S21CSE471: Statistical Methods in AI **Spring 2021**

Principle Component Analysis

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In this note, we start with introduction to Principle Component Analysis(PCA) and then formulate the problem mathematically. we also will see how PCA works, when should we use it and its use cases and extensions.

1 Introduction

Definition 1.1. *Principal component analysis (PCA) is a technique used for identification of a smaller number of uncorrelated variables known as principal components from a larger set of data. The technique is widely used to emphasize variation and capture strong patterns in a data set.*

2 What is PCA?

Let's say that you want to predict what the gross domestic product (GDP) of the United States will be for 2017. You have lots of information available: the U.S. GDP for the first quarter of 2017, the U.S. GDP for the entirety of 2016, 2015, and so on. You have any publicly-available economic indicator, like the unemployment rate, inflation rate, and so on. You have U.S. Census data from 2010 estimating how many Americans work in each industry and American Community Survey data updating those estimates in between each census. You know how many members of the House and Senate belong to each political party. You could gather stock price data, the number of IPOs occurring in a year, and how many CEOs seem to be mounting a bid for public office. Despite being an overwhelming number of variables to consider, this just scratches the surface.

If you've worked with a lot of variables before, you know this can present problems. Do you understand the relationships between each variable? Do you have so many variables that you are in danger of overfitting your model to your data or that you might be violating assumptions of whichever modeling tactic you're using?

You might ask the question, "How do I take all of the variables I've collected and focus on only a few of them?" In technical terms, you want to "reduce the dimension of your feature space." By reducing the dimension of your feature space, you have fewer relationships between variables to consider and you are less likely to overfit your model. (Note: This doesn't immediately mean that overfitting, etc. are no longer concerns — but we're moving in the right direction!)

Somewhat unsurprisingly, reducing the dimension of the feature space is called "dimensionality reduction." There are many ways to achieve dimensionality reduction, but most of these techniques fall into one of two classes:

- Feature Elimination
- Feature Extraction

Feature elimination is what it sounds like: we reduce the feature space by eliminating features. In the GDP example above, instead of considering every single variable, we might drop all variables except the three we think will best predict what the U.S.'s gross domestic product will look like. Advantages of feature elimination methods include simplicity and maintaining interpretability of your variables.

As a disadvantage, though, you gain no information from those variables you've dropped. If we only use last year's GDP, the proportion of the population in manufacturing jobs per the most recent American Community Survey numbers, and unemployment rate to predict this year's GDP, we're missing out on whatever the dropped variables could contribute to our model. By eliminating features, we've also entirely eliminated any benefits those dropped variables would bring.

Feature extraction, however, doesn't run into this problem. Say we have ten independent variables. In feature extraction, we create ten "new" independent variables, where each "new" independent variable is a combination of each of the ten "old" independent variables. However, we create these new independent variables in a specific way and order these new variables by how well they predict our dependent variable.

You might say, "Where does the dimensionality reduction come into play?" Well, we keep as many of the new independent variables as we want, but we drop the "least important ones." Because we ordered the new variables by how well they predict our dependent variable, we know which variable is the most important and least important. But — and here's the kicker — because these new independent variables are combinations of our old ones, we're still keeping the most valuable parts of our old variables, even when we drop one or more of these "new" variables!

Principal component analysis is a technique for feature extraction — so it combines our input variables in a specific way, then we can drop the "least important" variables while still retaining the most valuable parts of all of the variables! As an added benefit, each of the "new" variables after PCA are all independent of one another. This is a benefit because the assumptions of a linear model require our independent variables to be independent of one another. If we decide to fit a linear regression model with these "new" variables (see "principal component regression" below), this assumption will necessarily be satisfied.

3 When to use PCA?

- When we want to reduce the number of variables, but aren't able to identify variables to completely remove from consideration.
- When we want to ensure your variables are independent of one another.
- Are you comfortable making your independent variables less interpretable?

If the answer is "yes" to all three points, then PCA is a good method to use. If the answer to the third point is "no", then we should not use PCA.

4 How Does PCA works?

- We are going to calculate a matrix that summarizes how our variables all relate to one another.

