10-701: Introduction to Machine Learning Lecture 15: Dimensionality Reduction

Henry Chai

3/13/24

Front Matter

- Announcements
  - HW4 released 2/28, due 3/15 (Friday) at 11:59 PM
  - Midterm exam on 3/19 from **7 – 9 PM in DH A302**
    - If you have a conflict with this date/time fill out the conflict form on Piazza ASAP
  - Final exam date has been announced: Monday, May 6th from 1 – 4 PM
- Recommended Readings
  - Murphy, Chapters 12.2.1 - 12.2.3
  - Daumé III, Chapter 15: Unsupervised Learning

Midterm Exam Logistics

- Format of questions:
  - Multiple choice
  - True / False (with justification)
  - Derivations
  - (*Simple*) Proofs
  - Short answers
  - Drawing & Interpreting figures
  - Implementing algorithms on paper
- No electronic devices (you won’t need them!)
- You are allowed to bring one letter-/A4-size sheet of notes; you can put *whatever* you want on *both sides*

Midterm Exam Topics

- Covered material: Lectures 1 – 13
  - Decision Trees
  - k-NN
  - Linear Regression
  - MLE/MAP
  - Naïve Bayes
  - Logistic Regression
  - Regularization
  - Neural Networks & Backpropagation
  - CNNs & RNNs
  - Attention & Transformers

Midterm Exam Preparation

- Review the exam practice problems (released 3/12 on the course website, under the Recitations tab)
- Attend the dedicated exam 1 review recitation (3/15)
- Review HWs 1 - 4
- Review the key takeaways throughout the lecture slides
- Write your one-page cheat sheet (back and front)

Recipe for K-means

- Define a model and model parameters
  - Assume K clusters and use the Euclidean distance
  - Parameters: $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$ and $z^{(1)}, \ldots, z^{(N)}$
- Write down an objective function

$$\sum_{i=1}^{N} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{\mu}_{z^{(i)}} \right\|_2$$

- Optimize the objective w.r.t. the model parameters
  - Use (block) coordinate descent

K-means Algorithm

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

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:

    $$z^{(i)} = \underset{k}{\operatorname{argmin}} \left\|\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_k\right\|_2$$

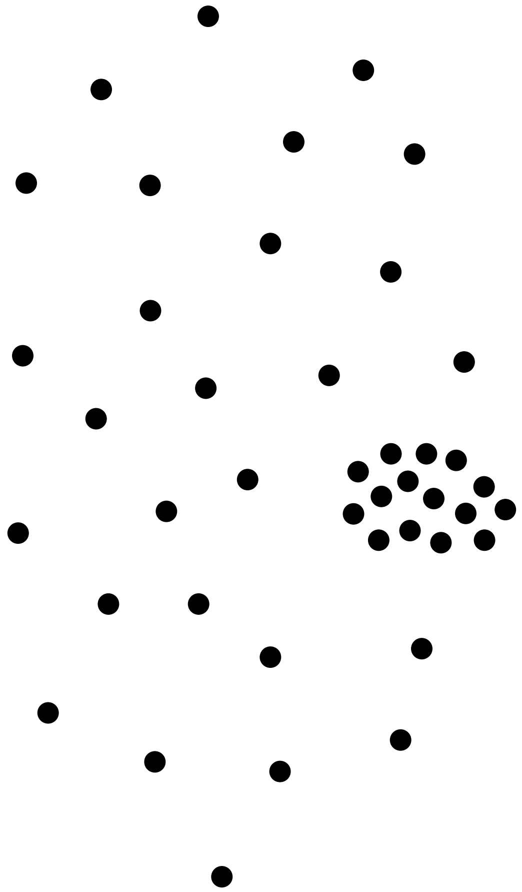
    b. Recompute the cluster centers:

    $$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i\,:z^{(i)}=k} \boldsymbol{x}^{(i)}$$

    where N_k is the number of data points in cluster k

- Output: cluster assignments $z^{(1)}, \ldots, z^{(N)}$

Shortcomings of K-means



- Clusters cannot overlap
- Clusters must all be of the same “width”
- Clusters must be linearly separable

Recipe for GMMs

- Define a model and model parameters
    - Assume K Gaussian clusters
    - Parameters: $\theta = \{\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \Sigma_1, \dots, \Sigma_K, \pi_1, \dots, \pi_K\}$
- Write down an objective function
    - Maximize the log marginal likelihood

$$\ell(\theta|\mathcal{D}) = \log \prod_{i=1}^{N} p\left(\boldsymbol{x}^{(i)} \middle| \theta\right)$$

- Optimize the objective w.r.t. the model parameters
    - Expectation-maximization

Expectation-Maximization for GMMs: Intuition

- Insight: if we knew the cluster assignments, $\boldsymbol{z}^{(i)}$, we could maximize the log complete likelihood instead of the log marginal likelihood
- Idea: replace $\boldsymbol{z}^{(i)}$ in the log complete likelihood with our "best guess" for $\boldsymbol{z}^{(i)}$ given the parameters and the data
- Observation: changing the parameters changes our "best guess" and vice versa
- Approach: iterate between updating our "best guess" and updating the parameters

Expectation-Maximization for GMMs

- Iterative algorithm that alternates between two steps
  - Expectation or E-step: for fixed parameters θ, compute the *expected* assignment vectors conditioned on θ and the data set $\mathcal{D}$

$$E\left[z_k^{(i)} | \boldsymbol{x}^{(i)}, \theta\right] = p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right) \ \forall\, i \text{ and } k$$

  - Maximization or M-step: for fixed assignment vectors $\boldsymbol{z}^{(i)}$, set the parameters θ to *maximize* the complete log likelihood of the data set $\mathcal{D}$
- Under the hood: EM performs block-coordinate ascent on a lower bound of the log marginal likelihood

E-Step for GMMs

$$p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right) = \frac{p\left(z_k^{(i)} = 1, \boldsymbol{x}^{(i)} | \theta\right)}{p(\boldsymbol{x}^{(i)} | \theta)}$$

$$= \frac{p\left(z_k^{(i)} = 1, \boldsymbol{x}^{(i)} | \theta\right)}{\sum_{j=1}^{K} p\left(z_j^{(i)} = 1, \boldsymbol{x}^{(i)} | \theta\right)}$$

$$= \frac{\pi_k N\left(\boldsymbol{x}^{(i)}; \mu_k, \Sigma_k\right)}{\sum_{j=1}^{K} \pi_j N\left(\boldsymbol{x}^{(i)}; \mu_j, \Sigma_j\right)} \ \forall\ i \text{ and } k$$

M-Step for GMMs

Let $N_k = \sum_{i=1}^{N} p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right)$

$$\pi_k = \frac{N_k}{N}$$

$$\mu_k = \frac{1}{N_k} \sum_{i=1}^{N} p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right) \boldsymbol{x}^{(i)}$$

$$\Sigma_k = \frac{1}{N_k} \sum_{i=1}^{N} p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right) \left(\boldsymbol{x}^{(i)} - \mu_k\right)\left(\boldsymbol{x}^{(i)} - \mu_k\right)^T$$

GMM Algorithm

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

1. Initialize all parameters $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \Sigma_1, \dots, \Sigma_K, \pi_1, \dots, \pi_K$
2. While NOT CONVERGED
    a. E-step: compute $p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right) \forall\, i$ and k
    b. M-step: update the parameters

- Output: parameters $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \Sigma_1, \dots, \Sigma_K, \pi_1, \dots, \pi_K$ and assignments probabilities $p\left(z_k^{(i)} = 1 \middle| \boldsymbol{x}^{(i)}, \theta\right) \forall\, i$ and k

