

# EEP 596: Adv Intro ML || Lecture 10

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Univ. of Washington, Seattle

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# Last Time

- tSNE
- Agglomerative Clustering

# Lectures and Programming Assignments

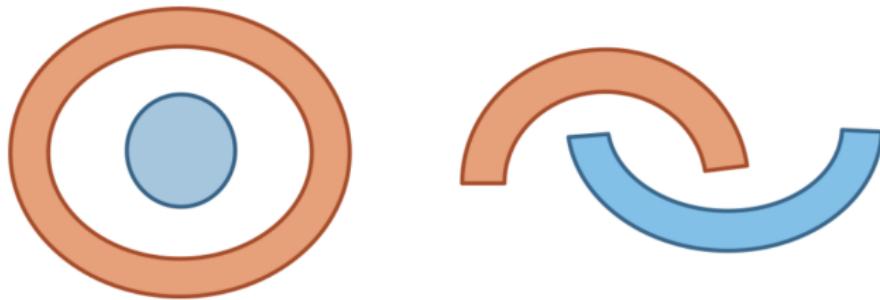
Week	Lecture Material	Assignment
1	Linear Regression	Housing Price Prediction
2	Classification	Spam classification (Kaggle)
3	Classification	Flower/Leaf classification
4	<b>Clustering</b>	MNIST digits clustering
5	Anomaly Detection	Crypto Prediction (Kaggle + P)
6	<b>Data Visualization and Embeddings</b>	Crypto Prediction (Kaggle + P)
7	Deep Learning	Visualizing 1000 images
8	Deep Learning (DL)	ECG Arrhythmia Detection
9	DL in NLP	TwitterSentiment Analysis (Kaggle + P)
10	DLs in Vision	TwitterSentiment Analysis (Kaggle + P)

# Today

- ⓐ Agglomerative Clustering Wrap up
- ⓑ SVD and Dimensionality Reduction
- ⓒ Word2Vec and X2Vec

# Agglomerative Clustering: Spiral and Donut!

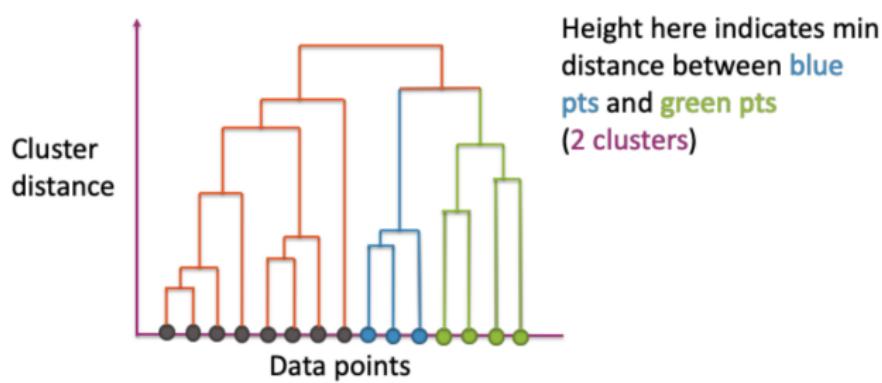
With agglomerative clustering, we are now very able to learn weirder clusterings like



# Dendrogram

x-axis shows the datapoints (arranged in a very particular order)

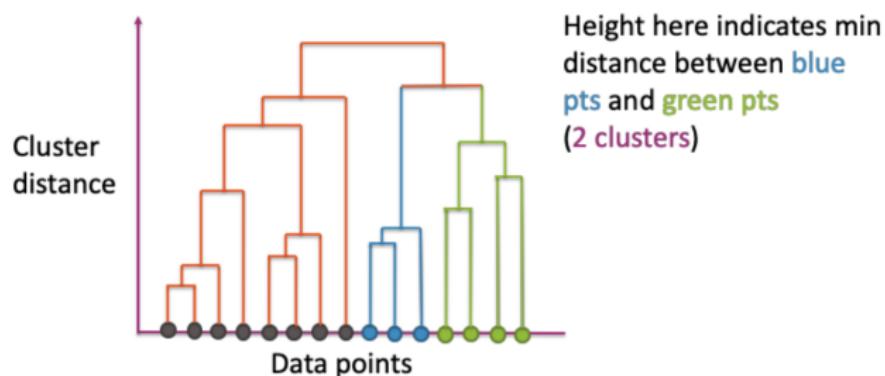
y-axis shows distance between pairs of clusters



# Dendrogram

x-axis shows the datapoints (arranged in a very particular order)

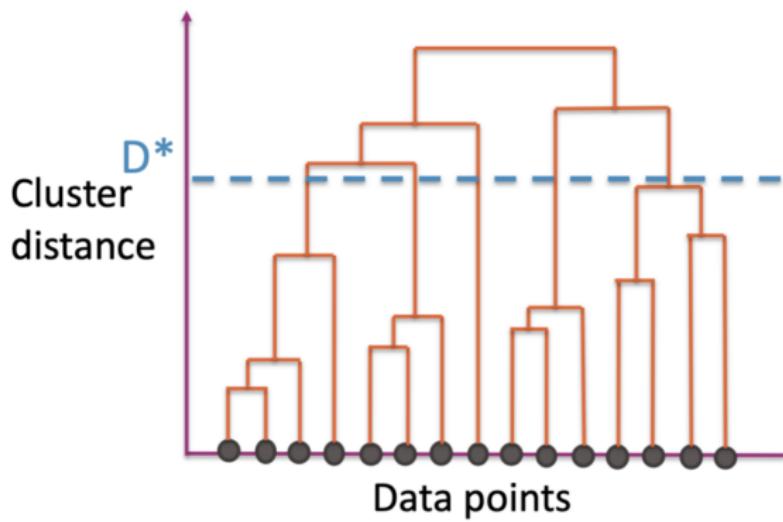
y-axis shows distance between pairs of clusters



