SDSC 3006 L02
Class 9. SVM and PCA

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Outline

- **Support Vector Machine**
- **Principal Components Analysis**
- **Principal Components Regression**

Support Vector Machine

Implementation

Notice:

1. SVM is an extension of the support vector classifier, using different kernels(non-linear).

2. Use the e1071 library to demonstrate the SVM on a two-dimensional example.

```
library(e1071)
##Generate data with nonlinear boundary
set.seed(1)
x=matrix(rnorm(200*2),ncol=2)
x[1:100,]=x[1:100,]+2
x[101:150,]=x[101:150,]-2
y=c(rep(1,150),rep(2,50))
dat=data.frame(x=x,y=as.factor(y))
plot(x,col=(3-y))
```

Implementation

##Use SVM with a radial kernel

```
train=sample(200,100)
svmfit=svm(y~.,data=dat[train,],kernel="radial",gamma=1,cost=1)
##"cost" is similar to tuning parameter C, but with opposite
##effects: small "cost", wide margin; large "cost", narrow margin

plot(svmfit,dat[train,])
summary(svmfit)
```

Implementation

```
##Select best values for "gamma" and "cost" by CV
tune.out=tune(svm,y~.,data=dat[train,],kernel="radial",ranges
=list(cost=c(0.1,1,10,100,1000),gamma=c(0.5,1,2,3,4)))
summary(tune.out)


##Use SVM with a polynomial kernel
svmfit=svm(y~.,data=dat[train,],kernel="polynomial" ,
degree=2,ranges=list(cost=c(0.001,0.01,0.1,1,5,10,100)))
plot(svmfit,dat[train,])
```

Principal Components Analysis

Details

- Objective:

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

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

- Notice: The principal components are the eigenvectors of a covariance matrix, and hence they are orthogonal. Importantly, the dataset on which PCA technique is to be used must be scaled. The results are also sensitive to the relative scaling.

Details

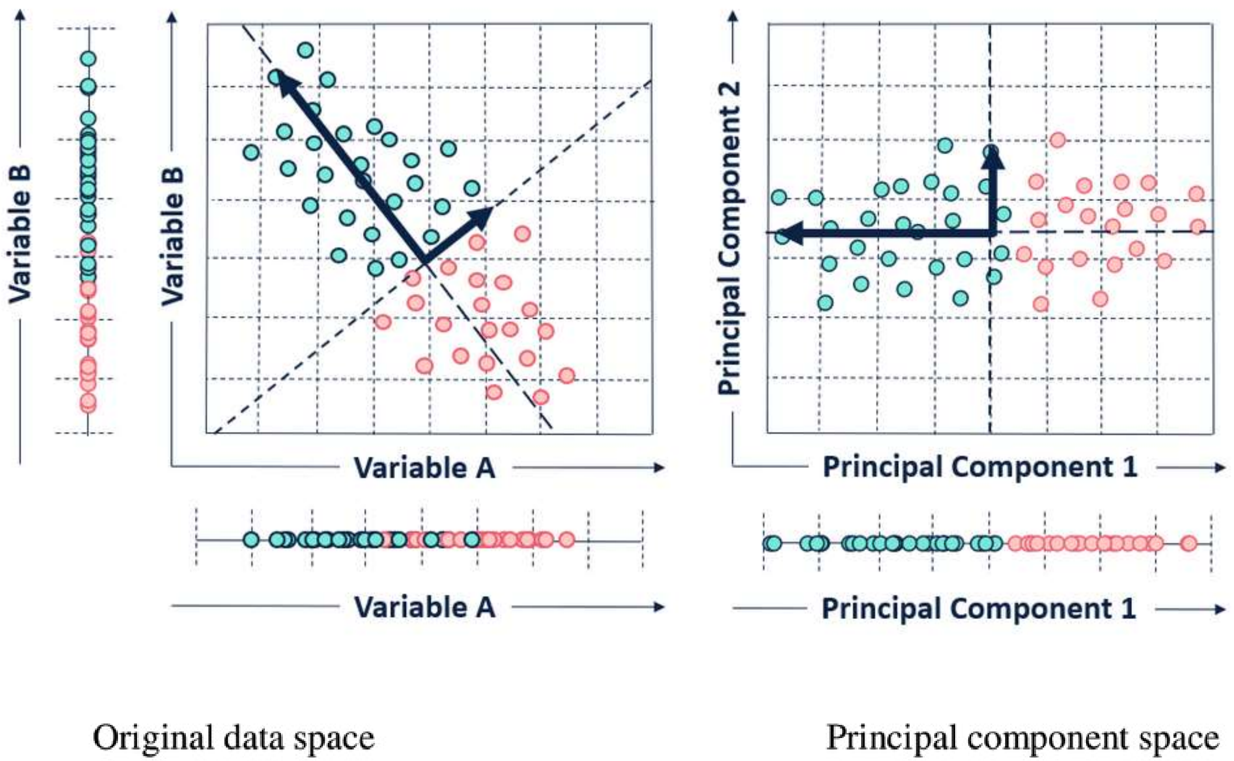
- The solution of PCA also could treat as:

$$Au = \lambda u$$

- Where $A \in R^{p*p}$, it is the covariance matrix of dataset X. $u\ and\ \lambda$ are eigen vector and eigen value respectively.
- It can easily show that eigen vectors are orthogonal with each other.

