Making Decisions in High Dimensions

Matt Taddy, Chicago Booth

faculty.chicagobooth.edu/matt.taddy/research

High Dimensional Decisions

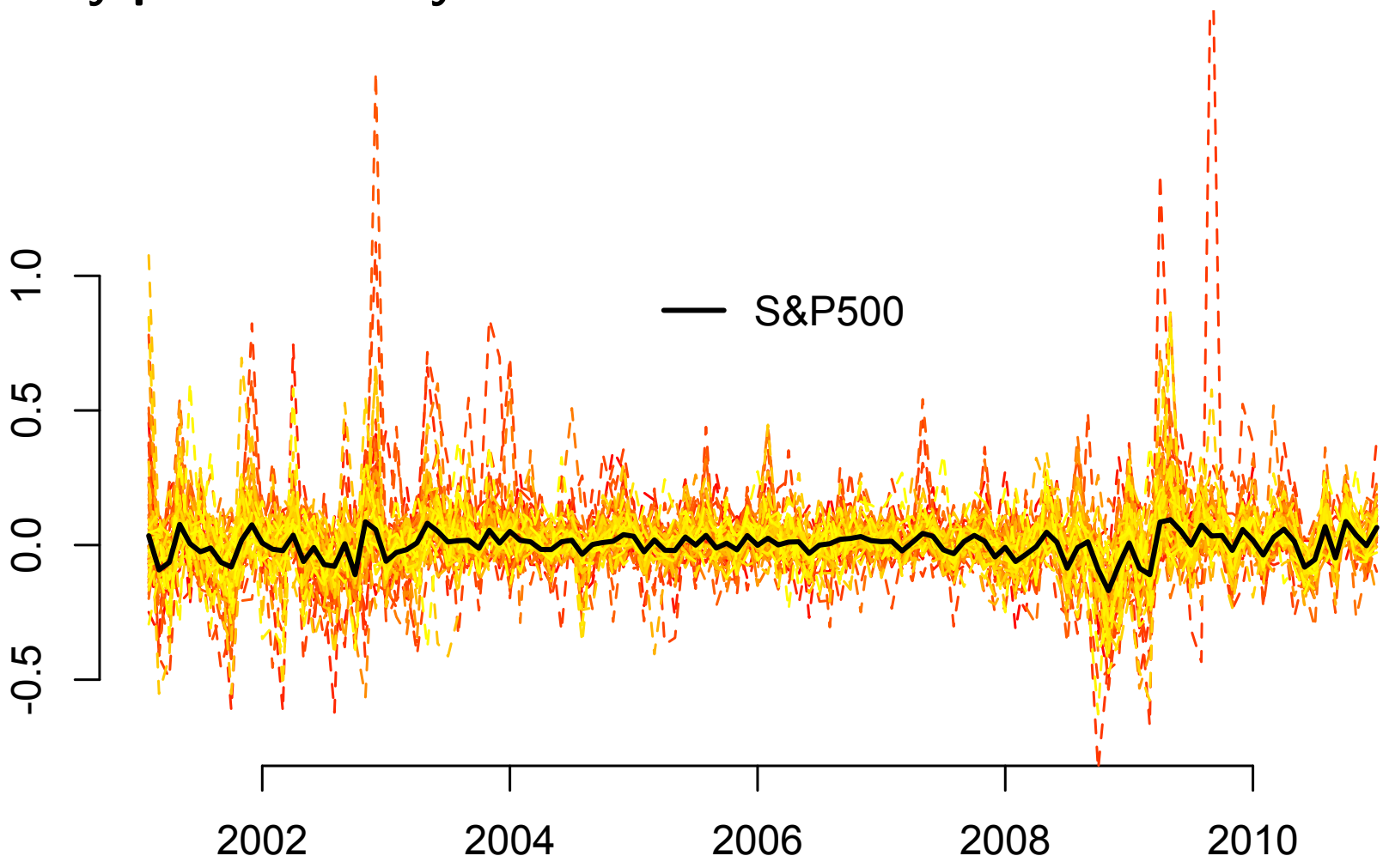
One of the ways that data is 'Big' is in the number of inputs.

This number often grows with the sample size (e.g., words in text, websites in browsers) and you never reach a statistically safe place.

For this type of Big, we need dimension reduction techniques: project from the full input set down to a useful low-D summary.

Crucially, this must be focused on the decisions you'd like to make.

Fancy plot: monthly stock returns



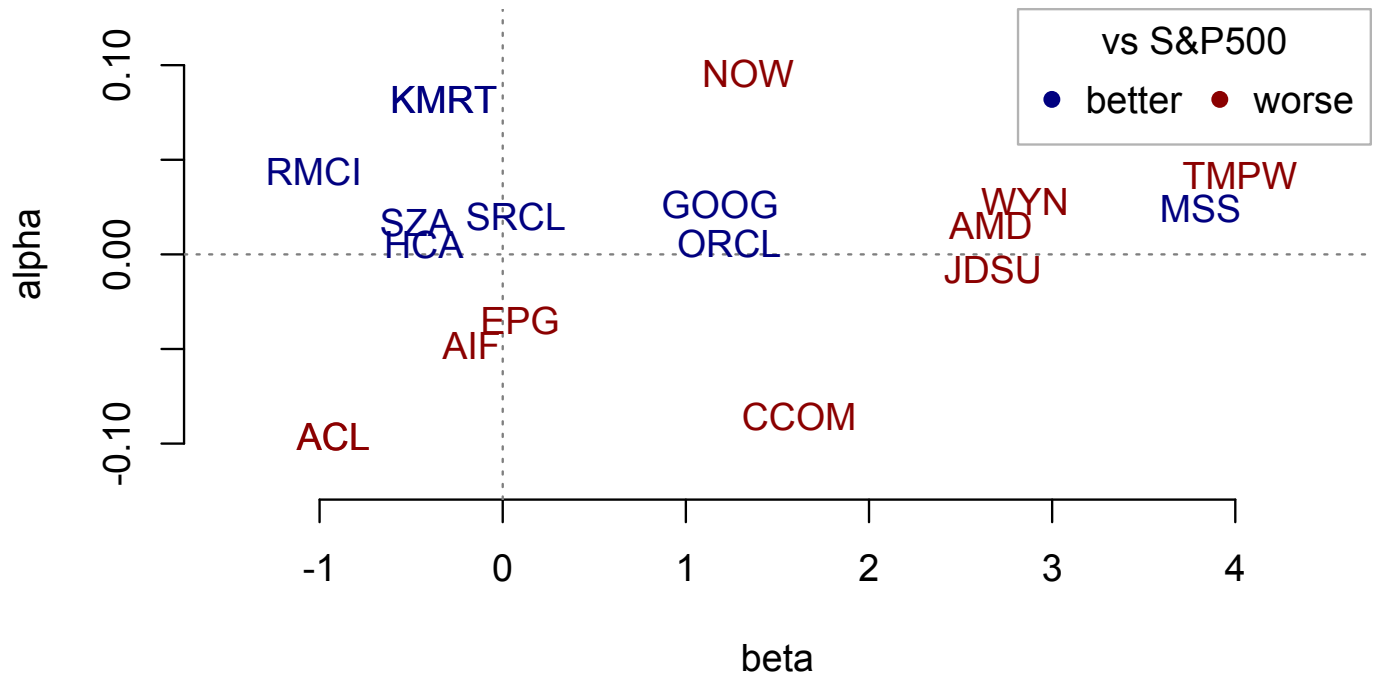
What do we learn?

