Data Mining
Lecture 3: Covariance, EVD, PCA & SVD

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Variance and Covariance - Expectation

Recap :

- Expectation and Variance
- Covariance
- Basis set
- PCA
- SVD, truncated SVD

Variance and Covariance - Expectation

A random variable takes on different values due to chance

The sample values from a single dimension of a featurespace can be considered to be a random variable

The expected value $E[X]$ is the most likely value a random variable will take.

If we assume that the values an element of a feature can take are all equally likely then the expected value is just the mean value.

Variance and Covariance - Variance

Variance = The expected squared difference from the mean

$$E[(X - E[X])^2]$$

i.e. the mean squared difference from the mean

$$\sigma^2(x) = \frac{1}{n} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

A measure of how spread out the data is

Variance and Covariance - Covariance

Covariance = the product of the expected difference between each feature and its mean

$$E[(x - E[x])(y - E[y])]$$

i.e. it measures how two variables change together

$$\sigma(x, y) = \frac{1}{n} \sum_{i=1}^{n} (x - \mu_x)(y - \mu_y)$$

When both variables are the same, covariance = variance, as $\sigma(x, x) = \sigma^2(x)$
If $\sigma^2 = 0$ then the variables are uncorrelated

Variance and Covariance - Covariance

A covariance matrix encodes how all features vary together
For two dimensions:

$$\begin{bmatrix} \sigma(x,x) & \sigma(x,y) \\ \sigma(y,x) & \sigma(y,y) \end{bmatrix}$$

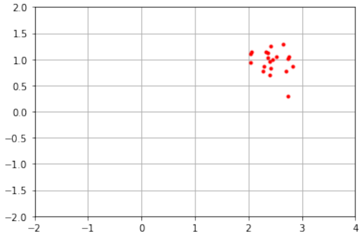
For *n* dimensions:

$$\begin{bmatrix} \sigma(x_1,x_1) & \sigma(x_1,x_2) & \dots & \sigma(x_1,x_n) \\ \sigma(x_2,x_1) & \sigma(x_2,x_2) & \dots & \sigma(x_2,x_n) \\ \vdots & \vdots & \ddots & \vdots \\ \sigma(x_n,x_1) & \sigma(x_n,x_2) & \dots & \sigma(x_n,x_n) \end{bmatrix}$$

This matrix must be square symmetric
(x cannot vary with y differently to how y varies with x!)
2d covariance demo

Variance and Covariance - Covariance

Mean Centering = subtract the of all the vectors from each vector
This gives centered data, with mean at the origin



Variance and Covariance - Covariance

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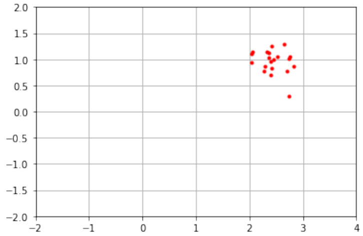
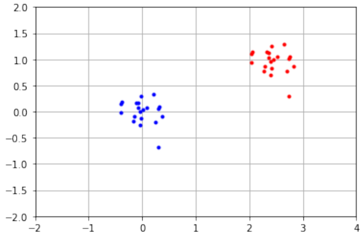




ipynb mean centering demo

Variance and Covariance - Covariance

If you have a set of mean centred data with d dimensions, where each row is your data point:

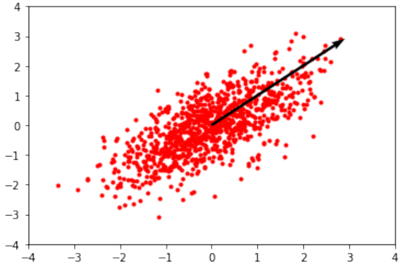
$$Z = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2d} \end{bmatrix}$$

Then its inner product is proportional to the covariance matrix

$$C \propto Z^T Z$$

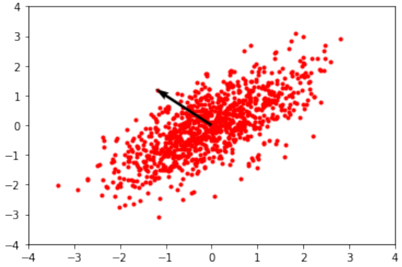
Variance and Covariance - Covariance

Principal axes of variation:
1st principal axis: direction of greatest variance



Variance and Covariance - Covariance

2nd Principal axis: direction orthogonal to 1st principal axis in direction of greatest variance



Variance and Covariance - Basis Set

In linear algebra, a basis set is defined for a space with the properties:

- They are all linearly independent
- They span the whole space

Every vector in the space can be described as a combination of basis vectors

Variance and Covariance - Basis Set

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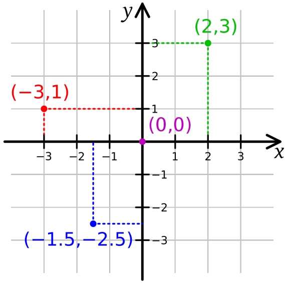


Using Cartesian coordinates, we describe every vector as a combination of x and y directions

Variance and Covariance - Basis Set

Eigenvectors and eigenvalues
An eigenvector is a vector that when multiplied by a matrix $\boldsymbol{A}$ gives a value that is a multiple of itself, i.e.:

$$\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$$

The eigenvalue λ is the multiple that it should be multiplied by.

eigen comes from German, meaning 'Characteristic' or 'Own'

for an $n \times n$ dimensional matrix $\boldsymbol{A}$ there are n eigenvector-eigenvalue pairs

Variance and Covariance - Basis Set

So if $\boldsymbol{A}$ is a covariance matrix, then the eigenvectors are its principal axes.

