

Software Development for Data Analysis

Principal Component Analysis (PCA)

- A statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components.
- The analyzed data consist in a table of observations, having n rows and m columns.

$$X = \begin{bmatrix} x_{11} & \dots & x_{1m} \\ \dots & & \\ x_{n1} & \dots & x_{nm} \end{bmatrix}, \text{ where } x_{ij} \text{ is the value taken by variable } j \text{ for the observation } i.$$

- The variables described by table X are also known as *initial*, *causal* or *observed variables*.

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- X_j is the column vector containing the values of variable j for n observations;
- The goal of the procedure is to describe table X through a reduced number of nonrelated variables: C_1, C_2, \dots, C_s .

Phase 1

Determine a new variable C_1 , the first principal component, as linear combination of variables X_j :

$$C_1 = a_{11}X_1 + \dots + a_{j1}X_j + \dots + a_{m1}X_m$$

The value taken by C_1 for a given observation i :

$$c_{i1} = a_{11}x_{i1} + \dots + a_{j1}x_{ij} + \dots + a_{m1}x_{im}$$

where $a_{j1}, j = \overline{1, m}$

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Phase k

Determine a new variable C_k , the k principal component, as linear combination of variables X :

$$C_k = a_{1k}X_1 + \dots + a_{jk}X_j + \dots + a_{mk}X_m ,$$

where a_k is the vector containing the multipliers a_{jk} , $j = \overline{1, m}$

The link between the causal variables (X) and the principal components (C) is given by:

$C_k = X \cdot a_k$, $k=1, s$, where s is the number of principal components.

Principal Component Analysis (PCA)

