Tools & Models for Data Science

Dimensionality Reduction

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Our Scenario

- We have high dimensional data and we want to make predictions on the data
- ... or we want to classify the data
- but, there’s too much data

? What can we do?

- Note: This is a “What” topic, not a “How” topic

Too much Data Problem

? What can we do?

1. We can use an approach that randomly samples from the data

   ... not today
2. We can throw away data points

   ... that's almost always a bad idea
3. We can throw away features

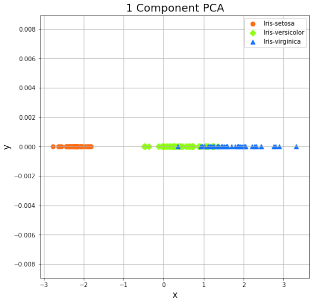
   ... let's explore this option

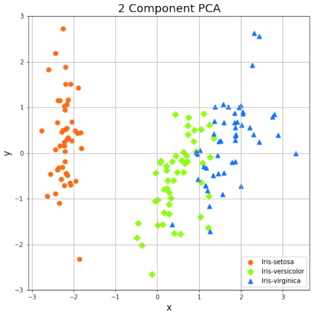
High Dimension Data

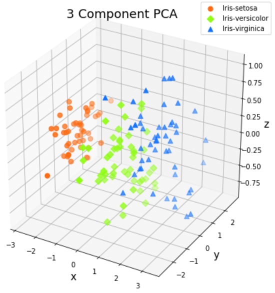
- What do we mean by “high dimension”?
  - Many, many features
  - Can be millions!
  - Lots of useless features obscure useful ones
  - Example: Genomic data
    - Comparing genome sequences
    - Classifying genomes

The Curse of Dimensionality

- "As the number of features or dimensions grows, the amount of data we need to generalize accurately grows exponentially."
  - Charles Isbell, Professor and Senior Associate Dean, School of Interactive Computing, Georgia Tech
- Data become sparse in high dimensions
- All points are basically the same distance from one another







Dimensionality Reduction: Basic Idea

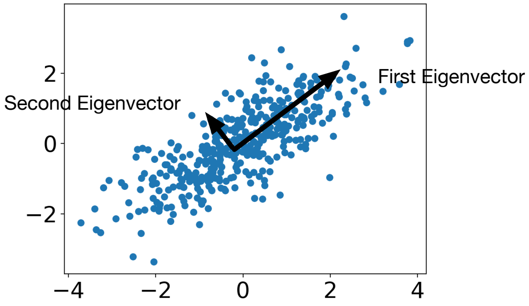
- Keep the dimensions that contain the most information
- Discard the least helpful dimensions
- Get the data down to a manageable size
- This is a type of feature extraction

Dimensionality Reduction vs. Feature Selection

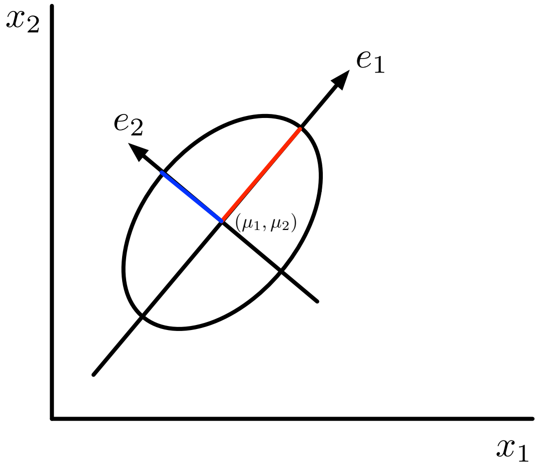
- Creates new, linear combinations of features vs. selecting subsets of features
- Built in attention to correlation
- New features may not be interpretable

How to do Dimensionality Reduction

- Goal: Find the line(s) on which to project the data to show most of the variability
- Approach: Compute a set of orthogonal (perpendicular) basis vectors
- We do this by computing the Eigenvalues and Eigenvectors of the data



Eigenvalues and Eigenvectors



- The ellipse describes the shape of the data
- The length of the red line is the value of the first Eigenvalue
- The length of the blue line is the value of the second Eigenvalue
- Each Eigenvector has direction based on the tilt of the data
- ...and the length is the Eigenvalue

What Does Our Data Look Like?

