

Principal Component Analysis

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https://warwick.ac.uk/fac/sci/dcs/teaching/material/cs909/

Accompanying Notebooks

• Please use:

https://github.com/foxtrotmike/PCA-Tutorial

Question?

Consider the vectors

$$-X_1=[1\ 2\ 1\ 4]^T$$

$$-X_2=[2\ 4\ 2\ 4]^T$$

$$-X_3 = [0\ 0\ 0\ 4]^T$$

$$-X_4=[3 6 3 4]^T$$

$$-X_5=[4844]^T$$

 To store each vector, how many dimensions (or variables) do we need?

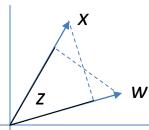
Motivation

- Having large number of related features is not informative
- Visualization of higher dimension data
- Can we reduce the number of features?
 - Dimensionality Reduction

Basics

Projections

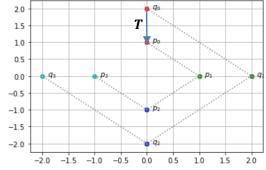
- Data can be projected onto a vector by taking its dot-product
 - The ith-component of a data point is the projection of the data onto the vector corresponding to the ith axis
- $z = w^T x$
 - Projection of x in the direction of w



Transformation

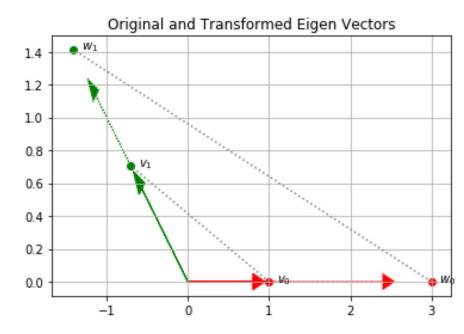
Multiplication of a vector with a matrix can be viewed as a geometric transformation of the vector

$$T = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$
, $x = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$
 $y = Tx = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$



- Eigen Values and Vectors
 - Those points that are characteristic to a given matrix that undergo only a change in scale are called Eigen vectors ${m w}={m T}{m v}=\lambda{m v}$
 - How to find them: $(T \lambda I)v = 0$ implies $|T \lambda I| = 0$
 - See: https://github.com/foxtrotmike/PCA-Tutorial/blob/master/Eigen.ipynb

•
$$T = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$$



• Eigen Vector: $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$, Eigen Value: 3

$$\begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- Note scaling only
- Eigen Vector: $\begin{bmatrix} -0.707 \\ 0.707 \end{bmatrix}$, Eigen Value: 2

$$\begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -0.707 \\ 0.707 \end{bmatrix} = \begin{bmatrix} -1.414 \\ 1.414 \end{bmatrix} = 2 \begin{bmatrix} -0.707 \\ 0.707 \end{bmatrix}$$

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then the characteristic equation is

and the two eigenvalues are

All that's left is to find the two eigenvectors. Let's find the eigenvector, \mathbf{v}_1 , associated with the eigenvalue, λ_1 =-1, first.

so clearly from the top row of the equations we get

Note that if we took the second row we would get

In either case we find that the first eigenvector is any 2 element column vector in which the two elements have equal magnitude and opposite sign.

 $\mathbf{v}_{\mathbf{1}} = \mathbf{k}_{\mathbf{1}} \begin{bmatrix} +1 \\ -1 \end{bmatrix}$

where k₁ is an arbitrary constant. Note that we didn't have to use +1 and -1, we could have used any two quantities of equal magnitude and opposite sign.

Going through the same procedure for the second eigenvalue:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix}$$

$$\begin{vmatrix} \mathbf{A} - \lambda \cdot \mathbf{I} \end{vmatrix} = \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} = 0$$
$$\begin{bmatrix} -\lambda & 1 \\ -2 & -3 - \lambda \end{bmatrix} = \lambda^2 + 3\lambda + 2 = 0$$

$$\lambda_1 = -1, \lambda_2 = -2$$

$$\begin{aligned} \boldsymbol{A} \cdot \boldsymbol{v}_1 &= \lambda_1 \cdot \boldsymbol{v}_1 \\ \left(\boldsymbol{A} - \lambda_1\right) \cdot \boldsymbol{v}_1 &= 0 \\ \begin{bmatrix} -\lambda_1 & 1 \\ -2 & -3 - \lambda_1 \end{bmatrix} \cdot \boldsymbol{v}_1 &= 0 \\ \begin{bmatrix} 1 & 1 \\ -2 & -2 \end{bmatrix} \cdot \boldsymbol{v}_1 &= \begin{bmatrix} 1 & 1 \\ -2 & -2 \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{V}_{1,1} \\ \boldsymbol{v}_{1,2} \end{bmatrix} = 0 \end{aligned}$$

