Data Science

Predictive and Descriptive Models

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Data Science

Module 1: Introduction to Data Science

Module 2 : Predictive and Descriptive Models

Module 3 : Evaluation and Methodology of Data Science

Module 4: Text Analytics and Recommendation system (RS)

Module 5 : Data Communication and Information Visualization

Module 6 : Scaling with Big Data

Data Science: Predictive and Descriptive Models

- Descriptive Modelling
  - PCA
  - SVD
  - Probabilistic PCA
  - EM Algorithm for PCA
  - ICA
- Predictive Modelling
  - Process
  - Parametric and non-Parametric models
  - BI
  - Challenges of Predictive Analysis
- Time Series Analysis

Data Science: Predictive and Descriptive Models

- Descriptive Modelling
- Data Mining Algorithms: “A data mining algorithm is a well-defined procedure that takes data as input and produces output in the form of models or patterns”
  - “well-defined”: can be encoded in software
  - “algorithm”: must terminate after some finite number of steps

Data Science: Predictive and Descriptive Models

Models

Prediction

- Linear regression
- Piecewise linear
- Nonparametric regression
- Classification

Probability Distributions

- Parametric models
- Mixtures of parametric models
- Graphical Markov models (categorical, continuous, mixed)

Structured Data

- Time series
- Markov models
- Mixture Transition Distribution models
- Hidden Markov models
- Spatial models

Data Science: Predictive and Descriptive Models

- Descriptive Modelling

Patterns

- Global
  - Clustering via partitioning
  - Hierarchical Clustering
  - Mixture Models
- Local
  - Outlier detection
  - Changepoint detection
  - Bump hunting
  - Scan statistics
  - Association rules

Data Science: Predictive and Descriptive Models

- What is a descriptive model?
  - “presents the main features of the data”
  - “a summary of the data”
  - Data randomly generated from a “good” descriptive model will have the same characteristics as the real data
  - Focus on techniques and algorithms for fitting descriptive models to data

- PCA Example

Q Transform following data from 2D space to 1D space using Dimensionality Reduction method (use P.C.A.)

	a_1	a_2
t_1	1	2
t_2	2	1
t_3	3	4
t_4	4	3

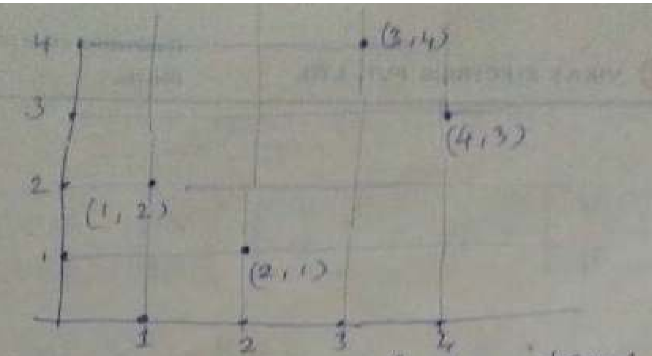
$\Rightarrow$ a_1 & a_2 are two attributes & 4 tuples

Solution:

Drawing the data-items of representing database in Matrix form as Matrix M

Data Science: Predictive and Descriptive Models

- PCA Example



plotting data items

$$M = \begin{vmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{vmatrix}$$

step 1: compute $M^t M$

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} = \begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix}$$

step 2: Find Eigenvalues

$$(30-\lambda)(30-\lambda)-(28)(28)=0$$

$$\therefore \lambda = 58, \quad \lambda = 2$$

- PCA Example

Step 3: Calculating EigenVector for $\lambda = 58$

$$\begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 58 \begin{bmatrix} x \\ y \end{bmatrix}$$

$$30x + 28y = 58x$$
$$28x + 30y = 58y$$

giving $x = y$

$\therefore$ assuming $x = y = 1$

So EV for $\lambda = 58 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$

(after Normalization)