# Cut Dendrogram

Choose a distance  $D^*$  to “cut” the dendrogram

- Use the largest clusters with distance  $< D^*$
- Usually ignore the idea of the nested clusters after cutting

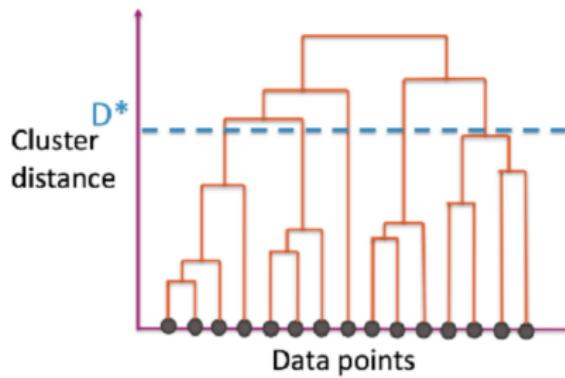


# Dendrogram ICE

## ICE #2

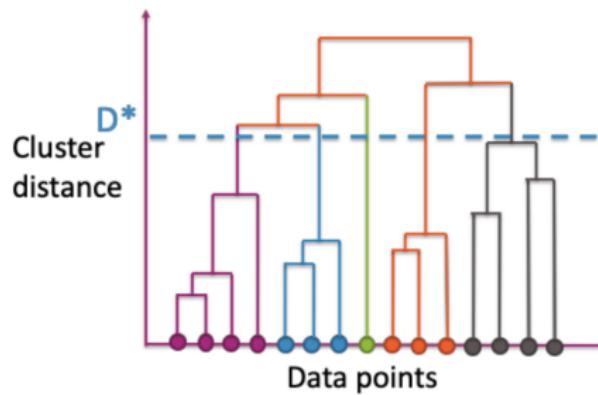
How many clusters would we have if we use this threshold to cut?

- a 4
- b 5
- c 6
- d 7



# Cut Dendrogram

Every branch that crosses  $D^*$  becomes its own cluster



# Agglomerative Clustering — Hyper-parameters

For agglomerative clustering, you need to make the following choices:

- Distance metric  $d(x_i, x_j)$

- Linkage function

- Single Linkage:

$$\min_{x_i \in C_1, x_j \in C_2} d(x_i, x_j)$$

- Complete Linkage:

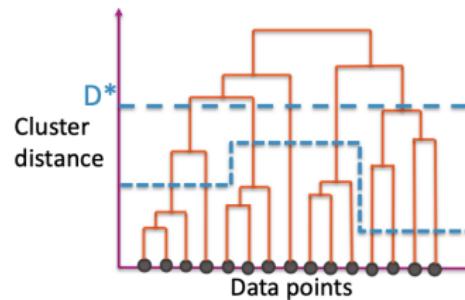
$$\max_{x_i \in C_1, x_j \in C_2} d(x_i, x_j)$$

- Centroid Linkage

$$d(\mu_1, \mu_2)$$

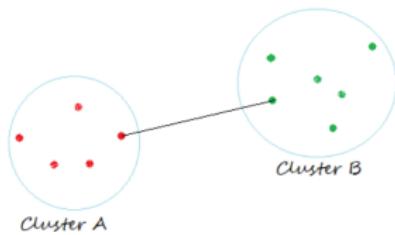
- Others

- Where and how to cut dendrogram

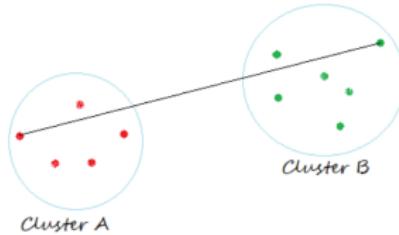


# Linkage examples

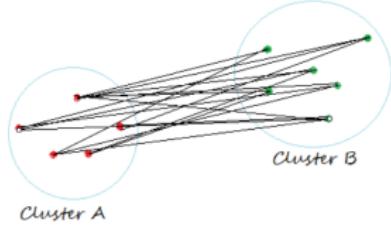
Single Linkage



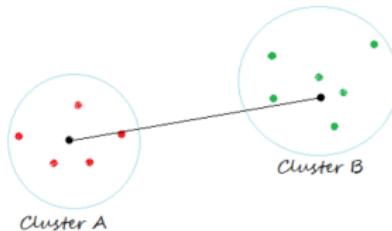
Complete Linkage



Average Linkage



Centroid Linkage



# Dendrogram ICE

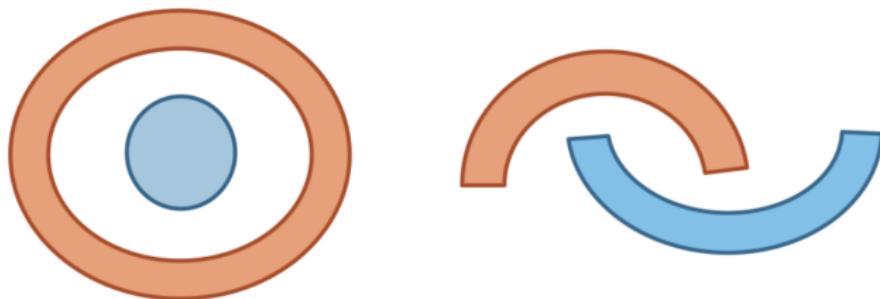
## ICE #1

Which linkage function is more likely to detect spiral clusters?