- We'll then break this matrix down into two separate components: direction and magnitude. We can then understand the "directions" of our data and its "magnitude" (or how "important" each direction is).
- The screenshot below, from the setosa.io applet, displays the two main directions in this data: the "red direction" and the "green direction." In this case, the "red direction" is the more important one. We'll get into why this is the case later, but given how the dots are arranged, can you see why the "red direction" looks more important than the "green direction?" (Hint: What would fitting a line of best fit to this data look like?)
- We will transform our original data to align with these important directions (which are combinations of our original variables). The screenshot below (again from setosa.io) is the same exact data as above, but transformed so that the x- and y-axes are now the "red direction" and "green direction." What would the line of best fit look like here?
- While the visual example here is two-dimensional (and thus we have two "directions"), think about a case where our data has more dimensions. By identifying which "directions" are most "important," we can compress or project our data into a smaller space by dropping the "directions" that are the "least important." By projecting our data into a smaller space, we're reducing the dimensionality of our feature space... but because we've transformed our data in these different "directions," we've made sure to keep all original variables in our model!

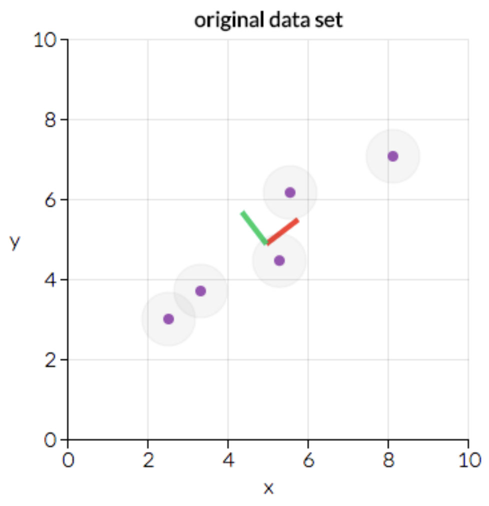


Figure 1: Original Data in xy plane

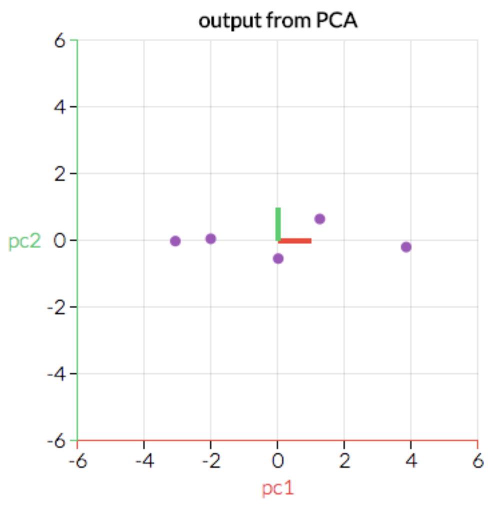


Figure 2: Output From PCA

5 Algorithm For PCA

Before starting, you should have tabular data organized with n rows and likely p+1 columns, where one column corresponds to your dependent variable (usually denoted Y) and p columns where each corresponds to an independent variable (the matrix of which is usually denoted X).

