APPLIED STATISTICS

Principal Components Analysis (PCA)

Dr Tao Zou

Research School of Finance, Actuarial Studies & Statistics
The Australian National University

Last Updated: Wed Oct 25 09:24:51 2017

Overview

Motivating Example

Linear Combination and PCA

PCA Usage

• When is it appropriate to use PCA?

References

- **1. F.L. Ramsey and D.W. Schafer** (2012) Chapter 17 of *The Statistical Sleuth*
- **2. J. Zhang** (2009) Chapter 4 of *Data Mining and Its Application*
- The slides are made by R Markdown. http://rmarkdown.rstudio.com

Example: Test Score Data

To illustrate PCA we will be using a dataset "testscores.txt". This dataset contains the results of qualifying examinations for 25 graduate students in mathematics at a U.S university.

```
rm(list=ls())
setwd('~/Desktop/Research/AppliedStat2017/L15')
testscores=read.table("testscores.txt",header=T)
head(testscores)
```

	_		_		_		
##	(diffgeom	complex	algebra	reals	statistics	
##	1	36	58	43	36	37	
##	2	62	54	50	46	52	
##	3	31	42	41	40	29	
##	4	76	78	69	66	81	
##	5	46	56	52	56	40	
##	6	12	42	38	38	28	

The students sat for examinations in differential geometry, complex analysis, algebra, real analysis, and statistics.

The differential geometry and complex analysis examinations where closed book, while the remaining exams were open book.

4/38

Multivariate Data

We can call the observations of the tuple (diffgeom, complex, algebra, reals, statistics) multivariate data.)

There are a lot of statistical tools to deal with the <u>multivariate data</u>. For instance, <u>PCA</u>, factor models, and cluster analysis. This course only instroduces <u>PCA</u>.

Combine Scores

It might be possible to reduce these five original vectors of test scores into one or two vectors that account for most of the information in the original dataset. This would be even more desirable if we had data on a larger number of different examinations.

One example is to use the mean test score, which is a linear combination of the five original scores with equal weights.

Do we have other methods to combine the five scores to produce an overall score?

PCA provides an answer to seek the linear combination of the original variables which contains the maximal variance (variation).

Principal Components Analysis (PCA)

PCA is potentially a way to select several linear combinations of the multivariate data that capture most of the variation information of the data.

This is most useful if relatively few linear combinations can explain most of the variation, and if the linear combinations can lend themselves to some useful interpretation.

Linear Combinations of Variables and Principal

A linear combination Z of variables X_1, X_2, \dots, X_k is given by:

Component Variables

$$Z = C_0 + C_1 X_1 + \cdots + C_k X_k.$$

In PCA, the original set of variables X_1, \dots, X_k is re-expressed in terms of a set of an equal number of principal component variables Z_1, \dots, Z_k , where

(inew combinations) Should Satisfy
$$Z_1 = C_{10} + C_{11}X_1 + \cdots + C_{1k}X_k;$$

$$Z_2 = C_{20} + C_{21}X_1 + \cdots + C_{2k}X_k;$$

$$\cdots$$

$$Z_k = C_{k0} + C_{k1}X_1 + \cdots + C_{kk}X_k.$$

We need **Requirement 1**: the principal component variables (Z_{j_1}) and (Z_{j_2}) are not correlated for $j_1 \neq j_2$. However, X_{j_1} and X_{j_2} are correlated for $j_1 \neq j_2$.

Linear Combinations of Variables and Principal Component Variables (Con'd)

We also need **Requirement 2**: the first principal component Z_1 is the linear combination of X_1, X_2, \dots, X_k that exhibits the maximum variance by choosing $C_{10} \cdots C_{1k}$.

Select the values of the maximise $C_{10} \cdots C_{1k}$.

By doing that, we are accounting for as much of the variation information contained in X_1, X_2, \dots, X_k as possible, such that Z_1 has the most of the variation information.

Select the values of Cook Cake

Requirement 3: the second principal component Z_2 is the linear combination of X_1, X_2, \dots, X_k that has the maximum variance subject to the constraint that the correlation between Z_2 and Z_1 is zero.

Requirement 4: the third principal component Z_3 is the linear combination of X_1, X_2, \dots, X_k that has the maximum variance subject to the constraint that the correlation between Z_3 and Z_1 and the correlation between Z_3 and Z_2 are both zeros.

. .

