## Recall from last time ...

## DBSCAN



## DBSCAN Clustering

- Core points: A point is a core point if there are at least MinPts within a distance of Eps, where MinPts and Eps are user-specified parameters.
- Border points: A border point is not a core point, but falls within the neighborhood of a core point.
- Noise points: A noise point is any point that is neither a core point nor a border point.

MinPts $=7$
border point
core point

epsilon $=1.00$
minPoints $=4$

Clustering Performance Eualuation

## Silhouette Coefficient

- The silhouette value is a measure of how similar a sample is to its own cluster (cohesion) compared to other clusters (separation).


Cohesion


Separation

## Silhouette Coefficient

- The silhouette value is a measure of how similar a sample is to its own cluster (cohesion) compared to other clusters (separation).
- The silhouette ranges from -1 to +1 .
- High value = the clustering configuration is appropriate
- Low value = the clustering configuration may have too many or too few clusters.


## Silhouette Coefficient

- The Silhouette Coefficient is defined for each sample and is composed of two scores:
- a: The mean distance between a sample and all other points in the same cluster.
- b: The mean distance between a sample and all other points in the next nearest cluster.


## Silhouette Coefficient

- The Silhouette Coefficient $s$ for a single sample is given as:

$$
s=\frac{b-a}{\max (a, b)}
$$

- The score is bounded between -1 for incorrect clustering and +1 for highly dense clustering $(a \ll b)$. Scores around zero indicate overlapping clusters.