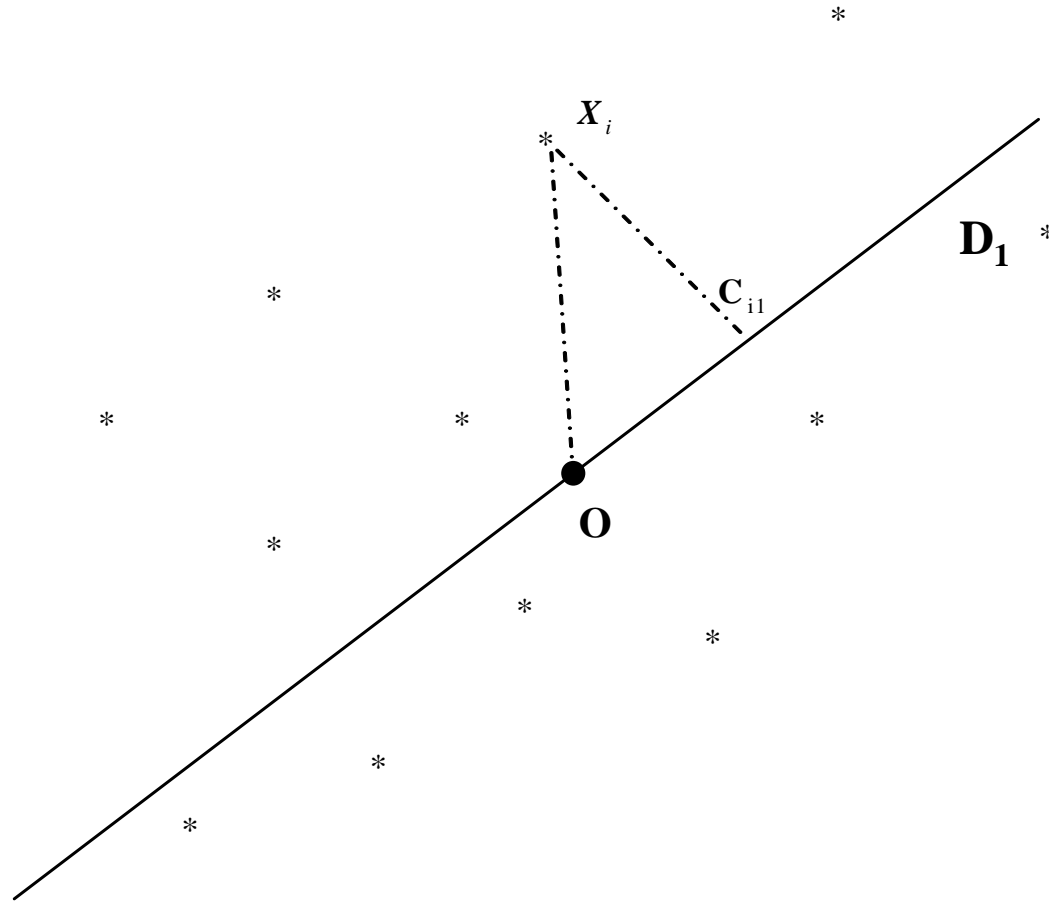
Observation driven approach

- The cloud of observations has n points within a m -dimensional space;
- Those m variables determine the m axis of coordinates;
- If the data is standardized, then the variables have the mean 0, and the standard deviation 1;
- Consider a system of orthonormal axes (it is orthogonal and having the norm 1) for those n points;
- Each axis corresponds to one principal component, and the vectors a_k are unit vectors (in a normed vector space, it is a vector, often a spatial vector, of length 1):

$$\sum_{j=1}^m a_{kj}^2 = 1, k = \overline{1, s}, \text{ where } s \text{ is the maximum number of axes}$$

Principal Component Analysis (PCA)

Observation driven approach: projection on D_1 axis



Principal Component Analysis (PCA)

Observation driven approach

Step 1

- Determine first axis, corresponding to the first principal component, so the component's variance is maxim;
- **O** is the center of gravity for the cloud of points;
- The distance from point (observation) X_i to the D_1 axis, corresponding to the first principal component is $d(i, D_1)$;
- The distance from X_i to origin **O** is $d(i, \mathbf{O})$.

Then we have the following relation between distances in the corresponding right-triangle:

$$d(i, \mathbf{O})^2 = d(i, D_1)^2 + c_{i1}^2, \quad \text{where } c_{i1} \text{ is the projection of } X_i \text{ on } D_1 \text{ axis.}$$

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Observation driven approach

- Therefore, for all the points in the cloud we have the following equality of sums:

$$\frac{1}{n} \sum_{i=1}^n d(i, O)^2 = \frac{1}{n} \sum_{i=1}^n d(i, D_1)^2 + \frac{1}{n} \sum_{i=1}^n c_{i1}^2$$

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Observation driven approach

- The sum of the distances toward the center of gravity (*barycenter*) does not depend on the chosen axis;
- The *variance explained through axis 1* is $\frac{1}{n} \sum_{i=1}^n c_{i1}^2$
- Which in terms of matrixes, knowing that $(Xa)^t = a^t X^t$, we then have:

$$\frac{1}{n} (C_1)^t C_1 = \frac{1}{n} (a_1)^t X^t X a_1$$

The problem is to dually (complementary) reach the same goal:

1. Maximize the explained variance on axis 1;
2. Minimize the sum point distances to axis 1.

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Observation driven approach

$$\begin{cases} \underset{a_1}{Max} \frac{1}{n} (a_1)^t X^t X a_1 \\ \text{subject of } (a_1)^t a_1 = 1 \end{cases}$$

Lagrange function (or Lagrangean) associated to the problem is defined by:

$$L(a_1, \lambda) = \frac{1}{n} (a_1)^t X^t X a_1 - \lambda ((a_1)^t a_1 - 1)$$

where λ is a Lagrange multiplier.

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Observation driven approach

Partial derivatives:

$$\frac{\partial L}{\partial a_1} = 2 \frac{1}{n} X^t X a_1 - 2 \lambda a_1 = 0 \quad \frac{\partial L}{\partial \lambda} = (a_1)^t a_1 - 1 = 0$$

Having then $\frac{1}{n} X^t X a_1 = \lambda a_1$.

Therefore a_1 is a *eigenvector* of the matrix $\frac{1}{n} X^t X$, corresponding to the *eigenvalue* (*characteristic value*) λ .