- **X** is $n \times d$
- $n \ll d$
  - Genomic data
  - Many more dimensions than data points
  - Each row is a patient
  - Each item is a feature: nucleotide, age, fasting blood glucose level, ...
  - Underconstrained / underspecified problem
- $n \gg d$
  - Netflix
  - Lots of users
  - Not so many movies
  - Not so many reviews
  - Not addressed by this approach
  - Overconstrained / overspecified problem

$$\mathbf{X} = n \left\{ \overbrace{\begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & \cdots & \cdots & \cdots & x_{1,d} \\ x_{2,1} & x_{2,2} & \cdots & \cdots & \cdots & \cdots & x_{2,d} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n,1} & x_{n,2} & \cdots & \cdots & \cdots & \cdots & x_{n,d} \end{bmatrix}}^{d} \right.$$

Dimensionality Reduction

- $\mathbf{X}$ can be too big to operate on directly
- We want a linear transform to compute data matrix $\mathbf{X}'$ with a reduced number of dimensions

$$X = n\left\{\overbrace{\begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & x_{1,d} \\ x_{2,1} & x_{2,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & x_{2,d} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n,1} & x_{n,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & x_{n,d} \end{bmatrix}}^{d}\right.$$

$$X' = n\left\{\overbrace{\begin{bmatrix} x'_{1,1} & x'_{1,2} & \cdots & x'_{1,m} \\ x'_{2,1} & x'_{2,2} & \cdots & x'_{2,m} \\ \cdots & \cdots & \cdots & \cdots \\ x'_{n,1} & x'_{n,2} & \cdots & x'_{n,m} \end{bmatrix}}^{m}\right.$$

Computing **X**’

- Linear transform realized by a mapping matrix **W** (d rows, m columns)
- So that $\mathbf{X}' = \mathbf{XW}$

$$\begin{bmatrix} \\ \\ \mathbf{X}' \\ \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \\ \quad\quad\quad\quad\quad\quad \mathbf{X} \quad\quad\quad\quad\quad\quad \\ \\ \\ \end{bmatrix} \times \begin{bmatrix} \\ \\ \\ \quad\quad \mathbf{W} \quad\quad \\ \\ \\ \\ \end{bmatrix}$$

How Big are these Matrices?

- $\mathbf{X}'$ is $n \times m$
- $m \ll d$
- Recall $\mathbf{X}' = \mathbf{X}\mathbf{W}$
- Want to compute **W** such that
- The columns of **W** are the basis functions in the reduced space

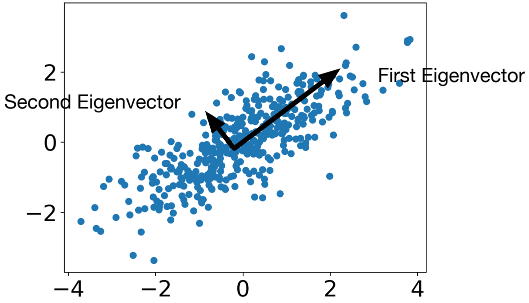
What can $\mathbf{W}$ do?

- $\mathbf{X}' = \mathbf{X}\mathbf{W}$
- It can weight columns by zero
- It can create new columns that are weighted sums of other columns
- $\ldots$

Classic Dimensionality Reduction Method: PCA

- Basic idea: Compute a set of orthogonal (perpendicular) basis vectors
- Then choose most important basis vectors (those with the most variance)
- Those become the rows of the mapping matrix **W**
- Then **XW** projects down onto that basis, giving us $\mathbf{X}'$

? If we want to draw a line that best describes the data, what line do we draw?



