Lecture 15: Dimensionality reduction

Reading: Sections 6.3, 6.4

STATS 202: Data mining and analysis

Jonathan Taylor, 10/29 Slide credits: Sergio Bacallado

Shrinkage methods

Ridge regression:

$$\min_{\beta} \ \mathsf{RSS}(\beta) + \lambda \sum_{j=1}^{p} \beta_j^2$$

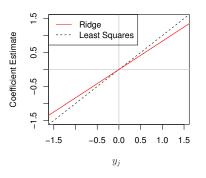
The Lasso:

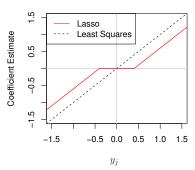
$$\min_{\beta} \ \mathsf{RSS}(\beta) + \lambda \sum_{j=1}^p |\beta_j|$$

As we increase λ we increase bias, but reduce variance.

Lasso and Ridge coefficients as a function of λ

Special case $\mathbf{X} = I$. Each coefficient $\hat{\beta}_j^R$, $\hat{\beta}_j^L$ depends only on y_j .

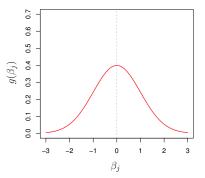


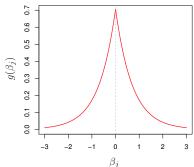


Bayesian interpretations

Ridge: $\hat{\beta}^R$ is the posterior mean, with a Normal prior on β .

Lasso: $\hat{\beta}^L$ is the posterior mode, with a Laplace prior on β .





Regularization methods

- Variable selection:
 - ▶ Best subset selection
 - Forward and backward stepwise selection

Regularization methods

- Variable selection:
 - ▶ Best subset selection
 - Forward and backward stepwise selection
- Shrinkage
 - Ridge regression
 - ► The Lasso (a form of variable selection)

Regularization methods

- Variable selection:
 - Best subset selection
 - Forward and backward stepwise selection
- Shrinkage
 - Ridge regression
 - ► The Lasso (a form of variable selection)
- Dimensionality reduction:
 - ▶ **Idea:** Define a small set of *M* predictors which *summarize* the information in all *p* predictors.

Recall: The loadings $\phi_{11}, \dots, \phi_{p1}$ for the first principal component define the directions of greatest variance in the space of variables.

Recall: The loadings $\phi_{11}, \dots, \phi_{p1}$ for the first principal component define the directions of greatest variance in the space of variables.

Example. USArrests dataset.

	UrbanPop			
Loading	$\phi_{11} = 0.28$	$\phi_{21} = 0.54$	$\phi_{31} = 0.59$	$\phi_{41} = 0.54$

Recall: The loadings $\phi_{11}, \dots, \phi_{p1}$ for the first principal component define the directions of greatest variance in the space of variables.

Example. USArrests dataset.

Variable	UrbanPop	Murder	Assault	Rape
Loading	$\phi_{11} = 0.28$	$\phi_{21} = 0.54$	$\phi_{31} = 0.59$	$\phi_{41} = 0.54$

Interpretation: The first principal component measures the overall rate of crime.

Recall: The scores z_{11}, \ldots, z_{n1} for the first principal component define the deviation of the samples along this direction.

$$z_{i1} = \sum_{j=1}^{p} \phi_{j1} x_{ij}$$

Recall: The scores z_{11}, \ldots, z_{n1} for the first principal component define the deviation of the samples along this direction.

$$z_{i1} = \sum_{j=1}^{p} \phi_{j1} x_{ij}$$

Example. USArrests dataset.

Sample	Alabama	Alaska	 Wyoming
Score	$z_{11} = 172$	$z_{21} = 196$	 $z_{n1} = 122$

Recall: The scores z_{11}, \ldots, z_{n1} for the first principal component define the deviation of the samples along this direction.

$$z_{i1} = \sum_{j=1}^{p} \phi_{j1} x_{ij}$$

Example. USArrests dataset.

