Principal Components

In this notebook, I will explore some aspects of principal components analysis that are not immediately obvious and review the basics of this method. We will use a small fabricated dataset of rent in Austin, where our goal is to predict rent prices based on eight explanatory variables:

```
df = read.csv("AustinApartmentRent.csv", fileEncoding = "UTF-8-BOM")
X = df[,-1]
y = df[,1]
```

```
head(df)
```

```
##   Rent Area Bedrooms Bathrooms Security Parking Distance Shuttle Age
## 1  519  725        1         1        0       0     10.5       1   9
## 2  765  995        2         2        0       0      6.5       1  17
## 3  475  481        1         1        0       0      6.5       1  17
## 4  575  925        2         2        0       1      4.0       1   9
## 5  415  600        1         1        0       0      5.0       1  30
## 6  530  668        1         1        0       0      6.5       1  19
```

First, I will run the principal components command in R, selecting the option to scale and center our data:

```
austin.pca = prcomp(X, center = TRUE, scale. = TRUE)
```

Let's be very clear about what is stored in the object that we have just created.

First, we have what are usually refered to as the "loadings" of PCA. This matrix of values represents the linear transformation that takes our original data to its new space. I will refer to this matrix as L

```
L = austin.pca$rotation
L
```

```
##                 PC1        PC2       PC3       PC4       PC5       PC6
## Area       0.585311 -0.0410293  0.071530  0.068055 -0.068786  0.306728
## Bedrooms   0.557811  0.0511387  0.017507  0.213885 -0.223945  0.365049
## Bathrooms  0.531719 -0.0089699  0.098242  0.078655  0.154635 -0.765108
## Security  -0.026968 -0.6394900  0.181997 -0.229136 -0.575143  0.034806
## Parking    0.229787  0.0948261 -0.119137 -0.841615  0.342038  0.212962
## Distance  -0.095461  0.1787124  0.712584  0.209221  0.309049  0.293231
## Shuttle    0.019668 -0.3816067 -0.563636  0.369681  0.413989  0.230631
## Age       -0.022467  0.6325502 -0.334884  0.046667 -0.454454  0.039086
##                  PC7       PC8
## Area      -0.0058366  0.739684
## Bedrooms   0.2441492 -0.630205
## Bathrooms -0.2833152 -0.108568
## Security  -0.4074434 -0.081782
## Parking   -0.1793672 -0.145534
## Distance  -0.4648192 -0.099232
## Shuttle   -0.4113293 -0.076622
## Age       -0.5259830  0.018337
```

We also have the transformed data itself, which I refer to as P:

```
P = austin.pca$x
head(P)
```

```
##          PC1       PC2      PC3      PC4      PC5       PC6      PC7
## [1,] -1.2267 -0.022926  1.87579  0.86879  1.63108  0.806210 -0.68146
## [2,]  1.6125  0.199470  0.18827  0.97408  0.41322 -0.752724 -0.43645
## [3,] -1.6118  0.236145 -0.21203  0.35499  0.51348 -0.152482 -0.11222
## [4,]  2.2776 -0.413837 -0.89040 -1.85563  1.43485 -0.690770  0.25717
## [5,] -1.2780  1.096197 -1.35575  0.28012 -0.53876 -0.197212 -0.56770
## [6,] -1.1675  0.364283 -0.24158  0.41909  0.34587  0.093196 -0.24949
##            PC8
## [1,]  0.0140261
## [2,] -0.0310040
## [3,] -0.4758023
## [4,] -0.5408935
## [5,]  0.0037877
## [6,]  0.0974940
```

This is our data, now transformed into a new coordinate system by the above loadings. With the loadings and our original data, we can perform this calculation manually:

```
head(as.matrix(scale(X)) %*% L)
```

```
##          PC1       PC2      PC3      PC4      PC5       PC6      PC7
## [1,] -1.2267 -0.022926  1.87579  0.86879  1.63108  0.806210 -0.68146
## [2,]  1.6125  0.199470  0.18827  0.97408  0.41322 -0.752724 -0.43645
## [3,] -1.6118  0.236145 -0.21203  0.35499  0.51348 -0.152482 -0.11222
## [4,]  2.2776 -0.413837 -0.89040 -1.85563  1.43485 -0.690770  0.25717
## [5,] -1.2780  1.096197 -1.35575  0.28012 -0.53876 -0.197212 -0.56770
## [6,] -1.1675  0.364283 -0.24158  0.41909  0.34587  0.093196 -0.24949
##            PC8
## [1,]  0.0140261
## [2,] -0.0310040
## [3,] -0.4758023
## [4,] -0.5408935
## [5,]  0.0037877
## [6,]  0.0974940
```