Useful plot: market model coefficients

Fit a line between stock returns R_t and market returns M_t (SP).

$$R_t \approx \alpha + \beta M_t$$

α is money you make regardless of what the market does.
β is the asset's sensitivity to broad market movements.



Many problems in BD involve a response of interest ('y')
and a set of covariates ('**x**') to be used for prediction.

If your 'decision' is to predict y for new $\mathbf{x}$, we need to reduce dimension in the direction of y. That is, we want to map $\mathbf{x} \rightarrow \hat{y}$.

A general tactic is to deal in averages and lines.
We'll model the conditional mean for y given $\mathbf{x}$,

$$\mathbb{E}[\ y \mid \mathbf{x}\ ] = f(\mathbf{x}'\boldsymbol{\beta})$$

$\mathbf{x} = [1, x_1, x_2, \ldots x_p]$ is your vector of covariates.

$\boldsymbol{\beta} = [\beta_0, \beta_1, \beta_2, \ldots \beta_p]$ are the corresponding coefficients.

Some basic facts about linear models

The model is always $\mathbb{E}[y|\mathbf{x}] = f(\mathbf{x}\boldsymbol{\beta})$.

- Gaussian (linear): $y \sim \mathrm{N}(\mathbf{x}\boldsymbol{\beta}, \sigma^2)$.
- Binomial (logistic): $\mathrm{p}(y = 1) = e^{\mathbf{x}\boldsymbol{\beta}}/(1 + e^{\mathbf{x}\boldsymbol{\beta}})$.

Likelihood (LHD) is $\mathrm{p}(y_1|\mathbf{x}_1) \times \mathrm{p}(y_2|\mathbf{x}_2) \cdots \times \mathrm{p}(y_n|\mathbf{x}_n)$.

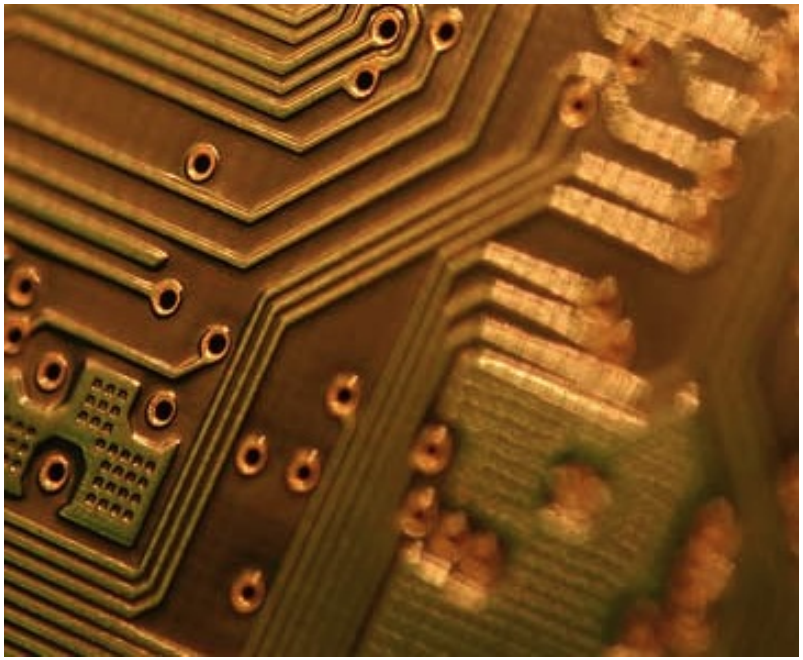
The Deviance (dev) is proportional to -log(LHD).

$\hat{\boldsymbol{\beta}}$ is commonly fit to maximize LHD $\Leftrightarrow$ minimize deviance.

Fit is summarized by $R^2 = 1 - \mathrm{dev}(\hat{\boldsymbol{\beta}})/\mathrm{dev}(\boldsymbol{\beta} = 0)$.

The only R^2 we ever really care about is out-of-sample R^2.

Example: Semiconductor Manufacturing Processes



Very complicated operation
Little margin for error.

Hundreds of diagnostics
Useful or debilitating?

We want to focus reporting and better predict failures.

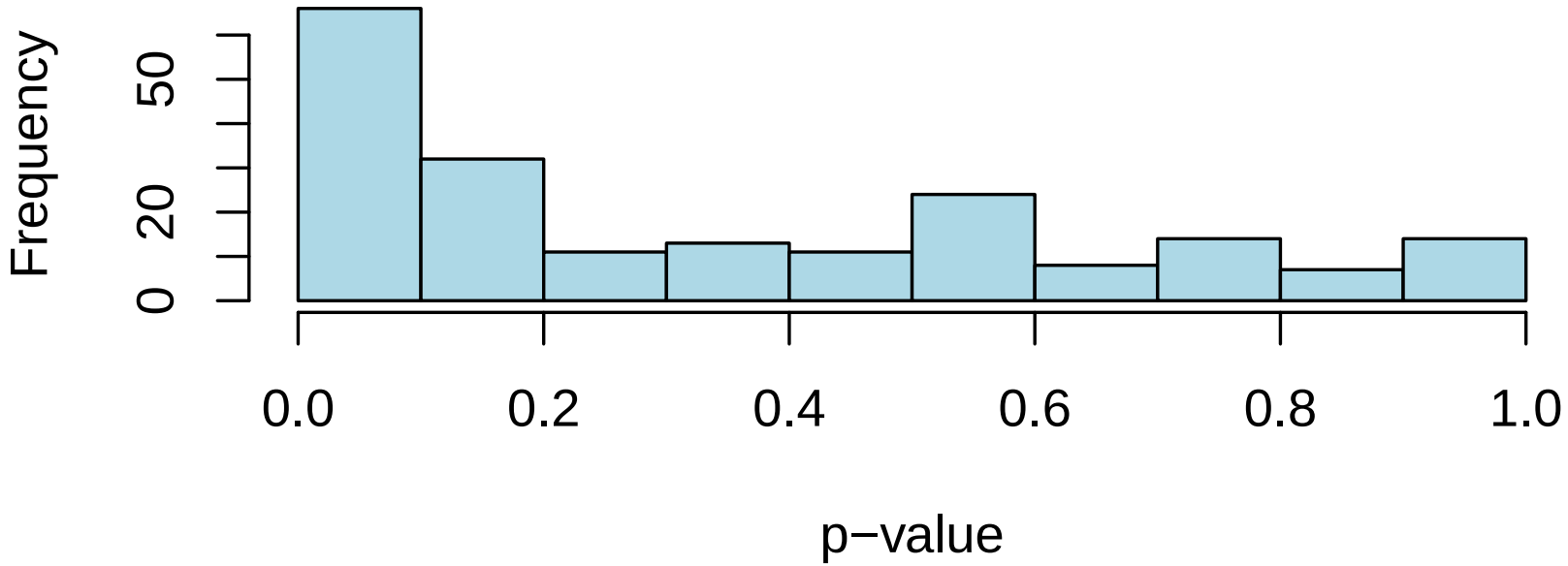
$\mathbf{x}$ is 200 input signals, y has 100/1500 failures.

