Lab 09: Principal Components Analysis (PCA)

PSTAT 131/231

Learning Objectives

- Review of PCA
- `prcomp()` and `biplot()` functions
- Visualization with PCAs
- Computing PCA using SVD

Data

In the lecture, we have used the `USArrests` dataset to illustrate the intuition behind PCA. In this lab, we will cover how to perform perform PCA on this dataset using R. Recall that each row of the dataset contains the number of arrests per 100,000 residents for each of the three crimes: `Assault`, `Murder`, and `Rape`. Each state also has a feature `UrbanPop`, which stands for the percent of the population in each state living in urban areas.

```
states=row.names(USArrests)
states
```

```
##  [1] "Alabama"        "Alaska"         "Arizona"        "Arkansas"
##  [5] "California"     "Colorado"       "Connecticut"    "Delaware"
##  [9] "Florida"        "Georgia"        "Hawaii"         "Idaho"
## [13] "Illinois"       "Indiana"        "Iowa"           "Kansas"
## [17] "Kentucky"       "Louisiana"      "Maine"          "Maryland"
## [21] "Massachusetts"  "Michigan"       "Minnesota"      "Mississippi"
## [25] "Missouri"       "Montana"        "Nebraska"       "Nevada"
## [29] "New Hampshire"  "New Jersey"     "New Mexico"     "New York"
## [33] "North Carolina" "North Dakota"   "Ohio"           "Oklahoma"
## [37] "Oregon"         "Pennsylvania"   "Rhode Island"   "South Carolina"
## [41] "South Dakota"   "Tennessee"      "Texas"          "Utah"
## [45] "Vermont"        "Virginia"       "Washington"     "West Virginia"
## [49] "Wisconsin"      "Wyoming"
```

The columns of the data set contain the four variables.

```
names(USArrests)
```

```
## [1] "Murder"   "Assault"  "UrbanPop" "Rape"
```

We first briefly examine the data.

```
summary(USArrests)
```

```
##      Murder          Assault         UrbanPop          Rape
##  Min.   : 0.800   Min.   : 45.0   Min.   :32.00   Min.   : 7.30
##  1st Qu.: 4.075   1st Qu.:109.0   1st Qu.:54.50   1st Qu.:15.07
##  Median : 7.250   Median :159.0   Median :66.00   Median :20.10
##  Mean   : 7.788   Mean   :170.8   Mean   :65.54   Mean   :21.23
##  3rd Qu.:11.250   3rd Qu.:249.0   3rd Qu.:77.75   3rd Qu.:26.18
```

```
## Max.   :17.400   Max.   :337.0   Max.   :91.00   Max.   :46.00
```

We notice that there are on average three times as many rapes as murders, and more than eight times as many assaults as rapes. We can also examine the variances of the four variables.

```
apply(USArrests, 2, var)
```

```
##     Murder    Assault   UrbanPop       Rape
##   18.97047 6945.16571  209.51878   87.72916
```

Not surprisingly, the variables also have vastly different variances: the `UrbanPop` variable measures the percentage of the population in each state living in an urban area, which is not a comparable number to the number of three crimes in each state per 100,000 individuals. If we failed to scale the variables before performing PCA, then most of the principal components that we observed would be driven by the `Assault` variable, since it has by far the largest mean and variance.

Recall that in the lecture we talked about whether standardization of the dataset should be performed before PCA. The short answer: that really depends on the application and dataset. From the discussion above, it is reasonable to standardize the four features in the `USArrests` to have mean zero and standard deviation one before performing PCA.