$$V_{1,1} + V_{1,2} = 0$$
, so $V_{1,1} = -V_{1,2}$

$$-2 \cdot V_{1,1} + -2 \cdot V_{1,2} = 0$$
, so again $V_{1,1} = -V_{1,2}$

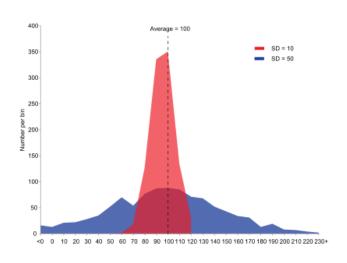
$$\begin{aligned} \boldsymbol{A} \cdot \boldsymbol{v}_2 &= \lambda_2 \cdot \boldsymbol{v}_2 \\ & \left(\boldsymbol{A} - \lambda_2\right) \cdot \boldsymbol{v}_2 = \begin{bmatrix} -\lambda_2 & 1 \\ -2 & -3 - \lambda_2 \end{bmatrix} \cdot \boldsymbol{v}_2 = \begin{bmatrix} 2 & 1 \\ -2 & -1 \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{v}_{21} \\ \boldsymbol{v}_{22} \end{bmatrix} = 0 \quad \text{so} \\ & 2 \cdot \boldsymbol{v}_{21} + 1 \cdot \boldsymbol{v}_{22} = 0 \quad \left(\text{or from bottom line: } -2 \cdot \boldsymbol{v}_{21} - 1 \cdot \boldsymbol{v}_{22} = 0 \right) \\ & 2 \cdot \boldsymbol{v}_{21} = -\boldsymbol{v}_{22} \\ & \boldsymbol{v}_2 = k_2 \begin{bmatrix} +1 \\ -2 \end{bmatrix} \end{aligned}$$

Again, the choice of +1 and -2 for the eigenvector was arbitrary; only their ratio is important. This is demonstrated in the MatLab code below.

Basics

Variance

- Mean of the spread of a variable around its mean
- $var(z) = \frac{1}{N} \sum_{i=1}^{N} (z_i \mu_z)^2 = \frac{1}{N} (\mathbf{z} \mu_z)^T (\mathbf{z} \mu_z)$
 - z is an N-dimensional vector composed of the values of all data points in the sample
- If mean is zero then $var(z) = \frac{1}{N} \mathbf{z}^T \mathbf{z} = \frac{1}{N} ||\mathbf{z}||^2$
- $var(z) = E[(z \mu_z)^2]$
- Variance as an information measure
 - How is variance related to information content?



https://www.khanacademy.org/math/ap-statistics/summarizing-quantitative-data-ap/more-standard-deviation/v/review-and-intuition-why-we-divide-by-n-1-for-the-unbiased-sample-variance

Covariance

Co-Variance

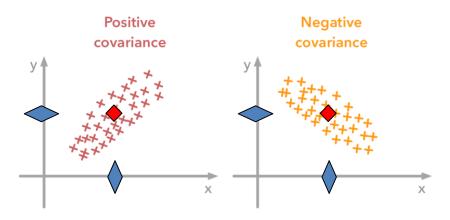
Given two random variables, to what extent are they linearly related to each other

$$- cov(x,y) = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu_x) (y_i - \mu_y) = \frac{1}{N} (x - \mu_x)^T (y - \mu_y)$$

- Covariance is positive if, on average,
 - When one variable is above its mean then the other variable is above its mean too
 - When one variable is below its mean then the other variable is below its mean too
- Covariance is negative if, on average,
 - When one variable is above the mean, the other is below its mean
- Assume that the means are zero: $cov(x, y) = \frac{1}{N}x^{T}y$
 - Maximum when the vectors are co-linear or parallel

$$- cov(x, y) = E[(y - \mu_y)(x - \mu_x)]$$

- Thus, var(z) = cov(z, z)