- a Single Linkage
- b Centroid Linkage
- c Complete Linkage
- d Any Linkage

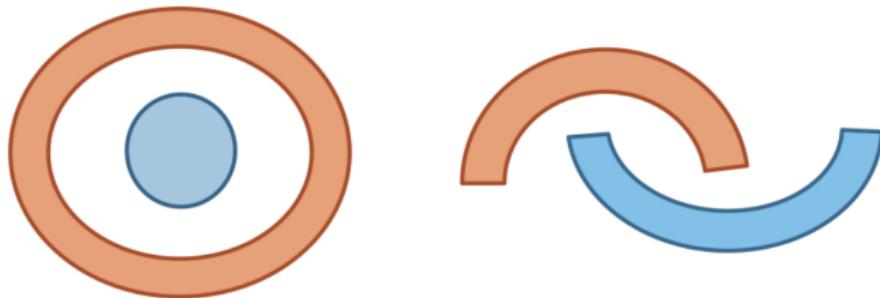
# Centroid Linkage Applied to Spiral

With agglomerative clustering, we are now very able to learn weirder clusterings like

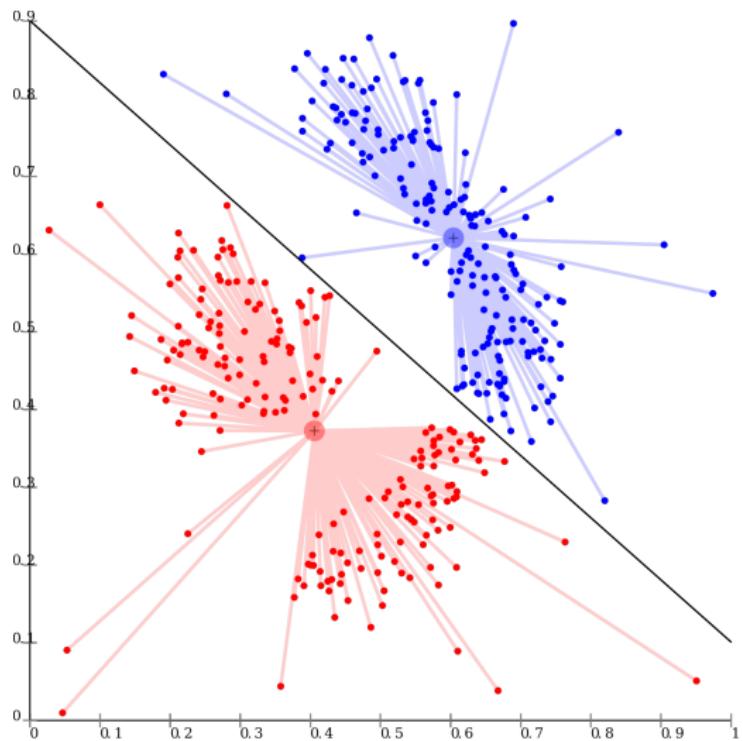


# Single Linkage Applied to Spiral

With agglomerative clustering, we are now very able to learn weirder clusterings like



# Where Centroid Linkage Works!



# Dendrogram

For visualization, generally a smaller # of clusters is better

For tasks like outlier detection, cut based on:

- Distance threshold
- Or some other metric that tries to measure how big the distance increased after a merge

No matter what metric or what threshold you use, no method is “incorrect”. Some are just more useful than others.

# Dendrogram

Computing all pairs of distances is pretty expensive!

- A simple implementation takes  $\mathcal{O}(n^2 \log(n))$

Can be much implemented more cleverly by taking advantage of the **triangle inequality**

- “Any side of a triangle must be less than the sum of its sides”

Best known algorithm is  $\mathcal{O}(n^2)$

# Comparison of Clustering Algorithms

## Quick comparison

	k-means	Agglomerative Clustering
Computation	$O(Ndk)$	$O(N^2d)$
Type	Spherical	Arbitrary shapes

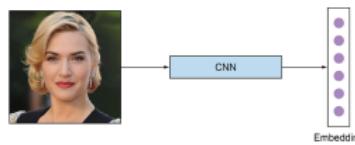
## Few more points..

- a) Weigh computational complexity with complexity of clustering - kmeans vs agglomerative
- b) Agglomerative distance choices yield different sets of clusters (single linkage vs centroid)
- c) Clustering in practice is an art
- d) However, quality of clustering can be evaluated - E.g. through Dunn Index!

# Dimensionality Reduction and Embeddings

## Basic Idea of Embeddings

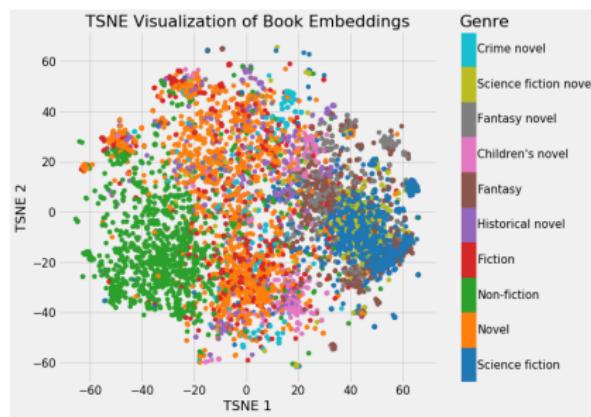
Can you capture information in an image concisely, in a vector? Perhaps a 500x500 pixel image can be reduced to a 256 dimensional vector,  $z$  and  $z$  may have most of the information about the original image that can help you make predictions on the image - Say image classification or object detection or image captioning! Say you have 300k words in a vocabulary. Can you capture the semantics and information contained in each word concisely, maybe through a 512 dimensional vector? Perhaps this representation can help you solve a word riddle such as: "*What is King - Man + Woman?*" Concise representations of this kind are referred to as Embeddings.



