Regularized regression

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Basic idea

1. Fit a regression model
2. Penalize (or shrink) large coefficients

Pros:

- Can help with the bias/variance tradeoff
- Can help with model selection

Cons:

- May be computationally demanding on large data sets
- Does not perform as well as random forests and boosting

A motivating example

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

where X_1 and X_2 are nearly perfectly correlated (co-linear). You can approximate this model by:

$$Y = \beta_0 + (\beta_1 + \beta_2) X_1 + \epsilon$$

The result is:

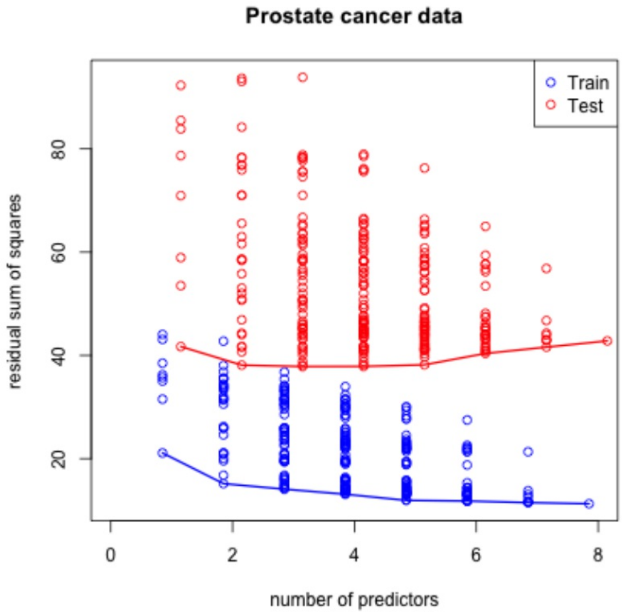
- You will get a good estimate of Y
- The estimate (of Y) will be biased
- We may reduce variance in the estimate

Prostate cancer

```r
library(ElemStatLearn); data(prostate)
str(prostate)
```

```
'data.frame':   97 obs. of  10 variables:
 $ lcavol : num  -0.58 -0.994 -0.511 -1.204 0.751 ...
 $ lweight: num  2.77 3.32 2.69 3.28 3.43 ...
 $ age    : int  50 58 74 58 62 50 64 58 47 63 ...
 $ lbph   : num  -1.39 -1.39 -1.39 -1.39 -1.39 ...
 $ svi    : int  0 0 0 0 0 0 0 0 0 0 ...
 $ lcp    : num  -1.39 -1.39 -1.39 -1.39 -1.39 ...
 $ gleason: int  6 6 7 6 6 6 6 6 6 6 ...
 $ pgg45  : int  0 0 20 0 0 0 0 0 0 0 ...
 $ lpsa   : num  -0.431 -0.163 -0.163 -0.163 0.372 ...
 $ train  : logi  TRUE TRUE TRUE TRUE TRUE TRUE ...
```

Subset selection

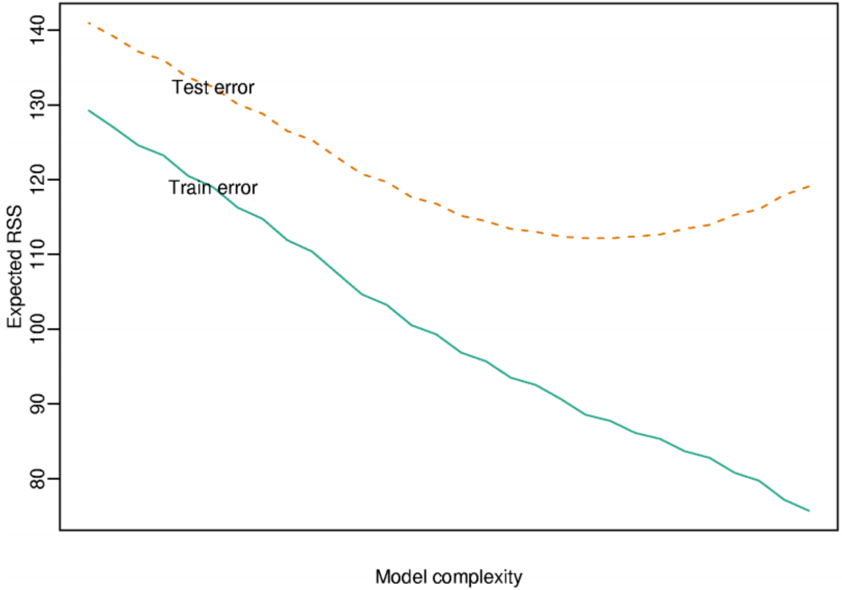


test set error goes first down with more predictors, but then up again: over-fitting!

training set error goes down as we include more predictors

Code here

Most common pattern



same pattern
as on previous slide

http://www.biostat.jhsph.edu/~ririzarr/Teaching/649/

Model selection approach: split samples

- No method better when data/computation time permits it
- Approach

1. Divide data into training/test/validation
2. Treat validation as test data, train all competing models on the train data and pick the best one on validation. `i.e. use validation dataset to select best model.`
   `But then we need the test dataset to actually estimate performance on new data:`
3. To appropriately assess performance on new data apply to test set
4. You may re-split and reperform steps 1-3

- Two common problems
  - Limited data `because we're splitting dataset into 3 groups`
  - Computational complexity

http://www.biostat.jhsph.edu/~ririzarr/Teaching/649/ http://www.cbcb.umd.edu/~hcorrada/PracticalML/