Initializing EM for GMMs

- Common heuristics for initialization
  - Cluster proportions typically initialized to be uniform
  - Cluster means
    - Randomly select data points to be cluster centers
    - Randomly sample locations in the range spanned by the data
  - Cluster covariances
    - Identity (or scaled identity) matrix
    - Random positive diagonal matrix
    - Randomly sample L, a lower triangular matrix with positive diagonal entries, and set to LL^{T}
    - Set to the empirical covariance of the data
  - Use multiple random restarts

Terminating EM for GMMs

- Common heuristics for termination
  - Stop if the log complete likelihood changes by less than some tolerance
  - Stop if the parameters and assignment probabilities change by less than some tolerance
  - Stop after a fixed number of iterations

GMMs: Example (Initial)

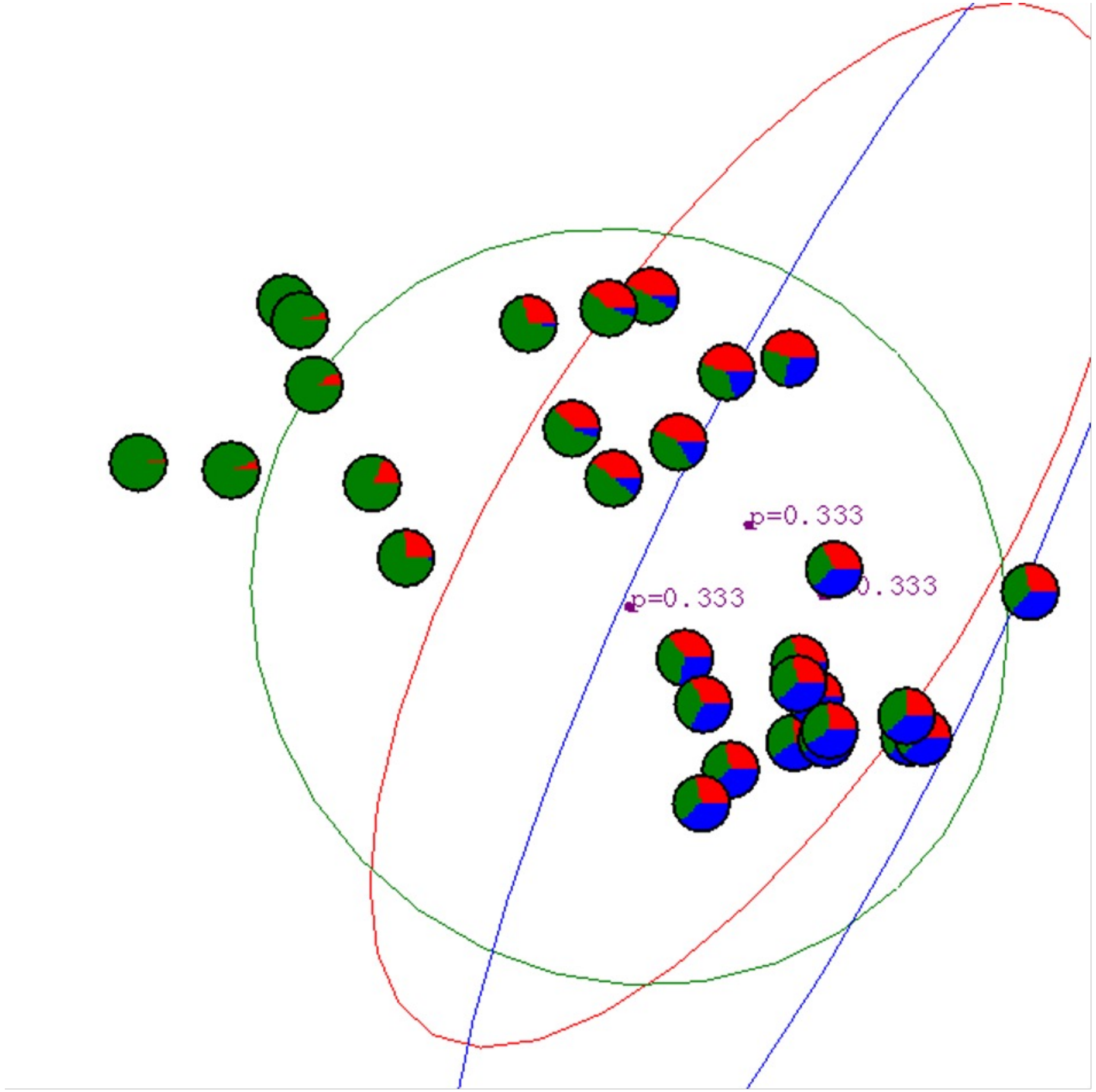


Figure courtesy of Pat Virtue

GMMs: Example (1 Iteration)

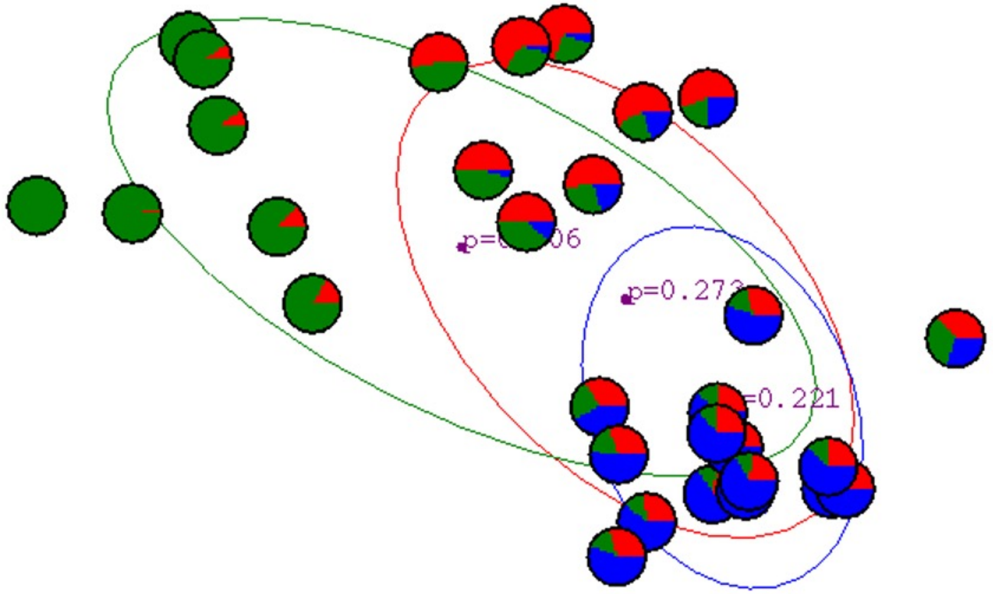


Figure courtesy of Pat Virtue

GMMs: Example (2 Iterations)