Principle Component Analysis

We now perform principal components analysis using the `prcomp()` function, which is one of several functions in R that perform PCA.

```
pr.out=prcomp(USArrests, scale=TRUE)
```

By default, the `prcomp()` function centers the variables to have mean zero. By using the option `scale=TRUE`, we scale the variables to have standard deviation one. The output from `prcomp()` contains a number of useful quantities.

```
names(pr.out)
```

```
## [1] "sdev"     "rotation" "center"   "scale"    "x"
```

The center and scale components correspond to the means and standard deviations of the variables that were used for scaling prior to implementing PCA.

```
pr.out$center
```

```
##   Murder  Assault UrbanPop     Rape
##    7.788  170.760   65.540   21.232
```

```
pr.out$scale
```

```
##    Murder   Assault  UrbanPop      Rape
##  4.355510 83.337661 14.474763  9.366385
```

The rotation matrix provides the principal component loadings; each column of `pr.out$rotation` contains the corresponding principal component loading vector

```
pr.out$rotation
```

```
##                 PC1        PC2        PC3         PC4
## Murder   -0.5358995  0.4181809 -0.3412327  0.64922780
## Assault  -0.5831836  0.1879856 -0.2681484 -0.74340748
## UrbanPop -0.2781909 -0.8728062 -0.3780158  0.13387773
## Rape     -0.5434321 -0.1673186  0.8177779  0.08902432
```

We see that there are four distinct principal components. This is to be expected because there are in general $min(n-1, p)$ informative principal components in a data set with n observations and p variables.

Using the `prcomp()` function, we do not need to explicitly multiply the data by the principal component loading vectors in order to obtain the principal component score vectors. Rather the 50×4 matrix x has as its columns the principal component score vectors. That is, the kth column is the kth principal component score vector.

```
dim(pr.out$x)
```

```
## [1] 50  4
```

