Soc504: Regularization and Hierarchical Models[1]

Brandon Stewart

Princeton

April 24-26, 2017

[1] I am grateful to Justin Grimmer, Marc Ratkovic and Dustin Tingley for sharing their slides with me. Some figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani."

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- Some notes on lecture structure for this week.

Readings

- Murphy (2012) *Machine Learning: a Probabilistic Perspective*

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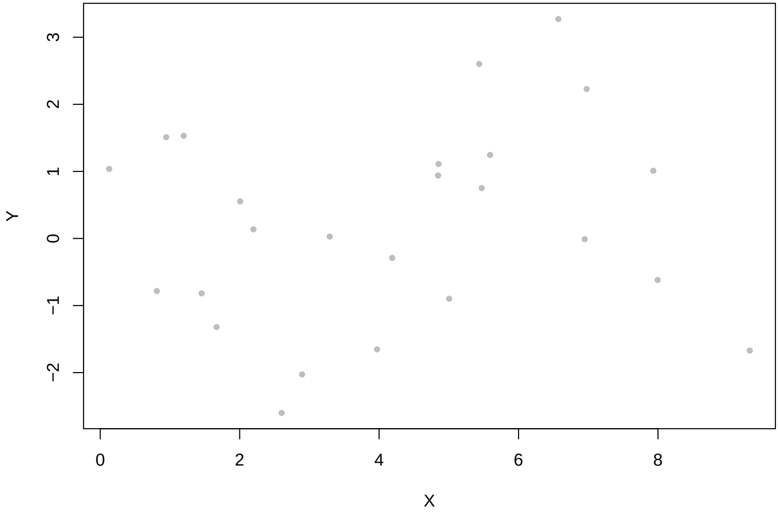
- Gelman and Hill (2008) *Data Analysis Using Regression and Multilevel/Hierarchical Models*

The Core Idea: Penalizing Complexity



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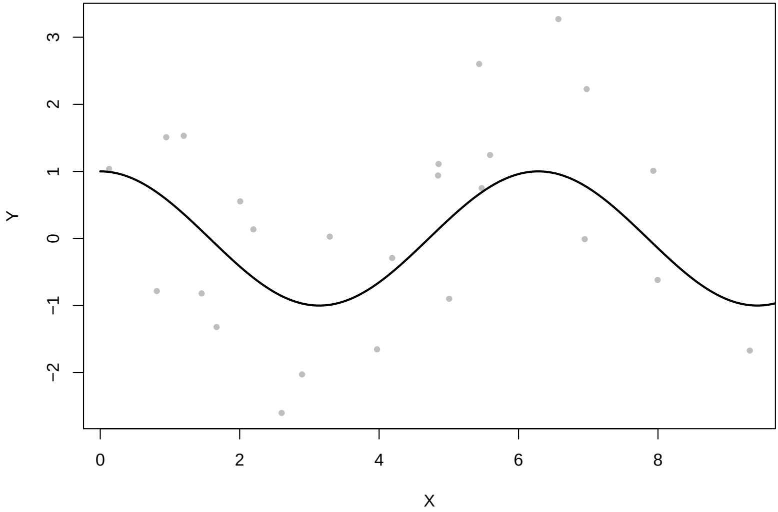

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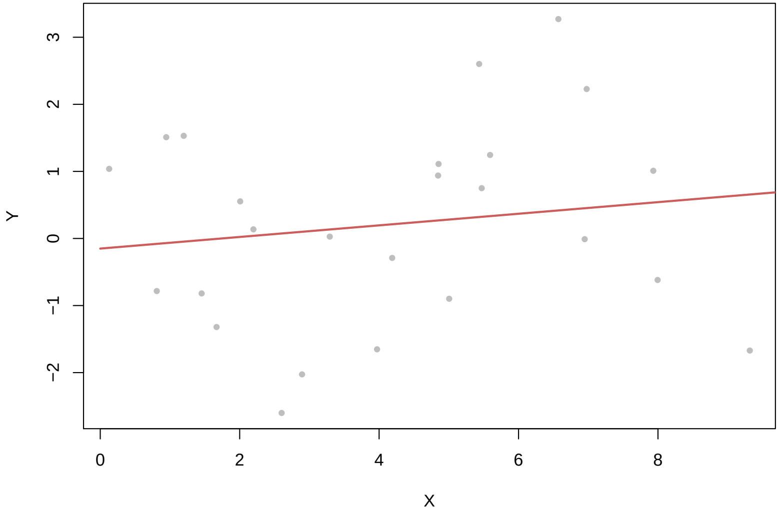

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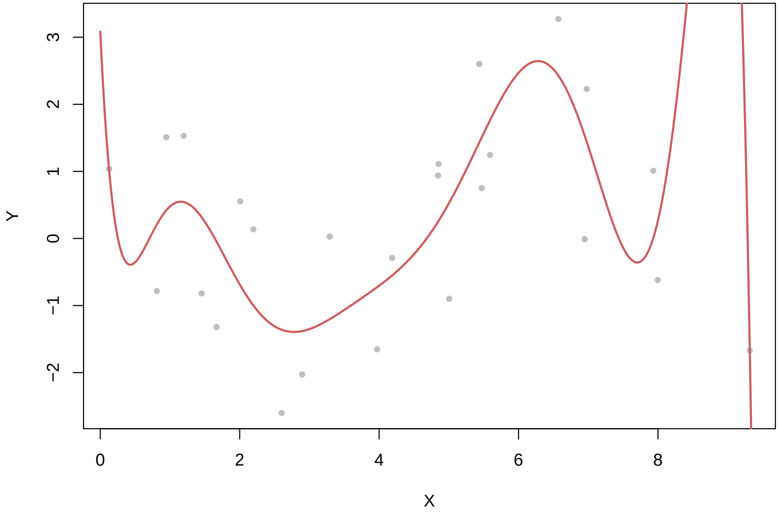

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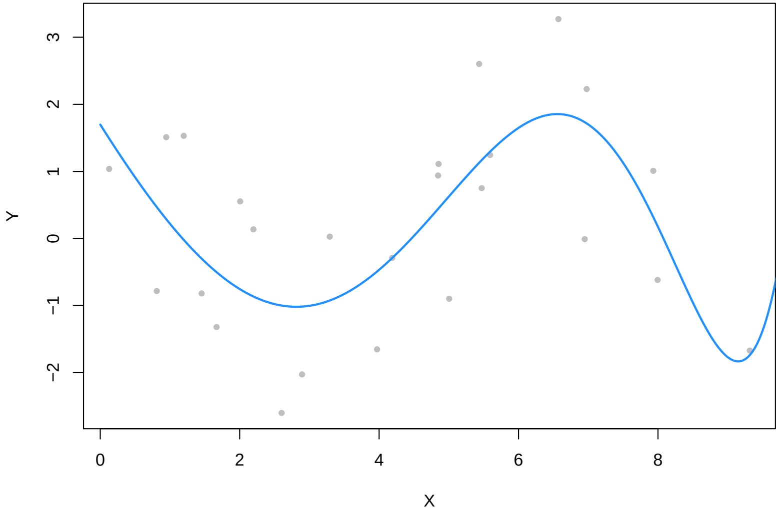