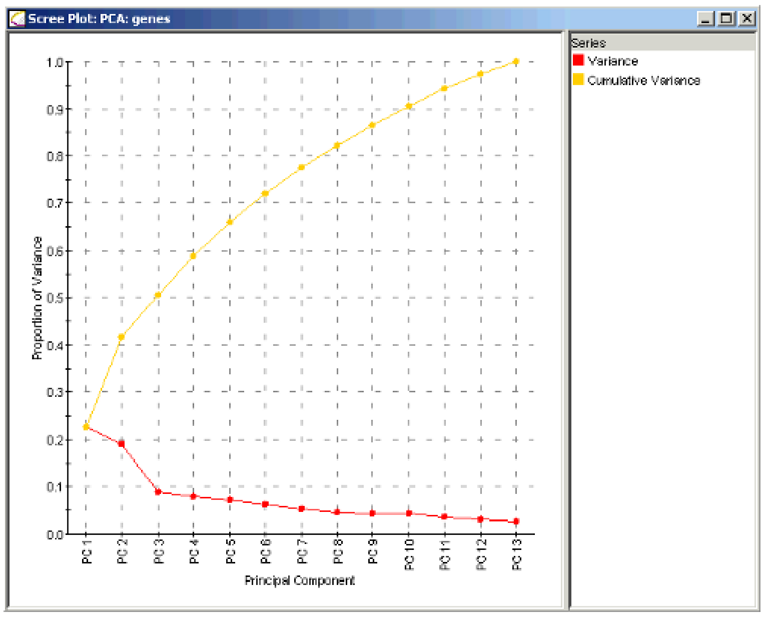
- If a Y variable exists and is part of your data, then separate your data into Y and X, as defined above — we'll mostly be working with X. (Note: if there exists no column for Y, that's okay — skip to the next point!)
- Take the matrix of independent variables X and, for each column, subtract the mean of that column from each entry. (This ensures that each column has a mean of zero.)
- Decide whether or not to standardize. Given the columns of X, are features with higher variance more important than features with lower variance, or is the importance of features independent of the variance? (In this case, importance means how well that feature predicts Y.) If the importance of features is independent of the variance of the features, then divide each observation in a column by that column's standard deviation. (This, combined with step 2, standardizes each column of X to make sure each column has mean zero and standard deviation 1.) Call the centered (and possibly standardized) matrix Z.
- Take the matrix Z, transpose it, and multiply the transposed matrix by Z. (Writing this out mathematically, we would write this as ZZ.) The resulting matrix is the covariance matrix of Z, up to a constant.
- (The toughest step to follow is to calculate the eigenvectors and their corresponding eigenvalues of ZZ. This is quite easily done in most computing packages— in fact, the eigendecomposition of ZZ is where we decompose ZZ into PDP¹, where P is the matrix of eigenvectors and D is the diagonal matrix with eigenvalues on the diagonal and values of zero everywhere else. The eigenvalues on the diagonal of D will be associated with the corresponding column in P — that is, the first element of D is and the corresponding eigenvector is the first column of P. This holds for all elements in D and their corresponding eigenvectors in P. We will always be able to calculate PDP¹ in this fashion. (Bonus: for those interested, we can always calculate PDP¹ in this fashion because ZZ is a symmetric, positive semidefinite matrix.)
- Take the eigenvalues $\lambda 1, \lambda 2, \ldots, \lambda p$ and sort them from largest to smallest. In doing so, sort the eigenvectors in P accordingly. (For example, if is the largest eigenvalue, then take the second

column of P and place it in the first column position.) Depending on the computing package, this may be done automatically. Call this sorted matrix of eigenvectors P*. (The columns of P* should be the same as the columns of P, but perhaps in a different order.) Note that these eigenvectors are independent of one another.

- Calculate Z* = ZP*. This new matrix, Z*, is a centered/standardized version of X but now each observation is a combination of the original variables, where the weights are determined by the eigenvector. As a bonus, because our eigenvectors in P* are independent of one another, each column of Z* is also independent of one another!
- If we plot a given dataset along PC axes, wer observe that the principal components are perpendicular to one another. In fact, every principal component will ALWAYS be orthogonal to every other principal. Because our principal components are orthogonal to one another, they are statistically linearly independent of one another, which is why our columns of Z* are linearly independent of one another component.
- Finally, we need to determine how many features to keep versus how many to drop. There are three common methods to determine this:

- **Method 1**: We arbitrarily select how many dimensions we want to keep. Perhaps I want to visually represent things in two dimensions, so I may only keep two features. This is use-case dependent and there isn't a hard-and-fast rule for how many features I should pick.
- **Method 2**: Calculate the proportion of variance explained (briefly explained below) for each feature, pick a threshold, and add features until you hit that threshold. (For example, if you want to explain 80
- **Method 3**: This is closely related to Method 2. Calculate the proportion of variance explained for each feature, sort features by proportion of variance explained and plot the cumulative proportion of variance explained as you keep more features. (This plot is called a scree plot, shown below.) One can pick how many features to include by identifying the point where adding a new feature has a significant drop in variance explained relative to the previous feature, and choosing features up until that point. (I call this the "find the elbow" method, as looking at the "bend" or "elbow" in the scree plot determines where the biggest drop in proportion of variance explained occurs.)

Because each eigenvalue is roughly the importance of its corresponding eigenvector, the proportion of variance explained is the sum of the eigenvalues of the features you kept divided by the sum of the eigenvalues of all features.



