MACHINE LEARNING

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1 Linear Discriminant Analysis

In linear algebra, the Singular Value Decomposition (SVD) of a matrix is a factorization of that matrix into three matrices. It has some interesting algebraic properties and conveys important geometrical and theoretical insights about linear transformations. It also has some important applications in data science.

To understand SVD we need to first understand the Eigenvalue Decomposition of a matrix. We can think of a matrix A as a transformation that acts on a vector x by multiplication to produce a new vector Ax. We use [A]ij or aij to denote the element of matrix A at row i and column j. If A is an m×p matrix and B is a p×n matrix, the matrix product C=AB (which is an m×n matrix) is defined as:

$$[\mathbf{C}]_{ij} = c_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj}$$

Figure 1: Lda.

For example, the rotation matrix in a 2-d space can be defined as:

Example Let us take a 2 Dimensional dataset: C1 X1 = (x1, x2) = (4, 1),(2, 4),(2, 3),(3, 6),(4, 4) C2 X2 = (x1, x2) = (9, 10),(6, 8),(9, 5),(8, 7),(10, 8)

1.1 Step1

Compute the within class scatter matrix Sw Sw = S1 + S2 S1 is the convariance matrix for the the class C1 S2 is the convariance matrix for the the class C2 Covariance matrix Covariance matrix = var(x) cov(y, x) cov(x, y) var(y) To calculate the covariance matrix we need to find x variance, y variance and the covariance of x and y

1.2 Scatter matrix

A scatter plot matrix is a grid (or matrix) of scatter plots used to visualize bivariate relationships between combinations of variables. Each scatter plot in the matrix visualizes the relationship between a pair of variables, allowing many relationships to be explored in one chart. A scatter matrix is a

$$\mathbf{VAR(X)} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - E(X))^2$$

$$\mathbf{COV(X, Y)} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - E(X))(y_i - E(Y))$$

$$\mathbf{COR(X, Y)} = \frac{\mathbf{COV(X, Y)}}{\sqrt{\mathbf{VAR(X)VAR(Y)}}}$$

$$\mathbf{R}^2 = 1 - \frac{\mathbf{VAR(X, Y)}_{FittedLine}}{\mathbf{VAR(X, Y)}_{Mean}}$$

estimation of covariance matrix when covariance cannot be calculated or costly to calculate. The scatter matrix is also used in lot of dimensionality reduction exercises. If there are k variables , scatter matrix will have k rows and k columns i.e k X k matrix.

The scatter matrix is computed by the following equation:

$$S = \sum_{k=1}^{n}(\boldsymbol{x}_k - \boldsymbol{m})(\boldsymbol{x}_k - \boldsymbol{m})^T$$

where $\boldsymbol{m}$ is the mean vector

$$\boldsymbol{m} = \frac{1}{n}\sum_{k=1}^{n}\boldsymbol{x}_k$$

1.3 In python scatter matrix can be computed using

The scatter matrix contains for each combination of the variable , the relation between them . Lets observe the scatter matrix for the following matrix

For k variables in the dataset, the scatter plot matrix contains k rows and k columns. Each row and column represents as a single scatter plot. Each individual plot (i, j) can be defined as:

Vertical Axis: Variable Xj Horizontal Axis: Variable Xi The plot lies on the diagonal is just a 45 line because we are plotting here Xi vs Xi. However, we can plot the histogram for the Xi in the diagonals or just leave it blank. Since Xi vs Xj is equivalent to Xj vs Xi with the axes reversed, we can also omit the plots below the diagonal. It can be more helpful if we overlay some line plot on the scattered points in the plots to give more understanding of the plot. The idea of the pair-wise plot can also be extended to different other plots such as quantile-quantile plots or bihistogram.