# Dimensionality Reduction and Embeddings

## Today

Today we will learn about embeddings learned through SVD and one specifically for words as well. Embeddings also overlap with the idea of dimensionality reduction - Which can also serve the purpose of compressing data. **What's an application of data compression that we use on a daily basis?**



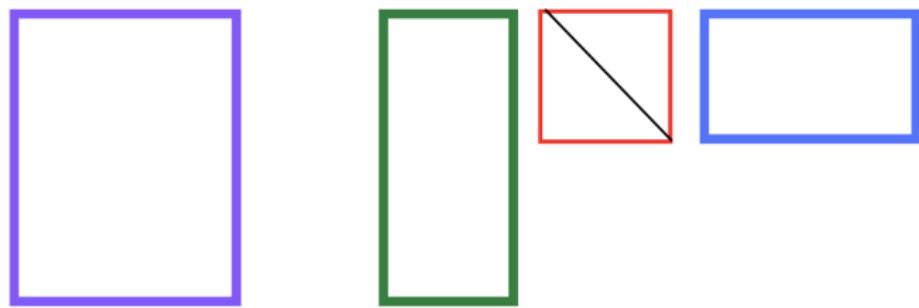
# SVD - Classic Method

## SVD

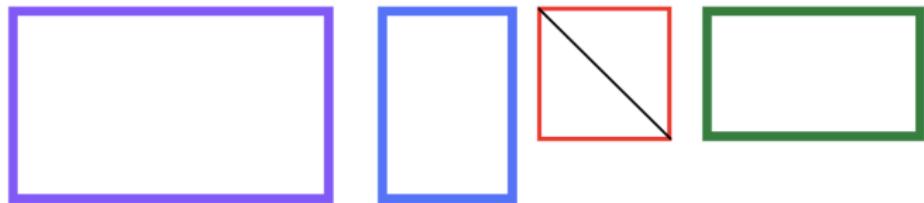
Every matrix  $X \in \mathcal{R}^{m \times n}$  has a Singular Value Decomposition:

$$X = U\Sigma V^T$$

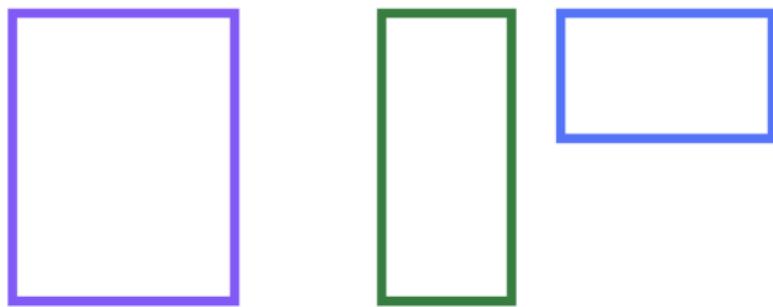
# SVD Example



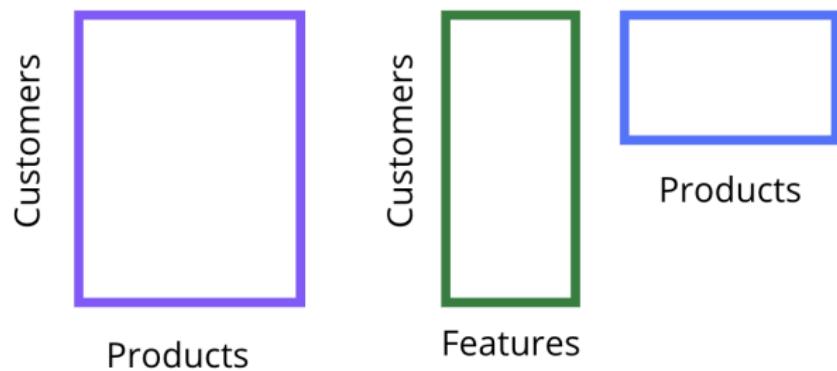
# SVD Example



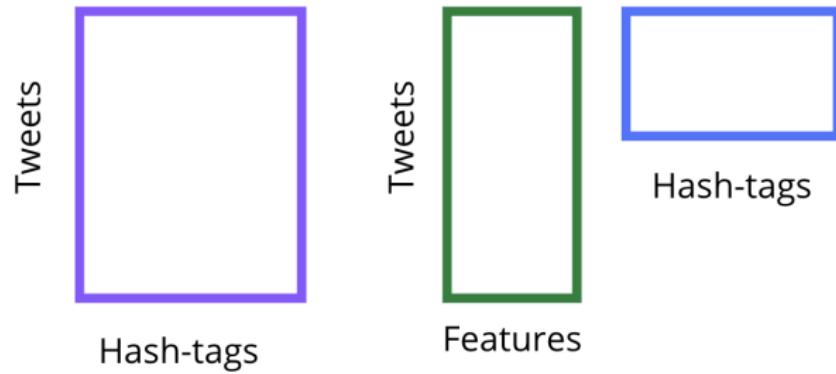
# SVD Example



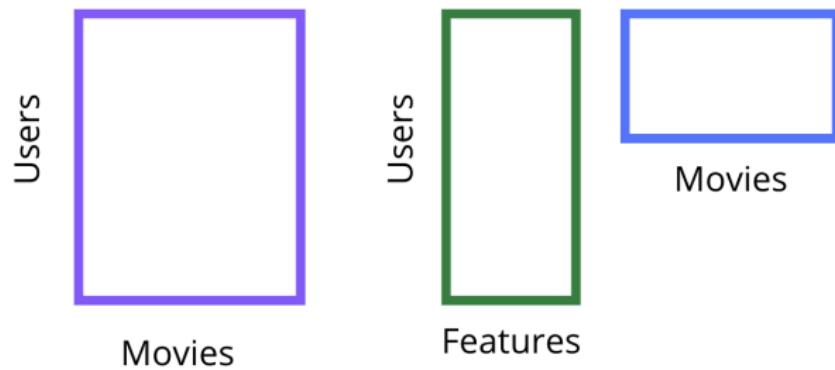
# SVD Example



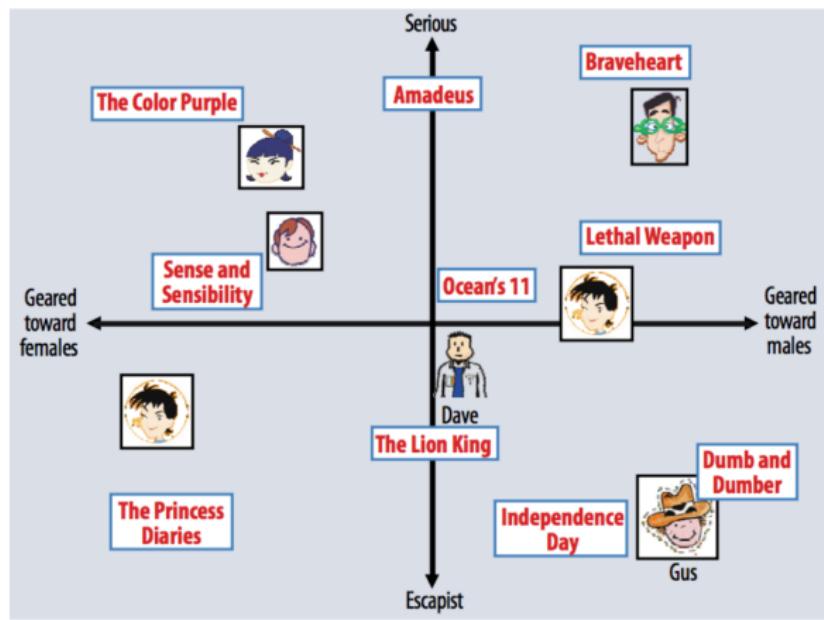
# SVD Example



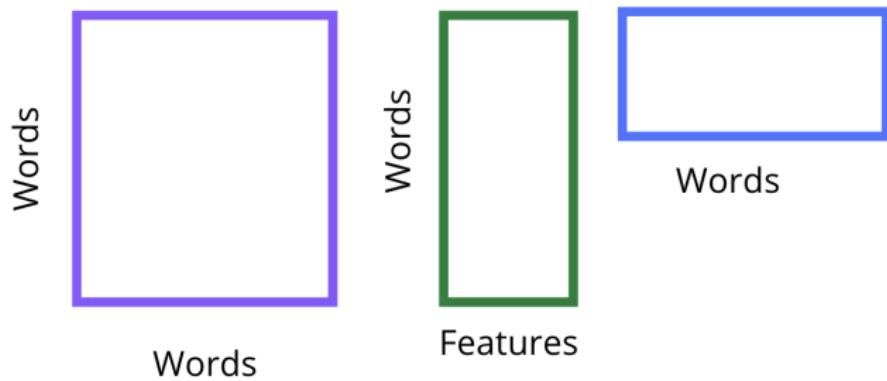
# SVD Example



# SVD Example



# SVD Example



# Word co-occurrence

## Example Sentence

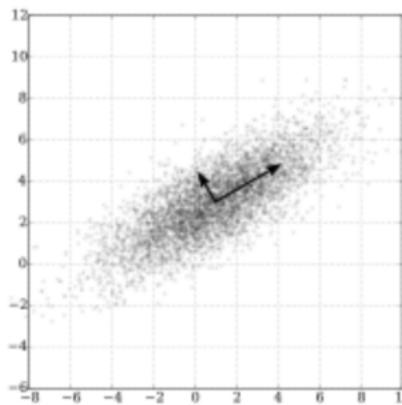
I like NLP. I enjoy flying. I like deep learning.

$$X = \begin{bmatrix} & I & like & enjoy & deep & learning & NLP & flying & . \\ I & 0 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ like & 2 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ enjoy & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ deep & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ learning & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ NLP & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ flying & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ . & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \end{bmatrix}$$

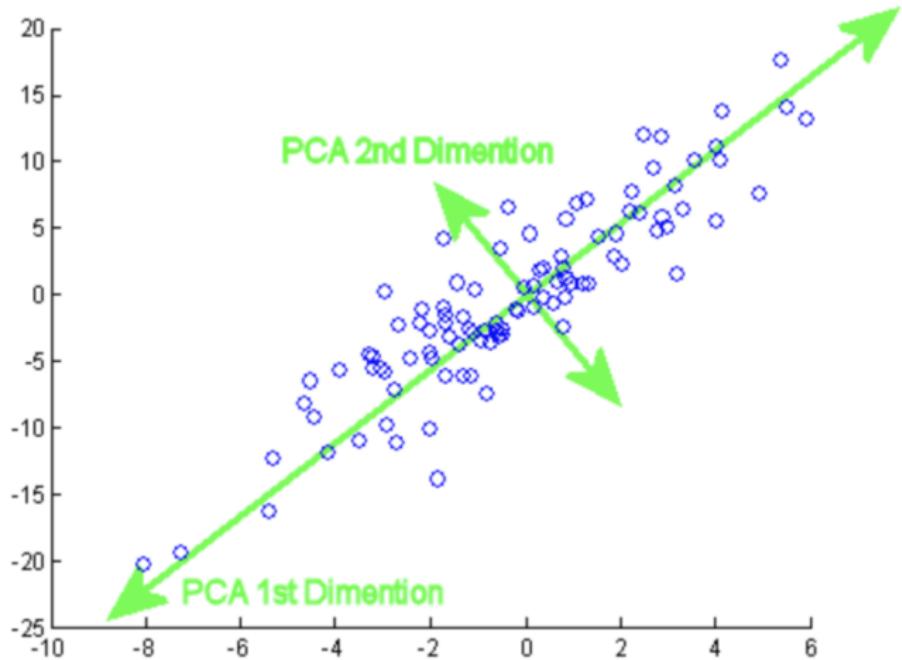
# Other Popular Low-dimensional Embeddings

## PCA

Principal components Analysis (based on SVD) tells us the direction of maximum variance in the data!