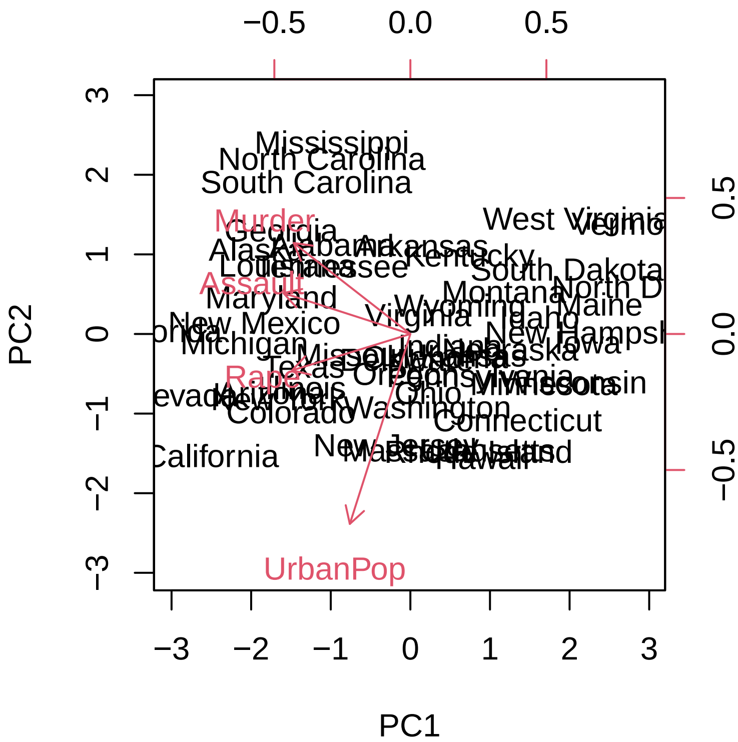
```
pr.out$x
```

```
##                        PC1         PC2         PC3          PC4
## Alabama        -0.97566045  1.12200121 -0.43980366  0.154696581
## Alaska         -1.93053788  1.06242692  2.01950027 -0.434175454
## Arizona        -1.74544285 -0.73845954  0.05423025 -0.826264240
## Arkansas        0.13999894  1.10854226  0.11342217 -0.180973554
## California     -2.49861285 -1.52742672  0.59254100 -0.338559240
## Colorado       -1.49934074 -0.97762966  1.08400162  0.001450164
## Connecticut     1.34499236 -1.07798362 -0.63679250 -0.117278736
## Delaware       -0.04722981 -0.32208890 -0.71141032 -0.873113315
## Florida        -2.98275967  0.03883425 -0.57103206 -0.095317042
## Georgia        -1.62280742  1.26608838 -0.33901818  1.065974459
## Hawaii          0.90348448 -1.55467609  0.05027151  0.893733198
## Idaho           1.62331903  0.20885253  0.25719021 -0.494087852
## Illinois       -1.36505197 -0.67498834 -0.67068647 -0.120794916
## Indiana         0.50038122 -0.15003926  0.22576277  0.420397595
## Iowa            2.23099579 -0.10300828  0.16291036  0.017379470
## Kansas          0.78887206 -0.26744941  0.02529648  0.204421034
## Kentucky        0.74331256  0.94880748 -0.02808429  0.663817237
## Louisiana      -1.54909076  0.86230011 -0.77560598  0.450157791
## Maine           2.37274014  0.37260865 -0.06502225 -0.327138529
## Maryland       -1.74564663  0.42335704 -0.15566968 -0.553450589
## Massachusetts   0.48128007 -1.45967706 -0.60337172 -0.177793902
## Michigan       -2.08725025 -0.15383500  0.38100046  0.101343128
## Minnesota       1.67566951 -0.62590670  0.15153200  0.066640316
## Mississippi    -0.98647919  2.36973712 -0.73336290  0.213342049
## Missouri       -0.68978426 -0.26070794  0.37365033  0.223554811
## Montana         1.17353751  0.53147851  0.24440796  0.122498555
## Nebraska        1.25291625 -0.19200440  0.17380930  0.015733156
## Nevada         -2.84550542 -0.76780502  1.15168793  0.311354436
## New Hampshire   2.35995585 -0.01790055  0.03648498 -0.032804291
## New Jersey     -0.17974128 -1.43493745 -0.75677041  0.240936580
## New Mexico     -1.96012351  0.14141308  0.18184598 -0.336121113
## New York       -1.66566662 -0.81491072 -0.63661186 -0.013348844
## North Carolina -1.11208808  2.20561081 -0.85489245 -0.944789648
## North Dakota    2.96215223  0.59309738  0.29824930 -0.251434626
## Ohio            0.22369436 -0.73477837 -0.03082616  0.469152817
## Oklahoma        0.30864928 -0.28496113 -0.01515592  0.010228476
## Oregon         -0.05852787 -0.53596999  0.93038718 -0.235390872
## Pennsylvania    0.87948680 -0.56536050 -0.39660218  0.355452378
## Rhode Island    0.85509072 -1.47698328 -1.35617705 -0.607402746
## South Carolina -1.30744986  1.91397297 -0.29751723 -0.130145378
## South Dakota    1.96779669  0.81506822  0.38538073 -0.108470512
```

```
## Tennessee      -0.98969377  0.85160534  0.18619262  0.646302674
## Texas          -1.34151838 -0.40833518 -0.48712332  0.636731051
## Utah            0.54503180 -1.45671524  0.29077592 -0.081486749
## Vermont         2.77325613  1.38819435  0.83280797 -0.143433697
## Virginia        0.09536670  0.19772785  0.01159482  0.209246429
## Washington      0.21472339 -0.96037394  0.61859067 -0.218628161
## West Virginia   2.08739306  1.41052627  0.10372163  0.130583080
## Wisconsin       2.05881199 -0.60512507 -0.13746933  0.182253407
## Wyoming         0.62310061  0.31778662 -0.23824049 -0.164976866
```

We can plot the first two principal components as follows:

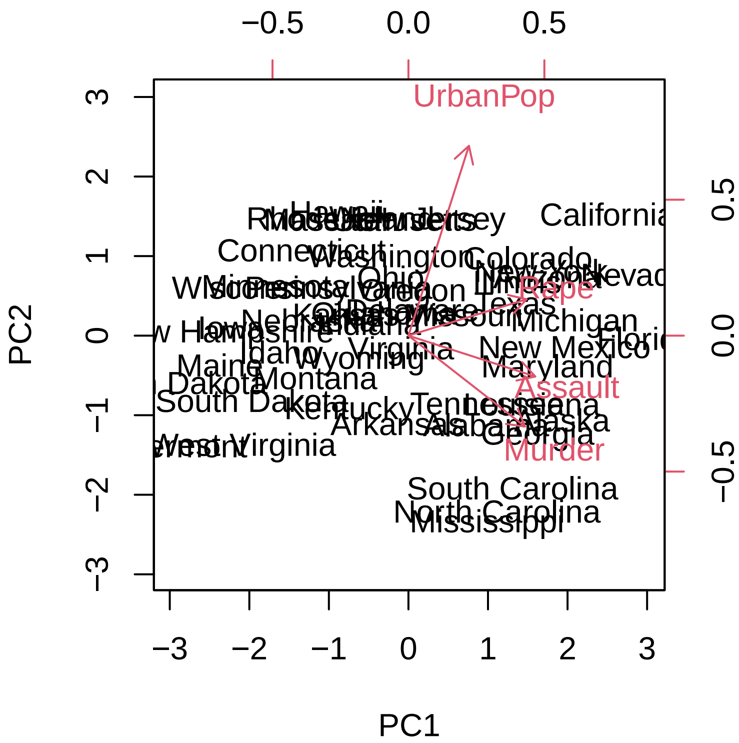
```
biplot(pr.out, scale=0)
```



The `scale=0` argument to `biplot()` ensures that the arrows are scaled to represent the loadings; other values for scale give slightly different biplots with different interpretations.

Notice that this figure is a mirror image of Figure 10.1. Recall that the principal components are only unique up to a sign change, so we can reproduce Figure 10.1 by making a few small changes:

```
pr.out$rotation=-pr.out$rotation
pr.out$x=-pr.out$x
biplot(pr.out, scale=0)
```



How many principal components are needed?

The `prcomp()` function also outputs the standard deviation of each principal component. For instance, on the USArrests data set, we can access these standard deviations as follows:

```
pr.out$sdev
```

```
## [1] 1.5748783 0.9948694 0.5971291 0.4164494
```

The variance explained by each principal component is obtained by squaring these:

```
pr.var=pr.out$sdev^2
pr.var
```

```
## [1] 2.4802416 0.9897652 0.3565632 0.1734301
```

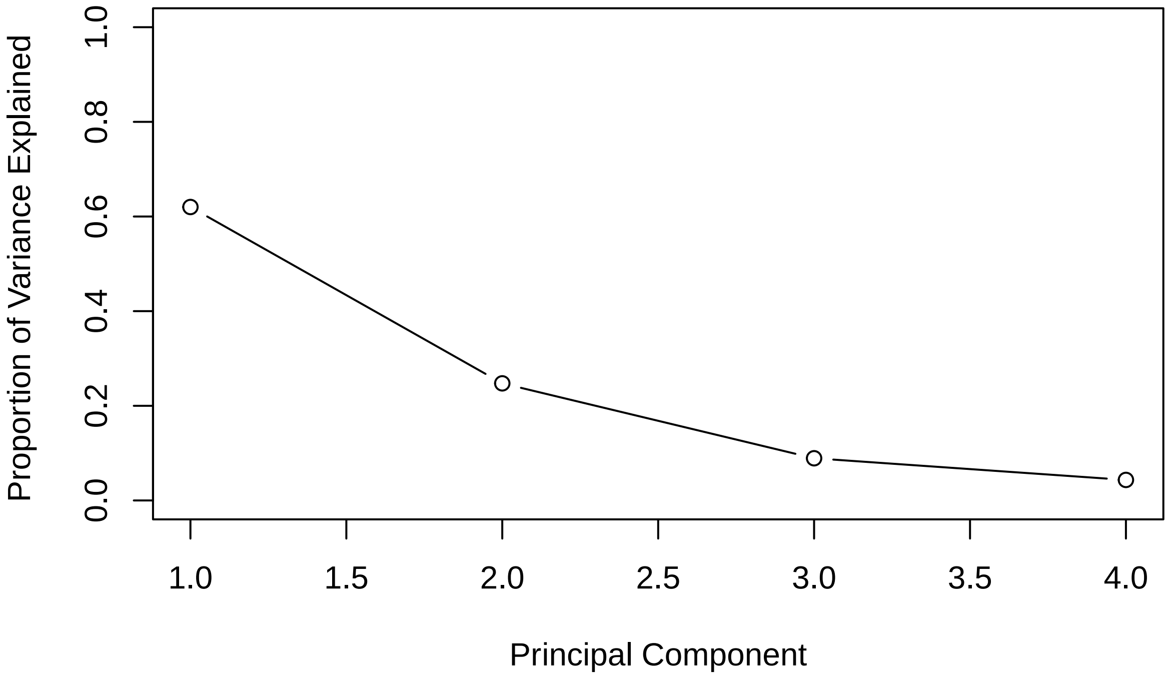
To compute the proportion of variance explained by each principal component, we simply divide the variance explained by each principal component by the total variance explained by all four principal components:

```
pve=pr.var/sum(pr.var)
pve
```