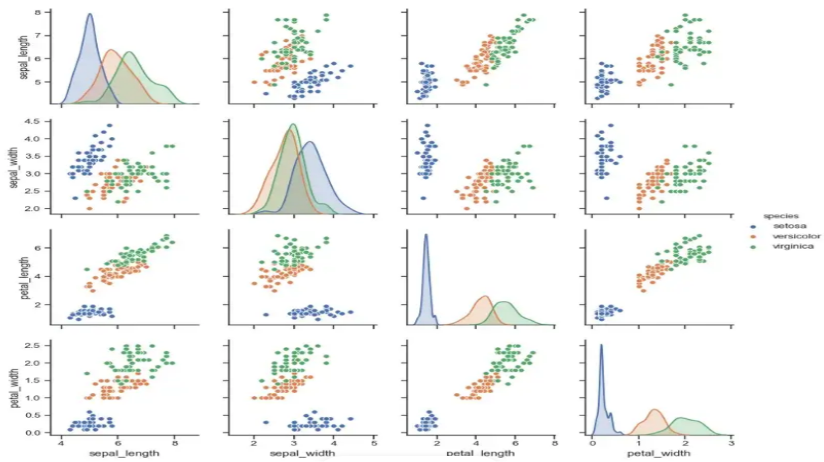
1.4 Dimension reduction

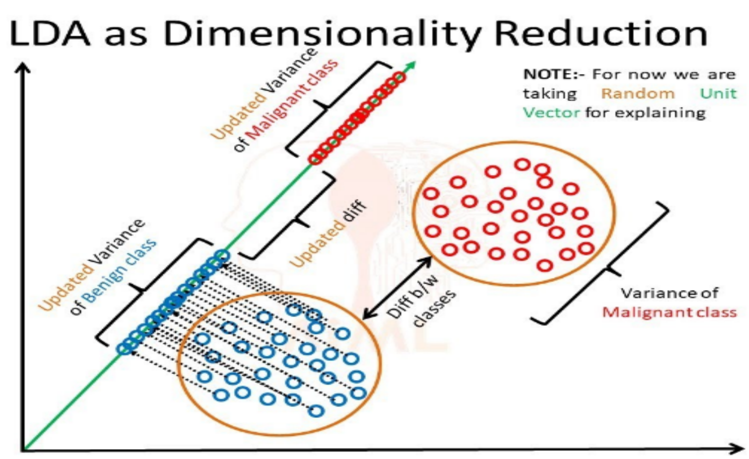
Dimension reduction In this step after obtaining the projection vector we use the input data to project the reduced data into a plot. y = V X . . .

Samples for class 1 : X1=(x1,x2)=(4,2),(2,4),(2,3),(3,6),(4,4) and Sample for class 2 : X2=(x1,x2)=(9,10),(6,8),(9,5),(8,7

STEP 1: Computing the d-dimensional mean vectors

$\mu_1 = 1/N_1 \sum_{x \epsilon w1} x$ =1/5 *[$\begin{bmatrix}4\\2\end{bmatrix} + \begin{bmatrix}2\\4\end{bmatrix} + \begin{bmatrix}2\\3\end{bmatrix} + \begin{bmatrix}3\\6\end{bmatrix} + \begin{bmatrix}4\\4\end{bmatrix}] = \begin{bmatrix}3\\3.8\end{bmatrix}$


sepal_length
sepal_width
petal_length
petal_width
species
setosa
versicolor
virginica


LDA as Dimensionality Reduction
Updated Variance of Malignant class
NOTE:- For now we are taking Random Unit Vector for explaining
Updated Variance of Benign class
Updated diff
Diff b/w classes
Variance of Malignant class

$\mu_2 = 1/N_2 \sum_{x \epsilon w2} x$ =1/5 *[$\begin{bmatrix} 9 \\ 10 \end{bmatrix} + \begin{bmatrix} 6 \\ 8 \end{bmatrix} + \begin{bmatrix} 9 \\ 5 \end{bmatrix} + \begin{bmatrix} 8 \\ 7 \end{bmatrix} + \begin{bmatrix} 10 \\ 8 \end{bmatrix}] = \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}$

class means are: $\boxed{\bar{\mu}_1 = \begin{bmatrix} 3 \\ 3.8 \end{bmatrix} \textit{ and } \bar{\mu}_2 = \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}}$

STEP 2 : Computing the Scatter Matrices

within-class scatter matrix S_W *is computed by the following equation* $S_W = \sum_{i=1}^{c} S_i$

where $S_i = \sum_{x \epsilon D_i}^{n} (x - \mu_i) - (x - \mu_i)^T$ Covariance matrix of the first class:

$S_i = \sum_{x \epsilon w1}^{n} (x - \mu_1) - (x - \mu_1)^T = \left[\begin{bmatrix} 4 \\ 2 \end{bmatrix} - \begin{bmatrix} 3 \\ 3.8 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 2 \\ 4 \end{bmatrix} - \begin{bmatrix} 3 \\ 3.8 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 2 \\ 3 \end{bmatrix} - \begin{bmatrix} 3 \\ 3.8 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 3 \\ 6 \end{bmatrix} - \begin{bmatrix} 3 \\ 3.8 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 4 \\ 4 \end{bmatrix} - \begin{bmatrix} 3 \\ 3.8 \end{bmatrix}\right]^2 = \begin{bmatrix} 1 & -0.25 \\ -0.25 & 2.2 \end{bmatrix}$