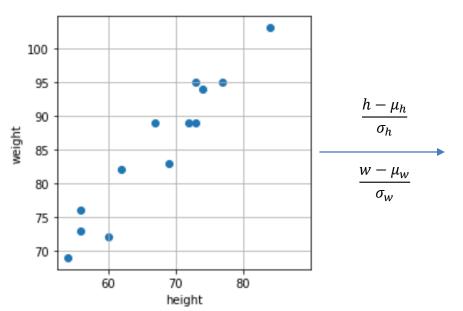
Basics

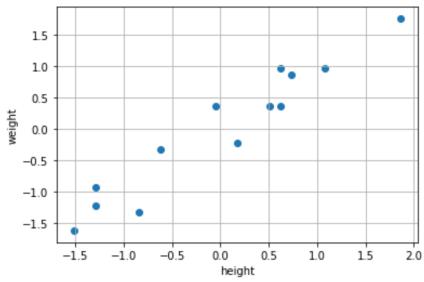
Why are we interested in covariance

- If two variables co-vary then they are redundant, or one can be linearly deduced from another
- Covariance matrix: matrix of all pairwise covariances of all variables

•
$$\boldsymbol{c} = \begin{bmatrix} cov(y,y) & cov(z,y) \\ cov(y,z) & cov(z,z) \end{bmatrix}$$

Covariance Matrix Example



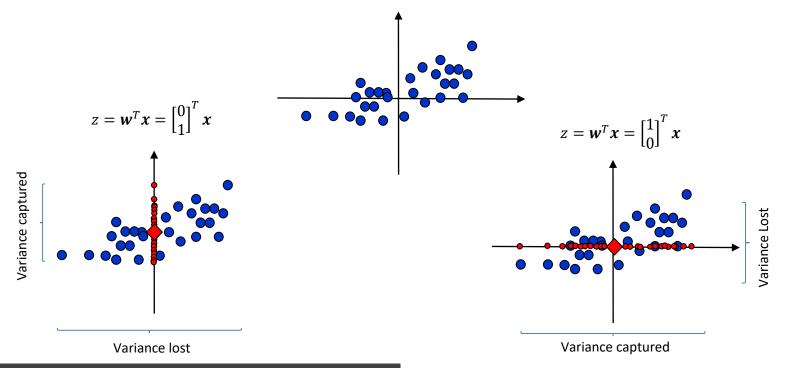


```
The mean is [67.46 \ 85.31]
The standard deviation is: [8.86 \ 10.06]
The variance is: [78.56 \ 101.14]
The co-variance matrix is: \begin{bmatrix} 78.56 \ 85.55 \\ 85.55 \ 101.14 \end{bmatrix}
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```
The mean is [0\ 0]
The standard deviation is: [1\ 1]
The variance is: [1\ 1]
Total variance: 1+1=2.0
The co-variance matrix is: \begin{bmatrix} 1 & 0.96 \\ 0.96 & 1 \end{bmatrix}
```

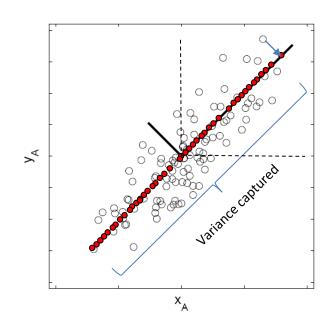
Data Dimensionality Reduction

- How can we reduce dimensions?
 - Drop features?
 - Equivalent to projecting data onto canonical axes
 - Loss in variance



Dimensionality Reduction as Projections

- Projections can be used for reducing dimensions
 - However, projecting data onto a vector loses information
 - We want to reduce the amount of information loss
 - Solution: Find and project along a direction along which information loss is minimum
 - A direction along which most of the variance is captured
 - How to do it?



How to do it: Naïve Implementation

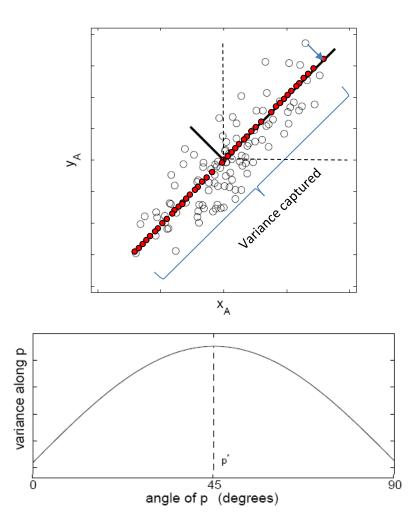
Data Mining

- Set p = 0
- For p from 0 to π in steps
 - Calculate projection vector

•
$$\mathbf{w}_p = \begin{bmatrix} \cos(p) \\ \sin(p) \end{bmatrix}$$

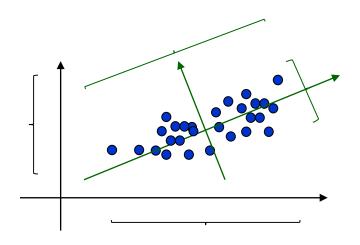
- Project your data onto $z_i = \boldsymbol{w}_p^T \boldsymbol{x}_i$
- Find the variance of the projected data
- Plot the variance across p
- Find the p that gives maximum variance





So what is PCA?

