Big Data Analysis

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Outline

What is [good] data mining? Discovery without overfit.
For most of today, it is variable selection in high dimensions.

Three ingredients to model building:

Model metrics: False Discovery proportion, Out-of-sample deviance, model probabilities.

Estimation of these metrics: FD Rate control, n-fold cross validation, and information criteria.

Building sets of candidate models: p-value cut-offs, stepwise regression, regularization paths.

If there is time we can discuss factor models and PCR.

An example: Comscore web data

Detailed information about browsing and purchasing behavior.
100k households, 60k where any money was spent online.
I've extracted info for the 8k websites viewed by at least 5%.

Why do we care? Predict consumption from browser history.

e.g., to control for base-level spending, say, in estimating advertising effectiveness. You'll see browser history of users when they land, but likely not what they have bought.
Thus predicting one from the other is key.

Potential regressions: $\mathrm{p}(\$ > 0|\mathbf{x})$ or $\mathbb{E}[\log \$|\$ > 0, \mathbf{x}]$.

$\mathbf{x}$ is just time spent on different domains. It could also include text or images on those websites or generated by the user (facebook) or their friends... data dimension gets huge fast.

DM is discovering patterns in high dimensional data

Data is usually big in both the number of observations ('n') and in the number of variables ('p'), but any $p \approx n$ counts.

In scientific applications, we want to summarize HD data in order to relate it to structural models of interest.

$\Rightarrow$ interpretable variables or factors, causal inference.

We also want to predict! If things don't change too much...

$\Rightarrow$ sparse or low-dimensional bases, ensemble learning.

The settings overlap and have one goal: Dimension Reduction.

Model Building: Prediction vs Inference

In some sense it is all about prediction.

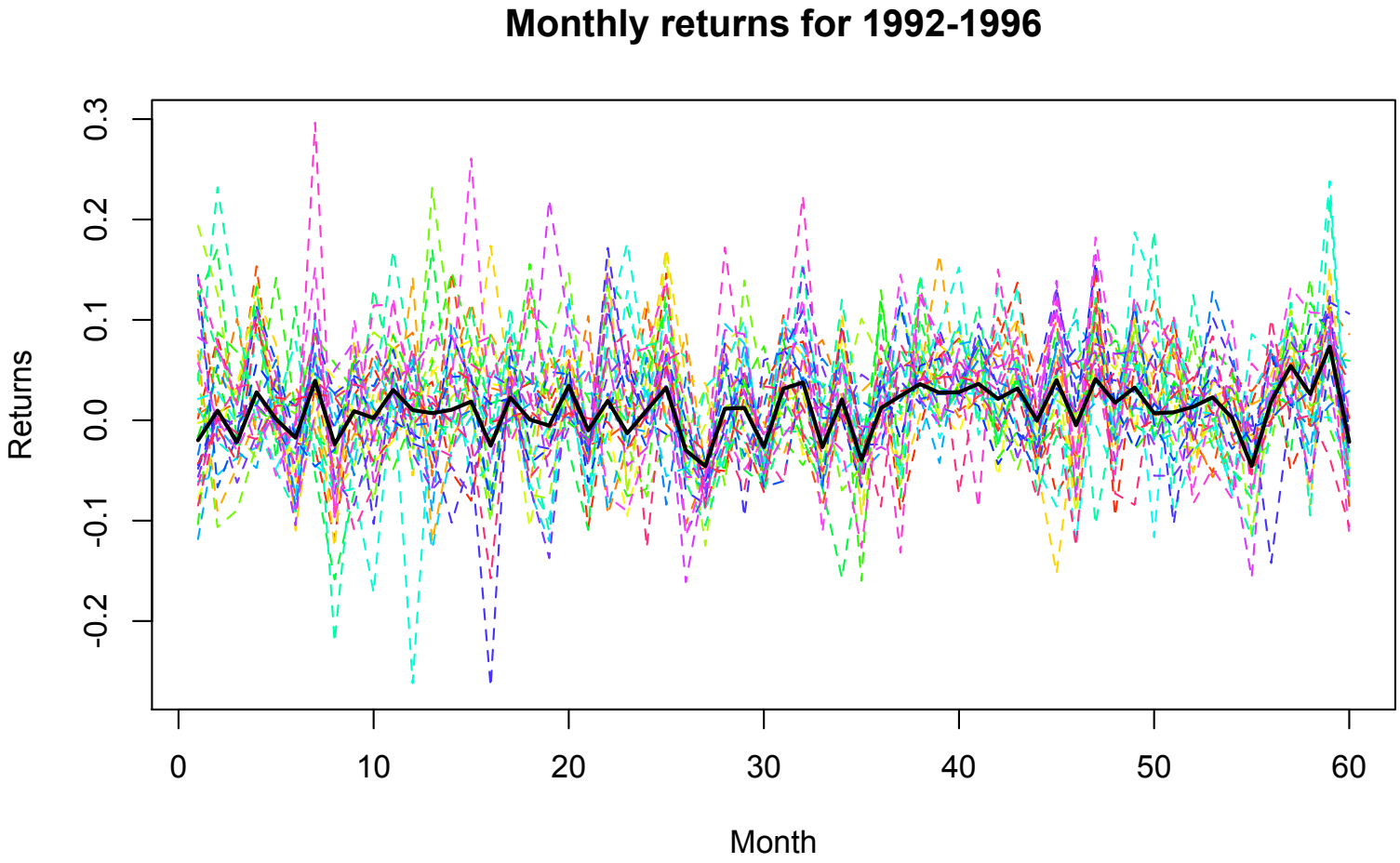
> Predictive modeling to forecast $y \mid \mathbf{x}$
> where both are drawn from some joint $\mathrm{p}(y, \mathbf{x})$.
>
> Causal modeling to forecast $y \mid d, \mathbf{x}$
> when d moves *but* $\mathbf{x}$ *is held constant*.

In the former, DR is 'in the direction' of y. In the latter, DR is in the direction of specific parameters in structural models.

You need to walk before you can run: good prediction is a pre-req for causal inference. For example, one 'controls for' $\mathbf{x}$ by building predictive each of $y|\mathbf{x}$ and $d|\mathbf{x}$.

Everything requires a different approach when $n \approx p$ are big.

A Fancy Plot: Monthly Stock Returns

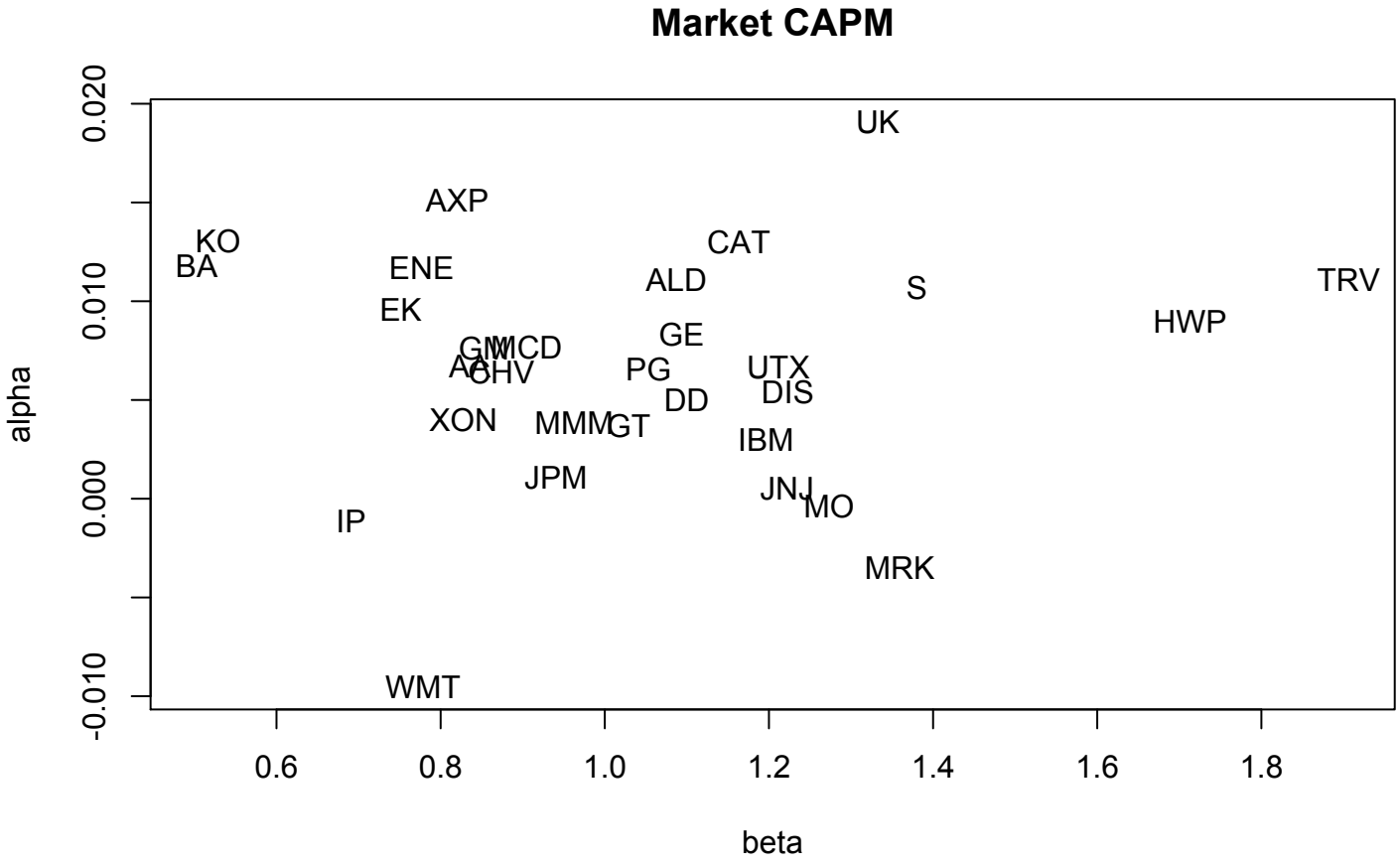


30 stocks, with the S&P 500 index in bold.

But what insight do we really gain?

A Powerful Plot: S&P Market Model Regression

CAPM regresses returns on the "market": $R \approx \alpha + \beta M$.



CAPM is great predicitive DM and, with factor interpretation through the efficient market story, it is also a structural model.

Model and Variable Selection

DM is the discovery of patterns in high dimensions.
Good DM is on constant guard against false discovery.

False Discovery = Overfit: you model idiosynchratic noise and the resulting predictor does very poorly on new data.

The search for *useful* real patterns is called model building. In linear models, this is a question of 'variable selection'.

$$\text{Given } \mathbb{E}[y|\mathbf{x}] = f(\mathbf{x}'\boldsymbol{\beta}), \text{ which } \beta_j \text{ are nonzero?}$$

Linear models dominate economics and we focus on variable selection. Since $\mathbf{x}$ can include arbitrary input transformations and interactions, this is less limiting than it might seem.

All there is to know 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): $\mathrm{p}(y = 1) = e^{\mathbf{x}\boldsymbol{\beta}}/(1 + e^{\mathbf{x}\boldsymbol{\beta}})$.
- Poisson (log): $\mathbb{E}[y] = \mathrm{var}(y) = \exp[\mathbf{x}'\boldsymbol{\beta}]$.

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

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

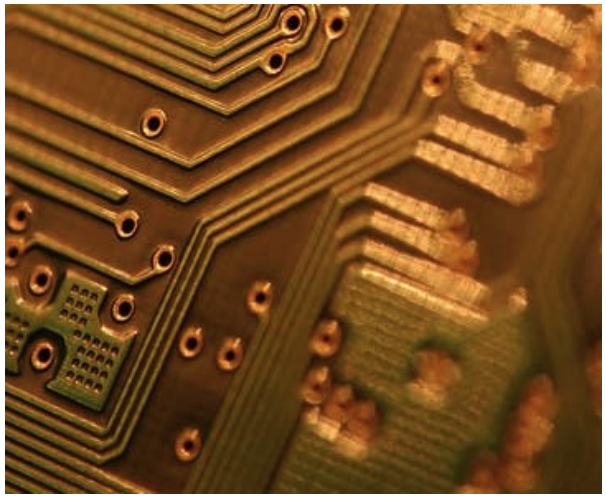
The deviance at $\hat{\boldsymbol{\beta}}$ is 2log(saturatedLHD) - 2 logLHD($\hat{\boldsymbol{\beta}}$).

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

EG, linear regression deviance is the sum of squares and $R^2 = 1 - \mathrm{SSE}/\mathrm{SST}$ is the 'proportion of variance explained'.

In DM the only R^2 we ever care about is out-of-sample R^2.

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

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

The x_{ij} inputs here are actually orthogonal: they are the first 200 Principal Component directions from an even bigger set.

Model fit and choice for the semiconductors

In-sample (IS) R^2 (i.e., the thing $\hat{\beta}$ was fit to maximize) is 0.56 for the full regression model (using all 200 signals).

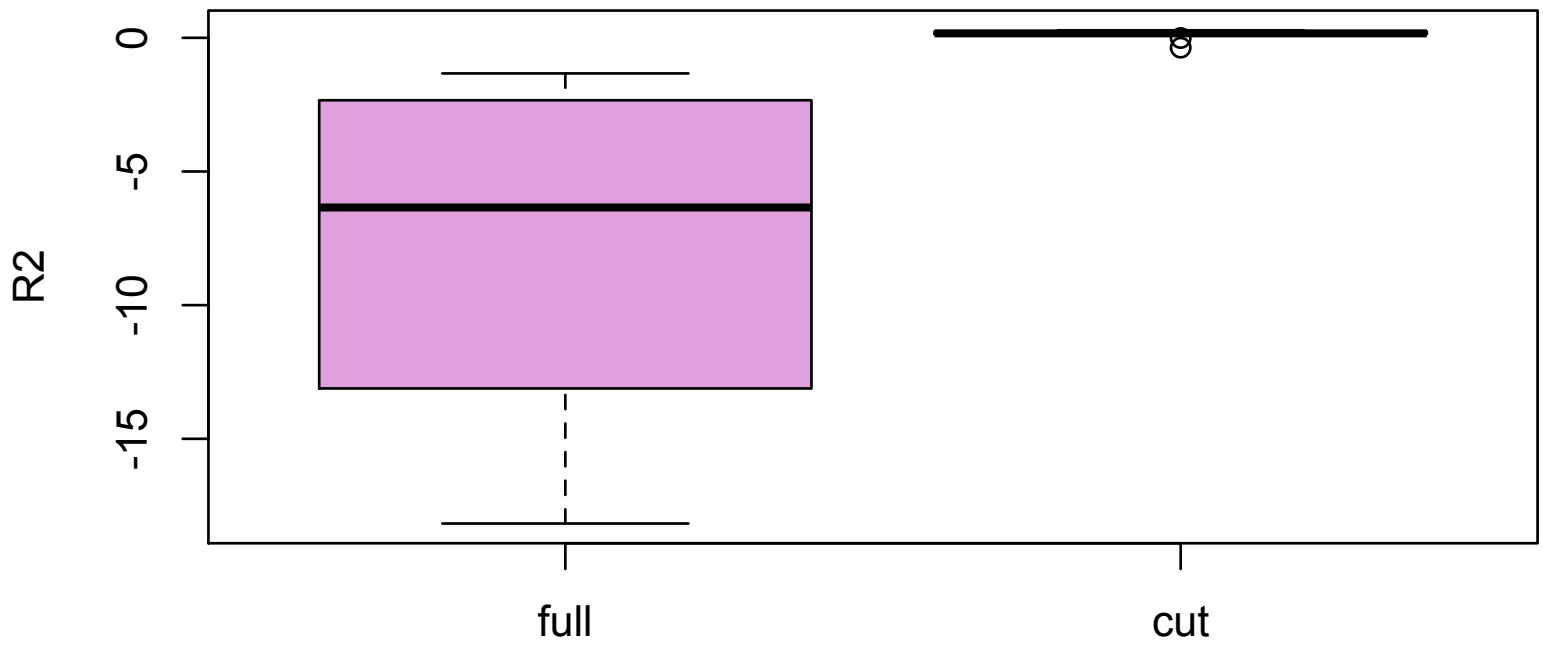
An alternative 'cut' model uses only the 25 signals of highest absolute correlation with `fail`. IS R^2 for this model is 0.24.

