Model Selection 1: Variable Selection

Lecture 5

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Today's Class

1. Quick Review
   - Deviance
   - Bootstrap
   - Out-of-Sample
2. Comparing Models – A primer
   - T-tests
   - F-tests
   - AIC/AICc/BIC
3. Stepwise Regression
4. Regularization and LASSO
5. Cross-Validation

Quick Review

Deviance

Deviance refers to the distance between our fit and the data. You generally want to minimize it.

$$Dev(\beta) = -2log(L(\beta|data)) + C$$

We can ignore C for now.

Deviance is useful for comparing models. It is a measure of GOF that is similar to the residual sum of squares, for a broader class of models (logistic regression, etc). It is closely related to R^2

$$R^2 = 1 - \frac{D}{D_0} = 1 - \frac{Dev(\hat{\beta}))}{Dev(\mathbf{0})}$$

Bootstrap

Basic Procedure for data with n observations.

1. Draw n observations (with replacement) from your data at random, forming a new sample $(X, Y)'$.
2. Estimate the parameter of interest (e.g. β) in the sample $(X, Y)'$. Save that value.
3. Repeat steps (1) and (2) 5k times.
4. Use distribution of values of $\hat{\beta}$ to calculate p-values, CIs, etc.

Out of Sample

We care about how well our model works out-of-sample.

One way to test this is to use a "validation sample".

1. Randomly split your data into two samples
   - usually named "testing" and "training".
2. Fit your model using the "training" data
3. Test predictions on the left-out "testing" data.

Out of Sample Deviances

The difference between in and out of sample deviance is about the sample.

Example Linear Regression

For In-Sample (IS) R^2, we have observations $[\mathbf{x}_1, y_1], ..., [\mathbf{x}_n, y_n]$, which we use to fit $\hat{\beta}_n$. The deviance is:

$$dev_{is}(\hat{\beta}_n) = \sum_{i=1}^{n}(y_i - \mathbf{x}_i'\hat{\beta}_n)^2$$

The Out-of-Sample (OOS) R^2, we keep the same observations $1..n$ to estimate $\hat{\beta}_n$, but the deviance is calculated using m new observations.

$$dev_{oos}(\hat{\beta}_n) = \sum_{i=n+1}^{n+m}(y_i - \mathbf{x}_i'\hat{\beta}_n)^2$$

Out of Sample Example 2: Semiconductors

Semiconductors manufacturing: extremely complicated, no margin for error, hundreds of diagnostics.

We want to focus on diagnostics that are predictive of failure.

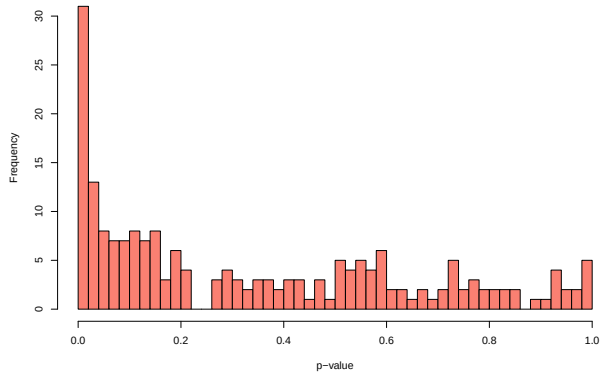
$\mathbf{x}_i$ is a vector of 200 diagnostic signals, y_i is a binary (Pass/Fail) for a chip batch. There are 100 failures out of 1477 batches.

Logistic regression for failure of chip i is

$$p_i = P[fail_i|\mathbf{x}_i] = exp(\alpha + \mathbf{x}_i'\beta)/(1 + exp(\alpha + \mathbf{x}_i'\beta))$$

Example 2: Semiconductors

Full model (non-interacted, jointly estimated) has an in-sample $R^2 \approx 0.56$ (based on binomial deviance).



Semiconductor + FDR

We could consider using FDR to slim down our model. $q = 0.1$ yields $\alpha \approx 0.012$ cutoff. That leaves 25 variables, of which ~2.5 are "false".

A 'cut' model using only those 25 variables has an $R^2 \approx 0.18$.

```
summary(cut.pvals)
```

```
##      Min.   1st Qu.    Median      Mean   3rd Qu.      Max.
## 0.000000 0.001762 0.030080 0.086693 0.092763 0.495039
```

But now we have a bunch of large pvalues again. One question: Should we repeat this process?

Semiconductors Cont.

We care about out of sample performance. Let's examine it.

In Sample R^2

- R^2 increases with more covariates.
  Larger model $\implies$ more flexible model $\implies$ better in-sample fit.
- Thus, we shouldn't use in-sample R^2 for model comparisons.

Out of Sample R^2.

- "How well can this model predict data it hasn't seen?"
- **K-Fold Cross-validation** will help us estimate the out-of-sample predictive performance. Details in 30(ish) slides.

OOS performance

We may gain predictive accuracy by dropping variables.