$\{$ i.e $\sqrt{1^2 + 1^2}$ $\}$

Step 4: Calculating EigenVector for $\lambda = 2$

$$\begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 2 \begin{bmatrix} x \\ y \end{bmatrix}$$

$$30x + 28y = 2x$$
$$28x + 30y = 2y$$

giving $x = -y$ $\therefore$ $x = -1, y = 1$

- PCA Example

So EV for $\lambda = 2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$

So $E = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$

Step 5: Finding Principal Components.

$$PC = M\,E = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

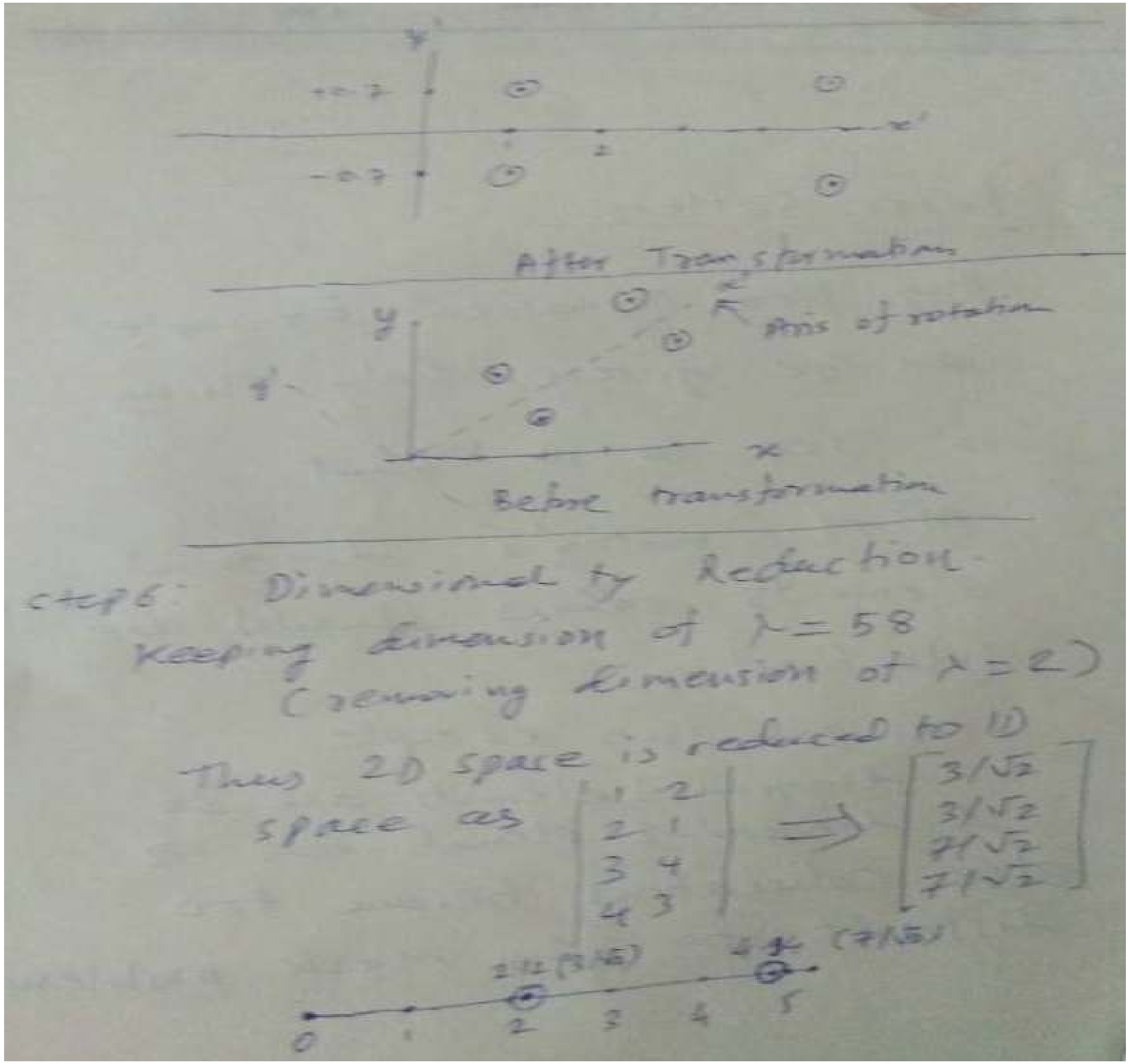
$$\begin{array}{cc} \lambda=58 & \lambda=2 \end{array}$$

