Linear Model Selection and Regularization

- Recall the linear model

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon.$$

- In the lectures that follow, we consider some approaches for extending the linear model framework. In the lectures covering Chapter 7 of the text, we generalize the linear model in order to accommodate *non-linear*, but still *additive*, relationships.
- In the lectures covering Chapter 8 we consider even more general *non-linear* models.

In praise of linear models!

- Despite its simplicity, the linear model has distinct advantages in terms of its *interpretability* and often shows good *predictive performance*.
- Hence we discuss in this lecture some ways in which the simple linear model can be improved, by replacing ordinary least squares fitting with some alternative fitting procedures.

lternatives to least squares?

- estimating regression coefficients to minimize residual sum-of-squares (RSS)
- RSS = training MSPE estimate
- training MSPE is not a good estimate of test MSPE

ecially when $p > n$, to control the

y removing irrelevant features —
rresponding coefficient estimates
a model that is more easily
ent some approaches for
feature selection.

p = # of predictors
n = sample size

least-squares estimation aims to solve the system of equations:

y = X \beta

- what happens when p > n? under-determined system of equations. we can't solve for \beta here!
- in fact, when p is close to n, the least-squares predictor will often have very high variance (because RSS = training MSPE, overfits)
- we want to find alternative ways to estimate regression coefficients (to reduce variance)

Three classes of methods

- *Subset Selection*. We identify a subset of the p predictors that we believe to be related to the response. We then fit a model using least squares on the reduced set of variables.
- *Shrinkage*. We fit a model involving all p predictors, but the estimated coefficients are shrunken towards zero relative to the least squares estimates. This shrinkage (also known as *regularization*) has the effect of reducing variance and can also perform variable selection.
- *Dimension Reduction*. We project the p predictors into a M-dimensional subspace, where $M < p$. This is achieved by computing M different *linear combinations*, or *projections*, of the variables. Then these M projections are used as predictors to fit a linear regression model by least squares.

Subset Selection

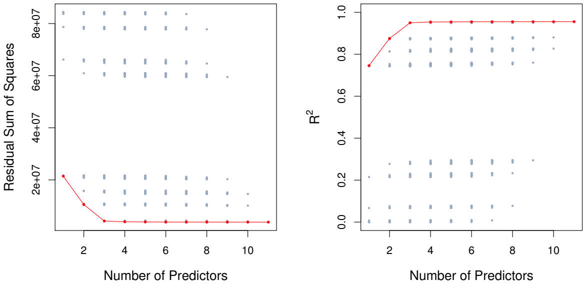
Best subset and stepwise model selection procedures

Best Subset Selection

1. Let $\mathcal{M}_0$ denote the *null model*, which contains no predictors. This model simply predicts the sample mean for each observation.
2. For $k = 1, 2, \ldots p$:
   (a) Fit all $\binom{p}{k}$ models that contain exactly k predictors.
   (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Here *best* is defined as having the smallest RSS, or equivalently largest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adj

can be interpreted as "surrogates" for the desired test MSPE criterion (which we do not have access to and thus need to estimate)

Example- Credit data set



For each possible model containing a subset of the ten predictors in the `Credit` *data set, the RSS and R^2 are displayed. The red frontier tracks the* best *model for a given number of predictors, according to RSS and R^2. Though the data set contains only ten predictors, the x-axis ranges from 1 to 11, since one of the variables is categorical and takes on three values, leading to the creation of two dummy variables*

Extensions to other models

- Although we have presented best subset selection here for least squares regression, the same ideas apply to other types of models, such as logistic regression.
- The *deviance*— negative two times the maximized log-likelihood— plays the role of RSS for a broader class of models.

there are 2^p models to compute RSS for!

Stepwise Selection

- For computational reasons, best subset selection cannot be applied with very large p. *Why not?*
- Best subset selection may also suffer from statistical problems when p is large: larger the search space, the higher the chance of finding models that look good on the training data, even though they might not have any predictive power on future data.
- Thus an enormous search space c high variance of the coefficient es

stepwise (forward & backward) selection are computational heuristics for navigating the large combinatorial model space.

- For both of these reasons, *stepwise* methods, which explore a far more restricted set of models, are attractive alternatives to best subset selection.

Forward Stepwise Selection

- Forward stepwise selection begins with a model containing no predictors, and then adds predictors to the model, one-at-a-time, until all of the predictors are in the model.
- In particular, at each step the variable that gives the greatest *additional* improvement to the fit is added to the model.