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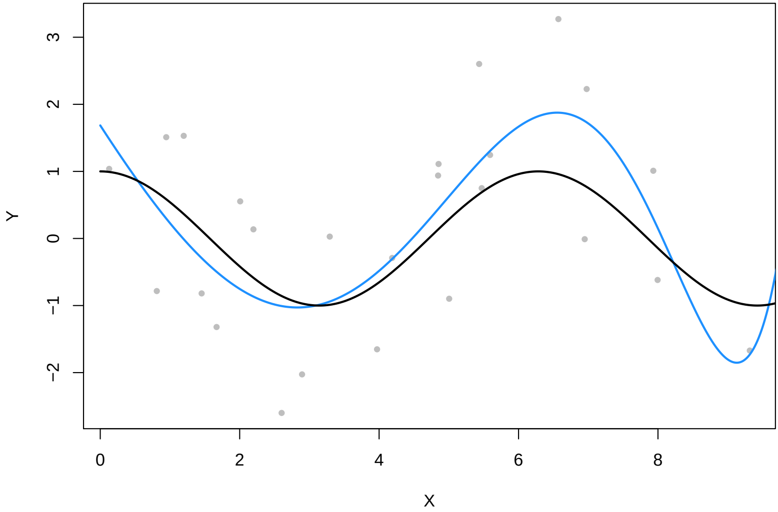

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- The core idea is that we may want to draw an estimate towards a particular point, generally inducing bias in exchange for a reduction in variance
- Hierarchical models induce regularization to draw a set of group specific coefficients towards each other.
- We will start with the simpler case of drawing coefficients towards zero (although later we will consider drawing estimates towards a data-driven point)

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- Regularizers which draw coefficients to exact zeroes are called sparsity-inducing regularizers
- Regularization attempts to improve the generalizability of the model by penalizing extreme solutions even if they fit the current dataset better.

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- In standard OLS we minimize the following criterion:

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- The math here is for least-squares but it also works for GLMs by replacing the RSS term with the negative log likelihood

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  - finding the maximum of the posterior (MAP inference) is equivalent to maximizing the likelihood with regularization

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- Assume squared loss, and an estimated function $\hat{f}$, and fixed X's. The pointwise expected prediction error is:

$$\begin{aligned}\mathcal{R}(x_0) &= \mathbb{E}[(Y-\hat{f}(x_0))^2|X=x_0] \\ &= \sigma_\epsilon^2 + (\mathbb{E}[\hat{f}(x_0)] - f(x_0))^2 + \mathbb{E}[\hat{f}(x_0) - \mathbb{E}\hat{f}(x_0)]^2 \\ &= \text{Irreducible error} + \text{Bias}^2 + \text{Variance}\end{aligned}$$

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To reduce MSE, we are willing to induce bias to decrease variance $\rightsquigarrow$ methods that shrink coefficients toward zero

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- We will cover two which come up frequently ridge regression and LASSO

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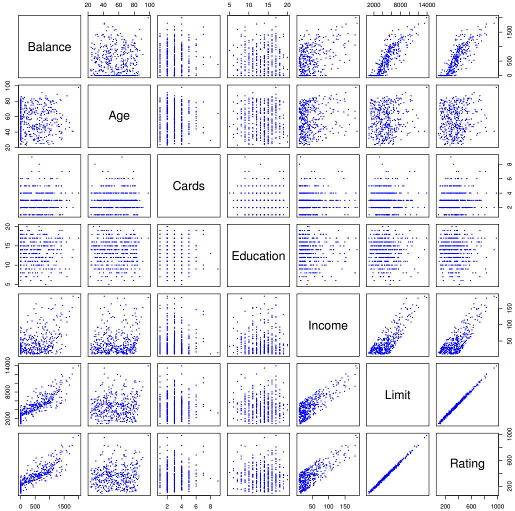
- We will use a running example of Credit Data which predicts credit card balance of a number of individuals using many predictors

Credit Data



Balance
Age
Cards
Education
Income
Limit
Rating
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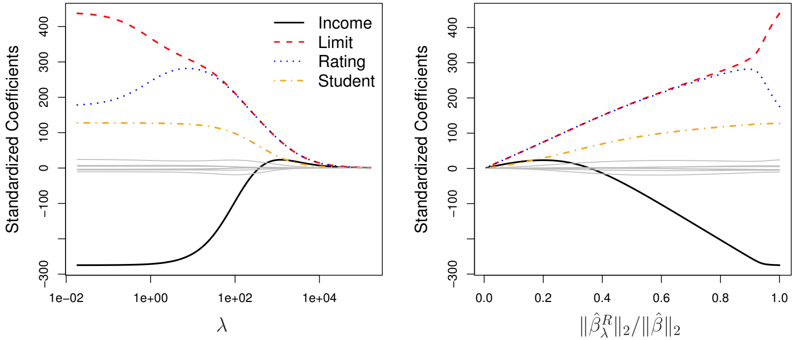
- We can visualize with a regularization path, a calculation across all values of λ

Regularization Path



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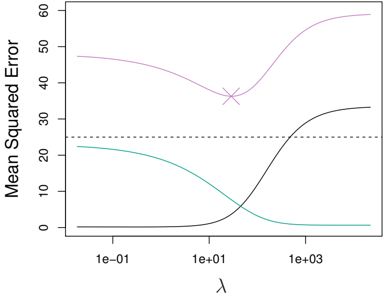

Squared bias (black), variance (green), test mean squared error (purple). Dashed line is the minimum possible MSE