Multiplying on the left with $(a_1)^t$ we have:

$$\frac{1}{n} (a_1)^t X^t X a_1 = \lambda$$

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Then

$\frac{1}{n} (a_1)^t X^t X a_1$ is the quantity we need to maximize.

Therefore:

- λ is the greatest characteristic value (eigenvalue), and a_1 is the corresponding characteristic vector (eigenvector);
- we shall assign λ to α_1 .

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Step 2

- Determine axis 2 described by vector a_2 so axis 2 is orthogonal with axis 1;
- Maximize the explained variance (the points are more scattered, disperse on the axis);
- The applied optimization is:

$$\begin{cases} \underset{a_2}{Max} \frac{1}{n} (a_2)^t X^t X a_2 \\ (a_2)^t a_2 = 1 \\ (a_2)^t a_1 = 0 \end{cases}$$

$$L(a_2, \lambda_1, \lambda_2) = \frac{1}{n} (a_2)^t X^t X a_2 - \lambda_1 ((a_2)^t a_2 - 1) - \lambda_2 (a_2)^t a_1$$

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Step 2

Set the partial derivative on a_2 to zero:

$$\frac{\partial L}{\partial a_2} = 2 \frac{1}{n} X^t X a_2 - 2 \lambda_1 a_2 - \lambda_2 a_1 = 0$$

Multiplying on the left with $(a_1)^t$ we obtain:

$$2 \frac{1}{n} (a_1)^t X^t X a_2 - 2 \lambda_1 (a_1)^t a_2 - \lambda_2 (a_1)^t a_1 = 0$$

Principal Component Analysis (PCA)

Step 2

Then we have: $(a_1)^t a_2 = 0$, since:

$\frac{1}{n} X^t X a_1 = \alpha_1 a_1$ through transposition, it implies that

$$(a_1)^t \frac{1}{n} X^t X = \alpha_1 (a_1)^t$$

since the matrix $X^t X$ is symmetrical. Then, multiplying with 2 and a_2 on the right hand side:

$$2 \frac{1}{n} (a_1)^t X^t X a_2 = 2 \frac{1}{n} \alpha_1 (a_1)^t a_2 = 0$$

Therefore $\lambda_2 = 0$.

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Step 2

Making the substitution in the derivative

$$\frac{1}{n} X^t X a_2 = \lambda_1 a_2$$

and therefore a_2 is eigenvector corresponding to eigenvalue λ_1 , and this eigenvalue is maximal having given the equality:

$$\frac{1}{n} (a_2)^t X^t X a_2 = \lambda_1$$

Since $\frac{1}{n} X^t X a_2 = \lambda_1 a_2$ it is maximized at this step, we shall assign λ_1 to α_2

Principal Component Analysis (PCA)

Step k

- Determine k axis of a_k vector, orthogonal on the previous axis and to maximize the explained variance;
- The optimum problem is as follows:

$$\left\{ \begin{array}{l} \underset{a^k}{Max} \frac{1}{n} (a_k)^t X^t X a_k \\ (a_k)^t a_k = 1 \\ (a_k)^t a_j = 0, j = \overline{1, k-1} \end{array} \right.$$

Principal Component Analysis (PCA)

Step k

The associated Lagrange function $L(a_k, \lambda_1, \lambda_2, \dots, \lambda_k)$ is as follows:

$$L(a_k, \lambda_1, \lambda_2, \dots, \lambda_k) = \frac{1}{n} (a_k)^t X^t X a_k - \lambda_1 ((a_k)^t a_k - 1) - \lambda_2 (a_k)^t a_1 - \dots - \lambda_k (a_k)^t a_{k-1}$$

Setting the derivative on zero:

$$\frac{\partial L}{\partial a_k} = 2 \frac{1}{n} X^t X a_k - 2 \lambda_1 a_k - \lambda_2 a_1 - \dots - \lambda_k a_{k-1} = 0$$

Then multiply the first relation successively with $(a_1)^t, (a_2)^t, \dots, (a_{k-1})^t$, and obtain $\lambda_2 = 0, \lambda_3 = 0, \dots, \lambda_k = 0$. Returning with these results to the first partial derivative we have:

$$\frac{1}{n} X^t X a_k = \lambda_1 a_k$$

Principal Component Analysis (PCA)

Step k

Therefore a_k is eigenvector of matrix $\frac{1}{n} X^t X$, corresponding to eigenvalue λ_1 , and since the quantity

$$\frac{1}{n} (a_k)^t X^t X a_k$$

it is the one maximized at this step, then λ_1 is eigenvalue of k order.