$\boxed{\bar{c}ovariance\ matrix\ of\ the\ first\ class\ S_1 = cov(X1)}$

$S_2 = \sum_{x \epsilon w2}^{n} (x - \mu_2) - (x - \mu_2)^T = \left[\begin{bmatrix} 9 \\ 10 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 6 \\ 8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 9 \\ 5 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 8 \\ 7 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right]^2 + \left[\begin{bmatrix} 10 \\ 8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right]^2 = \begin{bmatrix} 2.3 & -0.05 \\ -0.05 & 3.3 \end{bmatrix}$

$\boxed{\bar{c}ovariance\ matrix\ of\ the\ first\ class\ S_2 = cov(X2)}$

$Within - class\ scatter\ matrix : S_W = \sum_{i=1}^{c} S_i = S_1 + S_2 = \begin{bmatrix} 1 & -0.25 \\ -0.25 & 2.2 \end{bmatrix} + \begin{bmatrix} 2.3 & -0.05 \\ -0.05 & 3.3 \end{bmatrix} = \begin{bmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{bmatrix}$

$\boxed{\bar{W}ithin - class\ scatter\ matrix : S_W = \begin{bmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{bmatrix}}$

$Now\ compute\ Between - class\ scatter\ matrix : S_B$

$S_B = (\mu_1 - \mu_2) * (\mu_1 - \mu_2)^T = \left[\begin{bmatrix} 3 \\ 3.8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right] * \left[\begin{bmatrix} 3 \\ 3.8 \end{bmatrix} - \begin{bmatrix} 8.4 \\ 7.6 \end{bmatrix}\right]^T$

$= \begin{bmatrix} -5.4 \\ -3.8 \end{bmatrix} * \begin{bmatrix} -5.4 & -3.8 \end{bmatrix} = \begin{bmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{bmatrix}$

$Solving\ the\ generalized\ eigenvalue\ problem\ for\ the\ matrix\ S_W^{-1} * S_B$

$The\ LDA\ projection\ is\ then\ obtained\ as\ the\ solution\ of\ the\ generalized\ eigen\ value\ problem$

$i.e,\ S_W^{-1} * S_B = \lambda_W$

$|S_W^{-1} * S_B - \lambda_W| = 0$

$= \left| \begin{bmatrix} 3.3 & -0.3 \\ -0.3 & 5.5 \end{bmatrix}^{-1} * \begin{bmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{bmatrix} - \lambda * \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right|$

$$= | \begin{bmatrix} 0.3045 & 0.0166 \\ 0.0166 & 0.1827 \end{bmatrix} * \begin{bmatrix} 29.16 & 20.52 \\ 20.52 & 14.44 \end{bmatrix} - \lambda * \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} | = 0$$

$$= | \begin{bmatrix} 9.2213 - \lambda & 6.483 \\ 4.2339 & 2.9794 - \lambda \end{bmatrix} | = 0$$

$= (9.2213 - \lambda)(2.9794 - \lambda) - (6.483)(4.2339) = 0$
$= (\lambda)^2) - 12.2007 * \lambda = 0$
$i.e, \lambda_1 = 0 \ and \ \lambda_2 = 12.0027$

$STEP\ 4 : Selecting\ linear\ discriminant\ for\ the\ new\ feature\ subspace$

$Hence, \lambda_1 = 0$

$$\begin{bmatrix} 9.2213 & 6.483 \\ 4.2339 & 2.9794 \end{bmatrix} * W_1 = \lambda_1 * \begin{bmatrix} w1 \\ w2 \end{bmatrix} = \begin{bmatrix} 9.2213 & 6.483 \\ 4.2339 & 2.9794 \end{bmatrix} * W_1 = 0 * \begin{bmatrix} w1 \\ w2 \end{bmatrix}$$

$$and \begin{bmatrix} 9.2213 & 6.483 \\ 4.2339 & 2.9794 \end{bmatrix} * W_2 = \lambda_2 * \begin{bmatrix} w1 \\ w2 \end{bmatrix}$$

$$= \begin{bmatrix} 9.2213 & 6.483 \\ 4.2339 & 2.9794 \end{bmatrix} * W_1 = 12.0027 * \begin{bmatrix} w1 \\ w2 \end{bmatrix}$$

$$Thus W_1 = \begin{bmatrix} -0.5755 \\ 0.8178 \end{bmatrix}$$

$$and \boxed{\bar{W}_2 = \begin{bmatrix} 0.9088 \\ 0.4173 \end{bmatrix} = W^*}$$

2 Scalar Value Decompositon

LaTeX SVD is also a dimensional reduction technique. In this method the given matrix is decomposed into three distinct matrices. SVD of a m x n matrix is given as: A = UWVT U : mxn matrix of the orthonormal eigenvectors of AAT W : a nxn diagonal matrix of the singular values which are the square roots of the eigenvalues of AAT VT

denote their mean. Then as n approaches infinity, the random variables $\sqrt{n}(S_n - \mu)$ converge in distribution to a normal $\mathcal{N}(0, \sigma^2)$.