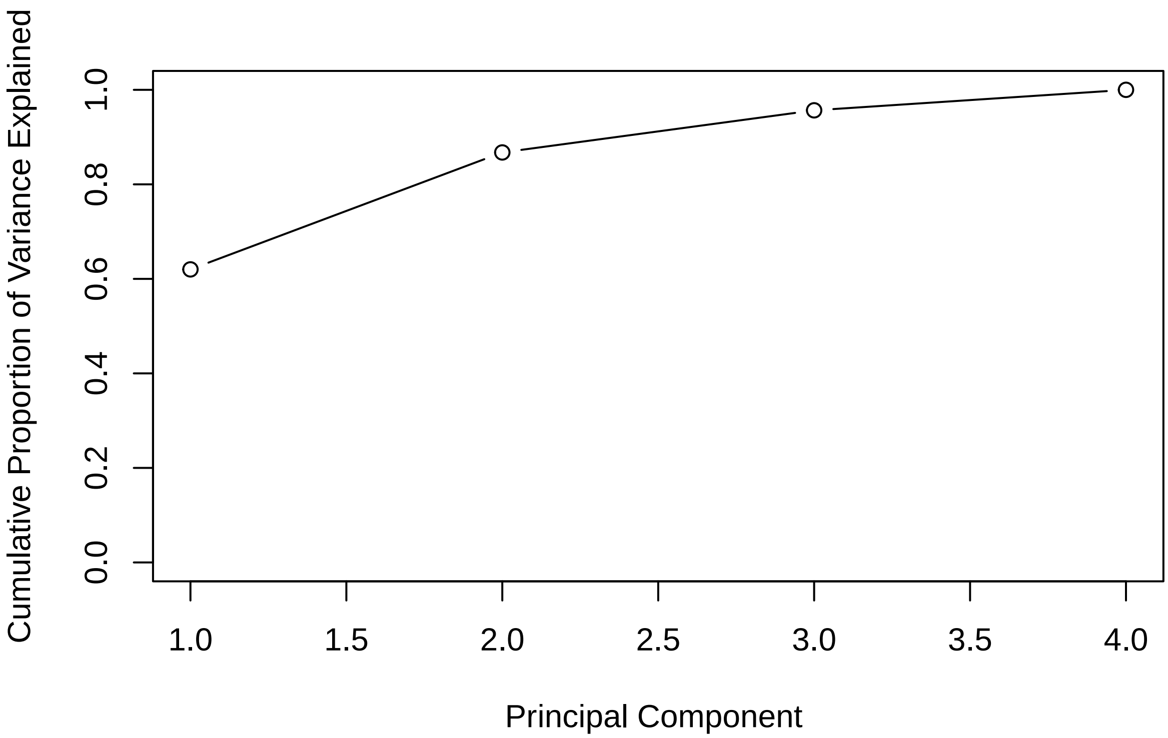
```
## [1] 0.62006039 0.24744129 0.08914080 0.04335752
```