In Detail

Forward Stepwise Selection

1. Let $\mathcal{M}_0$ denote the *null* model, which contains no predictors.
2. For $k = 0, \ldots, p-1$:
   2.1 Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor.
   2.2 Choose the *best* among these $p-k$ models, and call it $\mathcal{M}_{k+1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

More on Forward Stepwise Selection

- Computational advantage over best subset selection is clear.
- It is not guaranteed to find the best possible model out of all 2^p models containing subsets of the p predictors. *Why not? Give an example.*

Credit data example

# Variables	Best subset	Forward stepwise
One	rating	rating
Two	rating, income	rating, income
Three	rating, income, student	rating, income, student
Four	cards, income student, limit	rating, income, student, limit

The first four selected models for best subset selection and forward stepwise selection on the Credit *data set. The first three models are identical but the fourth models differ.*

Backward Stepwise Selection

- Like forward stepwise selection, *backward stepwise selection* provides an efficient alternative to best subset selection.
- However, unlike forward stepwise selection, it begins with the full least squares model containing all p predictors, and then iteratively removes the least useful predictor, one-at-a-time.

Backward Stepwise Selection: details

Backward Stepwise Selection

1. Let $\mathcal{M}_p$ denote the *full* model, which contains all p predictors.
2. For $k = p, p-1, \dots, 1$:
   - 2.1 Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
   - 2.2 Choose the *best* among these k models, and call it $\mathcal{M}_{k-1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \dots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

More on Backward Stepwise Selection

- Like forward stepwise selection, the backward selection approach searches through only $1 + p(p+1)/2$ models, and so can be applied in settings where p is too large to apply best subset selection
- Like forward stepwise selection, backward stepwise selection is not guaranteed to yield the *best* model containing a subset of the p predictors.
- Backward selection requires that the *number of samples n is larger than the number of variables p* (so that the full model can be fit). In contrast, forward stepwise can be used even when $n < p$, and so is the only viable subset method when p is very large.

Choosing the Optimal Model

- The model containing all of the predictors will always have the smallest RSS and the largest R^2, since these quantities are related to the training error.
- We wish to choose a model with low test error, not a model with low training error. Recall that training error is usually a poor estimate of test error.
- Therefore, RSS and R^2 are not suitable for selecting the best model among a collection of models with different numbers of predictors.

work well for simple models
(e.g., linear regression)

g test error: two approaches

can be used for a broader
variety of nonlinear models

- We can indirectly estimate test error by making an *adjustment* to the training error to account for the bias due to overfitting.
- We can *directly* estimate the test error, using either a validation set approach or a cross-validation approach, as discussed in previous lectures.
- We illustrate both approaches next.

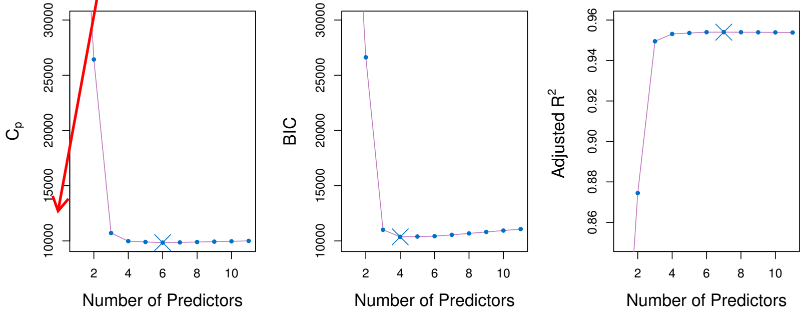
C_p, AIC, BIC, and Adjusted R^2

- These techniques adjust the training error for the model size, and can be used to select among a set of models with different numbers of variables.
- The next figure displays C_p, BIC, and adjusted R^2 for the best model of each size produced by best subset selection on the `Credit` data set.

all of these criteria provide an adjustment to training MSPE to correct for high variance (resulting from overfitting)

Credit data example

AIC / BIC curves are now U-shaped: they are better estimates of test MSE than RSS



r some deta

this penalty (adjustment) can be broken down into two parts:
- larger # of parameters d => higher model complexity
- \sigma^2: variance of the irreducible error (poll q 5.4), the variance adjustment needs to be greater when \sigma^2 is larger, because there's a greater risk of overfitting with complex models

Mallows (1973):
- smaller-the-better
- only for linear regression

$$\frac{1}{n}\left(\mathrm{RSS} + 2d\hat{\sigma}^2\right),$$

of parameters

estimate of the variance of the error h

response measurement.

Akaike information criterion (Akaike 1974):
- smaller-the-better
- equals the Cp criterion for linear regression
- can be defined for a broad class of parametric models (e.g., logistic regression)

- The *AIC* criterion is defined for a lar

  by maximum likelihood:

$$\mathrm{AIC} = -2\log L + 2\cdot d$$

  where L is the maximized value of the likelihood function for the estimated model.

- In the case of the linear model with Gaussian errors, maximum likelihood and least squares are the same thing, and C_p and AIC are equivalent. *Prove this.*

Bayesian information criterion (Schwartz 1978)

Details on BIC

BIC tends to favor less complex models

$$\mathrm{BIC} = \frac{1}{n}\left(\mathrm{RSS} + \log(n) d\hat{\sigma}^2\right).$$

- Like C_p, the BIC will tend to take on a small value for a model with a low test error, and so generally we select the model that has the lowest BIC value.
- Notice that BIC replaces the $2d\hat{\sigma}^2$ used by C_p with a $\log(n)d\hat{\sigma}^2$ term, where n is the number of observations.
- Since $\log n > 2$ for any $n > 7$, the BIC statistic generally places a heavier penalty on models with many variables, and hence results in the selection of smaller models than C_p. See Figure on slide 19.

