

# Variable Selection in Wide Data Sets

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# Overview

- Problem
  - Picking the features to use in a model
  - Wide data sets imply many choices
- Examples
  - Simulated idealized problems
  - Predicting credit risk
- Themes
  - Modifying familiar tools for data mining
  - Dealing with the problem of multiplicity

Collaboration with Dean Foster

# Questions

## **Credit scoring**

Who will repay the loan? Who will declare bankruptcy?

## **Identifying faces**

Is this a picture of a face?

## **Genomics**

Does a pattern of genes predict higher risk of a disease?

## **Text processing**

Which references were left out of this paper?

# Questions

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## **These are great statistics problems, so...**

Why not use our workhorse, regression?

Its familiar with diagnostics available.

# Regression Models

## Simple structure

- $n$  **independent** observations of  $m$  features
- $q$  predictors in model with error variance  $\sigma^2$ :

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_q X_q + \epsilon$$

## Calibrated predictions allow various link functions ...

- Linear regression has identity, logistic has logit link.

$$E(Y|X) = h(\beta_0 + \beta_1 X_1 + \cdots + \beta_q X_q)$$

## Rich feature space is key to the model

- Usual mix: continuous, categorical, dummy vars, ...
- Missing data indicators
- Combinations (principal components) and clusters
- Nonlinear terms, transformations (quadratics)

## Hard Question

If we allow for the possibility of **interactions** among the predictors, then the feature space becomes larger still.

*Which features generate the best predictions?*

Also hope to do this without cross-validation.

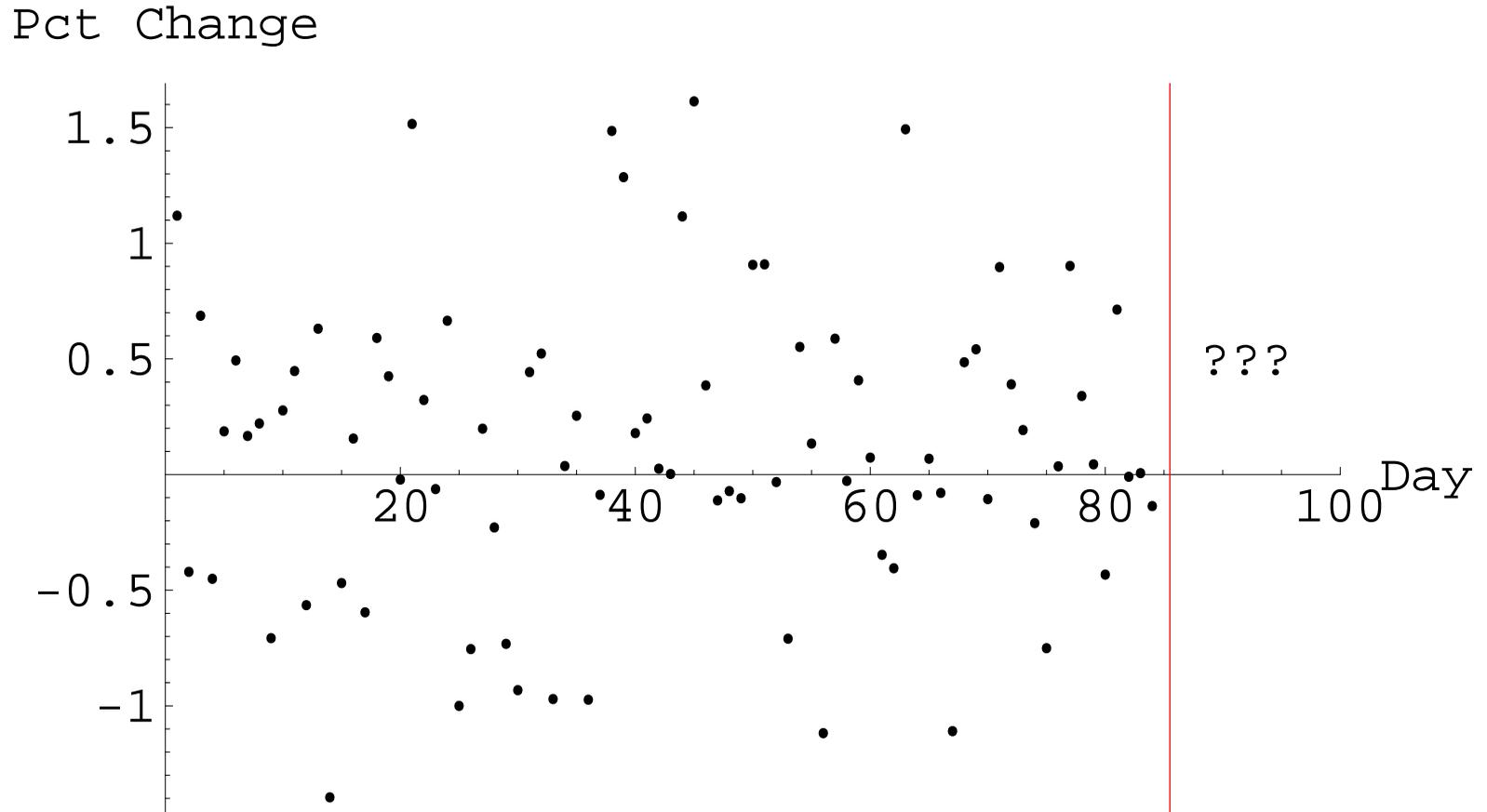
# A favorite example: Stock Market

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Daily percentage changes in the closing price of the S&P 500 during the last 3 months of 2004 (85 trading days) ...



# Predicting the Market

## Problem

Predict returns on S&P 500 in 2005 using features built from 12 *exogenous* factors (*a.k.a.*, technical trading rules).

## Regression model

$R^2 = 0.85$  using  $q = 28$  predictors.

With  $n = 85$ ,  $F = 12$  with p-value  $< 0.00001$ .