Lasso Regression Objective Function/Optimization

A different penalty $\rightsquigarrow$ different behavior

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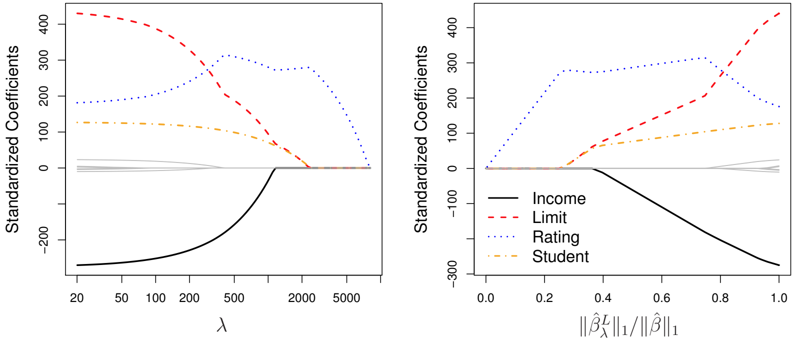
- Optimization is non-linear (due to the absolute value)
- Induces sparsity $\rightsquigarrow$ sets some coefficients to zero

Regularization Path: Lasso



Lasso Regression $\rightsquigarrow$ Soft Thresholding

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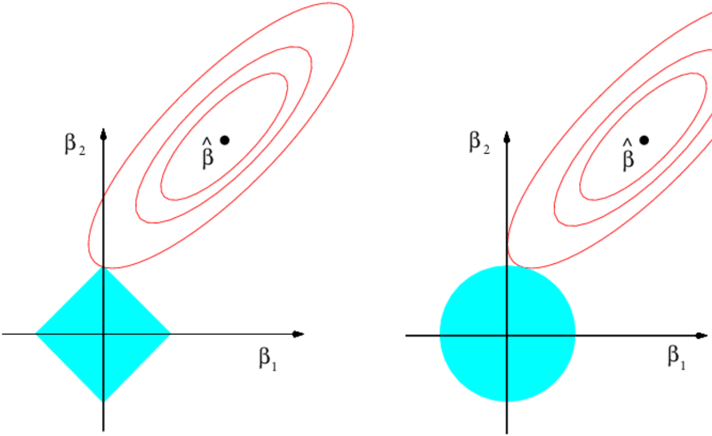
- Thus up to a particular value the coefficient remains 0.
- Where does the sparsity come from? and why doesn't ridge have it?

Lasso vs. Ridge



Origins of Sparsity

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- Let's do a quick mathematical example

Comparing Ridge and LASSO

Contrast $\beta = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ and $\tilde{\beta} = (1, 0)$

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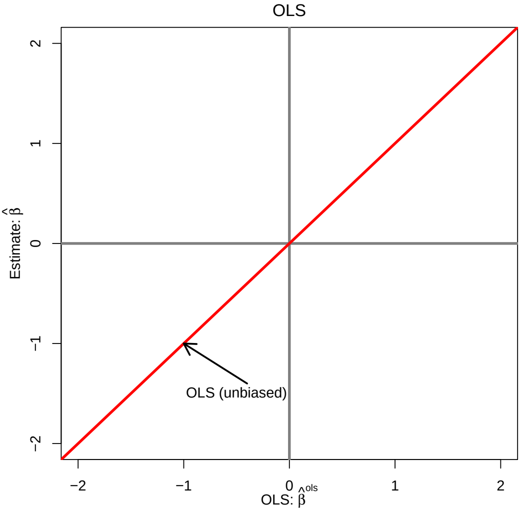

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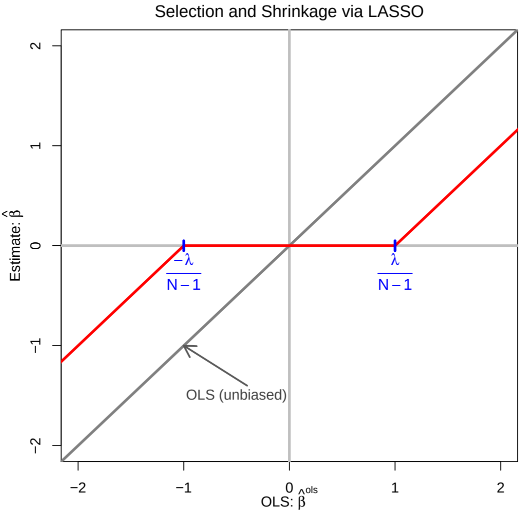

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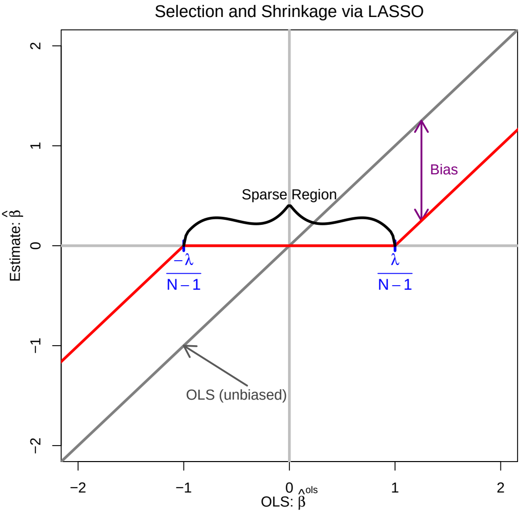

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Bias-Variance Tradeoff in Action

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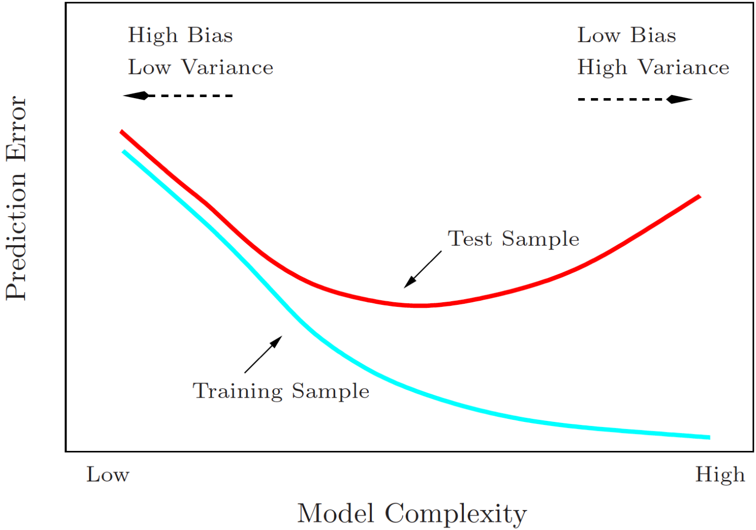
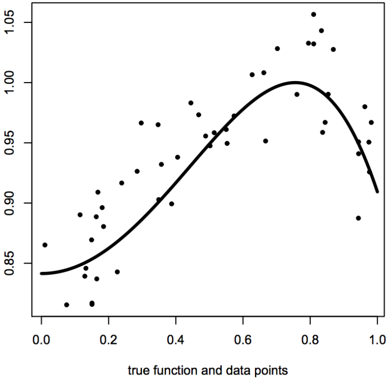


Example Synthetic Problem[2]

$$y = \sin(1 + x^2) + \epsilon$$



[2] These slides are adapted from material by Radford Neal.