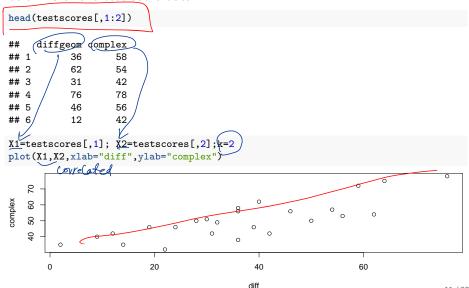
Linear Combinations of Variables and Principal Component Variables (Con'd)

We can keep working on the above procedures until we compute all the

$$\begin{pmatrix}
C_{10} & C_{11} & \cdots & C_{1k} \\
\vdots & \vdots & \vdots & \vdots \\
C_{k0} & C_{k1} & \cdots & C_{kk}
\end{pmatrix}$$

such that the above requirements are satisfied. The above figures are called loadings of principal components (PCs).

In this example we will find the principal components of the first two columns of the test score data.



11/38

To perform the PCA analysis the following R commands are used:

```
(m' 'g(m'
testscores.pca = princomp(testscores[, 1:k])
summary(testscores.pca, loadings = T)
                                                   2 Sd of 82
  Importance of components:
                                          Comp.2
##
                              Comp. 1(3)
   Standard deviation
                          20.9086650 6.12944765
                          0.9208621 0.07913793
  Proportion of Variance
## Cumulative Proportion
                           0.9208621 1.00000000
##
                                         81-92
   Loadings:
##
            Comp.1 Comp.2
## diffgeom -0.862
                    0.506
## complex -0.506 -0.862
```

This output gives us the two principal components.

Since we have two variables, we can only have two principal components.

The output also gives us the percentage of the total variation that is explained by each of the principal components.

92% of the variation in the differential geometry and complex analysis scores is accounted for by the first principal component.

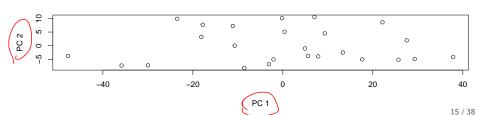
The second principal component accounts for the remaining 8% of the variation.

Suppose $X_1 = \text{diffgeom}, X_2 = \text{complex}.$

var(Z1)/(var(X1) + var(X2))

[1] 0.9208621

We can see that the two principal components are uncorrelated, while the original variables have a correlation of 0.81.



Recall that

$$\begin{cases}
Z_{1} = C_{10} + C_{11}X_{1} + C_{12}X_{2} \text{ and} \\
Z_{2} = C_{20} + C_{21}X_{1} + C_{22}X_{2}, & Page \ \ \ \ \ \end{cases}$$

by the definition of the PCs.

Based on R, we can obtain the values of $C_{i_1i_2}$, where

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} =$$

```
t(testscores.pca$loadings[,1/k])
```

We also have

$$\begin{pmatrix} \bar{X}_1 \\ \bar{X}_2 \end{pmatrix} =$$

testscores.pca\$center

```
## diffgeom complex
## 36.76 50.60
```

Hence,

$$\begin{pmatrix} C_{10} \\ C_{20} \end{pmatrix} =$$

-t(testscores.pca\$loadings[,1:k])%*%testscores.pca\$center

```
## Comp.1 57.31301
## Comp.2 25.03750
```

Hence

$$\begin{pmatrix} C_{10} & C_{11} & C_{12} \\ C_{20} & C_{21} & C_{22} \end{pmatrix} =$$

```
## Comp.1 57.31301 -0.8624793 -0.5060923 ## Comp.2 25.03750 0.5060923 -0.8624793
```

By using the above loadings, we can compute the Cs:

Use the information of Loadings

```
Z+t(cbind(-t(testscores.pca$loadings[,1:k])
%*%testscores.pca$center,
t(testscores.pca$loadings[,1:k]))%*%t(cbind(1,X1,X2)))
```

```
Compare
head(Z[,1])
## [1] -3.089599 -23.489692 9.320275 -47.710618 -10.702207 25.707382
                                                  new 8, 82
head(Z[,2])
## [1] -6.76697707 9.84134048 4.50223032 -3.77287054 0.01890475 -5.1135237
                                   new values of X, X,
head(testscores.pca$scores[,1])
   -3.089599 -23.489692 9.320275 -47.710618 -10.702207
                                   L 2,
head(testscores.pca$scores[,2])
##
## -6.76697707 9.84134048 4.50223032 -3.77287054
                                                0.01890475 -5.11352375
```