We shall assign λ_1 to α_k .

Principal Component Analysis (PCA)

PCA in variable spaces

Phase 1

Determine the first principal component C_1 so it is maximally correlated with initial, causal variables:

$$\sum_{j=1}^m R^2(C_1, X_j) \text{ to be maxim}$$

$$R^2(C_1, X_j) = \frac{\text{Cov}(C_1, X_j)^2}{\text{Var}(C_1)\text{Var}(X_j)} = \frac{1}{n} \frac{(C_1)^t X_j (X_j)^t C_1}{(C_1)^t C_1}$$

$$\sum_{j=1}^m R^2(C_1, X_j) = \frac{1}{n} \sum_{j=1}^m \frac{(C_1)^t X_j (X_j)^t C_1}{(C_1)^t C_1} = \frac{1}{n} \frac{(C_1)^t XX^t C_1}{(C_1)^t C_1}$$

Principal Component Analysis (PCA)

PCA in variable spaces

Phase 1

Solve the following problem:

$$\underset{C_1}{Maxim} \frac{1}{n} \frac{(C_1)^t X X^t C_1}{(C_1)^t C_1}$$

The solution is the eigenvector of matrix $\frac{1}{n} X X^t$, corresponding to the greatest eigenvalue β_1 :

$$\frac{1}{n} X X^t \cdot C_1 = \beta_1 \cdot C_1$$

Principal Component Analysis (PCA)

PCA in variable spaces

Phase 2

Determine the second principal component C_2 , maximally correlated with initial variables and not correlated at all with the first principal component C_1 .

$$\begin{cases} \underset{C_2}{\text{Maxim}} \frac{1}{n} \frac{(C_2)^t XX^t C_2}{(C_2)^t C_2} \\ R(C_1, C_2) = 0 \end{cases}$$

The solution is the eigenvector of the matrix $\frac{1}{n} XX^t$, corresponding to the second eigenvalue β_2 :

$$\frac{1}{n} XX^t \cdot C_2 = \beta_2 \cdot C_2$$

Principal Component Analysis (PCA)

PCA in variable spaces

Phase k

Determine the principal component C_k , maximally correlated with initial variables and not correlated at all with the components previously determined, $C_i, i=1, k-1$.

$$\left\{ \begin{array}{l} \underset{C^1}{Maxim} \frac{1}{n} \frac{(C_k)^t X X^t C_k}{(C_k)^t C_k} \\ R(C_k, C_i) = 0, i = 1, k-1 \end{array} \right.$$

The solution is the eigenvector of the matrix $\frac{1}{n} X X^t$, corresponding to the k eigenvalue β_k :

$$\frac{1}{n} X X^t \cdot C_k = \beta_k \cdot C_k$$

Principal Component Analysis (PCA)

The link between the two approaches

In the observation spaces, at step k it is determined the eigenvector a_k , which is the unit vector of k axis, corresponding to C_k component:

$$\frac{1}{n} X^t X \cdot a_k = \alpha_k a_k$$

Multiplying this equation on the left with X we obtain:

$$\frac{1}{n} XX^t X a_k = X \alpha_k a_k \Rightarrow \frac{1}{n} XX^t C_k = \alpha_k C_k$$

Principal Component Analysis (PCA)

The link between the two approaches

It is the same equality obtained in the variable spaces approach, if considered

$$\beta_k = \alpha_k$$

$$\frac{1}{n} XX^t C_k = \beta_k C_k$$

The maximum number of steps in the observation spaces may be ***m*** (the rank

of matrix $\frac{1}{n} X^t X$), while in the variable spaces, the maximum number of

steps may be ***n*** (the rank of matrix $\frac{1}{n} XX^t$).

The number of non-zero eigenvalues is ***min(m, n)***.