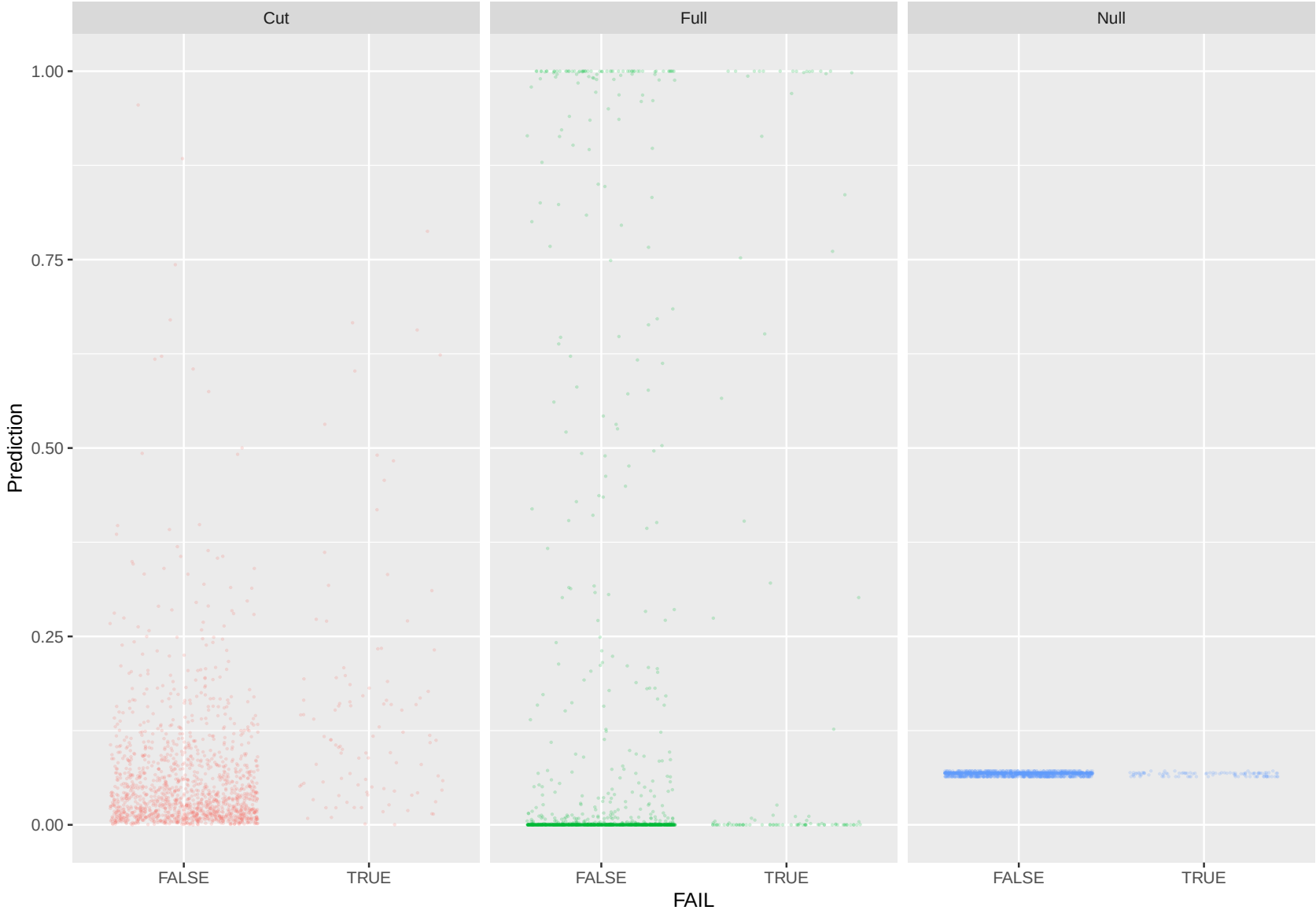
The OOS R^2 for the cut model: 0.10. ($\sim$50% of in-sample R^2)

The OOS R^2 for the full model: -5.87.

THIS IS NEGATIVE. Out-of-Sample, we would be much **BETTER** off predicting the mean than with the full model.

Estimated by using our testing-training split method – AKA cross-validation.

Fit plots



IN SAMPLE R^2 MISLEADS US

OOS

- In-sample measures of model fit can be misleading.
- More variables not necessarily better for out of sample performance

Cross validation uses OOS experiments to choose the best model. This is a big part of big data

Selection of 'the best' model is at the core of big data. We are moving into new territory here.

Before getting to selection, we need to come up with a good set of candidate models to choose from.

HOW?

Comparing Models – A Primer

How many models are we considering?

Suppose for the time being, we ignore interactions between variables, and nonlinearities. We are just interested in models which include some subset of our variables. With p variables, how many models are there?

- 2^p

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- If a computer can estimate 1 trillion/second, and we have 1 trillion computers, it would take more years than there are atoms in a human body to estimate every regression.
- So we will need to ignore a few of those

T-tests/FDR

T-tests are the source for the p-values we've been using for FDR control.

We could (as we did above), estimate the full joint model (or many marginal models) and use the pvalues from these t-tests to choose our covariates, ditching the covariates that are insignificant, either under standard rejection or FDR control frameworks.

But as we saw, the p-values shift as we change models. Do we iterate?

There are other problems, like independence of p-values, data with $p > n$ where we can't estimate p-values, and covariates that are useful only with or without other variables.

Is "variable significance" really what we care about?

Stepwise Regression

Stepwise regression is an important historical model building technique. Once we accept that we can't estimate every subsetted model, we ask "what if we start with an empty model and slowly build it up?"

Stepwise Algorithm (Forward)

1. Start with the null model – no variables.
2. Enumerate all models which contain 1 more variable.
3. Estimate those models
4. Compare each of those models to the current model.
5. Pick the best model, and make it the current model.
6. Repeat steps 2-5.

When to stop? Stop when your model selection rule prefers the current model to all candidate models. Model selection rules in a moment.

Stepwise Regression

This is a useful heuristic search procedure, which reduces the problem space significantly. $\implies$ can be easy to estimate.

There are many variants

- Backwards: start with some maximal model, and shrink it at each step
- Bidirectional: Start with some model, compare to all models one parameter smaller or larger at each step
- Large step size: Check all models with 2 variables more (or 10, etc) at each step

How do we choose?

F-tests

There is a standard tool for comparing two (nested) models in linear regression. The "F-test".

The F-test is purely a function of the R^2 and the number of variables.

You *could* build a procedure out of iteratively comparing two models.

But this will again mostly be selecting mostly for variables which are "significant" rather than optimizing for our predictive loss.

Again, this is not really what we want.

AIC

What we care about is Out-of-Sample predictive performance.

It turns out (after a lot of theoretical work) that we can estimate that using Akaike's Information Criterion. For a model M with k variables estimated to be $\hat{\beta}_M$

$$AIC = 2k + Dev(\hat{\beta}_M) = 2k - 2log(L(\hat{\beta}_M|data))$$

This was in our basic model output.

```
(Dispersion parameter for gaussian family taken to be 0.4829706)

    Null deviance: 30079  on 28946  degrees of freedom
Residual deviance: 13975  on 28935  degrees of freedom
AIC: 61094
```

AIC

The AIC actually estimates OOS deviance – what your deviance would be in another *independent sample of size n*.

In-sample deviance is too small, because the model minimizes that. Some incredible theory work shows us that $AIC \approx OOS\ Deviance$.

This approximation is good when $\frac{n}{k}$ is very big.

In big data, that may not apply. Often $k \approx n$ or is bigger. In that case, AIC overfits!

We want to minimize the AIC.

Information Criteria

There are many more information criteria. We'll cover two briefly.

- AICc
- BIC

AIC corrected: AICc

AIC struggles when the number of parameters is too big.

An improved approximation is:

$$AICc = Dev(\hat{\beta}_M) + 2k\frac{n}{n-k-1}$$

Notice that when $\frac{n}{k}$ is big, $AICc \approx AIC$. So we will generally prefer AICc. Nptice also that it is easy to calculate AICc given AIC.

Bayesian Information Criterion: BIC

$$BIC = Dev(\hat{\beta}_M) + k\ log(n)$$

This looks like AIC (swapping a $log(n)$ for a 2) but it comes from a very different place.