Linear Basis Function Models

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- In general the idea is to do a linear regression of y on $\phi_1(x), \phi_2(x), \ldots, \phi_{m-1}(x)$ where ϕ_j are basis functions.
- The model is now:

$$y = f(x, \beta) + \epsilon$$

$$f(x, \beta) = \beta_0 + \sum_{j=1}^{m-1} \beta_j \phi_j(x) = \beta^T \phi(x)$$

Polynomial Basis Functions

We can look at OLS fits with polynomial basis functions of increasing order.

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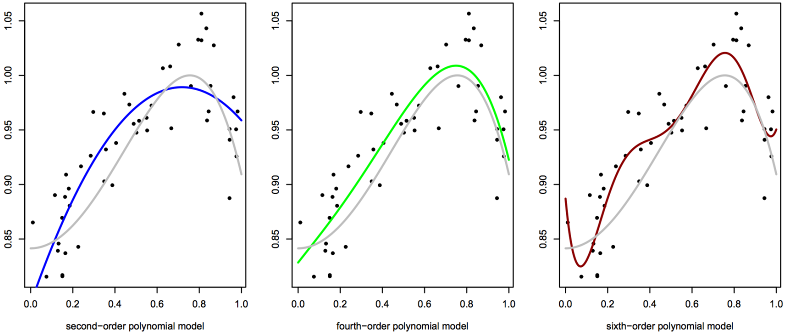

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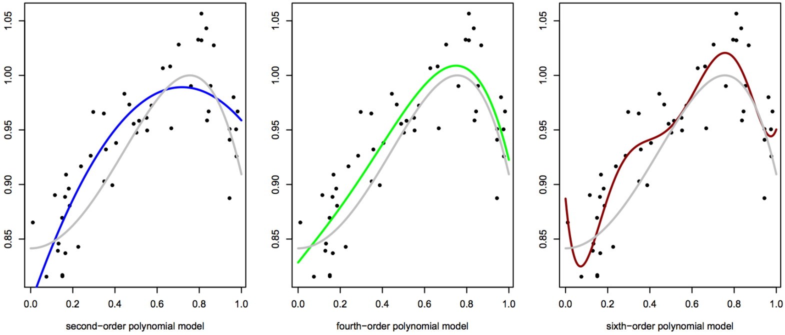

It appears that the last model is too complex and is overfitting a bit.

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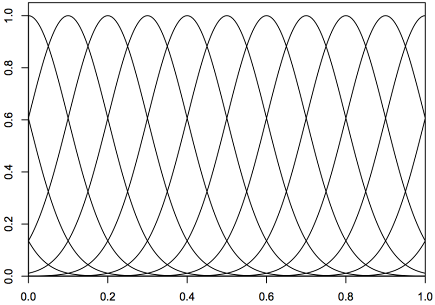
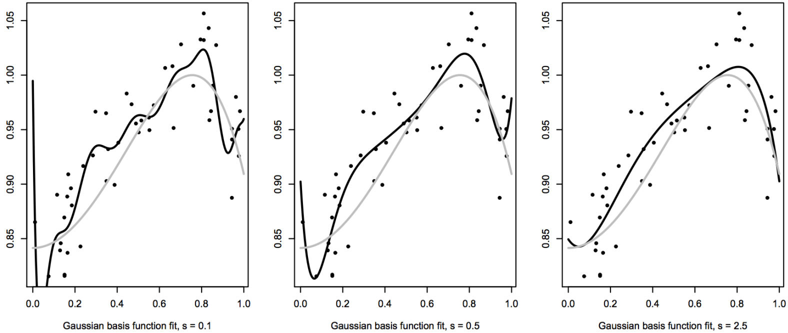


Gaussian basis functions, s = 0.1

Gaussian Basis Fits



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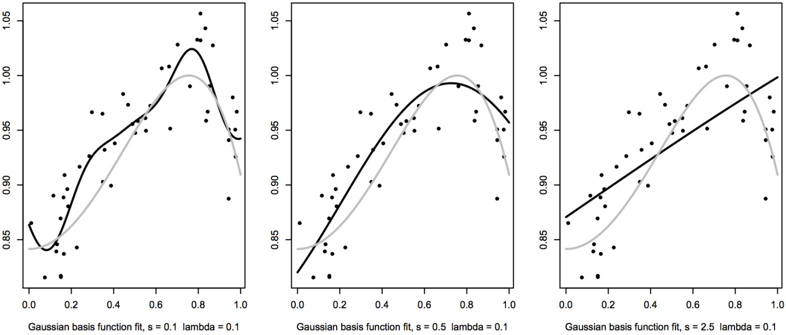
- Two ways to address: limit model flexibility or use a flexible model and regularize
- Regularization is the way to express preference for smoothness in our function
- Let's look at the ridge penalty $\lambda \sum_{j=1}^{m-1} \beta_j^2$ where λ controls the strength of the penalty.

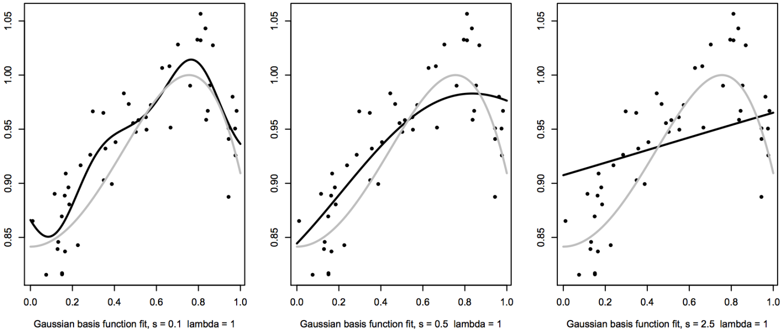
Results

Here are the results with $\lambda = 0.1$:



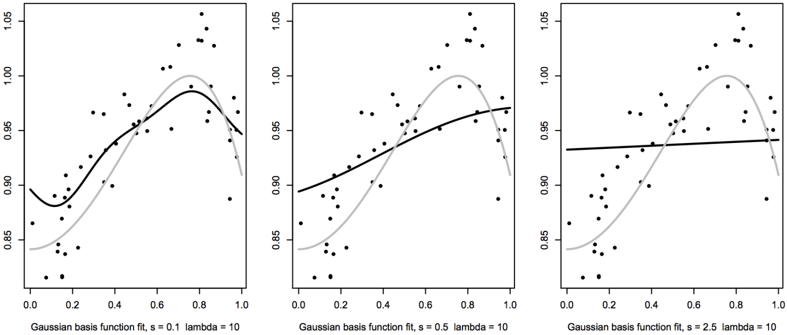
Results

Here are the results with $\lambda = 1$:



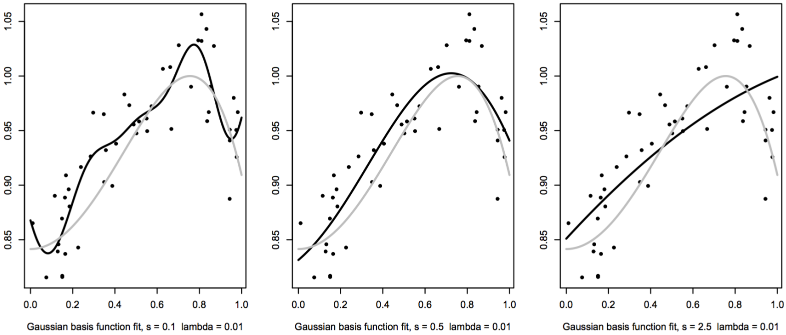
Results

Here are the results with $\lambda = 10$:



Results

Here are the results with $\lambda = 0.01$:



We've Seen Ridge Regression Before

- Generalized Additive Models (GAM's) from the `mgcv` package use ridge regression.

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- Also recall Kernel Regularized Least Squares (KRLS) Hainmueller and Hazlett (2013). "Kernel Regularized Least Squares: Reducing Misspecification Bias with a Flexible and Interpretable Machine Learning Approach" *Political Analysis*.

Paper

Ratkovic and Tingley (2017) "Sparse Estimation and Uncertainty with Application to Subgroup Analysis" *Political Analysis*.

Motivating Example: Subgroup Analysis

Moving past average treatment effects

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- conjoint analysis
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Proliferation of possible effects

Multiple hypothesis testing

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Majors problems with multiple hypothesis testing

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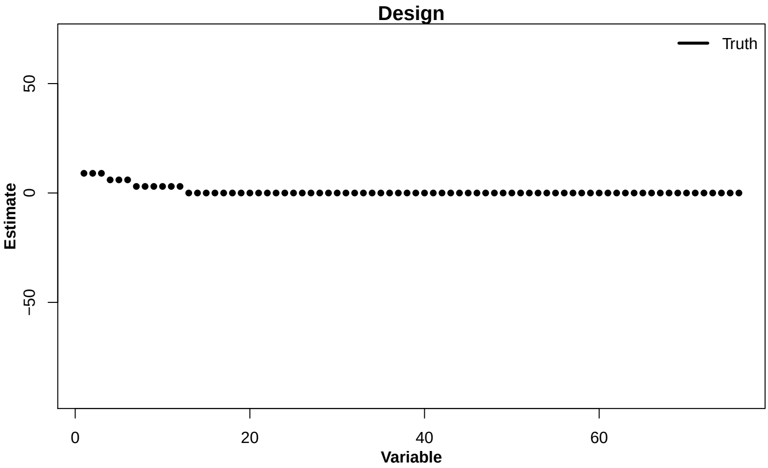
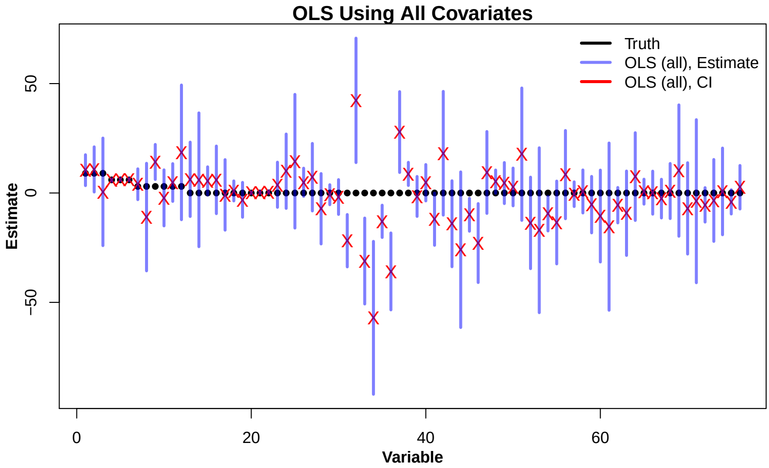
Subsetting data still requires specification hunting, and is also underpowered.

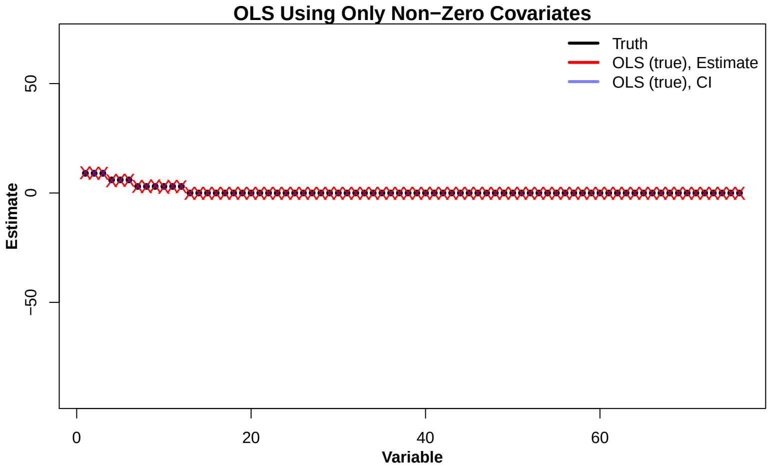
Design: $N = 10{,}000$; $K = 76$



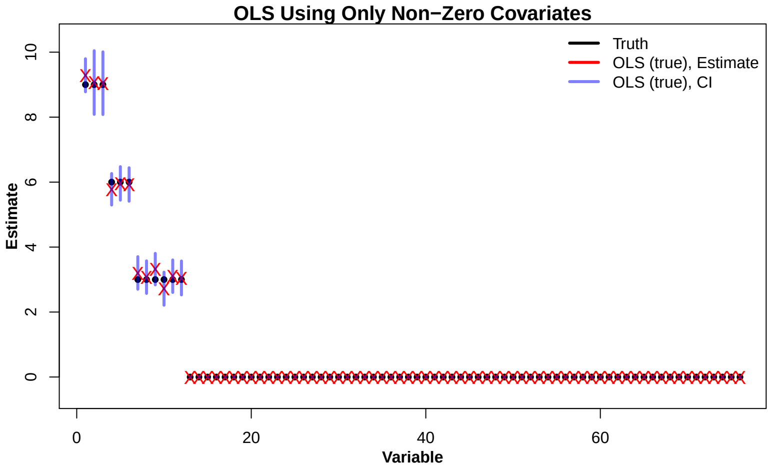
OLS


OLS Using All Covariates
Truth
OLS (all), Estimate
OLS (all), CI
Estimate
50
0
−50
0
20
40
60
Variable

