BIOS 635: Principal Components Regression and Partial Least Squares

Kevin Donovan

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Review

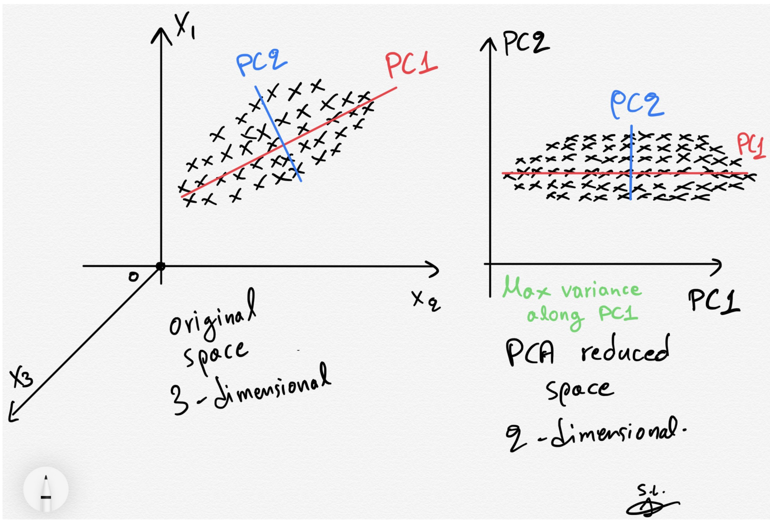
- Midterm assigned on Github Classroom, due on 3/19 by 11PM EST
- Article evaluation 3 assigned on Github Classroom, due on 3/23 by 11PM EST
- Last lecture: shrinkage and penalized regression

Model selection

- **Goal**: Choose/build model parameters and structure to create *optimal* model
- General methods:
    1. Subset Selection
    2. Shrinkage
    3. **Dimension Reduction**

Dimension Reduction

- For data with large p, may want to **reduce predictor set**
  - *Reduces chance of overfitting, estimation variance*
  - *Predictors may be highly correlated, but still important to assess*
  - *Traditional regression with $p > n$ not computationally possible*
- Idea: **project predictor space into reduced dimensional space**
  - *Use these new variables as regression model predictors*



Principal Components Regression

- Original predictors: $X_1, \ldots, X_p$
- New set: $Z_1, \ldots, Z_M$ where $M < p$
    - *Suppose Z_i are **linear combinations** of $X_1, \ldots, X_p$*

$$Z_m = \sum_{j=1}^{p} \phi_{jm} X_j$$

- Regression model:

$$Y_i = \theta_0 + \sum_{m=1}^{M} \theta_m Z_{im} + \epsilon_i$$

- Dimension of model reduced from $p+1$ to $M+1$
- **How do we decide on reduced set?**

    1. *How big should M be?*
    2. *How to estimate $\{\phi_{jm}\}$?*

Principal Components Analysis (PCA)

- PCA creates reduced set of predictors **equal to linear combos** of original set
- Method:
  - *First principal component (PC):*

$$
\begin{aligned}
Z_1 &= \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p \\
\hat{\phi}_1 &= \underset{||\phi_1||=1}{\text{argmax}}[\text{Var}(\phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p)] \\
&= \underset{||\phi_1||=1}{\text{argmax}}(\phi_{11}^2 + \phi_{21}^2 + \ldots + \phi_{p1}^2 + 2\phi_{11}\phi_{21}\rho_{12} + \ldots + 2\phi_{11}\phi_{p1}\rho_{1p} + \ldots + 2\phi_{p-1,1}\phi_{p1}\rho_{p-1,p})
\end{aligned}
$$

- $\rho_{ij} = \text{Cor}(X_i, X_j)$
- First PC = linear combo containing **maximum amount of variability between predictors**
- Weights ϕ_{ij} call *loadings*