Decomposing expected prediction error

Assume $Y_i = f(X_i) + \epsilon_i$

$EPE(\lambda) = E\left[\{Y - \hat{f}_\lambda(X)\}^2\right]$

```
EPE: expected prediction error = expected value of (difference of Y - predicted Y)^2
```

Suppose $\hat{f}_\lambda$ is the estimate from the training data and look at a new data point $X = x^*$

$$E\left[\{Y - \hat{f}_\lambda(x^*)\}^2\right] = \sigma^2 + \{E[\hat{f}_\lambda(x^*)] - f(x^*)\}^2 + var[\hat{f}_\lambda(x_0)]$$

$$= \text{Irreducible error} + \text{Bias}^2 + \text{Variance}$$

```
-> das wollen wir
   reduzieren.
   Kandidaten sind nur
   * Bias
   * Variance
```

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Another issue for high-dimensional data

```
small = prostate[1:5,]        nur 5 observations,
lm(lpsa ~ .,data =small)      aber viel mehr Prediktoren.
```

```
Call:
lm(formula = lpsa ~ ., data = small)
                                                              einige der Prediktoren kriegen keine
Coefficients:                                                 Koeffizienten
(Intercept)       lcavol      lweight          age         lbph          svi          lcp
     9.6061       0.1390      -0.7914       0.0952           NA           NA           NA
    gleason        pgg45    trainTRUE
    -2.0871           NA           NA
```

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Hard thresholding

- Model $Y = f(X) + \epsilon$
- Set $\hat{f}_\lambda(x) = x'\beta$ wir nehmen also an, das Modell sei linear
- Constrain only λ coefficients to be nonzero. fuer lambda=3: Modell mit nur 3 Koeffizienten
- Selection problem is after chosing λ figure out which $p - \lambda$ coefficients to make nonzero
  also: alle moegl Kombinationen von 3 Koeffizienten ausprobieren.

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Regularization for regression

If the β_j's are unconstrained:

- They can explode
- And hence are susceptible to very high variance

To control variance, we might $\boxed{\text{regularize/shrink the coefficients.}}$

$$PRSS(\beta) = \sum_{j=1}^{n} (Y_j - \sum_{i=1}^{m} \beta_{1i} X_{ij})^2 + P(\lambda; \beta)$$

P: Penalty term

where PRSS is a penalized form of the sum of squares. Things that are commonly looked for

- Penalty reduces complexity
- Penalty reduces variance
- Penalty respects structure of the problem

Ridge regression

Solve:

(minimize)

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

Regression-model

Penalty term

equivalent to solving

$\sum_{i=1}^{N}\left(y_i - \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j\right)^2$ subject to $\sum_{j=1}^{p} \beta_j^2 \leq s$ where s is inversely proportional to λ

Inclusion of λ makes the problem non-singular even if X^TX is not invertible.

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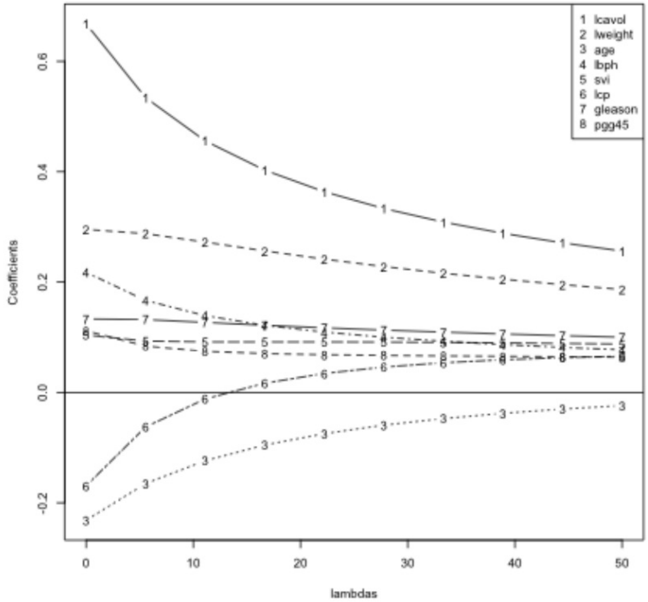
Ridge coefficient paths



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Tuning parameter λ

- λ controls the size of the coefficients
- λ controls the amount of {\bf regularization}
- As $\lambda \to 0$ we obtain the least square solution
- As $\lambda \to \infty$ we have $\hat{\beta}^{ridge}_{\lambda=\infty} = 0$

Optimal tuning parameter lambda could be found e.g. with cross validation.

Lasso

$\sum_{i=1}^{N}\left(y_i - \beta_0 + \sum_{j=1}^{p} x_{ij}\beta_j\right)^2$ subject to $\sum_{j=1}^{p} |\beta_j| \leq s$

also has a lagrangian form

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

For orthonormal design matrices (not the norm!) this has a closed form solution

$$\hat{\beta}_j = \text{sign}(\hat{\beta}_j^0)(|\hat{\beta}_j^0 - \gamma)^+$$

```
| = take absolute value
+ = take only the positive part

So coefficients are shrunk.
```

but not in general.

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Notes and further reading

- Hector Corrada Bravo's Practical Machine Learning lecture notes `good`
- Hector's penalized regression reading list
- Elements of Statistical Learning
- In `caret` methods are:
  - `ridge`
  - `lasso`
  - `relaxo`