$BIC \approx -log(P[M|data])$, the probability 'model b is true', in a bayesian setting.

Generally BIC will select for smaller models. Why?

Imperfect Rule of Thumb:
"AIC/AICc approximate deviance, BIC approximates truth"

Stepwise

Stepwise regression is not choosing the globally best subset of predictors.

Remember there are 2^k such models

Instead, it takes a "greedy" approach. Looking at the best option for the immediate step, and taking that. This is computationally much easier – but isn't likely to give you the 'globally' optimal model.

Its computationally easy?

Stepwise in R

```
null = glm(FAIL~1,data=SC,family=binomial)
full = glm(FAIL~.,data=SC,family=binomial)
stepwise = step(null,scope=formula(full),direction="forwar
```

```
length(coef(stepwise))
```

```
## [1] 63
```

Full is the largest model you would consider, and scope is it's formula. Feel free to include interactions to make it huge.

But be warned, even though stepwise is faster than ennumerating every possible model, it is not necessarily 'fast'.

Variable Selection Thus Far

Subset Selection Enumerate every possible model M, estimate $\hat{\beta}$ for each model, choose the best.
$\implies$ Completely infeasible even for small p like 50.

Stepwise Selection: A faster heuristic. Start with some base model, find the best 'adjacent' model, change to that, and continue iterating.

- Still not very fast (90+ seconds for semiconductor example)
- Not very stable. Small changes in a few observations can change your selected model a lot. With resulting big effects on your predictions.
- Inferential properties are extremely unclear.

What's next? Regularization

Regularization

The general idea: Impose restrictions on $\hat{\beta}$ to make them stable, purposeful, and quick to estimate.

Variable selection is achieved with Estimation, not p-values.

What are our goals?

- We would like $\hat{\beta}$ to be stable relative to small changes in data
- We would like $\hat{\beta}$ to give the best out of sample predictions possible
- We would like $\hat{\beta}$ to set some coefficients to exactly 0 (dropping variables from the model)

We will **penalize** solutions $\hat{\beta}$ that do not meet expectations.

Regularization

Using all predictors $x_1, ..., x_p$, the most likely (MLE) values $\hat{\beta}_{MLE}$ minimize deviance.

$$\hat{\beta}_{MLE} = \underset{\beta}{\text{argmin}}\ Dev(\beta) = \underset{\beta}{\text{argmin}} - 2log(L(\beta))/n$$

But $\hat{\beta}_{MLE}$ can only be estimated when $p < n$, may be unstable, and won't have exact 0s.

The penalized version of this adds a penalty $pen()$ which depends on the parameter β and is scaled by some weight $\lambda > 0$.

$$\hat{\beta}_{PMLE} = \underset{\beta}{\text{argmin}}\,(Dev(\beta) + \lambda\ pen(\beta))$$

Regularization

This penalty imposes a **cost** for solutions that don't meet our preferences. $\implies \hat{\beta}_{PMLE}$ is biased.

What costs should we impose? What costs do we face?

- *Estimation costs*: This is the deviance. As our model fit degrades, we penalize the model.

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  - A natural penalty then: $pen(\beta) = \sum_{j=1}^{p} 1(\beta \neq 0)$.
  - This is just best subset selection again though. We can't do it.
- *OOS costs*: Predictions near the unconditional mean of the data are 'safe'. Big coefficients push us far away from those predictions. So we should penalize big coefficients.

LASSO

LASSO is the most commonly used regularized (or penalized) regression model. The lasso penalty is the l_1 norm of our parameters: $pen(\beta) = \sum |\beta_j|$, which penalizes larger coefficients and non-zero coefficients. So our estimates are:

$$\hat{\beta}_\lambda = \underset{\beta}{\text{argmin}} \left(Dev(\beta) + \lambda \sum_{j=1}^{p} |\beta_j| \right)$$

For linear regression this simplifies dramatically:

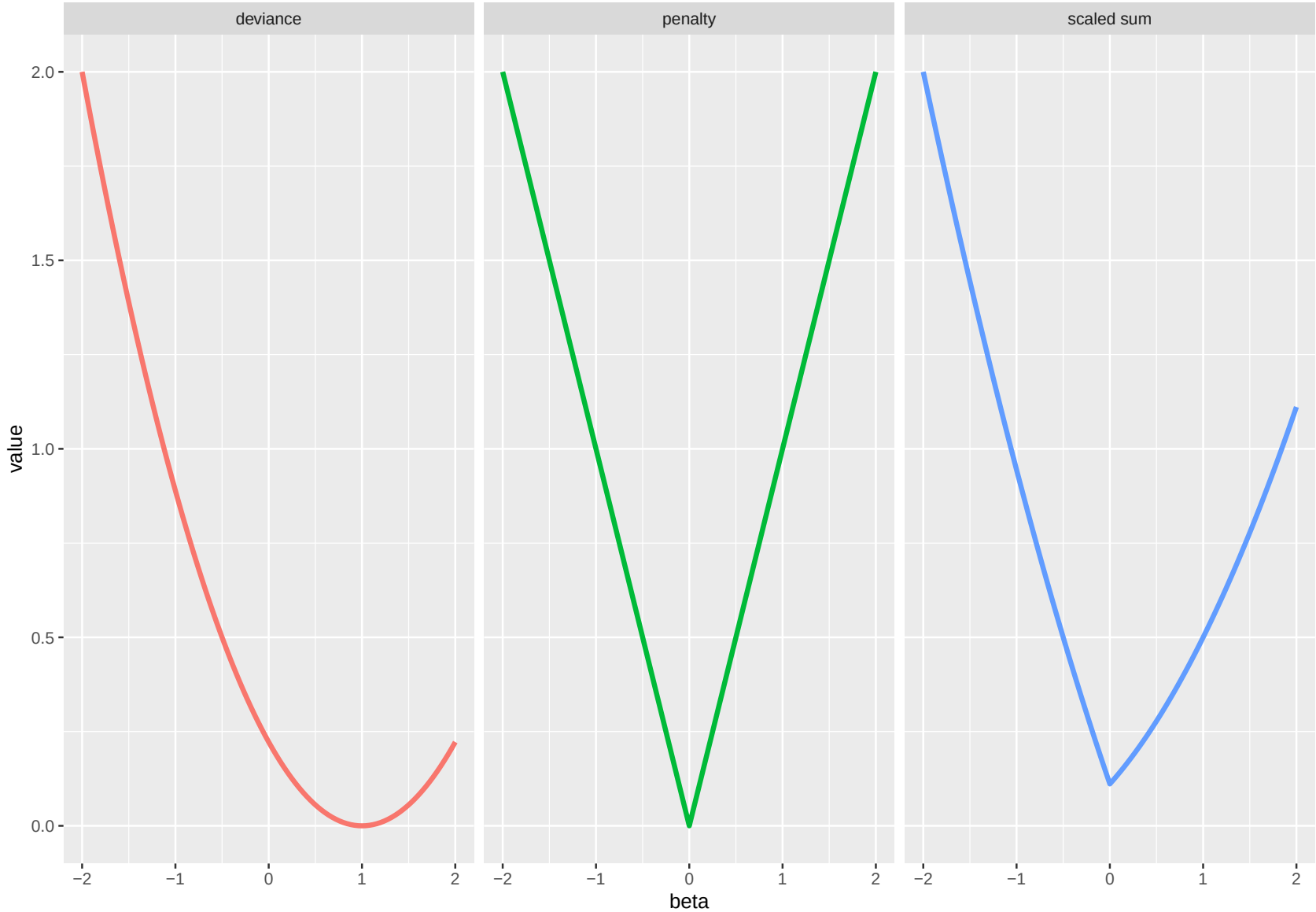
$$\hat{\beta}_\lambda = \underset{\beta}{\text{argmin}} \left(\sum_{i=1}^{n} (y - x'\beta)^2 + \lambda \hat{\sigma}^2 \sum_{j=1}^{p} |\beta_j| \right)$$