Sample	Alabama	Alaska	 Wyoming
Score	$z_{11} = 172$	$z_{21} = 196$	 $z_{n1} = 122$

Interpretation: The scores for the first principal component measure the overall rate of crime in each state.

Idea:

▶ Replace the original predictors, X_1, X_2, \ldots, X_p , with the first M score vectors Z_1, Z_2, \ldots, Z_M .

Idea:

- ▶ Replace the original predictors, $X_1, X_2, ..., X_p$, with the first M score vectors $Z_1, Z_2, ..., Z_M$.
- Perform least squares regression, to obtain coefficients $\theta_0, \theta_1, \dots, \theta_M$.

Idea:

- ▶ Replace the original predictors, $X_1, X_2, ..., X_p$, with the first M score vectors $Z_1, Z_2, ..., Z_M$.
- Perform least squares regression, to obtain coefficients $\theta_0, \theta_1, \dots, \theta_M$.

The model is:

$$y_i = \theta_0 + \theta_1 z_{i1} + \theta_2 z_{i2} + \dots + \theta_M z_{iM}$$

Idea:

- ▶ Replace the original predictors, $X_1, X_2, ..., X_p$, with the first M score vectors $Z_1, Z_2, ..., Z_M$.
- Perform least squares regression, to obtain coefficients $\theta_0, \theta_1, \dots, \theta_M$.

The model is:

$$y_{i} = \theta_{0} + \theta_{1}z_{i1} + \theta_{2}z_{i2} + \dots + \theta_{M}z_{iM}$$

$$= \theta_{0} + \theta_{1}\sum_{j=1}^{p} \phi_{j1}x_{ij} + \theta_{2}\sum_{j=1}^{p} \phi_{j2}x_{ij} + \dots + \theta_{M}\sum_{j=1}^{p} \phi_{jM}x_{ij}$$

Idea:

- ▶ Replace the original predictors, $X_1, X_2, ..., X_p$, with the first M score vectors $Z_1, Z_2, ..., Z_M$.
- Perform least squares regression, to obtain coefficients $\theta_0, \theta_1, \dots, \theta_M$.

The model is:

$$y_{i} = \theta_{0} + \theta_{1}z_{i1} + \theta_{2}z_{i2} + \dots + \theta_{M}z_{iM}$$

$$= \theta_{0} + \theta_{1}\sum_{j=1}^{p} \phi_{j1}x_{ij} + \theta_{2}\sum_{j=1}^{p} \phi_{j2}x_{ij} + \dots + \theta_{M}\sum_{j=1}^{p} \phi_{jM}x_{ij}$$

$$= \theta_{0} + \left[\sum_{m=1}^{M} \theta_{m}\phi_{1m}\right]x_{i1} + \dots + \left[\sum_{m=1}^{M} \theta_{m}\phi_{pm}\right]x_{ip}$$

Idea:

- ▶ Replace the original predictors, $X_1, X_2, ..., X_p$, with the first M score vectors $Z_1, Z_2, ..., Z_M$.
- Perform least squares regression, to obtain coefficients $\theta_0, \theta_1, \dots, \theta_M$.

Equivalent to a linear regression onto X_1, \ldots, X_p , with coefficients:

$$\beta_j = \sum_{m=1}^M \theta_m \phi_{jm}$$

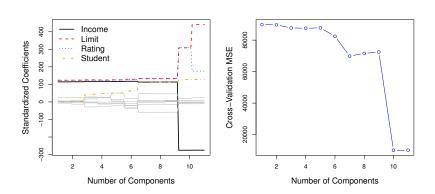
Idea:

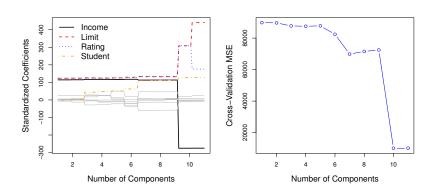
- ▶ Replace the original predictors, X_1, X_2, \ldots, X_p , with the first M score vectors Z_1, Z_2, \ldots, Z_M .
- Perform least squares regression, to obtain coefficients $\theta_0, \theta_1, \dots, \theta_M$.