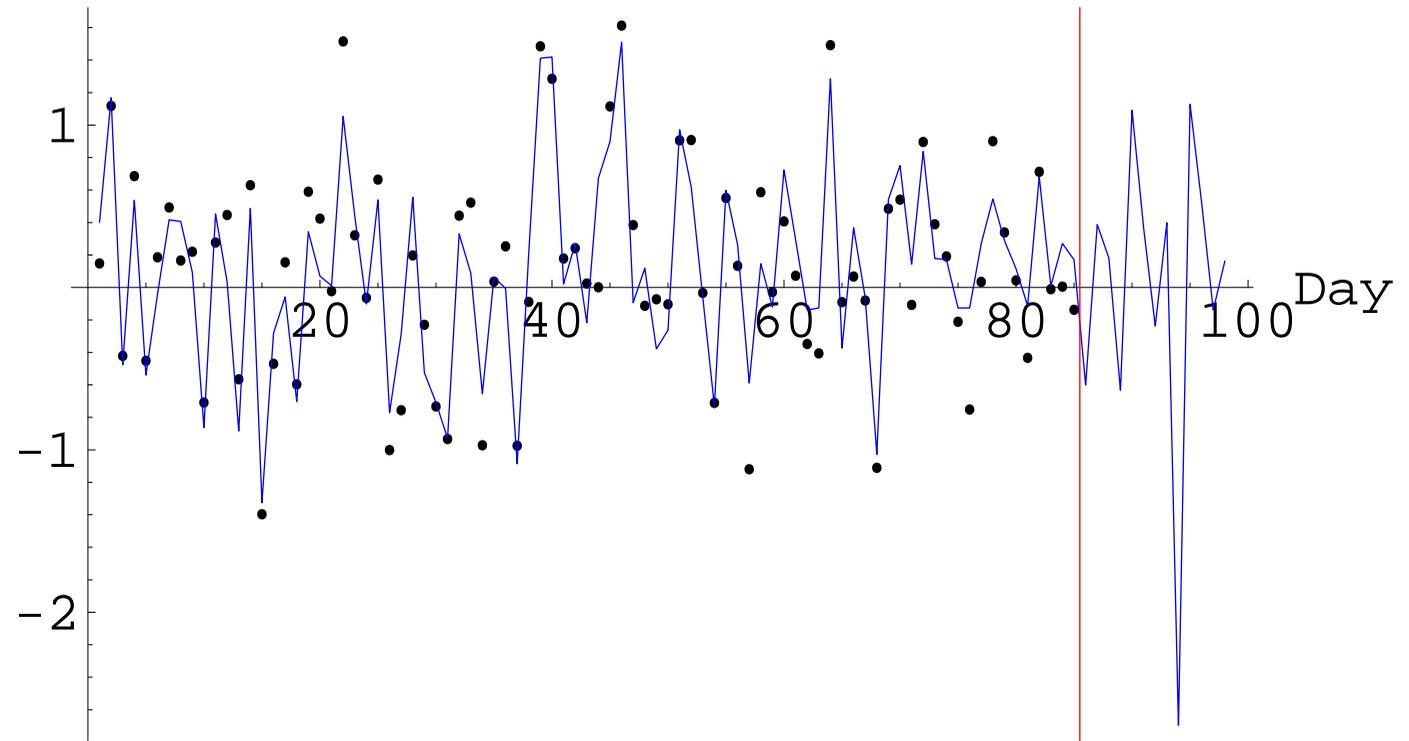
## Coefficients are impressive...

Term	Estimate	Std Error	t-Ratio	p-value
Intercept	0.323	0.078	4.14	0.0001
X4	0.172	0.040	4.34	0.0000
(X1)*(X1)	-0.202	0.039	-5.16	0.0000
(X1)*(X5)	0.256	0.048	5.34	0.0000
(X2)*(X6)	0.289	0.044	6.59	0.0000
(X7)*(X9)	0.249	0.046	5.37	0.0000

# Model Fit and Predictions

Predictions track the historical returns closely, even matching turning points.

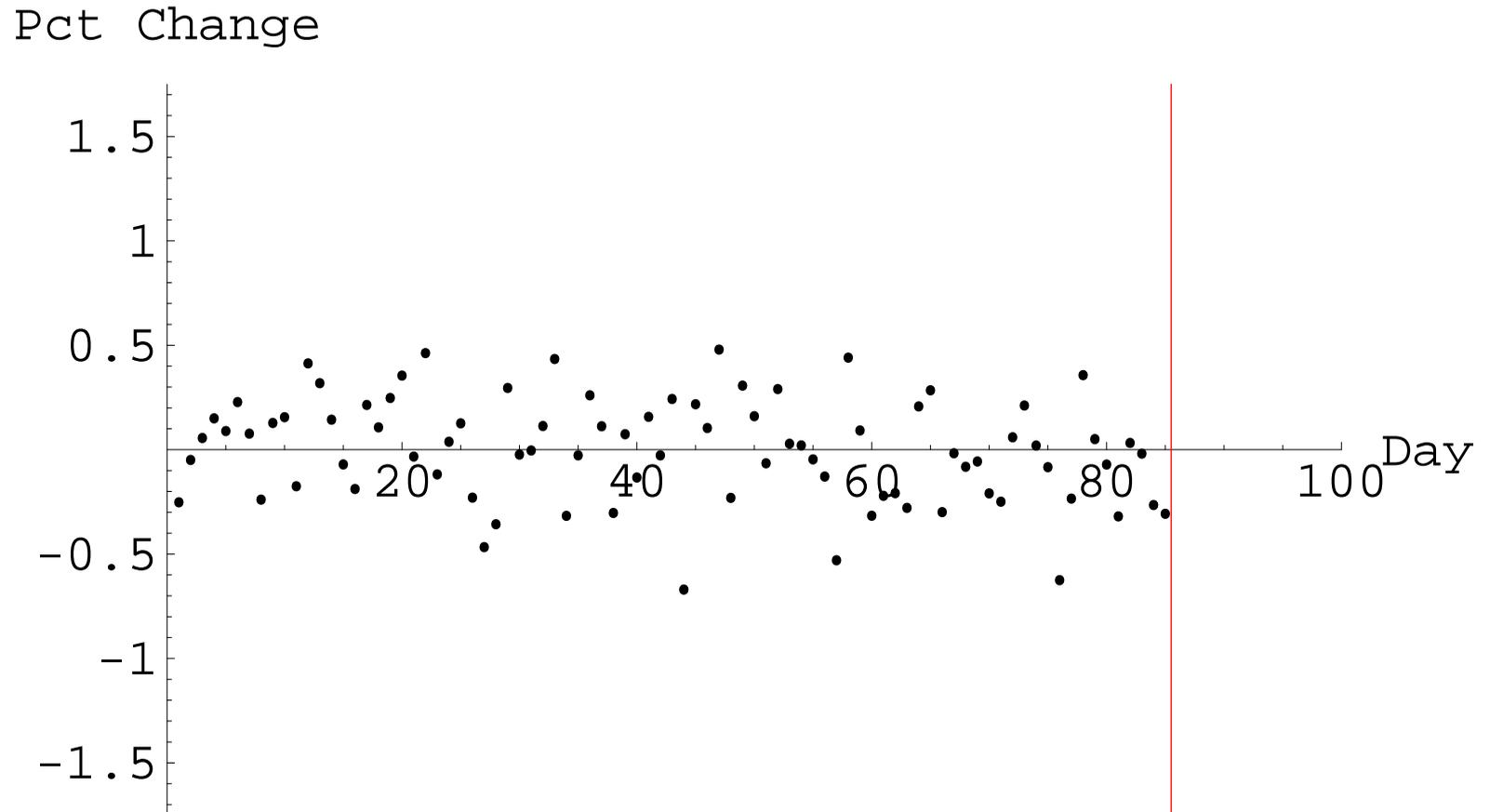
Daily Pct Change



Better short the market that day... No guts, no glory!