Logistic regression for failure of chip i is

$$p_i = \mathrm{p}(\mathtt{fail}_i|\mathbf{x}_i) = e^{\alpha+\mathbf{x}_i\boldsymbol{\beta}}/(1+e^{\alpha+\mathbf{x}_i\boldsymbol{\beta}})$$

The full model has $R^2 = 0.56$ (based on *binomial* deviance).

The p-values for these 200 coefficients:



Some are clustered at zero, the rest sprawl out to one.

FDR of $q = 0.1$ yields $\alpha = 0.0122$ p-value rejection cut-off.

Implies 25 'significant', of which approx 22-23 are true signals.

A *cut* model, using only these 25 signals, has $R^2_{cut} = 0.18$.
This is much smaller than the full model's $R^2_{full} = 0.56$.

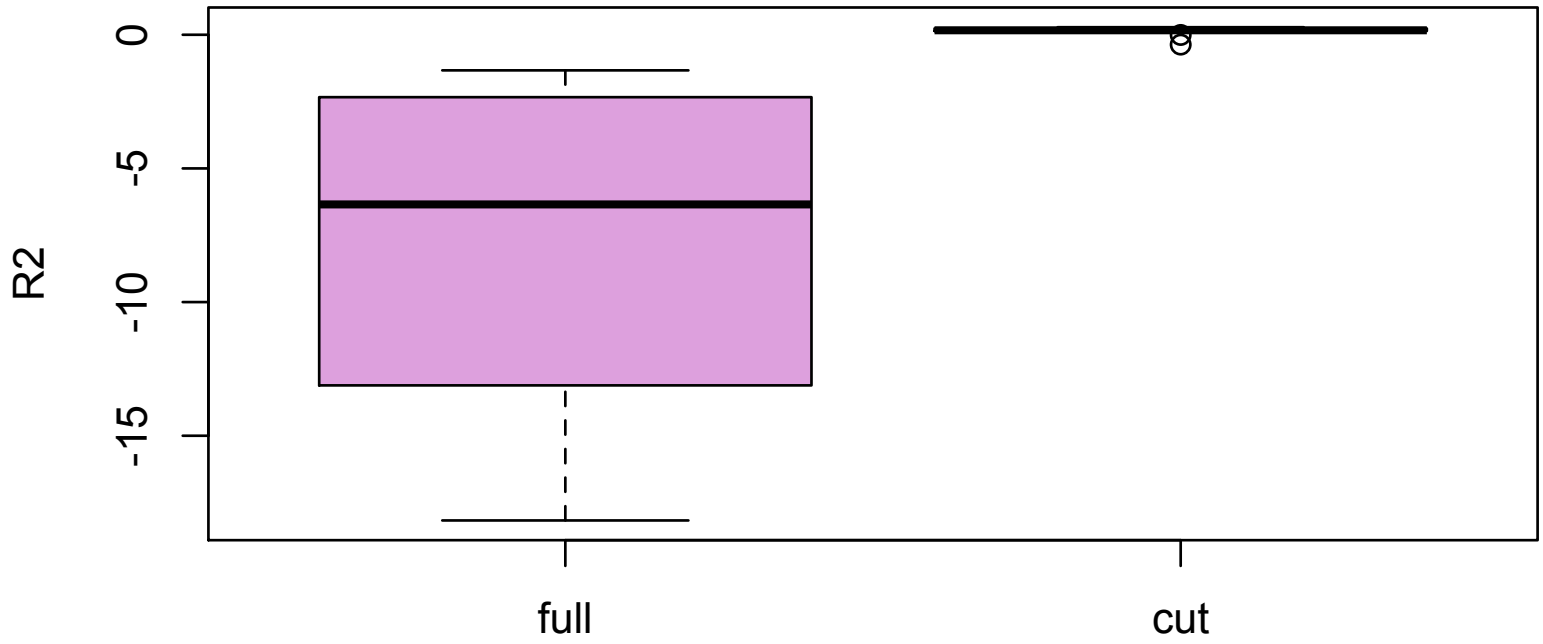
In-Sample (IS) R^2 *always* increases with more covariates.
This is exactly what MLE $\hat{\beta}$ is fit to maximize.
But how well does each model predict *new* data?

An out-of-sample (OOS) experiment

- split the data into 10 random subsets ('folds').
- Do 10x: fit model $\hat{\beta}$ using only 9/10 of data,
  and record R^2 on the left-out subset.

These OOS R^2 give us a sense of how well each
model can predict data that it has not already seen.

We gain predictive accuracy by *dropping* variables.



Cut model has mean OOS R2 of 0.09, about 1/2 in-sample R2.

The full model is terrible. It is overfit and worse than $\bar{y}$.
Negative R2 are more common than you might expect.

All that matters is Out-of-Sample R^2.
We don't care about In Sample R^2.

Using OOS experiments to choose the best model is called *cross validation*. It will be a big part of our big data lives.

Selection of 'the best' model is at the core of all big data.

But before getting to selection, we first need strategies to build good sets of candidate models to choose amongst.

Regularization

The key to contemporary statistics is regularization:

depart from optimality to stabilize a system.

Common in engineering: I wouldn't drive on an optimal bridge.

We minimize deviance

$$\min -\frac{2}{n}\log \mathrm{LHD}(\boldsymbol{\beta})$$

Regularization

The key to contemporary statistics is regularization:

depart from optimality to stabilize a system.

Common in engineering: I wouldn't drive on an optimal bridge.

We minimize deviance plus a cost on the size of coefficients.

$$\min -\frac{2}{n}\log \mathrm{LHD}(\boldsymbol{\beta}) + \lambda \sum_k |\beta_k|$$

This particular cost gives the 'lasso': the new least squares.

Decision theory: Cost in Estimation

Decision theory is based on the idea that choices have costs.
Estimation and hypothesis testing: what are the costs?

Estimation:

Deviance is the cost of distance between data and the model.
Recall: $\sum_i (y_i - \hat{y}_i)^2$ or $-\sum_i y_i \log(\hat{p}_i) - (1 - y_i) \log(1 - \hat{p}_i)$.