Adjusted R^2

larger-the-better

- For a least squares model with d variables, the adjusted R^2 statistic is calculated as

$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}.$$

  where TSS is the total sum of squares.
- Unlike C_p, AIC, and BIC, for which a *small* value indicates a model with a low test error, a *large* value of adjusted R^2 indicates a model with a small test error.
- Maximizing the adjusted R^2 is equivalent to minimizing $\frac{\text{RSS}}{n-d-1}$. While RSS always decreases as the number of variables in the model increases, $\frac{\text{RSS}}{n-d-1}$ may increase or decrease, due to the presence of d in the denominator.
- Unlike the R^2 statistic, the adjusted R^2 statistic *pays a price* for the inclusion of unnecessary variables in the model. See Figure on slide 19.

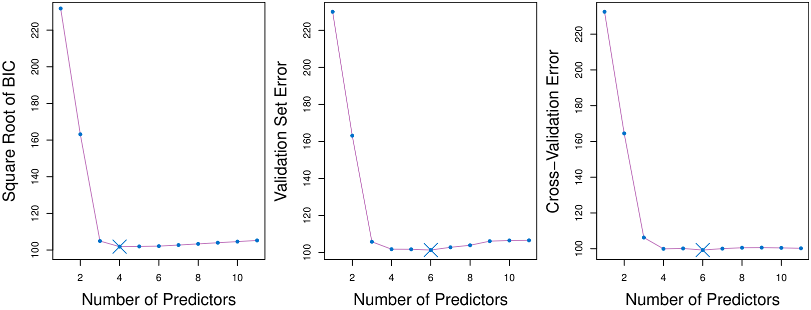
Validation and Cross-Validation

- Each of the procedures returns a sequence of models $\mathcal{M}_k$ indexed by model size $k = 0, 1, 2, \ldots$. Our job here is to select $\hat{k}$. Once selected, we will return model $\mathcal{M}_{\hat{k}}$

Validation and Cross-Validation

- Each of the procedures returns a sequence of models $\mathcal{M}_k$ indexed by model size $k = 0, 1, 2, \ldots$. Our job here is to select $\hat{k}$. Once selected, we will return model $\mathcal{M}_{\hat{k}}$
- We compute the validation set error or the cross-validation error for each model $\mathcal{M}_k$ under consideration, and then select the k for which the resulting estimated test error is smallest.
- This procedure has an advantage relative to AIC, BIC, C_p, and adjusted R^2, in that it provides a direct estimate of the test error, and *doesn't require an estimate of the error variance σ^2*.
- It can also be used in a wider range of model selection tasks, even in cases where it is hard to pinpoint the model degrees of freedom (e.g. the number of predictors in the model) or hard to estimate the error variance σ^2.

Credit data example



Advantages (adjustment-based approaches: Cp/AIC/BIC/aR^2):
- closed-form criterion: can be computed efficiently
- interpretable adjustment factor on training error

Advantages (K-fold CV):
- direct estimate of test error (instead of an approximation)
- no need to estimate irreducible noise variance \sigma^2
- generalizable to non-parametric (more complex) models

Details of Previous Figure

- The validation errors were calculated by randomly selecting three-quarters of the observations as the training set, and the remainder as the valid
- The cross-validation errors folds. In this case, the vali methods both result in a s
- However, all three approac and six-variable models ar their test errors.
- In this setting, we can select a model using the *one-standard-error rule*. We first calculate the standard error of the estimated test MSE for each model size, and then select the smallest model for which the estimated test error is within one standard error of the lowest point on the curve. *What is the rationale for this?*

complexity after K-fold CV estimate:
- min.cv: just take the model with lowest MSPE estimate
- 1se: take the smallest model for which (see below)
- 1se would always pick smaller (or equal sized) models

Implemented in many R packages (cv.glmnet$1se , cv.glmnet$min.cv)

Shrinkage M

many ways to varying model complexity:
- variable selection: change # of features considered
- nonlinear modeling: change the order of polynomials used
- shrinkage: shrinking our least-squares estimate to zero

Which trade-off is "best"? depends on the problem objectives, domain knowledge, and empirically trying out different trade-offs

Ridge regression and *Lasso*

- The subset selection methods us
linear model that contains a sub
- As an alternative, we can fit a model containing all p
predictors using a techn
the coefficient estimates
coefficient estimates tow
- It may not be immediat
should improve the fit, b
coefficient estimates can