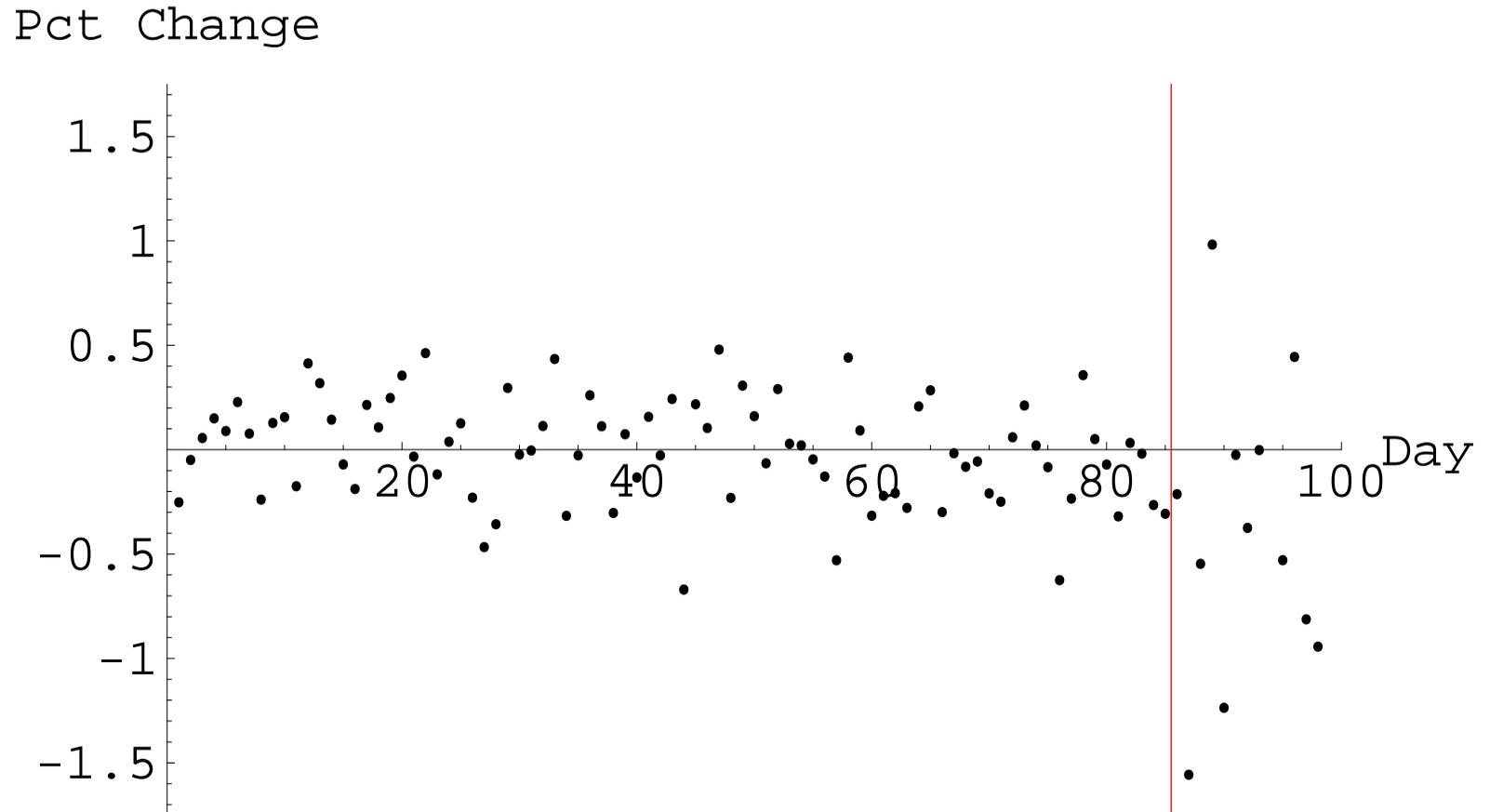
# Prediction Errors

In-sample prediction errors are small...



# Prediction Errors

How'd you lose the house? Even Bonferroni lost his house!



# What was that model?

## Exogenous base variables

12 columns of Gaussian noise.

**Null model** is the right model.

## Selecting predictors

Turn stepwise regression loose on  $m = 90$  features

12 linear + 12 Squares + 66 Interactions  
with “promiscuous” settings for adding variables,  
prob-to-enter = 0.16 (AIC)

Then run stepwise backward to remove extraneous effects.

## Why does this fool Bonferroni?

$s^2$  becomes biased, so remaining predictors appear more significant. Often “cascades” into a perfect fit.

Cannot fit saturated model to get unbiased estimate of  $\sigma^2$   
because  $m > n$ .

# Big Picture, 1

## **Moral**

Stepwise regression can make a silk purse from sow's ear.

## **Must control the fitting process**

Use Bonferroni from the start, not after the fact. No predictor joins model — the right answer.

## **So, how does one control the fitting process?**

Particularly when there are many possible choices.

# Second Example: Predicting Bankruptcy

## Predict onset of personal bankruptcy

Estimate probability customer declares bankruptcy.

## Challenge

Can **stepwise regression** predict as well as commercial “data-mining” tools or substantive models?

**Many features** About 350 “basic” variables

- Short time series for each account
- Spending, utilization, payments, background
- Missing data and indicators
- Interactions are important (cash advance in Vegas)

$m > 67,000$  predictors!

- **Transaction** history would vastly expand the problem.

# Complication: Sparse Response

**How much data do you really have?**

3 million months of activity, each with 67,000 predictors.

**Needle in many haystacks**

Observe only 2,244 bankruptcies.

**Further complication**

What loss function should be minimized?

Profitable customers look risky. Want to lose them?

Who is the ideal customer?

“Borrow lots of money and pay it back slowly.”

**Cross-validation**

Less appealing with so few events.

# Approach

## Forward stepwise search

Use p-values to determine whether to add predictors.

## Two questions

1. How to calculate a p-value?
2. Where to put the threshold for the p-value?

## Risk inflation criterion (RIC) ( $m = \#$ possible predictors)

Hard thresholding, Bonferroni, Fisher's method

$$\text{Add } X_j \iff t_j^2 > 2 \log m \iff p_j < \frac{1}{m}$$

Obtains RIC bound (Foster & George 1994)

$$\min_{\hat{\beta}} \max_{\beta} E \frac{\|Y - X\hat{\beta}\|^2}{|\beta| \sigma^2} \leq 2 \log m$$

where  $|\beta| = \#\{\beta_j \neq 0\}$ .