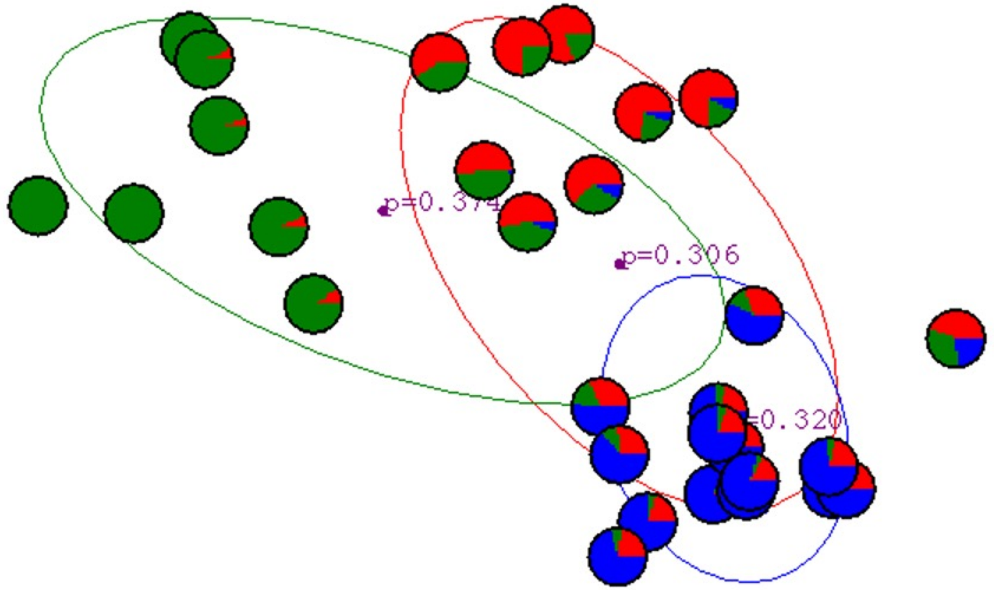


Figure courtesy of Pat Virtue

GMMs: Example (3 Iterations)

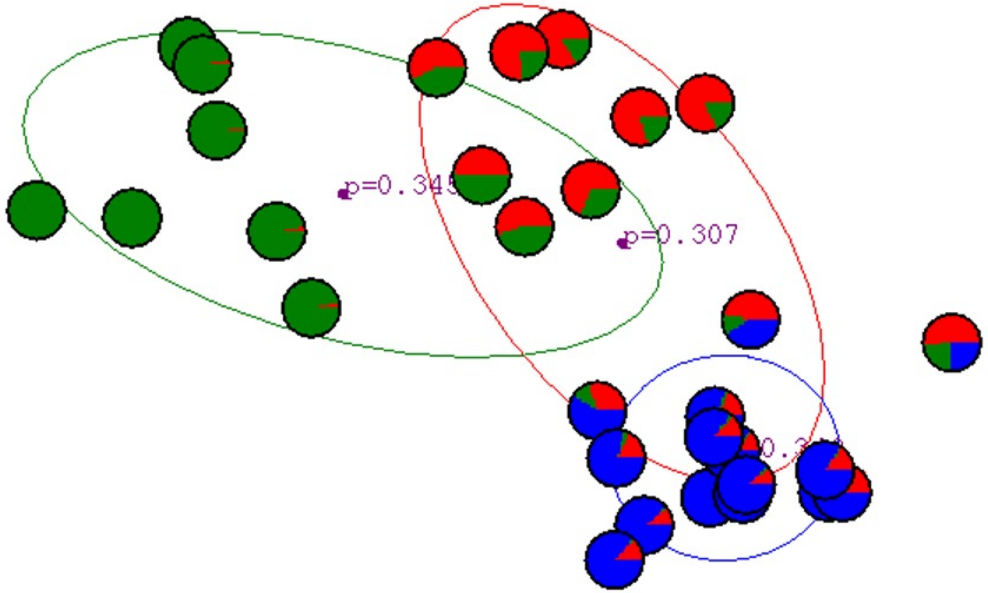


Figure courtesy of Pat Virtue

GMMs: Example (4 Iterations)

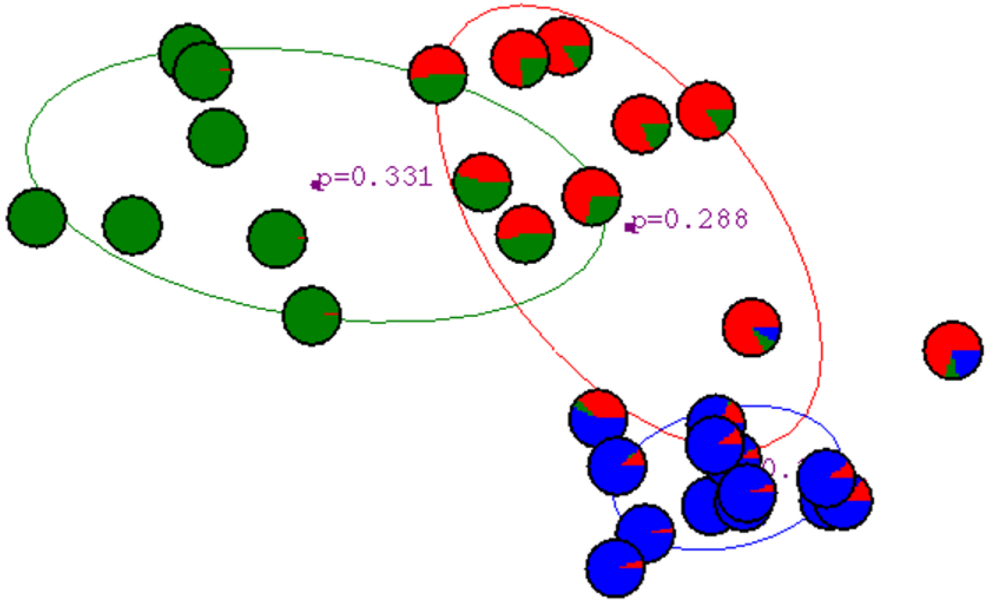


Figure courtesy of Pat Virtue

GMMs: Example (5 Iterations)

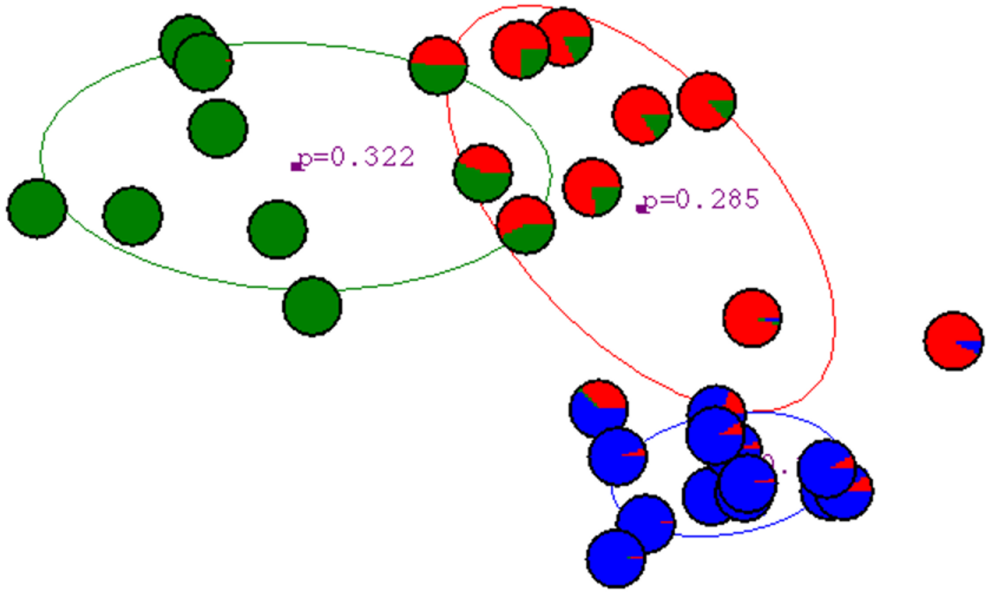


Figure courtesy of Pat Virtue

GMMs: Example (6 Iterations)