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.

Out-of-Sample prediction for semiconductor failure



We've gained OOS predictive accuracy by dropping variables.

The full model is very poor. It is overfit and worse than $\bar{y}$.

Negative R2 are more common than you might expect.

Cut model has mean OOS R2 of 0.12, about 1/2 in-sample R2.

Our standard tool to avoid false discovery is hypothesis testing.

Hypothesis Testing: a one-at-a-time procedure.

Recall: p-value is probability of getting a test statistic farther into the distribution tail than what you observe: $P(Z > z)$.

Testing procedure: Choose a cut-off 'α' for your p-value 'p', and conclude significance (e.g., variable association) for $p < \alpha$.

This is justified as giving only α probability of a false-positive. For example, in regression, $\hat{\beta} \neq 0$ only if its p-value is less than the accepted risk of a false discovery for each coefficient.

Contingency Tables:

discovering association / testing independence

Factor on factor comparisons in a contingency table

	Belief in an Afterlife	
Gender	Yes	No/Unsure
Females	509	116
Males	398	104

NORC: 1998 General Social Survey

This tabulates cross-classification of two factors.

If two factors are independent, then any level of one should have the same probability for each level of the other factor.

Review: Pearson chi-squared tests for independence

Consider a table with $i = 1...\mathrm{I}$ rows and $j = 1...\mathrm{J}$ columns.

If the two factors are independent, expected cell counts are $E_{ij} = \text{row.total}_i \times \text{column.total}_j / N$. and the statistic

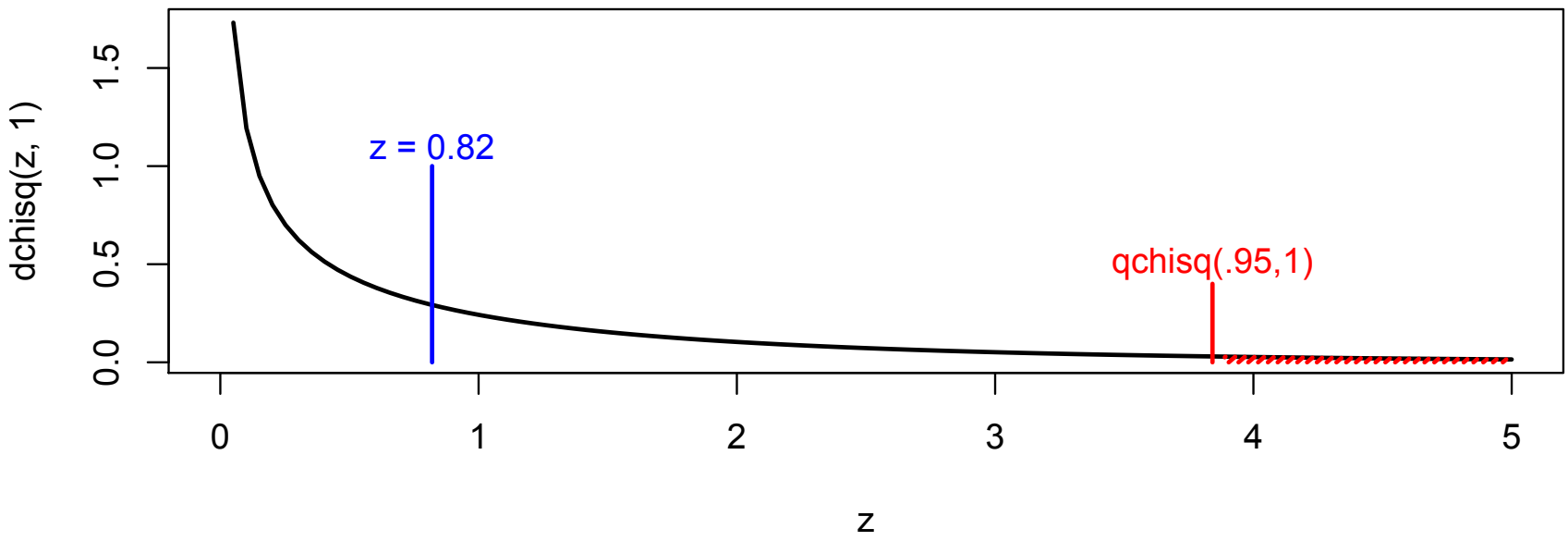
$$Z = \sum_i \sum_j \frac{(N_{ij} - E_{ij})^2}{E_{ij}}$$

has χ^2 distribution with $df = (I-1)(J-1)$ degrees of freedom.

The continuity approximation that requires $E_{ij} \geq 5$ish. Some software make small changes, but this is the basic formula.

Independence of Sex and the Afterlife

$$z = \frac{(509-503)^2}{503} + \frac{(398-404)^2}{404} + \frac{(116-122)^2}{122} + \frac{(104-98)^2}{98} \approx 0.8$$



No association between gender and afterlife beliefs.

The problem of multiplicity

α is for a single test. If you repeat many tests, about $\alpha \times 100\%$ of the null tests should erroneously pop up as significant.

Things are especially dire with rare signals:

Suppose that 5 of 100 regression coefficients are actually influential, and that you find all of them significant.

Test the rest of them at $\alpha = 0.05$:

Since you reject H_0 for 5% of the useless 95 variables, $4.75/9.75 \approx$ 50% of significant tests are false discoveries!

This is called the False Discovery Proportion (FDP).
For fixed α it gets smaller with 1-N_0/N (true non-Null rate).
Many examples have $\ll 1\%$ useful x's (genes, sites, words).

The False Discovery Rate

Instead of focusing on each test, we'll consider

$$\text{FD Proportion} = \frac{\#\text{ false positives}}{\#\text{ tests called significant}}$$

FDP is a property of our fitted model. We can't know it.
But we can derive its expectation under some conditions.

This is called the False Discovery Rate, FDR $= \mathbb{E}[\text{FDP}]$.

It is the multivariate (aggregate) analogue of α.

False Discovery Rate control

The Benjamini + Hochberg (BH) algorithm:

Rank your N p-values, smallest to largest, $p_{(1)} \dots p_{(N)}$.

Choose the q-value 'q', where you want FDR $\leq q$.
Set the p-value cut-off as $p^\star = \max\left\{p_{(k)} : p_{(k)} \leq q\frac{k}{N}\right\}$.

If your rejection region is p-values $> p^\star$, then FDR $\leq q$.

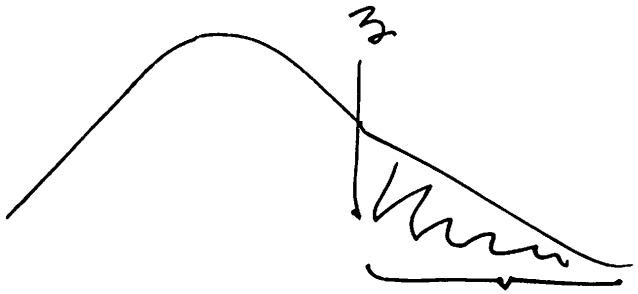
BH assumes independence between tests.

This condition can be weakened (only pos corr.) or replaced:
see empirical Bayes book by Efron, full Bayes papers by Storey.

Regardless, it's an issue for anything based on marginal p-vals.

Motivating FDR control

P-values are uniformly distributed under the Null.



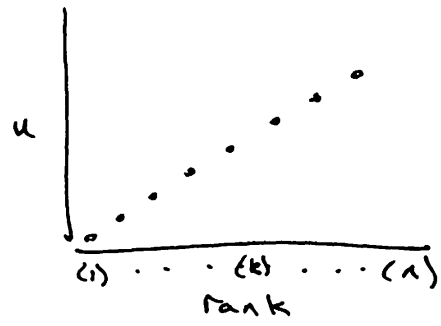
$\varphi(z) = P(Z > z)$

* Uniform CDF is $P(U < u) = u$
* $P(\varphi(Z) < \varphi(z)) = P(Z > z) = \varphi(z)$

$\Rightarrow \varphi(z) \sim$ Uniform.

Rank statistics from a uniform have Expectation $E[u_{(k)}] = \frac{k}{n}$ for sample size 'n'.

$\Rightarrow$ We can plot the mean w slope $\frac{1}{n}$



q is the slope of a shallower line defining our rejection region.

Demonstrating FDR control

Given our independence assumption the proof is simple.

N = total # tests, N_0 = # that are Null.

Say $R(u)$ is total w/ p-val $\le u$, & $r(u)$ is #Null w/ $p \le u$.

A cut-off equivalent to BH is

$$u^* = \max\left\{ u : u \le q \frac{R(u)}{N} \right\}$$

and then $\frac{1}{R(u^*)} \le q/N u^*$.

$\Longrightarrow$ FDP is $\frac{r(u^*)}{R(u^*)} \le q \frac{r(u^*)}{N u^*}$ w/ [Expectation $q \frac{N_0}{N}$]

(since $\mathbb{E}\left[\frac{r(u)}{u}\right] = N_0$ for unif. & indep. Null pvals.)

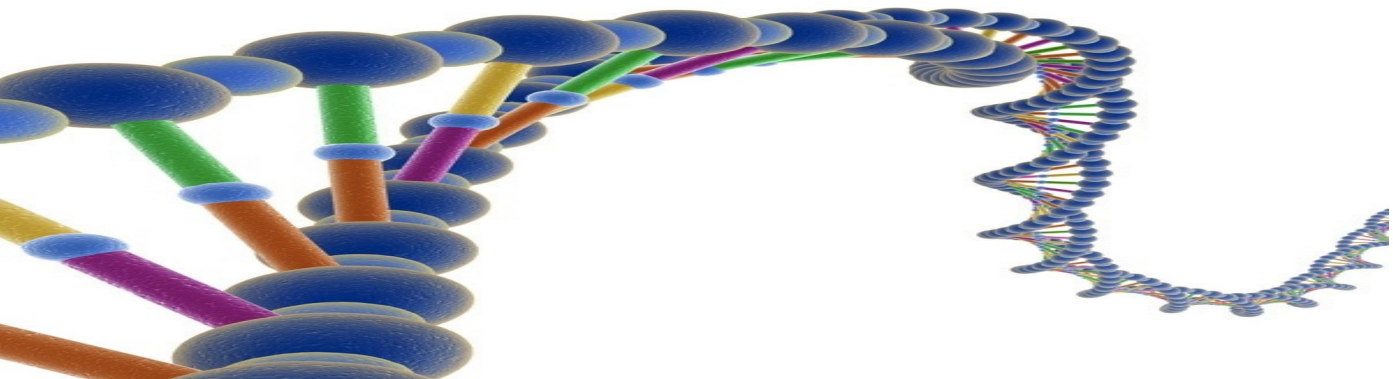
GWAS: genome-wide association studies

Given our weak understanding of the mechanisms, one tactic is to scan large DNA sequences for association with disease.

Single-nucleotide polymorphisms (SNPs) are paired DNA locations that vary across chromosomes. The allele that occurs most often is major (A), and the other is minor (a).

Question: Which variants are associated with increased risk?

Then investigate why + how.



Allele Association

A common SNP summary is Minor Allele Frequency (MAF):

$$\mathrm{AA} \to 0 \qquad \mathrm{Aa/aA} \to 1 \qquad \mathrm{aa} \to 2$$

Question: which MAF distributions vary with disease status?

Answer: a huge number of MAF×disease contingency tables.

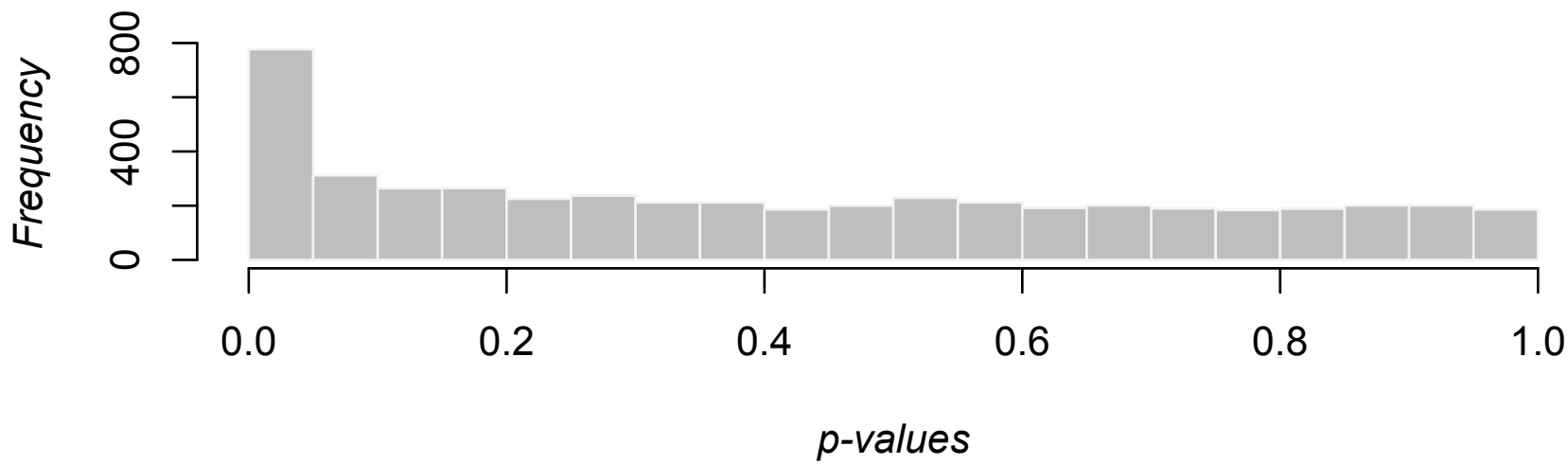
An example for type-2 Diabetes mellitus:

	MAF: `rs6577581`		
DM2 STATUS	0	1	2
case	357	72	27
control	428	54	1

χ^2 *stat is 32 on 2 df for* $p = 9{\times}10^{-8}$

Dataset has 1000 individuals, 1/2 diabetic, and 7597 SNPs.
Not all SNPs are recorded for all individuals, but most are.