$$= \begin{bmatrix} 3/\sqrt{2} & 1/\sqrt{2} \\ 3/\sqrt{2} & -1/\sqrt{2} \\ 7/\sqrt{2} & 1/\sqrt{2} \\ 7/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

$$= \begin{bmatrix} 2.12 & 0.707 \\ 2.12 & -0.707 \\ 4.94 & 0.707 \\ 4.94 & -0.707 \end{bmatrix}$$

Data Science: Predictive and Descriptive Models

- PCA Example



- Singular Value Decomposition (SVD):
  - A rectangular matrix A_{mn} can be broken down into the product of three matrices
    - an **orthogonal** matrix U,
    - a diagonal matrix S, called **singular** value and
    - the transpose of an **orthogonal** matrix V
    - $A_{mn} = U_{mm} S_{mn} V^T{}_{nn}$
  - Matrix Q is **orthogonal** if its transpose is equal to its inverse $Q^{-1} = Q^T$
  - Unitary if $Q^{-1} = Q^*$ and therefore normal $Q^*Q = QQ^*$
  - Symmetric if $Q = Q^T$
  - $U^TU = I$ and $V^TV = I$
  - Columns of U are orthonormal eigenvectors of AA^T
  - Columns of V are orthonormal eigenvectors of A^TA, and
  - S is a diagonal matrix containing the sqrts of eigenvalues from U or V in descending order

- SVD: Find the singular values of the matrix B

$$B = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}. \quad AA^T = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}$$

$\lambda^2 - 10\lambda + 9$, so $\lambda = 9$ and $\lambda = 1$ are the eigenvalues

the singular values are 3 and 1

- Example 2

Find the singular values of $A = \begin{bmatrix} 0 & 1 & 1 \\ \sqrt{2} & 2 & 0 \\ 0 & 1 & 1 \end{bmatrix}$ and find the SDV decomposition

$$AA^T = \begin{bmatrix} 2 & 2 & 2 \\ 2 & 6 & 2 \\ 2 & 2 & 2 \end{bmatrix} \qquad \begin{aligned} -\lambda^3 + 10\lambda^2 - 16\lambda &= -\lambda(\lambda^2 - 10\lambda + 16) \\ &= -\lambda(\lambda - 8)(\lambda - 2) \end{aligned}$$

eigenvalues of AA^T are $\lambda = 8, \lambda = 2, \lambda = 0$

singular values are $\sigma_1 = 2\sqrt{2}, \sigma_2 = \sqrt{2}$ (and $\sigma_3 = 0$).

- SVD: Example 2 (Contd.)
- To give the decomposition, we consider the diagonal matrix of singular values

$$\Sigma = \begin{bmatrix} 2\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

For $\lambda = 8$, we find an eigenvector $(1, 2, 1)$ - normalizing gives $p_1 = (\frac{1}{\sqrt{6}}, \frac{2}{\sqrt{6}}, \frac{1}{\sqrt{6}})$

For $\lambda = 2$ we find $p_2 = (-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}})$, and

For $\lambda = 0$ we get $p_3 = (\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}})$.

This gives the matrix $P = \begin{bmatrix} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} \\ \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$.

- Singular Value Decomposition (SVD): Defintion

Definition

- Any real mxn matrix A can be decomposed uniquely as

$$A = UDV^T$$

U is mxn and column orthogonal (its columns are eigenvectors of AA^T)
$$(AA^T = UDV^T VDU^T = UD^2U^T)$$

V is nxn and orthogonal (its columns are eigenvectors of $A^T A$)
$$(A^T A = VDU^T UDV^T = VD^2 V^T)$$

D is nxn diagonal (non-negative real values called *singular* values)

$$D = diag(\sigma_1, \sigma_2, \ldots, \sigma_n) \quad \text{ordered so that } \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$$
(if σ is a singular value of A, it's square is an eigenvalue of $A^T A$)