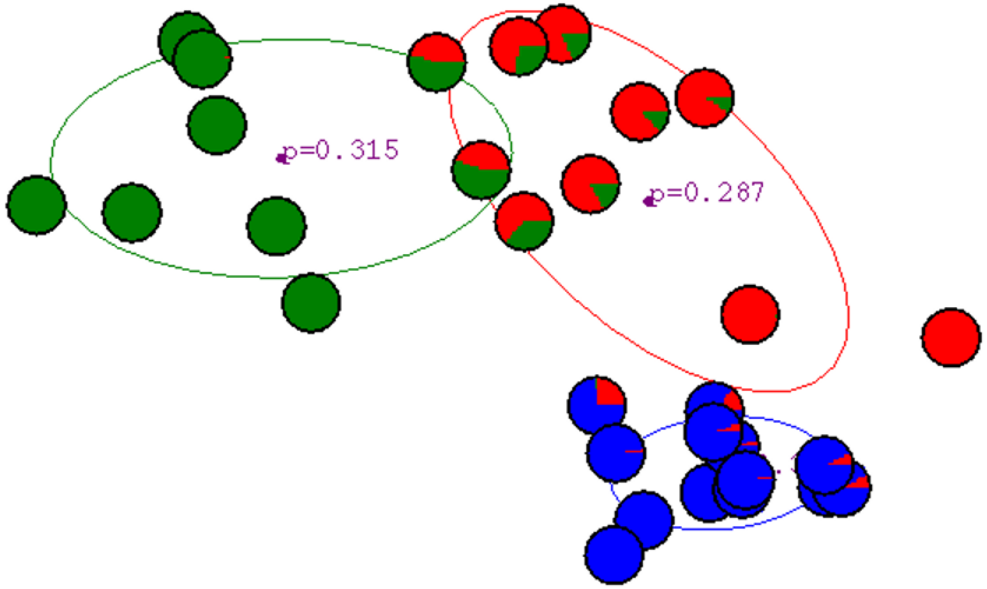


Figure courtesy of Pat Virtue

GMMs: Example (20 Iterations)

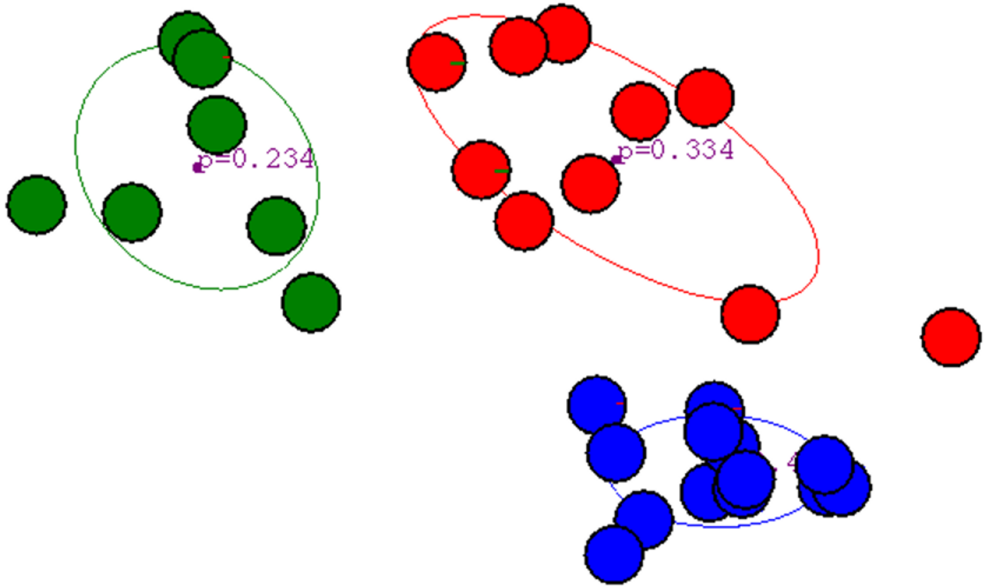


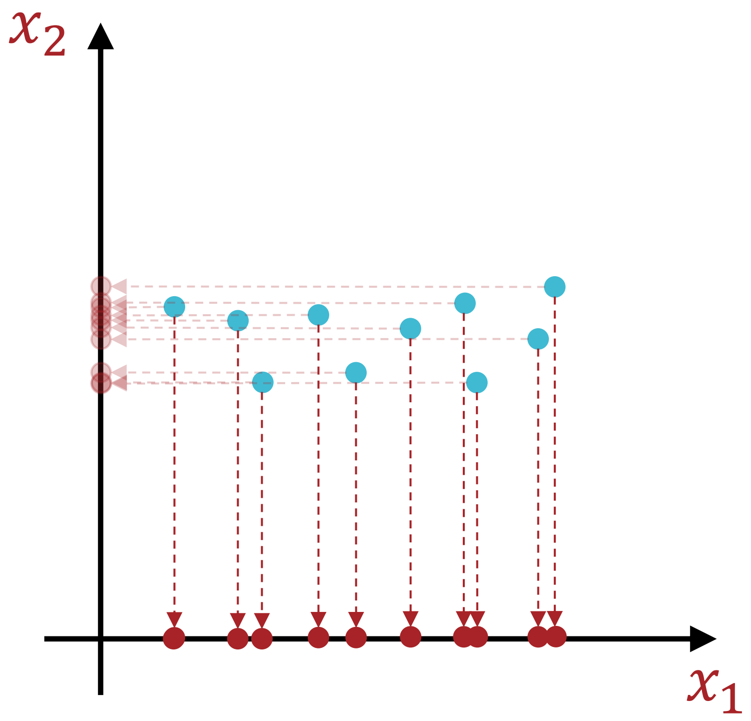
Figure courtesy of Pat Virtue

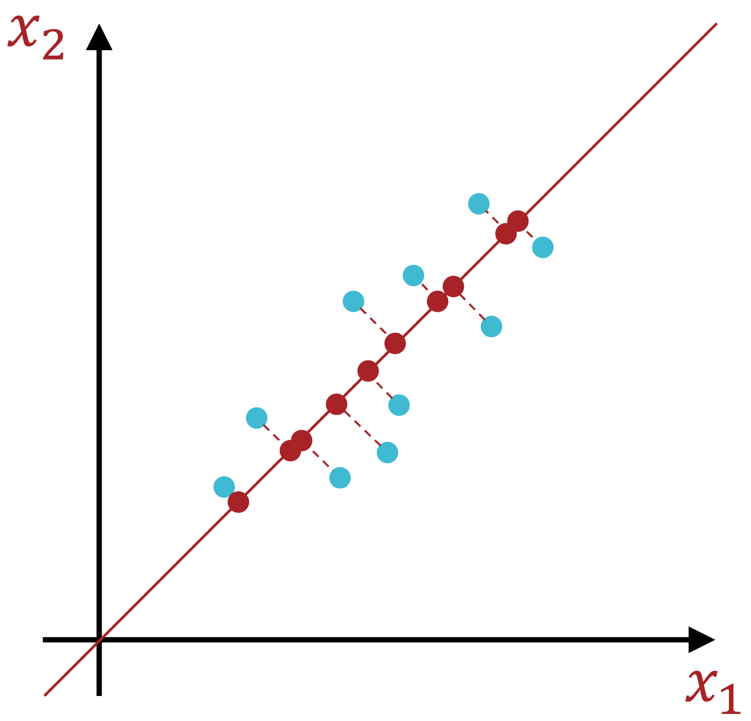
Key Takeaways

- Partition-based clustering
    - K-means (hard assignments)
        - Block-coordinate descent
        - Setting K
        - Initializing K means
    - Gaussian mixture models (probabilistic assignments)
        - Complete vs. marginal likelihood
        - Expectation-maximization for GMMs
        - Initializing EM for GMMs

