Recall from last time ...





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.





epsilon = 1.00 minPoints = 4

https://www.naftaliharris.com/blog/visualizing-dbscan-clustering

Restart

Clustering Performance Evaluation

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



 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.

- 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.

• 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



2.3.9. Clustering performance



Dimensionality Reduction Machine Learning

Prof. Sandra Avila

Institute of Computing (IC/Unicamp)

MC886, September 30, 2019

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

• Data Compression

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- Data Visualization

• Data Compression

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- 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



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



Optimal number of features

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



10 samples 1 dimension: 5 regions

Feature 1

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



10 samples 2 dimensions: 25 regions

Feature 1



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

10 samples 3 dimensions: 125 regions

Feature 1



- 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.

• Feature Selection

• Feature Extraction

- Feature Selection: choosing a subset of all the features (the ones more informative).
 - $\circ \quad \mathbf{x_1}, \mathbf{x_2}, \mathbf{x_3}, \mathbf{x_4}, \mathbf{x_5}$
- Feature Extraction

- Feature Selection: choosing a subset of all the features (the ones more informative).
 - $\circ \quad \mathbf{x_1}, \mathbf{x_2}, \mathbf{x_3}, \mathbf{x_4}, \mathbf{x_5}$
- Feature Extraction: create a subset of new features by combining the existing ones.

$$\circ \quad z = f(x_1, x_2, x_3, x_4, x_5)$$

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)


















 Reduce from 2-dimension to 1-dimension: Find a direction (a vector u⁽¹⁾ ∈ ℝⁿ) onto which to project the data so as to minimize the projection error.



 Reduce from *n*-dimension to *k*-dimension: Find *k* vectors *u*⁽¹⁾, *u*⁽²⁾, ..., *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 Σ
- **3**. Find eigenvectors u and eigenvalues λ
- 4. Sort eigenvalues and pick first *k* eigenvectors
- 5. Project data to *k* eigenvectors

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Data Preprocessing

Training set: $x^{(1)}, x^{(2)}, ..., x^{(m)}$

Preprocessing (feature scaling/mean normalization):

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

Replace each $x_{j}^{(i)}$ with $x_{j} - \mu_{j}$.

Center the data

If different features on different scales, scale features to have comparable range of values.

Data Preprocessing



Credit: http://cs231n.github.io/neural-networks-2/

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Reduce data from *n*-dimensions to *k*-dimensions

Compute "covariance matrix":

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

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Covariance of dimensions x_1 and x_2 :

- Do x_1 and x_2 tend to increase together?
- or does x_2 decrease as x_1 increases?

$$\begin{array}{c} x_1 & x_2 \\ x_1 & 2.0 & 0.8 \\ x_2 & 0.8 & 0.6 \end{array}$$

Multiple a vector by Σ :

 $\begin{bmatrix} 2.0 \ 0.8 \\ 0.8 \ 0.6 \end{bmatrix} \times \begin{bmatrix} -1 \\ 1 \end{bmatrix}$



Multiple a vector by Σ : $\begin{bmatrix} 2.0 \ 0.8 \\ 0.8 \ 0.6 \end{bmatrix} \times \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1.2 \\ -0.2 \end{bmatrix}$



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Multiple a vector by Σ :

Turns towards direction of variation



Want vectors u which aren't turned: $\Sigma u = \lambda u$ $u = eigenvectors of \Sigma$ $\lambda = eigenvalues$

Want vectors u which aren't turned: $\Sigma u = \lambda u$ x_2 X $u = eigenvectors of \Sigma$ X Х λ = eigenvalues X \mathcal{X}_{\cdot} X Principal components = $\mathcal{U}_{\mathcal{A}}$ u_{γ} eigenvectors w. largest eigenvalues

PCA in a Nutshell (Eigen Decomposition)

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

 $\det \begin{bmatrix} 2.0 - \lambda & 0.8\\ 0.8 & 0.6 - \lambda \end{bmatrix} =$

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$$\det\begin{bmatrix} 2.0 - \lambda & 0.8\\ 0.8 & 0.6 - \lambda \end{bmatrix} = (2.0 - \lambda)(0.6 - \lambda) - (0.8)(0.8)$$

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

$$det \begin{bmatrix} 2.0 - \lambda & 0.8 \\ 0.8 & 0.6 - \lambda \end{bmatrix} = (2.0 - \lambda)(0.6 - \lambda) - (0.8)(0.8) = \lambda^2 - 2.6\lambda + 0.56 = 0$$
$$\{\lambda_1, \lambda_2\} = \{2.36, 0.23\}$$

$$\begin{bmatrix} 2.0 \ 0.8 \\ 0.8 \ 0.6 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} = 2.36 \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix}$$

$$\begin{bmatrix} 2.0 \ 0.8 \\ 0.8 \ 0.6 \end{bmatrix} \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} = 2.36 \begin{bmatrix} u_{11} \\ u_{12} \end{bmatrix} \Rightarrow \begin{array}{c} 2.0u_{11} + 0.8u_{12} = 2.36u_{11} \\ 0.8u_{11} + 0.6u_{12} = 2.36u_{12} \end{bmatrix}$$

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Finding Principal Components

2. Find *i*th eigenvector by solving: $\Sigma u_i = \lambda_i u_i$



Finding Principal Components

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$$\begin{bmatrix} 2.0 \ 0.8 \\ 0.8 \ 0.6 \end{bmatrix} \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix} = 0.23 \begin{bmatrix} u_{21} \\ u_{22} \end{bmatrix} \Rightarrow u_{2} = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix} \qquad u_{1} \sim \begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

$$u_{1} \sim \begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

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$$W_{\text{ant } \|u_{1}\|=1}$$

$$\begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix} \text{ and } 2^{\text{nd}} \text{ PC: } \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

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- eigenvalue $\lambda_i = variance$ along u_i

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- 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

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0.95

- 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 Σ
- **3**. Find eigenvectors u and eigenvalues λ
- 4. Sort eigenvalues and pick first *k* eigenvectors
- 5. **Project data to** *k* **eigenvectors**

Principal Component Analysis (12 videos, 3-15min)

https://www.youtube.com/playlist?list=PLBv09BD7ez_5_yapAg86Od6JeeypkS4YM



https://www.youtube.com/playlist?list=PLZHQObOWTQDPD3MizzM2xVFitqF8hE_ab



chapter 14

16:46

MORE FROM YOUTUBE

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