## http://scikit-learn.org/stable/modules/clustering.html\#clustering

```
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```

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sclkit-learn v0.19.0 Other versions

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2.3. Clustering
2.3.1. Overview of clustering methods
2.3.2. K-means

- 2.3.2.1. Mini Batch K-Means
2.3.3. Affinity Propagation
2.3.4. Mean Shift
2.3.5. Spectral clustering
- 2.3.5.1. Different label assignment strategies
2.3.6. Hierarchical clustering
- 2.3.6.1. Different linkage type: Ward, complete and average linkage
- 2.3.6.2. Adding connectivity constraints
- 2.3.6.3. Varying the metric
2.3.7. DBSCAN
2.3.8. Birch
2.3.9. Clustering performance


### 2.3. Clustering

## Clustering of unlabeled data can be performed with the module sklearn.cluster .

Each clustering algorithm comes in two variants: a class, that implements the fit method to learn the clusters on train data, and a function, that, given train data, returns an array of integer labels corresponding to the different clusters. For the class, the labels over the training data can be found in the labels_ attribute.

## Input data

One important thing to note is that the algorithms implemented in this module can take different kinds of matrix as input. All the methods accept standard data matrices of shape [n_samples, $n \_f e a t u r e s$ ]. These can be obtained from the classes in the sklearn.feature_extraction module. For AffinityPropagation, Spectralclustering and DBSCAN one can also input similarity matrices of shape [n_samples, $n \_$samples]. These can be obtained from the functions in the sklearn.metrics.pairwise module.

### 2.3.1. Overview of clustering methods



## Dimensionality Reduction Machine Learning

Prof. Sandra Avila<br>Institute of Computing (IC/Unicamp)

## Why is Dimensionality Reduction useful?

## Why is Dimensionality Reduction useful?

- Data Compression
- Reduce time complexity: less computation required
- Reduce space complexity: less number of features
- More interpretable: it removes noise


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## Why is Dimensionality Reduction useful?

- Data Compression
- Reduce time complexity: less computation required
- Reduce space complexity: less number of features
- More interpretable: it removes noise
- Data Visualization
- To mitigate "the curse of dimensionality"


## Today's Agenda

- The Curse of Dimensionality
- PCA (Principal Component Analysis)
- PCA Formulation
- PCA Algorithm
- Choosing k


# The Curse of <br> Dimensionality 

## The Curse of Dimensionality



Even a basic 4D hypercube is incredibly hard to picture in our mind.

## The Curse of Dimensionality



Optimal number of features

## The Curse of Dimensionality

As the dimensionality of data grows, the density of observations becomes lower and lower and lower.


10 samples<br>1 dimension: 5 regions

Feature 1

## The Curse of Dimensionality

As the dimensionality of data grows, the density of observations becomes lower and lower and lower.


10 samples
2 dimensions: 25 regions


As the dimensionality of data grows, the density of observations becomes lower and lower and lower.

## 10 samples

3 dimensions: 125 regions


- 1 dimension: the sample density is $10 / 5=$ 2 samples/interval
- 2 dimensions: the sample density is $10 / 25=$ 0.4 samples/interval
- 3 dimensions: the sample density is $10 / 125=$ 0.08 samples/interval


## The Curse of Dimensionality: Solution?

## The Curse of Dimensionality: Solution?

- Increase the size of the training set to reach a sufficient density of training instances.


## The Curse of Dimensionality: Solution?

- Increase the size of the training set to reach a sufficient density of training instances.
- Unfortunately, the number of training instances required to reach a given density grows exponentially with the number of dimensions.


## How to reduce dimensionality?

## How to reduce dimensionality?

- Feature Selection

Feature Extraction

## How to reduce dimensionality?

- Feature Selection: choosing a subset of all the features (the ones more informative).