PCA details

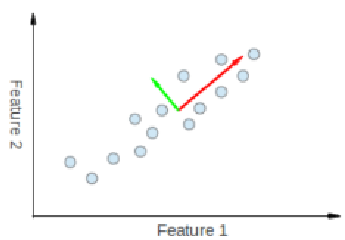
- $||\phi_1|| = 1 \rightarrow \sum_{j=1}^{p} \phi_{j1}^2 = 1$
- Above assumes X predictor matrix is *centered* (X_j have mean 0) and scaled (have variance 1)
- Can then compute PC values for each observation:

$$Z_{i1} = \phi_{11}X_{i1} + \phi_{21}X_{i2} + \ldots + \phi_{ip}X_{ip} \text{ for } 1 \leq i \leq n$$

- For next PC Z_2, same process is done but $\mathrm{Cor}(Z_1, Z_2) = 0$ assumed
  - $\rightarrow \phi_2$ *and* ϕ_1 *are orthogonal*

PCA recap

- PCA uses an **orthogonal transformation** to convert predictor set into new set of **uncorrelated** predictors equal to **linear combinations** of the original set
- Can compute new variables for each observation using **loadings**



First principal component: $\mathbf{Z}_1 = \phi_{11}\mathbf{X}_1 + \phi_{21}\mathbf{X}_2 + ... + \phi_{p1}\mathbf{X}_p$

PC loading vector: $\boldsymbol{\phi}_1 = \{\phi_{11}, \phi_{21}, ..., \phi_{p1}\}^T$, $\sum_{j=1}^{p} \phi_{j1}^2 = 1$

$\hat{\boldsymbol{\phi}}_1 = \underset{||\boldsymbol{\phi}_1||=1}{\text{argmax}}\{\boldsymbol{\phi}_1^T \mathbf{X}^T \mathbf{X} \boldsymbol{\phi}_1\}$ maximizes the variance of $\mathbf{Z}_1$.

$\boldsymbol{\phi}_1$ is the eigenvector corresponding to the largest eigenvalue of $\mathbf{X}^T\mathbf{X}$.

$\mathbf{Z}_2$ is restrained to be uncorrelated with $\mathbf{Z}_1$. Equivalently, $\boldsymbol{\phi}_2$ is orthogonal to $\boldsymbol{\phi}_1$.

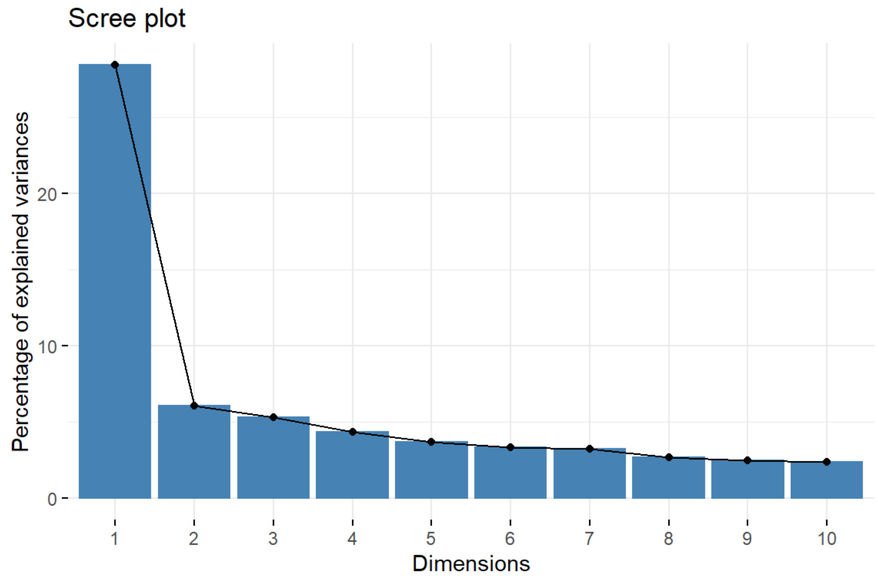
PCA example

- Suppose we have a large amount of regional brain activity measures on group of infants
- Want to see if this regional brain activity is related to diganosis of Autism (ASD)