- A method for transforming the data
 - Projecting the data onto orthogonal vectors such that the variance of the projected data is maximum
 - Projection of x on the direction of w: $z = w^T x$
 - Find w such that Var(z) is maximized



Principal Component Analysis

Relation between variance of projection and covariance matrix

$$Var(z) = Var(w^{T}x) = E[(w^{T}x - w^{T}\mu)^{2}]$$

$$= E[(w^{T}x - w^{T}\mu)(w^{T}x - w^{T}\mu)]$$

$$= E[w^{T}(x - \mu)(x - \mu)^{T}w]$$

$$= w^{T} E[(x - \mu)(x - \mu)^{T}]w = w^{T} C w$$
where $Cov(x) = E[(x - \mu)(x - \mu)^{T}] = C$

Maximizing variance

Thus, we want to find w such that the variance is maximized

$$max_{\mathbf{w}} var(\mathbf{w}^T \mathbf{x}) = \mathbf{w}^T \mathbf{C} \mathbf{w}$$

Another view is that we want to project the data such that the loss in variance after projection is minimized. Let's say the total variance is V, then what we want is:

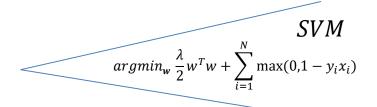
$$min_{\mathbf{w}} V - var(\mathbf{w}^T \mathbf{x}) = V - \mathbf{w}^T \mathbf{C} \mathbf{w}$$

Total Variance Variance along **w**

Using Structural Risk Minimization

- We have learned that machine learning models should reduce the structural risk
 - Regularization
 - Empirical Error Minimization

$$argmin_{w} \lambda R(w) + L(X; w)$$



 In case of dimensionality reduction, the empirical error is the loss in variance due to the projection

$$L(X; w) = V - var(\mathbf{w}^T \mathbf{x})$$

- Since V is a constant
 - $L(X; w) = -var(w^Tx) = w^TCw$

PCA with SRM

We can write the complete form as:

$$min_{\mathbf{w}} \ \alpha \mathbf{w}^T \mathbf{w} - \mathbf{w}^T \mathbf{C} \mathbf{w}$$

• Taking the derivative of $\alpha w^T w - w^T C w$ with respect to w and substituting it to zero, we get:

$$\frac{\partial}{\partial \mathbf{w}} \ \alpha \mathbf{w}^T \mathbf{w} - \mathbf{w}^T \mathbf{C} \mathbf{w} = \alpha \mathbf{w} - \mathbf{C} \mathbf{w} = \mathbf{0}$$

$$Cw = \alpha w$$

Connection to Eigen Vectors

- Note that $Cw = \alpha w$
- Thus, our solution means that ${\pmb w}$ is, in essence, an eigen vector of ${\pmb C}$ with eigen value ${\pmb \alpha}$

- The eigen vectors of the covariance matrix (Called Principal Components) of the given dataset are along the direction of maximum variance of the data!!
- Typically, the eigen vectors are normalized as unit vectors $\frac{w}{\|w\|}$

Let's see for our data

The co-variance matrix is: $\begin{bmatrix} 1 & 0.96 \\ 0.96 & 1 \end{bmatrix}$ Eigen vector 1:

$$w_1 = \begin{bmatrix} 0.7071 \\ 0.7071 \end{bmatrix}, \quad \alpha_1 = 1.96$$

Variance of data after projecting along W_1 : 1.96

Eigen vector 2:

$$w_2 = \begin{bmatrix} -0.7071 \\ 0.7071 \end{bmatrix}, \quad \alpha_2 = 0.04$$

Variance of data after projecting along w_1 : 0.04

Fraction of variance captured along each PC:

Using PC-1:
$$1.96/2 = 0.98$$

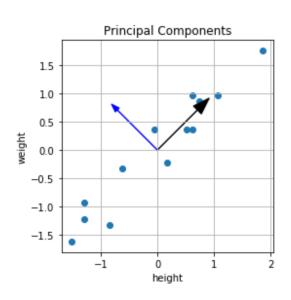
Using PC-1 and PC-2: $(1.96+0.04)/2 = 1.0$

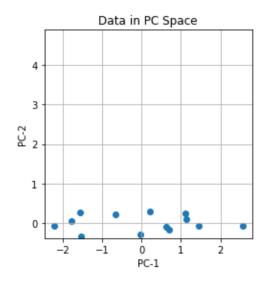
The two PC vectors are orthogonal to each other $w_1^T w_2 = 0$

The PC Matrix is
$$W = \begin{bmatrix} 0.7071 & -0.7071 \\ 0.7071 & 0.7071 \end{bmatrix}$$

The inverse of W is: $W^{-1} = \begin{bmatrix} 0.7071 & 0.7071 \\ -0.7071 & 0.7071 \end{bmatrix} = W^T$

Thus, $W^TW = I$

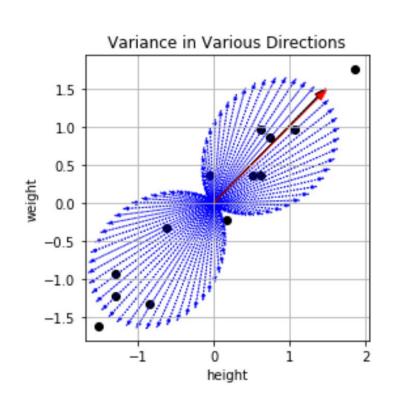


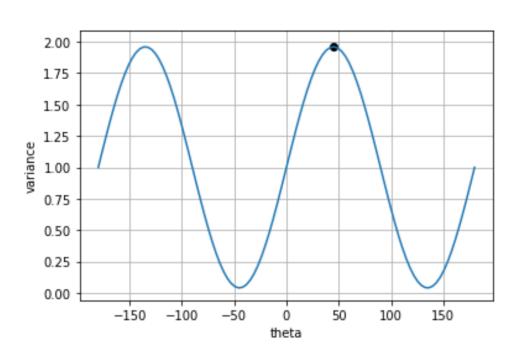


Things to note

- There are two principal components: The one with the largest variance (eigen value)
 is called the first principal component whereas the other one is called the second
 principal component.
- The variance along the first principal component is higher in comparison to the second.
- The variance along the first projected direction is higher than the variance along original features which is 1.0 after normalization. Thus, the principal component is a direction that captures more information than any of the original features alone.
- The norm of each of the principal components is 1.0.
- The two principal components are orthogonal to each other.
- The principle component matrix and its transpose are inverses of each other, i.e., $\mathbf{W}^T\mathbf{W} = \mathbf{I}$
- The eigen values correspond to the amount of captured variance: The fraction of variance captured along a direction is exactly equal to the fraction of eigen values. Thus, the first principal component corresponds to the largest eigen value and so on.
- The plot of the fraction of captured variance up to k principal components (called the scree plot) can be used to select how many principal components to retain when reducing dimensionality. For the original data used in this example, upto 98% variance is along the first principal component. Therefore, if the second principal component is dropped, the loss of information will be only ~2%.

Using the naïve implementation





Direction of Maximum Variance: [0.70, 0.71]

PCA for dimensionality reduction

- An eigen value of the covariance matrix is equal to the variance captured by projecting data along the direction of the corresponding principal component
- Thus, principal components with small eigen values have small contribution to the total variance of the data and these can be discarded without major loss of information
- We can retain 90% variance of the data by storing the largest eigen values and eigen vectors which contribute 90% of the variance and projecting our data on these bases
- Proportion of Variance (PoV) explained

$$PoV(k) = \frac{\lambda_1 + \lambda_2 + \dots + \lambda_k}{\lambda_1 + \lambda_2 + \dots + \lambda_k + \dots + \lambda_d}$$

when λ_i are sorted in descending order

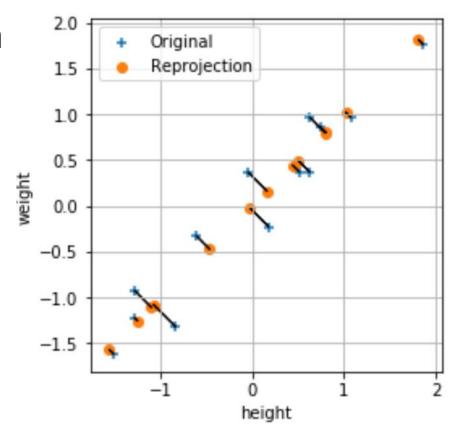
- Typically, stop at PoV > 0.9
- Scree graph plots of PoV vs k, stop at "elbow"