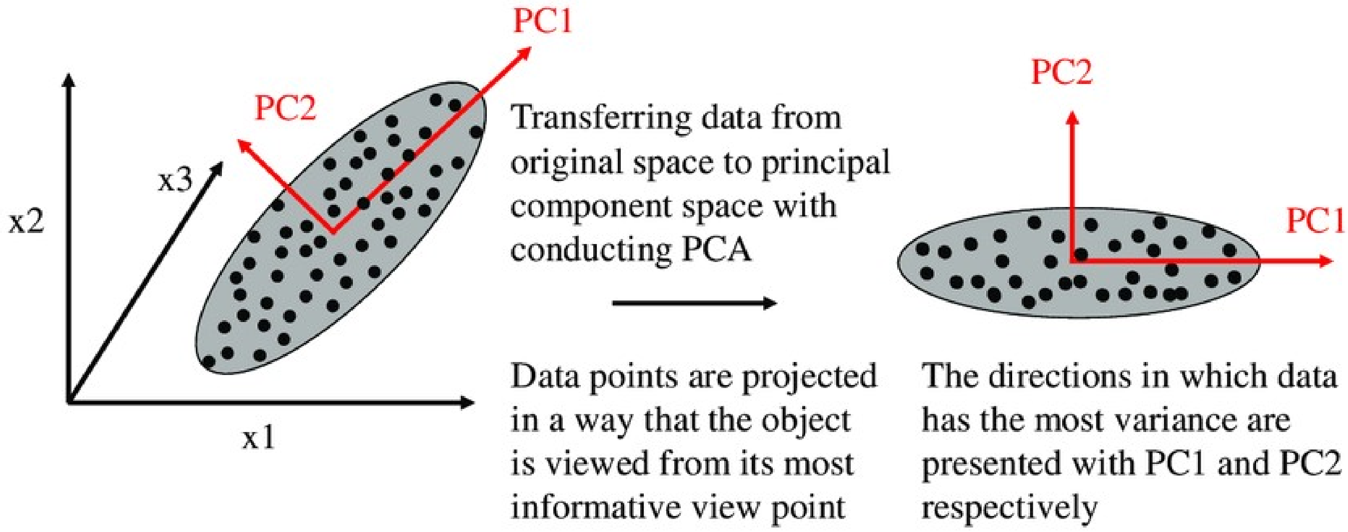
Examples

Example 1:
2D case:



PC1 will finc
make all poi
variance. In
points vary
direction.

Example 2:
3D case:



Implementation

Notice:

1. We perform PCA on the USArrests data set, which is part of the base R package.

2. Using the prcomp() function, which is one of several functions in R that perform PCA.

3. By default, the prcomp() function centers the variables to have mean zero. ‘Option scale = TRUE’ scale the variables to have sd 1.

Implementation

```
names (USArrests)
pr.out = prcomp (USArrests , scale = TRUE)
names (pr.out)
##rotation: principal component loadings
pr.out$rotation
biplot (pr.out , scale = 0)
##sdev: standard deviation of principal components
pr.out$sdev
pr.var = pr.out$sdev^2
```

Implementation

```
##compute the proportion of variance explained by each principal component
pve = pr.var / sum (pr.var)
par (mfrow = c(1, 2))
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")
```

Principal Components Regression

Details

- The principal components regression (PCR) approach involves constructing the first M principal components, $Z_1, \ldots, Z_M$, and then using these components as the predictors in a linear regression model that is fit using least squares.

Details

- If the assumption underlying PCR holds, then fitting a least squares model to $Z_1, \ldots, Z_M$ will lead to better results than fitting a least squares model to $X_1, \ldots, X_p$, since most or all of the information in the data that relates to the response is contained in $Z_1, \ldots, Z_M$, and by estimating only $M \ll p$ coefficients we can mitigate overfitting.

Implementation

Notice:

1. PCR can be performed using pcr() fuction in pls library
2. We now apply PCR to the Hitters data, in order to predict Salary.

```
install.packages('pls’)
library(ISLR)
library(pls)
attach(Hitters)
Hitters = na.omit (Hitters) ##remove rows with missing values
set.seed (2)
pcr.fit = pcr(Salary ~ ., data = Hitters , scale = TRUE, validation = "CV")
 ##10-fold cross-validation
summary (pcr.fit)
##plot the CV scores
validationplot(pcr.fit , val.type = "MSEP")
```

Implementation

```
##create training set and test set
x=model.matrix(Salary~.,Hitters)[,-1]
y=Hitters$Salary
train=sample(1:nrow(x), nrow(x)/2)
test=(-train)
y.test=y[test]
##perform PCR on training set
set.seed(1)
pcr.fit = pcr(Salary ~ ., data = Hitters , subset = train , scale = TRUE , validation = "CV")
validationplot (pcr.fit , val.type = "MSEP")  ##find the best M
##compute test MSE
pcr.pred = predict(pcr.fit , x[test , ], ncomp = 5)
mean ((pcr.pred - y.test)^2)   ##compare with shrinkage method?
##perform PCR on full data
pcr.fit = pcr (y ~ x, scale = TRUE , ncomp = 5)
```