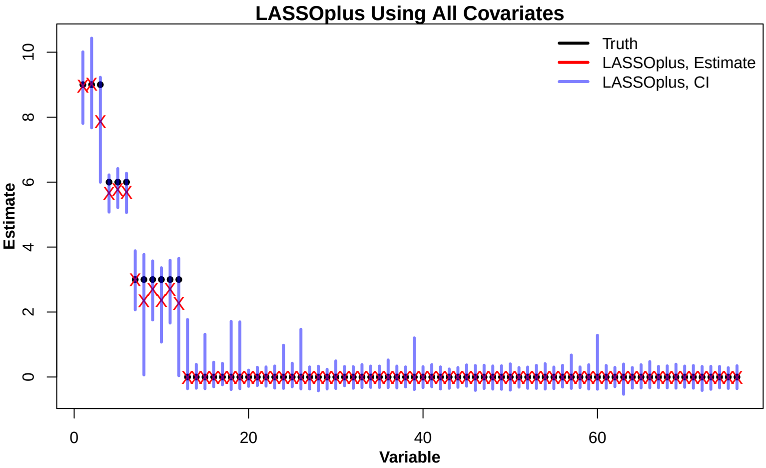
"Oracle:" OLS on only non-zero effects



"Oracle:" Zooming in



LASSOplus



LASSOplus Using All Covariates
Truth
LASSOplus, Estimate
LASSOplus, CI
Estimate
Variable
0
2
4
6
8
10
0
20
40
60

Introducing LASSOplus

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Practical properties

- Easy to implement

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s1<-sparsereg(y, X, cbind(t1, t2), scale.type="TX", EM=TRUE)
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```

- Flexibility
  - Up to three-way random effects
  - Continuous and binary outcomes

Contributions of LASSOplus

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1. Weakly informative prior structure
2. Sparse estimates
3. Approximate confidence intervals
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All implemented in `sparsereg` (Ratkovic and Tingley 2015) in **R**.

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- Data generating process

$$
\begin{aligned}
Y_i = & 3 + 2 \cdot X_{i2} + 2 \cdot \mathbf{1}(T_{i1} = a) - 2 \cdot \mathbf{1}(T_{i1} = b) \\
& - 2 \cdot X_{i2} \cdot \mathbf{1}(T_{i1} = b) + 2 \cdot X_{i2} \cdot \mathbf{1}(T_{i2} = c) + \epsilon_i
\end{aligned}
$$

where $\epsilon_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 4)$; $N = 500$

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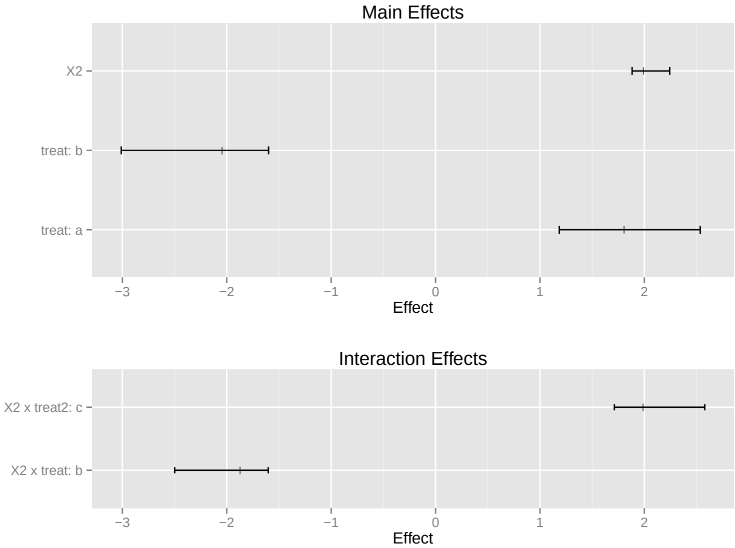
  where $\epsilon_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 4)$; $N = 500$

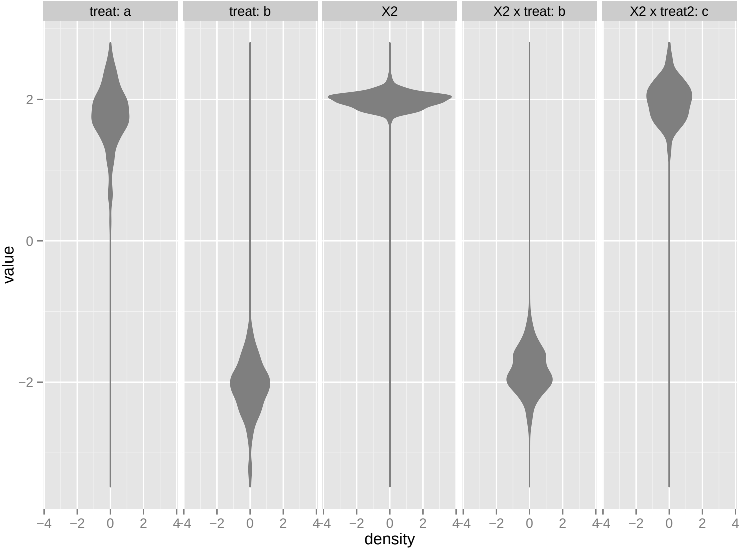
- $K = \underbrace{3 + 4 + 5}_{\text{main effects}} + \underbrace{5 \cdot (3 + 4)}_{\text{interaction terms}} = 47$

plot(s1)



Main Effects
X2
treat: b
treat: a
−3
−2
−1
0
1
2
Effect
Interaction Effects
X2 x treat2: c
X2 x treat: b
−3
−2
−1
0
1
2
Effect