LASSO

LASSO gives sparse solutions. It imposes a 'spiky' penalty for coefficients. The 'spike' at 0 yields a preference for coefficients that are 0. Non-zero coefficients need to be sufficiently informative to pay the penalty.

Even though the deviance (the other part of our maximation) is smooth, a smooth function plus a spiky one can be spiky. And the minimum can be at that spike.

LASSO



The LASSO ‘shrinks’ some coefficients to 0.

$\Longrightarrow$ Automatic variable selection.

LASSO Problems

But LASSO also shrinks the parameters that wind up being non-zero.

In particular, it can be shown that for a given λ,

$$\hat{\beta}_{j,\lambda} = \hat{\beta}_{j,OLS} \max\left(0, 1 - \frac{n\lambda}{|\hat{\beta}_{j,OLS}|}\right)$$

So when $\hat{\beta}_{j,\lambda}$ is non-zero, it is $\approx n\lambda$ closer to 0 than $\hat{\beta}_{j,OLS}$.

This, as well as the zeroing out of coefficients, induces the bias.

LASSO in R

Very easy to estimate in R, thanks to numerous useful packages.

```
library(glmnet)
mod = glmnet(as.matrix(SC[,-1]),SC$FAIL, family=binomial) #
sum(coef(mod, s=0.01) != 0) #s = 0.01 is setting lambda
```

```
## [1] 53
```

So 147 coefficients are 0 with $\lambda = 0.01$.

Other Regularizations

We chose the penalty to be the sum of absolute values of β. But there are other choices.

- Ridge regression: the l_2 norm: $pen(\beta) = \sum \beta^2$
  - This doesn't have a spike at 0, so it doesn't auto-select.
- Elastic Net: $pen(\beta) = \gamma \sum |\beta| + (1 - \gamma) \sum \beta^2$
  - This is 'between' LASSO and Ridge. It does some variable selection.
- Many more: 'spike and slab LASSO', 'gamma LASSO', etc

LASSO Details

LASSO finds $\hat{\beta}_\lambda$ which minimizes $Dev(\beta) + \lambda \sum |\beta|$. How do we pick λ?

R will estimate a sequence of $\lambda_1 < \lambda_2 < ... < \lambda_T$. We can apply model selection tools to choose the best $\hat{\lambda}$

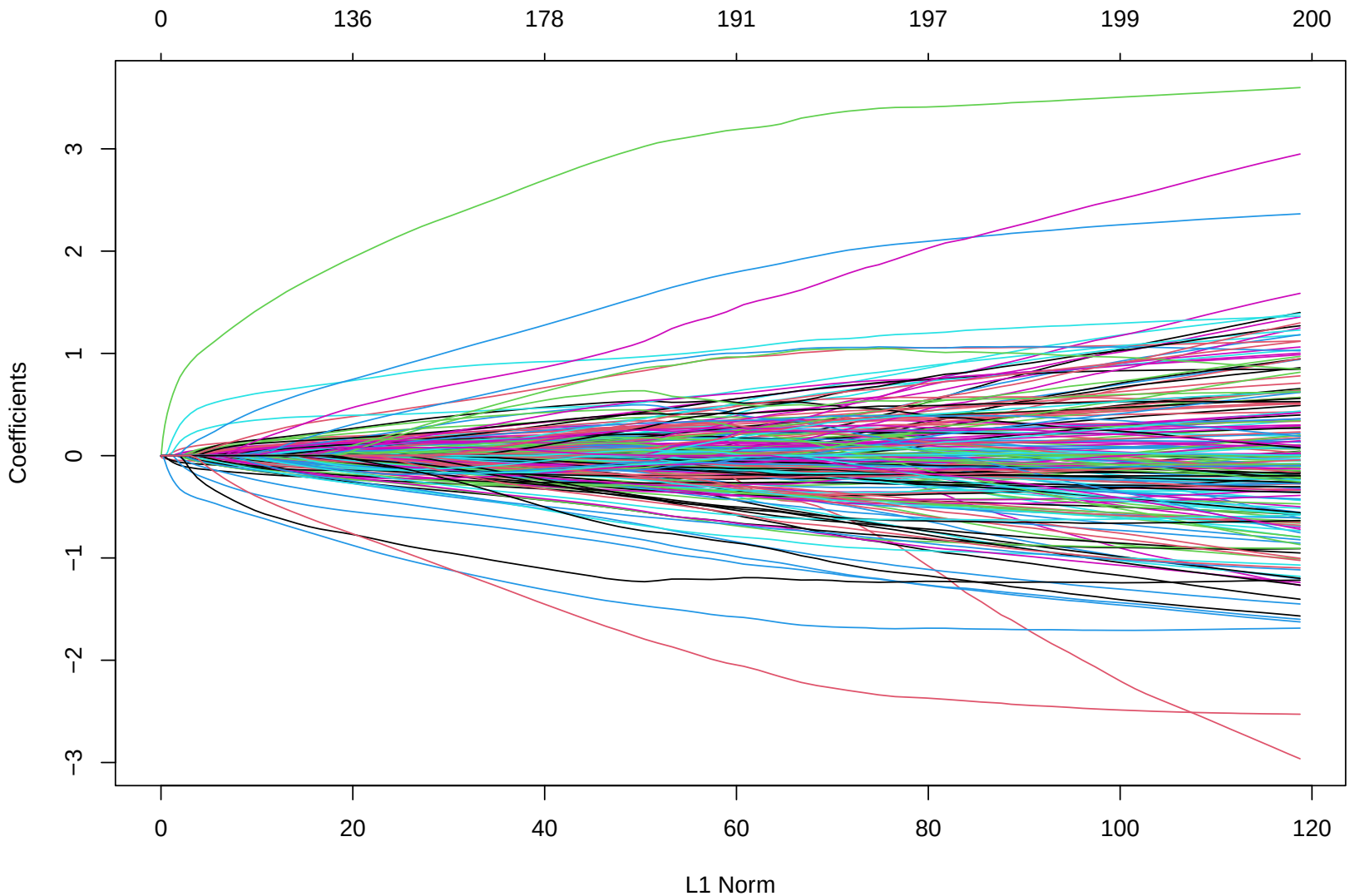
LASSO path estimation: R does the following:

1. Start with small $\lambda_1 \approx 0$ such that $\hat{\beta}_{\lambda_1} \approx \hat{\beta}_{MLE}$
2. Choose λ_2, compute $\hat{\beta}_{\lambda_2}$.
3. Keep increasing λ until you obtain the null model for some value, λ_T

- This is fast. Each update is easy.
- This is stable, optimal lambda may change slightly between samples, but not much.
- This is an improved 'stepwise' regression.

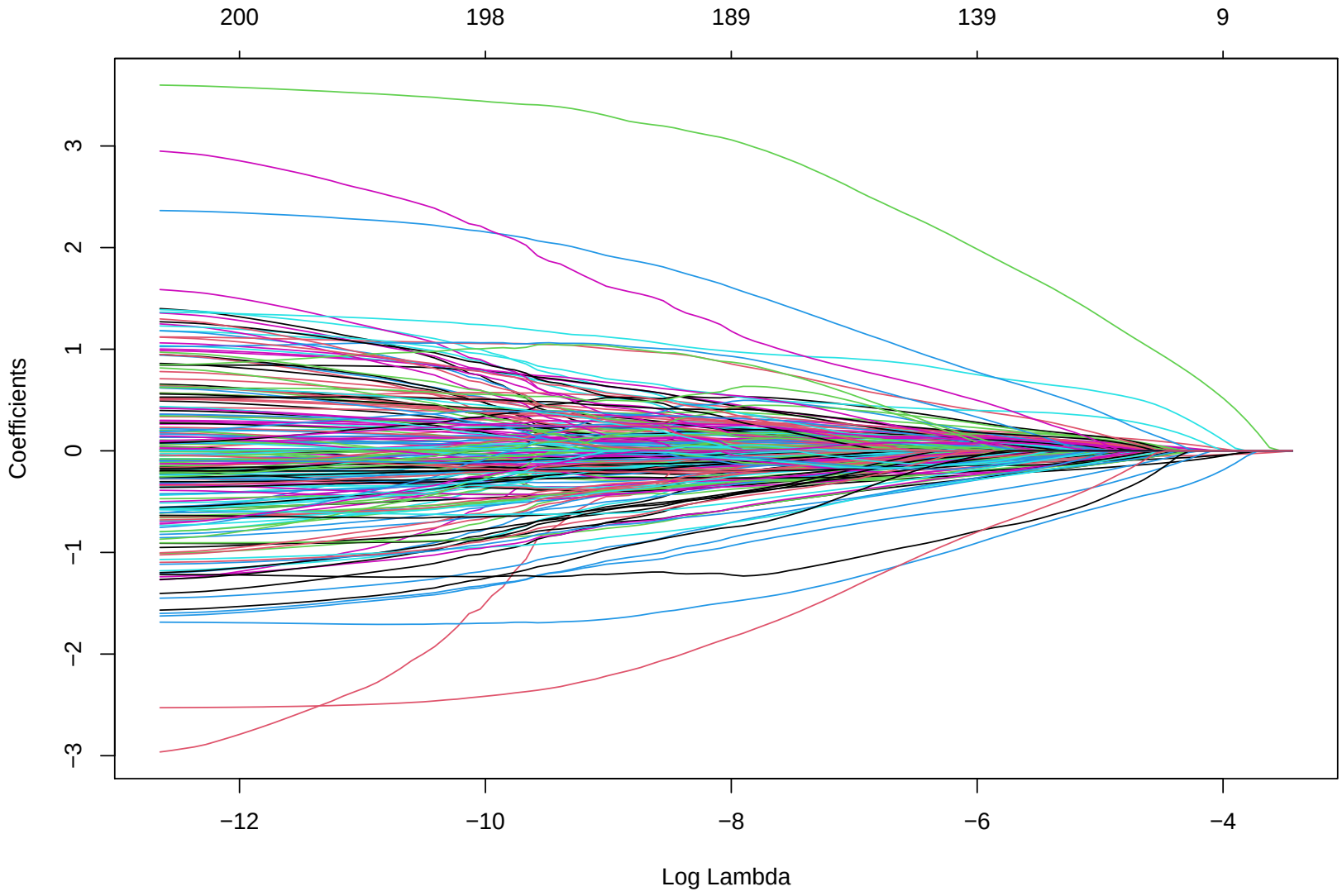
Classic Plot

Each lambda has a different series of coefficients. There is a classic plot illustrating. `plot(mod)`