James-Stein estimators:
- Suppose we observe data vectors X1, ... , Xn following N(\mu,I). We wish to use this to estimate the mean vector \mu.
- An intuitive estimator is the sample mean vector \bar{X}, which is unbiased for \mu
- But it turns out that a new shrunken estimator \alpha \bar{X} (for a carefully chosen \alpha) has lower MSE than the sample mean. This shows that by trading off a little bias, we can get much reduction in variance here.
- Similar phenomenon occurs for estimating \beta in linear regression:
    - least-squares estimate is unbiased, but can have high variance (when n ~ p, or multicollinearity, etc)

Ridge regression

- Recall that the least squares ... nates $\beta_0,$

high variance, but unbiased

\lambda = 0 (least-squares, unshrunken):
- high variance
- unbiased (zero bias)

\lambda large (fully shrunk, very close to 0):
- low variance
- high bias

This is a bias-varian

We will choose the c ... via using

shrinkage penalty:
- larger \beta makes the criterion larger
- since we're minimizing the objective function, ridge regression discourages larger \beta's (shrinkage)
- \lambda: penalty parameter (tuning parameter)

- In ... are

$$\sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2=\mathrm{RSS}+\lambda\sum_{j=1}^{p}\beta_j^2,$$

where $\lambda \geq 0$ is a *tuning parameter*, ... separately.

note: intercept \beta_0 is not shrunken, since it just measures the mean response

Ridge regression: continued

\lambda = 0 (least-squares, unshrunken):
- high variance
- unbiased (zero bias)

\lambda large (fully shrunk, very close to 0):
- low variance
- high bias

This is a bias-variance trade-off!

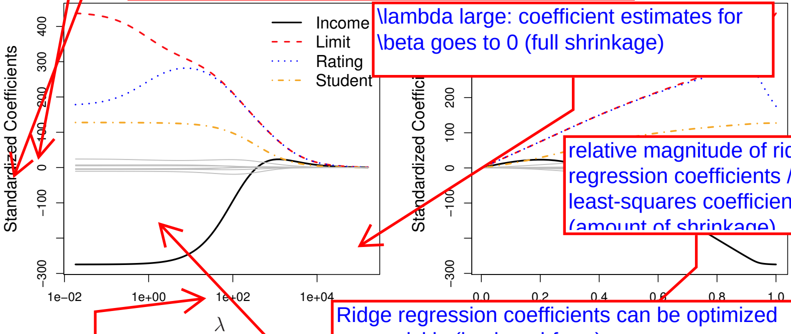
We will choose the optimal \lambda for estimation / prediction via using

- As
  esti
- How
  pen t
  has .
- The
  imp
  estimates.
- Selecting a good value for λ is critical; cross-validation is used for this.

Credit data example

solution path

\lambda close to 0 => least-squares solution (no shrinkage)



\lambda large: coefficient estimates for \beta goes to 0 (full shrinkage)

relative magnitude of ridge regression coefficients / least-squares coefficients (amount of shrinkage)

we can show that the ridge regression coefficient estimates, while shrunken, will never equal 0 exactly (HW3 Q1)

Ridge regression coefficients can be optimized very quickly (in closed-form):
- computational work it takes to compute the least-squares solution = computational work for computing the ridge regression estimator over all \lambdas

Details of Previous Figure

- In the left-hand panel, each curve corresponds to the ridge regression coefficient estimate for one of the ten variables, plotted as a function of λ.
- The right-hand panel displays the same ridge coefficient estimates as the left-hand panel, but instead of displaying λ on the x-axis, we now display $\|\hat{\beta}^R_\lambda\|_2 / \|\hat{\beta}\|_2$, where $\hat{\beta}$ denotes the vector of least squares coefficient estimates.
- The notation $\|\beta\|_2$ denotes the ℓ_2 norm (pronounced "ell 2") of a vector, and is defined as $\|\beta\|_2 = \sqrt{\sum_{j=1}^{p} {\beta_j}^2}$.

Euclidean norm

Ridge regression: scaling of predictors

e.g., if we measure income in $ instead of $1000, then estimated \beta from the linear regression will be increased by 1000x

- Th t estimates are *scale equ*: multiplying X_j by a constant c simply leads to a scaling of the least squares coefficient estimates by a factor of $1/c$. In other words, regardless of how the jth predictor is scaled, $X_j\hat{\beta}_j$ will remain the same.

ridge regression penalty treats all variables on the same scale

- In contrast, the ridge regression coefficient estimates can chang multiplying a given predictor by a cons of squared the penalty part of the ridge regressio

scaling (dividing) each predictor by its standard deviation:
- standardized predictors will all have sd=1
- treat all predictors " equally"

- Therefore, it is best to apply ridge regr *standardizing the predictors*, using the

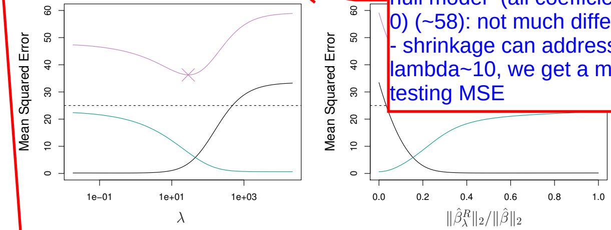
$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \overline{x}_j)^2}}$$

Why Does Ridge Regression Improve Over Least Squares?

all predictors are "active": true regression coefficients are nonzero

e tradeoff

- \lambda = 0 (least squares), \lambda large (full shrinkage, \beta close to 0)
- note: test error for least squares (~48) is almost as high as test error for the " null model" (all coefficients are close to 0) (~58): not much difference!
- shrinkage can address this issue: \ lambda~10, we get a much lower testing MSE



Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients. Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of λ and $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$. The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.