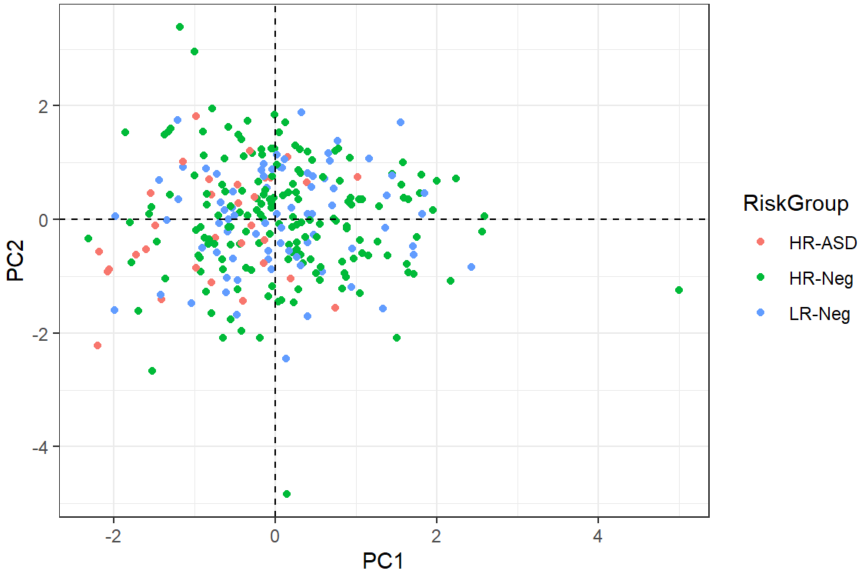
```
brain_data <- read_csv("../data/IBIS_brain_data_ex.csv")

brain_data <- brain_data %>%
  select("CandID", "RiskGroup", names(brain_data)[grepl("V12", names(brain_data))]) %>%
  select(CandID:Uncinate_R_V12) %>%
  drop_na()

dim(brain_data)
```

```
## [1] 278 120
```

```
# Run PCA on brain variables
pca_brain <- prcomp(brain_data %>%
                      select(LeftAmygdala_V12, RightAmygdala_V12,
                             PreCG_L_V12:Uncinate_R_V12) %>% as.data.frame(),
                    cor=TRUE, scores=TRUE)

# Scree plot
fviz_eig(pca_brain)
```



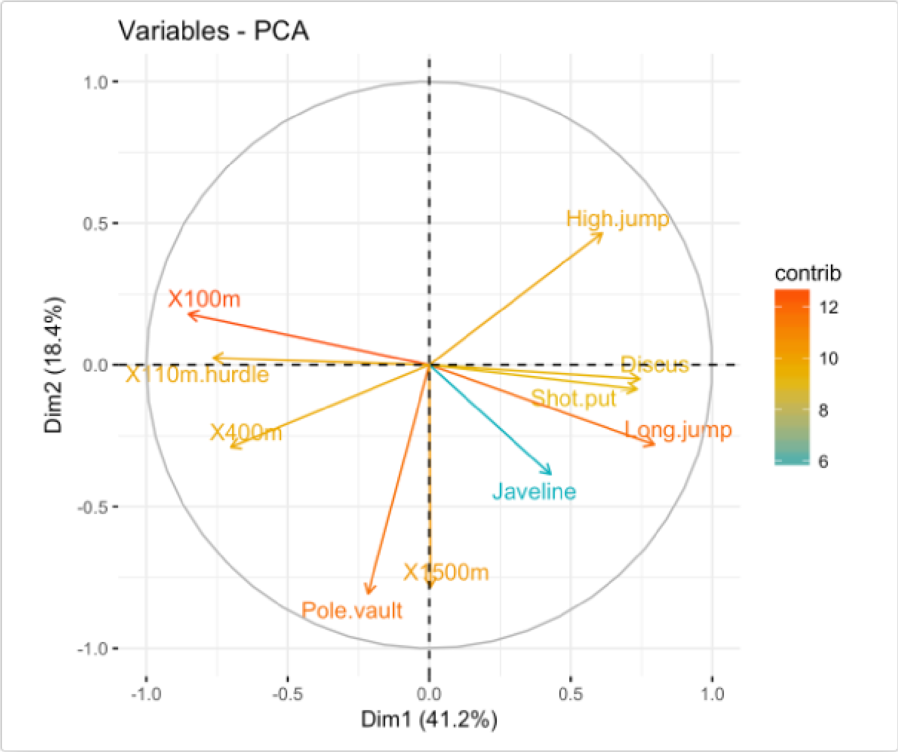

```r
# Plot PC scores
# First will center and scale PC2
data_for_plot <- scale(pca_brain$x)

# Add in diagnosis back
data_for_plot <- data.frame(data_for_plot,
                     "RiskGroup"=brain_data$RiskGroup,
                     "CandID"=brain_data$CandID)

ggplot(data = data.frame(data_for_plot),
       mapping = aes(x=PC1, y=PC2, color=RiskGroup))+
  geom_point()+
  geom_hline(yintercept=0, linetype="dashed")+
  geom_vline(xintercept=0, linetype="dashed")+
  theme_bw()
```