Classic Plot - In Lambda

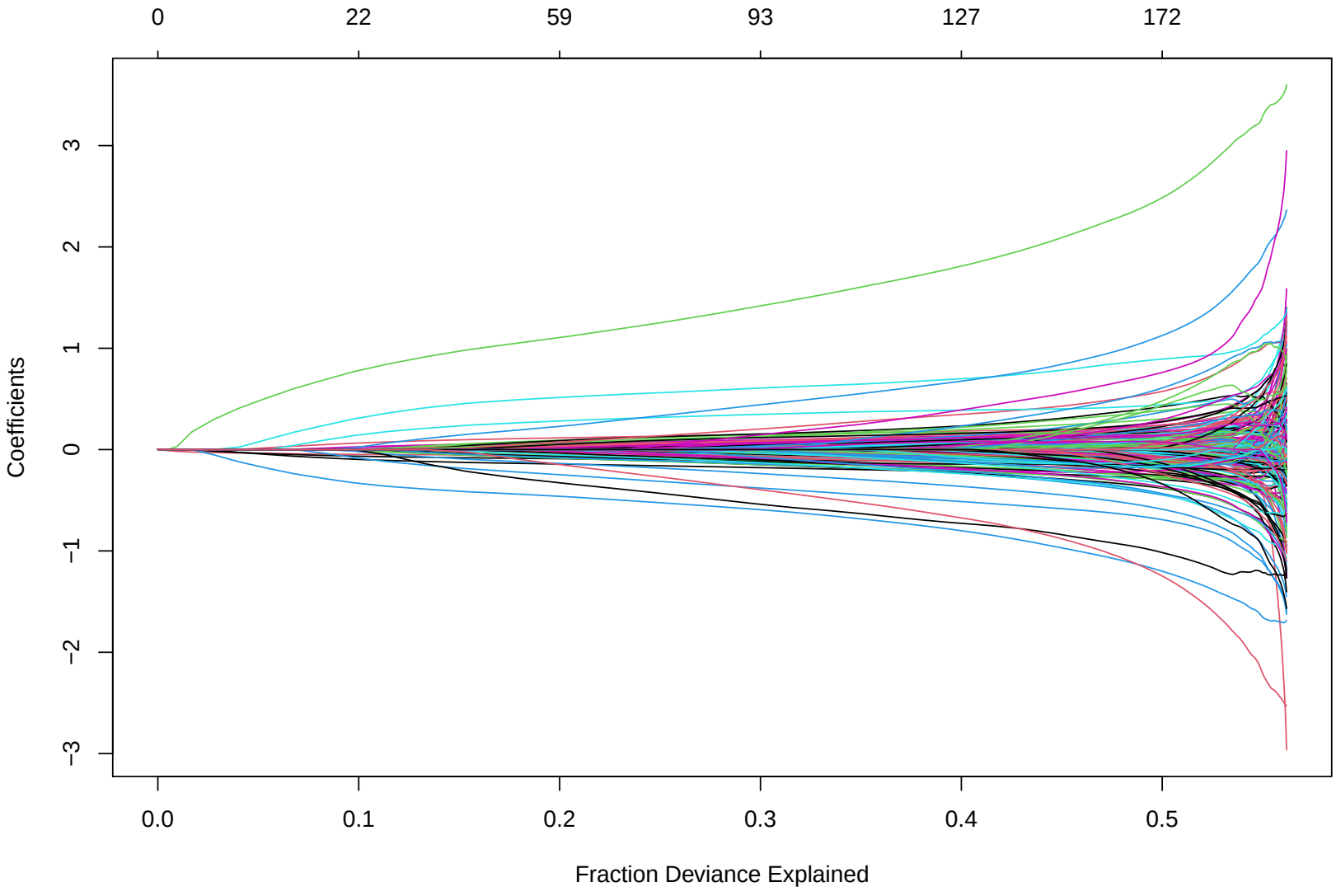
That was against the sum of coefficients, we can also plot against λ. `plot(mod,xvar="lambda")`



Classic Plot - In Deviance Shares

Or we can plot in shares of deviance – pseudo-R^2.

```
plot(mod,xvar="dev")
```



LASSO Details pt 2 – SCALE

Covariate scale matters here. This is because $x'\beta$ has the same effect in predictions as $2x'\beta/2$, but $|\beta|$ is twice as large a penalty as $|\beta/2|$.

We can recenter and rescale our covariates so that they all are mean 0 and standard deviation 1. This will eliminate any problems here.

Most major stats packages will do this for you.

Picking λ

We can now estimate an entire path of coefficients for every value of λ. But we still need to choose one.

Think of λ as a signal-to-noise filter.

If there is lots of signal in your data, you want a low λ. If there is lots of noise, you want high λ.

We will use Cross Validation to pick the best λ, but you could also use some information criterion.

This works well because the path algorithms are relatively stable and fast. We can quickly enumerate many candidate models, and the one that 'looks best' is going to be quite near the one that is best.

Prediction vs Interpretation

Testing frameworks are about *is this model true?*
We want to know *what is my best guess?*

None of your models will be 'true' for complicated high dimensional systems. We just want a model that makes good predictions.

Parsimony or **Occams Razor**: If two models do similarly well in unseen data, choose the simpler one.

- Overly simple models will 'underfit' the data (λ too big)
- Overly complicated models will 'overfit' the data (λ too small)

The goal is to find the sweet spot.

OOS Prediction based Model Selection

The recipe:

1. Find a manageable set of candidate models (such that fitting them is fast)
2. Choose the one with best predictive performance on unseen data

LASSO path algorithms give us (1)
OOS prediction error methods give us (2)

In particular, K-FOLD CROSS VALIDATION

Naive OOS/Cross-validation flaws

We need to estimate the prediction accuracy on unseen future data. We've seen that we can split our sample into a 'test' and 'training' data sets to do this.

But this is inefficient. If your test data has 10% of the observations:

- You only check the prediction errors with 10% of your observation space
- You only estimate your model with 90% of the data
- How do we pick 10%? Last class – I said its a rule-of-thumb. Unsatisfying.

K-Fold Cross-validation systematically improves on this.

K-Fold Cross Validation

We could, like the bootstrap, repeat our testing-training procedure many times. But we want to guarantee each observation gets used as an 'out-of-sample' observation at least once.

Instead, we will "fold" the data. We will partition it (split into exclusive and exhaustive groups) into K different groups of observations. Then, `for k=1:K`

- Use observations in group k as test data.
- Train the models on the remaining data (for every λ)
- Predict the observations in group k using those models
- Record the prediction errors for each lambda

This guarantees that each observation is left out once, and improves the performance of our routine.

Picking K

There are several options:

- Leave-one-out Cross-validation: AKA $K = n$ is great, but much slower (fits every model under consideration n times)
- $K = 5$ corresponds to 5 different 20% leave-out samples.
- $K = 20$ corresponds to 20 different 5% leave-out samples.

Most people set $K \in [5, 20]$. I'll mostly use 10.

$\implies$ Optimizing K is very 3rd order. Not worth worrying about too much beyond time considerations and some preference for larger K.

All Together.

We have a LASSO path indexed by $\lambda_1 < \lambda_2 < ... < \lambda_T$.

Cross-Validation for λ:
For each of $k = 1, ..., K$ folds:

1. Fit the path $\hat{\beta}^k_{\lambda_1}, ..., \hat{\beta}^k_{\lambda_T}$ using the data not in fold k.
2. Get the fitted deviance for new data: $-log\ P[y^k | X^k, \hat{\beta}^k_{\lambda_t}]$ where k denotes fold membership.

This gives us K draws of the OOS deviance for each λ_t.