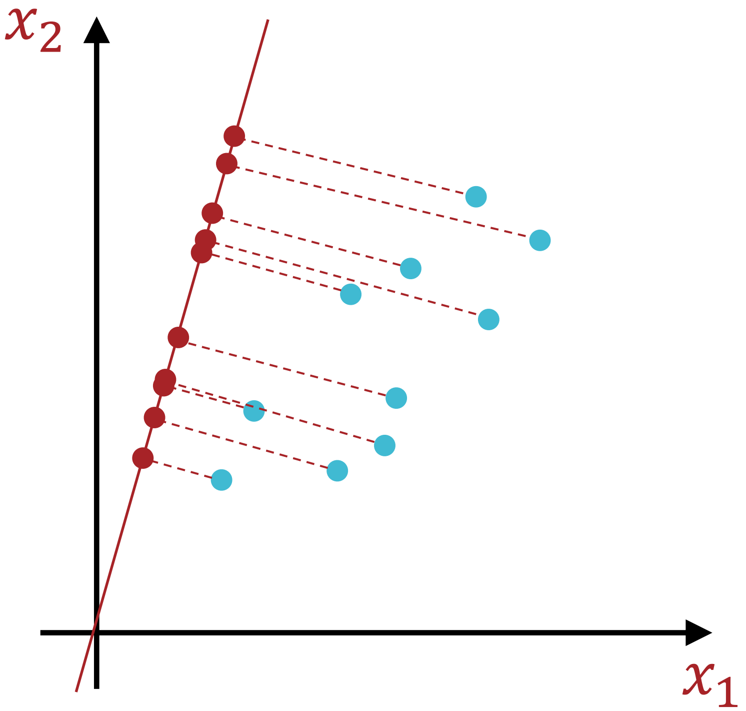
Unsupervised Learning

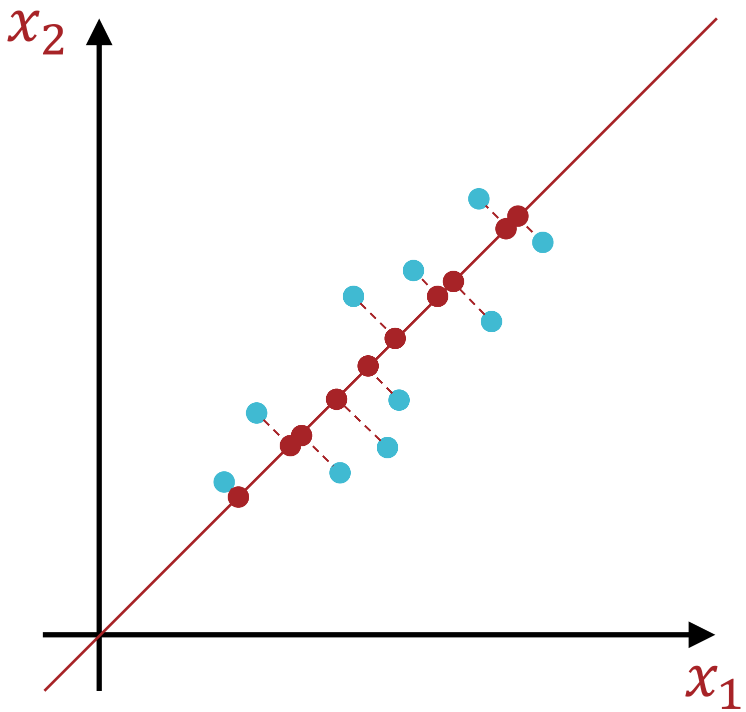
- Clustering: split an unlabeled data set into groups or partitions of “similar” data points
    - Use cases:
        - Organizing data
        - Discovering patterns or structure
        - Preprocessing for downstream tasks
- Dimensionality Reduction: given some unlabeled data set, learn a latent (typically lower-dimensional) representation
    - Use cases:
        - Decreasing computational costs
        - Improving generalization
        - Visualizing data



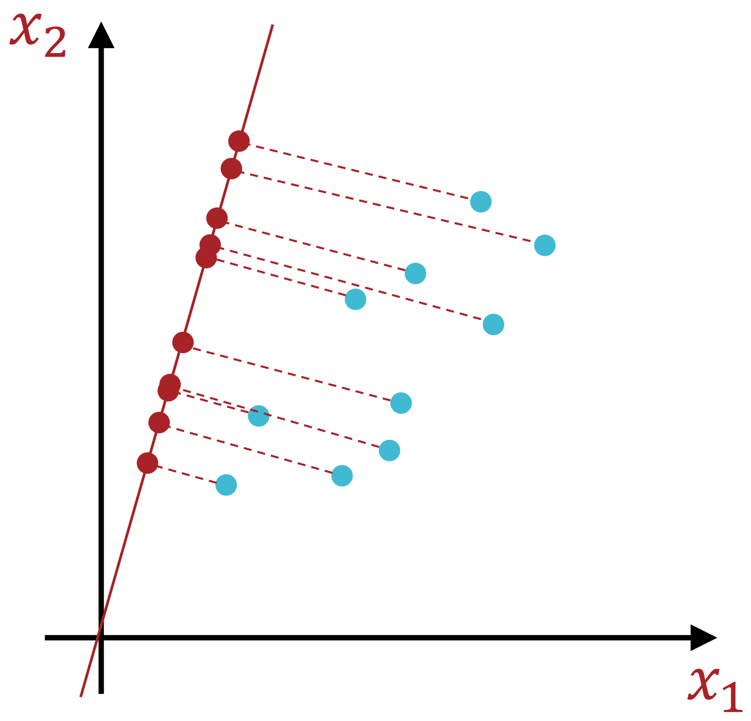


Feature Elimination

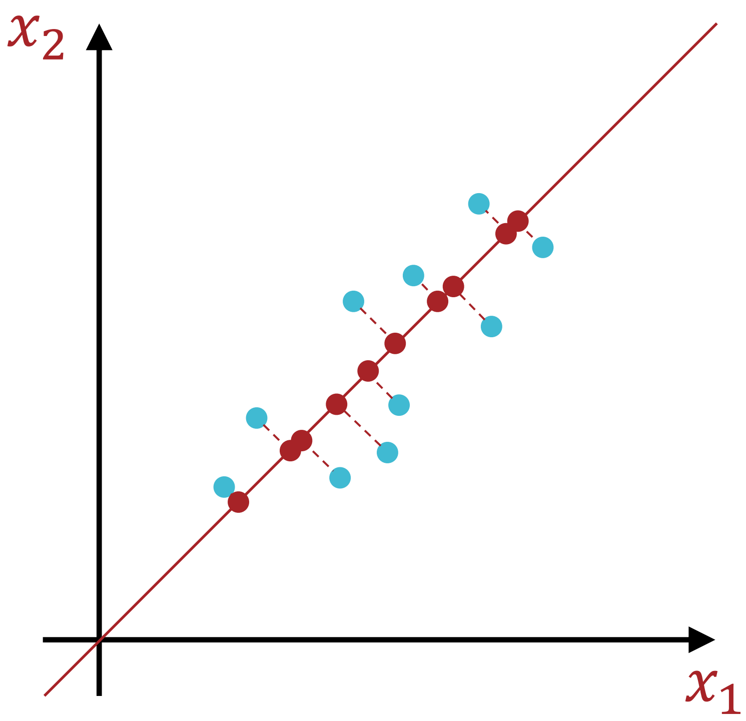




Feature Reduction



Option A



Option B

Which projection do you prefer?

