

Syllabus for the Datamining Class

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Chapter 1

Introduction

This course is taught in the *Maestría y Doctorado en Ciencias e Ingeniería* (MyDCI) program of Facultad de Ingeniería, Arquitectura y Diseño of Universidad Autónoma de Baja California in the Ensenada Campus.

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Chapter 2

Principal Components Analysis

2.1 What does PCA do?

This methods tries to explain the correlation structure of a set of predictor variables using a smaller set o linear combinations of these variables called **components**, note that components are not variables, rather indicators of linear combinations between variables. Given a dataset with m variables a set of k linear combinations can be used to represent it (meaning that k contains almost as much information as the m variables), also $k \ll m$.

2.2 PCA Step by Step

2.2.1 1. Getting the dataset and things ready.

Before starting the process of dimensionality reduction one should make sure the data is standardized, this is done to avoid biased in the results by values to large or to small when compared to each other.

2.2.2 2. Centering the points

- The **standardization process** is accomplished when the mean for each variable = 0 and the standard deviation = 1. The following formula can be followed to accomplish this process:

$$Z_i = \frac{(X_i - \mu_i)}{\sigma_{ii}}$$

Where: μ_i equals the mean of X_i and σ_{ii} equals the standard deviation of X_i .

- If the values are given as a set of points the process can be accomplished with the following formula:

$$x_{i,a} = x_{i,a} - \mu_a$$

This move will facilitate the calculations down the road.

2.2.3 3. Compute covariance ($\sigma_{X,Y}$) matrix

The **covariance** is a measure of the degree to which two variables vary together. Positive covariance indicates that when one variable increases, the other tends to increase. Negative covariance indicates that when one variable increases, the other tends to decrease. The covariance measure **is not scaled**.

In a 2×2 matrix:

$$\begin{vmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{vmatrix}$$

Since the mean (μ) is equal to 0 thanks to centering the values in the previous step, the formula to calculate the covariance of the values in the matrix is:

$$\text{cov}(x_1, x_2) = \frac{1}{n} \sum_{i=1}^n x_{i,1} x_{i,2}$$

The way to interpret covariance is to understand its results as information about how one attribute changes as the other one changes.

It is important to remember that, if we multiply a vector by the covariance matrix or \sum the resulting vector will turn towards the direction of the variance.

Changing the units of measure would change the results, this is an inconvenience and is addressed by calculating the **correlation coefficient** r_{ij} :

r_{ij} scales the covariance by each of the standard deviations:

$$r_{ij} = \frac{\sigma_{ij}^2}{\sigma_{ii}\sigma_{jj}}$$

The r_{ij} gives us a value with reference to know how much of a correlation exists between two variables.

2.2.4 4. Eigenvectors + Eigenvalues

Define a **new set of dimensions** by:

1. Taking the dataset and looking for the direction of the data, looking to draw a line in which, along it, there is the **greatest amount of variance** σ^2 in the data, this line will be called the **principal component 1 (PC1)**.

$$\sigma^2 = \frac{\sum (X - \mu)^2}{N} \text{ or } \sigma^2 = \frac{\sum X^2}{N} - \mu^2$$

In the previous formula σ^2 is defined as the sum of the squared distances of each term in the distribution from the mean (μ^2) divided by the number of terms in the distribution (N). In simple words: σ^2 measures **how far a set of random numbers are spread out from their mean**.

2. Once PC1 is determined, it will establish the next dimension by drawing an **orthogonal** (perpendicular) line in relation to PC1, the exact area where the line will be drawn is determined by the same process of finding the greatest σ^2 of the remaining data, once this is done PC2 is ready.
3. This will be done iteratively until all the dimensions (d) of the dataset are covered and components (m) are generated for every single d .
 - The first $m \ll d$ components become m new dimensions.
 - Coordinates from every datapoint will be changed to these “new” dimensions.
 - **Greatest variability** is pursued to maintain the smoothness assumption of dimensions.

Eigenvectors and eigenvalues are mathematically expressed as:

$$A\vec{v} = \lambda\vec{v}$$

Where A represents transformation, \vec{v} , a vector, also known as **eigenvector**, that comes out of the matrix being analysed and λ , a scalar value also known as **eigenvalue**.