The eigenvalues are proportional to the variance of the data along each eigenvector

The eigenvector corresponding to the largest eigenvalue is the first principal axis

Variance and Covariance - Basis Set

To find eigenvectors and eigenvalues for smaller matrices, there are algebraic solutions, and all values can be found
For larger matrices, numerical solutions are found, using eigendecomposition.
Eigen - Value - Decomposition (EVD):

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}$$

Where $\boldsymbol{Q}$ is a matrix where the columns are the eigenvectors, and $\boldsymbol{\Lambda}$ is a matrix with eigenvalues along the corresponding diagonal

Covariance matrices are real symmetric, so $Q^{-1} = Q^T$ Therefore:

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{\boldsymbol{T}}$$

This diagonalisation of a covariance matrix gives the principal axes and their relative magnitudes

Variance and Covariance - Basis Set

$$\boldsymbol{A} = \boldsymbol{Q}\Lambda\boldsymbol{Q}^{\boldsymbol{T}}$$

This diagonalisation of a covariance matrix gives the principal axes and their relative magnitudes

Usually the implementation will order the eigenvectors such that the eigenvalues are sorted in order of decreasing value.
Some solvers only find the top k eigenvalues and corresponding eigenvectors, rather than all of them.
Java demo: EVD and component analysis

Variance and Covariance - PCA

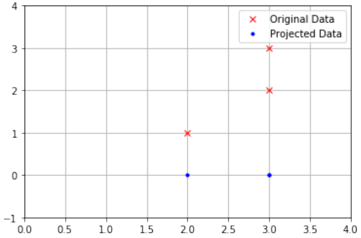
Principal Component Analysis - PCA

Projects the data in to a lower dimensional space, while keeping as much of the information as possible.

$$X = \begin{bmatrix} 2 & 1 \\ 3 & 2 \\ 3 & 3 \end{bmatrix}$$

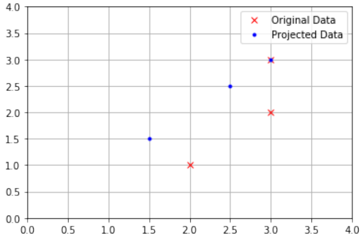
For example: data set X can be transformed so only information from the x dimension is retained using a projection matrix P:

$X_p = XP$



Variance and Covariance - PCA

However if a different line is chosen, more information can be retained.



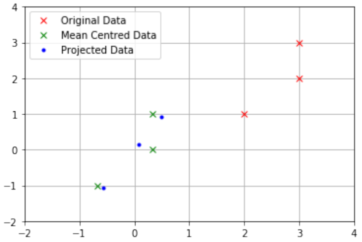
This process can be reversible, (Using $\hat{X} = X_p P^{-1}$) but this is lossy if the dimensionality has been changed.

Variance and Covariance - PCA

In PCA, a line is chosen that minimises the orthogonal distances of the data points from the projected space.

It does this by keeping the dimensions where it has the most variation, i.e. using the directions provided by the eigenvectors corresponding to the largest eigenvalues of the estimated covariance matrix

It uses the mean centred data to give the matrix proportional to the covariance matrix



(ipynb projection demo)

Variance and Covariance - PCA

Algorithm 1: PCA algorithm using EVD

```
**Data:** $N$ data points with feature vectors $X_i$ $i = 1 \dots N$
$Z = \text{meanCentre}(X)$;
$eigVals$, $eigVects = \text{eigendecomposition}(Z^T Z)$;
take $k$ $eigVects$ corresponding to $k$ largest $eigVals$;
make projection matrix $P$;
Project data $Xp = ZP$ in to lower dimensional space;
```

(Java PCA demo)

Variance and Covariance - SVD

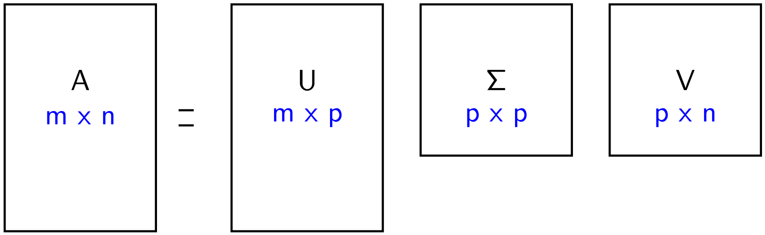
Eigenvalue Decomposition, EVD, $A = Q\Lambda Q^T$ only works for symmetric matrices.
Singular value decomposition - SVD

$$A = U\Sigma V^T$$

where U and V are both different orthogonal matrices, and Σ is a diagonal matrix
Any matrix can be factorised this way.