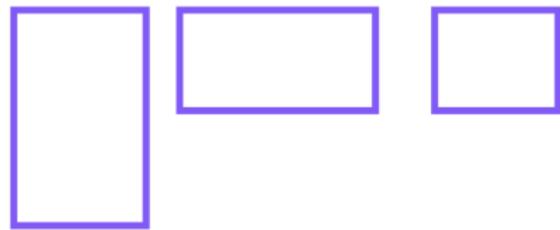
# PCA



# PCA

## PCA model

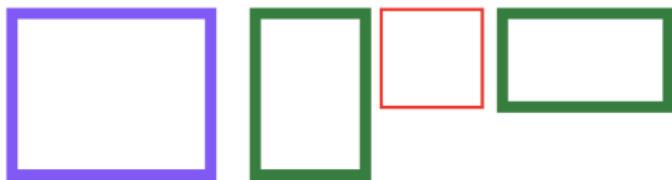
Obtained through the eigen-decomposition of the sample covariance matrix


$$\begin{matrix} X & X' & X'X \end{matrix}$$

# SVD and PCA

## PCA model

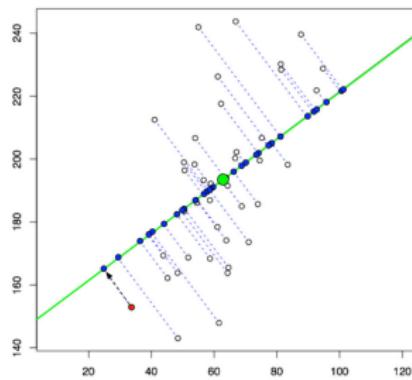
SVD on the covariance matrix is the same as Eigen-decomposition of covariance matrix.



# PCA Embeddings

## PCA Embeddings

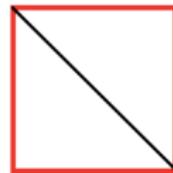
Projecting data onto the PCA directions also gives us low-dimensional embeddings.



# Principal Components and Embeddings!

## Principal Components

If  $X^T X = V \Sigma^2 V^T$  is the co-variance matrix, then  $V$  represents the principal components and  $V^T X^T$  represents the embeddings or compressed representation of the data points!



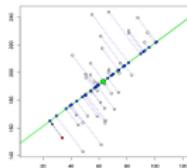
## ICE #3

### SVD manipulations

Let  $X = U\Sigma V^T$ . The projection of the data onto the principal components is given by  $V^T X^T$ . If  $X$  is  $N \times d$ , what's the dimension of the projection matrix with 3 principal components?

- a  $3 \times d$
- b  $3 \times N$
- c  $N \times 3$
- d  $d \times N$

# ICE #4



## Projection Dimension

Consider the figure above. Let  $V_1 \in \mathcal{R}^d$  be the first principal component and the project of a data point  $x \in \mathcal{R}^d$  onto  $V_1$  is given by  $V_1^T x$ . Now let  $V \in \mathcal{R}^{d \times k}$  be the entire set of principal components. When  $x \in \mathcal{R}^d$  gets projected onto all the principal components, what's the dimension of the projected vector?

- ① d
- ② k
- ③ N
- ④ 1

## ICE #5

### Images PCA (Work in groups of 2)

If you have 1000 face images and did a PCA on these images and found that 10 Eigen faces would be sufficient to reconstruct the images accurately. You stored compressed representations of the images on your laptop and to reconstruct the image, you send it to a server that then gives you back a re-constructed image. What would be the compression factor for the compressed representation you have on your laptop and obtained from PCA? Assume that each image is  $1000 \times 1000$  pixels?

- a 1000x
- b 10000x
- c 100000x
- d 1MMx

# PCA for Images



# PCA for Images - Eigen Faces



# PCA for Images - Re-construction



## SVD PCA - One main Issue

- ① Not scalable!
- ② Imagine millions of movies and millions of people watching it - How do you compute the SVD for it?
- ③ Complexity is  $O(N^2k)$  where  $k$  is the latent dimension of the matrix.
- ④ Not very flexible
- ⑤ Also not robust to outliers
- ⑥ Uses a bi-linear model instead of a non-linear model

# Word2Vec

## Skip Gram Model

Is based on the skip-gram model! How is training done? It's semi-supervised!!

### Source Text

The quick brown fox jumps over the lazy dog. →

### Training Samples

(the, quick)  
(the, brown)

The quick brown fox jumps over the lazy dog. →

(quick, the)  
(quick, brown)  
(quick, fox)

The quick brown fox jumps over the lazy dog. →

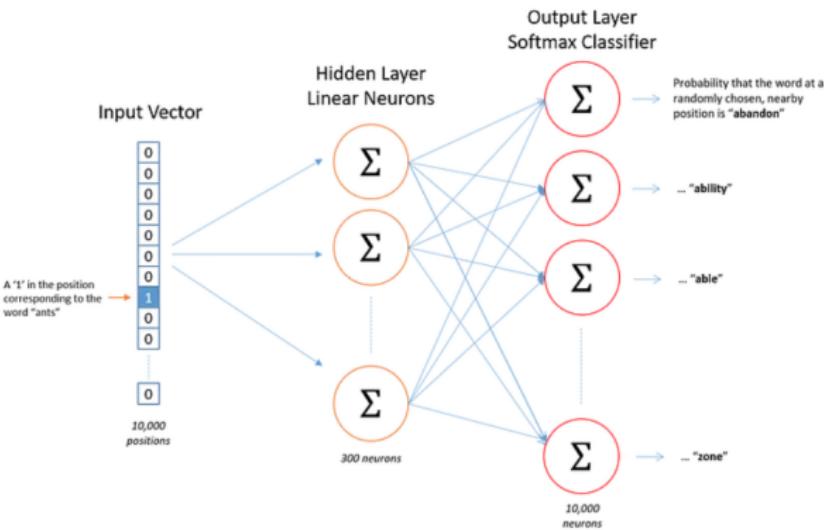
(brown, the)  
(brown, quick)  
(brown, fox)  
(brown, jumps)