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

Reconstruction Error

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

$$\boldsymbol{z}^{(n)} = \underbrace{\left(\frac{\boldsymbol{v}^T \tilde{\boldsymbol{x}}^{(n)}}{\|\boldsymbol{v}\|_2}\right)}_{\text{Length of projection}} \underbrace{\frac{\boldsymbol{v}}{\|\boldsymbol{v}\|_2}}_{\text{Direction of projection}}$$

Reconstruction Error

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

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

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

$$\left\|\tilde{\boldsymbol{x}}^{(n)} - \left(\boldsymbol{v}^T\tilde{\boldsymbol{x}}^{(n)}\right)\boldsymbol{v}\ \right\|_2^2$$

$$= \tilde{\boldsymbol{x}}^{(n)^T}\tilde{\boldsymbol{x}}^{(n)} - 2\left(\boldsymbol{v}^T\tilde{\boldsymbol{x}}^{(n)}\right)\boldsymbol{v}^T\tilde{\boldsymbol{x}}^{(n)} + \left(\boldsymbol{v}^T\tilde{\boldsymbol{x}}^{(n)}\right)\left(\boldsymbol{v}^T\tilde{\boldsymbol{x}}^{(n)}\right)\boldsymbol{v}^T\boldsymbol{v}$$

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

$$= \left\|\tilde{\boldsymbol{x}}^{(n)}\right\|_2^2 - \left(\boldsymbol{v}^T\tilde{\boldsymbol{x}}^{(n)}\right)^2$$

Minimizing the Reconstruction Error $\Updownarrow$ Maximizing the Variance

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

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

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

Variance of projections ($\tilde{\boldsymbol{x}}^{(n)}$ are centered)

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

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

Maximizing the Variance

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

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

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

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

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

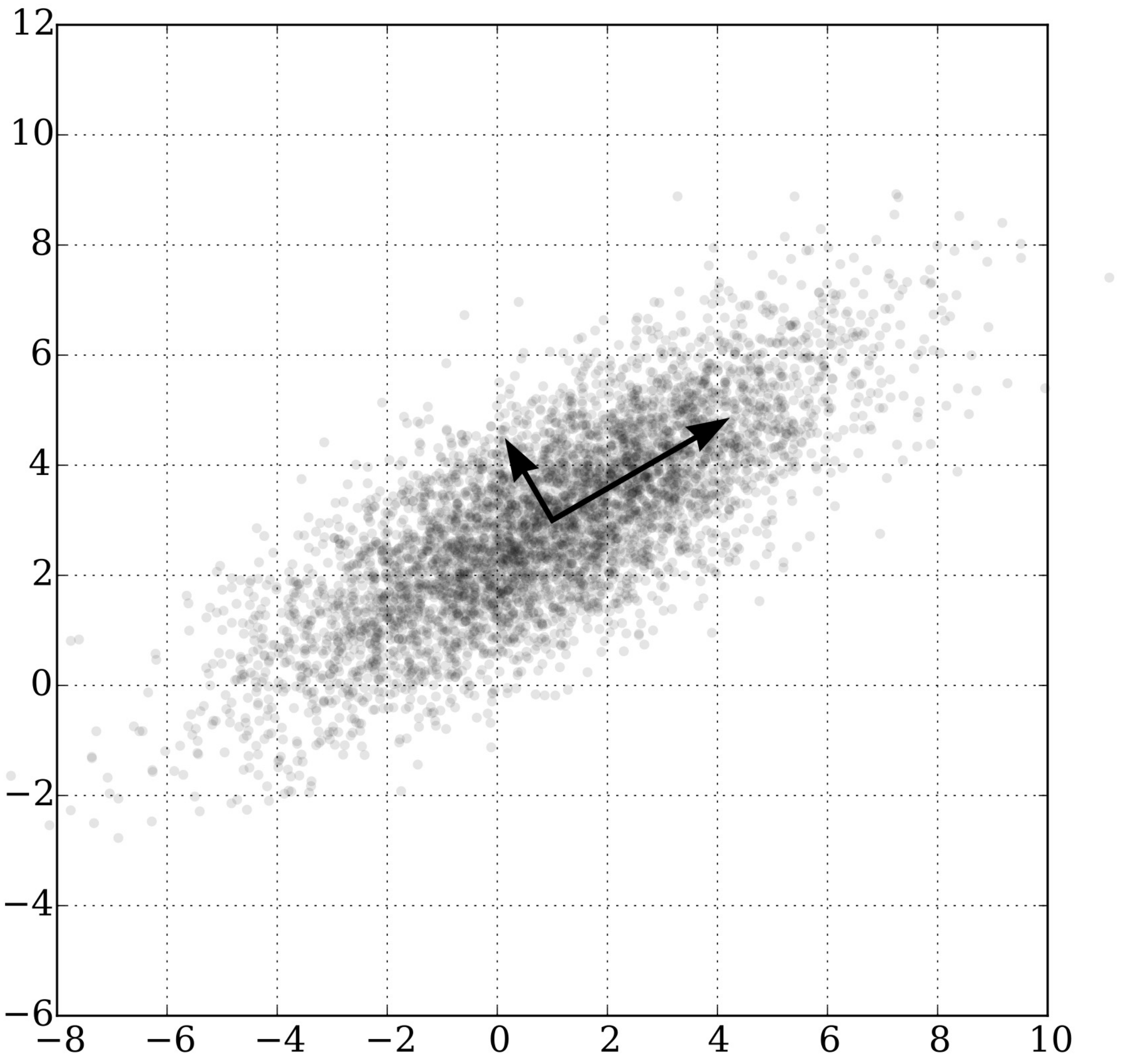
Maximizing the Variance

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

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

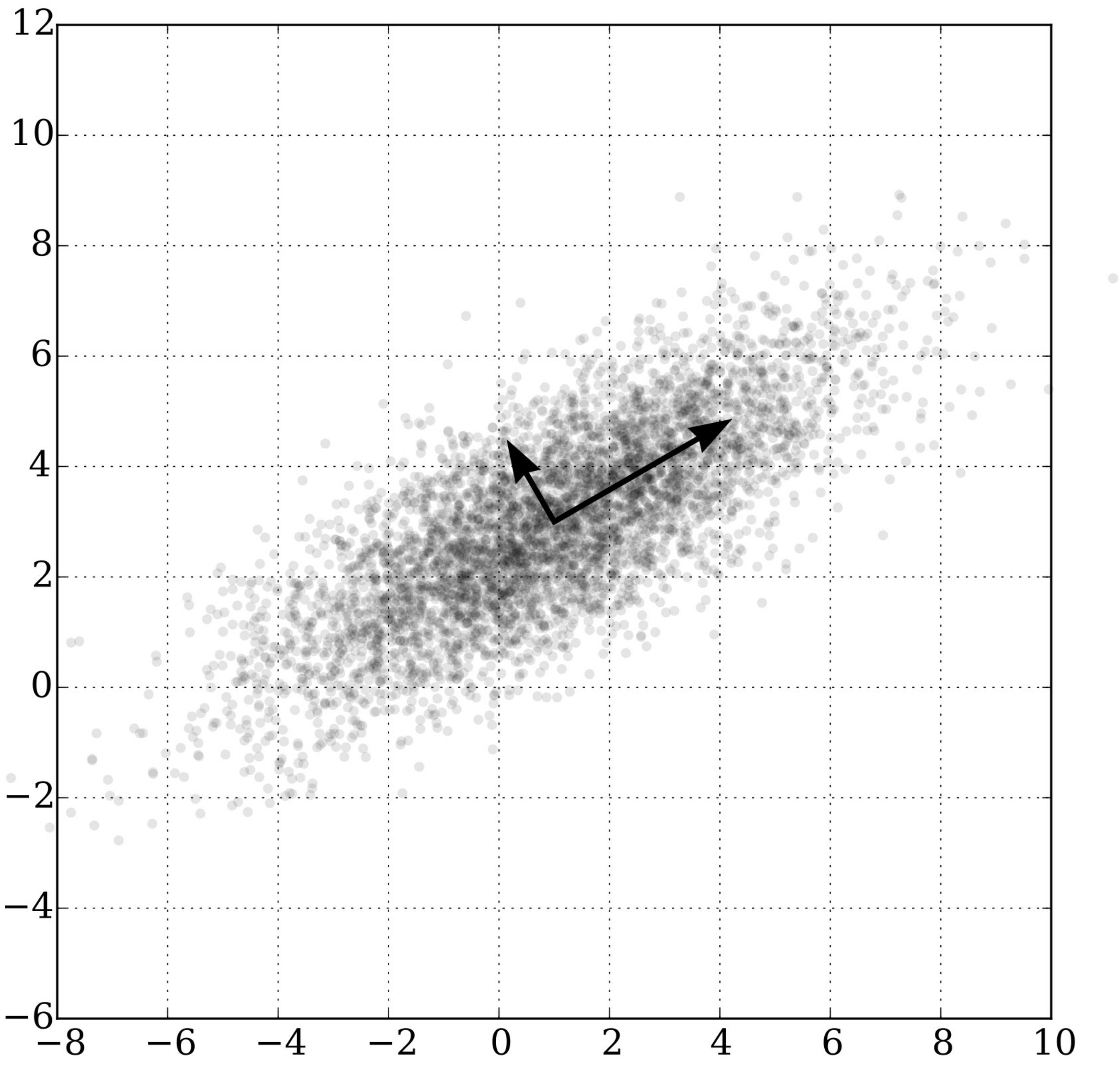
- The first principal component is the eigenvector $\hat{\boldsymbol{v}}_1$ that corresponds to the largest eigenvalue λ_1
- The second principal component is the eigenvector $\hat{\boldsymbol{v}}_2$ that corresponds to the second largest eigenvalue λ_1
  - $\hat{\boldsymbol{v}}_1$ and $\hat{\boldsymbol{v}}_2$ 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)?