# Adaptive Variable Selection

## Sparse models

RIC best when “truth” is sparse, but lacks power if much signal. **False discovery rate** motivates an alternative.

**Adaptive threshold** If you’ve added  $q$  predictors,

$$\text{Add } X_j \iff p_j < \frac{q+1}{m}$$

## Further motivation

- Half-normal plot (Cuthbert Daniel?)
- Generalized degrees of freedom (Ye 1998, 2002)
- Empirical Bayes (George & Foster 2000)
- Information theory (Foster, Stine & Wyner 2002)

**Universal prior** Which predictors minimize this ratio?

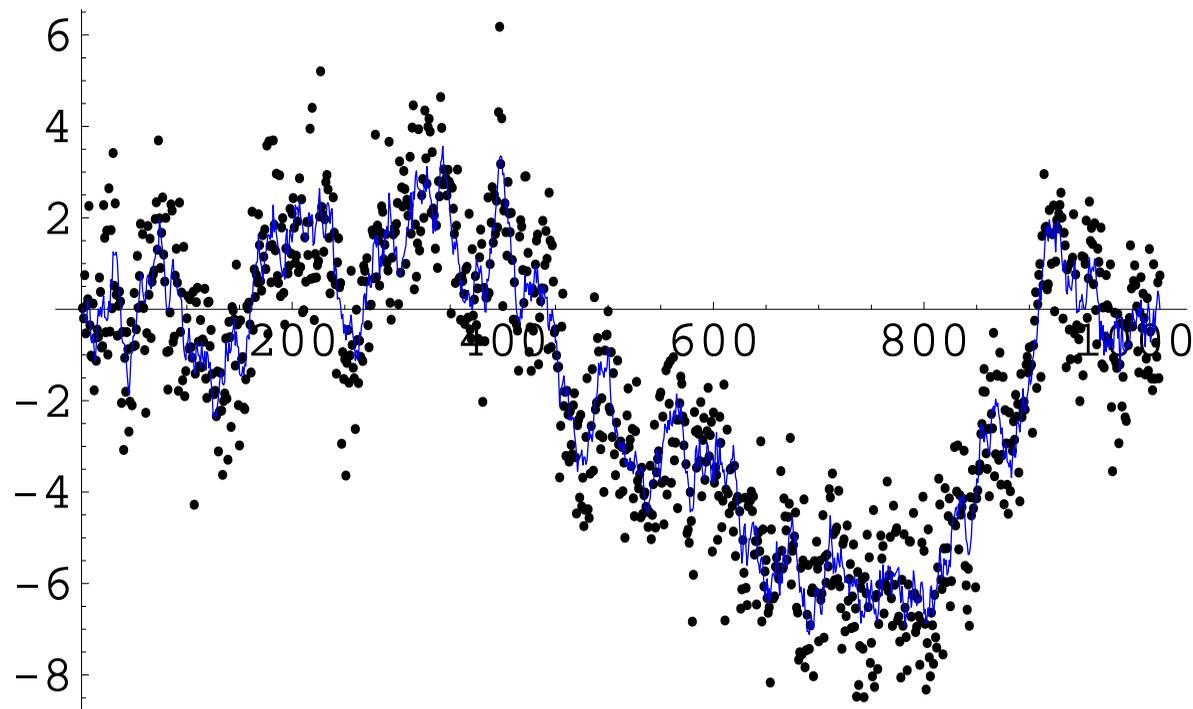
$$\min_{\hat{q}} \max_{\pi} \frac{E \|Y - \hat{Y}(\hat{q})\|^2}{E \|Y - \hat{Y}(\pi)\|^2} \text{ for } \beta \sim \pi$$

# Example: Finding Subtle Signal

Signal is a **Brownian bridge**

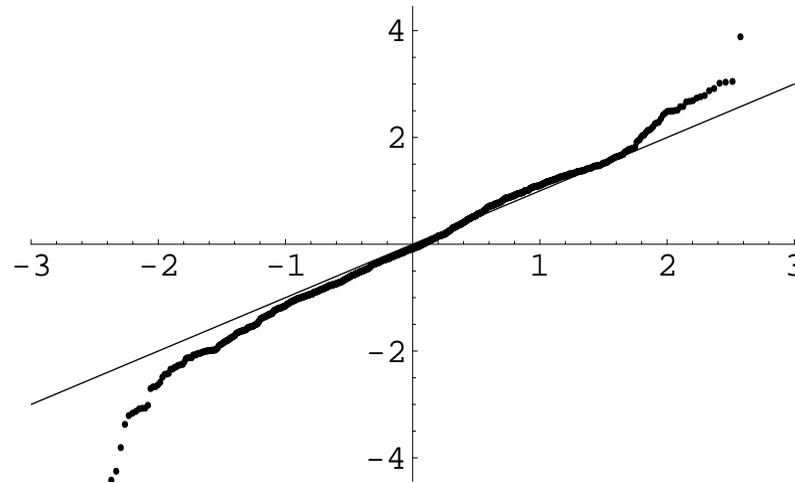
Stylized version of financial volatility.

$$Y_t = BB_t + \sigma \epsilon_t$$

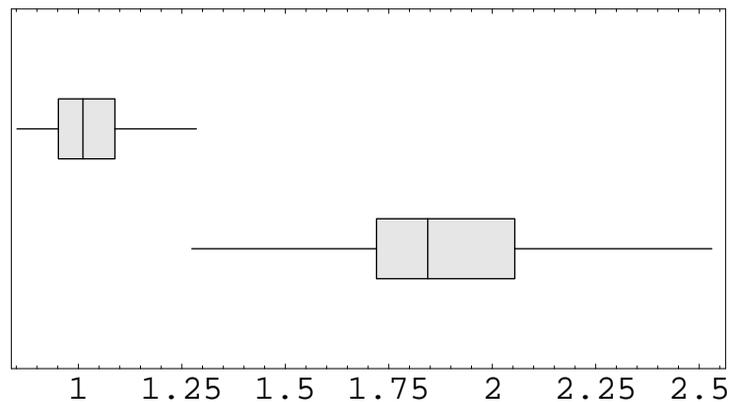


# Example: Finding Subtle Signal

Wavelet transform has many coefficients but none is very large relative to the others.



**MSE** with adaptive (top) vs. hard (bottom)



# But it fails for bankruptcy!

**Thresholding classical p-values does not work**

Fit on 600,000, predict 2,400,000.