PCA for dimensionality reduction

- Once we find k, we drop smaller eigen values
- Projections along a vector w is $z = w^Tx$
- In matrix form, the projections along k Principal Components can be written as $Z_{N\times\,k}=X_{N\times d}W_{d\times k}$

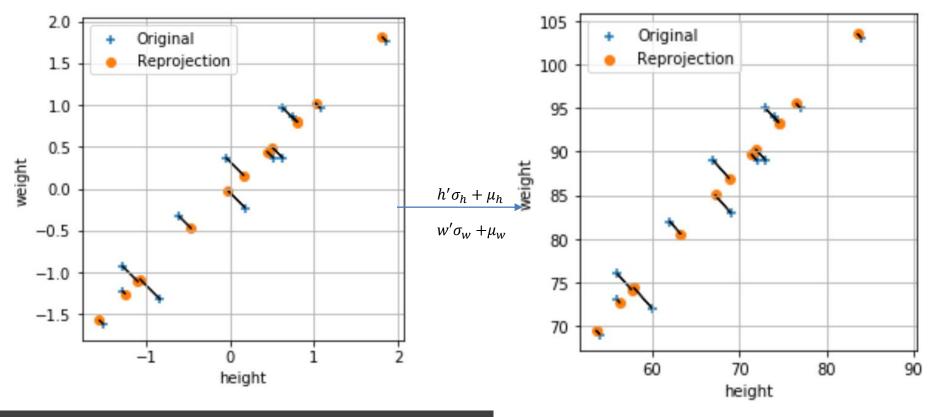
Reconstruction

- It is possible to reconstruct the data from lower dimensional representation
- Since, Z = XW
- Thus
- $X^r = ZW^{-1} = ZW^T$



Unnormalization

- We will still need to unnormalize the data
 - Multiply the re-projected data by standard deviation and add the mean



Reconstruction Error

The reconstruction error can be written as:

•
$$E(X; W) = \frac{1}{N} \sum_{i=1}^{N} ||x_i - x_i^r||^2 = \frac{1}{N} ||X - X^r||_F^2 = \frac{1}{N} ||X - ZW^T||_F^2 = \frac{1}{N} ||X - XWW^T||_F^2$$

- For our case:
- The average reconstruction error is: 0.402
- Which is exactly equal to the Eigen value of the dimension which was dropped

PCA Interpretation

PCA

- Finds directions of maximum variance and projects the data along those direction
- Finds the directions that minimize reconstruction error

$$\min_{\mathbf{W}} \frac{1}{N} ||\mathbf{X} - \mathbf{X} \mathbf{W} \mathbf{W}^{\mathsf{T}}||_{F}^{2}$$
Such that
$$\mathbf{W}^{\mathsf{T}} \mathbf{W} = \mathbf{I}$$

An algorithmic view of how PCA Works

- Input: $X_{N \times d}$
- Output: A transformation matrix W which can be used for dimensionality reduction
- **Parameters**: Selection of principal components
 - Proportion of variance
 - Number of principal components (k)
 - Which principal components to retain

Internal Working

- Normalize data
 - Calculate feature wise mean and standard deviation and normalize data to zero mean and unit standard deviation
- Find Covariance Matrix
- Find Principal Components (Eigen Value Problem)
- Select Principal Components
 - Using Scree Graph
 - Intuition
- Reduce dimensionality by Projection along selected components

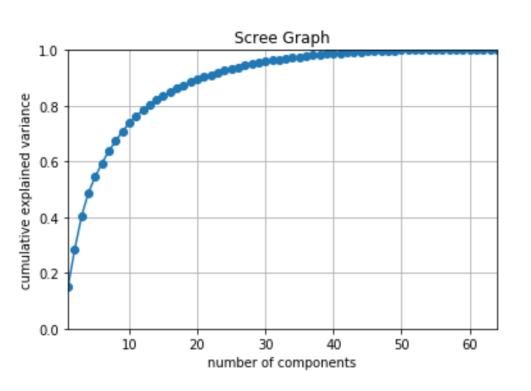
How to code?