Consider this scree plot for genetic data. The red line indicates the proportion of variance explained by each feature, which is calculated by taking that principal component's eigenvalue divided by the sum of all eigenvalues. The proportion of variance explained by including only principal component 1 is $\lambda_1/(\lambda_1 + \lambda_2 + \ldots + \lambda_p)$, which is about 23%. The proportion of variance explained by including only principal component 2 is $\lambda_2/(\lambda_1 + \lambda_2 + \ldots + \lambda_p)$, or about 19%.

The proportion of variance explained by including both principal components 1 and 2 is $\lambda_1 + \lambda_2/(\lambda_1 + \lambda_2 + \ldots + \lambda_p)$, which is about 42%. This is where the yellow line comes in; the yellow line indicates the cumulative proportion of variance explained if you included all principal components up to that point. For example, the yellow dot above PC2 indicates that including principal components 1 and 2 will explain about 42% of the total variance in the model. Now let's go through some examples:

- **Method 1**: We arbitrarily select a number of principal components to include. Suppose I wanted to keep five principal components in my model. In the genetic data case above, these five principal components explains about 66% of the total variability that would be explained by including all 13 principal components.
- **Method 2**: Suppose I wanted to include enough principal components to explain 90% of the total variability explained by all 13 principal components. In the genetic data case above, I would include the first 10 principal components and drop the final three variables from Z*.
- **Method 3**: Here, we want to "find the elbow." In the scree plot above, we see there's a big drop in proportion of variability explained between principal component 2 and principal component 3. In this case, we'd likely include the first two features and drop the remaining features. As you can see, this method is a bit subjective as "elbow" doesn't have a mathematically precise definition and, in this case, we'd include a model that explains only about 42% of the total variability.

Note: Some scree plots will have the size of eigenvectors on the Y axis rather than the proportion of variance. This leads to equivalent results, but requires the user to manually calculate the proportion of variance. Once we've dropped the transformed variables we want to drop, we're done. That's PCA.

Why does PCA work?

- While PCA is a very technical method relying on in-depth linear algebra algorithms, it's a relatively intuitive method when you think about it. First, the covariance matrix ZZ is a matrix that contains estimates of how every variable in Z relates to every other variable in Z. Understanding how one variable is associated with another is quite powerful.
- Second, eigenvalues and eigenvectors are important. Eigenvectors represent directions. Think of plotting your data on a multidimensional scatterplot. Then one can think of an individual eigenvector as a particular "direction" in your scatterplot of data. Eigenvalues represent magnitude, or importance. Bigger eigenvalues correlate with more important directions.
- Finally, we make an assumption that more variability in a particular direction correlates with explaining the behavior of the dependent variable. Lots of variability usually indicates signal, whereas little variability usually indicates noise. Thus, the more variability there is in a particular direction is, theoretically, indicative of something important we want to detect.

Thus, PCA is a method that brings together:

- A measure of how each variable is associated with one another (Covariance matrix).
- The directions in which our data are dispersed (Eigenvectors).
- The relative importance of these different directions (Eigenvalues).

6 Extensions of PCA

6.1 Principal Components Regression

Principal Components Regression is a technique for analyzing multiple regression data that suffer from multicollinearity. When multicollinearity occurs, least squares estimates are unbiased, but their variances are large so they may be far from the true value. By adding a degree of bias to the regression estimates, principal components regression reduces the standard errors. It is hoped that the net effect will be to give more reliable estimates. Another biased regression technique, ridge regression, is also available in NCSS. Ridge regression is the more popular of the two methods.

Multicollinearity Multicollinearity is discussed both in the Multiple Regression chapter and in the Ridge Regression chapter, so we will not repeat the discussion here. However, it is important to understand the impact of multicollinearity so that you can decide if some evasive action (like pc regression) would be beneficial.

Principal Components Regression Models Following the usual notation, suppose our regression equation may be written in matrix form as $\underline{Y} = X\underline{B} + \underline{e}$ where Y is the dependent variable, X represents the independent variables, B is the regression coefficients to be estimated, and e represents the errors or residuals.