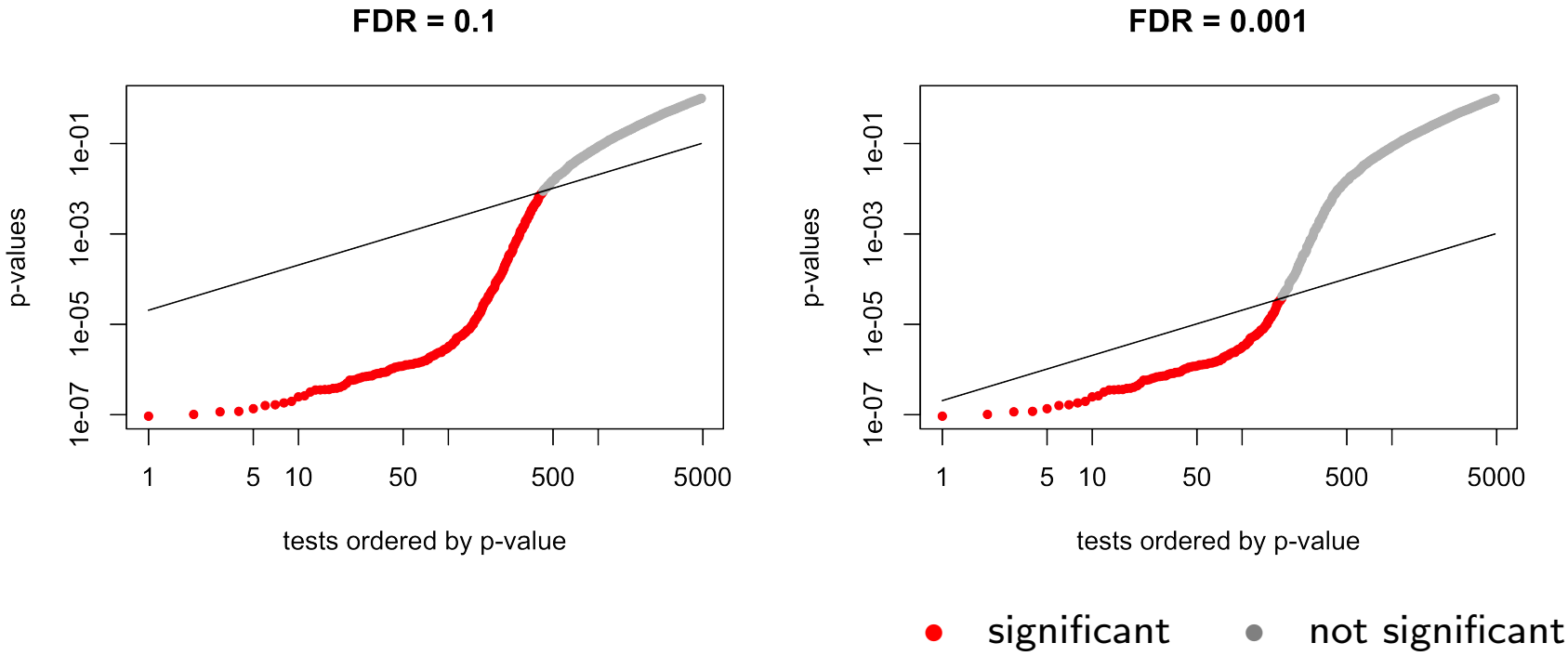
2712 of the tables have cell expectations < 5,
so the χ^2 approximation is invalid: drop them.
This leaves us with 4875 χ^2-test p-values.



Which are significant? We'll choose a cut-off to control FDR.

Controlling the False Discovery Rate

The slope of the FDR-cut line is q/[# of variables].

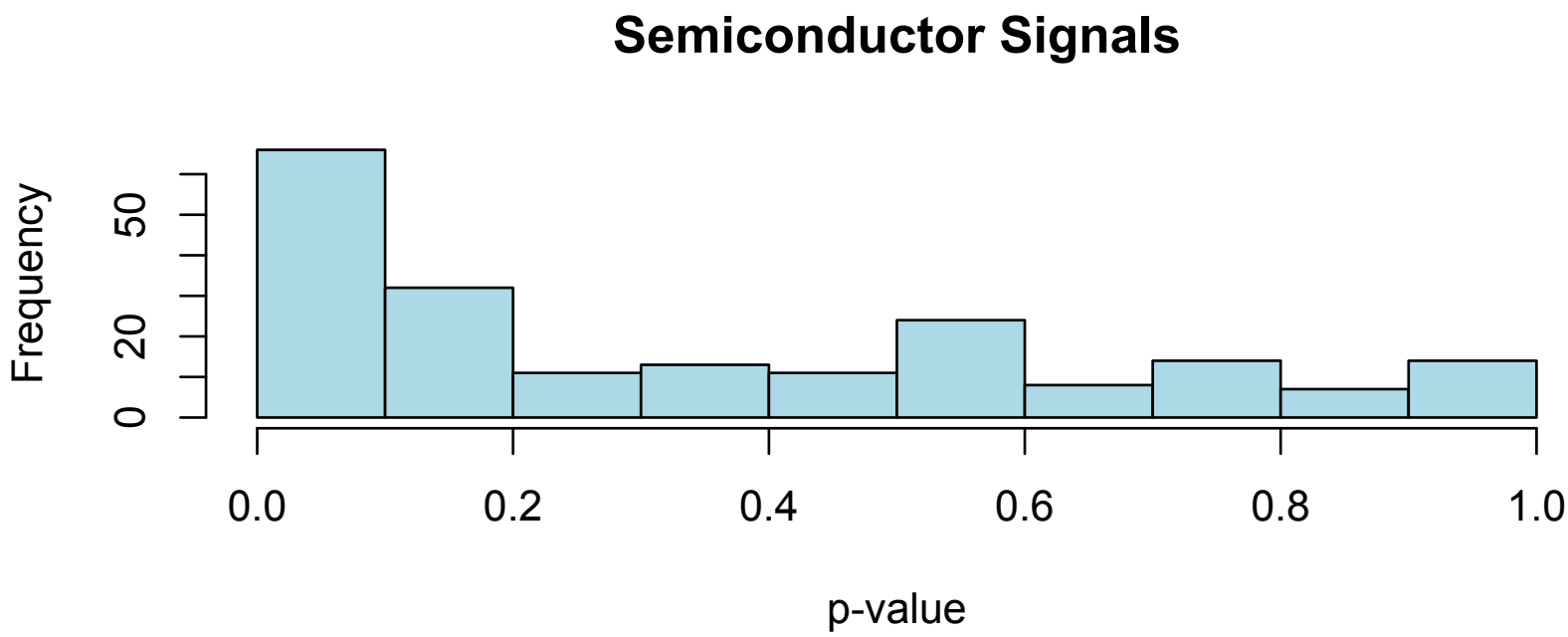


Lots of action!

183 significant tests at FDR of 1e−3. This is (for genetics) a massive sample, and these SNP locations were targeted.

Much GWAS is not as rich: e.g., Chabris+ Psych Sci 2012.

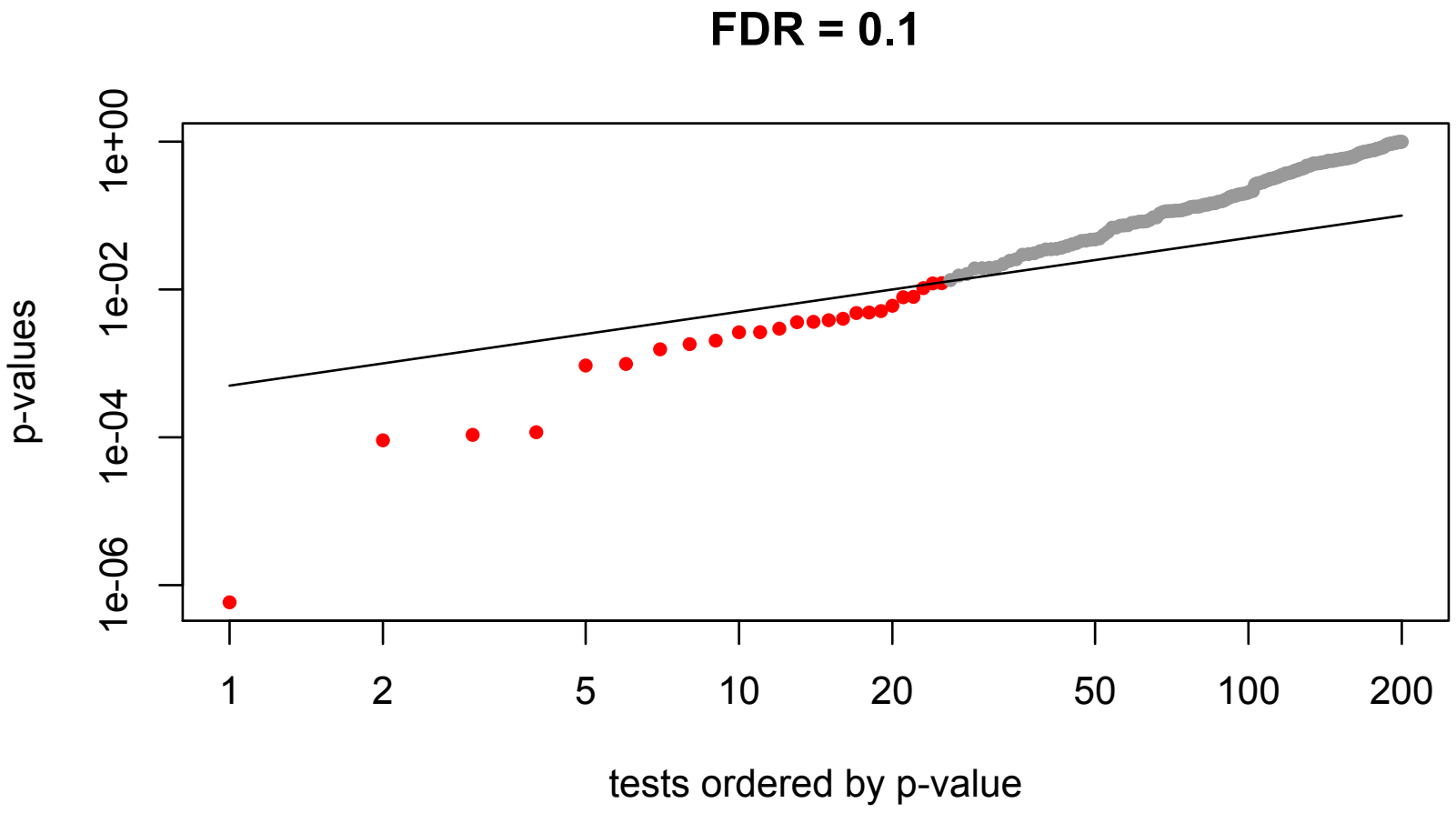
Back to the semiconductors



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

Which come from null $\beta_j = 0$? Which are significant?

The $q = 0.1$ line yields 25 'significant' signals.



Since the inputs are orthogonal, these are the same 25 most highly correlated-with-y from earlier.

The problem with FDR: test dependence

The tests in these examples are plausibly independent:

SNPs are far apart, and PCs are orthogonal.

This seldom holds. Even here: related genes, estimated PCs.

In regression, multicollinearity causes problems: Given two highly correlated x's the statistician is unsure which to use. You then get big p-values and neither variable is significant.

Even with independence, FDR control is often impractical

- Regression p-values are conditional on all other x_j's being 'in the model'. This is probably a terrible model.
- p-values only exist for $p < n$, and for p anywhere near to n you are working with very few degrees of freedom.

But if you are addicted to p-values, its the best you can do.

Prediction vs Evidence

Hypothesis testing is about evidence: what can we conclude?

Often, you really want to know: what is my best guess?

False Discovery proportions are just one possible model metric.
As an alternative, predictive performance can be easier to measure and more suited to the application at hand.

This is even true in causal inference:
most of your model components need to predict well for you to claim structural interpretation for a few chosen variables.

Model Building: it is all about prediction.

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 hard. We'll discuss how this is done...

2. Seems impossible! We need to define some measures of predictive performance and estimators for those metrics.

Metrics of predictive performance

How useful is my model for forecasting unseen data?

Crystal ball: what is the error rate for a given model fitting routine on new observations from the same DGP as my data?

Bayesian: what is the posterior probability of a given model? IE, what is the probability that the data came from this model?

These are very closely linked: posteriors are based on integrated likelihoods, so Bayes is just asking 'what is the probability that this model is best for predicting new data?'.

We'll estimate crystal ball performance with cross validation, and approximate model probabilities with information criteria.

Out-of-sample prediction experiments

We already saw an OOS experiment with the semiconductors. Implicitly, we were estimating crystal ball R^2.

The procedure of using such experiments to do model selection is called Cross Validation (CV). It follows a basic algorithm:

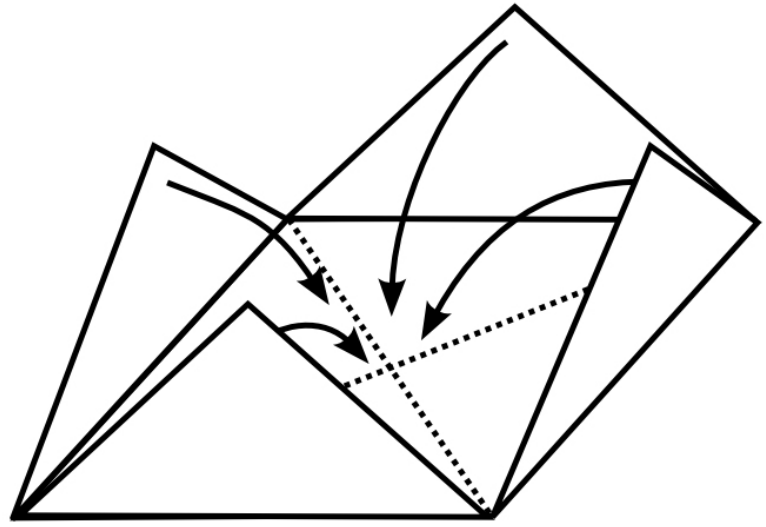
For $k = 1 \ldots K$,

- Use a subset of $n_k < n$ observations to 'train' the model.
- Record the error rate for predictions from this fitted model on the left-out observations.

Error is usually measured in deviance. Alternatives include MSE, misclass rate, integrated ROC, or error quantiles.

You care about both average and spread of OOS error.

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.

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 huge 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.

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

Alternatives to CV: Information Criteria

There are many 'Information Criteria' out there: AIC, BIC, ...
These IC are approximations to -log model probabilities.
The *lowest* IC model has *highest* posterior probability.

Think Bayes rule for models M_1,M_2,...M_B:

$$\mathrm{p}(M_b|\mathrm{data}) = \frac{\mathrm{p}(\mathrm{data}, M_b)}{\mathrm{p}(\mathrm{data})} \propto \underbrace{\mathrm{p}(\mathrm{data}|M_b)}_{\text{LHD}} \underbrace{\mathrm{p}(M_b)}_{\text{prior}}$$

The 'prior' is your probability that a model is best *before* you saw any data. Given Ockham's razor, p(M_b) should be high for simple models and low for complicated models.

$\Rightarrow$ exp(-IC) is *proportional* to model probability.

IC and model priors

IC are distinguished by what prior they correspond to.
The two most common are AIC (Akaike's) and BIC (Baye's).

These are both proportional to Deviance + k # parameters.

This comes from a Laplace approximation to the integral

$$-\log \mathrm{p}(\mathbf{y}, M_b) = \int -\log \mathsf{LHD}(\mathbf{y}|\boldsymbol{\beta}_b) d\mathrm{P}(\boldsymbol{\beta}_b)$$

Akaike uses $k = 2$ and Bayes uses $k = \log(n)$. So BIC uses a prior that penalizes complicated models more than AIC's does.

BIC uses a unit-information prior: $\mathrm{N}\left(\hat{\boldsymbol{\beta}}, -\frac{1}{n}\frac{\partial^2 \mathsf{logLHD}}{\partial \boldsymbol{\beta}^2}\right)$

AIC's integrates $\propto \exp\left[\frac{\mathrm{p}_b}{2}(\log(n) - 1)\right]$.

Example: IC for Semiconductors

Consider AIC and BIC for full (p=200) and cut (p=25) `glms`.

```
> BIC(full)
[1] 1787.184
> BIC(cut)
[1] 744.0906
```

```
> AIC(full)
[1] 722.3321
> AIC(cut)
[1] 606.3487
```

Here they agree: cut model wins. Usually they will not.
Preference is controversial, but you'll find which you prefer.