- $x_{1}, x_{2}, x_{3}, x_{4}, x_{5}$
- Feature Extraction


## How to reduce dimensionality?

- Feature Selection: choosing a subset of all the features (the ones more informative).
- $x_{1}, x_{2}, x_{3}, x_{4}, x_{5}$
- Feature Extraction: create a subset of new features by combining the existing ones.
- $z=f\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)$

PCA: Principal
Component Analysis

## Principal Component Analysis (PCA)

- The most popular dimensionality reduction algorithm.
- PCA have two steps:
- It identifies the hyperplane that lies closest to the data.
- It projects the data onto it.


## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)



## Problem Formulation (PCA)

- Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^{n}$ ) onto which to project the data so as to minimize the projection error.



## Problem Formulation (PCA)

- Reduce from $n$-dimension to $k$-dimension: Find $k$ vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.


# PCA Algorithm By Eigen Decomposition 

## PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
3. Find eigenvectors $u$ and eigenvalues $\lambda$
4. Sort eigenvalues and pick first $k$ eigenvectors
5. Project data to $k$ eigenvectors

## PCA in a Nutshell (Eigen Decomposition)

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## Data Preprocessing

Training set: $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$
Preprocessing (feature scaling/mean normalization):

$$
\mu_{j}=\frac{1}{m} \sum_{i=1}^{m} x_{j}^{(i)}
$$

## Center the data

Replace each $x_{j}^{(i)}$ with $x_{j}-\mu_{j}$.
If different features on different scales, scale features to have comparable range of values.

## Data Preprocessing



## PCA in a Nutshell (Eigen Decomposition)

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## PCA Algorithm

Reduce data from $n$-dimensions to $k$-dimensions
Compute "covariance matrix":

$$
\Sigma=\frac{1}{m} \sum_{i=1}^{n}\left(x^{(i)}\right)\left(x^{(i)}\right)^{\mathrm{T}} \square n \times n \text { matrix }
$$

## PCA Algorithm

Reduce data from $n$-dimensions to $k$-dimensions
Compute "covariance matrix":

$$
\Sigma=\frac{1}{m} \sum_{i=1}^{n}\left(x^{(i)}\right)\left(x^{(i)}\right)^{\mathrm{T}} \square n \times n \text { matrix }
$$

Covariance of dimensions $x_{1}$ and $x_{2}$ :

- Do $x_{1}$ and $x_{2}$ tend to increase together?



## PCA Algorithm

Multiple a vector by $\mathbf{\Sigma}$ :
$\left[\begin{array}{ll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right] \times\left[\begin{array}{c}-1 \\ 1\end{array}\right]$


## PCA Algorithm

Multiple a vector by $\mathbf{\Sigma}$ :
$\left[\begin{array}{ccc}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right] \times\left[\begin{array}{c}-1 \\ 1\end{array}\right]=\left[\begin{array}{l}-1.2 \\ -0.2\end{array}\right]$


## PCA Algorithm

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$\left[\begin{array}{lll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right] \times\left[\begin{array}{l}-2.5 \\ -1.0\end{array}\right]=\left[\begin{array}{l}-6.0 \\ -2.7\end{array}\right]$
$\left[\begin{array}{ll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right] \times\left[\begin{array}{c}-6.0 \\ -2.7\end{array}\right]=\left[\begin{array}{c}-14.1 \\ -6.4\end{array}\right]$

## PCA Algorithm

Multiple a vector by $\mathbf{\Sigma}$ :
$\left[\begin{array}{lll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right] \times\left[\begin{array}{c}-1 \\ 1\end{array}\right]=\left[\begin{array}{l}-1.2 \\ -0.2\end{array}\right]$
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$\left[\begin{array}{ll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right] \times\left[\begin{array}{l}-6.0 \\ -2.7\end{array}\right]=\left[\begin{array}{c}-14.1 \\ -6.4\end{array}\right]$
Turns towards direction of variation

## PCA Algorithm

Want vectors $u$ which aren't turned: $\boldsymbol{\Sigma} u=\lambda u$


$$
\begin{aligned}
& u=\text { eigenvectors of } \Sigma \\
& \lambda=\text { eigenvalues }
\end{aligned}
$$

## PCA Algorithm

Want vectors $u$ which aren't turned: $\boldsymbol{\Sigma} u=\lambda u$


$$
