{\boldsymbol{v}}_2$ are orthogonal
- Etc …
- λ_i is a measure of how much variance falls along $\hat{\boldsymbol{v}}_i$

Principal Components: Example



Source: https://en.wikipedia.org/wiki/Principal_component_analysis#/media/File:GaussianScatterPCA.svg

How can we efficiently find principal components (eigenvectors)?



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Singular Value Decomposition (SVD) for PCA

- Every real-valued matrix $X \in \mathbb{R}^{N \times D}$ can be expressed as

$$X = USV^T$$

where:

1. $U \in \mathbb{R}^{N \times N}$ - columns of U are eigenvectors of XX^T
2. $V \in \mathbb{R}^{D \times D}$ - columns of V are eigenvectors of $X^T X$
3. $S \in \mathbb{R}^{N \times D}$ - diagonal matrix whose entries are the eigenvalues of $X \rightarrow$ squared entries are the eigenvalues of XX^T and $X^T X$

PCA Algorithm

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}\right)\right\}_{n=1}^{N}, \rho$

1. Center the data
2. Use SVD to compute the eigenvalues and eigenvectors of $X^T X$
3. Collect the top ρ eigenvectors (corresponding to the ρ largest eigenvalues), $V_\rho \in \mathbb{R}^{D \times \rho}$
4. Project the data into the space defined by V_ρ, $Z = XV_\rho$

- Output: Z, the transformed (potentially lower-dimensional) data

How many PCs should we use?

- Input: $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}\right)\right\}_{n=1}^{N}, \rho$

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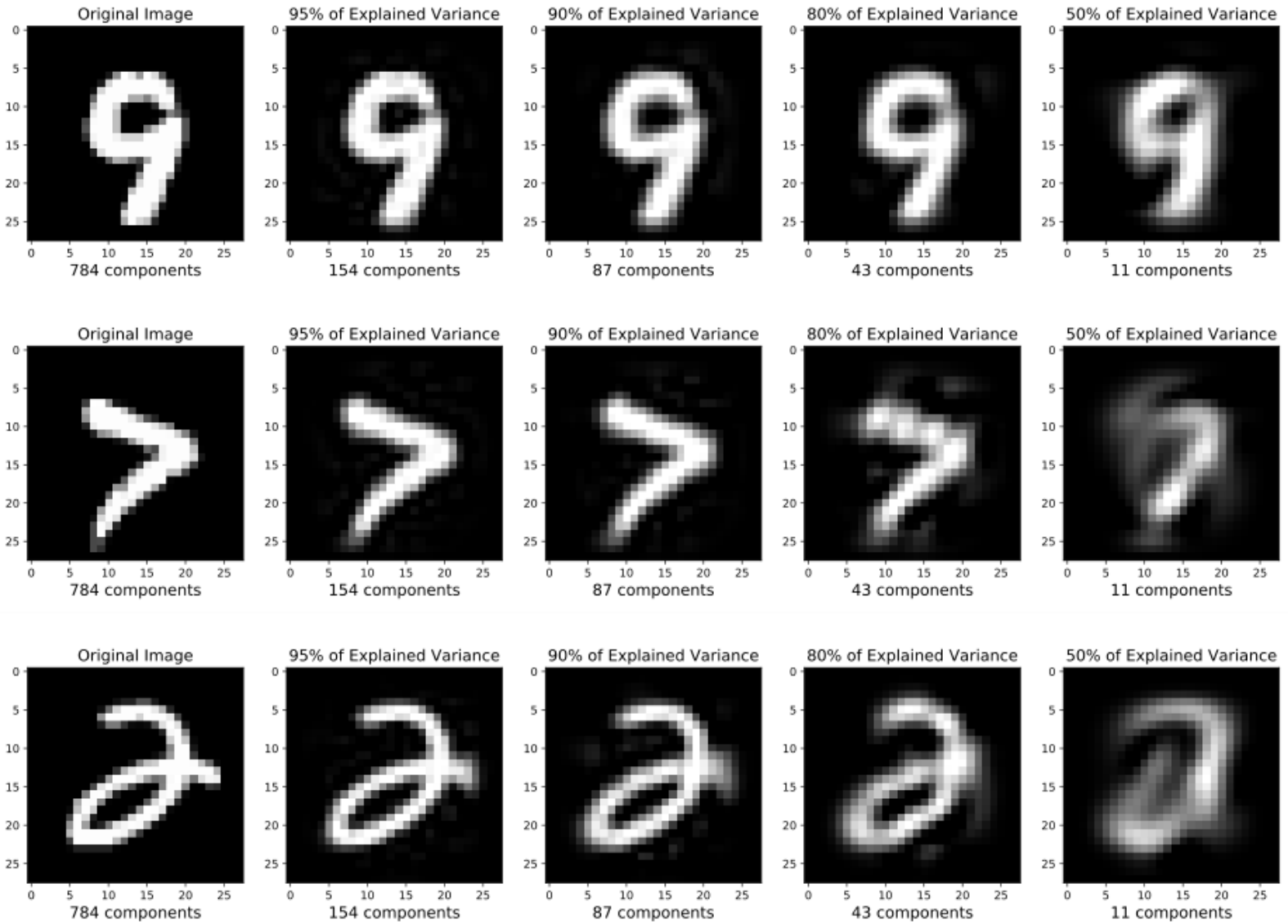
Choosing the number of PCs