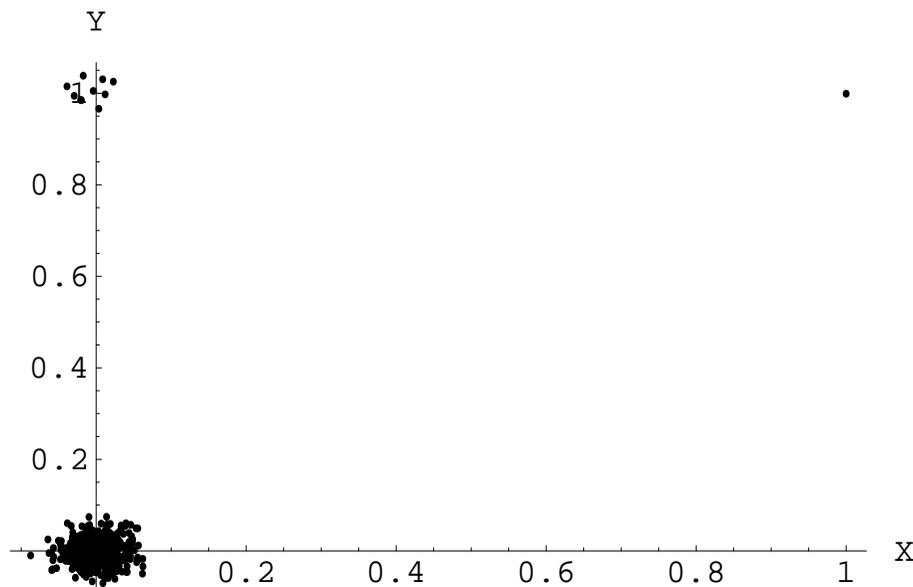
As fitting proceeds, out-of-sample error shows sudden spike.

Diagnostic **plots** revealed the problem.

**Stylized problem**  $n = 10,000$ , dithered

$X_1 = 1, X_2, \dots, X_{10,000} \sim N(0, 0.025)$

$P(Y = 1) = 1/1000$ , independent of  $X$ .



$t = 14$ , but common sense suggests  $p \approx 1/1000$ .

# What went wrong?

## Theory implies p-values are known

- Normal distribution on error (thin tailed).
- Know “true” error variance  $\sigma^2$ , plus its constant.
- Predictors are orthogonal.

$$\Rightarrow \hat{\beta}_j \stackrel{\text{iid}}{\sim} N(\beta_j, \text{SE}_j)$$

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## In practice...

- Is any data ever normally distributed?
  - Don't believe there's a true model, much less fixed error variance.
  - Collinear features, frequently with  $m > n$ .
- $\Rightarrow$  At best, can only guess p-values.

# Honest p-values

## Concern from stock example

Must avoid “false positives” that lead to inaccurate predictions, cascade of mistakes.

## Robustness of validity

Rank regression would also protect you to some extent, but has problems dealing with extreme heteroscedasticity.

## Alternatives

Method	Requires
Robust estimator (e.g. ranks)	Homoscedastic
White estimator	Symmetry
Bennett bounds	Bounded $Y$

## Bounded influence estimators

Another possibility, but can it be computed fast enough?

# White Estimator

$$Y = \hat{\beta}_0 + \hat{\beta}_{q,1}X_{q,1} + \cdots + \hat{\beta}_{q,q}X_{q,q} + \epsilon$$

**Sandwich formula** (H. White, 1980, *Econometrica*)

$$\text{Var}(\hat{\beta}_q) = (X'_q X_q)^{-1} X'_q \underbrace{\text{Var}(\epsilon)} X_q (X'_q X_q)^{-1}$$

Estimate variance using the residuals from **prior** step:

$$\text{Var}(\hat{\beta}_q) = (X'_q X_q)^{-1} X'_q \underbrace{\text{Diag}(e^2_{q-1})} X_q (X'_q X_q)^{-1}$$

## Result in stylized problem

Estimated SE is 10 times larger, more appropriate p-value.

**Moral: Watch your null hypothesis!**

Only test  $H_0 : \beta_{q,q} = 0$  rather than

$$H_0 : \beta_{q,q} = 0 \quad \& \quad \text{Var}(\epsilon_i) = \sigma^2$$

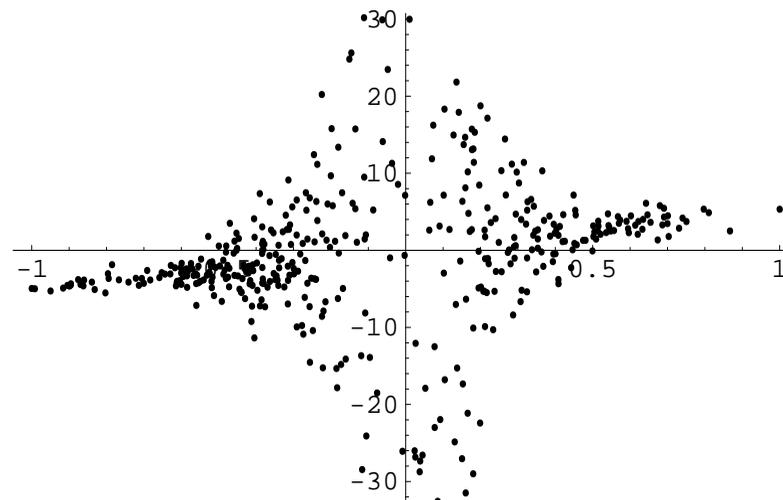
# Example: Finding Missed Signal

## Question

Does White estimator ever find an effect that OLS misses?  
Usually OLS underestimates SE.

## Heteroscedastic data

High variance at 0 obscures the differences at extremes.



## Least squares

Standard OLS reports  $SE = 3.6$  giving  $t = 1.2$ .  
White  $SE \approx 0.9$  and finds the underlying effect.

# Honest p-values for Testing $H_0 : \beta = 0$

## Three methods

Each method makes some assumption about the data in order to produce reliable p-value.

Method	Requires
Robust estimator (e.g. ranks) White estimator <b>Bennett bounds</b>	Homoscedastic Symmetry <b>Bounded <math>Y</math></b>

# Bennett Inequality

## Think differently

Sampling distribution of  $\hat{\beta}$  is not normal because huge leverage contributes “Poisson-like” variation.