What is special about this particular transformation is that is orthonormal, meaning it preserves all lengths and angles (i.e. the inner product) and more specifically, maximizes the variance among each principal component. We can visualize this by comparing the correlation matrix of our original data with our tansformed principal components.

```
X.scale = scale(X)
round(cor(X.scale), digits = 5)
```

```
##               Area Bedrooms Bathrooms Security  Parking Distance  Shuttle
## Area       1.00000  0.85959   0.72787  0.02549  0.26884 -0.05888  0.02325
## Bedrooms   0.85959  1.00000   0.65614 -0.07261  0.12736 -0.09617  0.00910
## Bathrooms  0.72787  0.65614   1.00000 -0.05164  0.22646 -0.02342  0.00000
## Security   0.02549 -0.07261  -0.05164  1.00000 -0.04385 -0.08628  0.04385
## Parking    0.26884  0.12736   0.22646 -0.04385  1.00000 -0.21480 -0.13462
## Distance  -0.05888 -0.09617  -0.02342 -0.08628 -0.21480  1.00000 -0.43717
## Shuttle    0.02325  0.00910   0.00000  0.04385 -0.13462 -0.43717  1.00000
## Age       -0.07832  0.04920  -0.09309 -0.48575  0.02704 -0.16145 -0.13938
##                Age
## Area      -0.07832
## Bedrooms   0.04920
## Bathrooms -0.09309
## Security  -0.48575
## Parking    0.02704
## Distance  -0.16145
## Shuttle   -0.13938
## Age        1.00000
```

```
round(cor(P), digits = 5)
```

```
##     PC1 PC2 PC3 PC4 PC5 PC6 PC7 PC8
## PC1   1   0   0   0   0   0   0   0
## PC2   0   1   0   0   0   0   0   0
## PC3   0   0   1   0   0   0   0   0
## PC4   0   0   0   1   0   0   0   0
## PC5   0   0   0   0   1   0   0   0
## PC6   0   0   0   0   0   1   0   0
## PC7   0   0   0   0   0   0   1   0
## PC8   0   0   0   0   0   0   0   1
```

In the original data, there is correlation between our different variables, as would be expected. PCA takes the original data and "rotates" it to the point where there is no correlation between each direction, maximizing the variance in each new coordinate. We can also look at the sample covariance matrix to understand how much variance each principal components contains:

$$\frac{1}{n-1}(P^T P)$$

in R this is:

```
(1/59)*round(t(P) %*% P, digits = 5)
```

```
##        PC1   PC2   PC3    PC4     PC5     PC6     PC7     PC8
## PC1 2.5982 0.000 0.000 0.0000 0.00000 0.00000 0.00000 0.00000
## PC2 0.0000 1.544 0.000 0.0000 0.00000 0.00000 0.00000 0.00000
## PC3 0.0000 0.000 1.424 0.0000 0.00000 0.00000 0.00000 0.00000
## PC4 0.0000 0.000 0.000 1.0238 0.00000 0.00000 0.00000 0.00000
## PC5 0.0000 0.000 0.000 0.0000 0.64572 0.00000 0.00000 0.00000
## PC6 0.0000 0.000 0.000 0.0000 0.00000 0.34819 0.00000 0.00000
## PC7 0.0000 0.000 0.000 0.0000 0.00000 0.00000 0.30743 0.00000
## PC8 0.0000 0.000 0.000 0.0000 0.00000 0.00000 0.00000 0.10864
```

What we see is that our transformation has eliminated any correlation between our considered variables, as shown by the fact that entries only appear in the diagonals of our sample covariance matrix. In fact, these are what our refered to as the eigenvalues of our PCA, which represent the amount of variance in each principal component:

```
austin.pca$sdev^2
```

```
## [1] 2.59819 1.54398 1.42404 1.02382 0.64572 0.34819 0.30743 0.10864
```

Since these are the elements of the diagonal covariance matrix, we can see that these eigenvalues are also equal to the amount of variance in each principal component, which are ordered by decreasing variance.