- Define a percentage of explained variance for the i^{th} PC:

$$\lambda_i \Big/ \sum \lambda_j$$

- Select all PCs above some threshold of explained variance, e.g., 5%
- Keep selecting PCs until the total explained variance exceeds some threshold, e.g., 90%
- Evaluate on some downstream metric

PCA Example: MNIST Digits



Figures courtesy of Matt Gormley

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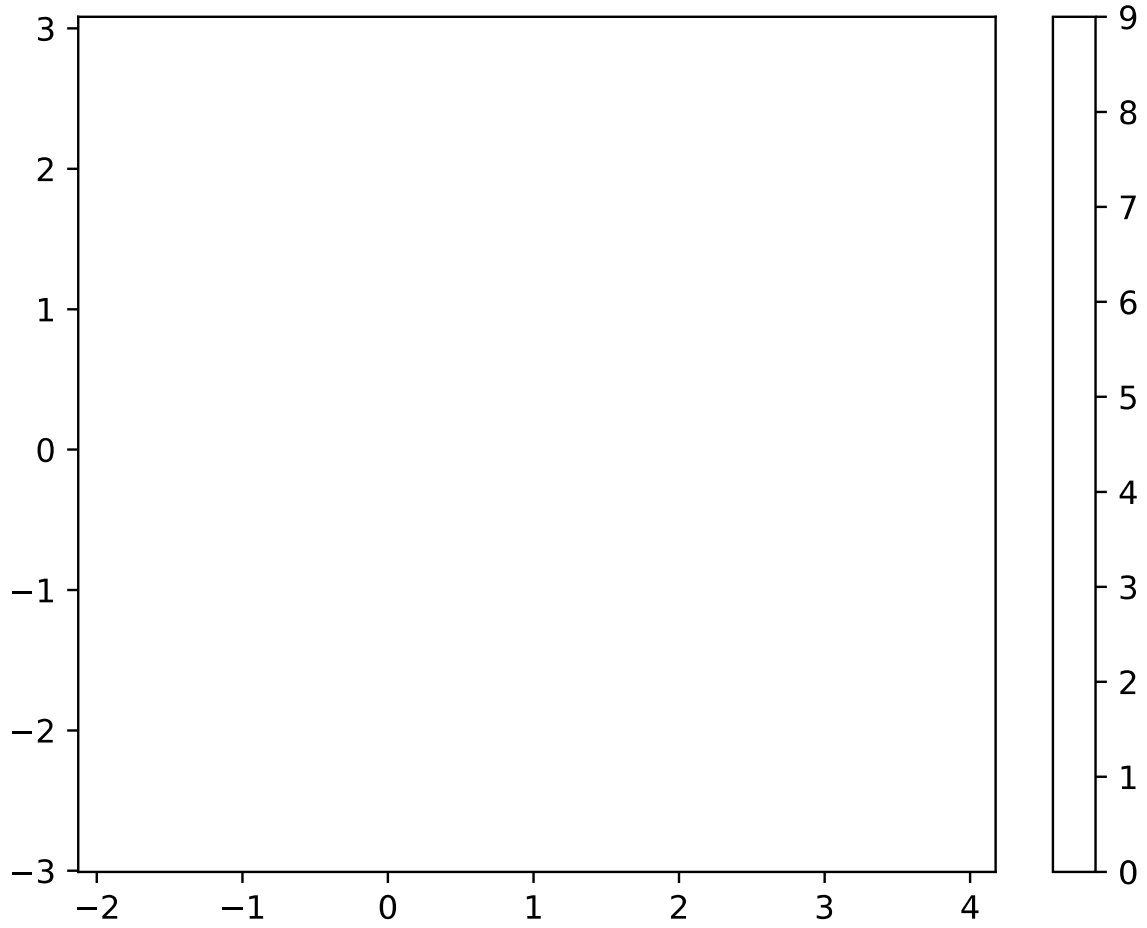


