Shrinkage

November 29, 2018

Large *p* problems

More and more statistical datasets have *p* large, sometimes much larger than *n*.

- What variations in genome are associated with disease?

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- Even if $p < n$ we will get a lot of variability in our estimates of $\hat{\beta}$ if both p and n are large. Model selection can help – i.e. reduce the number of variables – but the methods we've discussed so far are not going to be very compelling in the face of hundreds of variables, as 2^p can be very large.

Multiple Testing

- With a large number of tests, one for each variable, we are likely to get a great number of false positives. If we have a hundred variables, we get, on average, 5 significant variables, even if there is absolutely no relationship between the variables and the response, and that number grows with the number of variables.

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- If we have a set of p-values (e.g. 1 per variable) that are each individually valid, then there are multiple testing corrections that we can do on the p-values to be able to make joint decisions that as a group will control the number of false positives we make. We will not cover this in detail, other than to note an obvious one: if we make *k* tests, then if each p-value is multiplied by *k* and compared to our level α, the total probability of a single false positive remains $\leq \alpha$. This is called the Bonferroni method.

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- This can be done even if $p >> n$. In this setting the joint relationship is less important than finding single variables of interest (e.g. genes). In this case, the number of variables could be in the thousands, while the number of observations in the tens. Often in this case we control for the false positive rate – the proportion of discoveries that are FP, rather than the absolute number. Otherwise we would never find anything.

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- If we want to limit the contributions of variable $\boldsymbol{X}_j$ to the model, we can think of wanting $|\hat{\beta}_j|$ to be small. We don't know which variables we want to limit, though, so we want to write down some condition that is global on the vector β and then algorithmically let the data tell me which variables should get to contribute the most.

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We can make different choices as to what is the allowable 'size' of β, e.g.

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- As $c \rightarrow \infty$ we are putting on less constraint, so we get closer to the standard least squares model. Another way we can formulate this problem

  $$\min_{\beta} ||y - \mathbf{X}\beta||^2 + \lambda\mathcal{S}(\beta)$$

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- **Relationship to Model Subsets** If we wanted to make 0/1 choices about β, then we could write $\mathcal{S}(\beta) = \sum_j I(\beta_j > 0)$ and $\mathcal{S}(\beta) \leq c$ would limit us to *c* variables in our model. This is clearly a choice of $\mathcal{S}$ that will be untractable.

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- Before we saw model selection criteria as the error of a model (RSS) plus a penalty that depended on $p(m)$ of the model. This makes sense if we consider our 0/1 size evaluation. But now, we can allow for smoother versions.

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- The reason is that for those constraints, this is a convex problem – no local optimum – for which there are algorithms that efficiently search the space of β and can guarantee that they will find the global optimum.
- $p > n$

  By putting an appropriate constraint on the space of β we consider, we now can solve this even when $p > n$.

Ridge Regression

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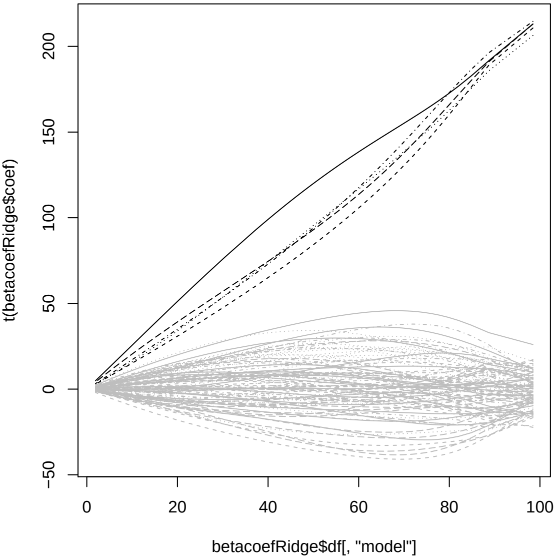
- Notice that $\hat{\beta}_{RR}$ is biased,

$$E(\hat{\beta}_{RR}) = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^T\mathbf{X}\beta$$


t(betacoefRidge$coef)
200
150
100
50
0
−50
0
20
40
60
80
100
betacoefRidge$df[, "model"]