With all this in mind, we can now look at regression using these principal components:

```r
data  = as.data.frame(cbind(y, austin.pca$x))
model.pca.full = lm(y ~ ., data = data)
summary(model.pca.full)
```

```
##
## Call:
## lm(formula = y ~ ., data = data)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -164.32  -44.29    6.88   42.54  121.34
##
## Coefficients:
##             Estimate Std. Error t value            Pr(>|t|)
## (Intercept)   572.27       8.31   68.89 <0.0000000000000002 ***
## PC1            75.07       5.20   14.44 <0.0000000000000002 ***
## PC2            -7.75       6.74   -1.15              0.2554
## PC3             2.44       7.02    0.35              0.7292
## PC4            21.48       8.28    2.59              0.0123 *
## PC5            -3.13      10.43   -0.30              0.7653
## PC6            -4.32      14.20   -0.30              0.7624
## PC7           -24.38      15.11   -1.61              0.1128
## PC8            83.44      25.42    3.28              0.0019 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 64.3 on 51 degrees of freedom
## Multiple R-squared:  0.819,  Adjusted R-squared:  0.79
## F-statistic: 28.8 on 8 and 51 DF,  p-value: 0.000000000000000238
```

Notice that our standard errors of the coefficients of this regression are strictly increasing. This is because:

$$\widehat{\text{var}}(\hat{\beta}) = s^2(X^TX)^{-1}$$

where s is the standard error of our residuals. In the case of principal components, we saw that the term X^TX is equal to exactly the diagonal matrix of eigenvalues multiplied by (n-1):

$$\widehat{\text{var}}(\hat{\beta}) = s^2 \begin{bmatrix} (n-1)\lambda_1 & & \\ & \ddots & \\ & & (n-1)\lambda_j \end{bmatrix}^{-1}$$

Simplifying:

$$\widehat{\text{var}}(\hat{\beta}) = \begin{bmatrix} \dfrac{s^2}{(n-1)\lambda_1} & & \\ & \ddots & \\ & & \dfrac{s^2}{(n-1)\lambda_j} \end{bmatrix}$$

recalling that

$$\lambda_1 \geq \cdots \geq \lambda_j$$

we can see that each successive variance is increasing, thus explaining why the variance of coefficients is increasing in our regression. It is interesting to note that this is independent of the response variable!

We could alternatively note that:

$$\widehat{\text{var}}(\hat{\beta}_j) = \frac{s^2}{(n-1)\widehat{\text{var}}(X_j)} \cdot \frac{1}{1-R_j^2}$$

where R_J^2 is the is the multiple R^2 for the regression of X_j on the other covariates. However, we already established that the variance of each principal component is its corresponding eigenvalue, and that this R^2 value is zero. So we have:

$$\widehat{\text{var}}(\hat{\beta}_j) = \frac{s^2}{(n-1)\lambda_j}$$

We can compute this in R:

```
sum = summary(model.pca.full)
s = sum$sigma
eigenvalues = austin.pca$sdev^2
```

```
sqrt(s^2/(59*eigenvalues))
```

```
## [1]  5.1973  6.7420  7.0202  8.2794 10.4253 14.1971 15.1092 25.4167
```

And see that we get the same standard errors that R calculated in the above regression:

```
sum$coefficients[-1,2]
```