## Bennett inequality (Bennett, 1962, *JASA*)

Bounded independent r.v.  $U_1, \dots, U_n$  with  $\max |U_i| < 1$ ,  
 $E U_i = 0$ , and  $\sum_i E U_i^2 = 1$ ,

$$P\left(\sum_i U_i \geq \tau\right) \leq \exp\left(\frac{\tau}{M} - \left(\frac{\tau}{M} + \frac{1}{M^2}\right) \log(1 + M\tau)\right)$$

If  $M\tau$  is small,  $\log(1 + M\tau) \approx M\tau - M^2\tau^2/2$

## Allows heteroscedastic data

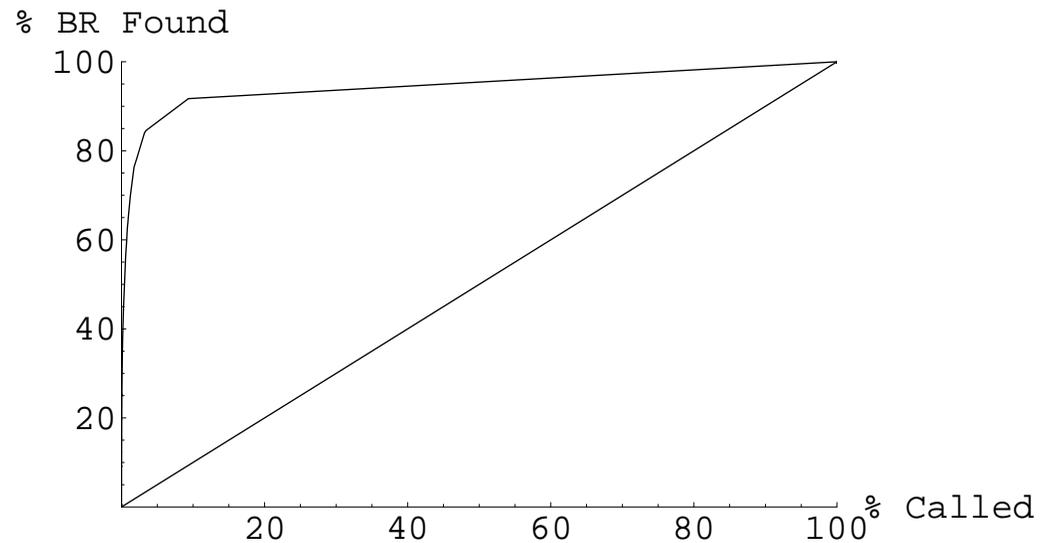
Free to divy up the variances as you choose, albeit only for bounded random variables.

**In stylized example** assigns p-value  $\approx 1/100$ .

# Classification Results

## Success!

Not only does the model obtain smaller costs than C4.5 (w/wo boosting), it has huge lift:





# Big Picture, 2

## Moral

Better get the right p-values

## Successful

Carefully computed standard errors and p-values

+

Adaptive thresholding rules

= Competitive procedure

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## Downside

- Know that we're not leveraging domain knowledge.
- Model is more complicated than need be.
- Took forever to run.

# Obesity

The issues arising the bankruptcy application only get worse as the data set gets wider...

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The issues arising the bankruptcy application only get worse as the data set gets wider...

and data sets seem to be getting wider and wider.

<i>Application</i>	<i>Number of Cases</i>	<i>Number Raw Features</i>
Bankruptcy	3,000,000	350
Faces	10,000	1,400
Genetics	1,000	10,000
CiteSeer	500	10,000,000

# Sequential Selection

## Simple idea

Search features in *some* order rather than all at once.

## Opportunities

- Incorporate substantive knowledge into search order
- Sequential selection of features based on current status
- Open vs. closed view of space of predictors
- Run faster

## Heuristics

- Theory from adaptive selection suggests that if you can order predictors, then little to be gained from knowing  $\beta$ .
- Alpha spending rules in clinical trials.
- Depth-first rather than breath-first search.

# Multiple Hypothesis Testing

**Test**  $m$  null hypotheses  $\{H_1, \dots, H_m\}$ ,  $H_j : \theta_j = 0$ .

		Accept $H_0$	Reject $H_0$	
True	$H_0$	$U^\theta(m)$	$V^\theta(m)$	$m_0$
State	$H_0^c$	$T^\theta(m)$	$S^\theta(m)$	$m - m_0$
		$m - R(m)$	$R(m)$	$m$

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**Classical criterion** Family wide error rate

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**Classical criterion** Family wide error rate

$$\text{FWER}(m) = P_0(V^\theta(m) \geq 1)$$

**Classical procedure** Bonferroni

Test each  $H_j$  at level  $\alpha_j$  so that

$$P_0(V_j^\theta = 1) \leq \alpha_j, \quad \sum_j \alpha_j \leq \alpha$$

# False Discovery Rate

**Approach** Control testing procedure once it rejects.

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**FDR criterion** (Benjamini & Hochberg 1995, *JRSSB*)

Proportion of false positives among rejects

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**Step-down testing** (procedure)

Order p-values of  $m$  **independent** tests of hypotheses

$$p_{(1)} \leq p_{(2)} \leq \cdots \leq p_{(m)}$$

Starts with Bonferroni comparison  $p_{(1)} \leq \alpha/m$ , then gradually raises threshold as more hypotheses are rejected.

Reject  $H_{(j)}$  if  $p_{(j)} \leq \alpha j/m$ .

**Controls FWER and FDR** with more power.

## An Alternative to FDR

Count the number of *correct* rejections  $S^\theta(m)$  in excess of a fraction of the total number rejected.

$$\text{EDC}_{\alpha,\gamma}(m) = E_\theta[S^\theta(m) - \gamma R(m)] + \alpha, \quad 0 < \alpha, \gamma < 1.$$

Heuristically,  $\alpha$  controls FWER and  $\gamma$  controls FDR.

Testing procedure “controls EDC”  $\iff \text{EDC} \geq 0$

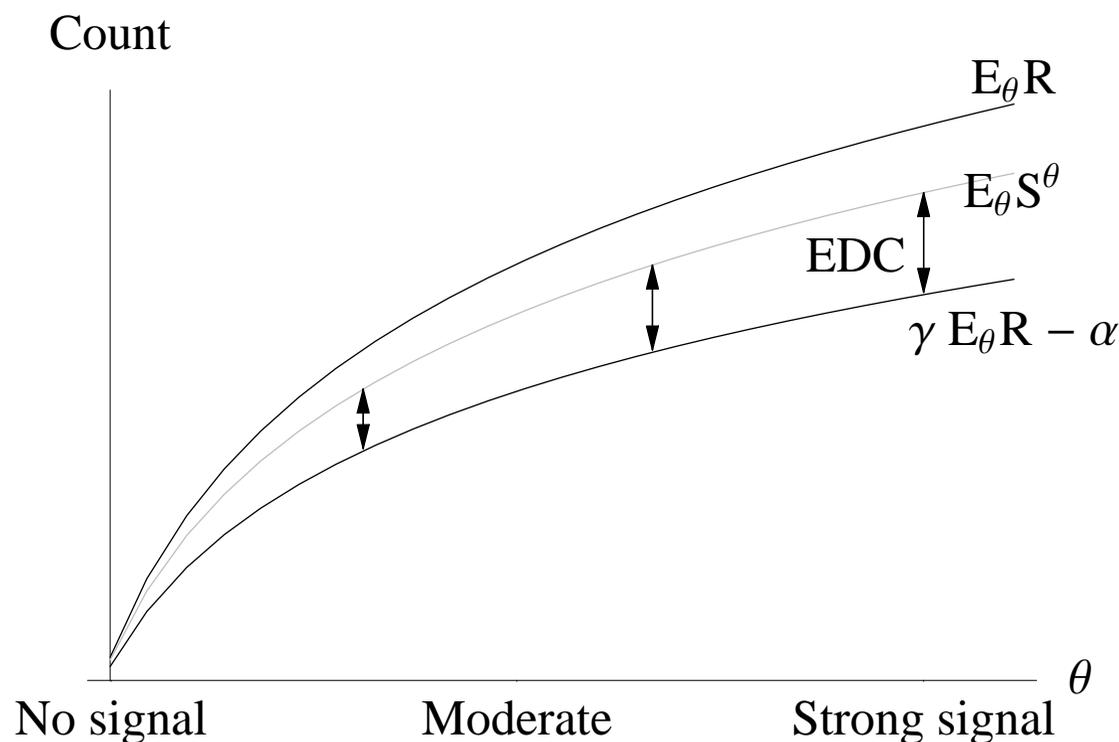
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# Comparison to FDR