- If $U = (u_1 \; u_2 \; \cdots \; u_n)$ and $V = (v_1 \; v_2 \; \cdots \; v_n)$, then

$$A = \sum_{i=1}^{n} \sigma_i u_i v_i^T$$

(actually, the sum goes from 1 to r where r is the rank of A)

- Singular Value Decomposition (SVD) Computation Example
- Step1: To Find U, find AA^T

$$A = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix} \quad A^T = \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} \quad AA^T = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 11 & 1 \\ 1 & 11 \end{bmatrix}$$

- Step2: To find the eigenvalues and corresponding eigenvectors of AA^T

$$A\vec{v} = \lambda\vec{v}, \begin{bmatrix} 11 & 1 \\ 1 & 11 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$11x_1 + x_2 = \lambda x_1 \qquad x_1 + 11x_2 = \lambda x_2$$

$$(11 - \lambda)x_1 + x_2 = 0 \qquad x_1 + (11 - \lambda)x_2 = 0$$

$$\begin{vmatrix} (11-\lambda) & 1 \\ 1 & (11-\lambda) \end{vmatrix} = 0 \quad (11-\lambda)(11-\lambda) - 1 \cdot 1 = 0 \quad (\lambda - 10)(\lambda - 12) = 0 \quad \lambda = 10, \lambda = 12$$

$$\text{For } \lambda = 10 \quad (11-10)x_1 + x_2 = 0 \quad x_1 = -x_2 \qquad \text{For } \lambda = 12 \quad (11-12)x_1 + x_2 = 0 \quad x_1 = x_2$$

- Eigenvector for λ = 12 is column 1 & eigenvector for λ = 10 is column 2

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- Singular Value Decomposition (SVD) Computation Example $\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
- Step3: Gram-Schmidt orthonormalization process to the column vectors

$$\text{normalize} \quad \vec{u_1} = \frac{\vec{v_1}}{|\vec{v_1}|} = \frac{[1,1]}{\sqrt{1^2+1^2}} = \frac{[1,1]}{\sqrt{2}} = [\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}]$$

$$\text{Compute} \quad \vec{w_2} = \vec{v_2} - \vec{u_1} \cdot \vec{v_2} * \vec{u_1} =$$

$$[1,-1] - [\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}] \cdot [1,-1] * [\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}] =$$

$$[1,-1] - 0 * [\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}] = [1,-1] - [0,0] = [1,-1]$$

$$\text{normalize} \quad \vec{u_2} = \frac{\vec{w_2}}{|\vec{w_2}|} = [\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}] \qquad U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

- Similarly calculate V where V is based on A^TA

$$V = \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{30}} \\ \frac{2}{\sqrt{6}} & \frac{-1}{\sqrt{5}} & \frac{2}{\sqrt{30}} \\ \frac{1}{\sqrt{6}} & 0 & \frac{-5}{\sqrt{30}} \end{bmatrix} \qquad V^T = \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix}$$

- Singular Value Decomposition (SVD) Computation Example
- Step4:
  - S is the sqrts of the non-zero eigenvalues and
  - populate the diagonal with them, putting the largest in s_{11}, the next largest in s_{22} and so on until the smallest value ends up in s_{mn}

$$S = \begin{bmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{bmatrix}$$

$$A_{mn} = U_{mm} S_{mn} V_{nn}^T = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\sqrt{12}}{\sqrt{2}} & \frac{\sqrt{10}}{\sqrt{2}} & 0 \\ \frac{\sqrt{12}}{\sqrt{2}} & \frac{-\sqrt{10}}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & \frac{-1}{\sqrt{5}} & 0 \\ \frac{1}{\sqrt{30}} & \frac{2}{\sqrt{30}} & \frac{-5}{\sqrt{30}} \end{bmatrix} = \begin{bmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{bmatrix}$$

  - The diagonal entries in *S* are the singular values of *A*, the columns in *U* are called left singular vectors, and the columns in *V* are called right singular vectors

Data Science: Predictive and Descriptive Models

- Application of SVD to document classification

Data Science: Predictive and Descriptive Models

- Descriptive Modelling

References

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