Equivalent to a linear regression onto X_1, \ldots, X_p , with coefficients:

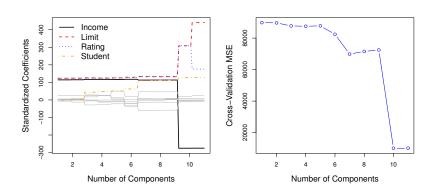
$$\beta_j = \sum_{m=1}^M \theta_m \phi_{jm}$$

This constraint in the form of β_j introduces *bias*, but it can lower the *variance* of the model.

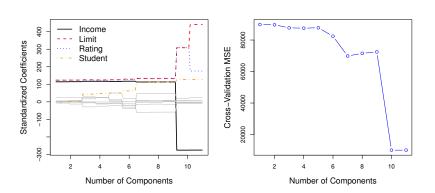




► A model with 11 components is equivalent to least-squares regression



- ► A model with 11 components is equivalent to least-squares regression
- ▶ Best error is achieved with 10 components (almost no dimensionality reduction)



The left panel shows the coefficients β_j estimated for each M. The coefficients shrink as we decrease M!

Least squares regression: want to minimize

$$RSS = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta)$$

Least squares regression: want to minimize

$$RSS = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta)$$

$$\frac{\partial RSS}{\partial \beta} = -2\mathbf{X}^T(y - \mathbf{X}\beta) = 0$$

Least squares regression: want to minimize

$$RSS = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta)$$

$$\frac{\partial RSS}{\partial \beta} = -2\mathbf{X}^T(y - \mathbf{X}\beta) = 0$$

$$\implies \hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T y$$

Least squares regression: want to minimize

$$RSS = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta)$$

$$\frac{\partial RSS}{\partial \beta} = -2\mathbf{X}^T(y - \mathbf{X}\beta) = 0$$

$$\implies \hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T y$$

Solve the singular value decomposition: $\mathbf{X} = UD^{1/2}V^T$, where $D^{1/2} = \mathrm{diag}(\sqrt{d_1},\dots,\sqrt{d_p})$; then

$$(\mathbf{X}^T \mathbf{X})^{-1} = V D^{-1} V^T$$

where $D^{-1} = diag(1/d_1, 1/d_2, \dots, 1/d_p)$.

Ridge regression: want to minimize

$$RSS + \lambda \|\beta\|_2^2 = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta) + \lambda \beta^T \beta$$

Ridge regression: want to minimize

$$RSS + \lambda \|\beta\|_2^2 = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta) + \lambda \beta^T \beta$$

$$\frac{\partial (RSS + \lambda \|\beta\|_2^2)}{\partial \beta} = -2\mathbf{X}^T(y - \mathbf{X}\beta) + 2\lambda\beta = 0$$

Ridge regression: want to minimize

$$RSS + \lambda \|\beta\|_{2}^{2} = (y - \mathbf{X}\beta)^{T}(y - \mathbf{X}\beta) + \lambda \beta^{T}\beta$$
$$\frac{\partial (RSS + \lambda \|\beta\|_{2}^{2})}{\partial \beta} = -2\mathbf{X}^{T}(y - \mathbf{X}\beta) + 2\lambda\beta = 0$$
$$\implies \hat{\beta}_{\lambda}^{R} = (\mathbf{X}^{T}\mathbf{X} + \lambda I)^{-1}\mathbf{X}^{T}y$$