The Lasso

- antage:
  ect models
  e regression

recall prediction vs interpretation:
- Ridge regression can yield good predictive models but they are not very interpretable (\beta's can never be 0 for any \lambda)
- Lasso aims to get the best of both worlds: it performs shrinkage while also providing variable selection

- The *Lasso* is a relatively recent alternative to ridge
  sso

shrinkage penalty:
- large \beta's make the penalty larger
- since we are minimizing the objective, lasso discourages large \beta's (shrinkage)

key difference with ridge regression is how we measure the size of the \beta:
- ridge regression: l2-norm
- lasso: l1-norm (Manhattan distance)

$$\sum_{j=1}^{p} |\beta_j|.$$

- In statistical parlance, the lasso uses an ℓ_1 (pronounced "ell 1") penalty instead of an ℓ_2 penalty. The ℓ_1 norm of a coefficient vector β is given by $\|\beta\|_1 = \sum |\beta_j|$.

The Lasso: continued

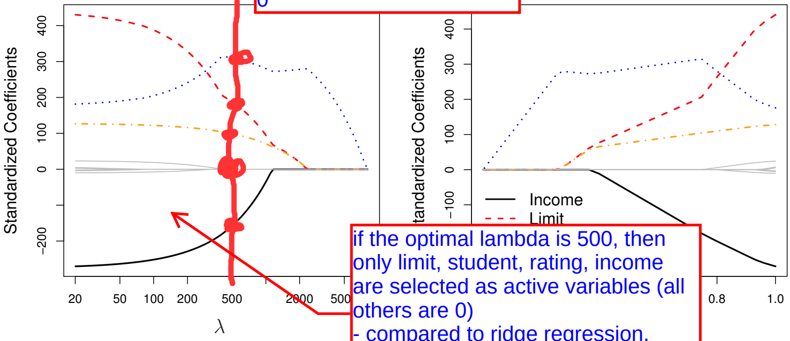
- Lasso can select active predictors (those with nonzero coefficient) and inert predictors (those with coefficients 0)
- Lasso can perform variable selection, but ridge cannot

- o shrinks the coefficient estimates towards zero.
- However, in the case of the lasso, the ℓ_1 effect of forcing some of the coefficient e exactly equal to zero when the tuning parameter λ is sufficiently large.

from a thresholding perspective:
- ridge regression: proportional shrinkage
- lasso regression: soft thresholding

- Hence, much like best subset selection, the lasso performs *variable selection*.
- We say that the lasso yields *sparse* models — that is, models that involve only a subset of the variables.
- As in ridge regression, selecting a good value of λ for the lasso is critical; cross-validation is again the method of choice.

Example: Credit dataset



\lambda very small: least squares
- \lambda very large: all coefficients become exactly 0

if the optimal lambda is 500, then only limit, student, rating, income are selected as active variables (all others are 0)
- compared to ridge regression, Lasso can perform both shrinkage and variable selection

The Variable Selection Property of the Lasso

Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?

The Variable Selection Property of the Lasso

rearrange the penalty as a constraint in the optimization problem (lagrange multiplier, optimization duality)
- \lambda larger: smaller s
- \lambda smaller: larger s

lasso, unlike ridge regression, results in
s that are exactly equal to zero?

the lasso and ridge regression coefficient
problems

$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s$$

and

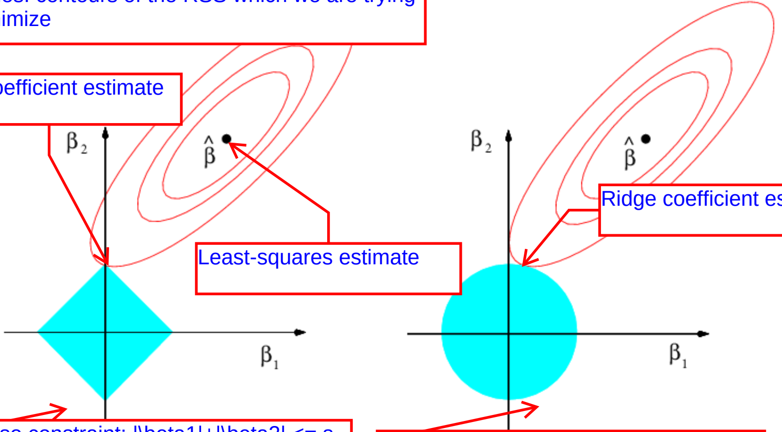
$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s,$$

respectively.