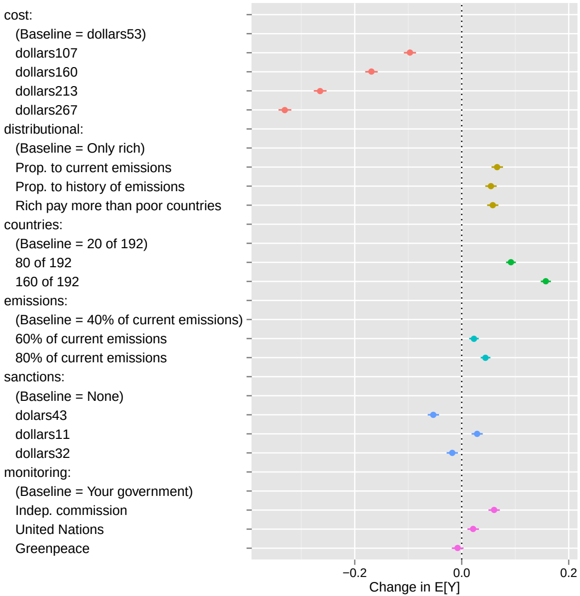
violinplot(s1)

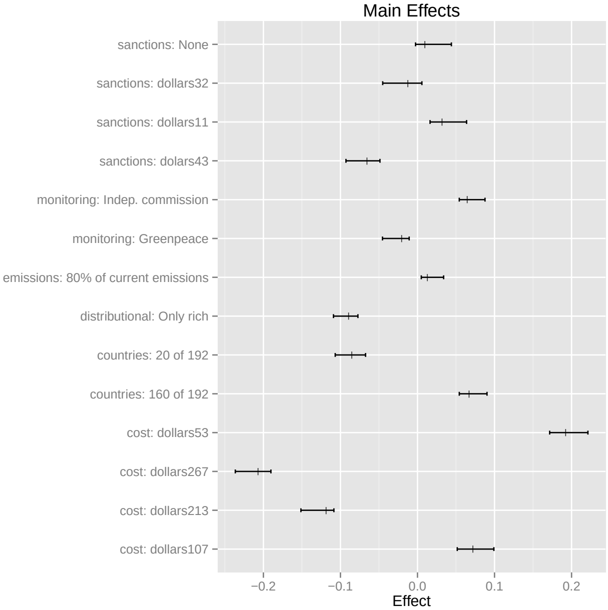


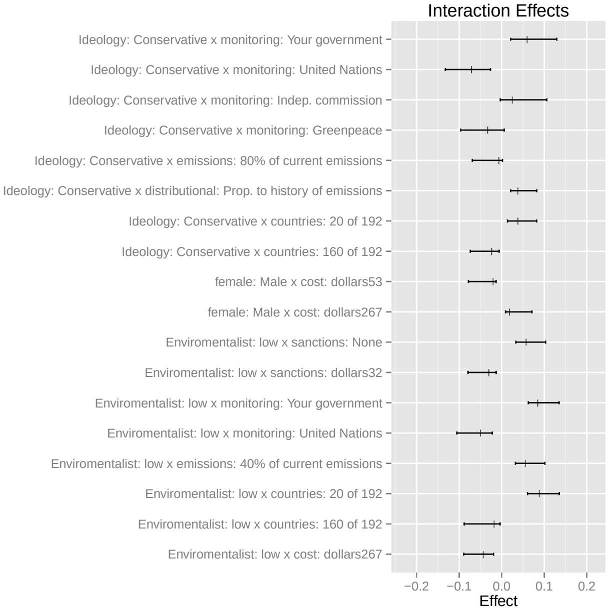
Application

Study: Bechtel and Scheve 2013

- Effect of international treaty on climate design on support
- Conjoint experiment across four countries
- Treatment conditions: cost, extent of other countries participating, extent of sanctions, who monitors
- 215 total effects
  - 16 covariates; 31 main effects; 6 treatments, 23 levels; 184 treatment $\times$ covariate effects
- Investigated sub-group effects by multiple split sample analyses


cost:
(Baseline = dollars53)
dollars107
dollars160
dollars213
dollars267
distributional:
(Baseline = Only rich)
Prop. to current emissions
Prop. to history of emissions
Rich pay more than poor countries
countries:
(Baseline = 20 of 192)
80 of 192
160 of 192
emissions:
(Baseline = 40% of current emissions)
60% of current emissions
80% of current emissions
sanctions:
(Baseline = None)
dolars43
dollars11
dollars32
monitoring:
(Baseline = Your government)
Indep. commission
United Nations
Greenpeace
−0.2
0.0
0.2
Change in E[Y]


Main Effects
sanctions: None
sanctions: dollars32
sanctions: dollars11
sanctions: dolars43
monitoring: Indep. commission
monitoring: Greenpeace
emissions: 80% of current emissions
distributional: Only rich
countries: 20 of 192
countries: 160 of 192
cost: dollars53
cost: dollars267
cost: dollars213
cost: dollars107
−0.2
−0.1
0.0
0.1
0.2
Effect


Interaction Effects
Ideology: Conservative x monitoring: Your government
Ideology: Conservative x monitoring: United Nations
Ideology: Conservative x monitoring: Indep. commission
Ideology: Conservative x monitoring: Greenpeace
Ideology: Conservative x emissions: 80% of current emissions
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female: Male x cost: dollars53
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Enviromentalist: low x sanctions: None
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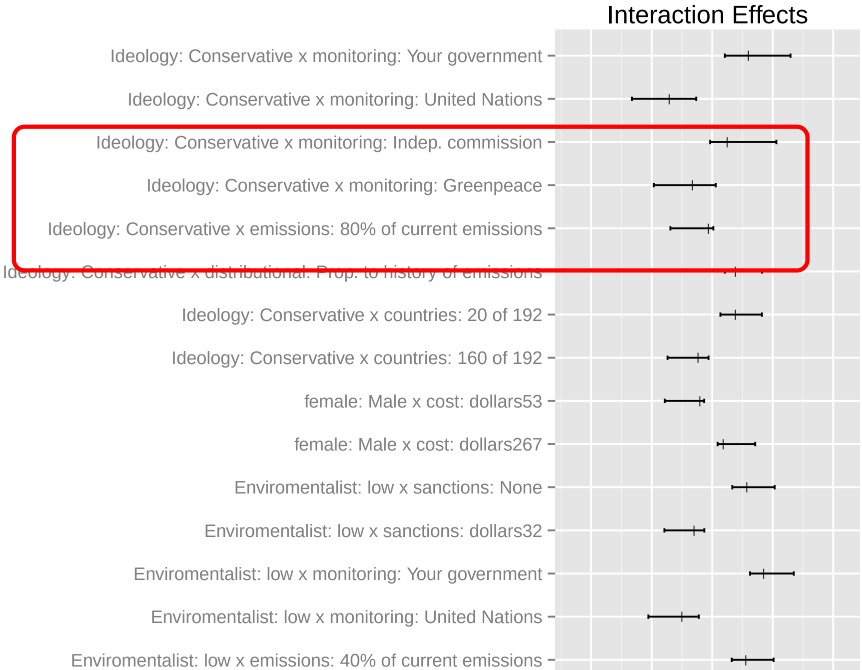
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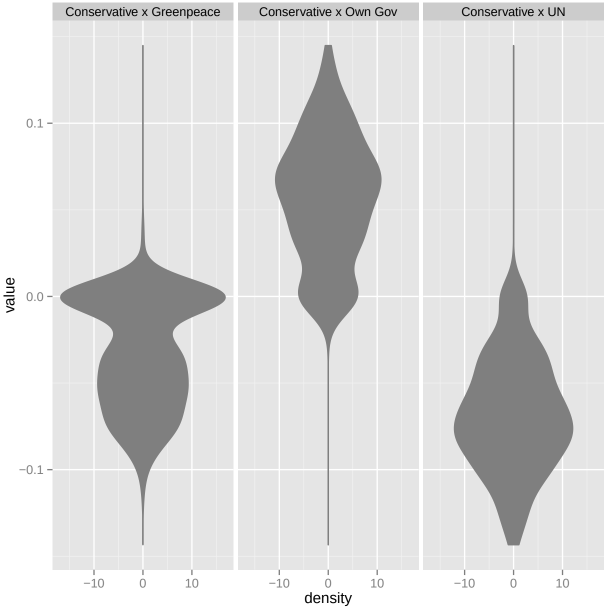
Conservative x Greenpeace
Conservative x Own Gov
Conservative x UN
value
0.1
0.0
−0.1
−10
0
10
density