Figure courtesy of Matt Gormley

PCA Example: MNIST Digits

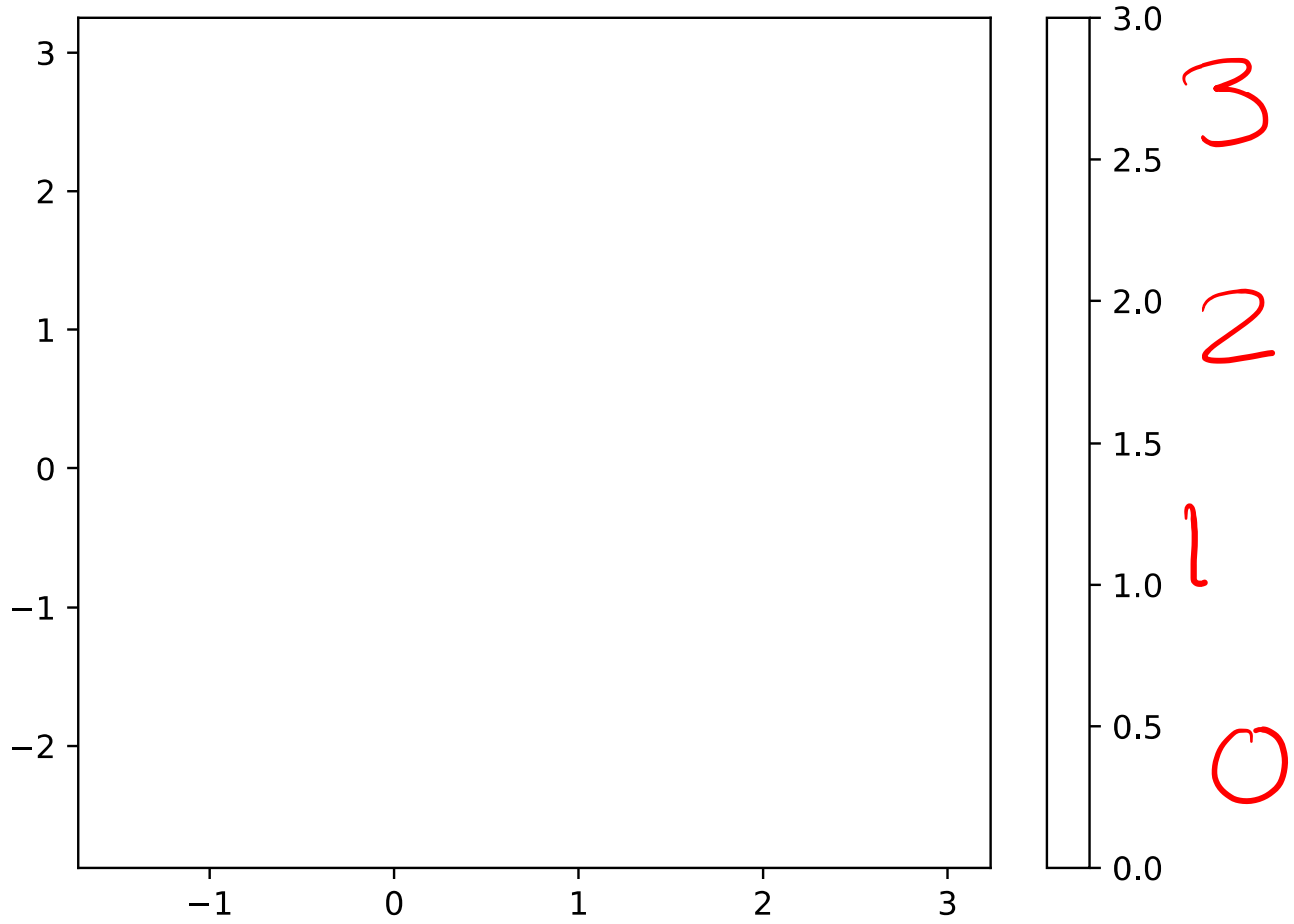
