18) Principal Components Analysis

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March 2018

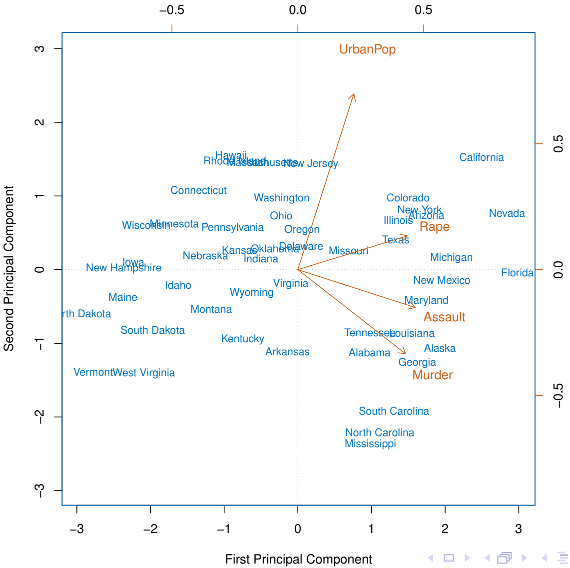
Reference

Tables, Graphics, and Figures from

James et al. (2017): Chapters: 10.2, and 10.4

Hastie et al. (2017): Chapter: 14.5

USArrests Data



Principal Component Analysis (PCA)

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + ... + \phi_{p1}X_p$$

$$z_{i1} = \phi_{11}x_{i1} + \phi_{21}x_{i2} + ... + \phi_{p1}x_{ip}$$

$$\max_{\phi_{11},\dots,\phi_{p1}} \left\{\frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{j1}x_{ij}\right)^2\right\}$$

$$\text{subject to } \sum_{j=1}^{p}\phi_{j1}^2 = 1$$

$$z_{i2} = \phi_{12}x_{i1} + \phi_{22}x_{i2} + ... + \phi_{p2}x_{ip}$$

Singular Value Decomposition (SVD)

$$X_{n\times p} = U_{n\times p} D_{p\times p} V_{p\times p}^T$$

U and V are Orthogonal

$$U^T U = I_{n\times n} \text{ and } V^T V = I_{p\times p}$$

$$S = X^T X = VD^2 V^T$$

$$XX^T = UD^2 U^T$$

$$(S - \delta I)v = 0$$

Maximum Variance

$$z_1 = Xv_1 = u_1 d_1$$

$$Var(z_1) = \frac{d_1^2}{n}$$

Subsequent Principal Components z_j have maximum variance $\frac{d_j^2}{n}$, subject to being orthogonal to the earlier ones

OLS and Ridge Fitted Vector

$$
\begin{aligned}
X\hat{\beta}^{ls} &= X(X^TX)^{-1}X^Ty \\
&= UU^Ty
\end{aligned}
$$

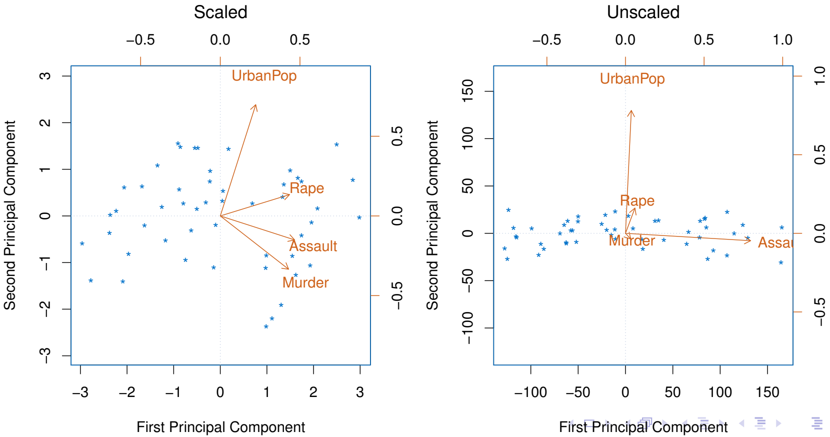
$$
\begin{aligned}
X\hat{\beta}^{ridge} &= X(X^TX+\lambda I)^{-1}X^Ty \\
&= UD(D^2+\lambda I)^{-1}DU^Ty \\
&= \sum_{j=1}^{p} u_j \frac{d_j^2}{d_j^2+\lambda} u_j^T y
\end{aligned}
$$

First and Second Principal Component

	PC1	PC2
Murder	0.5358995	−0.4181809
Assault	0.5831836	−0.1879856
UrbanPop	0.2781909	0.8728062
Rape	0.5434321	0.1673186