Testing:

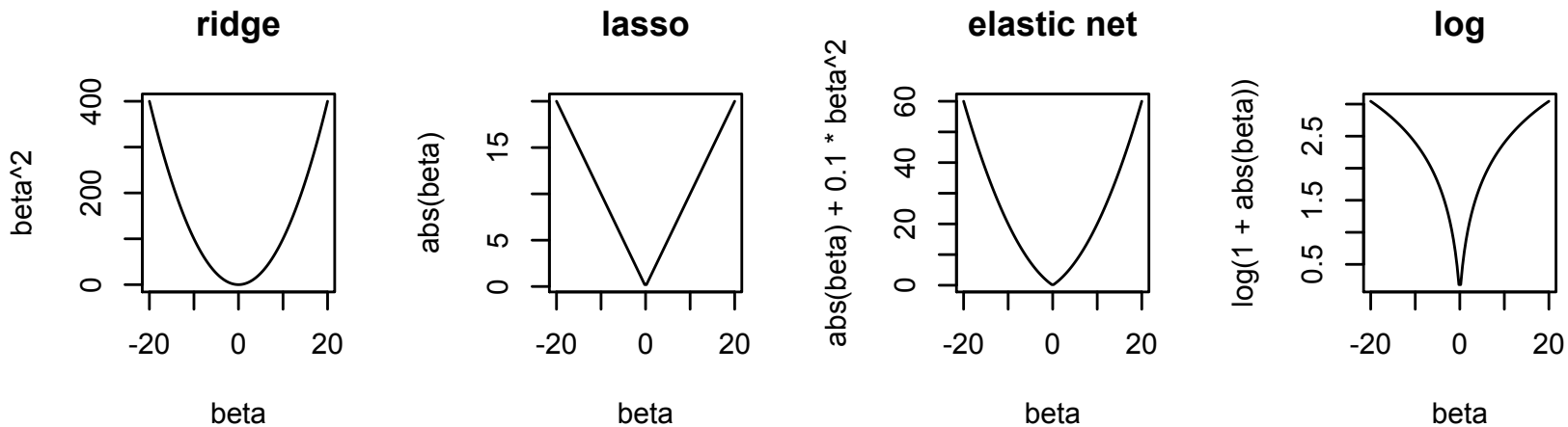
Since $\hat{\beta}_j = 0$ is *safe*, it should cost us to decide otherwise.

$\Rightarrow$ The cost of $\hat{\beta}$ is deviance plus a penalty away from zero.

[Sparse] Regularized Regression

$$\min \left\{ -\frac{2}{n} \log \mathrm{LHD}(\boldsymbol{\beta}) + \lambda \sum_j c(\beta_j) \right\}$$

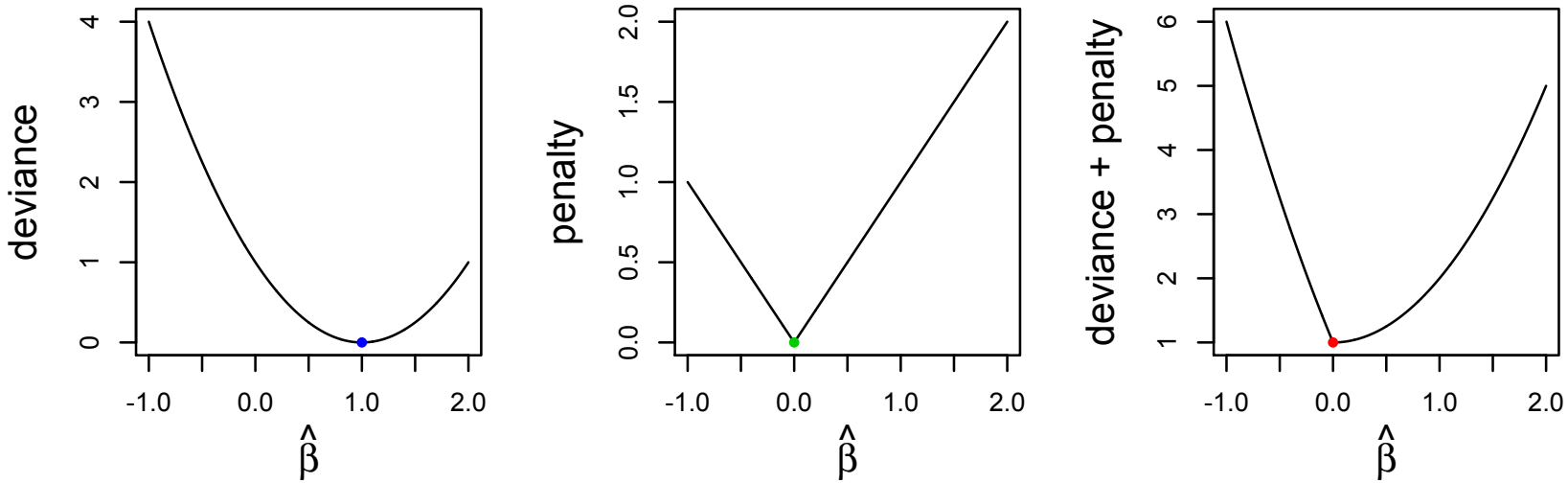
$\lambda > 0$ is the penalty weight, c is a cost (penalty) function.
$c(\beta)$ will be lowest at $\beta = 0$ and we pay more for $|\beta| > 0$.



Options: ridge β^2, lasso $|\beta|$, elastic net $\alpha\beta^2 + |\beta|$, $\log(1 + |\beta|)$.

Penalization can yield automatic variable selection

The minimum of a smooth + pointy function can be at the point.



Anything with an absolute value (e.g., lasso) will do this.

There are MANY penalty options and far too much theory.

Think of lasso as a baseline, and others as variations on it.

Lasso Regularization Paths

The lasso fits $\hat{\boldsymbol{\beta}}$ to minimize $-\frac{2}{n}\log \text{LHD}(\boldsymbol{\beta}) + \lambda \sum_j |\beta_j|$.

We'll do this for a *sequence* of penalties $\lambda_1 > \lambda_2 ... > \lambda_T$.

Then we can apply model selection tools to choose best $\hat{\lambda}$.

Path estimation:

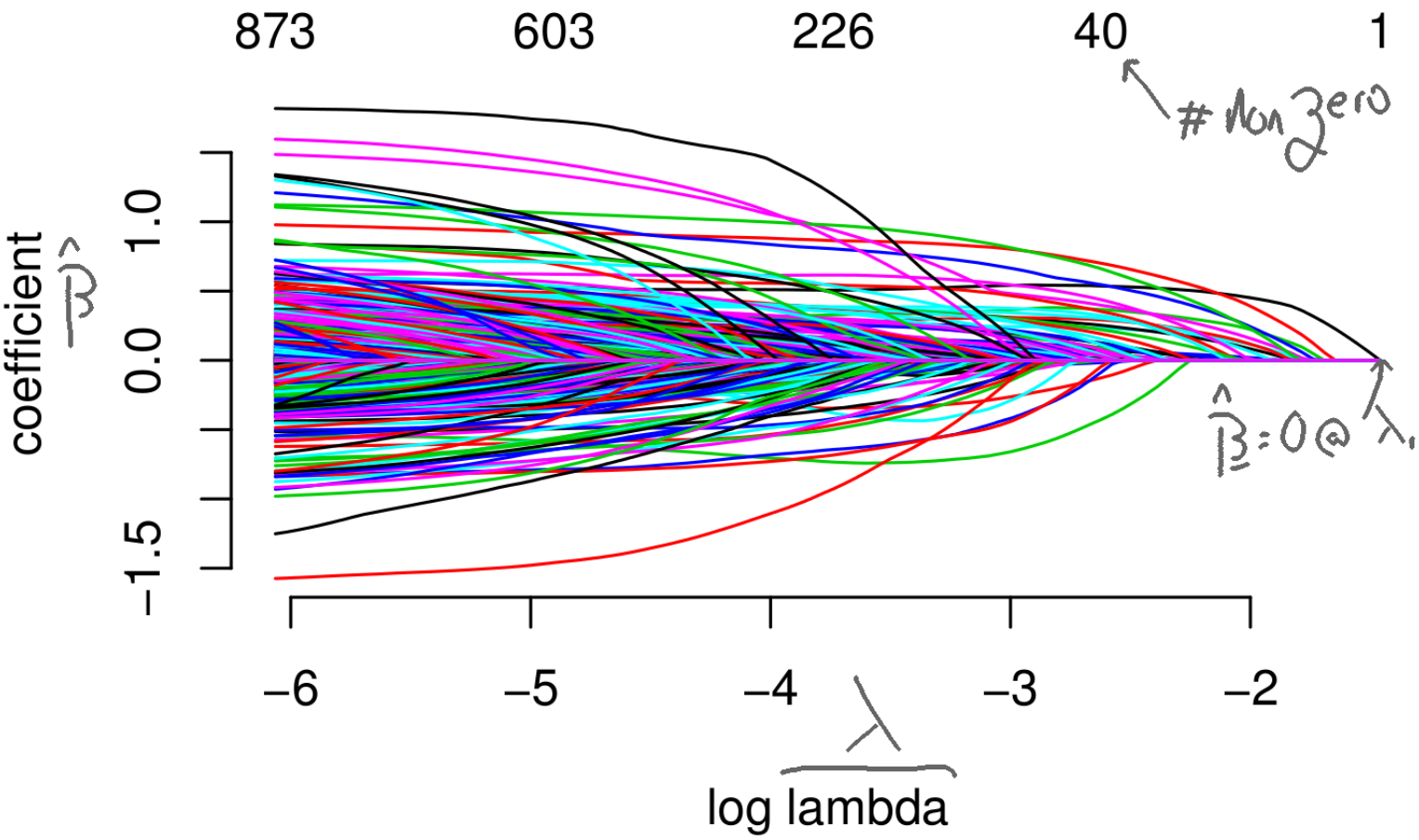
Start with big λ_1 so big that $\hat{\boldsymbol{\beta}} = \mathbf{0}$.

For $t = 2 \dots T$: update $\hat{\boldsymbol{\beta}}$ to be optimal under $\lambda_t < \lambda_{t-1}$.

Since estimated $\hat{\boldsymbol{\beta}}$ changes smoothly along this path:

- It's fast! Each update is easy.
- It's stable: optimal λ_t may change a bit from sample to sample, but that won't affect the model much.

The whole enterprise is easiest to understand visually.



The algorithm moves *right to left*.

The y-axis is $\hat{\boldsymbol{\beta}}$ (each line a different $\hat{\beta}_j$) as a function of λ_t.

Example: web browser data

The previous plot is household log-online-spend regressed onto % of time spent on various websites (each β_j a different site).

Browsing and purchasing behavior for households:

I've extracted 2006 data for the 1000 most heavily trafficked websites and for 10,000 households that spent at least 1$.

Why do we care? Predict consumption from browser history.

faculty.chicagobooth.edu/matt.taddy/teaching/comscore.R

There are many packages for fitting lasso regressions in R.

`glmnet` is most common. `gamlr` is my contribution.
These two are very similar, and they share syntax.

Big difference is what they do beyond a simple lasso:.

- `glmnet` does an 'elastic net': $c(\beta) = |\beta| + \nu\beta^2$.
- `gamlr` does a 'gamma lasso': $c(\beta) \approx \log(\nu + |\beta|)$.

Both use the `Matrix` library representation for sparse matrices.

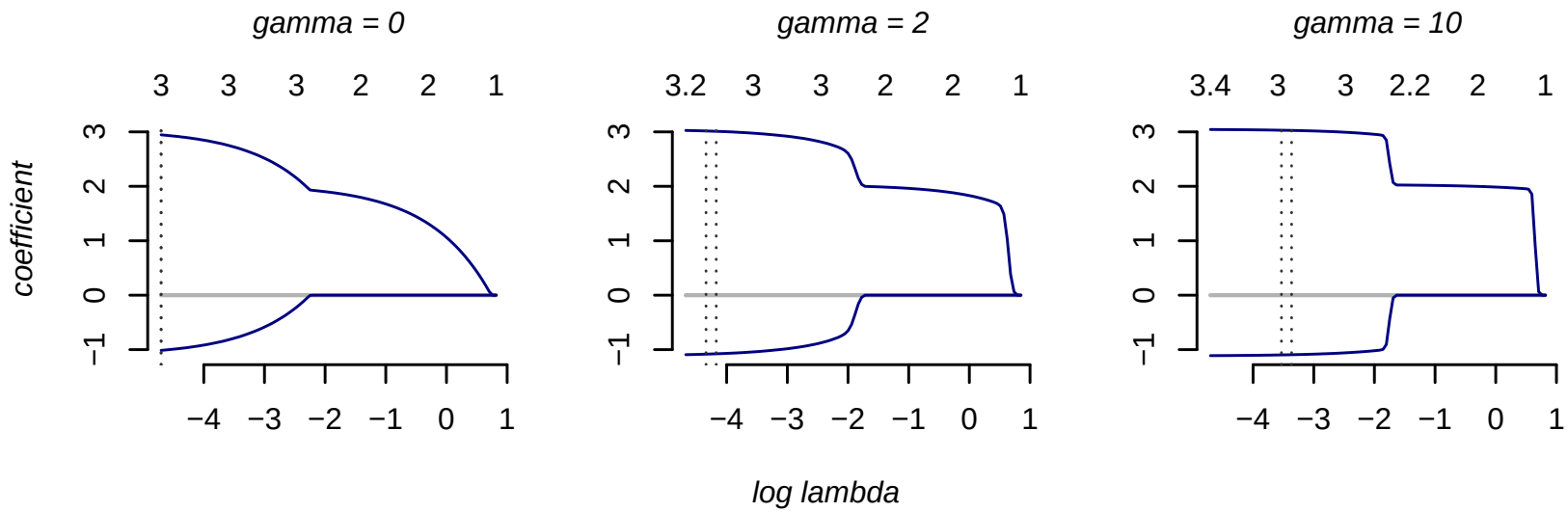
A little bit more info on `gamlr`:

it actually applies a weighted L_1 penalty: $\lambda \sum_j \omega_j |\beta_j|$.

These weights adapt along the regularization path as a function of the previous segment's solution

$$\omega_j^t = \left(1 + \gamma |\hat{\beta}_j^{t-1}|\right)^{-1} \quad j = 1 \dots p \tag{1}$$

This lets you measure large signals with less bias.



See *Paths of One-Step Estimators* on my website.

Regularization and Selection

The lasso minimizes $-\frac{2}{n}\log \mathrm{LHD}(\boldsymbol{\beta}) + \lambda \sum_j |\beta_j|$.

This 'sparse regularization' auto-selects the variables.

Sound too good to be true? You need to choose λ.