Principal components = eigenvectors with largest eigenvalues.

2.2.4.1 Finding Eigenvalues and Eigenvectors

In order to exemplify the process of finding these values and vector steps are presented for a 2×2 matrix, but this can be done with any matrix of $n \times n$ dimensions following the rules of matrix algebra.

To begin with the example we will declare a matrix:

$$A = \begin{bmatrix} 7 & 3 \\ 3 & -1 \end{bmatrix}$$

Now the steps:

1. **Multiply an $n \times n$ identity matrix by the scalar λ : $I\lambda$**

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} * \lambda = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}$$

2. **Subtract the identity matrix multiple from matrix A : $A - \lambda I$**

$$\begin{bmatrix} 7 & 3 \\ 3 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 7 - \lambda & 3 \\ 3 & -1 - \lambda \end{bmatrix}$$

3. **Find the determinant of the matrix obtained in previous step: $\det(A - \lambda I)$**

$$\begin{aligned} \det \begin{bmatrix} 7 - \lambda & 3 \\ 3 & -1 - \lambda \end{bmatrix} &= (7 - \lambda)(-1 - \lambda) - (3 * 3) \\ &= -7 - 7\lambda + \lambda + \lambda^2 = -16 - 6\lambda + \lambda^2 \\ &= \lambda^2 - 6\lambda - 16 \end{aligned}$$

4. **Solve for the values of λ that satisfy the equation $\det(A - \lambda I) = 0$** Solving for $\lambda^2 - 6\lambda - 16 = 0$ will result in:

$$(\lambda - 8)(\lambda + 2) = 0$$

Therefore $\lambda_1 = 8$ and $\lambda_2 = -2$ these are the eigenvalues for matrix A .

5. **Solve for the corresponding vector to each λ**

Solving for $\lambda = 8$, in this process we will call the matrix with substituted values: B .

$$\begin{bmatrix} 7 - (8) & 3 \\ 3 & -1 - (8) \end{bmatrix} = \begin{bmatrix} -1 & 3 \\ 3 & -9 \end{bmatrix}$$

We will assume the following $B\vec{X} = 0$.

$$\begin{bmatrix} -1 & 3 \\ 3 & -9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Applying row reduction $3R_1 + R_2 = R_2$ to:

$$\left[\begin{array}{cc|c} -1 & 3 & 0 \\ 3 & -9 & 0 \end{array} \right] = \left[\begin{array}{cc|c} -1 & 3 & 0 \\ 0 & 0 & 0 \end{array} \right] \therefore -x_1 + 3x_2 = 0$$

From the previous operation we obtain $3x_2 = x_1$, at this point we can choose a value for any x , we will go for $x_2 = 1$ to keep it simple.

$$3x_2 = x_1 \therefore 3(1) = x_1 \therefore x_1 = 3$$

Now we know that the eigenvalue $\lambda = 8$ corresponds to the eigenvector $\bar{X} = (3, 1)$.

Solving for $\lambda - 2$, generating matrix C .

$$C = \left[\begin{array}{cc} 7 - (-2) & 3 \\ 3 & -1 - (-2) \end{array} \right]$$

$$C\bar{X} = 0 \therefore$$

$$\left[\begin{array}{cc} 9 & 3 \\ 3 & 1 \end{array} \right] \left[\begin{array}{c} x_1 \\ x_2 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \end{array} \right]$$

Applying row reduction $3R_2 - R_1 = R_1$:

$$\left[\begin{array}{cc|c} 0 & 0 & 0 \\ 3 & 1 & 0 \end{array} \right] \therefore 3x_1 + x_2 = 0$$

Assigning $x_1 = 1$:

$$x_2 = -3x_1 \therefore x_2 = -3(1)$$

The eigenvalue $\lambda = 8$ corresponds to the eigenvector $\bar{X} = (1, -3)$

2.2.5 5. Pick $m < d$ eigenvectors with highest eigenvalues.

In other words, usually the **2** eigenvectors with the highest scalars, or λ , will be selected to represent the whole dataset as Principal Component 1 and Principal Component 2.