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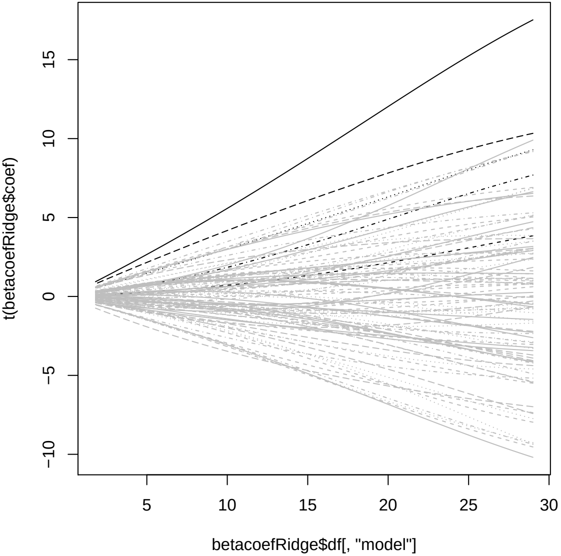
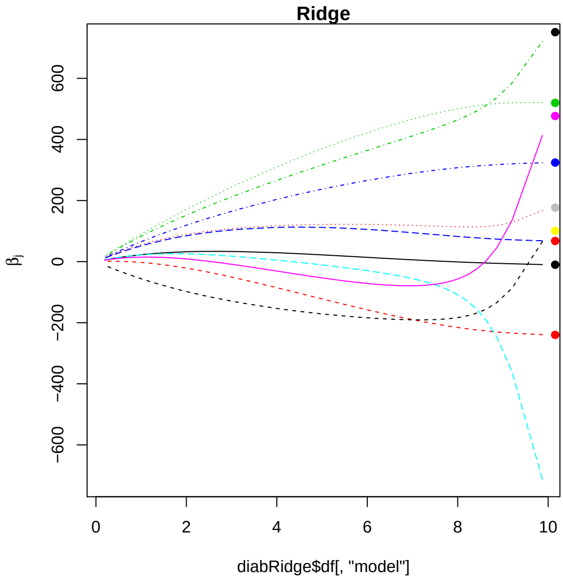
- You can fit it with less observations than variables.



Do model selection after this, like cross-validation


Ridge
600
400
200
0
−200
−400
−600
β_j
0
2
4
6
8
10
diabRidge$df[, "model"]

- Note that our prediction of y is still linear combination of the y,

  $$y = \mathbf{H}_\lambda y = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I}_p)^{-1}\mathbf{X}^T y$$

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- **Stabilizing** $(\mathbf{X}^T\mathbf{X})^{-1}$ Notice that even if $(\mathbf{X}^T\mathbf{X})^{-1}$ is not invertible (e.g. $p > n$),

$$(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}_p)^{-1}$$

  is always invertible if $\lambda > 0$. Why?

- Choosing $\mathcal{S}(\beta) = \sum_j |\beta_j|$ is called **Lasso** (Least Absolute Shrinkage and Selection Operator). Our measure of size $(\mathcal{S})$ is also a norm on $\mathbb{R}^p$ and is called the L_1 norm,