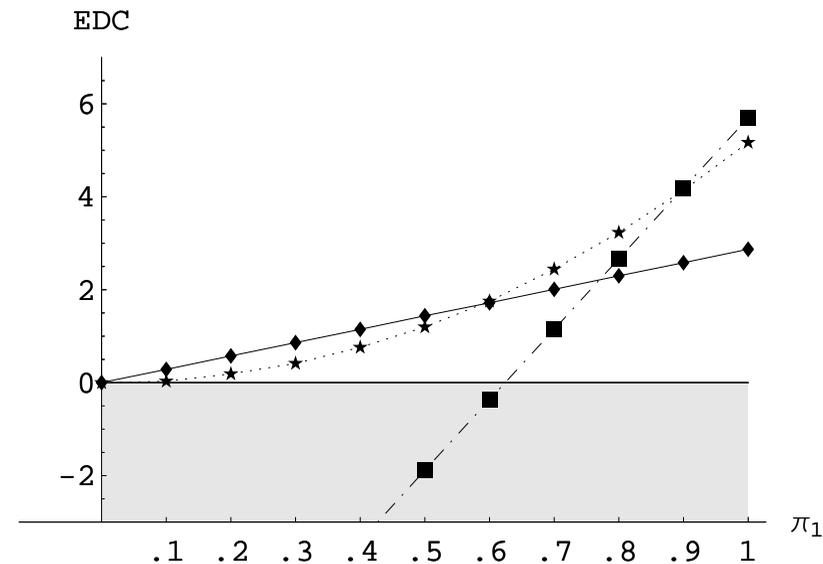
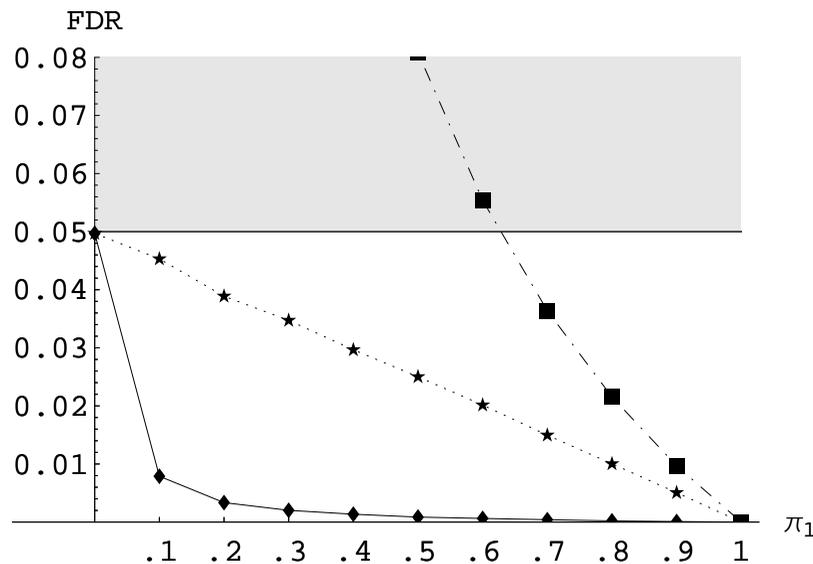
Simulate tests of  $m = 200$  hypotheses with

$$\mu_j \sim \begin{cases} 0 & w.p. \quad 1 - \pi_1 \\ N(0, \sigma^2) & w.p. \quad \pi_1 \end{cases}$$

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Three methods: naive fixed  $\alpha$  level, step-down, Bonferroni.

# Alpha-Investing Rules

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## P-value

Determines how alpha-wealth changes:

$$W(j) \approx W(j - 1) + \begin{cases} \omega - p_j & \text{if } p_j \leq \alpha_j, \\ -\alpha_j & \text{if } p_j > \alpha_j. \end{cases}$$

## Payout

If the test rejects, the rule “earns” payout  $\omega$  toward future tests. Otherwise, its wealth decreases by  $\alpha_j$ .

# Alpha-investing Controls EDC

## Benefit of EDC

Because it uses differences in counts rather than expected ratio, we can prove alpha investing satisfies EDC criterion.

## Theorem

An alpha-investing rule with initial wealth  $W(0) \leq \alpha$  and payoff  $\omega \leq 1 - \gamma$  controls EDC,

$$\inf_M \inf_{\theta} E_{\theta} \text{EDC}_{\alpha, \gamma}(M) \geq 0$$

for any stopping time  $M$ .

## Generality

The tests need not be independent, just “honest” in the sense that

$$E(V_j | R_1, \dots, R_{j-1}) \leq \alpha_j \quad \text{under } H_j$$

# Comparison to Step-Down Testing

## Simulation

Same setup.

200 hypotheses, varying proportion of signal  $\pi_1$ .

## Testing procedures

- Step-down testing
- Alpha-investing: “conservative” and “aggressive”

## Two scenarios: What is known?

Order of testing differs in the two cases:

**Nothing:** random order.

**Lots:** order of  $|\mu_j|$  (not  $\bar{Y}_j$ )

# Approaches to Alpha-Investing

## Conservative

Micro-investing matches performance of FDR.

Suppose FDR rejects  $k$  hypotheses, and  $\alpha = \omega = W(0)$ .

- Test all  $m$  hypotheses at Bonferroni level  $\alpha/m$ .  
Rejects  $H_{(1)}$ : pay  $\alpha = m \times \alpha/m$  to earn  $\alpha$ .
- Test other  $m - 1$  hypotheses given  $p_j > \alpha/m$ .  
Rejects  $H_{(2)}$ : pays  $\alpha$  and earns  $\alpha$ .
- Continue...

Rejects at least those FDR rejects, and perhaps more.

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## Aggressive

Spend more  $\alpha$  testing leading hypotheses since these should have the most signal — if your science is right.