My take:

BIC tends to move with OOS error, so that the model with lowest BIC is close to that with lowest OOS deviance.
For big n, AIC does not and will over-fit.

Forward stepwise regression

Both CV and IC methods require a set of 'candidate models'.
How do we find a manageable group of good candidates?

Forward stepwise procedures: start from a simple 'null' model, and incrementally update fit to allow slightly more complexity.

Better than backwards methods

- The 'full' model can be expensive or tough to fit, while the null model is usually available in closed form.
- Jitter the data and the full model can change dramatically (because it is overfit). The null model is always the same.

Stepwise approaches are 'greedy': they find the best solution at each step without thought to global path properties.
Many ML algorithms can be understood in this way.

Naive stepwise regression

The `step()` function in R executes a common routine

- Fit all univariate models. Choose that with highest R^2 and put that variable – say $x_{(1)}$ – in your model.
- Fit all bivariate models including $x_{(1)}$ ($y \sim \beta_{(1)}x_{(1)} + \beta_j x_j$), and add x_j from one with highest R^2 to your model.
- Repeat: max R^2 by adding one variable to your model.

The algorithm stops when IC is lower for the current model than for any of the models that add one variable.

Two big problems with this algorithm

Cost: it takes a very long time to fit all these models.
3 min to stop at AIC's $p = 68$, 10 sec to stop at BIC's $p = 10$.

Stability: sampling variance of the naive routine is very high.

Penalized estimation

Stepwise is a great way to build candidate sets,
but the naive algorithm is slow and unstable.
CV is impractical if one fit on a tiny dataset takes 3 minutes.

Modern stepwise algorithms use deviance penalties.
Instead of MLE, fit $\hat{\boldsymbol{\beta}}$ to minimize -logLHD$(\boldsymbol{\beta}) + \lambda \sum_j c(\beta_j)$.

$\lambda > 0$ is a penalty weight, c is a cost function with min at zero.
Cost functions look something like $|\beta|^\alpha$, for $\alpha \in 0, 1, 2$.

λ indexes candidate models.

A forward stepwise algorithm: start from λ big enough that all $\beta_j = 0$. Incrementally decrease λ and update $\hat{\boldsymbol{\beta}}$ at each step.

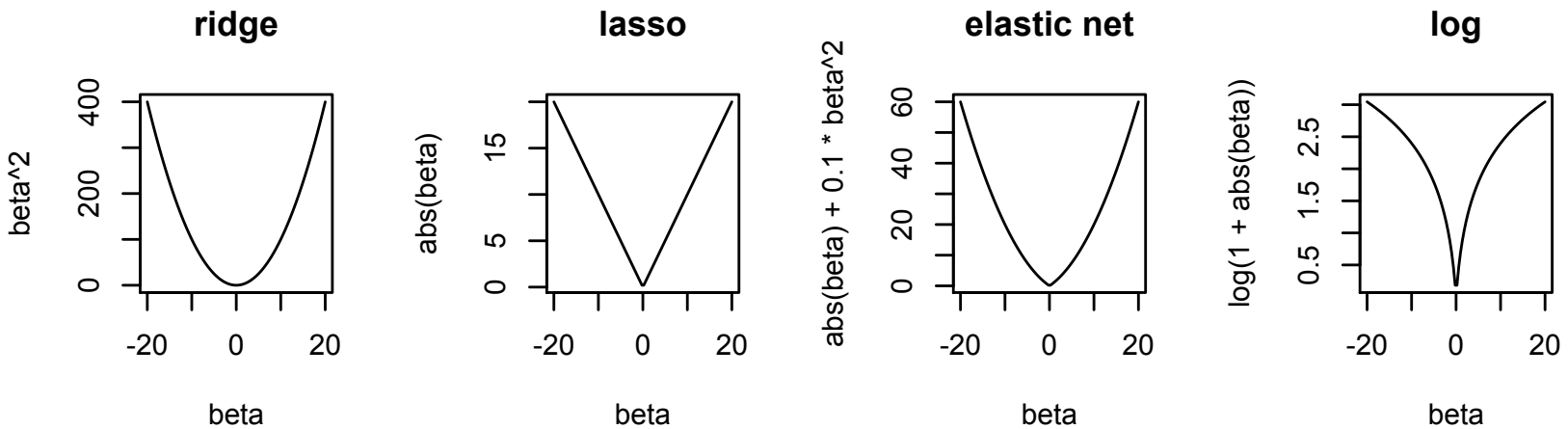
Cost functions

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

Estimation: Deviance is cost of distance from data to model.

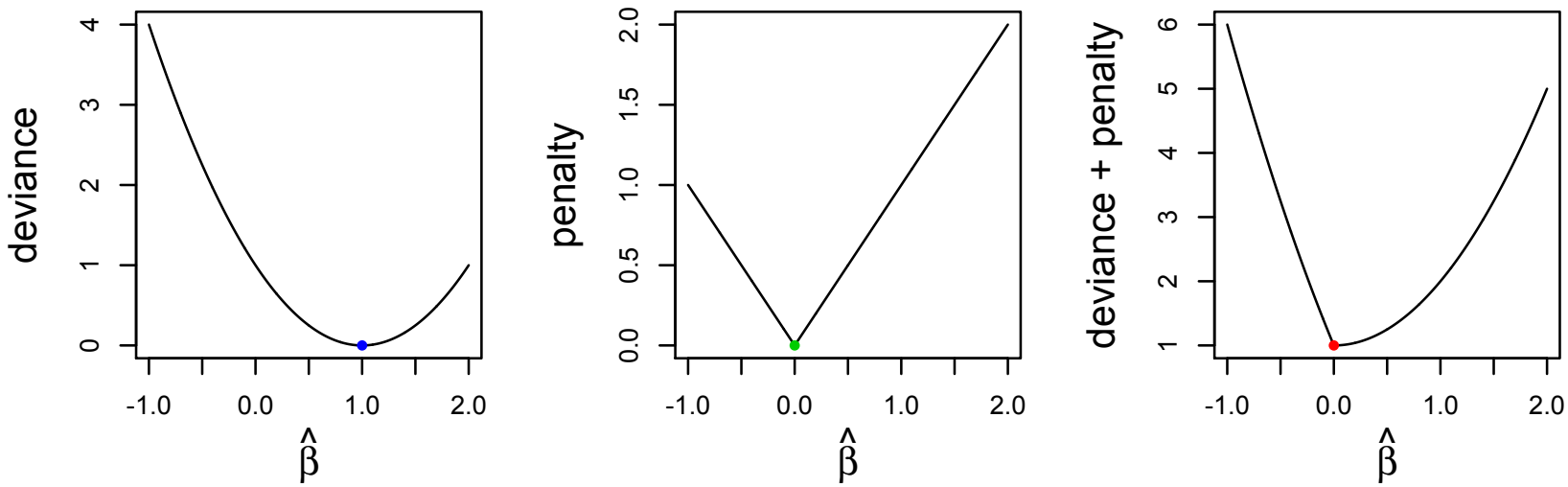
Testing: $\hat{\beta}_j = 0$ is safe, so it should cost to decide otherwise.

$\Rightarrow$ c should 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



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

There are MANY penalty options; think of lasso as a baseline.

Important practical point:

Penalization means that scale matters. Most software will multiply β_j by sd(x_j) in the cost function to standardize.

Cost function properties

Ridge is a James-Stein estimator, with the associated squared-error-loss optimality for dense signals. It shrinks the coefficients of correlated variables towards each other.

Concave penalties have oracle properties: $\hat{\beta}_j$ for 'true nonzero coefficients' converge to MLEs for the true model (Fan+, 200+).

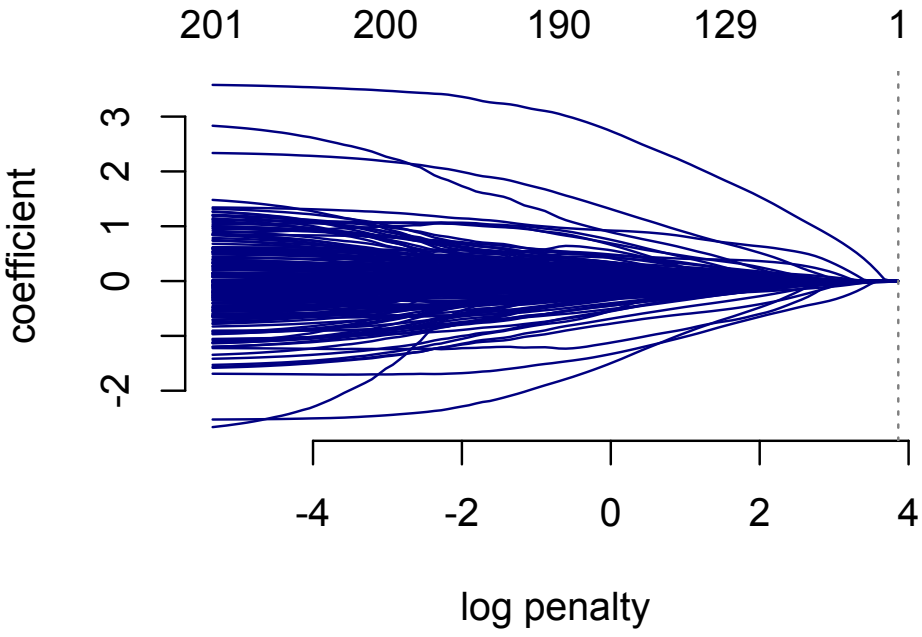
Lasso is a middle ground. It tends to choose a single input amongst correlated signals but also has a non-diminishing bias.

The lasso does not have Oracle properties.
It gains them if the coefficients are weighted by signal strength (Zou 2006), and predicts as well as the Oracle if λ is chosen via CV (Homrighausen + McDonald, 2013).

Regularization: depart from optimality to stabilize a system.

Common in engineering: I wouldn't fly on an optimal plane.

Fitted $\boldsymbol{\beta}$ for decreasing λ is called a **regularization path**.



The New Least Squares

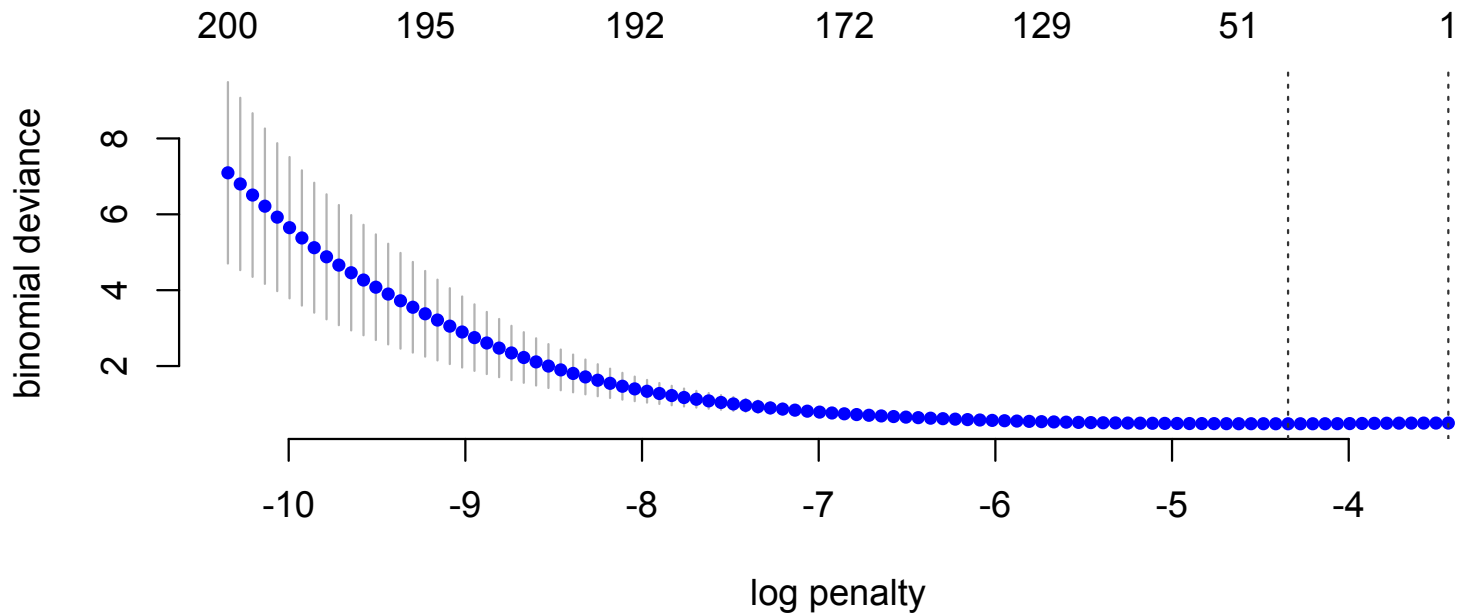
For big p, a path to $\lambda = 0$ is faster than a single full OLS fit.

For the semiconductors ($\leftarrow$) it takes ≈ 4 seconds.

The genius of lasso: $\hat{\boldsymbol{\beta}}$ changes smoothly (i.e., very little) when λ moves, so updating estimates from $\lambda_{t-1} \to \lambda_t$ is crazy fast.

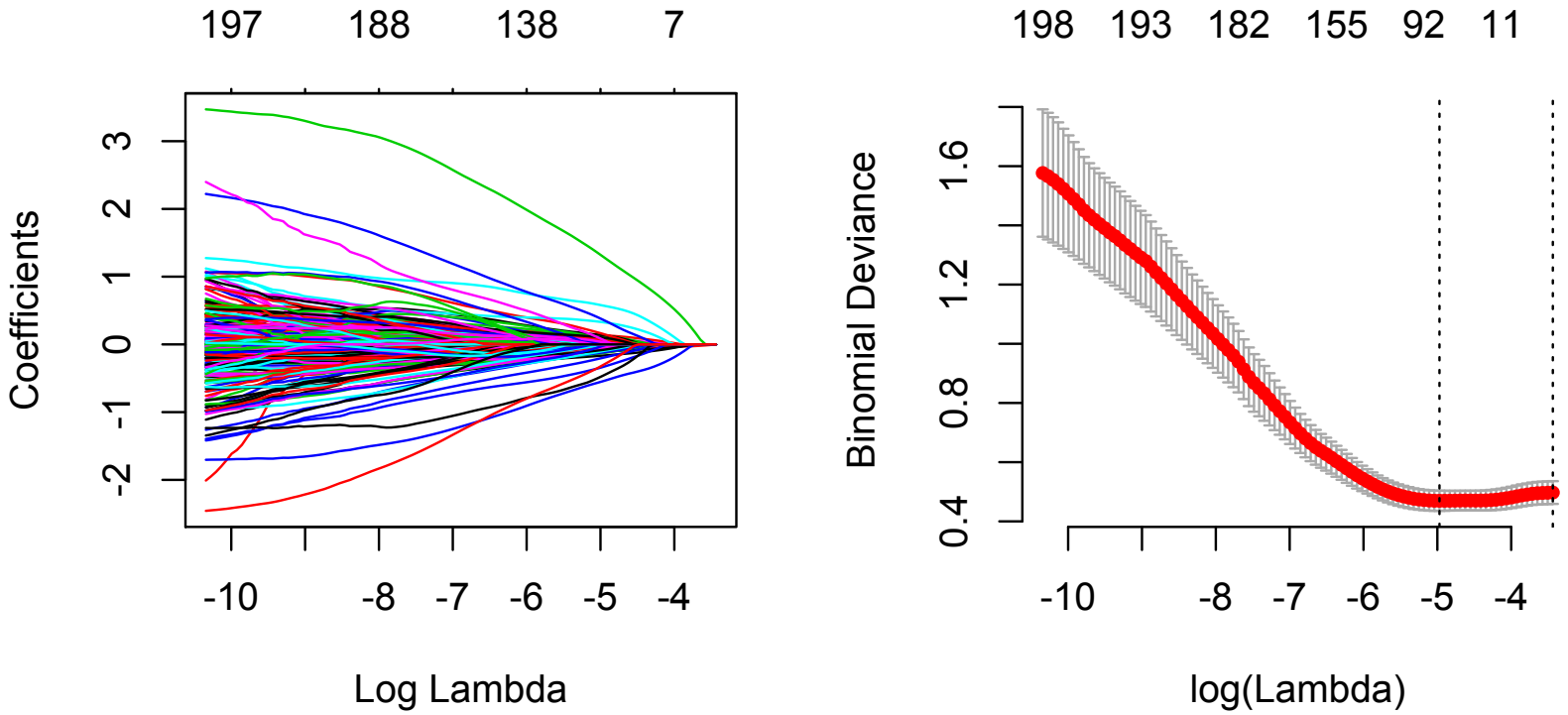
Sound too good to be true? You need to choose λ.

