Machine Learning

Dimensionality Reduction using PCA

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Outline

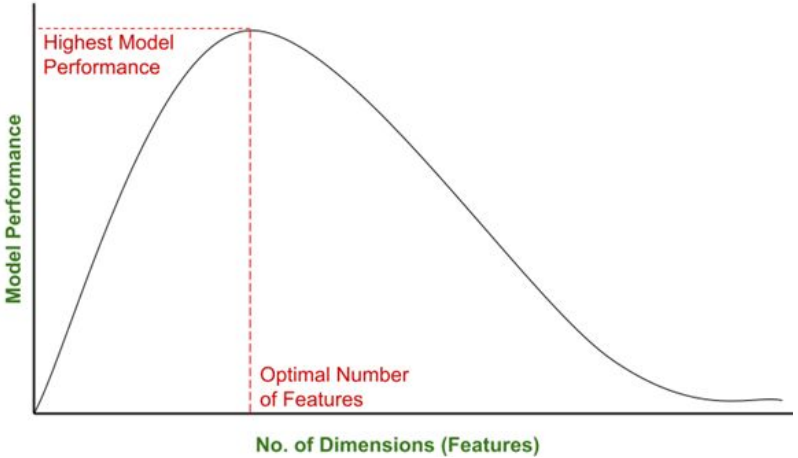
- Dimensionality Reduction
  - Dimensionality Reduction Techniques
    - Principal Components Analysis (Eigenvalues, Eigen vectors, Orthogonality)
    - Independent Component Analysis
    - Single Value Decomposition

Dimensionality Reduction

- Introduction
- Data Science and ML helps to solve several complex regression and classification problems.
- However, the performance of all these models depends on the input dataset.
- So, It is important to provide optimal dataset to ML models.
- Large dataset leads to increased computational demands
- Large dataset leads to overfitting.
- If we provide large dataset (with a large no. of features/columns) to ML models
  - it gives rise to the problem of overfitting,
  - wherein the model starts getting influenced by outlier values and noise.
  - This is called the Curse of Dimensionality.

Dimensionality Reduction

- Dimensionality Reduction is a statistical/ML-based technique
- It helps to reduce the number of features in our dataset.
- It helps to obtain a dataset with an optimal number of dimensions.
- It is useful in Feature Extraction
  - By reduce the number of dimensions by mapping a higher dimensional feature space to a lower-dimensional feature space.
- Effect of the change in model performance with the increase in the number of dimensions of the dataset.
- The model performance is best only at an option dimension, beyond which it starts decreasing.
- Technique of Dimensionality Reduction (Feature Extraction)
  - Principal Component Analysis (PCA)
  - Independent Component Analysis (ICA)
  - Singular Value Decomposition (SVD)
  - Linear Discriminant Analysis (LDA)



Dimensionality Reduction

- Application of DR wrt the type of datasets
  - Image Data: Compressing high-resolution images for efficient storage and retrieval.
  - Audio Data: Simplifying speech recordings for speaker recognition.
  - Audio Data: Reducing music audio data for genre classification.
  - Video Data: Compressing video for faster processing in surveillance systems.
  - Video Data: Reducing video sequences to key frames for action recognition.
  - Time Series Data: Reducing the complexity of financial time series data to reveal major trends.
  - Spatial Data: Reducing GPS data to visualization or summarizing geographic locations.
  - Graph Data: Reducing social network data to identify key communities.
  - Text Data: Efficient sentiment analysis.
  - Numerical Data: Reducing the number of variables in a dataset to predict housing prices.
  - Categorical and Ordinal Data: Reducing customer preferences for easier interpretation.

Principal Components Analysis

- PCA is unsupervised algorithms
- Used for data analysis, data compression, de-noising, reducing the dimension of data.
- It helps to reduce or eliminate similar data.
- PCA analysis reduces dimensionality without any data loss.
- It is a method of factor analysis.
- PCA is also called a dimensionality-reduction method.
- It helps you find out the most common dimensions of our dataset.
- It makes result analysis faster, easier and accurate.
- Dataset contains significant variables and dimensions.
- However, not all these variables will be critical.
- Some variables are primary key variables, whereas others are not.
- So, it helps to eliminate a few extra less important variables, without any data loss.
- Reduced data and dimensions help to achieve results faster and easy visualization.
- PCA helps to analyze all the dimensions and reducing them by maintaining the exact information.