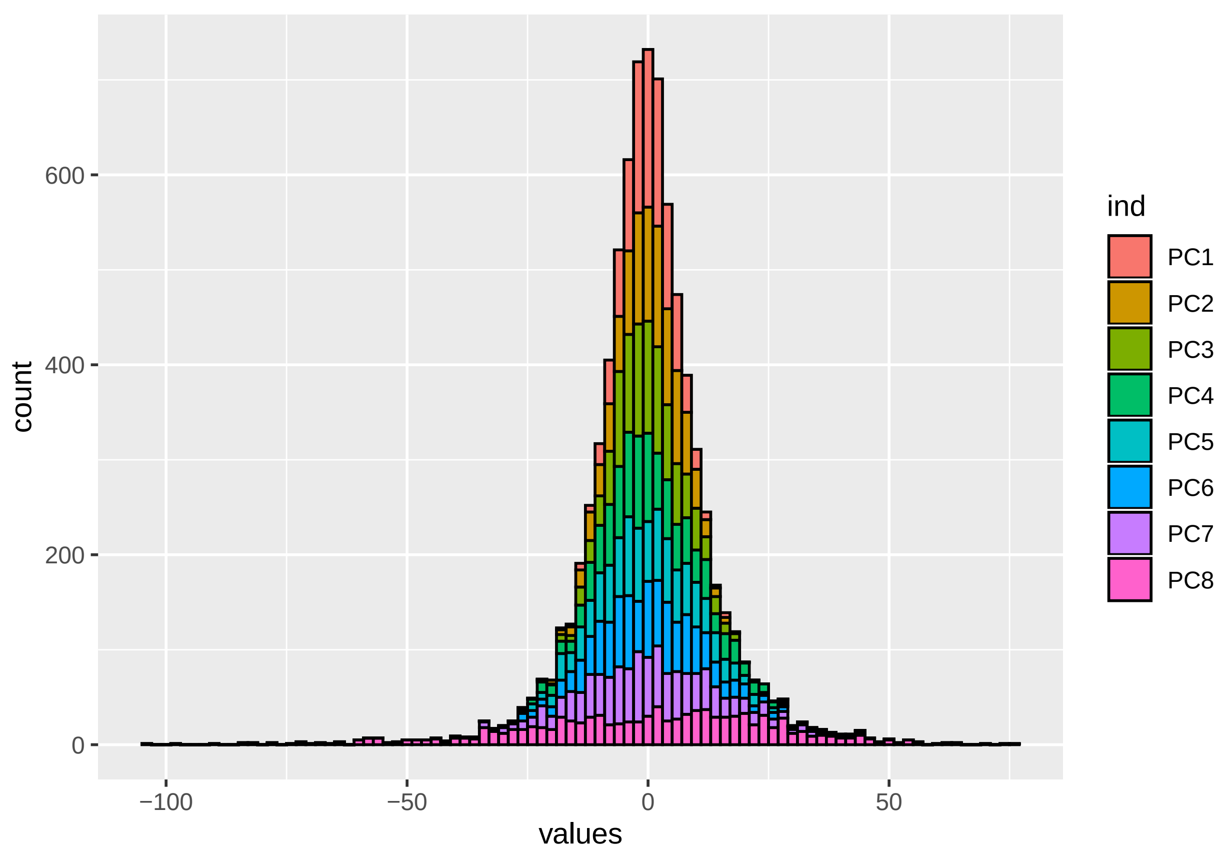
```
##     PC1     PC2     PC3     PC4     PC5     PC6     PC7     PC8
##  5.1973  6.7420  7.0202  8.2794 10.4253 14.1971 15.1092 25.4167
```

Finally, we can graphically view how these differing variances of our coefficients appear in a simulation. Below I have have 1000 random samples of our data:

```
model.pca.full.coef = matrix(data = 0, nrow = 1000, ncol = 8)


for (i in 1:1000){
  sample  = sample(1:60, 40)
  model.pca.full.coef[i,] = as.numeric(summary(lm(y ~ ., data = data[sample,]))$coefficients[-1,1])

}
```

Below I plot a histogram of our esimate of each coefficient for each of our simulations, centering the data so that we can compare:

```
model.pca.full.coef = as.data.frame(model.pca.full.coef)
colnames(model.pca.full.coef) = paste("PC", 1:8, sep = "")

library(ggplot2)
pca.center = as.data.frame(apply(model.pca.full.coef, 2, scale, scale = FALSE, center = TRUE))
ggplot(stack(pca.center), aes(x=values, fill = ind))+ geom_histogram(binwidth = 2, color = "black")
```



We see the expected result, that as we look at each successive coefficient of our principal components that we observe a higher varience for our estimate.

For what may be a more clear picture, we can compare PC1, PC6, and PC8:

```
ggplot(stack(pca.center)[c(1:1000, 5001:6000, 7001:8000),], aes(x=values, fill = ind))+ geom_histogram(
```