\begin{aligned}
& u=\text { eigenvectors of } \Sigma \\
& \lambda=\text { eigenvalues }
\end{aligned}
$$

Principal components = eigenvectors $\mathbf{W}$. largest eigenvalues

## PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
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4. Sort eigenvalues and pick first $k$ eigenvectors
5. Project data to $k$ eigenvectors

## Finding Principal Components

1. Find eigenvalues by solving: $\operatorname{det}(\boldsymbol{\Sigma}-\lambda \mathrm{I})=0$
$\operatorname{det}\left[\begin{array}{cc}2.0-\lambda & 0.8 \\ 0.8 & 0.6-\lambda\end{array}\right]=$

## Finding Principal Components

1. Find eigenvalues by solving: $\operatorname{det}(\Sigma-\lambda I)=0$
$\operatorname{det}\left[\begin{array}{cc}2.0-\lambda & 0.8 \\ 0.8 & 0.6-\lambda\end{array}\right]=(2.0-\lambda)(0.6-\lambda)-(0.8)(0.8)$

## Finding Principal Components

1. Find eigenvalues by solving: $\operatorname{det}(\Sigma-\lambda I)=0$

$$
\begin{aligned}
\operatorname{det}\left[\begin{array}{cc}
2.0-\lambda & 0.8 \\
0.8 & 0.6-\lambda
\end{array}\right]= & (2.0-\lambda)(0.6-\lambda)-(0.8)(0.8)=\lambda^{2}-2.6 \lambda+0.56=0 \\
& \left\{\lambda_{1}, \lambda_{2}\right\}=\{2.36,0.23\}
\end{aligned}
$$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

$$
\left[\begin{array}{ll}
2.0 & 0.8 \\
0.8 & 0.6
\end{array}\right]\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]=2.36\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]
$$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

$$
\left[\begin{array}{ll}
2.0 & 0.8 \\
0.8 & 0.6
\end{array}\right]\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]=2.36\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right] \Rightarrow \begin{aligned}
& 2.0 u_{11}+0.8 u_{12}=2.36 u_{11} \\
& 0.8 u_{11}+0.6 u_{12}=2.36 u_{12}
\end{aligned}
$$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

$$
\left[\begin{array}{c}
2.0 \\
0.8 \\
0.8 \\
0.6
\end{array}\right]\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]=2.36\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right] \Rightarrow \begin{aligned}
& 2.0 u_{11}+0.8 u_{12}=2.36 u_{11} \\
& 0.8 u_{11}+0.6 u_{12}=2.36 u_{12}
\end{aligned} \Rightarrow u_{11}=2.2 u_{12}
$$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

$$
\left[\begin{array}{ll}
2.0 & 0.8 \\
0.8 & 0.6
\end{array}\right]\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]=2.36\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right] \Rightarrow \begin{aligned}
& 2.0 u_{11}+0.8 u_{12}=2.36 u_{11} \\
& 0.8 u_{11}+0.6 u_{12}=2.36 u_{12}
\end{aligned} \Rightarrow u_{11}=2.2 u_{12}
$$

$$
\mathrm{u}_{1} \sim\left[\begin{array}{c}
2.2 \\
1
\end{array}\right]
$$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

$$
\left[\begin{array}{ll}
2.0 & 0.8 \\
0.8 & 0.6
\end{array}\right]\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]=2.36\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right] \Rightarrow \begin{aligned}
& 2.0 u_{11}+0.8 u_{12}=2.36 u_{11} \\
& 0.8 u_{11}+0.6 u_{12}=2.36 u_{12}
\end{aligned} \Rightarrow u_{11}=2.2 u_{12}
$$

$$
\mathrm{u}_{1} \sim\left[\begin{array}{c}
2.2 \\
1
\end{array}\right]
$$

Want $\left\|u_{1}\right\|=1$

$$
\left[\begin{array}{c}
0.91 \\
0.41
\end{array}\right]
$$

## Finding Principal Components

2．Find $i^{\text {th }}$ eigenvector by solving： $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$

$$
\begin{aligned}
& {\left[\begin{array}{ll}
2.0 & 0.8 \\
0.8 & 0.6
\end{array}\right]\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right]=2.36\left[\begin{array}{l}
u_{11} \\
u_{12}
\end{array}\right] \Rightarrow \begin{array}{l}
2.0 u_{11}+0.8 u_{12}=2.36 u_{11} \\
0.8 u_{11}+0.6 u_{12}=2.36 u_{12}
\end{array} \Rightarrow u_{11}=2.2 u_{12} } \\
& {\left[\begin{array}{ll}
2.0 & 0.8 \\
0.8 & 0.6
\end{array}\right]\left[\begin{array}{l}
u_{21} \\
u_{22}
\end{array}\right]=0.23\left[\begin{array}{l}
u_{21} \\
u_{22}
\end{array}\right] \Rightarrow u_{2}=\left[\begin{array}{c}
-0.41 \\
0.91
\end{array}\right] } u_{1} \sim\left[\begin{array}{c}
2.2 \\
1
\end{array}\right] \\
& \text { Want \|u⿱卄一} \|=1
\end{aligned}
$$