Principal Components Analysis

- **Applications of PCA Analysis**
  - PCA in ML is used to visualize multidimensional data.
  - Healthcare data: To explore the factors important in increasing the risk of any chronic disease.
  - You can also use PCA to analyze patterns when you are dealing with high-dimensional data sets.
  - PCA helps to resize an image.
  - PCA is used to analyze stock data and forecasting data.
- **Domain of PCA Applications:**
  - Data cleaning;
  - Data preprocessing;
  - Denoise the information
  - Analyzing different dimensions.
  - Visualize multidimensional data.
  - Compress the information and transmit the same without any loss in quality.
  - Applied for face recognition, image identification, pattern identification.
  - PCA in ML helps in simplifying complex business algorithms.

Principal Components Analysis

- **When to use PCA**
  - To reduce the number of dimensions in the dataset.
  - To decide the critical variables.
  - To categorize the dependent and independent variables in the dataset.
  - To eliminate the noise components in our dimension analysis.
- Principle components with greater amount of variance are grouped under one category.
- Principle components with smaller variance are grouped under the second category.
- Note:
  - Vectors calculated in the Principal Component Method of factor analysis are not calculated at random.
  - All the calculated components can be combined as linear components and
  - so a single straight vector of each component helps identify difference in features much easier than ever.

Principal Components Analysis

- **Advantages of Principal Component Analysis**
  - Easy to calculate and compute.
  - Prevents predictive algorithms from data overfitting issues.
  - Speeds up machine learning computing processes and algorithms.
  - PIncreases performance of ML algorithms by eliminating unnecessary correlated variables.
  - Principal Component Analysis results in high variance and increases visualization.
  - Helps reduce noise that cannot be ignored automatically.
- **Disadvantages of Principal Component Analysis**
  - Sometimes, PCA is difficult to interpret.
    - Sometimes difficult to identify the most important features even after computing the PCs.
  - You may face some difficulties in calculating the covariances and covariance matrices.
  - Sometimes, the PCAs can be more difficult to read rather than the original set of components.

Principal Components Analysis

- Example: Steps to perform PCA
- 1. Standardize the range of continuous initial variables
- 2. Compute the covariance matrix to identify correlations
- 3. Compute the eigenvectors and eigenvalues of the covariance matrix to identify the Principal Components
- 4. Create a feature vector to decide the Principal Components
- 5. Recast the data along the Principal Components axes

Principal Components Analysis

- Example 1: Find the eigenvalues and eigenvectors of the matrix $A = \begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix}$

The eigenvalues and eigenvectors are found by solving the eigenvalue probelm

$$AX = \lambda X \qquad X = \begin{bmatrix} x \\ y \end{bmatrix} \quad \text{i.e.} \quad (A - \lambda I)X = 0.$$

Non-trivial solutions will exist if $\det(A - \lambda I) = 0$

that is, $\det\left\{\begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right\} = 0, \quad \therefore \quad \begin{vmatrix} 1-\lambda & 0 \\ 1 & 2-\lambda \end{vmatrix} = 0,$

expanding this determinant: $(1-\lambda)(2-\lambda) = 0$. Hence the solutions for λ are: $\lambda = 1$ and $\lambda = 2$.

So we have found two values of λ for this 2×2 matrix A. Since these are unequal they are said to be **distinct** eigenvalues.

To each value of λ there corresponds an eigenvector. We now proceed to find the eigenvectors.

Principal Components Analysis

- Example 2: Find the eigenvalues and eigenvectors of the matrix

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix}$$

$\lambda = 1$ (smaller eigenvalue). Then our original eigenvalue problem becomes: $AX = X$.

$$\begin{aligned} x &= x \\ x + 2y &= y \end{aligned} \qquad \text{Simplifying} \qquad \begin{aligned} x &= x \\ x + y &= 0 \end{aligned}$$

All we can deduce here is that $x = -y$ $\quad \therefore \quad X = \begin{bmatrix} x \\ -x \end{bmatrix}$ for any $x \neq 0$

(We specify $x \neq 0$ as, otherwise, we would have the trivial solution.)

So the eigenvectors corresponding to eigenvalue $\lambda = 1$ are all proportional to $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$, e.g. $\begin{bmatrix} 2 \\ -2 \end{bmatrix}$, $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ etc.

Sometimes we write the eigenvector in **normalised** form that is, with modulus or magnitude 1. Here, the normalised form of X is $\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$ which **is unique**.

Principal Components Analysis

- Example 1: Find the eigenvalues and eigenvectors of the matrix

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix}$$

Now we consider the larger eigenvalue $\lambda = 2$. Our original eigenvalue problem $AX = \lambda X$ becomes $AX = 2X$ which gives the following equations:

$$\begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = 2\begin{bmatrix} x \\ y \end{bmatrix} \quad \text{i.e.} \quad \begin{aligned} x &= 2x \\ x + 2y &= 2y \end{aligned}$$

These equations imply that $x = 0$ whilst the variable y may take any value whatsoever (except zero as this gives the trivial solution).