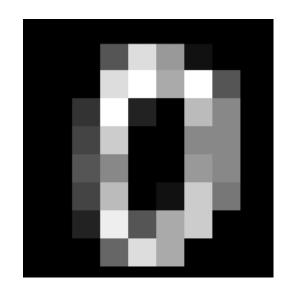
- Fitting PCA to training data
- from sklearn.decomposition import PCA
- pca = PCA(n_components=4)
- pca.fit(X)
- Projection
- Z = pca.transform(X)
- Visualization
- Screen Graph
- plt.plot(np.cumsum(pca.explained_variance_ratio_),'o-')
- Reconstruction
- Xr = pca.inverse_transform(Z)

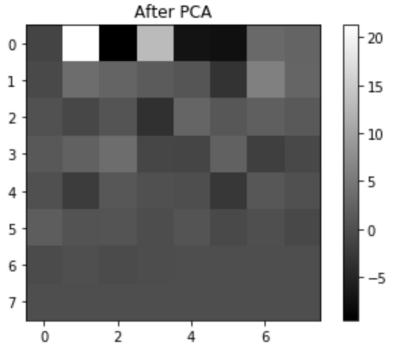
Example

MNIST visualization

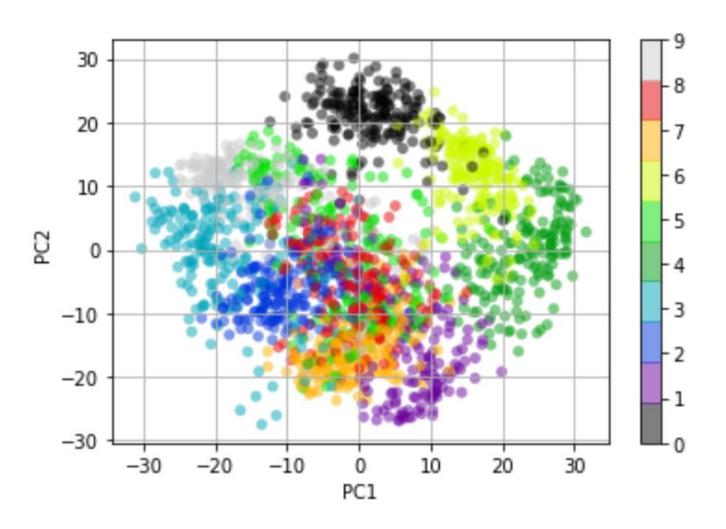
• X: 1797x64







Visualization



Algorithm for PCA: Classical Method

• Each of the N samples is stored as a d-dimensional vector

$$x^i = \begin{bmatrix} x_1^i & \cdots & x_d^i \end{bmatrix}^T$$

• The data matrix is formed as

$$X = \begin{bmatrix} x^1 & \cdots & x^N \end{bmatrix}$$

• Compute the mean $m=[m_1 ... m_d]^T$ from X using

$$m_i = \frac{1}{N} \sum_{j=1}^P x_i^j$$

Centralize each sample in the data as

$$\overline{x}^i = x^i - m \quad \overline{X} = \begin{bmatrix} \overline{x}^1 & \cdots & \overline{x}^N \end{bmatrix}$$

• Compute Covariance Matrix

$$S = \frac{\overline{X}\overline{X}^T}{N-1}$$

- Find the Eigen Values λ_1 , λ_2 ... λ_d & d-dimensional Eigen Vectors w_1 , w_2 ... w_{d_1} of S using $S\lambda = w\lambda$ and sort the eigen values in decreasing magnitudes. Normalize the eigen vectors.
- Calculate the required dimension k based on proportion of variance based approach explained earlier for a given threshold
- Form $W = [w_1 w_2 ... w_k]_{(d \times k)}$
- A vector x can be projected using $z = W^T(x-m)$

Algorithm for PCA: Snapshot Method

- If the input dimension (d) is large then the size of the covariance matrix is also large making its calculations computationally demanding
- It is known that for a d x N matrix the maximum number of non-zero eigenvectors is min(d-1,N-1)
- If N < d, then we can compute the eigen vectors
 w_i' of