The quick brown fox jumps over the lazy dog. →

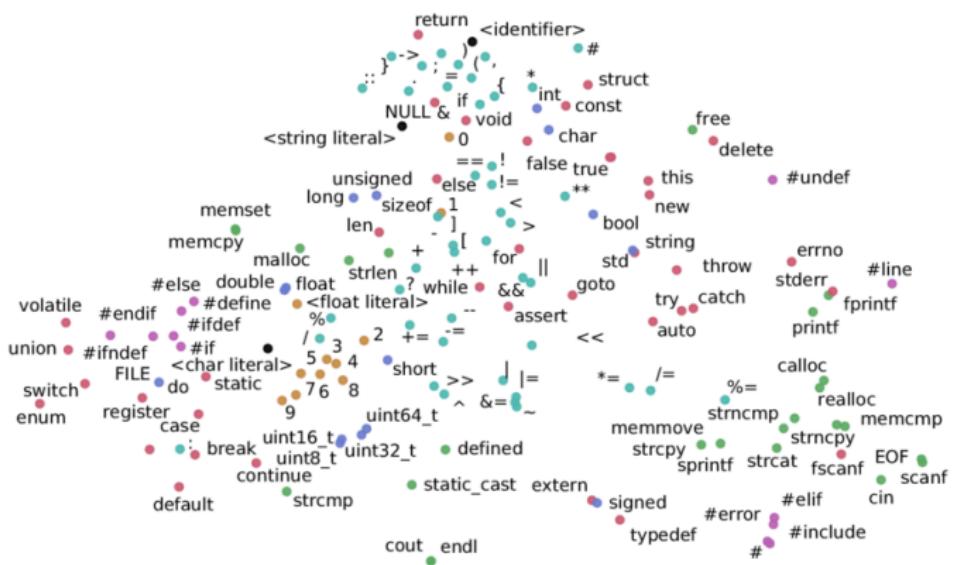
(fox, quick)  
(fox, brown)  
(fox, jumps)  
(fox, over)

# Word2Vec

## Architecture



## Word2Vec representation



# Product2Vec

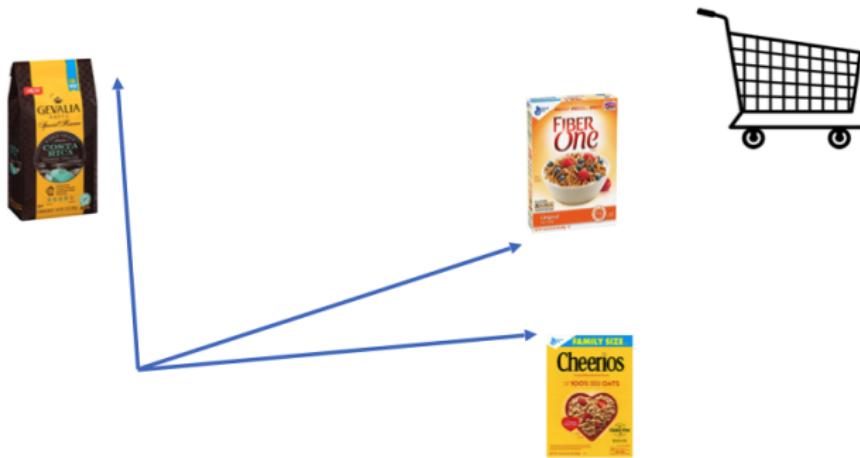


Represent products in product space  
with a large matrix of embedding  
coordinate vectors “ $L$ ”

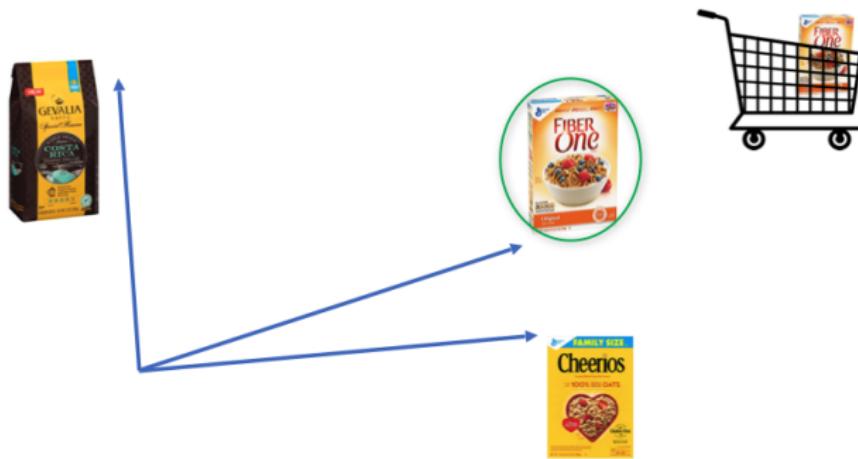
$$L = \begin{pmatrix} 1.5 & 1.9 & 1.8 & 1.4 & \cdots & 0.4 \\ 0.6 & 0.1 & 1.0 & 1.6 & \cdots & 1.9 \\ 0.6 & 1.6 & 1.6 & 1.6 & \cdots & 1.8 \\ 0.6 & 1.0 & 0.1 & 1.6 & \cdots & 0.6 \\ 0.8 & 1.4 & 1.9 & 0.8 & \cdots & 0.7 \end{pmatrix}$$

We obtain these embedding vectors from the  
[Product2Vec service](#) [London et al, 2017]