Orthogonal matrices are where each column is a vector pointing in an othogonal direction to each other, $U^T U = UU^T = I$

Variance and Covariance - SVD



Where p is rank of matrix A

U called *left singular vectors*, contains the eigenvectors of AA^T,
V called *right singular vectors*, contains the eigenvectors of A^TA
Σ contains square roots of eigenvalues of AA^T and A^TA

If A is matrix of mean centred featurevectors, V contains principal components of the covariance matrix

Variance and Covariance - SVD

```
**Algorithm 2:** PCA algorithm using SVD
**Data:** $N$ data points with feature vectors $X_i$ $i = 1 \dots N$
$Z = \text{meanCentre}(X)$;
$U, \Sigma, V = \text{SVD}(Z)$;
take $k$ columns of $V$ corresponding to the largest $k$ values of $\Sigma$;
make projection matrix $P$;
Project data $Xp = ZP$ in to lower dimensional space;
```

Better than using EVD of $Z^T Z$ as:

- has better numerical stability
- can be faster

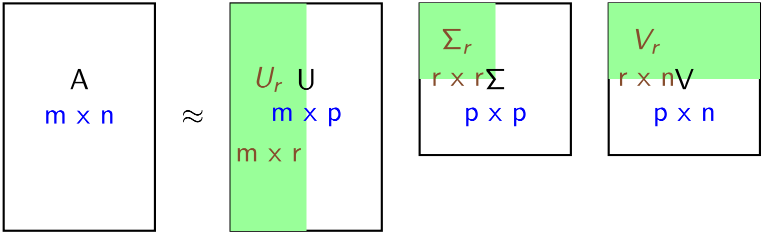
Variance and Covariance - SVD

SVD has better numerical stability:
E.g. Läuchli matrix:

$$X^T X = \begin{bmatrix} 1 & \epsilon & 0 & 0 \\ 1 & 0 & \epsilon & 0 \\ 1 & 0 & 0 & \epsilon \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{bmatrix} = \begin{bmatrix} 1+\epsilon^2 & 1 & 1 \\ 1 & 1+\epsilon^2 & 1 \\ 1 & 1 & 1+\epsilon^2 \end{bmatrix}$$

If ϵ is very small, $1+\epsilon^2$ will be counted as 1, so information is lost

Variance and Covariance - Truncated SVD



Uses only the largest r singular values (and corresponding left and right vectors)

This can give a *low rank approximation* of A, $\tilde{A} = U_r \Sigma_r V_r$

has the effect of minimising the Frobenius norm of the difference between A and $\tilde{A}$

Variance and Covariance - SVD

SVD can be used to give a Pseudoinverse:

$$A^{+} = V\Sigma^{-1}U^{T}$$

This is used to solve $\boldsymbol{A}x = b$ for x where $||\boldsymbol{A}x - b||_2$ is minimised
i.e. in least squares regression $x = \boldsymbol{A}^{+}b$
Also useful in solving homogenous linear equations $\boldsymbol{A}x = 0$
SVD has also found application in:

- model based CF recommender systems
- latent factors
- image compression
- and much more..

Variance and Covariance - EVS / SVD computation

Eigenvalue algorithms are iterative, using *power iteration*

$$b_{k+1} = \frac{Ab_k}{||Ab_k||}$$

Vector b_0 is either an approximation of the dominant eigenvector of A or a random vector.
At every iteration, the vector b_k is multiplied by the matrix A and normalized
If A has an eigenvalue that is greater than its other eigenvalues and the starting vector b_0 has a non zero component in the direction of the associated eigenvector, then the following b_k will converge to the dominant eigenvector.

After the dominant eigenvector is found, the matrix can be rotated and truncated to remove the effect of the dominant eigenvector, then repeated to find the next dominant eigenvector, etc.

Variance and Covariance - EVS / SVD computation

More efficient (and complex) algorithms exist

- Using Raleigh Quotient
- Arnoldi Iteration
- Lanczos Algorithm

Can also use *Gram-Schmidt* to find the orthonormal basis of the top r eigenvectors

Variance and Covariance - EVS / SVD computation

In practice, we use the library implementation, usually from LAPACK (numpy matrix operations usually involve LAPACK underneath)

These algorithms work very efficiently for small to medium sized matrices, as well as for large, sparse matrices, but not really massive matrices (e.g. in pageRank)
There are variations to find the smallest non-zero eigenvectors.

Variance and Covariance - Summary

Covariance measures how different dimensions change together:

- Represented by a matrix
- Eigenvalue decomposition gives eigenvalue - eigenvector pairs
- The dominant eigenvector gives the principal axis
- The Eigenvalue is proportional to the variance along that axis
- The principal axes give a basis set, describing the directions of greatest variance

PCA: aligns data with its principal axes, allows dimensional reduction losing the least information by discounting axes with low variance

SVD: a general matrix factorisation tool with many uses.