Choose the best $\hat{\lambda}$, and fit your model to all the data with that $\hat{\lambda}$.

In R

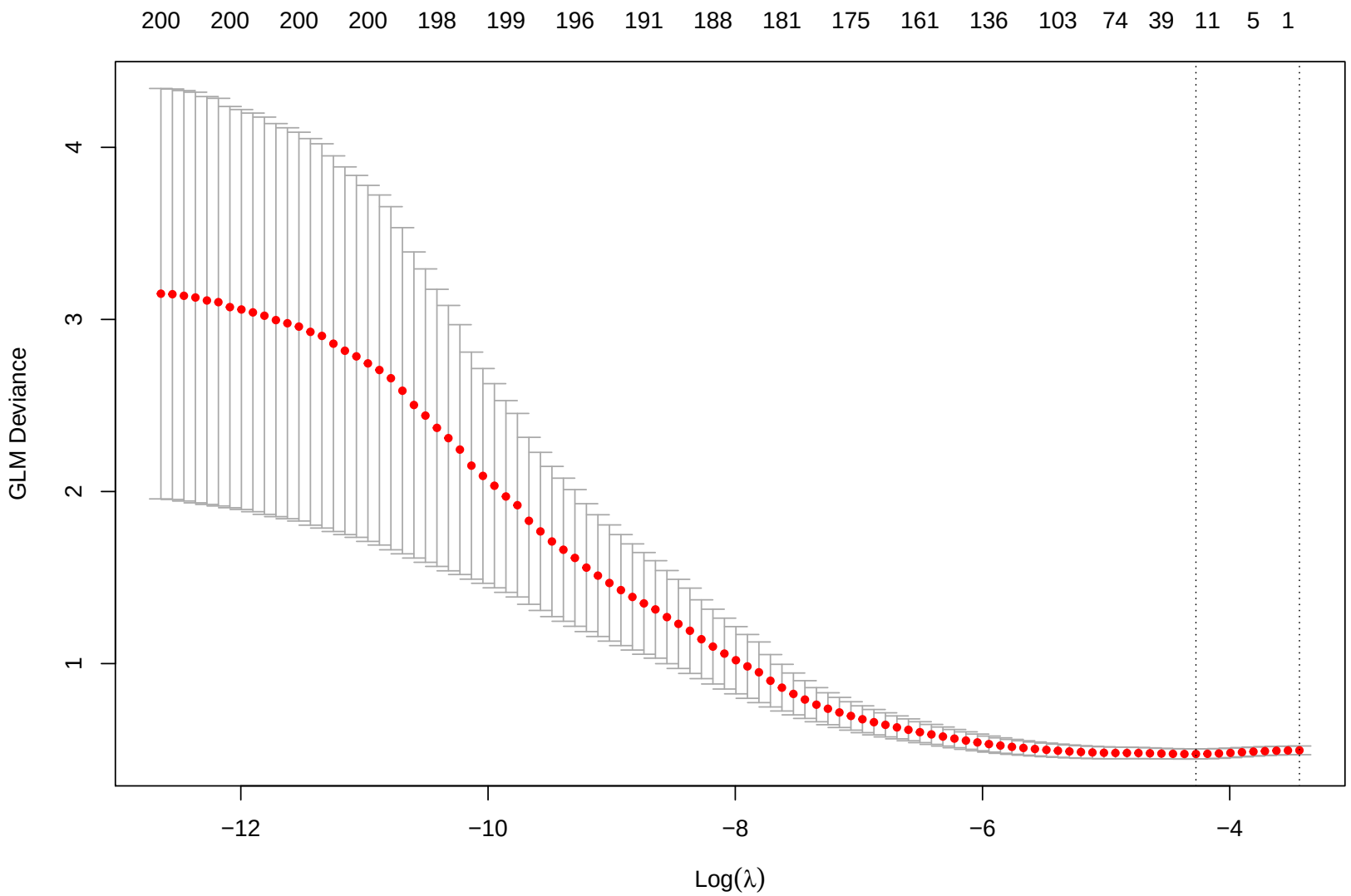
Again, Cross-validation is very easy and relatively fast for LASSO in R.

```
mod = cv.glmnet(as.matrix(SC[,-1]),SC$FAIL,family=binomial)
```

And there is a nice plot for it too

CV LASSO plot

```
plot(mod)
```



LASSO Outputs

Once we've done the cross-validation its easy to pick out our coefficients.

```
sum(coef(mod,s="lambda.1se") != 0)
```

```
## [1] 1
```

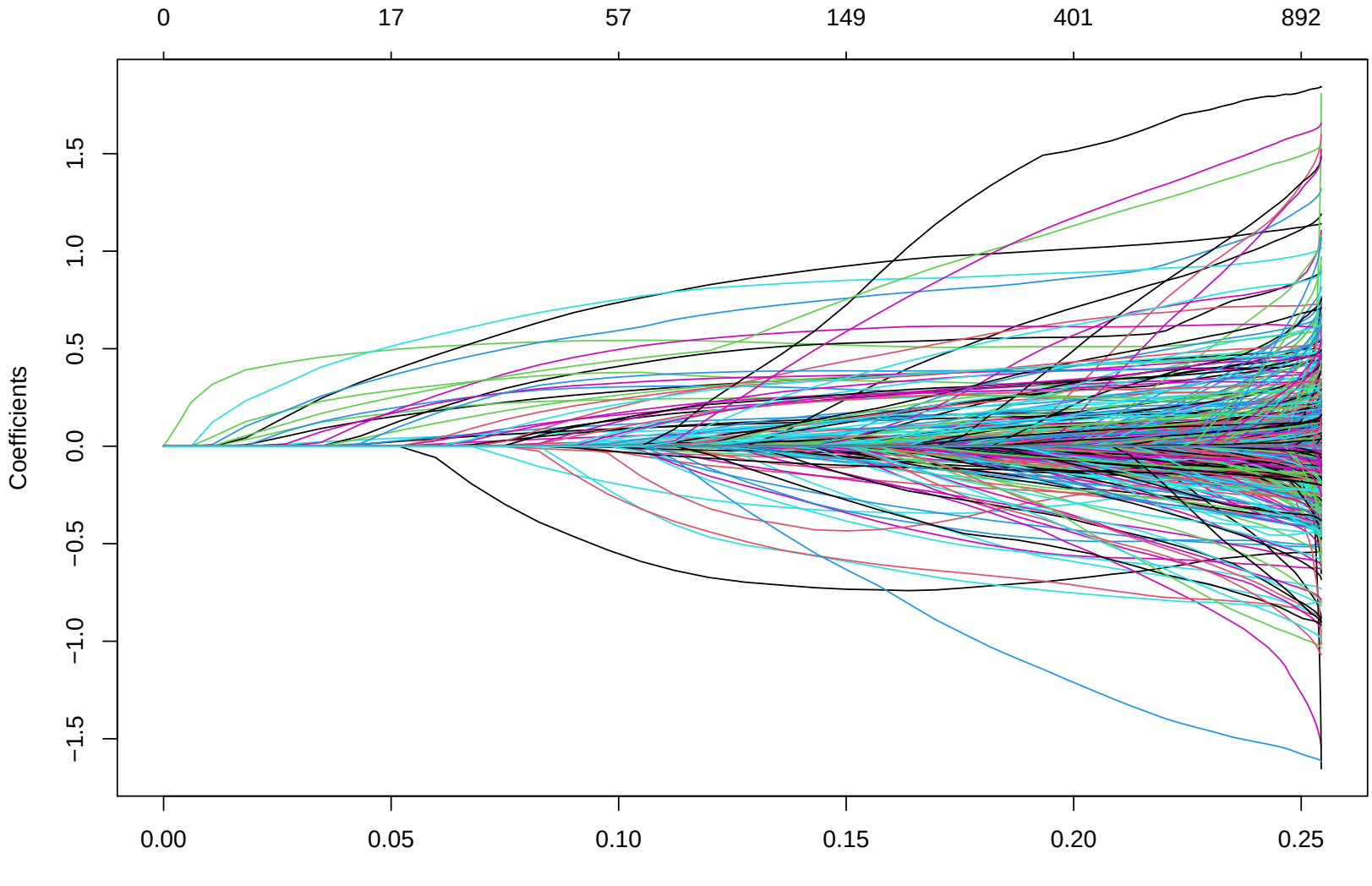
```
sum(coef(mod,s="lambda.min") != 0)
```

```
## [1] 15
```