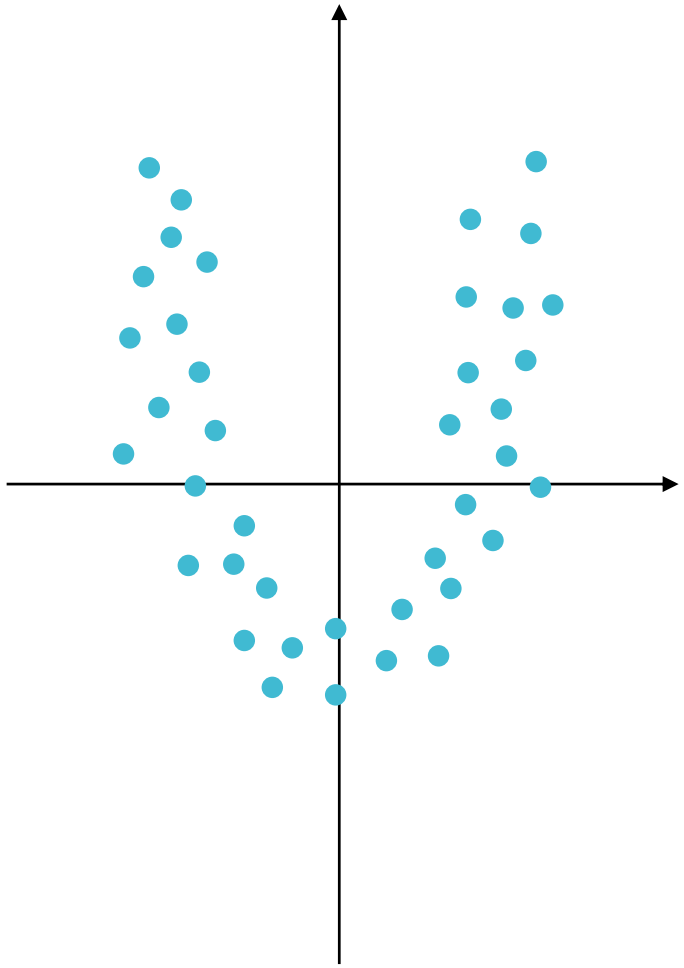
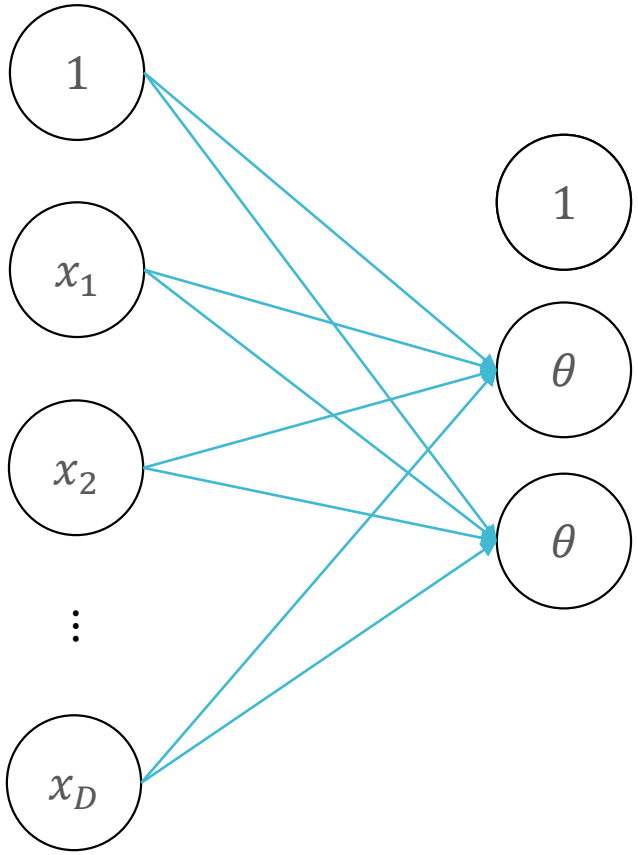