 $S_{(N\times N)}' = \frac{X^T X}{N-1}$

instead of S. The eigen values for both S and S' are same and the eigen vectors of S can be obtained from those of S' using

$$w_{i_{(d\times 1)}} = \overline{X}_{(d\times N)} w_{i_{(N\times 1)}}$$

Algorithm for PCA: Snapshot Method

Each of the N samples is stored as a d-dimensional vector

$$x^i = \begin{bmatrix} x_1^i & \cdots & x_d^i \end{bmatrix}^T$$

The data matrix is formed as

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Compute the mean m=[m₁ ... m_d]^T from X using $m_i = \frac{1}{N} \sum_{i=1}^{P} x_i^j$

$$m_i = \frac{1}{N} \sum_{j=1}^{P} x_i^j$$

Centralize each sample in the data as

$$\overline{x}^i = x^i - m \quad \overline{X} = \begin{bmatrix} \overline{x}^1 & \cdots & \overline{x}^N \end{bmatrix}$$

Compute Covariance Matrix $S' = \frac{\overline{X}^T \overline{X}}{N-1}$

$$S' = \frac{\overline{X}^T \overline{X}}{N-1}$$

- Find the Eigen Values (sorted in decreasing values) λ'_1 , λ'_2 ... λ'_d & d-dimensional Eigen Vectors w'_1 , w'_2 ... w'_d , of S using $S\lambda'=w'\lambda'$.
- Calculate the required dimension k based on proportion of variance based approach explained earlier for a given threshold
- Form $W = [w_1 w_2 ... w_k]_{(d \times k)}$ $w_i^* = \overline{X} w_i^*, \qquad w_i = \frac{w_i^*}{|w_i^*|}$

$$w_i^* = \overline{X}w_i^{'},$$

$$w_i = \frac{w_i^*}{|w_i^*|}$$

A vector x can be projected using $z = W^T(x-m)$

Principal Component Analysis: Another view

• Maximize $Var(z_1)$ subject to $||\mathbf{w}_1|| = 1$

$$\max_{\mathbf{w}_1} \ \mathbf{w}_1^T \mathbf{C} \mathbf{w}_1 - \alpha_1 (\mathbf{w}_1^T \mathbf{w}_1 - 1)$$

$$Cw_1 = \alpha_1 w_1$$

Differentiating w.r.t w₁

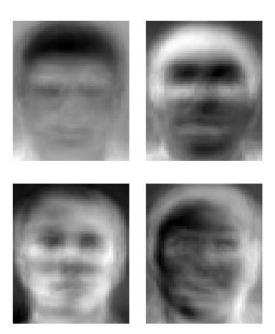
- w₁ is an eigenvector of C
- Choose the one with the largest eigenvalue for $Var(z_1)$ to be max
- Second principal component: Max $Var(z_2)$, s.t., $\|\mathbf{w}_2\| = 1$ and orthogonal to \mathbf{w}_1

$$\max_{\mathbf{w}_2} \mathbf{w}_2^T \mathbf{C} \mathbf{w}_2 - \alpha_2 (\mathbf{w}_2^T \mathbf{w}_2 - 1) - \beta (\mathbf{w}_2^T \mathbf{w}_1 - 0)$$

 And so on. The Eigen values are sorted in decreasing order and the eigen vectors with positive eigen values are kept

Practical Use

- Face Recognition
 - Eigen Faces
 - Turk and Pentland
 - https://en.wikipedia.org/wiki/Eigenface



How to use it in your work

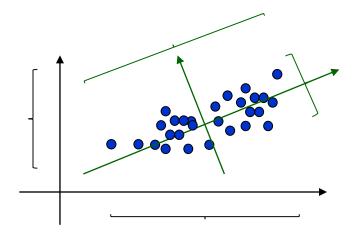
- Dimensionality reduction
- Visualization
- Selecting which dimensions are more informative for classification

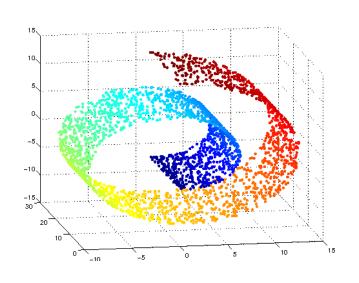
Issues

- Slow
- Iterative Implementations
- Robustness
- Does not consider label information: Unsupervised technique
- Linear Projections only
- Other techniques
 - tSNE
 - UMAP

Important Conceptual Note

- A number of variables can be correlated in real datasets
- Thus, the effective dimensionality of the dataset can be lower than what you see in terms of number of features
- Thus, data lives on a "manifold"
- That is why dimensionality reduction models help
- Sometimes these manifolds may not be linear





Quiz Time: Find Principal Components

 What are the principal components for each data set below?

