Data Analysis and Model Classification Guidesheet VII: PCA and regression

Fumiaki Iwane Ping-Keng Jao Ricardo Chavarriaga Bastien Orset — Julien Rechenmann José del R. Millán

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Introduction

The purpose of this exercise is to get familiar with regression techniques.

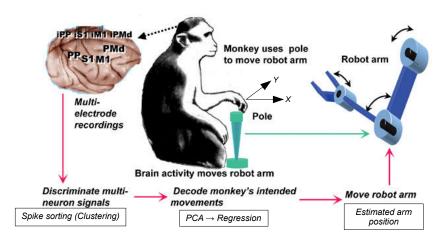


Figure 1: Objective of this guidesheet.

With regards to the Fig. 1, we will work on decoding monkey's intended movements.

Dataset partitioning and PCA

Partition your dataset (Data) into two different sets that will be used respectively for training and testing. The recorded signal is said to be non-stationary (changing over time), which means that the samples are correlated in time. Therefore, it is crucial to keep chronological order of the data when partitioning. Take the first k% of the data for training and (100-k)% for testing (with k belonging to the interval [0,100]). Try, for example, with a 70% - 30% data partitioning. Then, apply PCA properly.

General questions

- On which data partition will you apply PCA for finding the coefficients of the PCs?
- Do you need to perform any transformation of your data before applying the PCA?
- Will you reuse the coefficient of the PCs or estimate a new one on the other partition?

In order to find the coefficients of the PCs, we apply the PCA on the train set. Before applying PCA, we need to standardize our data. This is done because we don't know of how many neurons our neuronal groups are composed. Some may represent 1 neuron, other 100; thus, the dimensions will be extremely different. Once we get the PCs coefficients, we use them in order to rotate the test set (after having standardized it using the mean and the SD of the train set).

Regression

The purpose of this task is to provide an introduction to Linear Regression. This method attempts to predict the value of an output variable y (dependent variable), given the values of one or more input (independent) variables $\mathbf{x} = \{x_1, x_2, ..., x_N\}$. Therefore, it attempts to define a mapping $f: y \leftarrow f(\mathbf{x})$ such that the error between \mathbf{Y} and $f(\mathbf{X})$ is minimized, where \mathbf{X} is a set of given samples and \mathbf{Y} is their known respective output values.

Regression is a supervised learning methodology, since the known values \mathbf{Y} act as the "Labels" that will help define the mapping f. The difference with respect to classification methods is that y in this case is a continuous variable whose value we wish to predict given input sample x we measured, while in a classification problem, y is a discrete variable denoting the type of class we want to assign to a sample x. For additional information on the concepts and equations used in regression, take a look at the supplementary material.

In this task, we will assess the performance of univariate and polynomial regression models for predicting two different variables **PosX** and **PosY** from **Data**. In particular, we will evaluate the results of the regression as a function of the number of features used for training the regressor and with respect to the polynomial order of the regressor.

General questions

• On which data partition will you train the regressor on?

The regressor will be trained on the train set. The regressor will be trained on the feature matrix projected on the PCs, because otherwise

• On which feature matrix will you train the regressor on? On the original feature matrix (**Data**) or on the one projected on the PCs (**DataPCA**)? Why?

Hands on Use the MATLAB function b = regress(y(dataPartition), X(dataPartition, chosenFeatures)) to learn a regressor. b are the coefficients of the learned regressor, y is the target to be regressed and X is the data used for the regression.

Let's define I = ones(size(y(dataPartition),1),1) and FM = FeatureMatrix(dataPartition,chosenFeatures). For training a linear model we have to define X as:

X = [IFM].

For learning a 2nd-order regressor, X has to be defined as follows:

 $X = [IFMFM.^2]$

Similarly, for n-th order polynomials, the corresponding columns FM. n have to be added to X.

- Use all of your chosen feature matrix to train a linear regressor for the data vector y (PosX) by y = PosX(dataPartition). Then, use the MATLAB function immse(y,X*b) to evaluate the performance of the regression (the function calculates the mean-squared error between the y vector and the regressed one X*b), both on the train and test partitions. Is there any difference between the errors on the train sets and those on the test sets? Why?
- Repeat the previous step for the **PosY** data vector.
- For both **PosX** and **PosY**, plot the real vectors and the regressed ones, both for the train and test partitions. You can compare the vectors using the MATLAB "Zoom in" plot tool and interpret the goodness of the fit.
- Using all the features of your chosen feature matrix, train now a 2nd order polynomial regressor on your data and compare the results on the train and test sets to those obtained with the linear regression. Are there any differences? If yes, how do you interpret them? How do you think the regression will perform by increasing the order of the polynomial?
- Implement now a loop to gradually include features when training your regressors. Inside the loop, train a linear regressor and a 2nd order regressor for both PosX and PosY, and evaluate their performances on the train and test partitions. At the end of the training, plot the results of your regressors (differentiating between train/test errors and polynomial order of the regressor) w.r.t.

The train error with 2nd order decreases but the test error increases: overfitting!! We should stop at 1st order.

 $^{^1}$ Instead of including the features one by one, you can include features by steps of $50 \sim 100$ for accelerating the computation.

the number of features used. Which trend do you see when increasing the number of features used? How do you explain it?

• By looking at these plots, which number of features would you eventually use for regressing the provided data? Is this number comparable with the one found when looking at the variance explained by each feature in the PCA section of the exercise? What are the cons of choosing this number based on these results? Which technique learned during the course could be used to properly tune this hyperparameter?

Usefull features: 100 max, compared to 741 with 90% variance. And with 741 features there is overfitting.