Thus the eigenvector corresponding to eigenvalue $\lambda = 2$ has the form $\begin{bmatrix} 0 \\ y \end{bmatrix}$, e.g. $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$, $\begin{bmatrix} 0 \\ 2 \end{bmatrix}$ etc.

The normalised eigenvector here is $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

In conclusion: the matrix $A = \begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix}$ has two eigenvalues and two associated normalised eigenvectors:

$$\lambda_1 = 1, \qquad \lambda_2 = 2 \qquad X_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} \qquad X_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Principal Components Analysis

- Example 2: Obtain the eigenvalues and the eigenvectors of the symmetric 2 × 2 matrix

$$A = \begin{bmatrix} 4 & -2 \\ -2 & 1 \end{bmatrix}$$

The characteristic equation for A is

$$(4-\lambda)(1-\lambda)+4=0 \qquad \text{or} \qquad \lambda^2 - 5\lambda = 0$$

giving $\lambda = 0$ and $\lambda = 5$, both of which are of course real and also unequal (i.e. distinct). For the larger eigenvalue $\lambda = 5$ the eigenvector $X = \begin{bmatrix} x \\ y \end{bmatrix}$ satisfy

$$\begin{bmatrix} 4 & -2 \\ -2 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 5x \\ 5y \end{bmatrix} \quad \text{i.e.} \quad -x-2y=0, \qquad -2x-4y=0$$

Both equations tell us that $x = -2y$ so an eigenvector for $\lambda = 5$ is $X = \begin{bmatrix} 2 \\ -1 \end{bmatrix}$ or any multiple of this. For $\lambda = 0$ the associated eigenvectors satisfy

$$4x - 2y = 0 \qquad -2x + y = 0$$

i.e. $y = 2x$ (from both equations) so an eigenvector is $Y = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ or any multiple.

Principal Components Analysis

- Example 3: Prove that the X and Y matrix are orthogonal.

$$X^TY = [2, \quad -1] \begin{bmatrix} 1 \\ 2 \end{bmatrix} = 2 \times 1 - 1 \times 2 = 2 - 2 = 0$$

$X^TY = 0$ means are X and Y are **orthogonal**.

Principal Components Analysis

- Example 4: Show that these three eigenvectors X, Y,Z are mutually orthogonal.

$$X = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \qquad Y = \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}$$

$$X^T Y = [1, \quad 0, \quad -1] \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} = 1 - 1 = 0$$

$$Y^T Z = [1, \quad -\sqrt{2}, \quad 1] \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix} = 1 - 2 + 1 = 0$$

$$Z^T X = [1, \quad \sqrt{2}, \quad 1] \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} = 1 - 1 = 0$$

Covariance Matrix

- It is a type of matrix that is used to represent the covariance values
  - between pairs of elements given in a random vector.
- It can also be referred to as the variance covariance matrix.
- This is because the variance of each element is represented along the main diagonal of the matrix.
- It is always a square matrix.
- It is positive semi-definite, and symmetric.
- This matrix is very useful in stochastic modeling and principal component analysis.
- It displays the variance exhibited by elements of datasets and covariance between a pair of datasets.
- Variance is a measure of dispersion and can be defined as the spread of data from the mean of the given dataset.
- Covariance is calculated between two variables and is used to measure how the two variables vary together.
- It is a square matrix where diagonal elements represent the variance and the off-diagonal elements represent the covariance.
- The covariance between two variables can be positive, negative, and zero.
- A positive covariance indicates that the two variables have a positive relationship whereas negative covariance shows that they have a negative relationship.
- If two elements do not vary together then they will display a zero covariance.

Covariance Matrix

- Example: Covariance Matrix 2 × 2

Covariance Matrix Example

$$\begin{bmatrix} Var(x_1) & \cdots\cdots & Cov(x_n,x_1) \\ \vdots & \cdot & \vdots \\ \vdots & \cdot & \vdots \\ Cov(x_n,x_1) & \cdots\cdots & Var(x_n) \end{bmatrix}$$

Population Var: $var(x) = \frac{\sum_1^n (x_i-\mu)^2}{n}$ Sample Var: $var(x) = \frac{\sum_1^n (x_i-\bar{x})^2}{n-1}$

Population Cov: $cov(x, y) = \frac{\sum_1^n (x_i-\mu_x)(y_i-\mu_y)}{n}$ Sample Cov: $cov(x, y) = \frac{\sum_1^n (x_i-\bar{x})(y_i-\bar{y})}{n-1}$

μ = mean of population data. n = number of observations in the dataset.

$\bar{x}$ = mean of sample data. x_i = observations in dataset x.