We will now use PCA on the full test score data.

statistics -0.519 -0.570 0.607

```
testscores.pca=princomp(testscores)
summary(testscores.pca,loadings=T)
## Importance of components:
                                        Comp. 2
##
                             Comp.1
                                                   Comp.3
                                                              Comp.4
  Standard deviation
                         28.4896795 9.03547104 6.60095491 6.13358179
                         0.8212222 0.08260135 0.04408584 0.03806395
## Proportion of Variance
                          0.8212222 (0.90382353 0.94790936 0.98597332
## Cumulative Proportion
##
                             Comp.5
  Standard deviation
                         3.72335754
## Proportion of Variance 0.01402668
                         1.00000000
## Cumulative Proportion
##
## Loadings:
##
             Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## diffgeom
             -0.598 0.675 0.185 0.386
## complex
             -0.361
                     0.245 -0.249 -0.829 -0.247
## algebra -0.302 -0.214 -0.211 -0.135
                                          0.894
## reals
             -0.389 -0.338 -0.700 0.375 -0.321
```

-0.179

The first principal component explains 82% of the variance, and the first two principal components contain 90% of the variance.

In this example we might consider retaining only the first two principal components. This would mean we have only two variables instead of the original five.

These first two principal components give the "best" two dimensional view of the data.

Looking at the loadings (k = 5 in this case)

$$\begin{pmatrix} C_{10} & C_{11} & \cdots & C_{1k} \\ \vdots & \vdots & \vdots & \vdots \\ C_{k0} & C_{k1} & \cdots & C_{kk} \end{pmatrix} =$$

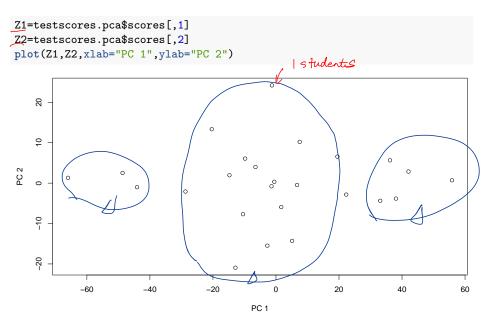
```
k=5
cbind(-t(testscores.pca$loadings[,1:k])
     %*%testscores.pca$center,
     t(testscores.pca$loadings[,1:k]))
                    diffgeom
                                         algebra
                               complex
##
  Comp.1 96 20039 -0 59827824 0 3607532 -0 3021774 -0 3890403 -0 51889947
                  Comp.2
         14.18709
         22.12546
                  0.18525556 - 0.2490064 - 0.2114109 - 0.6999921
  Comp.3
## Comp.4
         20.44037
                  0.38597894 -0.8287185 -0.1348456
                                                 0.3753787 - 0.07178665
## Comp.5 -12.45426
                  0.06131111 - 0.2470174 \ 0.8944144 - 0.3212995 - 0.17892129
```

A reasonable interpretation for the first principal component is the average score of the five examinations. The second principal component contrasts the two closed book exams with the three open book exams.

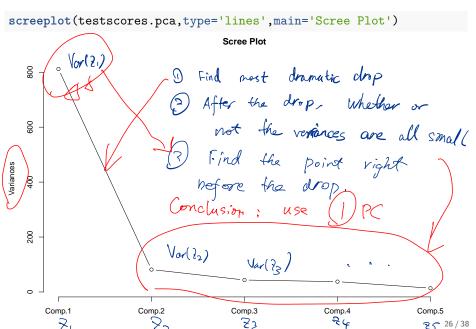
Similarly by using the above loadings, we can compute the PCs

Compare

```
head(Z[,1])
##
##
     7.540322 -20.361037 19.503154 -65.965273 -9.778056
head(Z[,2])
## 10.216765 13.346034 6.555244 1.313665 6.068014 -4.372231
head(testscores.pca$scores[,1])
##
##
     7.540322 -20.361037 19.503154 -65.965273 -9.778056
head(testscores.pca$scores[,2])
  10.216765 13.346034 6.555244 1.313665 6.068014 -4.372231
```