Figure courtesy of Matt Gormley

Shortcomings of PCA

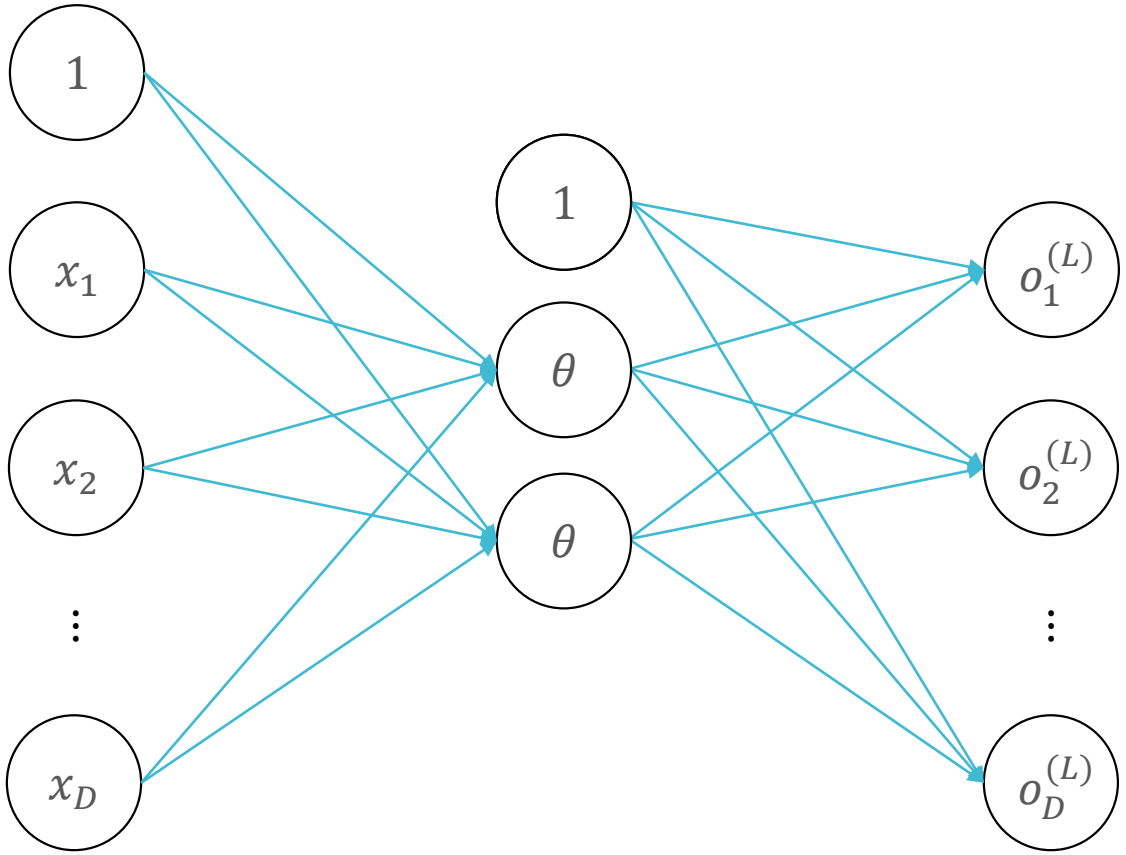


Autoencoders



Insight: neural networks implicitly learn low-dimensional representations of inputs in hidden layers