We see that the first principal component explains 62.0% of the variance in the data, the next principal component explains 24.7% of the variance, and so forth. We can plot the PVE explained by each component, as well as the cumulative PVE, as follows:

```
plot(pve, xlab="Principal Component",
     ylab="Proportion of Variance Explained ", ylim=c(0,1),type='b')
```




```
plot(cumsum(pve), xlab="Principal Component ",
     ylab=" Cumulative Proportion of Variance Explained ", ylim=c(0,1), type='b')
```



The result is shown in Figure 10.4. Note that the function `cumsum()` computes the cumulative sum of the elements of a numeric vector. For instance:

```
a=c(1,2,8,-3)
cumsum(a)
```

```
## [1]  1  3 11  8
```

Computing PCA using singular value decomposition

Recall in lecture we talked about that computing PCA is equivalent to the singular value decomposition (SVD). Actually, `prcomp` is doing SVD internally. In this section, we just verify this fact.

Recall that the singular value decomposition of a data matrix is the following form:

$$\mathbf{X} = UDV^T,$$

where $\mathbf{X} \in \mathbb{R}^{n\times p}$ is the data matrix with n rows (observations) and p columns (features). The SVD writes $\mathbf{X}$ as a product of three matrices, where $U \in \mathbb{R}^{n\times p}$, $V \in \mathbb{R}^{p\times p}$, and $D \in \mathbb{R}^{p\times p}$ is a diagonal matrix.

We now verify that PCA can be computed using SVD. We first standardize the data matrix by using `scale`, and pass it into the function `svd`, which computes the singular value decomposition.

```
dat = scale(USArrests, center = TRUE, scale = TRUE)
decomp = svd(dat)
names(decomp)
```

```
## [1] "d" "u" "v"
```

The result of the SVD contains three parts: `u`, `v`, and `d`, which correspond to the matrix U, the matrix V, and the diagonal elements of the diagonal matrix D, respectively.

In lecture, we mentioned that the columns of V are the loadings of PCs (again, recall that the loadings of PCs are unique up to a sign change):

```
decomp$v
```

```
##            [,1]       [,2]       [,3]        [,4]
## [1,] -0.5358995  0.4181809 -0.3412327  0.64922780
## [2,] -0.5831836  0.1879856 -0.2681484 -0.74340748
## [3,] -0.2781909 -0.8728062 -0.3780158  0.13387773
## [4,] -0.5434321 -0.1673186  0.8177779  0.08902432
```

```
pr.out$rotation
```

```
##                PC1        PC2        PC3         PC4
## Murder   0.5358995 -0.4181809  0.3412327 -0.64922780
## Assault  0.5831836 -0.1879856  0.2681484  0.74340748
## UrbanPop 0.2781909  0.8728062  0.3780158 -0.13387773
## Rape     0.5434321  0.1673186 -0.8177779 -0.08902432
```

and that the percentage of variance explained (PVE) by the m-th PC is $d_m^2 / \sum_j d_j^2$, which can be verified as below:

```
decomp$d^2 / sum(decomp$d^2)
```

```
## [1] 0.62006039 0.24744129 0.08914080 0.04335752
```

```
pve
```

```
## [1] 0.62006039 0.24744129 0.08914080 0.04335752
```

Bibliography

Note: The material in the first two sections of this lab was obtained from ISLR Section 10.4

[1] James et. al. - An Introduction to Statistical Learning with Applications in R, Eigth Edition. Available at: http://www-bcf.usc.edu/~gareth/ISL/