Ridge regression: want to minimize

$$RSS + \lambda \|\beta\|_2^2 = (y - \mathbf{X}\beta)^T (y - \mathbf{X}\beta) + \lambda \beta^T \beta$$

$$\frac{\partial (RSS + \lambda \|\beta\|_2^2)}{\partial \beta} = -2\mathbf{X}^T(y - \mathbf{X}\beta) + 2\lambda\beta = 0$$

$$\implies \hat{\beta}_{\lambda}^{R} = (\mathbf{X}^{T}\mathbf{X} + \lambda I)^{-1}\mathbf{X}^{T}y$$

Solve the singular value decomposition: $\mathbf{X} = UD^{1/2}V^T$, where $D^{1/2} = \mathrm{diag}(\sqrt{d_1},\dots,\sqrt{d_p})$; then

$$(\mathbf{X}^T\mathbf{X} + \lambda I)^{-1} = VD_{\lambda}^{-1}V^T$$

where $D_{\lambda}^{-1} = \text{diag}(1/(d_1 + \lambda), 1/(d_2 + \lambda), \dots, 1/(d_p + \lambda)).$

Predictions of least squares regression:

$$\hat{y} = \mathbf{X}\hat{\beta} = \sum_{j=1}^p u_j u_j^T y, \qquad u_j \text{ is the } j \text{th column of } U$$

Predictions of least squares regression:

$$\hat{y} = \mathbf{X}\hat{\beta} = \sum_{j=1}^{p} u_j u_j^T y, \qquad u_j \text{ is the } j \text{th column of } U$$

Predictions of Ridge regression:

$$\hat{y} = \mathbf{X}\hat{\beta}_{\lambda}^{R} = \sum_{j=1}^{p} u_{j} \frac{d_{j}}{d_{j} + \lambda} u_{j}^{T} y$$

The projection of y onto a principal component is shrunk toward zero. The smaller the principal component, the larger the shrinkage.

Predictions of least squares regression:

$$\hat{y} = \mathbf{X}\hat{\beta} = \sum_{j=1}^{p} u_j u_j^T y, \qquad u_j \text{ is the } j \text{th column of } U$$

Predictions of Ridge regression:

$$\hat{y} = \mathbf{X}\hat{\beta}_{\lambda}^{R} = \sum_{j=1}^{p} u_{j} \frac{d_{j}}{d_{j} + \lambda} u_{j}^{T} y$$

The projection of y onto a principal component is shrunk toward zero. The smaller the principal component, the larger the shrinkage.

Predictions of PCR:

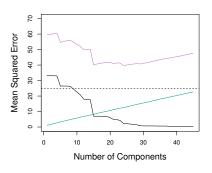
$$\hat{y} = \mathbf{X}\hat{\beta}^{\mathsf{PC}} = \sum_{j=1}^{p} u_j \mathbf{1}(j \le M) u_j^T y$$

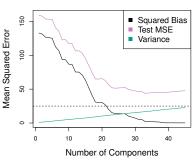
The projections onto small principal components are shrunk to zero.

Simulated example

In each case n = 50, p = 45.

- ▶ Left: Response is a function of all the predictors.
- ▶ Right: Response is a function of 2 predictors (good for Lasso).

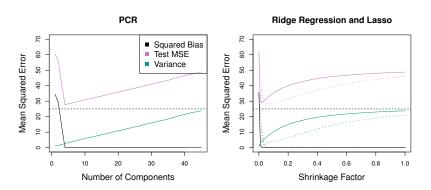




Simulated example

Again, n = 50, p = 45.

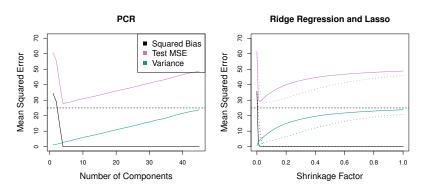
The response is a function of the first 5 principal components.



Simulated example

Again, n = 50, p = 45.

The response is a function of the first 5 principal components.



▶ Principal components regression derives $Z_1, ..., Z_M$ using only the predictors $X_1, ..., X_p$.