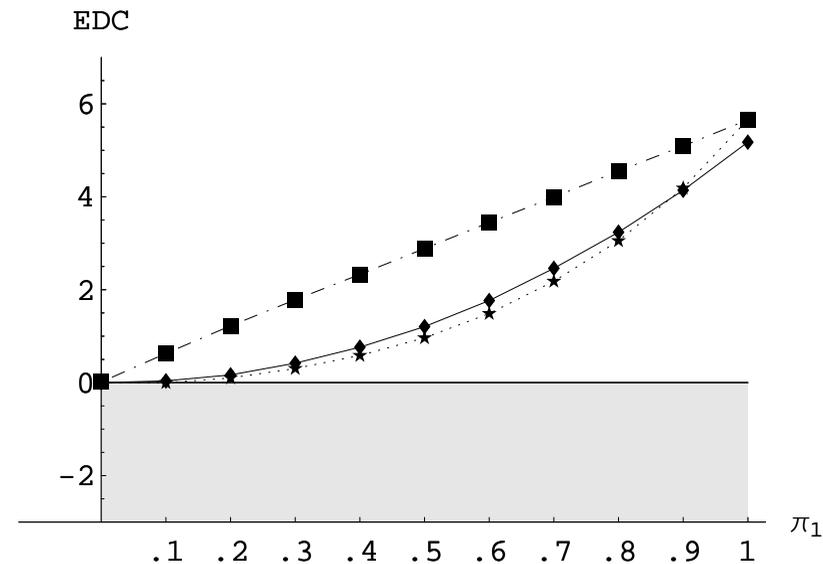
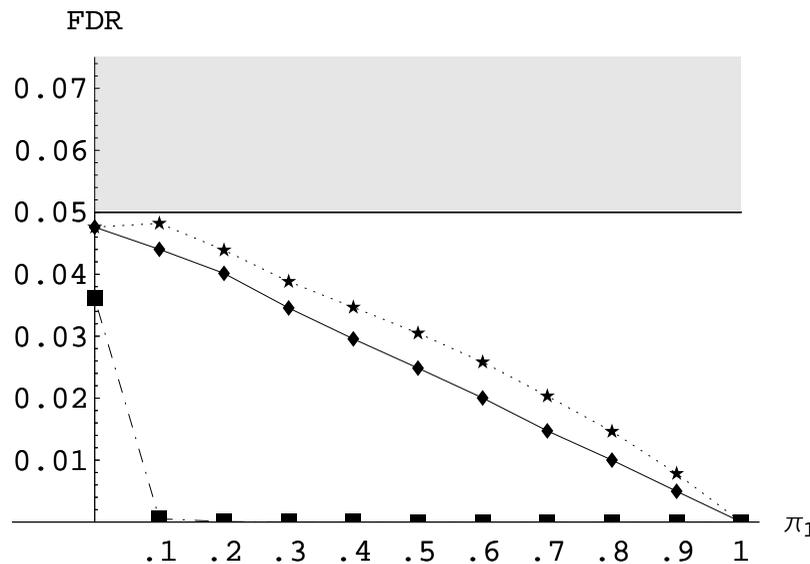
*e.g.*, Set level as

$$\alpha_j = \frac{cW(0)}{j^2}, \quad j = 1, 2, \dots$$

# Results of Simulation

Simulate tests of  $m = 200$  hypotheses with

$$\mu_j \sim \begin{cases} 0 & w.p. \ 1 - \pi_1 \\ N(0, \sigma^2) & w.p. \ \pi_1 \end{cases}$$



Step-down testing . . .

Alpha-investing (conservative —, aggressive - · -)

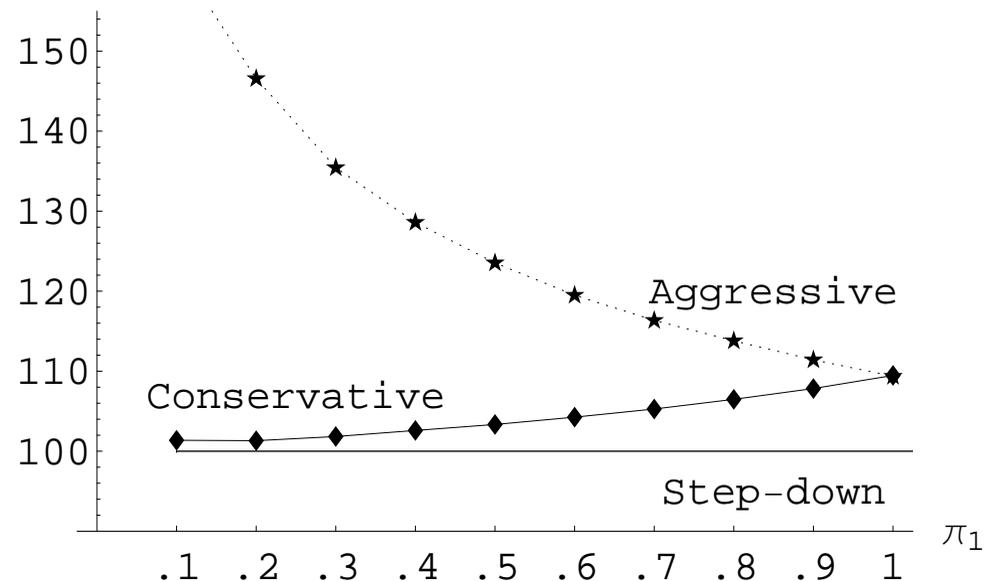
# Knowledge = Power

**Percentage rejection** relative to step-down testing.

$$100 \frac{S^\theta(m, \text{aggressive investing})}{S^\theta(m, \text{step-down})} > 150\%$$

**Aggressive alpha investing** works well when the information it uses is accurate.

% Rejected vs Step-Down



# Going Further

## In for a penny, in for a pound

EDC and alpha-investing provide framework for testing a *stream* of hypotheses using *several* investing rules.

## Multiple predictor streams

- Start with raw variables as basic stream.
- Once select  $X_1$  and  $X_2$ , try  $X_1 * X_2$ .

## Auction = Multiple alpha-investing rules

- Two rules, one for  $X$ 's and second for interactions.
- Each starts with wealth  $\alpha/2$ .
- Easy to wager more for  $m$   $X$ 's than  $m^2$  interactions.
- Best strategy accumulates wealth, makes most choices.

## It works!

- Have run auctions through 1,000,000 predictors.
- Finds linear effects *and* high-order interactions.

# Discussion

## Variable selection

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## Strategies for feature creation

- Room for serious improvement
- Substantive expert can order features (chemist)
- Parasitic rules that exploit substantive rules

# Discussion

## Variable selection

- Importance of p-values (which not all methods have).
- Role for cross-validation.
- Provably as good as class of Bayes estimators.

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## Multiple testing using EDC

- Adaptive sequential trials
- Universal wagering