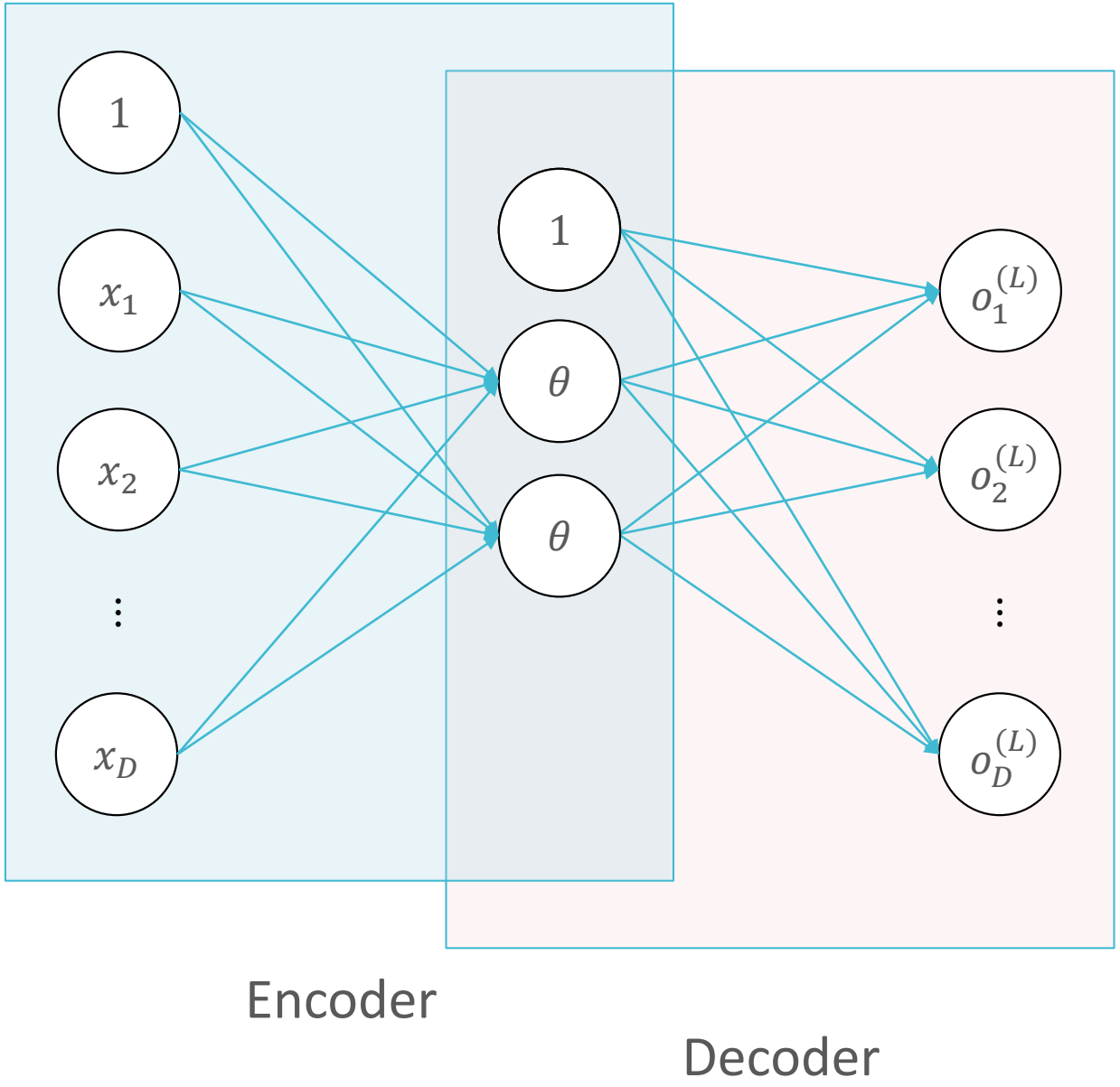
Autoencoders



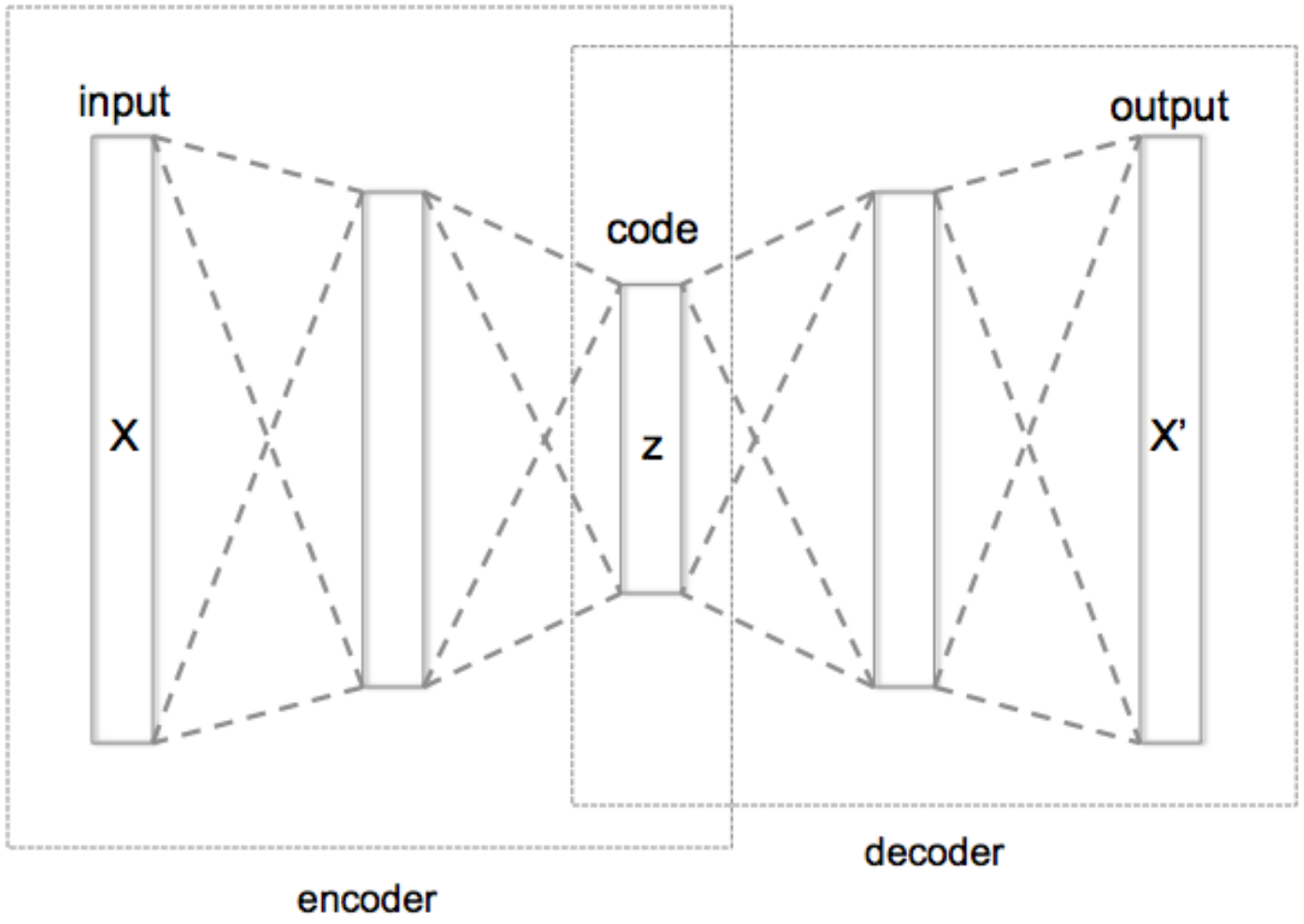
- Learn the weights by minimizing the reconstruction loss:

$$e(\boldsymbol{x}) = \left\| \boldsymbol{x} - \boldsymbol{o}^{(L)} \right\|_2^2$$