PC2
PC1
2
0
-2
-4
-2
0
2
4
RiskGroup
HR-ASD
HR-Neg
LR-Neg

PCA example

- Explain overall track and field athlete performance using results in many events

```
fviz_pca_var(res.pca,
             col.var = "contrib", # Color by contributions to the PC
             gradient.cols = c("#00AFBB", "#E7B800", "#FC4E07"),
             repel = TRUE     # Avoid text overlapping
             )
```



Sparse PCA

- Some predictors may not be very useful in principal components
  - *However, loadings **won't be exactly 0***
  - ***Idea**: apply penalized regression idea to PCA*
  - *Called sparse PCA*

First principal component: $\mathbf{Z}_1 = \phi_{11}\mathbf{X}_1 + \phi_{21}\mathbf{X}_2 + ... + \phi_{p1}\mathbf{X}_p$

PC loading vector: $\boldsymbol{\phi}_1 = \{\phi_{11}, \phi_{21}, ..., \phi_{p1}\}^T$, $\sum_{j=1}^{p} \phi_{j1}^2 = 1$

$\hat{\boldsymbol{\phi}}_1 = \underset{||\boldsymbol{\phi}_1||=1, ||\boldsymbol{\phi}_1||_0 \leq k}{\text{argmax}} \{\boldsymbol{\phi}_1^T \mathbf{X}^T \mathbf{X} \boldsymbol{\phi}_1\}$ maximizes the variance of $\mathbf{Z}_1$.

If $k = p$, this reduces to ordinary PCA.

Sparse PCA in R

```
# Run sparse PCA on brain variables
spca_data <- brain_data %>%
                      select(LeftAmygdala_V12, RightAmygdala_V12,
                             PreCG_L_V12:Uncinate_R_V12) %>% as.data.frame()

sparsepca_brain <- spca(x=spca_data,
                    K=4,
                    para = rep(1, dim(spca_data)[2]),
                    sparse="penalty",
                    use.corr=TRUE)

# Look at loadings
apply(X=sparsepca_brain$loadings, MARGIN=2, function(x){sum(x==0)})
```

```
## PC1 PC2 PC3 PC4
##   1   2  10   6
```

Principal Components Regression

- Regression Model: Y=outcome, $Z_1, \ldots, Z_M$=predictors
  - Y *not used in creation of predictors, thus unsupervised*
  - $\rightarrow$ *PCs may best explain predictors but may* ***not*** *be best set at also* ***predicting response***
- Solution: *partial least squares* (PLS)

Partial Least Squares

- **Goal**: Find set of $Z_1, \ldots, Z_M$ that best summarizes $X_1, \ldots, X_p$ **and** their relationship to outcome Y
- Method:
  1. *Standardize p predictors*
  2. *For first component Z_1 :*
     - Set each ϕ_{1j} from PCA equal to β from regression of Y onto X_j
     - Results in $Z_1 = \sum_{j=1}^{p} \phi_{1j} X_j$
     - Then compute residuals of regressing Y onto Z_1
  3. *Repeat for desired number of components*
- Fit in R: `pls` package