Standardization The first step is to standardize the variables (both dependent and independent) by subtracting their means and dividing by their standard deviations. This causes a challenge in notation, since we must somehow indicate whether the variables in a particular formula are standardized or not. To keep the presentation simple, we will make the following general statement and then forget about standardization and its confusing notation. As far as standardization is concerned, all calculations are based on standardized variables. When the final regression coefficients are displayed, they are adjusted back to their original scale.

PC Regression Basics In ordinary least squares, the regression coefficients are estimated using the formula

$$\underline{\hat{B}} = (X'X)^{-1}.X'\underline{Y}$$

Note that since the variables are standardized, X'X = R, where R is the correlation matrix of independent variables. To perform principal components (PC) regression, we transform the independent variables to their principal components. Mathematically, we write

$$X'X = PDP' = Z'Z$$

where D is a diagonal matrix of the eigenvalues of X'X, P is the eigenvector matrix of X'X, and Z is a data matrix (similar in structure to X) made up of the principal components. P is orthogonal so that P'P = I. We have created new variables Z as weighted averages of the original variables X. This is nothing new to us since we are used to using transformations such as the logarithm and the square root on our data values prior to performing the regression calculations. Since these new variables are principal components, their correlations with each other are all zero. If we begin with variables X1, X2, and X3, we will end up with Z1, Z2, and Z3. Severe multicollinearity will be detected as very small eigenvalues. To rid the data of the multicollinearity, we omit the components (the z's) associated with small eigenvalues. Usually, only one or two relatively small eigenvalues will be obtained. For example, if only one small eigenvalue were detected on a problem with three independent variables, we would omit Z3 (the third principal component). When we regress Y on Z1 and Z2, multicollinearity is no longer a problem. We can then transform our results back to the X scale to obtain estimates of B. These estimates will be biased, but we hope that the size of this bias is more than compensated for by the decrease in variance. That is, we hope that the mean squared error of these estimates is less than that for least squares. Mathematically, the estimation formula becomes

$\underline{\hat{A}} = (Z'Z)^{-1}Z'\underline{Y} = D^{-1}Z'\underline{Y}$

because of the special nature of principal components. Notice that this is ordinary least squares regression applied to a different set of independent variables. The two sets of regression coefficients, A and B, are related using the formulas

$\underline{A}$ = P'$\underline{B}$ and $\underline{B}$ = P$\underline{A}$

Omitting a principal component may be accomplished by setting the corresponding element of $\underline{A}$ equal to zero. Hence, the principal components regression may be outlined as follows:

1. Complete a principal components analysis of the X matrix and save the principal components in Z.

2. Fit the regression of Y on Z obtaining least squares estimates of A.

3. Set the last element of A equal to zero.

4. Transform back to the original coefficients using $\underline{B}$ = P$\underline{A}$.

6.2 Kernel PCA

Kernel PCA extends conventional principal component analysis (PCA) to a high dimensional feature space using the "kernel trick". It can extract up to n (number of samples) nonlinear principal components without expensive computations.

Making PCA Non-Linear Suppose that instead of using the points we would first map them to some nonlinear feature space ψx_i e.g. using polar coordinates instead of cartesian coordinates would help us deal with the circle. We then extract principal component in that space (PCA). The result will be non-linear in the original data space.

Steps: 1. Pick a kernel

2. Construct the normalized kernel matrix of the data (this will be of dimension m × m)

3. Find the eigenvalues and eigenvectors of this matrix λ_j, a_j

4. For any data point (new or old), we can represent it as the following set of features:

$y_j = \sum_{i=1}^{m} a_{ji}K(x, x_i), j = 1, ...m$

5. We can limit the number of components to k ¡ m for a more compact representation (by picking the a's corresponding to the highest eigenvalues)

Thus,

- Kernel PCA can give a good re-encoding of the data when it lies along a non-linear manifold
- The kernel matrix is m × m, so kernel PCA will have difficulties if we have lots of data points
- In this case, we may need to use dictionary methods to pick a subset of the data
- For general kernels, we may not be able to easily visualizethe image of a point in the input space, though visualization still works for simple kernels

7 Conclusion

Thus, PCA combines our predictors and allows us to drop the eigenvectors that are relatively unimportant. We can also extend it to principal component regression, where we take our untransformed Y and regress it on the subset of Z* that we didn't drop. The other commonly-seen variant is kernel PCA.

References

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