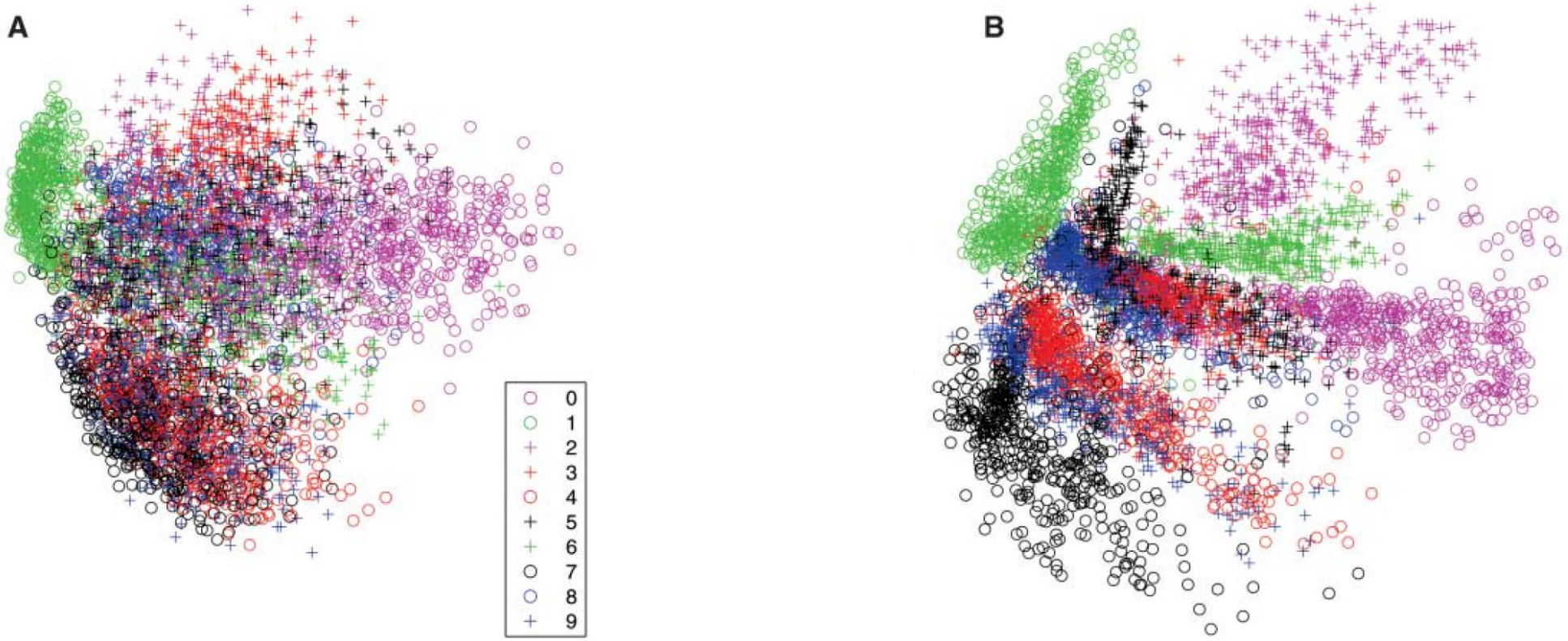
Autoencoders



Deep Autoencoders



Source: https://en.wikipedia.org/wiki/Autoencoder#/media/File:Autoencoder_structure.png



PCA (A) vs. Autoencoders (B) (Hinton and Salakhutdinov, 2006)

Source: https://www.science.org/doi/10.1126/science.1127647

PCA Learning Objectives

You should be able to…

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