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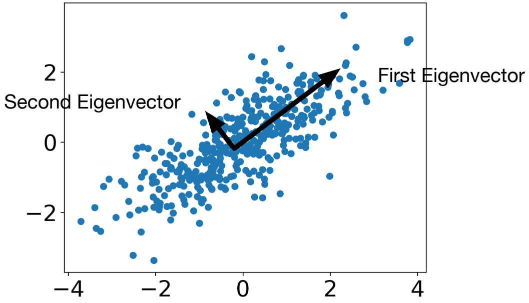
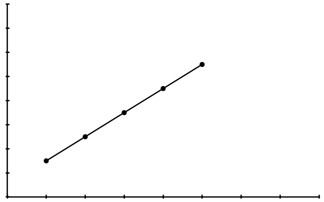
- If we want to draw a line that best describes the data, what line do we draw?
- We draw the first Eigenvector



An Extreme Data Set

- Here there is no variability along the second dimension
- In the extreme case, we could completely drop it
- Note: When $d \gg n$ there will be some dimensions with Eigenvalue = 0



Classic Dimensionality Reduction Method: PCA

- Principal Component Analysis
- We want to lose the least amount of information
- So we remove the dimensions with NO variability
- Note that the number of principle components = the number of dimensions in our data
- We want to drop out the low variance ones that aren't helpful
- For example:
  - If all of our data points are about people who are ages 18 - 19
  - ... or have a fasting blood glucose value in a very narrow, equivalent range
  - That piece of information is highly unlikely to be useful in discriminating between people

Consider the Case of the Multivariate Normal Distribution

- **Z** is an equation variable
- From the data matrix, **X** we get
  - μ is the vector of means, 1 for each dimension
  - Σ is the covariance matrix of **X**
- Each entry, $\sigma_{i,j} = E[(\mathbf{X}_i - \mu_i)(\mathbf{X}_j - \mu_j)]$
- Σ is a symmetric matrix
- If Σ is diagonal
  - The dimensions of **X** are independent
- We leverage the covariance matrix to figure out which dimensions are most important

$$\text{pdf}(\mathbf{Z}) = \frac{exp^{(-\frac{1}{2}(\mathbf{Z}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{Z}-\boldsymbol{\mu}))}}{\sqrt{(2\pi)^k|\Sigma|}}$$

$$\Sigma = \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \cdots & \sigma_{1,d} \\ \sigma_{2,1} & \sigma_{2,2} & \cdots & \sigma_{2,d} \\ \cdots & \cdots & \cdots & \cdots \\ \sigma_{d,1} & \sigma_{d,2} & \cdots & \sigma_{d,d} \end{bmatrix}$$

Consider the Case of the Multivariate Normal Distribution

- From Linear Algebra, we know
  - The Eigenvectors of Σ describe the direction of the spread in **X**
  - The Eigenvalues of Σ describe the magnitude of the Eigenvectors

  - Now we know why we need them
    - To project data onto them to form the mapping matrix **W**
  - We also know what they are
    - They determine the shape and spread of the data cloud

  ? How do we determine the Eigenvalues & Eigenvectors?

How do we determine the Eigenvalues & Eigenvectors?

1. Eigenvalue Decomposition
2. Singular Value Decomposition

Computing the Eigenvalues & Eigenvectors

- Method 1: EVD
- The covariance matrix Σ can be decomposed into $\Sigma = \mathbf{VLV}^T$
- This is the **Eigenvalue Decomposition** of Σ
- Where **L** is a diagonal matrix of values, typically sorted in decreasing order, from left to right
- These values are called Eigenvalues
- The top left value is the largest / most significant
- The columns of **V** are Eigenvectors
- ...and will be sorted by Eigenvalue magnitude
- Each Eigenvalue is how much variance exists across the Eigenvector

Why EVD Doesn’t Work in High Dimensions

- It decomposes the covariance matrix Σ, which is $d \times d$, to get the Eigenvalues and Eigenvectors
- Recall that the $d \gg n$
- Computationally difficult
- The covariance matrix is $d \times d$, so taking the inverse is $O(d^3)$
- This can be done while $d < 50K$ or so
- Once the data gets “big” we can’t use closed form approaches

Why use the Covariance Matrix?

- Because it's square
- Because it describes the relationships between the different dimensions
- It solves the Normal Equation from Linear Regression (closed form solution)
  - $\mathbf{X}r = b$
  - Where r is the vector of regression coefficients
  - and b is the vector of intercept terms
  - Note that we are not guaranteed to have a solution to this equation
  - Because the problem is underconstrained

Why use the Covariance Matrix?