Determining the Number of Principal Components



PCA on explanatory variables prior to Regression

In multiple linear regression, PCA can be used to select a small number of uncorrelated variables for use in the regression model.

```
library(Sleuth3)
SATdata=case1201
head(SATdata)
                                                             / X1 1 1 X4
         State (SAT Takers Income Years Public Expend Rank
          Towa 1088
                            326 16.79
                                        87.8
                                             25.60 89.7
## 2 SouthDakota 1075
                            264 16.07
                                       86.2 19.95 90.6
    NorthDakota 1068
                            317 16.57
                                       88.3 20.62 89.8
## 4
         Kansas 1045
                            338 16 30
                                       83 9 27 14 86 3
## 5
       Nebraska 1045
                            293 17.25
                                       83.6 21.05.88.5
      Montana 1033
                            263 15.91
                                       93.7 29.48 86.4
## 6
SATdata=SATdata[-29.]
                   /#removing Alaska
n=length(SATdata[.1])
n
## [1] 49
#Randomly choose the training data and test data
set.seed(1)
                                                  draw 4 balls from
TestIndex=sample(1:n.floor(n*0.1),replace=F)
TestIndex -
                                                   holls labeled by
                   49×0-1=4.4
## [1] 14 18 27 42
                                                         1,2,3, ~~ 4)
SATdataTest=SATdata[TestIndex.]
SATdataTraining=SATdata[-TestIndex,]
YTraining <- SATdataTraining[,2]
XTraining<-SATdataTraining[,-c(1,2)]
```

```
fit=lm(YTraining~..data=XTraining)
summary(fit)
 ##
## Call:
## lm(formula = YTraining ~ ., data = XTraining)
 ## Residuals:
               10 Median
       Min
                          30
                                     Max
 ## -50.553 -13.803 0.426 14.014 51.252
 ##
## Coefficients:
 ##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept) -241.08294 208.14437 -1.158 0.253990
## Takers
                 0.08336 0.69408 0.120 0.905040
 ## Income
                0.20985 0.15995 1.312 0.197390
 ## Years
               17.31698 6.36423 2.721 0.009765 **
## Public
              -0.33927 0.56556 -0.600 0.552148
## Expend
              3.68170 0.92470 3.981 0.000298 ***
 ## Rank
                            2 08782 4 729 3 09e-05 ***
                 9 87277
 ## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
 ##
## Residual standard error: 24.66 on 38 degrees of freedom
## Multiple R-squared: 0.9023, Adjusted R-squared: 0.8869
## F-statistic: 58.52 on 6 and 38 DF, p-value: < 2.2e-16
library(car)
vif(fit)
      Takers
                Income
                          Years
                                   Public
                                            Expend
                                                        Rank
## 17.530307
             3.168006 1.494717 2.288297 1.504407 14.290468
```

One way to solve the multicollinearity problem is to use PCA.

```
pca = princomp(XTraining)
summary(pca,loadings=T)
```

```
## Importance of components:
##
                                       Comp.2
                                                  Comp.3
                            Comp.1
                                                             Comp.4
## Standard deviation 44.5887106 15.9482569 8.15348132 4.232637337
## Proportion of Variance 0.8532103 0.1091523 0.02852939 0.007688266
## Cumulative Proportion 0.8532103 0.9623626 0.99089198 0.998580248
##
                             Comp.5 Comp.6
## Standard deviation 1.725883075 0.5741415323
## Proportion of Variance 0.001278289 0.0001414634
## Cumulative Proportion 0.999858537 1.0000000000
##
## Loadings:
##
         Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6
## Takers 0.397 0.828 -0.210 0.149 0.300
## Income -0.907 0.367 -0.194
## Years
                                            0.994
## Public
              -0.288 -0.926 0.207
## Expend
                       -0.247 - 0.962
## Rank
                -0.296
                                     0.946
```

Looking at the loadings (k = 6 in this case)

$$\begin{pmatrix} C_{10} & C_{11} & \cdots & C_{1k} \\ \vdots & \vdots & \vdots & \vdots \\ C_{k0} & C_{k1} & \cdots & C_{kk} \end{pmatrix} =$$

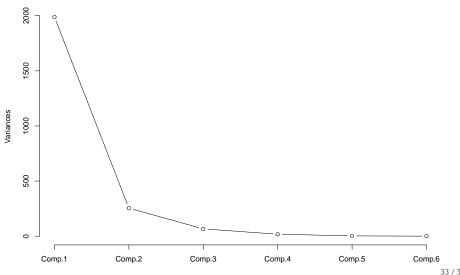
```
##
                   Takers
                           Income
                                   Years Public
                                                  Expend
                                                            Rank
  Comp.1 253.8407
                   0.3972 -0.9073 -0.0036 0.0945 0.0206 -0.0987
## Comp. 2 -83.8376 0.8281
                         0.3668 0.0068 -0.2883 0.0950 -0.2957
## Comp.3 142.4120 -0.2101 -0.1936
                                  0.0232 -0.9257 -0.2465 -0.0046
## Comp.4 -16.6089 0.1491 0.0666 -0.0651 0.2070 -0.9623 -0.0121
## Comp.5 -84.8807 0.2996 0.0200 0.0896 -0.0781 0.0130 0.9463
## Comp.6 -11.5686 -0.0166 0.0013
                                  0.9935 0.0445 -0.0591 -0.0844
```

Any reasonable interpretations for the first principal component and the second principal component?