Think of λ as a signal-to-noise filter: like squelch on a radio.
CV: fit training-sample paths and use λ that does best OOS.



Two common rules for 'best': min average error, or the largest λ with mean error no more than 1SE away from the minimum.

Any serious software will fit lasso paths and do CV.



These plots for semiconductor regression are from `glmnet` in `R`.

It's as simple as `fit = cv.glmnet(x,y,family=binomial)`.

IC and the lasso

What are the degrees of freedom for penalized regression?
Think about L_0 cost (subset selection): we have $\hat{p}$ parameters in a given model, but we've looked at all p to choose them.

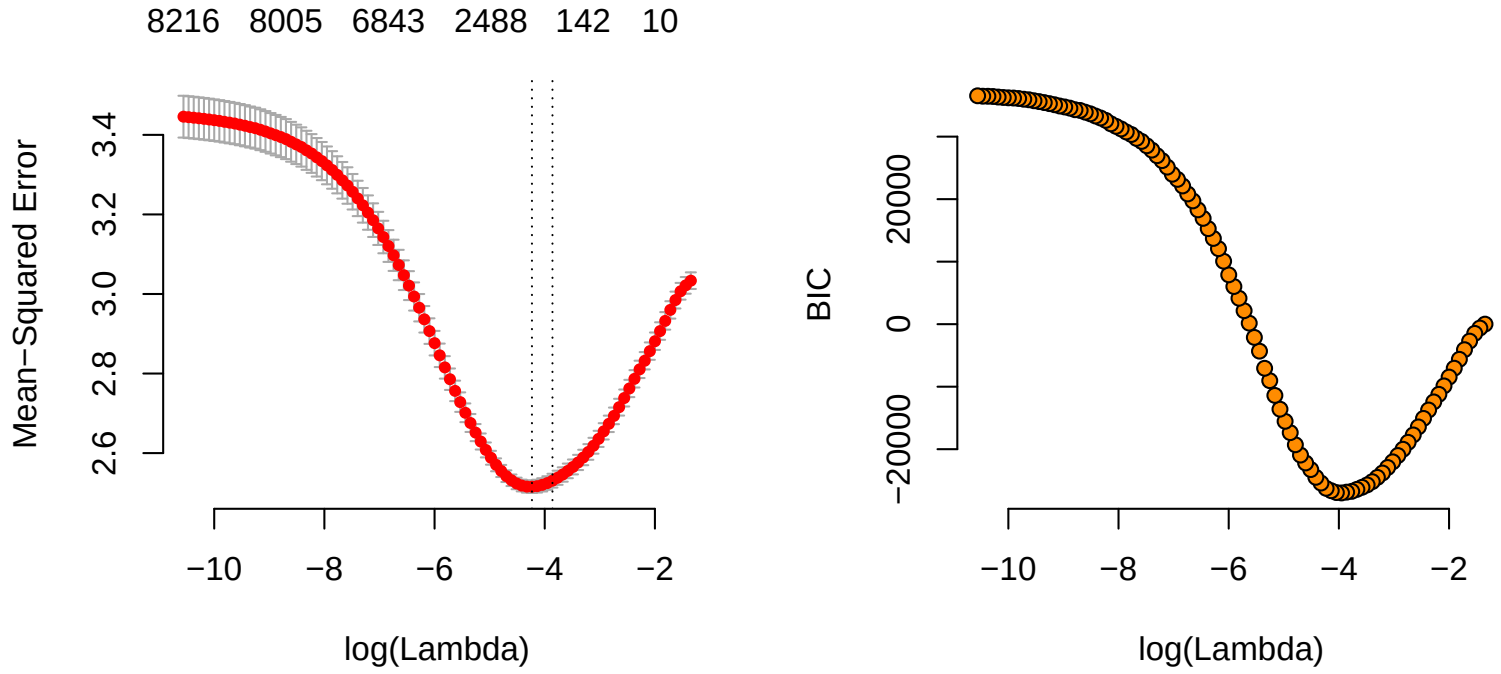
A fantastic and surprising result about the lasso is that $\hat{p}_\lambda$, the number of nonzero parameters at λ, is an unbiased estimate of the degrees of freedom (in Stein sense, $\sum_i \mathrm{cov}(\hat{y}_i, y_i)/\sigma^2$).
See Zou, Hastie, + Tibshrani 2007, plus Efron 2004 on df.

So the BIC for lasso is just deviance + $\hat{p}_\lambda \log(n)$.
This is especially useful when CV takes too long.
(For semiconductors, it agrees with the 1SE rule that $\hat{p} = 1$.)

Lasso and the Comscore data

Recall web browsing example: y is log spend for 60k online consumers, and $\mathbf{x}$ is the % of visits spent at each of 8k sites.

Lasso path minimizes $\sum_i \frac{1}{2}(y_i - \alpha - \mathbf{x}'\boldsymbol{\beta})^2 + \lambda \sum_j |\beta_j|$.



The BIC mirrors OOS error. This is why practitioners like BIC.

Comscore regression coefficients

The BIC chooses a model with around 400 nonzero $\hat{\beta}$.

Some of the large absolute values:

shoppingsnap.com	onlinevaluepack.com	bellagio.com
3.5011219	2.2230610	1.3548940
scratch2cash.com	safer-networking.org	cashunclaimed.com
-2.0384024	-1.8353769	-1.3052399
tunes4tones.com	winecountrygiftbaskets.com	marycy.org
-1.5433389	1.4545323	-1.1138126
finestationery.com	columbiahouse.com-o01	harryanddavid.com
1.4125547	1.3916690	1.0512341
bizrate.com	frontgate.com	victoriassecret.com
1.3359164	1.2803210	0.9578552

Note that the most raw dollars were spent on travel sites (`united.com`,`oribtz.com`,`hotels.com`,...) but these don't have the largest coefficients (changes if you scale by sd).

Non-convex penalties

The concave penalties – e.g., $s \log(r + |\beta_j|)$ – are tempting:
If a variable is *in-the-model*, you get a low bias estimate for it.

However you need to be careful:
Bias improves prediction by lowering estimation variance.
See Breiman, 1996 for a classic discussion of the issue.

For us, bias is what makes the regularization paths continuous.

Discontinuity implies instability (jitter data = big fit changes).

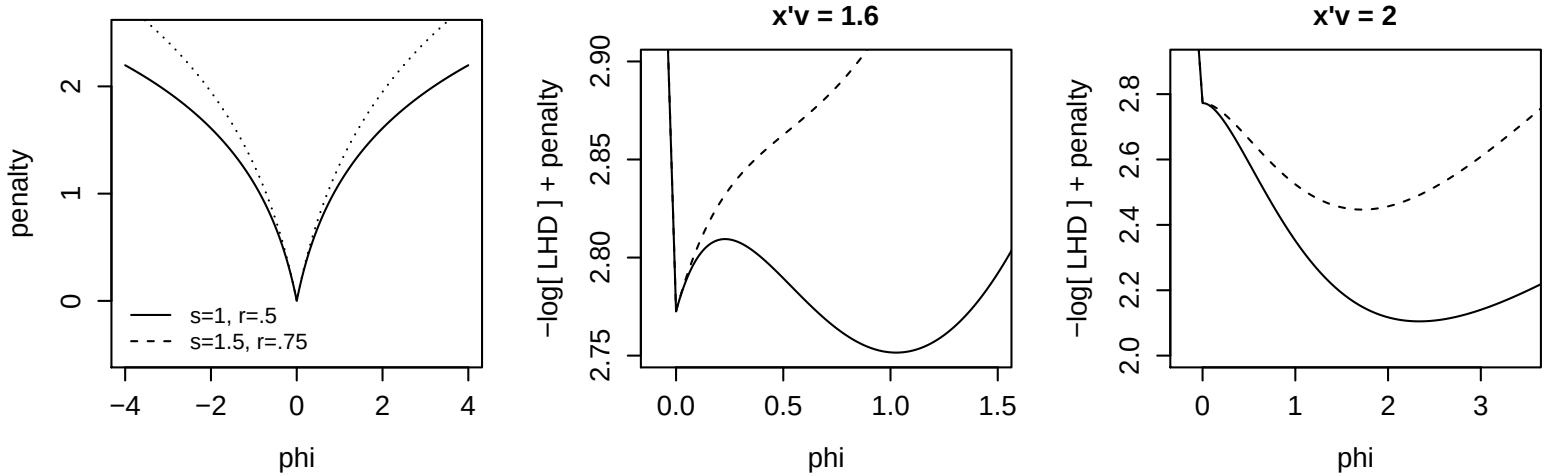
It also has big practical implications on computation time.

Continuity and curvature

There is space between L_1 and discontinuity.
Jumps are caused by concavity at the origin.

For orthogonal $\mathbf{X}$, this happens if $\dfrac{\lambda d^2 c}{d\beta^2} < \left.\dfrac{\partial^2 \text{logLHD}}{\partial \boldsymbol{\beta}^2}\right|_{\beta_j=0}$

Log penalty curve at zero is s/r^2.
For linear regression $v \sim x$:



Bayesian Lasso and gamma-Lasso

I call this s/r^2 curvature the 'variance of lambda'.
That's because it is, if you derive the log penalty from a gamma(s, r) prior on unique L1 penalties for each β_j.

More generally, all penalized MLEs can be interpreted as posterior maxima (MAPs) under some Bayesian prior.

The classics: ridge implies a Gaussian prior on β, and lasso is a Laplace prior (carlin,polson,stoffer, 1992, park+casella 2008).

The log penalty corresponds to joint solution under the prior

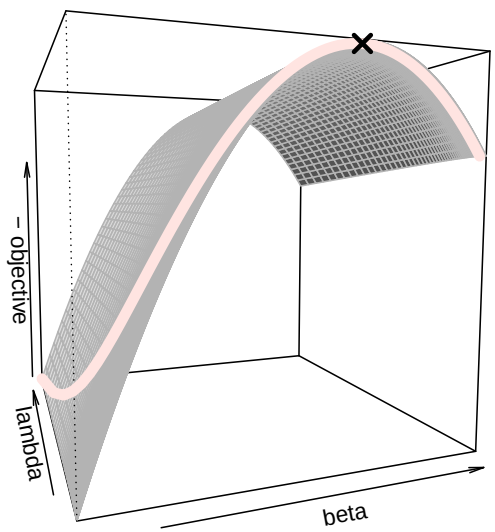
$$\pi(\beta_j, \lambda_j) = \mathrm{La}(\beta_j; \lambda_j)\mathrm{Ga}(\lambda_j; s, r) = \frac{r^2 \lambda_j^s}{2\Gamma(s)} e^{-\lambda_j (r + |\beta_j|)}.$$

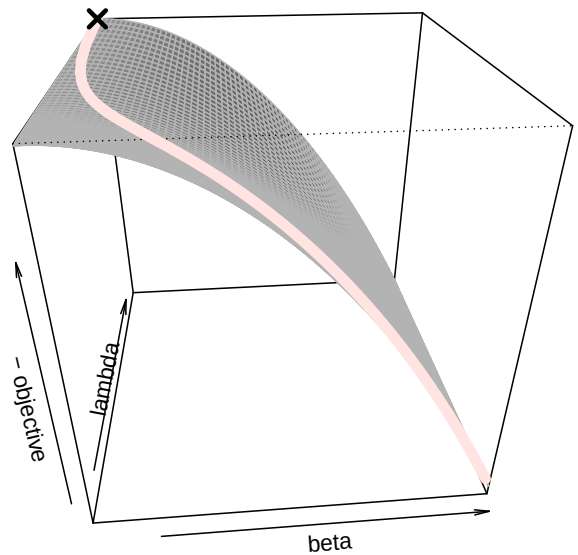
Armagan+Dunson 2013, Taddy 2012, and others similar.

A useful way to think about penalization

The log penalty is a conjugate prior relaxation of the lasso...

The joint problem is convex, so we get fast globally convergent estimation under non-convex penalties.

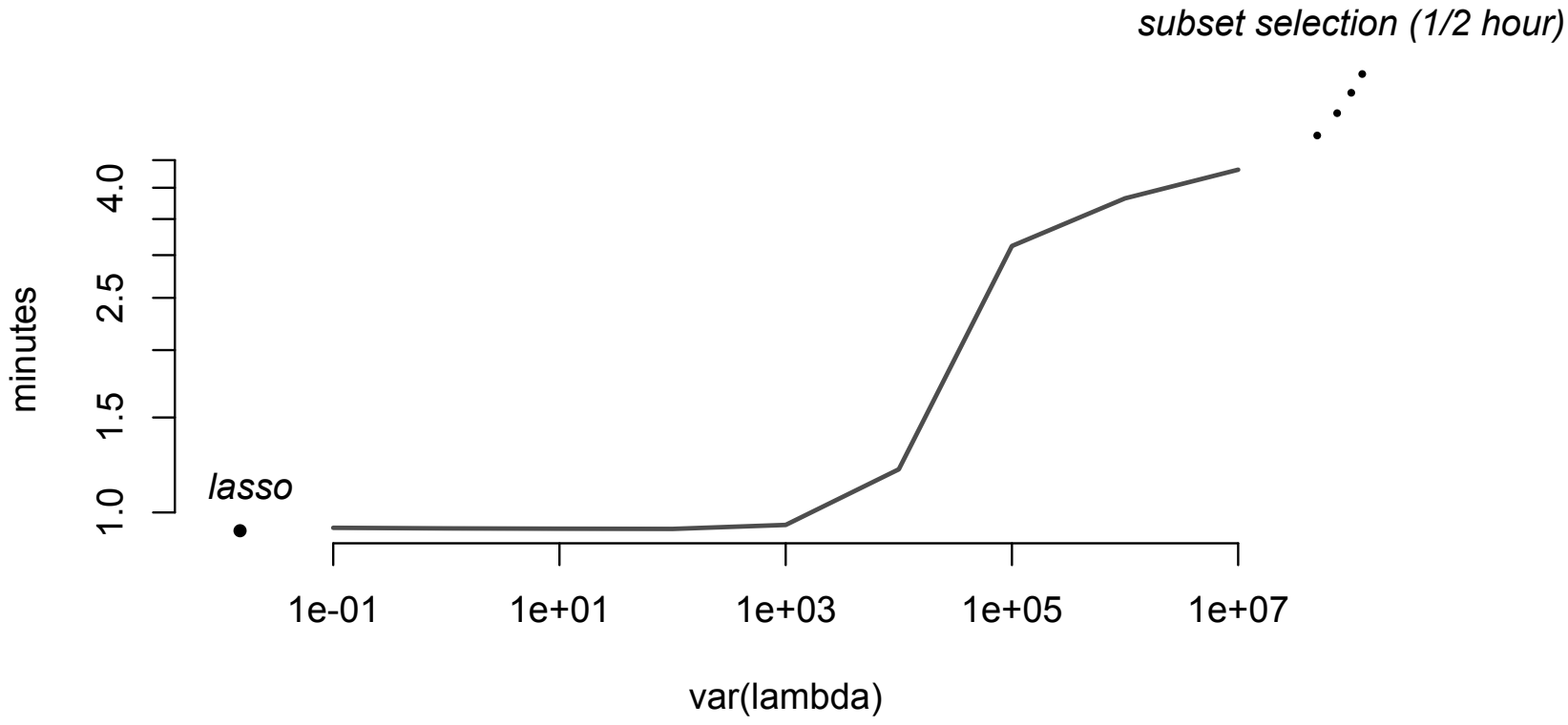




Continuity as a function of prior variance is a nice bonus.