Scaling the Variables

Variance for Murder, Rape, Assault, and UrbanPop:
18.97, 87.73, 6945.16, and 209.5



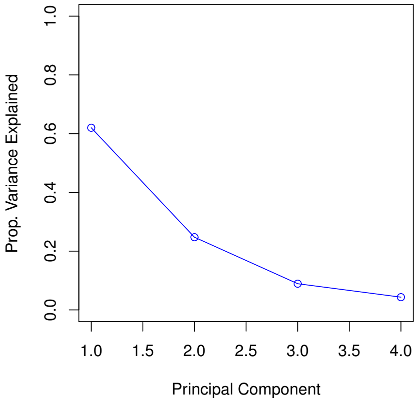
Proportion of Variance Explained (PVE)

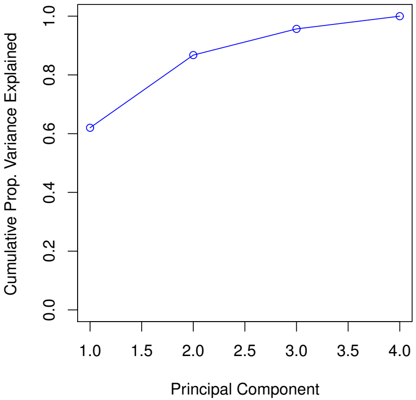
$$PVE = \frac{\frac{1}{n}\sum_{i=1}^{n} z_{im}^2}{\sum_{j=1}^{p} Var(X_j)}$$

$$\sum_{j=1}^{p} Var(X_j) = \sum_{j=1}^{p} \frac{1}{n} \sum_{i=1}^{n} x_{ij}^2$$

$$\frac{1}{n} \sum_{i=1}^{n} z_{im}^2 = \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{jm} x_{ij}\right)^2$$

Cumulative Proportion of Variance Explained





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

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
```

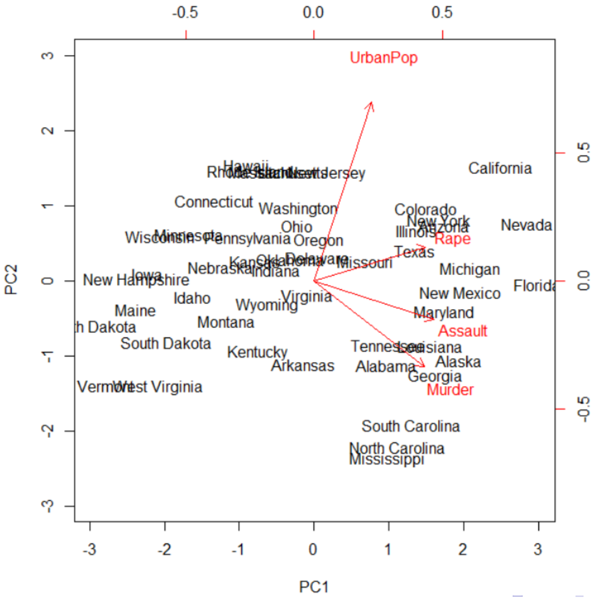
pr.out$rotation=-pr.out$rotation

pr.out$x=-pr.out$x

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

biplot(pr.out, scale=0)



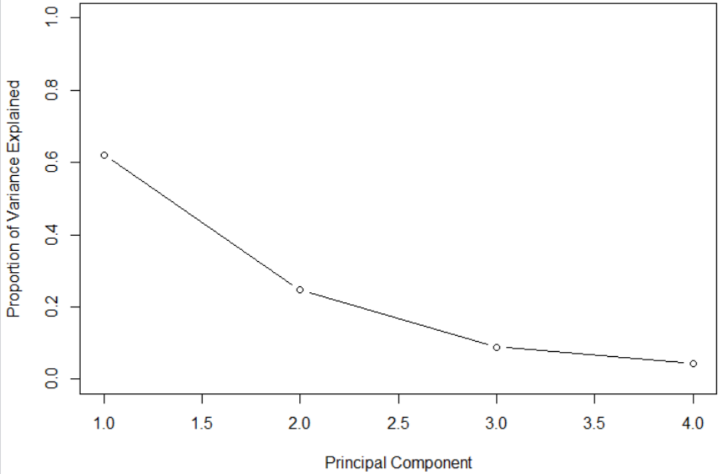
pr.var=pr.out$sdev^2; pr.var

```
2.4802416 0.9897652 0.3565632 0.1734301
```

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

```
0.62006039 0.24744129 0.08914080 0.04335752
```

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')