Similarly by using the above loadings, we can compute the PCs of the training dataset.

screeplot(pca,type='lines',main='Scree Plot')

Scree Plot



We might decide to run a regression of Y on the first two principal components, which account for 96% of the total variance.

```
ZTraining.pca2=data.frame(ZTraining[.1:2])
fit.pca2=lm(YTraining~..data=ZTraining.pca2)/
summary(fit.pca2)
## Call:
## lm(formula = YTraining ~ .. data = ZTraining.pca2)
## Residuals:
              10 Median 30
      Min
                                     Max
## -90.781 -22.925 -1.853 23.448 68.606
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 947.9778
                         5.7406 165.135 < 2e-16 ***
## Comp.1 (-1.1509) 0.1287 -8.939 2.86e-11 ***
## Comp.2
             -2.2085
                          0.3600 -6.136 2.53e-07 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 38.51 on 42 degrees of freedom
## Multiple R-squared: 0.7368, Adjusted R-squared: 0.7242
## F-statistic: 58.78 on 2 and 42 DF, p-value: 6.713e-13
vif(fit.pca2)
## Comp.1 Comp.2
##
```

By using the loadings, we can also compute the PCs of the test dataset:

Compare the mean squared prediction error (MSPE) for the model with the multicollinearity problem and the model constructed by the two principle components.

```
YPred=predict(fit,XTest)
MSPE=mean((YTest-YPred)^2)
MSPE

## [1] 121.3127

ZTest.pca2=data.frame(ZTest[,1:2])
YPred.pca2=predict(fit.pca2,ZTest.pca2)
MSPE.pca2=mean((YTest-YPred.pca2)^2)
MSPE.pca2

## [1] 215.0987
```

Try to use all of the principal components:

```
ZTraining.pca6=data.frame(ZTraining)
fit.pca6=lm(YTraining~.,data=ZTraining.pca6)
summary(fit.pca6)
```

```
##
## Call:
## lm(formula = YTraining ~ ., data = ZTraining.pca6)
##
## Residuals:
      Min
             10 Median
                                   Max
## -50.553 -13.803 0.426 14.014 51.252
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 947.97778 3.67590 257.890 < 2e-16 ***
## Comp.1 -1.15091 0.08244 -13.961 < 2e-16 ***
## Comp.2
          -2.20854 0.23049 -9.582 1.10e-11 ***
## Comp.3
             -0.29594 0.45084 -0.656
                                        0.516
## Comp.4
            -4.83419 0.86846 -5.566 2.24e-06 ***
            10.99797 2.12986 5.164 7.95e-06 ***
## Comp.5
            16.13864 6.40242 2.521 0.016 *
## Comp.6
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 24.66 on 38 degrees of freedom
## Multiple R-squared: 0.9023, Adjusted R-squared: 0.8869
## F-statistic: 58.52 on 6 and 38 DF, p-value: < 2.2e-16
```

```
vif(fit.pca6)
```

```
## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 ## 1 1 1 1 1 1 1
```

Compare MSPE for the model constructed by all of the principle components:

```
ZTest.pca6=data.frame(ZTest)
YPred.pca6=predict(fit.pca6, ZTest.pca6)
MSPE.pca6=mean((YTest-YPred.pca6)^2)
MSPE.pca6
```

```
## [1] 121.3127
```

When is it appropriate to use PCA?

Typically, PCA is used when we have a large number of correlated variables.

In such situations PCA may be able to reduce a large set of variables to a small set that still contains most of the variation information in the large set.

Another advantage of PCA is that the principal components are uncorrelated, so we can talk about one principal component without referring to the others.

One disadvantage of PCA is that the principal components are often difficult to interpret. In such situations it may not be desirable to use the principal components in future analyses such as regression. Also it cannot provide better prediction in regression.