Taddy 2013 'the gamma lasso'

Comscore: time for a single log penalty path fit



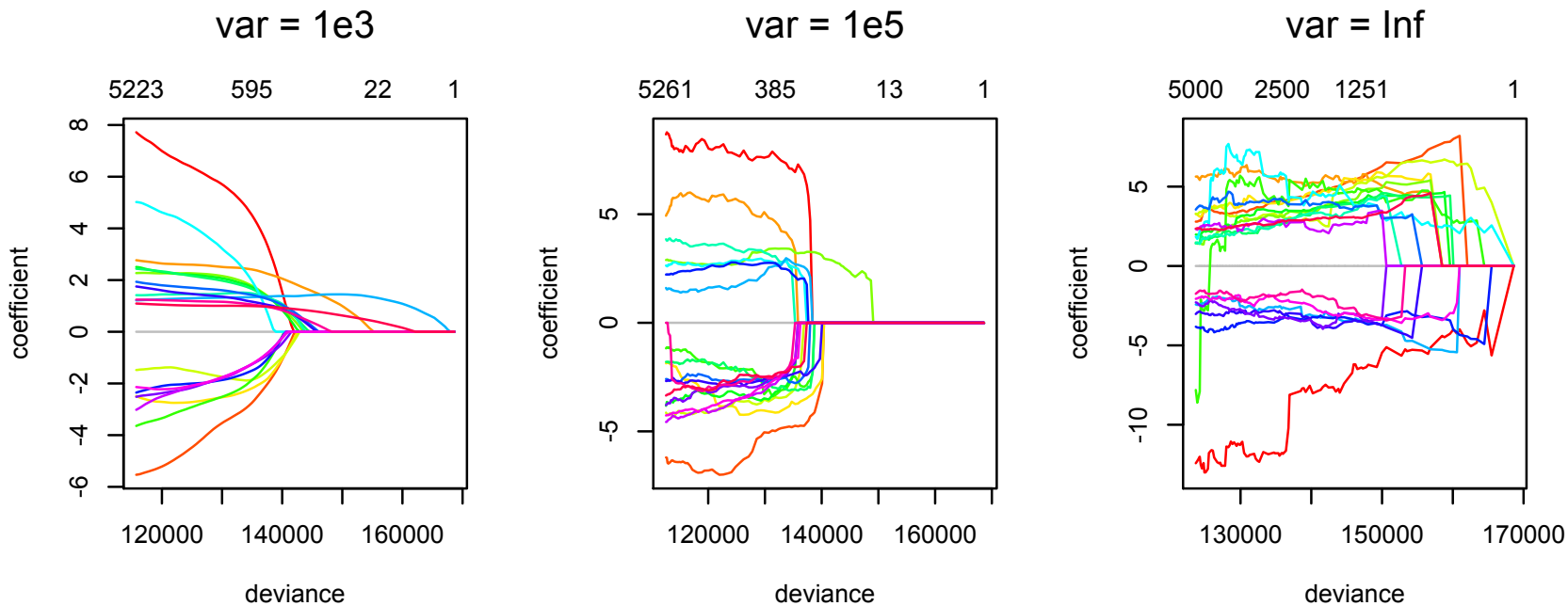
Paths are in s/r with s/r^2 constant. SS is greedy forward.

The paths here (including SS) all go out to $\approx$ 5k df.

Full OLS ($p \approx$ 8k) takes $>$3 hours on a fast machine.

Comscore: path continuity

A quick look at the paths explains our time jumps.
Plotting only the 20 biggest BIC selected β:



Algorithm cost explodes with discontinuity.
(var = Inf is subset selection).

Factor models: PCA and PCR.

Setting things to zero is just one way to reduce dimension.

Another useful approach is a factor model:

$$\mathbb{E}[\mathbf{x}] = \mathbf{v}'\mathbf{\Phi}, \text{ where } K = \dim(\mathbf{v}) \ll \dim(\mathbf{x}).$$

Factor regression then just fits $\mathbb{E}[y] = \mathbf{v}'\boldsymbol{\beta}$.

For our semiconductors example, the covariates are PC directions. So we've been doing this all along.

It is best to have both y and $\mathbf{x}$ inform estimation of $\mathbf{v}$.
This is 'supervised' factorization (also inverse regression).
We'll just start with the (unsupervised) two stage approach.

Factor models: PCA and PCR.

Most common routine is principal component (PC) analysis.

Columns of $\mathbf{\Phi}$ are eigenvectors of the covariance $\mathbf{X}'\mathbf{X}$, so $\mathbf{z} = \mathbf{x}'\mathbf{\Phi}$ is a projection into the associated ortho subspace.

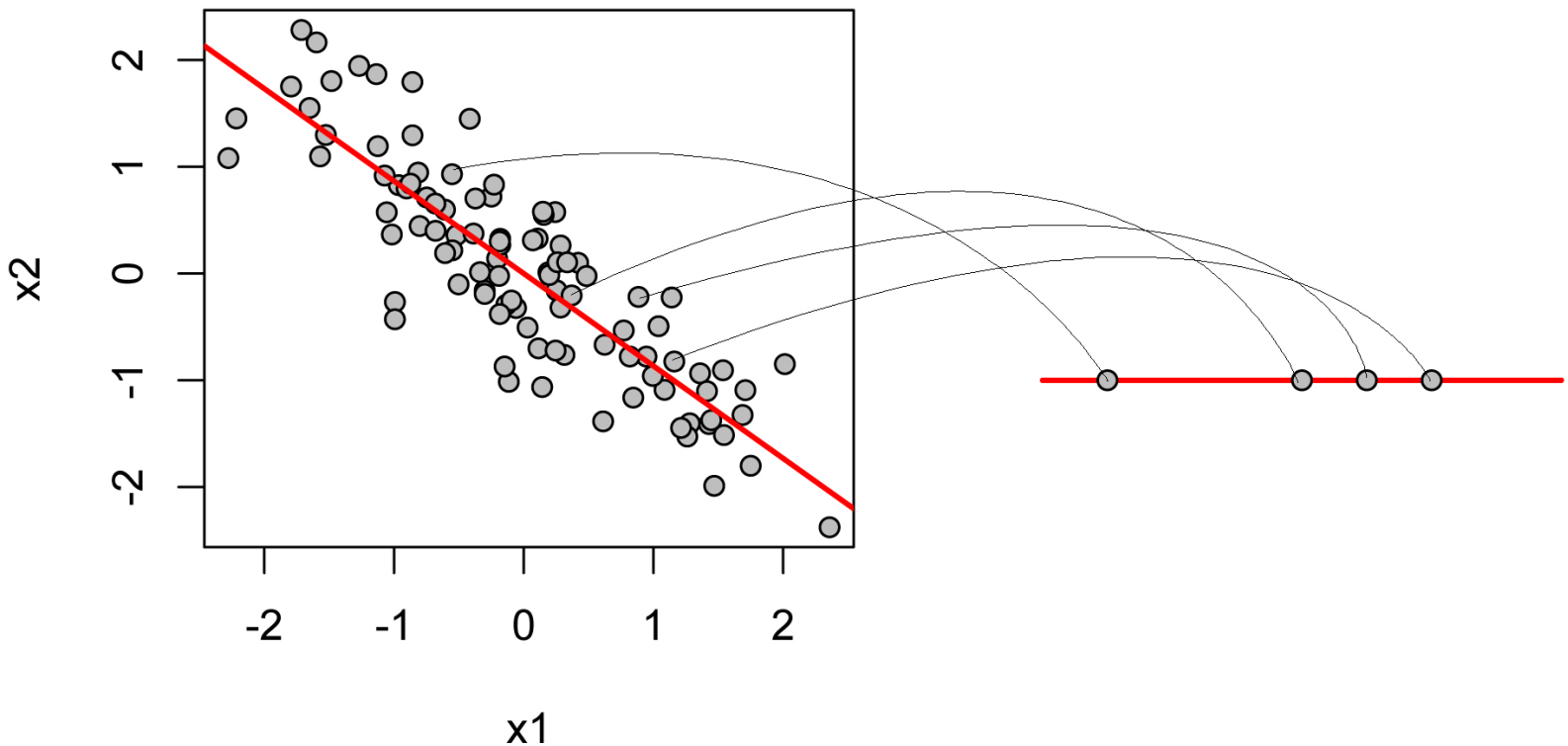
Recall: the actual model is $\mathbb{E}[\mathbf{x}] = \mathbf{v}'\mathbf{\Phi}$.
$\mathbf{z} = \mathbf{x}'\hat{\mathbf{\Phi}} \propto \hat{\mathbf{v}}$ is the projection of $\mathbf{x}$ onto our factor space.
If this is confusing you can equate the two without problem.

Full spectral decomposition has `ncol(`$\mathbf{\Phi}$`) = min(n,p)`, but a factor model uses only the $K \ll p$ with largest eigenvalues.

PCA: projections into latent space

Another way to think about factors, in a 2D example:

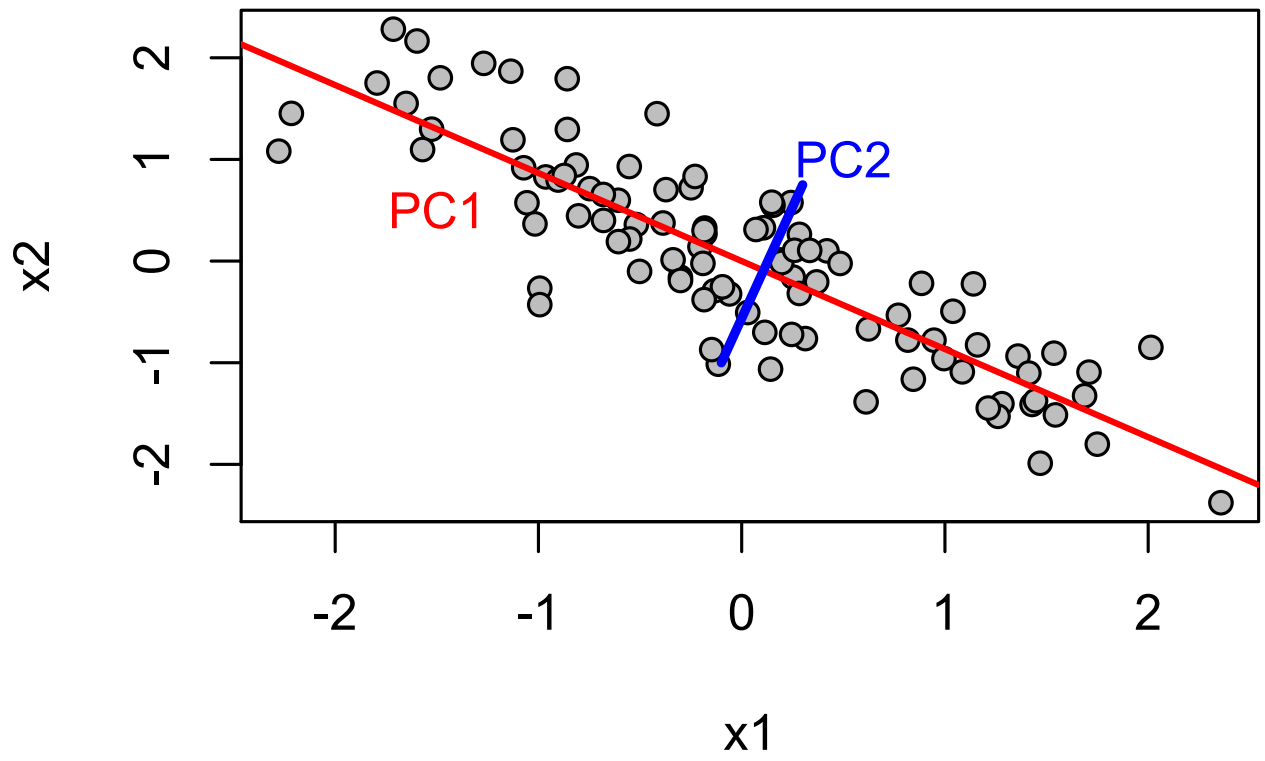
PCA equivalent to finding the line that fits through x_1 and x_2, and seeing where each observation lands (projects) on the line.



We've projected from 2D onto a 1D axis.

Fitting Principal Components via Least Squares

PCA looks for high-variance projections from multivariate $\mathbf{x}$ (i.e., the long direction) and finds the least squares fit.



Components are ordered by variance of the fitted projection.

A greedy algorithm

Suppose you want to find the first set of factors, $\mathbf{v} = v_1 \dots v_n$.
We can write our system of equations (for $i = 1...n$)

$$\begin{aligned} \mathbb{E}[x_{i1}] &= \mathrm{cor}(x_1, v)v_i \\ &\vdots \\ \mathbb{E}[x_{ip}] &= \mathrm{cor}(x_p, v)v_i \end{aligned}$$

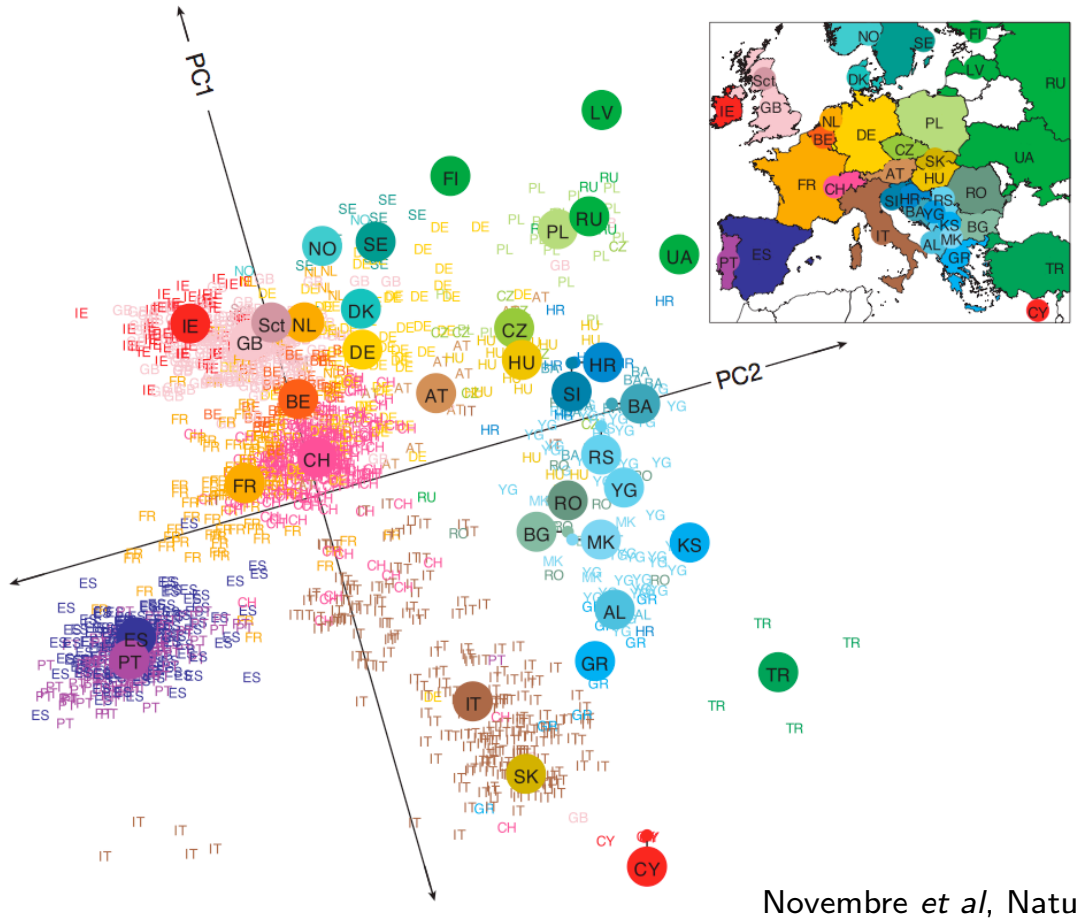
The factors $\mathbf{v}_1$ are fit to maximize average R^2 in this equation.