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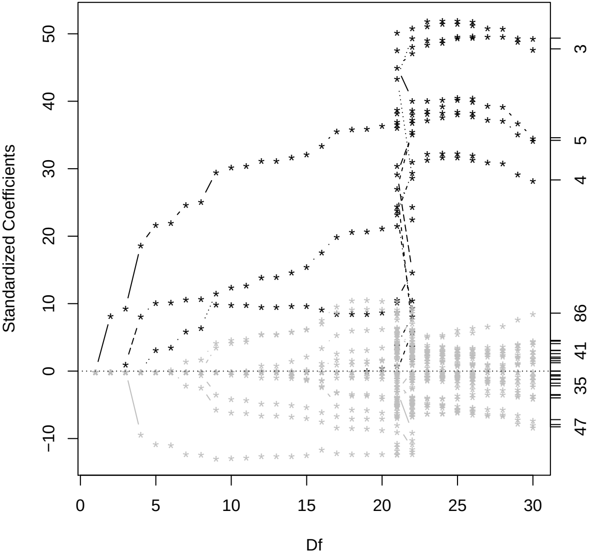
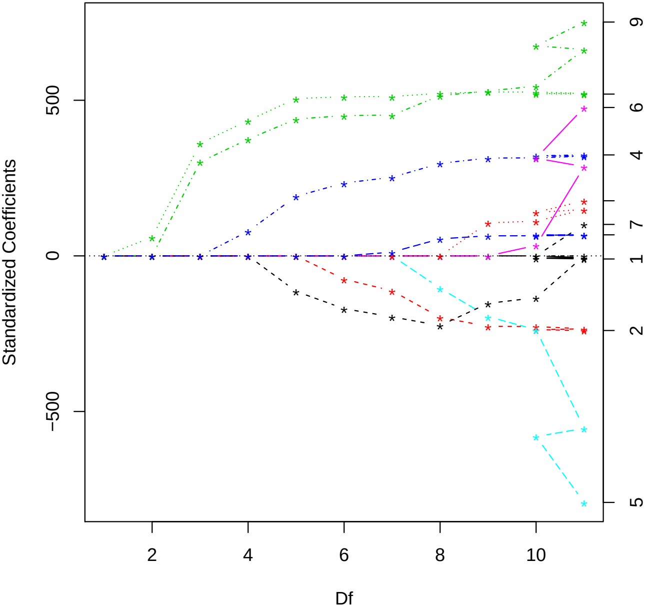
- **Subset Selection** There is a lot of theoretical work on Lasso, and Lasso (i.e. L_1 penalties) actually can be shown to often mimic all subset selection.
- And you can have less observations than variable.


Standardized Coefficients
Df
−10
0
10
20
30
40
50
0
5
10
15
20
25
30
3
5
4
86
41
35
47



Standardized Coefficients
500
0
−500
2
4
6
8
10
Df
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4
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1
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5

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- If $\lambda > 0$, then every solution $\hat{\beta}$, has the same ℓ_1 norm, $\|\hat{\beta}\|_1$.
- Lasso is a nonlinear estimator, meaning we can't express $\hat{y} = \mathbf{A}y$.

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- Lasso is setting some coefficients to zero, ridge is just decreasing them.

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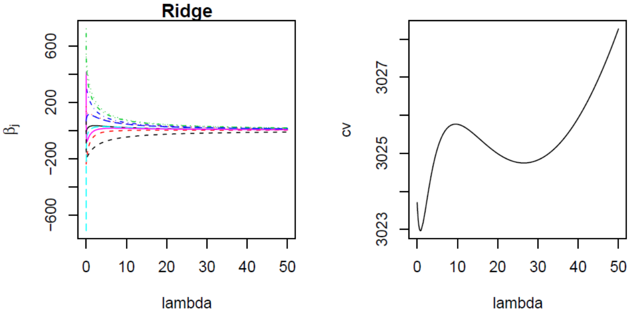
- There are ways to do Mallow's cp or BIC model selection for LASSO, but this require using an estimate the number of parameters.
- Cross-Validation can also be used. We have parameterized our problem so that for each λ we have a model defined by $\hat{\boldsymbol{\beta}}_\lambda$ so we just need to pick between λ values. Specifically, we can choose a grid of λ values, and for each λ value do cross-validation.


Ridge
600
200
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βj
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30
40
50
lambda
3027
3025
3023
cv
0
10
20
30
40
50
lambda