Think of $\lambda > 0$ as a signal-to-noise filter: *like squelch on a radio.*

We'll use cross validation or information criteria to choose.

Path algorithms are key to the whole framework:

⋆ They let us quickly enumerate a set of candidate models.

⋆ This set is stable, so selected 'best' is probably pretty good.

A recipe for model selection.

1. Find a manageable set of candidate models (i.e., such that fitting all models is fast).
2. Choose amongst these candidates the one with best predictive performance *on unseen data*.

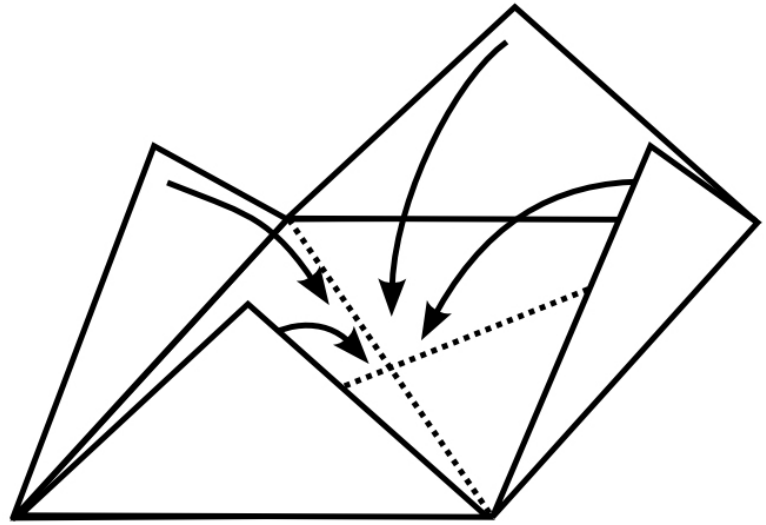
1. is what the lasso paths provide.
2. Seems impossible! But it's not ...

First, define predictive performance via 'deviance'.

Then, we need to *estimate* deviance for a fitted model applied to *new independent observations* from the true data distribution.

K-fold Cross Validation

One option is to just take
repeated random samples.
It is better to 'fold' your data.



- Sample a random ordering of the data
  (important to avoid order dependence)
- Split the data into K folds: 1st 100/K%, 2nd 100/K%, etc.
- Cycle through K CV iterations with a single fold left-out.

This guarantees each observation is left-out for validation,
and lowers the sampling variance of CV model selection.

Leave-one-out CV, with $K = n$, is nice but takes a long time.
$K = 5$ to 10 is fine in most applications.

CV Lasso

The lasso path algorithm minimizes $-\frac{2}{n}\log \text{LHD}(\boldsymbol{\beta}) + \lambda_t \sum_j |\beta_j|$ over the sequence of penalty weights $\lambda_1 > \lambda_2 \ldots > \lambda_T$.

This gives us a path of T fitted coefficient vectors, $\hat{\boldsymbol{\beta}}_1 \ldots \hat{\boldsymbol{\beta}}_T$, each defining deviance for new data: $-\log \text{p}(\mathbf{y}^{new} \mid \mathbf{X}^{new}\hat{\boldsymbol{\beta}}_t)$.

Set a sequence of penalties $\lambda_1 \ldots \lambda_T$.
Then, for each of $k = 1 \ldots K$ folds,

- Fit the path $\hat{\boldsymbol{\beta}}^k_1 \ldots \hat{\boldsymbol{\beta}}^k_T$ on all data *except* fold k.
- Get fitted deviance *on left-out data*: $-\log \text{p}(\mathbf{y}^k \mid \mathbf{X}^k\hat{\boldsymbol{\beta}}_t)$.

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

Finally, use the results to choose the 'best' $\hat{\lambda}$, then re-fit the model to *all of the data* by minimizing $-\frac{2}{n}\log \text{LHD}(\boldsymbol{\beta}) + \hat{\lambda} \sum_j |\beta_j|$.

CV Lasso

Both `gamlr` and `glmnet` have functions to wrap this all up.
The syntax is the same; just preface with `cv.`.

```
cv.spender <- cv.gamlr(xweb, log(yspend))
```

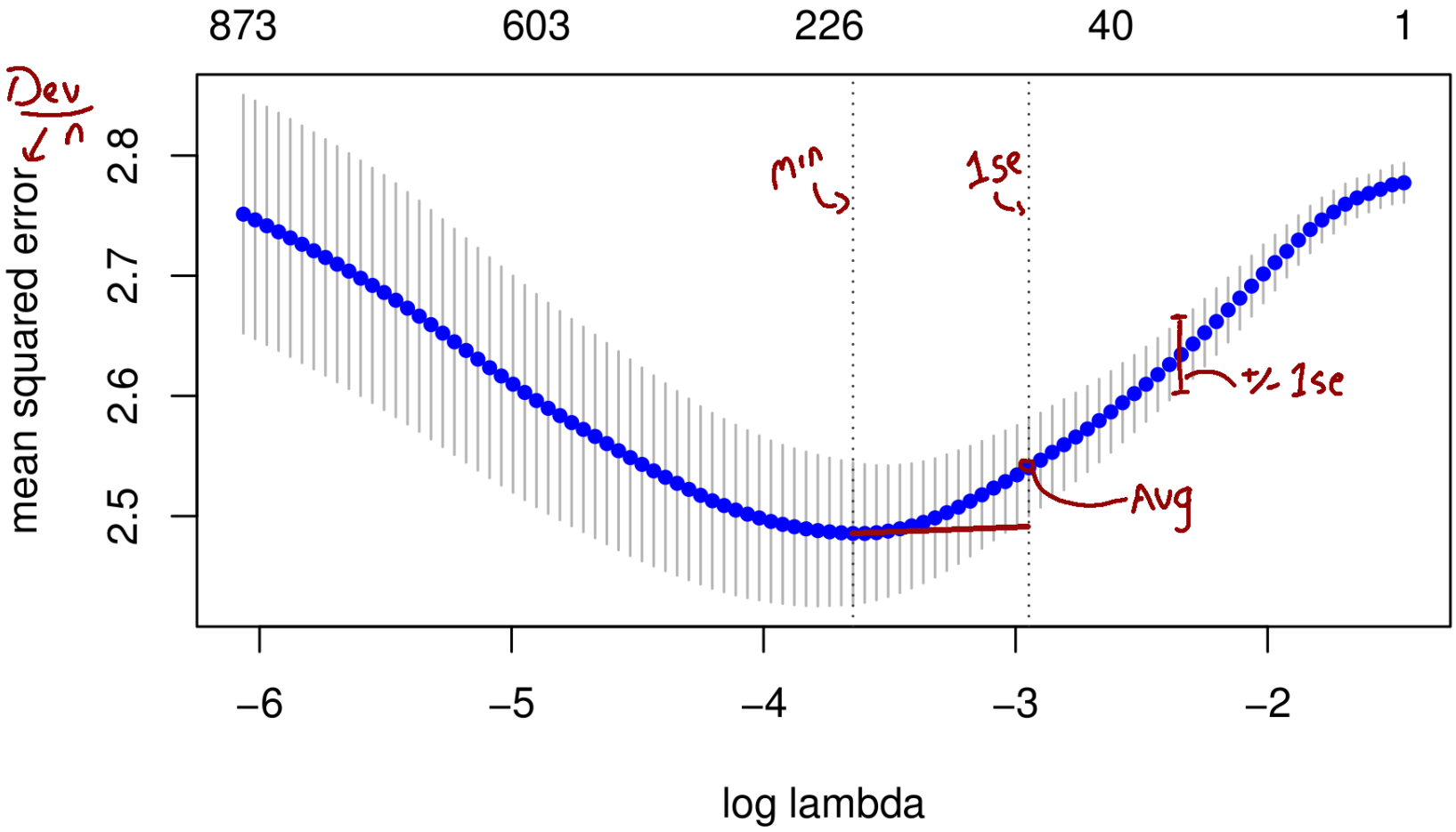
Then, `coef(cv.spender)` gives you $\hat{\beta}_t$ at the 'best' λ_t