- ▶ Principal components regression derives $Z_1, ..., Z_M$ using *only* the predictors $X_1, ..., X_p$.
- \blacktriangleright In partial least squares, we will use the response Y as well.

- ▶ Principal components regression derives $Z_1, ..., Z_M$ using *only* the predictors $X_1, ..., X_p$.
- ▶ In partial least squares, we will use the response Y as well.

Algorithm:

1. Define $Z_1 = \sum_{j=1}^p \phi_{j1} X_j$, where ϕ_{j1} is the coefficient of a simple linear regression of Y onto X_j .

- ▶ Principal components regression derives $Z_1, ..., Z_M$ using *only* the predictors $X_1, ..., X_p$.
- ▶ In partial least squares, we will use the response Y as well.

- 1. Define $Z_1 = \sum_{j=1}^p \phi_{j1} X_j$, where ϕ_{j1} is the coefficient of a simple linear regression of Y onto X_j .
- 2. Let $X_j^{(2)}$ be the residual of regressing X_j onto Z_1 .

- ▶ Principal components regression derives $Z_1, ..., Z_M$ using only the predictors $X_1, ..., X_p$.
- ▶ In partial least squares, we will use the response Y as well.

- 1. Define $Z_1 = \sum_{j=1}^p \phi_{j1} X_j$, where ϕ_{j1} is the coefficient of a simple linear regression of Y onto X_j .
- 2. Let $X_j^{(2)}$ be the residual of regressing X_j onto Z_1 .
- 3. Define $Z_2 = \sum_{j=1}^p \phi_{j2} X_j^{(2)}$, where ϕ_{j2} is the coefficient of a simple linear regression of Y onto $X_j^{(2)}$.

- ▶ Principal components regression derives $Z_1, ..., Z_M$ using *only* the predictors $X_1, ..., X_p$.
- ▶ In partial least squares, we will use the response Y as well.

- 1. Define $Z_1 = \sum_{j=1}^p \phi_{j1} X_j$, where ϕ_{j1} is the coefficient of a simple linear regression of Y onto X_j .
- 2. Let $X_j^{(2)}$ be the residual of regressing X_j onto Z_1 .
- 3. Define $Z_2 = \sum_{j=1}^p \phi_{j2} X_j^{(2)}$, where ϕ_{j2} is the coefficient of a simple linear regression of Y onto $X_j^{(2)}$.
- 4. Let $X_j^{(3)}$ be the residual of regressing $X_j^{(2)}$ onto Z_2 .

- ▶ Principal components regression derives $Z_1, ..., Z_M$ using only the predictors $X_1, ..., X_p$.
- ▶ In partial least squares, we will use the response Y as well.

- 1. Define $Z_1 = \sum_{j=1}^p \phi_{j1} X_j$, where ϕ_{j1} is the coefficient of a simple linear regression of Y onto X_j .
- 2. Let $X_j^{(2)}$ be the residual of regressing X_j onto Z_1 .
- 3. Define $Z_2 = \sum_{j=1}^p \phi_{j2} X_j^{(2)}$, where ϕ_{j2} is the coefficient of a simple linear regression of Y onto $X_j^{(2)}$.
- 4. Let $X_j^{(3)}$ be the residual of regressing $X_j^{(2)}$ onto Z_2 .
- 5. ...

▶ At each step, we try to find the linear combination of predictors that is highly correlated to the response (the highest correlation is the least squares fit).

- ▶ At each step, we try to find the linear combination of predictors that is highly correlated to the response (the highest correlation is the least squares fit).
- ► After each step, we transform the predictors such that they are *uncorrelated* from the linear combination chosen.

- ▶ At each step, we try to find the linear combination of predictors that is highly correlated to the response (the highest correlation is the least squares fit).
- After each step, we transform the predictors such that they are uncorrelated from the linear combination chosen.
- Compared to PCR, partial least squares has less bias and more variance (a stronger tendency to overfit).