## Finding Principal Components

2. Find $i^{\text {th }}$ eigenvector by solving: $\boldsymbol{\Sigma} u_{i}=\lambda_{i} u_{i}$
$\left[\begin{array}{ll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right]\left[\begin{array}{l}u_{11} \\ u_{12}\end{array}\right]=2.36\left[\begin{array}{l}u_{11} \\ u_{12}\end{array}\right] \Rightarrow \begin{aligned} & 2.0 u_{11}+0.8 u_{12}=2.36 u_{11} \\ & 0.8 u_{11}+0.6 u_{12}=2.36 u_{12}\end{aligned} \Rightarrow u_{11}=2.2 u_{12}$
$\left[\begin{array}{ll}2.0 & 0.8 \\ 0.8 & 0.6\end{array}\right]\left[\begin{array}{l}u_{21} \\ u_{22}\end{array}\right]=0.23\left[\begin{array}{l}u_{21} \\ u_{22}\end{array}\right] \Rightarrow u_{2}=\left[\begin{array}{c}-0.41 \\ 0.91\end{array}\right]$
3. $1^{\text {st }} P C:\left[\begin{array}{l}0.91 \\ 0.41\end{array}\right]$ and $2^{\text {nd }} P C:\left[\begin{array}{c}-0.41 \\ 0.91\end{array}\right]$

Want $\left\|u_{1}\right\|=1$
$\left[\begin{array}{l}0.91 \\ 0.41\end{array}\right]$

## PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
3. Find eigenvectors $u$ and eigenvalues $\lambda$
4. Sort eigenvalues and pick first $k$ eigenvectors
5. Project data to $k$ eigenvectors

## How many PCs?

Have eigenvectors $u_{1}, u_{2}, \ldots, u_{n}$, want $k<n$ eigenvalue $\lambda_{i}=$ variance along $u_{i}$

## How many PCs?

- Have eigenvectors $u_{1}, u_{2}, \ldots, u_{n}$, want $k<n$
- eigenvalue $\lambda_{i}=$ variance along $u_{i}$
- Pick $u_{i}$ that explain the most variance:
- Sort eigenvectors s.t. $\lambda_{1}>\lambda_{2}>\lambda_{3}>\ldots>\lambda_{n}$
- Pick first $k$ eigenvectors which explain 95\% of total variance


## How many PCs?

- Have eigenvectors $u_{1}, u_{2}, \ldots, u_{n}$, want $k<n$
- eigenvalue $\lambda_{i}=$ variance along $u_{i}$

Pick $u_{i}$ that explain the most variance:

$$
\frac{\sum_{i=1}^{k} \lambda_{i}}{\sum_{i=1}^{n} \lambda_{i}} \leq 1
$$

- Sort eigenvectors s.t. $\lambda_{1}>\lambda_{2}>\lambda_{3}>\ldots>\lambda_{n}$
- Pick first $k$ eigenvectors which explain 95\% of total variance


## How many PCs?

- Have eigenvectors $u_{1}, u_{2}, \ldots, u_{n}$, want $k<n$
- eigenvalue $\lambda_{i}=$ variance along $u_{i}$
- Pick $u_{i}$ that explain the most variance:

- Sort eigenvectors s.t. $\lambda_{1}>\lambda_{2}>\lambda_{3}>\ldots>\lambda_{n}$
- Pick first $k$ eigenvectors which explain 95\% of total variance

■ Typical threshold: 90\%, 95\%, 99\%


## PCA in a Nutshell (Eigen Decomposition)

1. Center the data (and normalize)
2. Compute covariance matrix $\mathbf{\Sigma}$
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4. Sort eigenvalues and pick first $k$ eigenvectors
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# Principal Component Analysis (12 uideos, 3-15min) 

https://www.youtube.com/playlist?list=PLBu09BD7ez_5_yapAg860d6JeeypkS4YM


Principal Component Analysis
12 videos • 119,895 views • Last updated on May 21, 2014

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Victor Lavrenko
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PCA 2: dimensionality reduction
Victor Lavrenko

PCA 3: direction of greatest variance
Victor Lavrenko

PCA 4: principal components = eigenvectors
Victor Lavrenko

PCA 5: finding eigenvalues and eigenvectors

2



https://www.youtube.com/playlist?list=PLZHQObOWTQDPD3MizzM2xVFitgF8hE_ab

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10


3BLUE1BROWN SERIES S1•E10


Cross products | Essence of linear algebra, Chapter 10
3Blue1Brown
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$\equiv \quad$ Neural Networks ...
Essence of linear algebra



3BLUE1BROWN SERIES S1•E12
Change of basis | Essence of linear algebra, chapter 12

3Blue1Brown


A geometric understanding of matrices, determinants, eigen-stuffs and more.

## References

## Machine Learning Books

- Hands-On Machine Learning with Scikit-Learn and TensorFlow, Chap. 8
"Dimensionality Reduction"
- Pattern Recognition and Machine Learning, Chap. 12 "Continuous Latent Variables"
- Pattern Classification, Chap. 10 "Unsupervised Learning and Clustering"


## Machine Learning Courses

- https://www.coursera.org/learn/machine-learning, Week 8