Next, calculate residuals $e_{ij} = x_{ij} - \mathrm{cor}(x_j, v_1)v_{1i}$.
Then find $\mathbf{v}_2$ to maximize R^2 for these residuals.

This repeats until residuals are all zero ($\min(p, n)$ steps).

This is not actually done in practice, but the intuition is nice.

Geo-Genes Example: two interpretable factors.



Novembre *et al*, Nature 456 (2008)

The $\mathbf{x}$ for each individual is a giant vector of SNPs. They've reduced it into two factors that explain most of the variation.

Turns out that location in this 2-D space looks geographical.

Congress and Roll Call Voting

Votes in which names and positions are recorded are called 'roll calls'.

The site `voteview.com` archives vote records and the R package `pscl` has tools for this data.

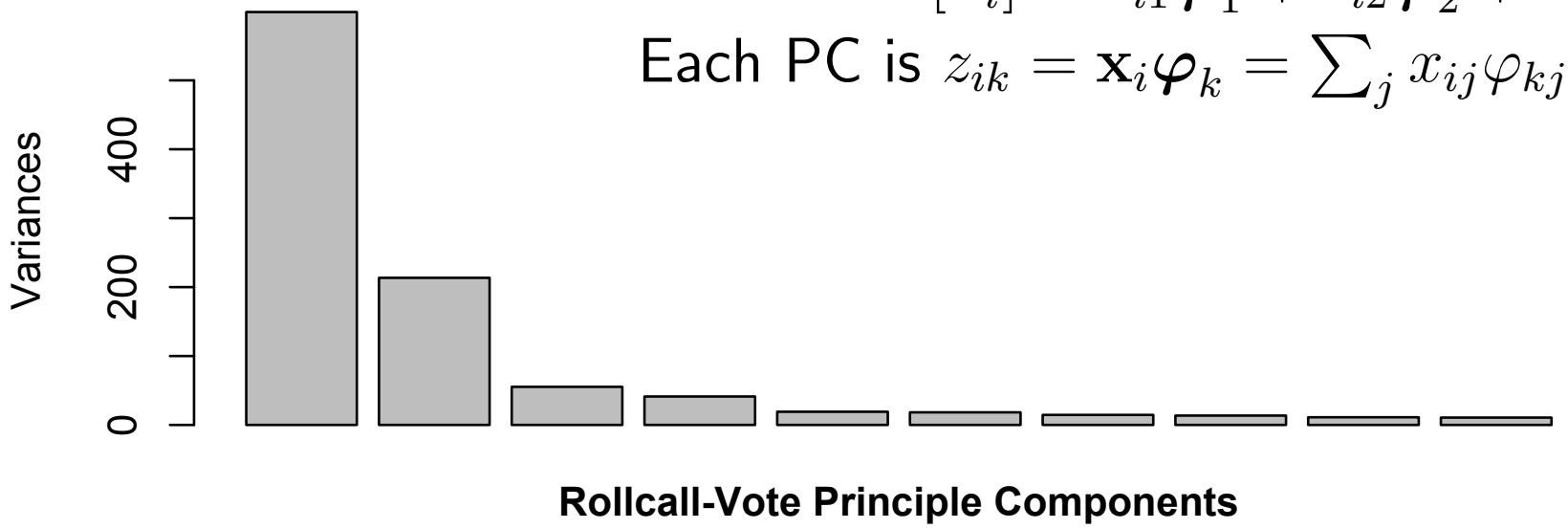
445 members in the last US House (the 111^{th})
1647 votes: nea = -1, yea=+1, missing = 0.

This leads to a large matrix of observations that can probably be reduced to simple factors (party).

Vote components in the 111^{th} house

The model is $\mathbb{E}[\mathbf{x}_i] = v_{i1}\boldsymbol{\varphi}_1 + v_{i2}\boldsymbol{\varphi}_2 + \ldots$

Each PC is $z_{ik} = \mathbf{x}_i\boldsymbol{\varphi}_k = \sum_j x_{ij}\varphi_{kj}$

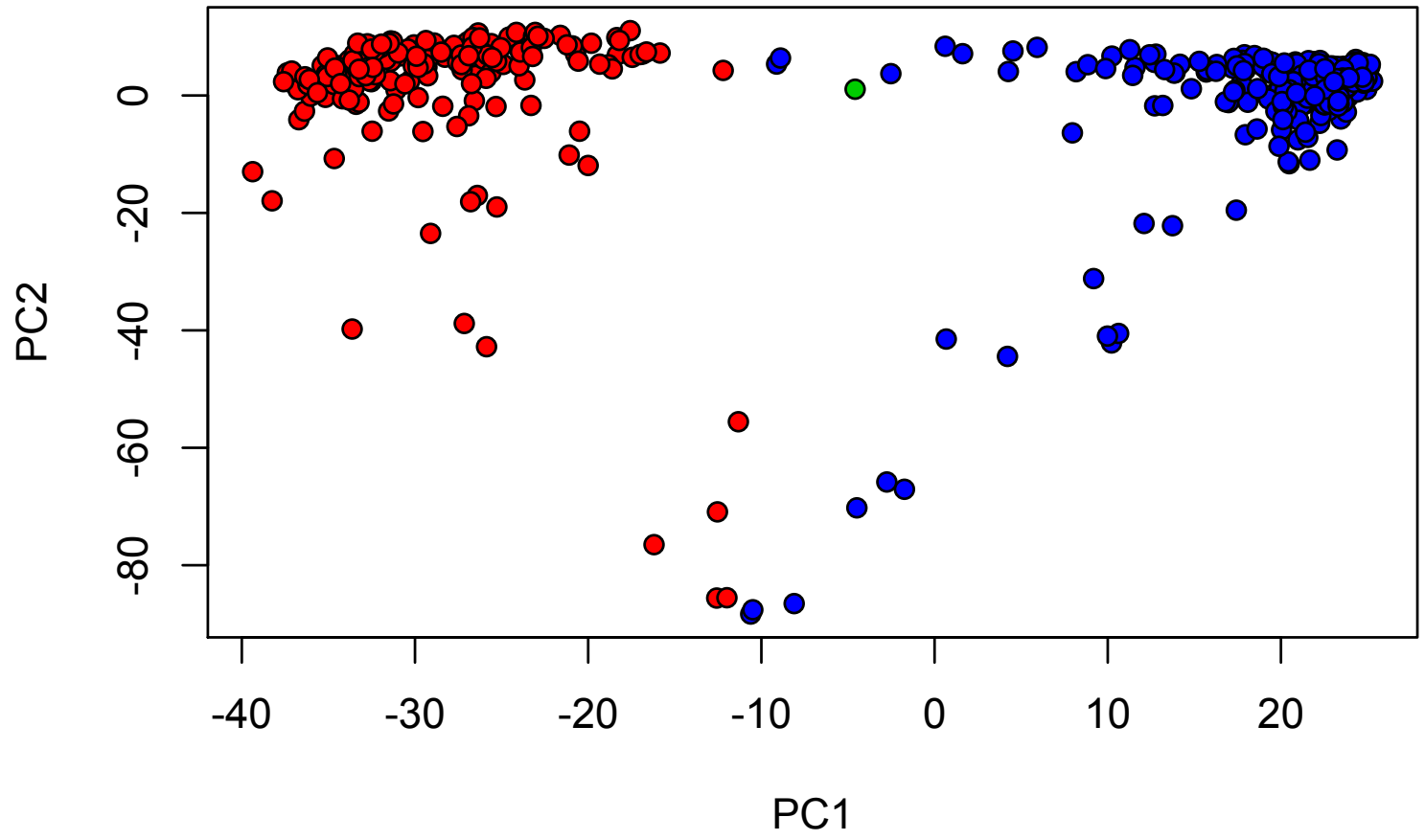


Huge drop in variance from 1^{st} to 2^{nd} and 2^{nd} to 3^{rd} PC.

Poli-Sci holds that PC1 is usually enough to explain congress.

2nd component has been important twice: 1860's and 1960's.

Top two PC directions in the 111^{th} house



Republicans in red and Democrats in blue:

- Clear separation on the first principal component.
- The second component looks orthogonal to party.

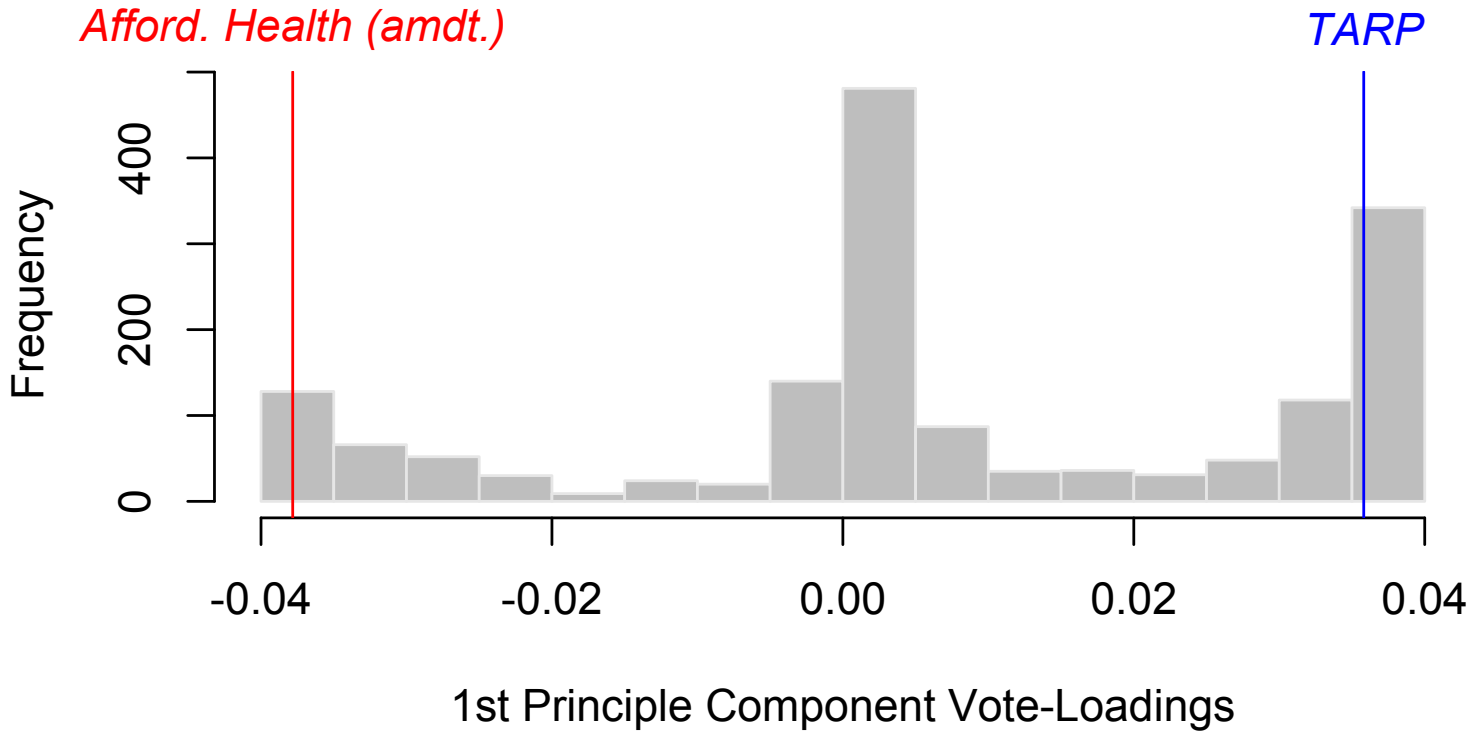
Interpreting the principal components

```
## Far right (very conservative)
> sort(votepc[,1])
     BROUN (R GA-10)       FLAKE (R AZ-6)   HENSARLIN (R TX-5)
         -39.3739409          -38.2506713          -37.5870597

## Far left (very liberal)
> sort(votepc[,1], decreasing=TRUE)
    EDWARDS (D MD-4)   PRICE (D NC-4)    MATSUI (D CA-5)
         25.2915083        25.1591151         25.1248117

## social issues?  immigration?  no clear pattern
> sort(votepc[,2])
     SOLIS (D CA-32) GILLIBRAND (D NY-20)      PELOSI (D CA-8)
        -88.31350926         -87.58871687         -86.53585568
   STUTZMAN (R IN-3)       REED (R NY-29)      GRAVES (R GA-9)
        -85.59217310         -85.53636319         -76.49658108
```

PC1 is easy to read, PC2 is ambiguous (is it even meaningful?)

High PC1-loading votes are ideological battles.

These tend to have informative voting across party lines.



A vote for Republican amendments to 'Affordable Health Care for America' strongly indicates a negative PC1 (more conservative), while a vote for TARP indicates a positive PC1 (more progressive).

Look at the largest loadings in φ_2 to discern an interpretation.

```
> loadings[order(abs(loadings[,2]), decreasing=TRUE)[1:5],2]
 Vote.1146   Vote.658  Vote.1090  Vote.1104  Vote.1149
0.05605862 0.05461947 0.05300806 0.05168382 0.05155729
```

These votes all correspond to near-unanimous symbolic action.

For example, 429 legislators voted for resolution 1146:
'Supporting the goals and ideals of a Cold War Veterans Day'
If you didn't vote for this, you weren't in the house.

Mystery Solved: **the second PC is just attendance!**

```
> sort(rowSums(votes==0), decreasing=TRUE)
     SOLIS (D CA-32) GILLIBRAND (D NY-20)       REED (R NY-29)
                1628                  1619                 1562
  STUTZMAN (R IN-3)      PELOSI (D CA-8)      GRAVES (R GA-9)
                1557                  1541                 1340
```

PCR: Principal Component Regression

The concept is very simple: instead of regressing onto $\mathbf{x}$, use a lower dimension set of principal components $\mathbf{z}$ as covariates.

This works well for a few reasons:

- PCA reduces dimension, which is always good.
- The PCs are independent: no multicollinearity.