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

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^TX
3. $S \in \mathbb{R}^{N \times D}$ - diagonal matrix whose entries are the eigenvalues of X → squared entries are the eigenvalues of XX^T and X^TX

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

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, $Z = X V_\rho$

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

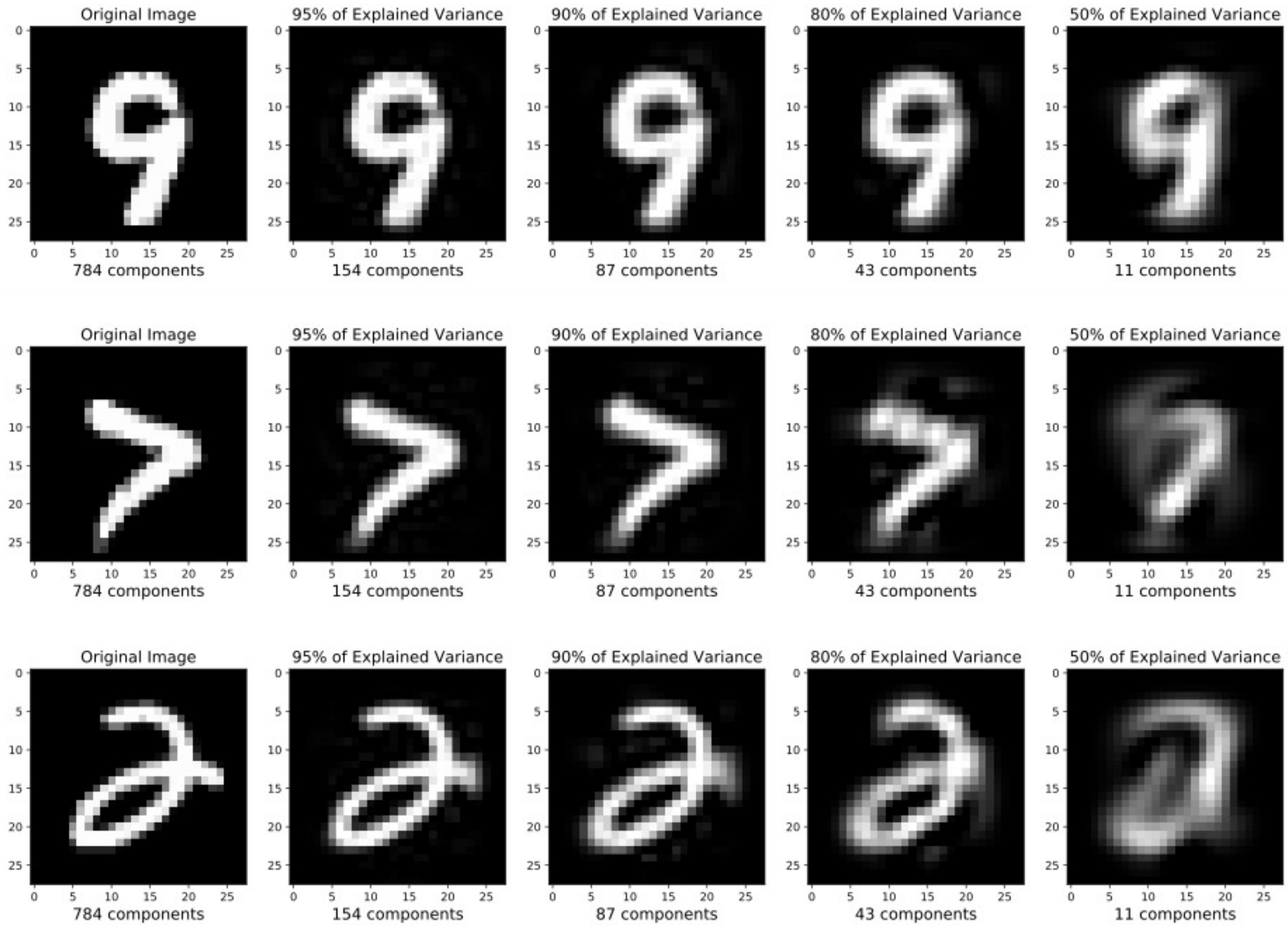