2.2.6 6. Project datapoints to those eigenvectors.

One or the algorithm has to project the datapoints to these new set of dimensions so they can be analyzed.

2.2.7 7. Perform analysis as needed according to study.

2.3 Pros and Cons of PCA

This algorithm, as all, is better suited for specific circumstances and performs poorly in others. The following list tries to summarize this idea:

2.3.0.1 Pros

- Reduction in size of data.
- Allows estimation of probabilities in high-dimensional data.
- It renders a set of components that are uncorrelated.

2.3.0.2 Cons

- It has a high computational cost, therefore it cannot be applied to very large datasets.
- Not good when working with fine-grained classes.

Chapter 3

Canonical Correlation Analysis (CCA)

3.1 What is CCA?

- Seeks the weighted linear composite for each variate (sets of D.V. or I.V.) to maximize the overlap in their distributions.
- Labeling of DV and IV is arbitrary. The procedure looks for relationships and not causation.
- Goal is to **maximize the correlation** (not the variance extracted as in most other techniques).
- Lacks specificity in interpreting results, that may limit its usefulness in many situations.

CCA helps us answer the questions:

- *What is the best way to understand how the variables in two sets are related?* , mathematically speaking:
 - *what linear combinations of the set X variables (u) and the set Y variables (t) will maximize their correlation?*

3.1.1 Canonical R (R_c)

It represents the overlapping variance between two variates which are linear composites of each set of variables.

3.2 Assumptions for CCA

- Multiple continuous variables for DVs and IVs or categorical with dummy coding.
- Assumes **linear relationship** between any two variables and between variates.
- Multivariate normality is necessary to perform CCA.
- Multicollinearity in either variate **confounds** interpretation of canonical results.

3.3 Objectives of CCA

- Determine the magnitude of the relationships that may exist between two sets of variables.

- Derive a variate(s) for each set of criterion and predictor variables such that the variate(s) of each set is maximally correlated.
- Explain the nature of whatever relationships exist between the sets of criterion and predictor variables.
- Seek the max correlation of shared variance between the two sides of the equation.

3.4 Terms used in the context of a CCA analysis

- **Canonical correlation:** Correlation between two sets; the largest possible correlation that can be found between linear combinations.
- **Canonical variate:** The linear combinations created from the IV set and DV set.
- **Canonical weights:** weights used to create the linear combinations; interpreted like regression coefficients.
- **Canonical loadings:** correlations between each variable and its variate; interpreted like loadings in PCA.
- **Canonical cross-loadings:** Correlation of each observed independent or dependent variable with opposite canonical variate.

3.5 Interpreting canonical variates

- Canonical weights
 - larger weight contributes more to the function.
 - negative weight indicates an inverse relationship with other variables.
 - always look out for multicollinearity, it can skew the whole analysis.
- Canonical Loadings.
 - A direct assessment of each variable's contribution to its respective canonical variate.
 - Larger loadings are interpreted as more important to deriving the canonical variate.
 - Correlation between the original variable and its canonical variate.
- Canonical Cross-Loadings
 - Measure of correlation of each original D.V. with the independent canonical variate.
 - Direct assessment of the relationship between each D.V. and the independent variate.
 - Provides a more pure measure of the dependent and independent variable relationship.
 - Preferred approach to interpretation.

3.6 Considerations when working with CCA

- Small samples sizes may have an adverse effect.
- Suggested minimum sample size = $10 * \#$ of values.
- Selection of variables to be included:
- Select them with domain knowledge or theoretical basis.
- Inclusion of irrelevant or deletion of relevant variables may adversely affect the entire canonical solution.
- All I.V.s must be interrelated and all D.V.s must be interrelated.
- Composition of D.V. and I.V. variates is critical to producing practical results.

3.7 Limitations of CCA

- R_c (canonical R) reflects only the variance shared by the linear composites, not the variances extracted from the variables.
- Canonical weights are subject to a great deal of instability, particularly when there is multicollinearity.

- Interpretation difficult because rotation is not possible.
- Precise statistics have not been developed to interpret canonical analysis.

This chapter is under construction.



Figure 3.1:

Bibliography