- `select="min"` gives λ_t with *min average OOS deviance*.
- `select="1se"` defines best as *biggest* λ_t *with average OOS deviance no more than 1SD away from the minimum.*

`1se` is default, and balances prediction against false discovery.
`min` is purely focused on predictive performance.

CV Lasso

Again, the routine is most easily understood visually.



Both selection rules are good; `1se` has extra bias for simplicity.

Problems with Cross Validation

It is time consuming: When estimation is not instant, fitting K times can become unfeasible even K in 5-10.

It can be unstable: imagine doing CV on many different samples. There can be large variability on the model chosen.

It is hard not to cheat: for example, with the FDR cut model we've already used the full n observations to select the 25 strongest variables. It is not surprising they do well 'OOS'.
The rules: if you do something to the data, do it *inside* CV.

Still, some form of CV is used in most DM applications.

Alternatives to CV: **Information Criteria**

Many 'Information Criteria' out there: AICc, AIC, BIC, ...
These approximate distance between a model and 'the truth'.
You can apply them by choosing the model with minimum IC.

Most common is Akaike's AIC $=$ Deviance $+ 2df$.

$df =$ 'degrees of freedom' used in your model fit.
For lasso and MLE, this is just the # of nonzero $\hat{\beta}_j$.

AIC overfits in high dimensions

The AIC is atually estimating OOS deviance: what your deviance would be on another *independent* sample of size n.

IS deviance is too small, since the model is tuned to this data.
Some deep theory shows that IS - OOS deviance $\approx 2df$.

$$\Rightarrow \text{AIC} \approx \text{OOS deviance.}$$

Its common to claim this approx (i.e., AIC) is good for 'big n'.
Actually, its only good for big n/df.

In Big Data, df (# parameters) can be huge. Often $df \approx n$.
In this case the AIC will be a bad approximation: it overfits!

AIC corrected: AICc

AIC approximates OOS deviance, but does a bad job for big df.

In linear regression an improved approx to OOS deviance is

$$\text{AICc} = \text{Deviance} + 2df\,\mathbb{E}\left[\frac{\sigma^2}{\hat{\sigma}^2}\right] = \text{Deviance} + 2df\,\frac{n}{n - df - 1}$$

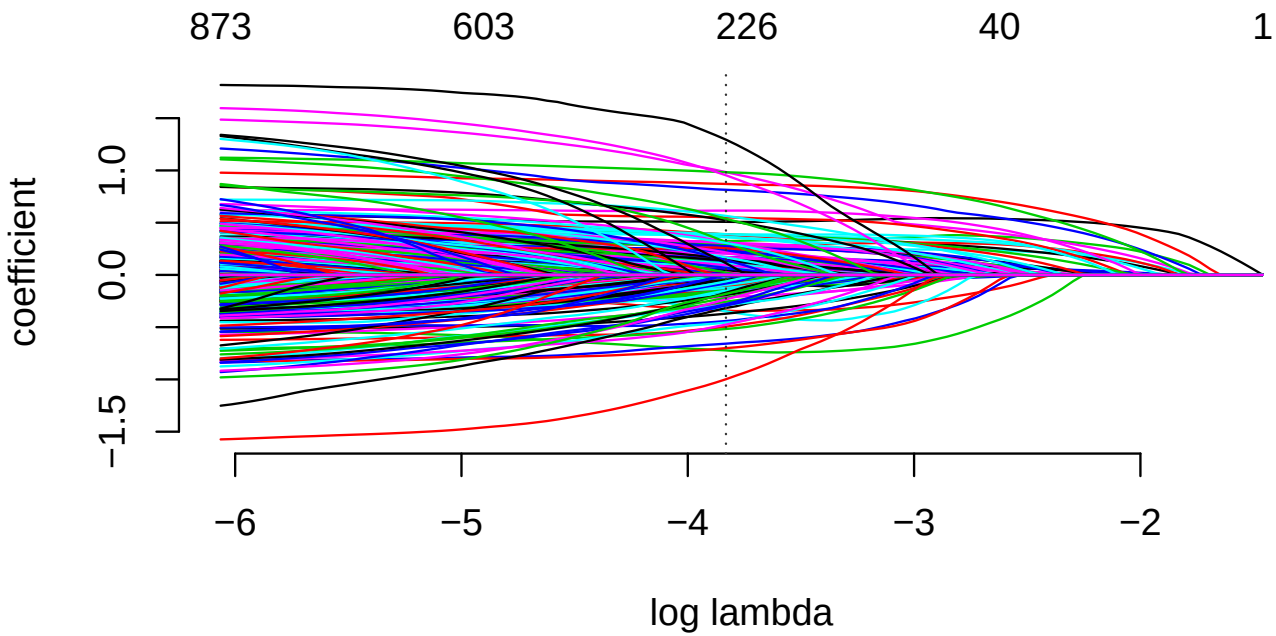
This is the corrected AIC, or AICc.

It also works nicely in logistic regression, or for any `glm`.

Notice that for big n/df, AICc $\approx$ AIC. So *always* use AICc.