The Lasso Picture

blue region: constrained regions for optimization (l1-ball on the left, l2-ball on the right)

red lines: contours of the RSS which we are trying to minimize



Lasso coefficient estimate

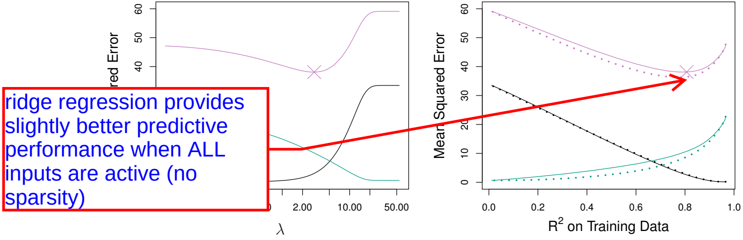
Least-squares estimate

Ridge coefficient estimate

Lasso constraint: |\beta1|+|\beta2| <= s

Ridge constraint: beta1^2+\beta2^2 <= s

Comparing the Lasso and Ridge Regression

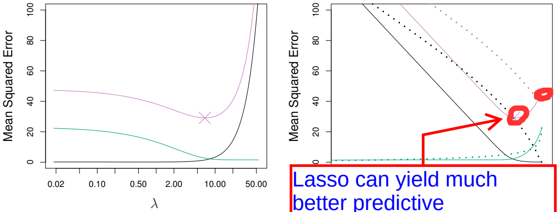


ridge regression provides slightly better predictive performance when ALL inputs are active (no sparsity)

Left: *Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data set of Slide 32.* *Right:* *Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed).* *against their R^2 on the training data, as a common form of indexing. The crosses in both plots indicate the lasso model for which the MSE is smallest.*

all 45 predictors active: true coefficients are non-zero

Comparing the Lasso and Ridge Regression: continued



Lasso can yield much better predictive performance when only some inputs are active (sparsity: a sparse number of inputs are truely active)

Left: *Plots of squared bias (black* [illegible] *and test MSE (purple) for the lasso. The* [illegible] *milar to that in Slide 38, except that now only two predictors are related to the response.* *Right:* *Comparison of squared bias, variance and test MSE between* [illegible] *lasso (solid) and ridge (dashed). Both a* [illegible] *eir R^2 on the training data, as a common form of indexing. The crosses in both plots indicate the lasso model for which the MSE is smallest.*

only 2 out of 45 predictors are active

Conclusions

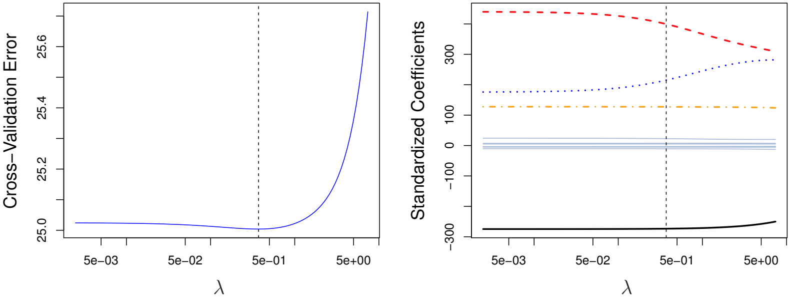
domain knowledge of the problem:
- millions of genes are predictors for a disease. biologists wish to find only a few effective genes: Lasso
- a physicist worked for many years to pick out 3 predictors which they are certain are influential for the system: Ridge

- These two examples illustra nor the lasso will universall
- In general, one might expect the lasso to perform better when the response is a function of only a relatively small number of predictors.
- However, the number of predictors that is related to the response is never known *a priori* for real data sets.
- A technique such as cross-validation can be used in order to determine which approach is better on a particular data set.

Selecting the Tuning Parameter for Ridge Regression and Lasso

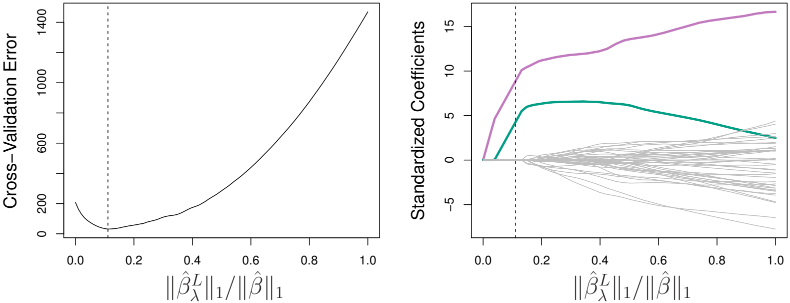
- As for subset selection, for ridge regression and lasso we require a method to determine which of the models under consideration is best.
- That is, we require a method selecting a value for the tuning parameter λ or equivalently, the value of the constraint s.
- *Cross-validation* provides a simple way to tackle this problem. We choose a grid of λ values, and compute the cross-validation error rate for each value of λ.
- We then select the tuning parameter value for which the cross-validation error is smallest.
- Finally, the model is re-fit using all of the available observations and the selected value of the tuning parameter.