1. $\mathbf{X}r = b$
2. $\mathbf{X}^T\mathbf{X}r = \mathbf{X}^T b$
3. $\frac{1}{n-1}\mathbf{X}^T\mathbf{X}r = \mathbf{X}^T b \frac{1}{n-1}$

1. Normal Equation
2. Multiply both sides by $\mathbf{X}^T$
3. Multiply both sides

- Note that $\frac{1}{n-1}\mathbf{X}^T\mathbf{X}$ is the definition of a covariance matrix, Σ for data with mean 0
- The $n-1$ term gives us a bias free estimator

Solve

$$\frac{1}{n-1}\mathbf{X}^T\mathbf{X}r = \mathbf{X}^T b\frac{1}{n-1}$$

- To solve for r, compute $(\mathbf{X}^T\mathbf{X})^{-1}$
- But this is very expensive to compute
- Instead we can approximate the calculation
- EVD gives the best approximation
- So, we do an EVD of Σ to learn which dimensions are important

Computational Complexity

- Eigenvalue decomposition is $O(d^3)$
- Which leads us to Method 2: Singular Value Decomposition (SVD) of **X**
- In SVD, we operate on **X** directly, instead of Σ because it is smaller
- **X** is $n \times d$ and Σ is $d \times d$
- Recall $n \ll d$

SVD Decomposition

- We want to avoid computing and using covariance matrix Σ because it is $\mathbf{X}^T\mathbf{X}$ and is of size $d \times d$

? Can we get the Eigenvalues and Eigenvectors of Σ by using $\mathbf{X}$ instead?

SVD Decomposition

- We want to avoid computing and using covariance matrix Σ because it is $\mathbf{X}^T\mathbf{X}$ and is of size $d \times d$
- Can we get the Eigenvalues and Eigenvectors of Σ by using $\mathbf{X}$ instead?
- The SVD of $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T$
  - $\mathbf{U}$ is a unitary matrix $(\mathbf{U}\mathbf{U}^T = 1)$
  - $\mathbf{V}$ is matrix of right singular vectors
  - $\mathbf{S}$ is a diagonal matrix of singular values
- Idea is that we can factorize $\mathbf{X}$ instead of Σ
- We can reduce the number of dimensions by projecting onto the space determined by the right singular vectors with the largest values
- In this case, the biggest singular values correspond to the Eigenvalues with the largest magnitude

Using the SVD of $\mathbf{X}$

$$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T$$
$$\mathbf{X}^T\mathbf{X} = (\mathbf{V}\mathbf{S}^T\mathbf{U})(\mathbf{U}\mathbf{S}\mathbf{V}^T)$$
$$= \mathbf{V}\mathbf{S}^T\mathbf{S}\mathbf{V}^T$$

- Where $\mathbf{S}^T\mathbf{S}$ is $\mathbf{L}$ from EVD
- Where $\mathbf{L}$ is a diagonal matrix of values, typically sorted in decreasing order, from left to right

Dimensions & Complexity, Revisited

- $\mathbf{X}$ is $n \times d$
- $\mathbf{X}^T\mathbf{X}$ is $d \times d$
- When $d \gg n$
- EVD is $O(d^3)$, operating on a $d \times d$ covariance matrix
- SVD is $O(\min(d^2n, n^2d))$, because we are operating on $\mathbf{X}$, instead of Σ

How Do We Find the Dimensions with the Most Variance?

- Options
  1. Traditional approach: Eigenvalue Decomposition (EVD)
  2. More efficient approach: Singular Value Decomposition (SVD)
  3. Highly efficient approach: Random Matrix
- Taking into consideration
  - $\mathbf{X}$ is not square
  - So, it can’t have Eigenvalues / Eigenvectors
  - So, we use the covariance matrix Σ instead

Which Dimensions Matter?

- AKA How to Compute the Basis Vectors?