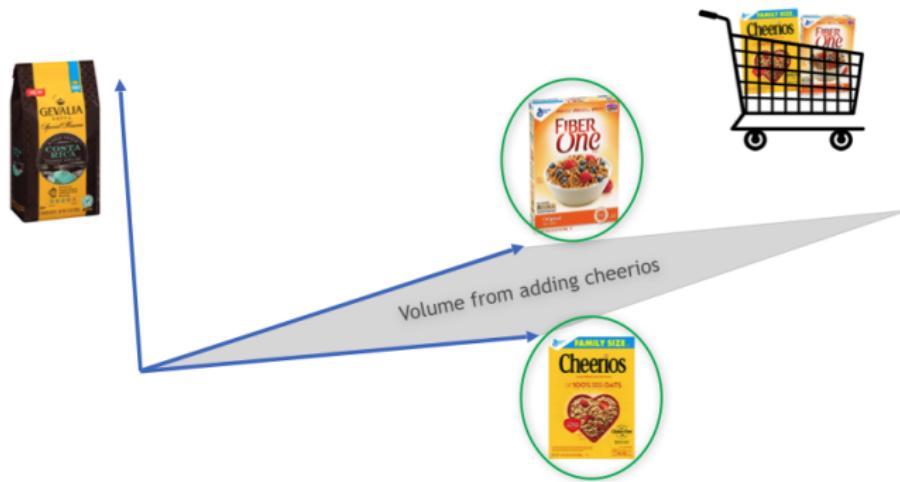
# Product2Vec application



# Product2Vec application



# Product2Vec application



# Product2Vec application



## Breakout: Discuss your favorite X2Vec!

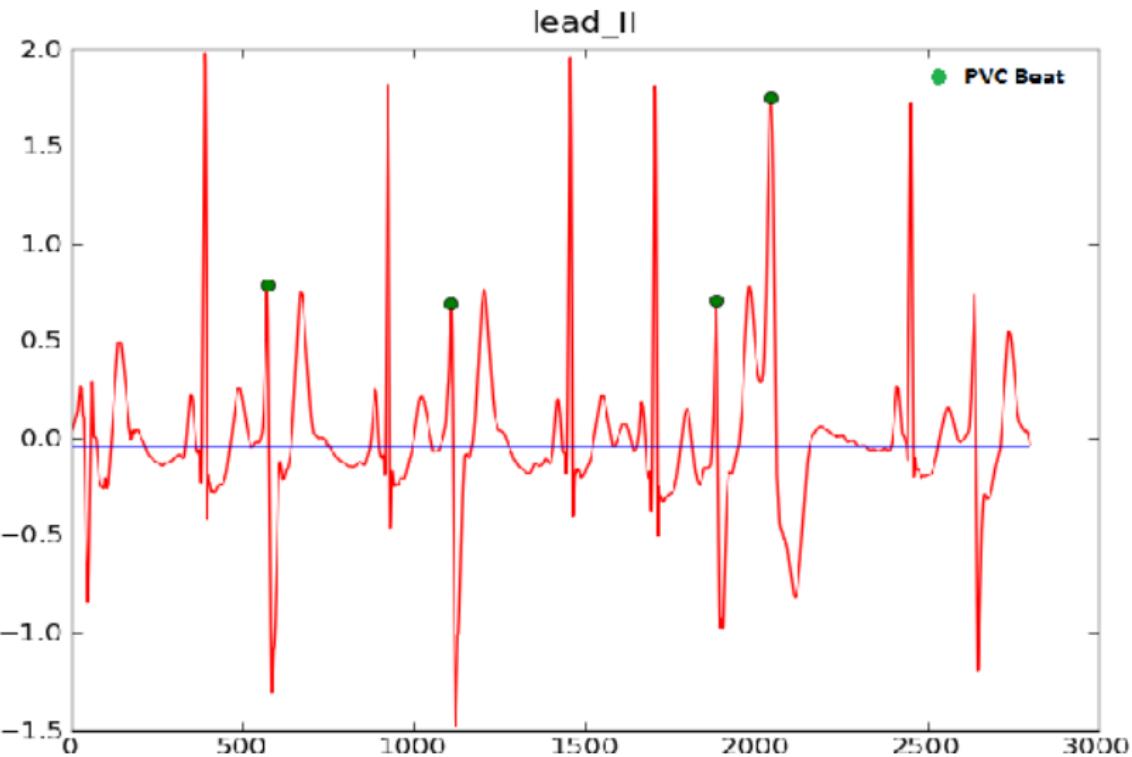
### X2Vec

In your group - Discuss an application that requires machine learning. Be specific about it - Example, data, features, the type of problem (classification, clustering, etc). Can you see how X2Vec would benefit your application. What would be your X in this case? How would you learn X2vec for your application? And how would you use it?

# Comparison of Dimensionality Reduction Methods

Method	Utility	Pros	Cons
SVD	Low-dim embeddings	Easily available	Scalability
PCA	Same as SVD	EigenFaces	Accuracy Outlier issues
Word2Vec	Semantic understanding	Non-linear	
Sentence2Vec	Comparing sentences		
Tweet2Vec	Understanding Tweets		
Product2Vec	Recommending products		
X2Vec			

# Anomaly Detection: Arrhythmia



# Broad list of methods

## Categorization

- Offline anomaly detection
- Real-time anomaly detection

# Broad list of methods

## Categorization

- Offline anomaly detection
- Real-time anomaly detection

## Categorization

- Time-series data anomaly detection
- Regular anomaly detection

# Summary

- a SVD - Bi-linear model
- b PCA application of SVD to understand variation in data
- c Application of PCA to images - Eigen faces
- d PCA can be used to compress images
- e Non-linear models more accurate and flexible
- f Word2vec uses a skip-gram non-linear model
- g Word2vec an example of context based learning (semi-supervised learning)
- h Can construct X2Vec for any X provided you have sufficient data
- i Introduction to Anomaly detection