gamlr uses AICc

It's marked on the path plot

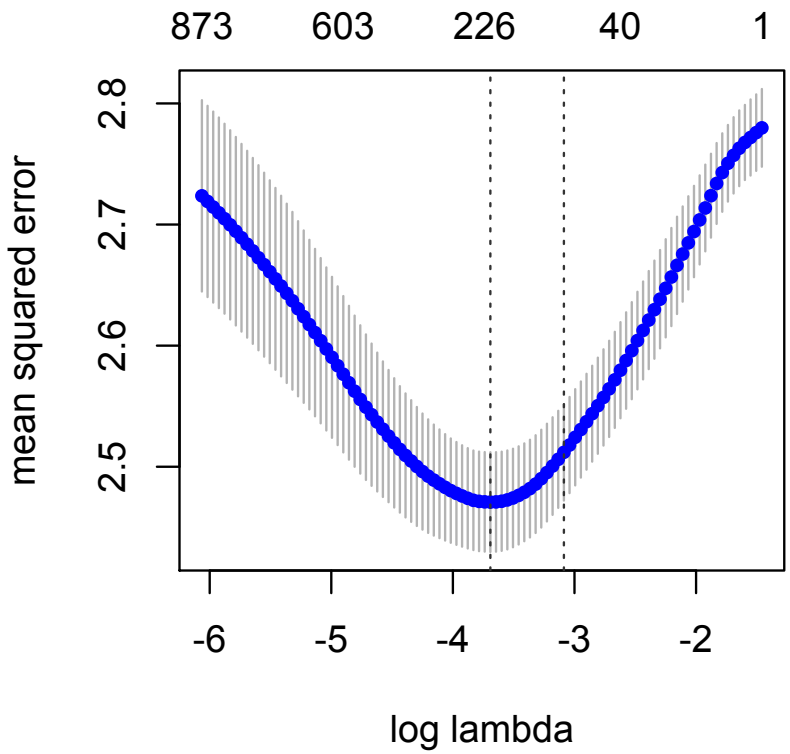


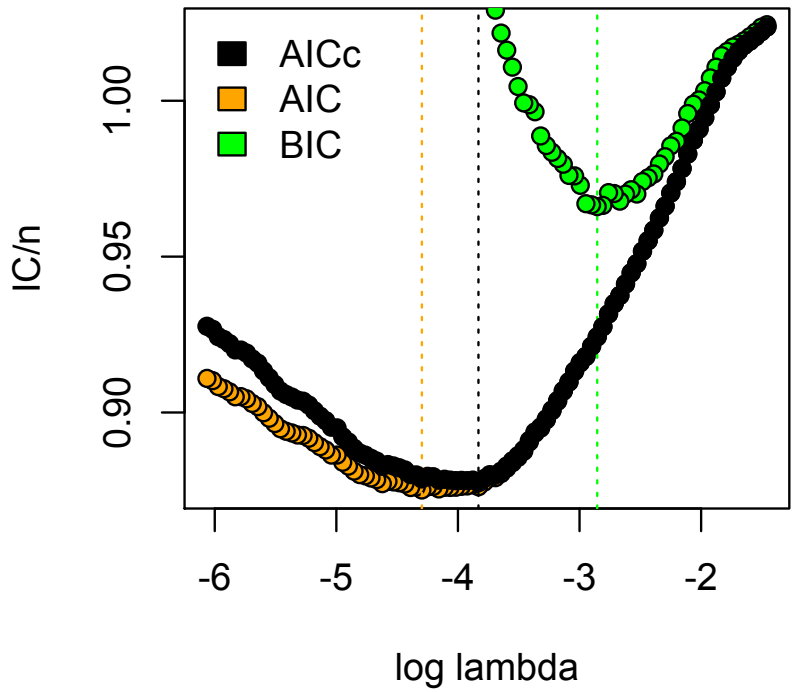
And it is the default for `coef.gamlr`

```
B <- coef(spender)[-1,]
B[c(which.min(B),which.max(B))]
```

```
    cursormania.com shopyourbargain.com
          -0.998143             1.294246
```

IC and CV on the Comscore Data

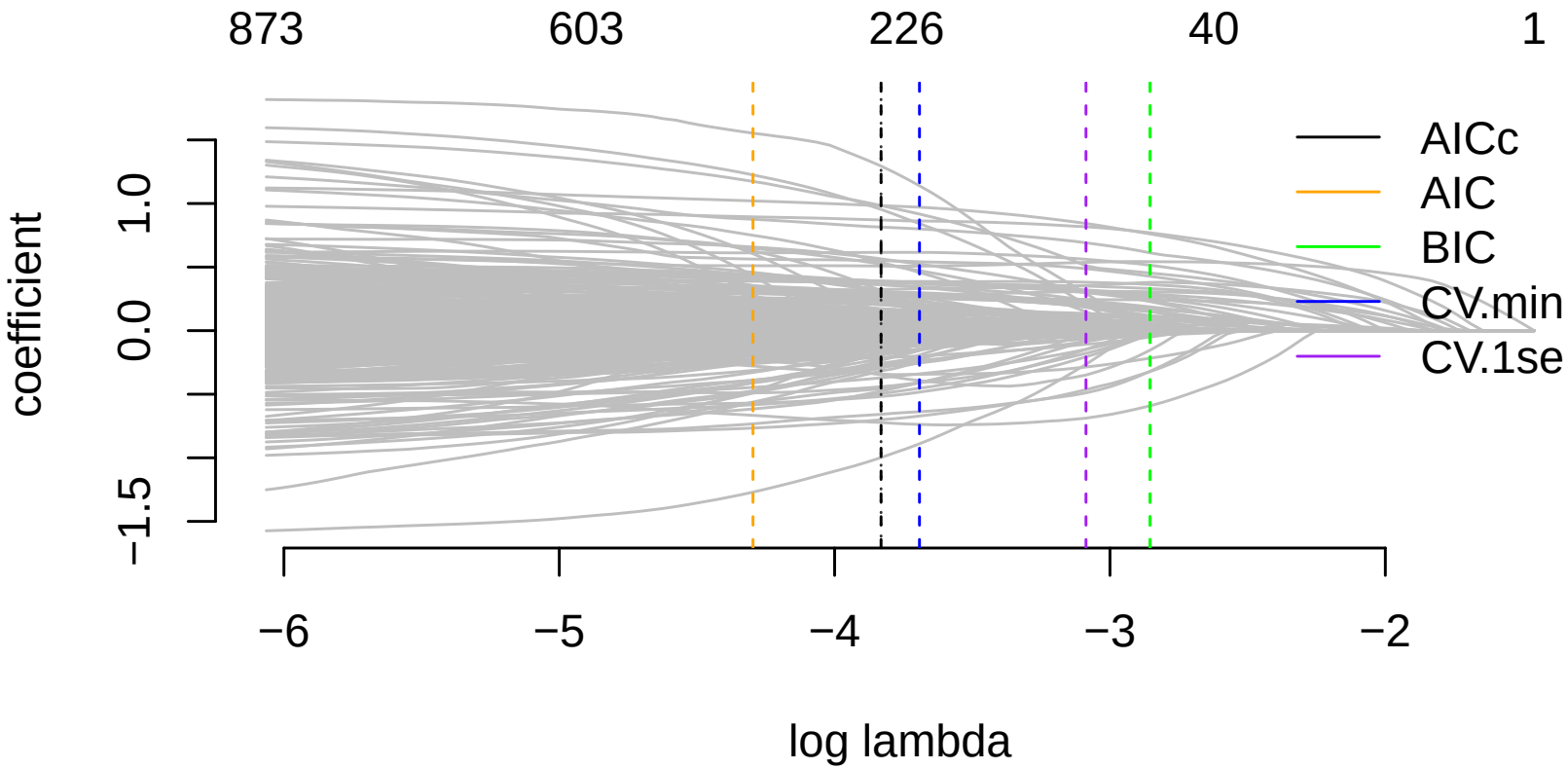




The take home message: AICc curve looks like CV curve.

In practice, BIC works more like the 1se CV rule.
But with big n it chooses too simple models (it underfits).

IC and CV on the Comscore Data



With all of these selection rules, you get a range of answers.

If you have time, do CV. But AICc is fast and stable.

If you are worried about false discovery, tend towards BIC/1se.