1. Center your data
   - Subtract out the mean in each dimension
   - So the data has mean 0
2. Compute Σ
3. Do the EVD of $\Sigma = \mathbf{V}\mathbf{L}\mathbf{V}^T$
   - Then the basis vectors are the Eigenvectors of data covariance matrix, Σ

$$\Sigma = \frac{\mathbf{X}^T\mathbf{X}}{(n-1)}$$

   - Where Σ is a $d \times d$ matrix
4. Get $\mathbf{W}$ from the vectors in $\mathbf{V}$, using the largest values in $\mathbf{L}$

How to Compute the Basis Vectors?

- From the EVD of $\Sigma = \mathbf{V}\mathbf{L}\mathbf{V}^T$
- Construct mapping matrix $\mathbf{W}$ from the m most important Eigenvectors
- That is, the leftmost columns of $\mathbf{V}$

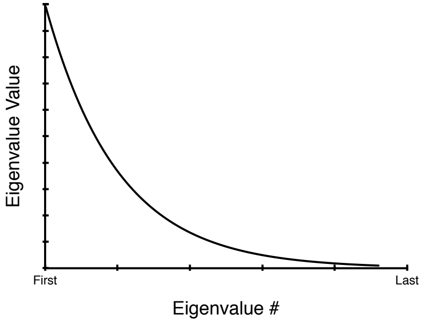
$$\begin{bmatrix} \\ \mathbf{X}' \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \quad\quad\quad \mathbf{X} \quad\quad\quad \\ \\ \end{bmatrix} \times \begin{bmatrix} \\ \\ \quad \mathbf{W} \quad \\ \\ \\ \end{bmatrix}$$

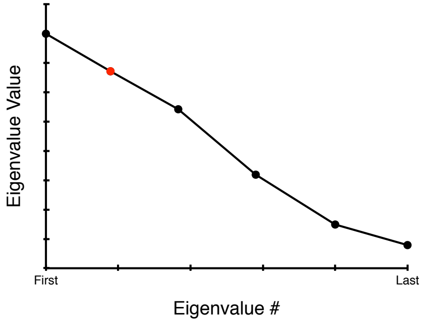
Dimensions

- $\mathbf{X}$ is $n \times d$
- $\mathbf{X}^T\mathbf{X}$ is $d \times d$
- When $d \gg n$
- EVD is $O(d^3)$, operating on a $d \times d$ covariance matrix
- SVD is $O(\min(d^2n, n^2d))$, because we are operating on $\mathbf{X}$, instead of Σ

How Many Eigenvectors to Use?

- There's no magic number
- Look at the values
- Decide how many you can handle, computationally
- Red point is probably not a good choice to stop including Eigenvectors





Even SVD Can Be Too Expensive

- In practice, just fill **W** with samples from Normal$(0, 1)$
  - Known as a random projection[1]
  - Often does a very nice job in practice!
  - Johnson-Lindenstrauss Lemma
    - Basic premise is that the distances between points in a high dimensional space are “nearly preserved” when they are projected on to a large enough random subspace

[1] Bingham E, Mannila H, editors. Random projection in dimensionality reduction: applications to image and text data. Proceedings of the seventh ACM SIGKDD international conference on Knowledge discovery and data mining; 2001: ACM.

Summary Motivation

- Why do it at all?
  - Counteract the Curse of Dimensionality
  - Reduce computational burden

Summary of Methods

- PCA via Eigenvalue decomposition
  - Classic approach
  - Can be difficult for even good software to do the math correctly (consider ill-conditioned matrices)
- PCA via SVD
  - Avoids the covariance matrix entirely, we operate directly on $\mathbf{X}$
  - Considered more stable numerically
  - Computationally faster
  - But still very expensive
  - Results in the same $\mathbf{W}$
- Random Projections
  - Not as precise
  - May not get the dimensions with the most variance
  - But is computationally feasible

Questions?

- What do we know now that we didn’t know before?
  - We know what the curse of dimensionality is and why it is a problem
  - We know that it’s possible to reduce the dimensions of our data
  - We know some approaches to perform dimensionality reduction
  - We know some trade-offs between the approaches
- How can we use what we learned today?
  - We can choose an appropriate method for dimensionality reduction