We'll do exactly this for comscore: just replace $\mathbb{E}[y|\mathbf{x}] = \mathbf{z}'\boldsymbol{\beta}$

Factor regressions are especially popular in social science, because people like to interpret the latent factors.

Be careful though: if you end up needing a large number of factors it could just be that you don't have a factor structure.

Choosing the number of factors

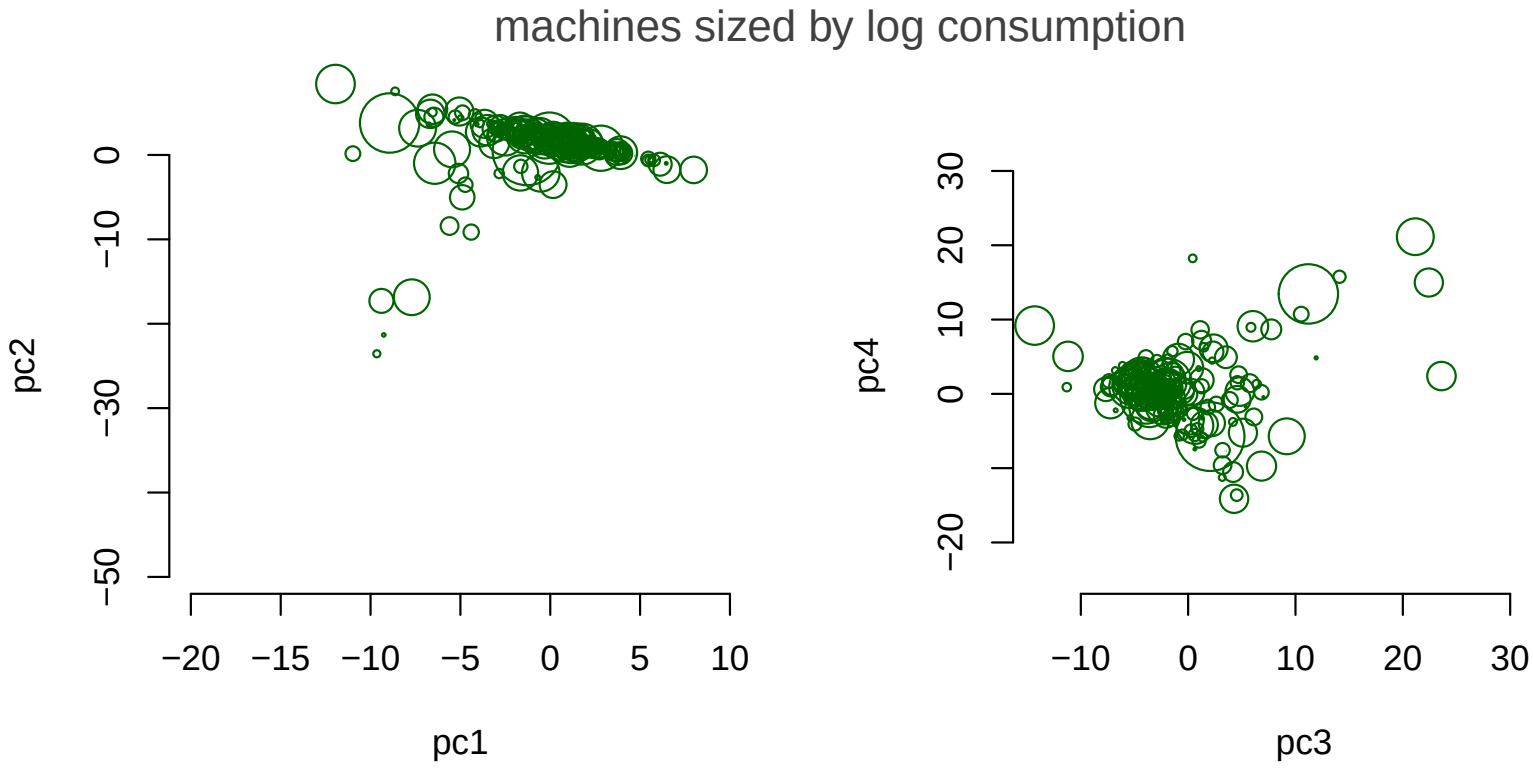
Without supervision this is tough, but for PCR we can use CV.

1. Regress onto factors 1 through K for a few K, and choose the model with lowest CV error.
2. Lasso-CV (or other penalty) through all p factors.

The standard routine is to do '1', but this is unnecessary given our alternative ways to build regularized candidate sets.

NB: unfortunately the approximations that go into BIC don't work with factor models (K factor parameters in addition to the coefficients). It often works, but will break for large K.
(Roeder + Wasserman 1997 for BIC justification in such context)

Comscore PC factors

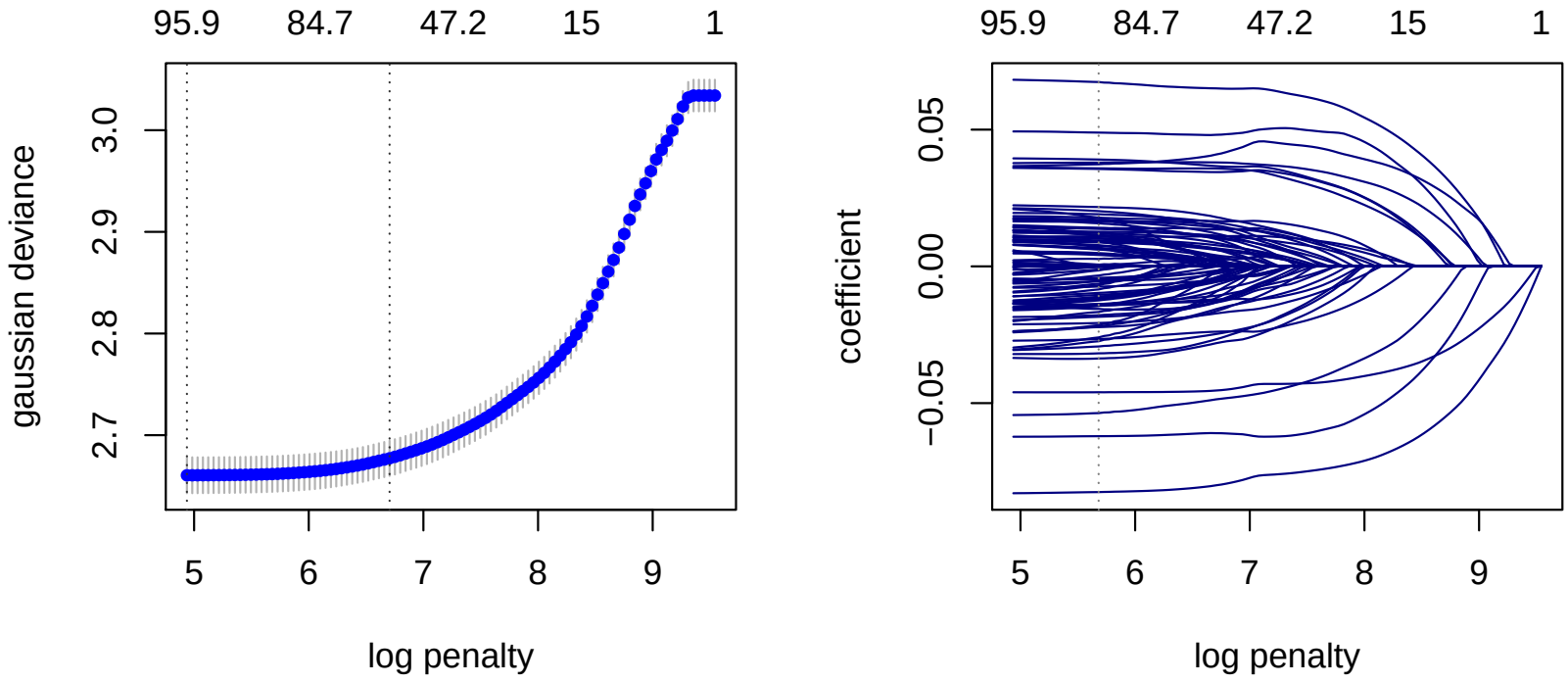


PC1 has big loadings on ad trackers and providers (`atdmt.com`, `zedo.com`, `googlesyndication.com`),
PC2 is all just big negatives on porn (I'll shield you), ...

Mixing methods: CV, penalization, and PCs.

How to choose the number of factors?

We can do lasso-CV for y on $\mathbf{z}$.



Even though we've done variable (factor) selection,

every model for $\lambda < \lambda_0$ is dense: $\beta_1 z_{ik} = \beta_1 \varphi_{jk} x_{ij}$.

Large absolute value coefficients on scaled x_j/s_j

lillianvernon.com	victoriassecret.com	liveperson.net
0.010568003	0.010467798	0.010457976
neimanmarcus.com	revresda.com	oldnavy.com
0.010402899	0.010313770	0.010199234
homedecorators.com	kohls.com	richfx.com
0.009989661	0.009960027	0.009864902

And on raw x_j

thestationerystudio.com	diamond.com	ordermedia.com
0.7397097	0.7378156	0.7320079
raffaello-network.com	visitlasvegas.com	spafinder.com
0.7279747	0.7247268	0.7170530
onewayfurniture.com	finestationery.com	mandalaybay.com
0.7136429	0.7064830	0.6880314

In the PC regression, biggest β were on factors 18, 35, 22.

Pretty deep: is factorization useful?

Nope: compare to original lasso OOS deviance.

Alternative Factor Models

When $> 99\%$ of your data are zero, assuming they are independent and normal (i.e. using least squares) can break. These are the cases where functional form actually matters.

Recall our factorization $\mathbb{E}[\mathbf{x}_i] = \boldsymbol{\varphi}_1 v_{i1} + \ldots \boldsymbol{\varphi}_K v_{iK}$.
The count-data version is a topic model

$$\mathbf{x}_i \sim \mathsf{MN}(v_{i1}\boldsymbol{\theta}_1 + \ldots + v_{iK}\boldsymbol{\theta}_K, m)$$

Topics $\sum_{j=1}^{p} \theta_{kj} = 1$ and weights $\sum_{k=1}^{K} v_{ik} = 1$,
so an observation $(\mathbf{x})$ is drawn from a multinomial with probabilities that are a mixture of topics $\boldsymbol{\theta}_1 \ldots \boldsymbol{\theta}_K$.

Also 'LDA': latent Dirichlet allocation `Blei,Ng,Jordan` 2003.

Topic Models: factors for count data

They really can lead to better factorizations (e.g. Taddy 2013 techno), but because of the nonlinearity they take longer to fit.

Taddy 2012 describes fast numeric approximation to the model probabilities $\int \text{LHD}(\mathbf{X}|\mathbf{\Theta}, \mathbf{V}) d\text{P}(\mathbf{\Theta}, \mathbf{V})$.

Hoffman, Blei, Wang, Paisley 2013 use stochastic gradient approximation to just fit the model faster (enough for CV).

There is a big literature on topic model approximation...
Generally when working with topic models and big data you give up precision in exchange for a better functional form.

Topic modeling Comscore

Instead of looking at proportion of time spent on each site, we'll use raw machine-domain counts (# of visits) as $\mathbf{x}$.

Since it takes so long (a common refrain) I just fit for K=25.

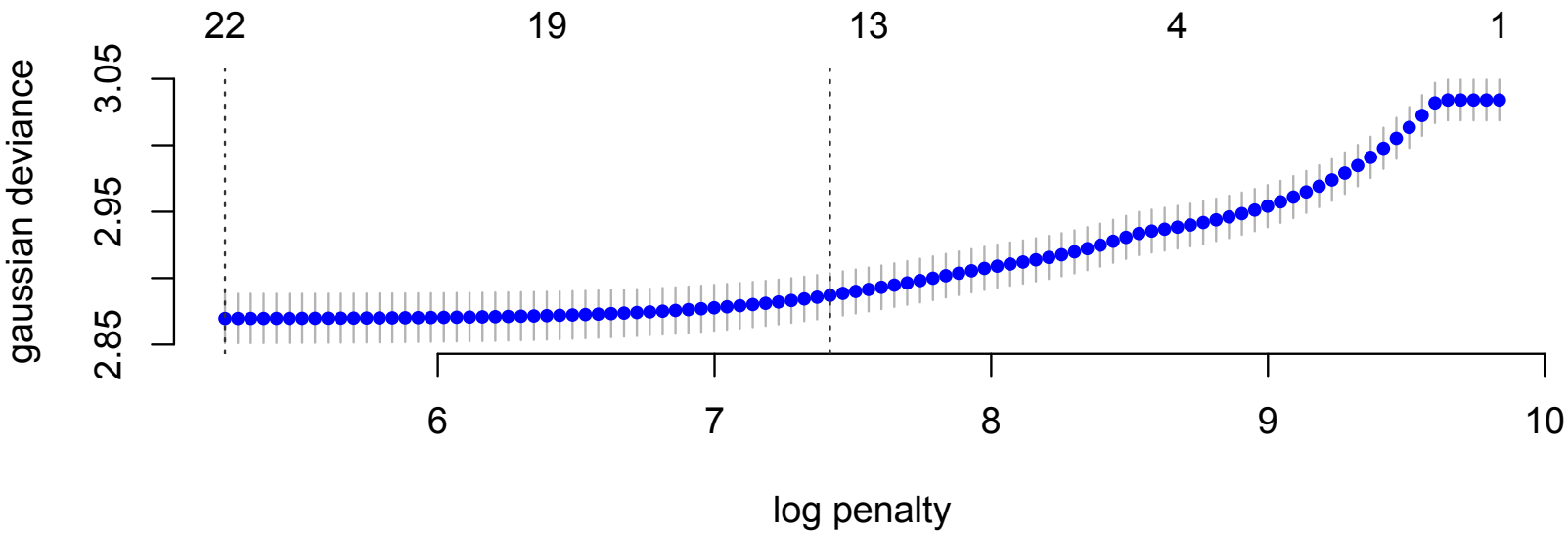
```
> tpc <- topics(x, K=25)
> summary(tpc)

Top phrases by topic-over-null term lift (and usage %):

[2] meegos.com, footprint.net, passport.net, passport.com
[3] regionsnet.com, gwu.edu, drexel.edu, ku.edu, regions.com
[4] catcha10.com, treborwear.com, whateverlife.com, webgavel.com
[5] waol.exe, acsd.exe, aolacsd.exe, aol.com-o07, aoltpspd.exe
[8] worldofwarcraft.com, mininova.org, beboframe.com, runescape.com
[9] drudgereport.com, eproof.com, mercuras.com, breitbart.com
[10] eimg.net, paviliondownload.com, wachoviabillpay.com, marykayintouch.com
[11] freeslots.com, iwon.com-o04, jigzone.com, luckysurf.com
....
```

Topic regression

Just like PCR: put the topic weights in regression.

Since $\sum_j v_{ij} = 1$, we regress y on $\mathbf{v}_{i,-1}$.
(the factors are ordered by decreasing average).

Again, we can use cv-lasso to choose the number of topics.



Still no better than straight lasso.

In conclusion, the Recipe:

Build a forward stepwise path of candidate regularized models, then select the best via CV (or BIC if you are pressed on time).
If you think you have factor structure, try fitting that first.

There is a ton more to 'data science'.

- Supervised factor models and inverse regression: model $\mathbf{x}|\mathbf{y}$ for efficient 'weak signal' factorization.
- Trees and forests: decision trees, and techniques for averaging many possible trees: bagging and MCMC.
- More generally: model averaging and ensemble methods; e.g. predicting $\hat{y}$ as a weighted average across different λ.
- MapReduce and distributed algorithms...

Have fun with it!