"Min" vs "1se" is to do with a concern about overfitting. The 1SE model is the smallest model that has predictions which perform very similarly to the true model.

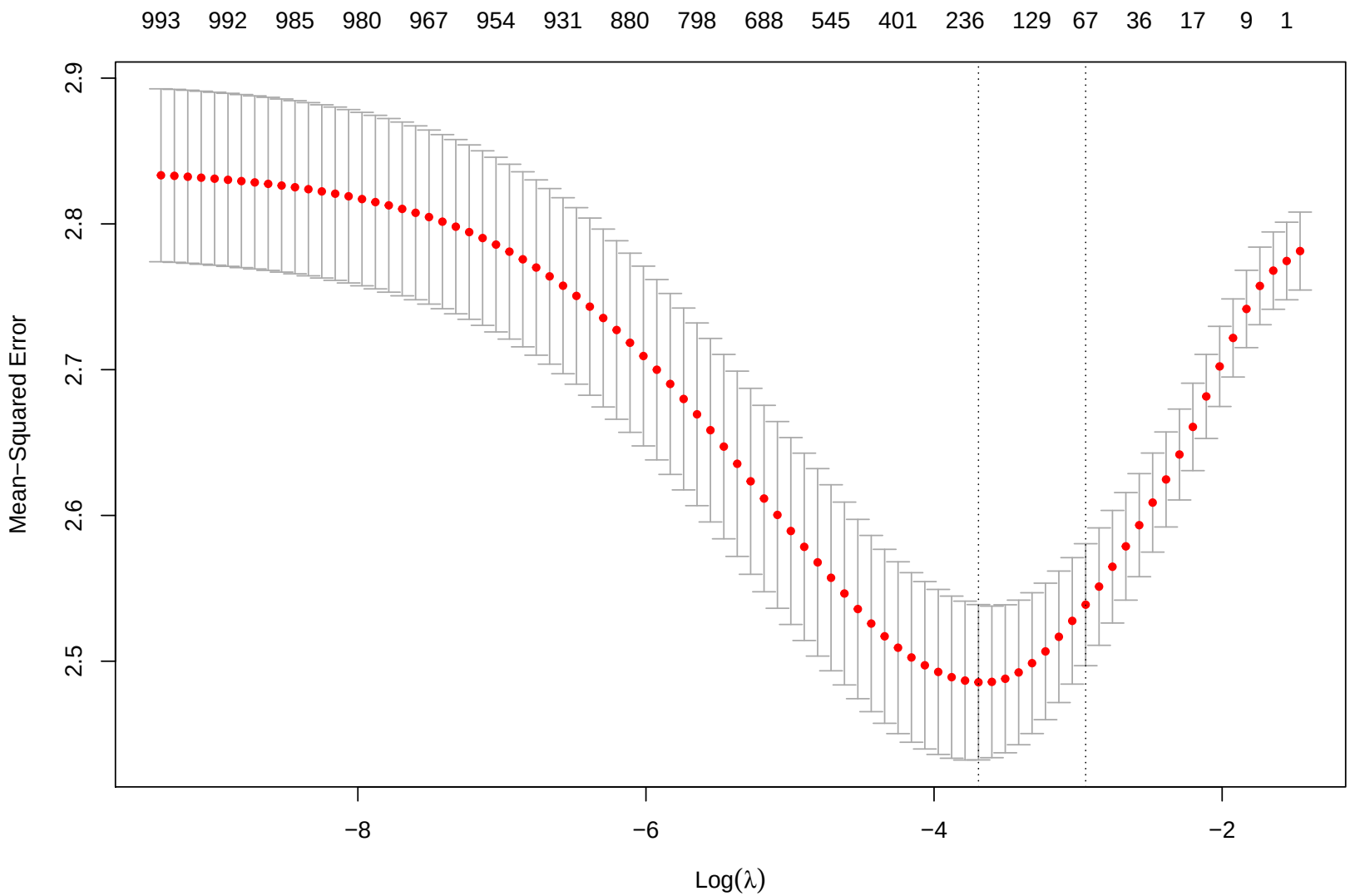
Example 2: Comscore

That plot wasn't the most lovely. This is from a new example looking at Comscore data. This data is about consumer spending on websites.



Comscore

```
plot(cv.spender)
```



Wrap up

Things to do

Before Wednesday:

- HW 2

Before Thursday:

- Nothing

Rehash

- Long history of variable selection, starting with F and T-tests
- Moving into Stepwise "greedy" procedures using AIC or BIC as guides
- Modern techniques: LASSO is a powerful tool for doing automatic variable selection
  - But it doesn't fully solve the 'out-of-sample' problem.
- We use K-Fold Cross Validation to do this
  - In essence, trading computational power for theoretical work and assumptions

Bye!