Dataset	X	Y
	3	6
	2	4
Sum (∑)	5	10
Mean ($\bar{x}$)	2.5	5

	$x_i-\bar{x}$	$y_i-\bar{y}$	$(x_i-\bar{x})(y_i-\bar{y})$	$(x_i-\bar{x})^2$	$(y_i-\bar{y})^2$
	0.5	1	0.5	0.25	1
	-0.5	-1	0.5	0.25	1
Sum (∑)	0	0	1	0.5	2
Sample Var				0.5	2
Sample Cov			1		

Covariance Matrix 2 × 2

var(x)	cov(x, y)
cov(x, y)	var(x)

Covariance Matrix 2 × 2

0.5	1
1	2

Covariance Matrix

- Example:
- Covariance Matrix 3 × 3

$$\begin{bmatrix} Var(x_1) & \cdots\cdots & Cov(x_n,x_1) \\ \vdots & \ddots & \vdots \\ Cov(x_n,x_1) & \cdots\cdots & Var(x_n) \end{bmatrix}$$

Population Var: $var(x) = \frac{\sum_1^n (x_i-\mu)^2}{n}$ Sample Var: $var(x) = \frac{\sum_1^n (x_i-\bar{x})^2}{n-1}$

Population Cov: $cov(x, y) = \frac{\sum_1^n (x_i-\mu_x)(y_i-\mu_y)}{n}$ Sample Cov: $cov(x, y) = \frac{\sum_1^n (x_i-\bar{x})(y_i-\bar{y})}{n-1}$

μ = mean of population data. n = number of observations in the dataset.

$\bar{x}$ = mean of sample data. x_i = observations in dataset x.

Dataset	Math (X)	Science (Y)	English (Z)
1	70	80	50
2	65	30	40
3	90	70	60
Sum (∑)	**225**	**180**	**150**
Mean ($\bar{x}$)	**75**	**60**	**50**

	$x_i-\bar{x}$	$y_i-\bar{y}$	$z_i-\bar{z}$	$(x_i-\bar{x})(y_i-\bar{y})$	$(x_i-\bar{x})(z_i-\bar{z})$	$(y_i-\bar{y})(z_i-\bar{z})$	$(x_i-\bar{x})^2$	$(y_i-\bar{y})^2$	$(z_i-\bar{z})^2$
	-5	20	0	-100	0	0	25	400	0
	-10	-30	-10	300	100	300	100	900	100
	15	10	10	150	150	100	225	100	100
Sum (∑)	**0**	**0**	**0**	**350**	**250**	**400**	**350**	**1400**	**200**
Sample Var							**175**	**700**	**100**
Sample Cov				**175**	**125**	**200**			

Covariance Matrix 3 × 3

var(x)	cov(x, y)	cov(x,z)
cov(x, y)	var(y)	cov(y,z)
cov(x,z)	cov(y,z)	var(z)

Covariance Matrix 3 × 3

175	175	125
175	700	200
125	200	100

Covariance Matrix

- **Properties of Covariance Matrix**
- It is a very important tool used by data scientists to understand and analyze multivariate data.
- It depicts the variance of datasets and covariance of a pair of datasets in matrix format.
- The diagonal elements represent the variance of a dataset and
  - the off-diagonal terms give the covariance between a pair of datasets.
- The variance covariance matrix is always square, symmetric, and positive semi-definite.
- Extremely useful properties of Covariance Matrix:
  - It is always a square matrix. That is # of rows of the matrix will be equal to the number of columns.
  - The matrix is symmetric. Suppose M is the cov.mat. then MT = M.
  - It is positive semi-definite.
    - Let u be a column vector, uT is the transpose of that vector and M be the cov.mat. then uTMu ≥ 0.
  - All eigenvalues of the variance covariance matrix are real and non-negative.

Covariance Matrix

- **Interpretation of the variance covariance matrix:**
- 1) The diagonal elements 500, 340 and 800 indicate the variance in data sets X, Y and Z respectively.
  - Y shows the lowest variance whereas Z displays the highest variance.
- 2) The covariance for X and Y is 320.
  - As this is a positive number it means that when X increases (or decreases) Y also increases (or decreases)
- 3) The covariance for X and Z is –40.
  - As it is a negative number it implies that when X increases Z decreases and vice – versa.
- 4) The covariance for Y and Z is 0.
  - This means that there is no predictable relationship between the two data sets.

Covariance Matrix 3 × 3

var(x)	cov(x, y)	cov(x,z)
cov(x, y)	var(y)	cov(y,z)
cov(x,z)	cov(y,z)	var(z)

Covariance Matrix 3 × 3

500	320	–40
320	340	0
–40	0	800

References

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Thank You.