$$AA^T = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix} . \begin{bmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{bmatrix} = \begin{bmatrix} 17 & 8 \\ 8 & 17 \end{bmatrix}$$

Applying the characteristic equation for the above matrix is $W - \lambda I = 0$
$AA^T - \lambda I = 0$

$\lambda^2 - 34\lambda + 225 = 0$

$= (\lambda - 25)(\lambda - 9)$

so our singular values are: $\sigma_1 = 5\,; \sigma_2 = 3$ Now we find the right singular vectors i.e orthonormal set of eigenvectors of AA^T. The eigenvalues of AA^T are 25, 9, and 0, and since AA^T.is symmetric we know that the eigenvectors will be orthogonal.
For $\lambda = 25$,

$$AA^T - 25I = \begin{bmatrix} -12 & 12 & 2 \\ 12 & -12 & -2 \\ 2 & -2 & -17 \end{bmatrix}$$

which can be row-reduces to : $\begin{bmatrix} 1 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$

Singular value decomposition is an extension *eigenvalue decomposition* (see Fig. 6.2) to nonsquare matrices. For $d \times m$ matrix $\boldsymbol{A}$, a d-dimensional nonzero vector $\boldsymbol{\psi}$, an m-dimensional nonzero vector $\boldsymbol{\varphi}$, and a non-negative scalar κ such that

$$\boldsymbol{A}\boldsymbol{\varphi} = \kappa\boldsymbol{\psi}$$

are called a *left singular vector*, a *right singular vector*, and a *singular value* of $\boldsymbol{A}$, respectively. Generally, there exist c singular values $\kappa_1, \ldots, \kappa_c$, where

$$c = \min(d, m).$$

Singular vectors $\boldsymbol{\varphi}_1, \ldots, \boldsymbol{\varphi}_c$ and $\boldsymbol{\psi}_1, \ldots, \boldsymbol{\psi}_c$ corresponding to singular values $\kappa_1, \ldots, \kappa_c$ are mutually orthogonal and are usually normalized, i.e., they are *orthonormal* as

$$\boldsymbol{\varphi}_k^\top \boldsymbol{\varphi}_{k'} = \begin{cases} 1 & (k = k') \\ 0 & (k \neq k') \end{cases} \quad \text{and} \quad \boldsymbol{\psi}_k^\top \boldsymbol{\psi}_{k'} = \begin{cases} 1 & (k = k'), \\ 0 & (k \neq k'). \end{cases}$$

A matrix $\boldsymbol{A}$ can be expressed by using its singular vectors and singular values as

$$\boldsymbol{A} = \sum_{k=1}^{c} \kappa_k \boldsymbol{\psi}_k \boldsymbol{\varphi}_k^\top.$$

In MATLAB, singular value decomposition can be performed by the svd function.

Figure 2: Flock of birds.

unit vector in the direction of it is:

$v_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$

Similarly, for $\lambda = 9, v_2 = \begin{bmatrix} \frac{1}{\sqrt{18}} \\ \frac{-1}{\sqrt{18}} \\ \frac{4}{\sqrt{18}} \end{bmatrix}$

For the 3rd eigenvector, we could use the property that it is perpendicular to v1 and v2 such that:

$v_1^T v_3 = 0$

$v_2^T v_3 = 0$

Solving the above equation to generate the third eigenvector

$v_3 = \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} a \\ -a \\ -a/2 \end{bmatrix} = \begin{bmatrix} \frac{2}{3} \\ \frac{-2}{3} \\ \frac{-1}{3} \end{bmatrix}$ Now, we calculate U using the formula $u_i = \frac{1}{\sigma} A v_i$ and this gives U $= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$.

Hence, our final SVD equation becomes:

$A = A = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{18}} & \frac{-1}{\sqrt{18}} & \frac{4}{\sqrt{18}} \\ \frac{2}{3} & \frac{-2}{3} & \frac{1}{3} \end{bmatrix}$