Credit data example



Left: *Cross-validation errors that result from applying ridge regression to the* `Credit` *data set with various values of λ.*
Right: *The coefficient estimates as a function of λ. The vertical dashed lines indicates the value of λ selected by cross-validation.*

Simulated data example



Left: *Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data set from Slide 39.* Right: *The corresponding lasso coefficient estimates are displayed. The vertical dashed lines indicate the lasso fit for which the cross-validation error is smallest.*

Dimension Reduction Methods

- The methods that we have discussed so far in this chapter have involved fitting linear regression models, via least squares or a shrunken approach, using the original predictors, $X_1, X_2, \ldots, X_p$.
- We now explore a class of approaches that *transform* the predictors and then fit a least squares model using the transformed variables. We will refer to these techniques as *dimension reduction* methods.

Dimension Reduction Methods: details

- Let $Z_1, Z_2, \ldots, Z_M$ represent $M < p$ *linear combinations* of our original p predictors. That is,

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

  for some constants $\phi_{m1}, \ldots, \phi_{mp}$.

- We can then fit the linear regression model,

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \epsilon_i, \quad i = 1, \ldots, n, \tag{2}$$

  using ordinary least squares.

- Note that in model (2), the regression coefficients are given by $\theta_0, \theta_1, \ldots, \theta_M$. If the constants $\phi_{m1}, \ldots, \phi_{mp}$ are chosen wisely, then such dimension reduction approaches can often outperform OLS regression.

- Notice that from definition (1),

$$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{mj} x_{ij} = \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{mj} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij},$$

  where

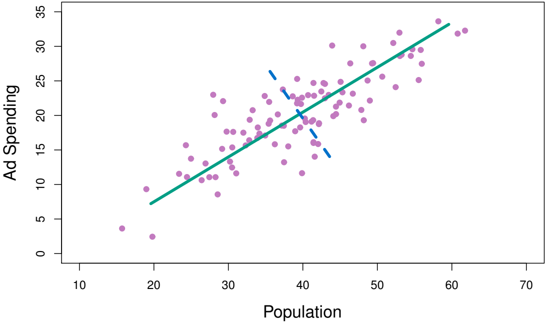
$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}. \tag{3}$$

- Hence model (2) can be thought of as a special case of the original linear regression model.
- Dimension reduction serves to constrain the estimated β_j coefficients, since now they must take the form (3).
- Can win in the bias-variance tradeoff.

Principal Components Regression

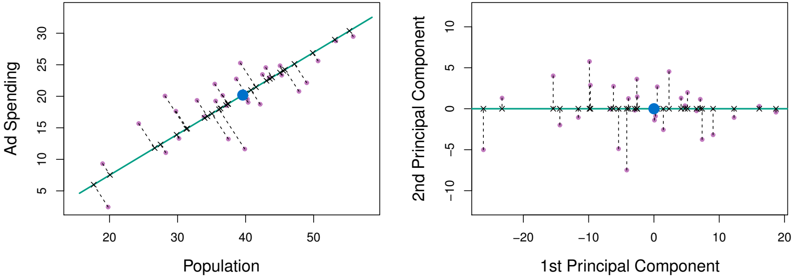
- Here we apply principal components analysis (PCA) (discussed in Chapter 10 of the text) to define the linear combinations of the predictors, for use in our regression.
- The first principal component is that (normalized) linear combination of the variables with the largest variance.
- The second principal component has largest variance, subject to being uncorrelated with the first.
- And so on.
- Hence with many correlated original variables, we replace them with a small set of principal components that capture their joint variation.

Pictures of PCA



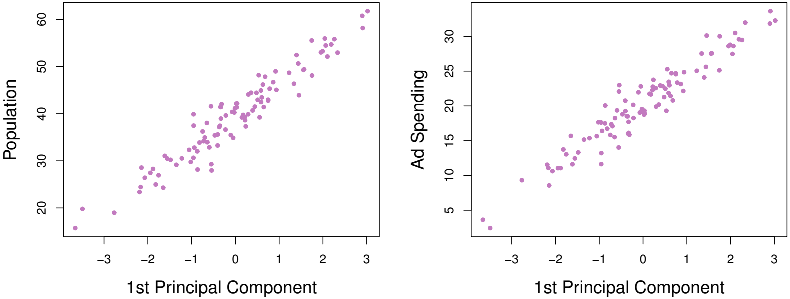
The population size (`pop`*) and ad spending (*`ad`*) for* 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