Choosing the number of PCs

- 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

PCA Example: MNIST Digits

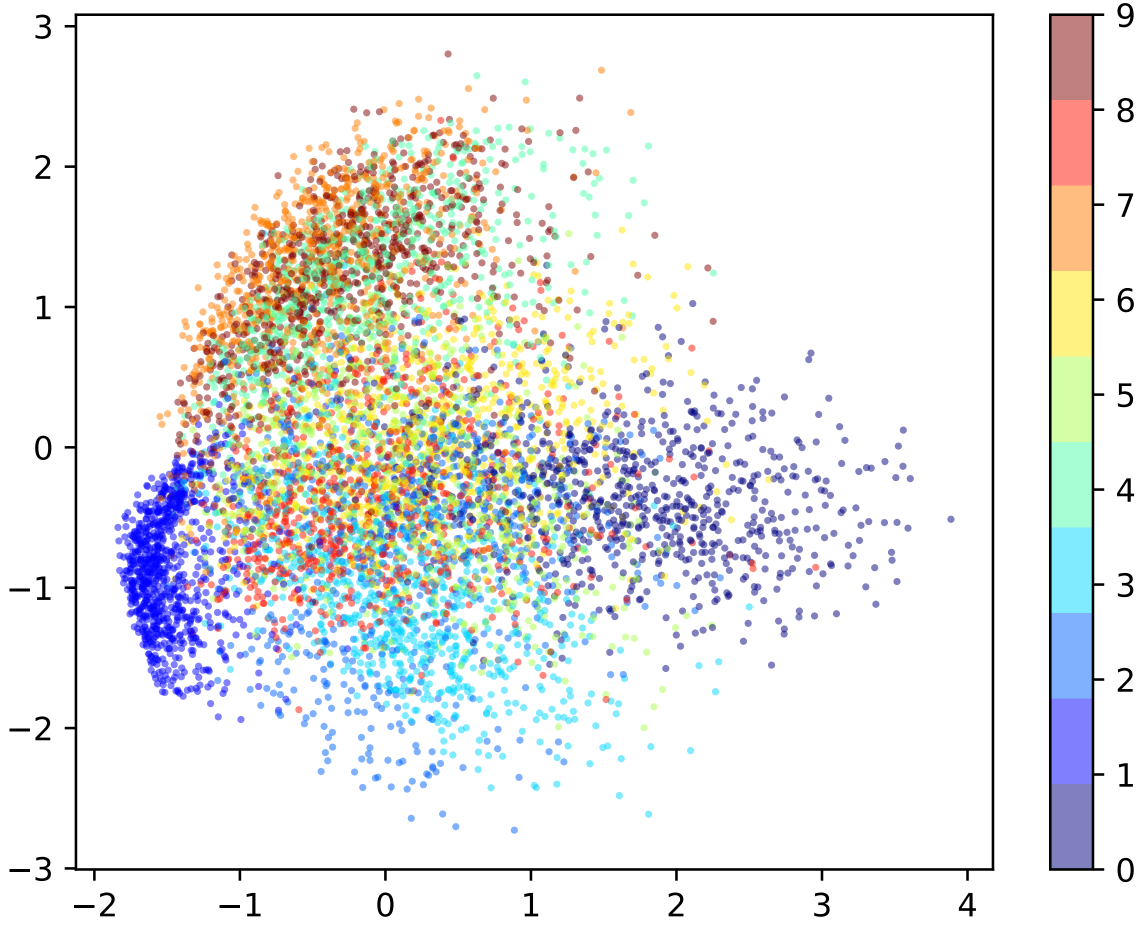


Figure courtesy of Matt Gormley

PCA Example: MNIST Digits

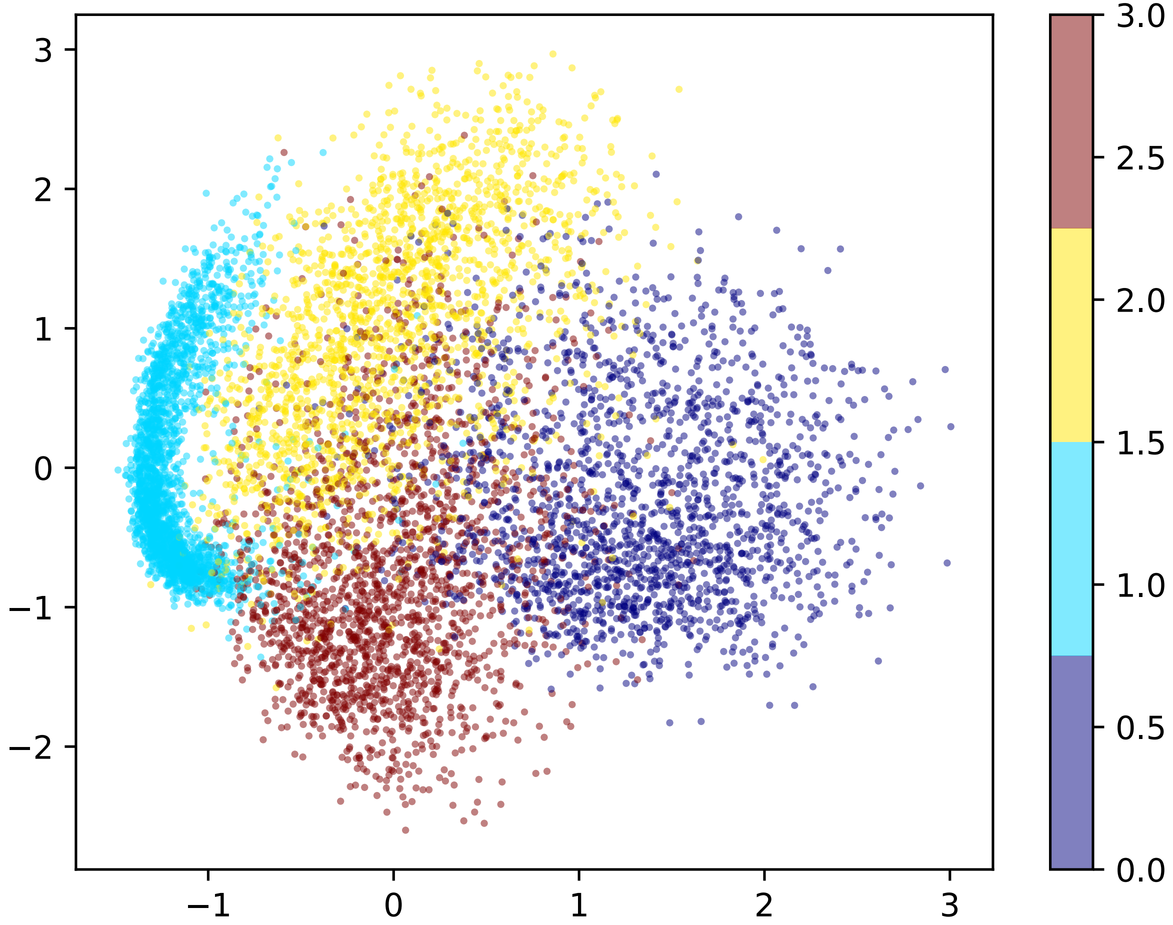
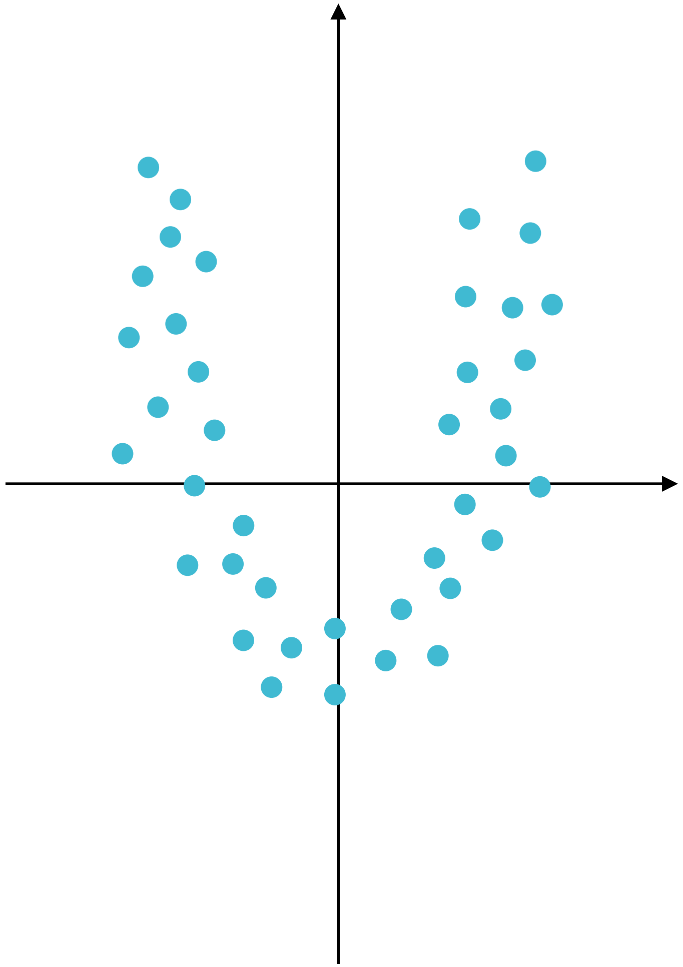


Figure courtesy of Matt Gormley

Shortcomings of PCA



- Principal components are orthogonal (unit) vectors
- Principal components can be expressed as linear combinations of the data