Pictures of PCA: continued



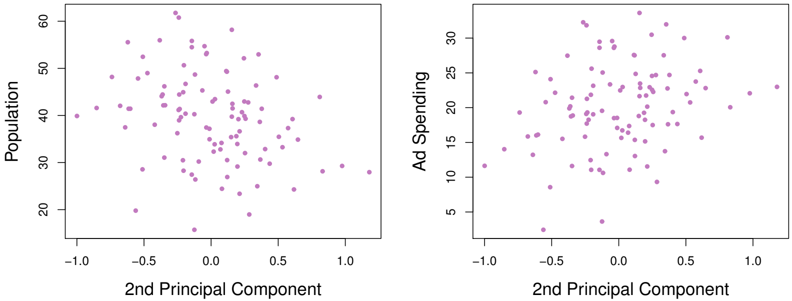
A subset of the advertising data. Left: *The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments.* Right: *The left-hand panel has been rotated so that the first principal component lies on the x-axis.*

Pictures of PCA: continued



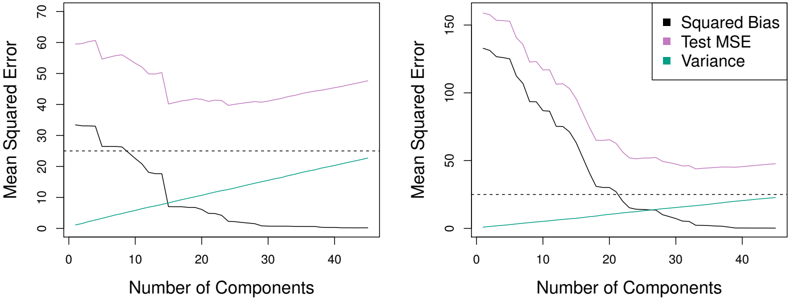
Plots of the first principal component scores z_{i1} versus `pop` *and* `ad`*. The relationships are strong.*

Pictures of PCA: continued



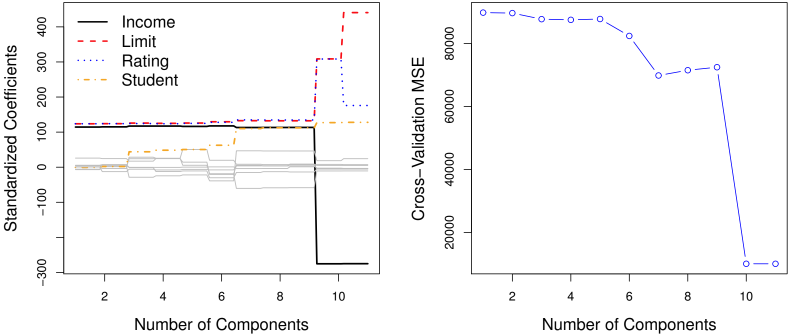
Plots of the second principal component scores z_{i2} versus `pop` *and* `ad`*. The relationships are weak.*

Application to Principal Components Regression



PCR was applied to two simulated data sets. The black, green, and purple lines correspond to squared bias, variance, and test mean squared error, respectively. Left: *Simulated data from slide 32.* Right: *Simulated data from slide 39.*

Choosing the number of directions M



Left: *PCR standardized coefficient estimates on the* `Credit` *data set for different values of M.* Right: *The* 10*-fold cross validation MSE obtained using PCR, as a function of M.*

Partial Least Squares

- PCR identifies linear combinations, or *directions*, that best represent the predictors $X_1, \ldots, X_p$.
- These directions are identified in an *unsupervised* way, since the response Y is not used to help determine the principal component directions.
- That is, the response does not *supervise* the identification of the principal components.
- Consequently, PCR suffers from a potentially serious drawback: there is no guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response.

Partial Least Squares: continued

- Like PCR, PLS is a dimension reduction method, which first identifies a new set of features $Z_1, \ldots, Z_M$ that are linear combinations of the original features, and then fits a linear model via OLS using these M new features.
- But unlike PCR, PLS identifies these new features in a supervised way – that is, it makes use of the response Y in order to identify new features that not only approximate the old features well, but also that *are related to the response*.
- Roughly speaking, the PLS approach attempts to find directions that help explain both the response and the predictors.

Details of Partial Least Squares

- After standardizing the p predictors, PLS computes the first direction Z_1 by setting each ϕ_{1j} in (1) equal to the coefficient from the simple linear regression of Y onto X_j.
- One can show that this coefficient is proportional to the correlation between Y and X_j.
- Hence, in computing $Z_1 = \sum_{j=1}^{p} \phi_{1j} X_j$, PLS places the highest weight on the variables that are most strongly related to the response.
- Subsequent directions are found by taking residuals and then repeating the above prescription.

Summary

- Model selection methods are an essential tool for data analysis, especially for big datasets involving many predictors.
- Research into methods that give *sparsity*, such as the *lasso* is an especially hot area.
- Later, we will return to sparsity in more detail, and will describe related approaches such as the *elastic net*.