Conclusion on LASSOplus

LASSOplus is an estimator that

1. possesses the Oracle property
2. achieves a low FDR
3. identifies non-zero effects
4. returns approximate confidence intervals

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- Let's consider a single example of a hierarchical model: eight schools

Eight Schools Background

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- (Analysis is from Rubin 1981, treatment via Gelman et al 2015)

Eight Schools Data

School	Est. Effect	SE
A	28	15
B	8	10
C	-3	16
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- It is the "same course" in every school, but they are different schools.

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   - the pooled estimate is 7.7 with standard error of 4.1. Thus the confidence interval is $[-.5, 15.9]$

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- This model contains both the separate and pooled estimates as limiting special cases. If we force the standard deviation of the true effects to be zero, then all school get the same estimate, if we let it go to infinity we get the separate estimates

The Model

$$\bar{y}_j|\theta_j \sim \text{Normal}(\theta_j, \sigma_j^2)$$
$$\theta_j|\mu, \tau \sim \text{Normal}(\mu, \tau^2)$$
$$p(\mu, \tau) = p(\mu|\tau)p(\tau) \propto p(\tau)$$

Known: $\bar{y}_j, \sigma_j^2$
Unknown: τ, μ, θ

A General Hierarchical Model Form

First Stage: p(data | process, parameters)
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$$
\begin{aligned}
Y|X,\beta &\sim N(X\beta, \Sigma_Y) \\
\beta|Z,\alpha &\sim N(z\alpha, \Sigma_\beta) \\
\alpha &\sim N(\alpha_0, \Sigma_\alpha)
\end{aligned}
$$

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$$\theta_j|\mu, \tau, y \sim \mathrm{N}(\hat{\theta}_j, V_j)$$

$$\hat{\theta}_j = \frac{\frac{1}{\sigma_j^2}\bar{y}_j + \frac{1}{\tau^2}\mu}{\frac{1}{\sigma_j^2} + \frac{1}{\tau^2}}$$

$$V_j = \frac{1}{\frac{1}{\sigma_j^2} + \frac{1}{\tau^2}}$$

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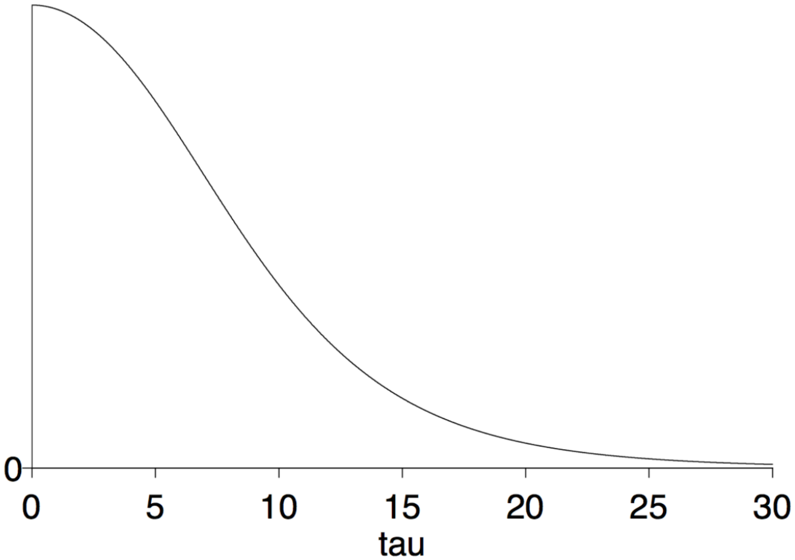
- Our final guess is that the median effect for school A is about 10 points with 50% probability between 7 and 16

Results



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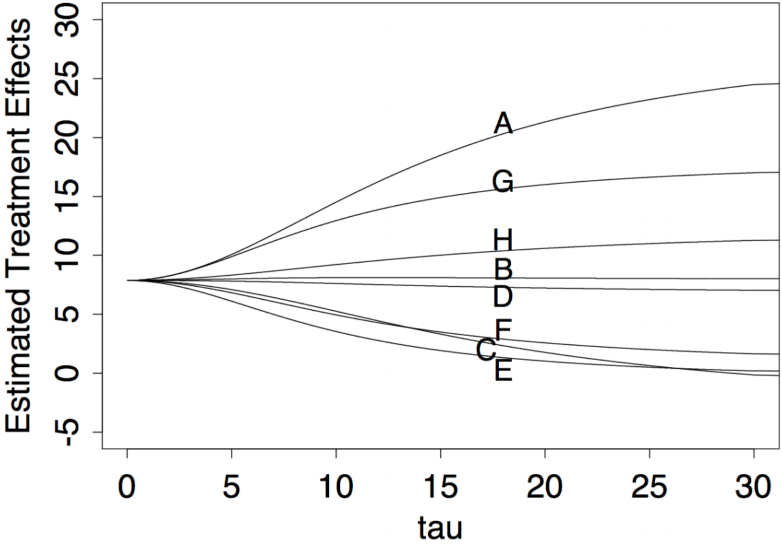
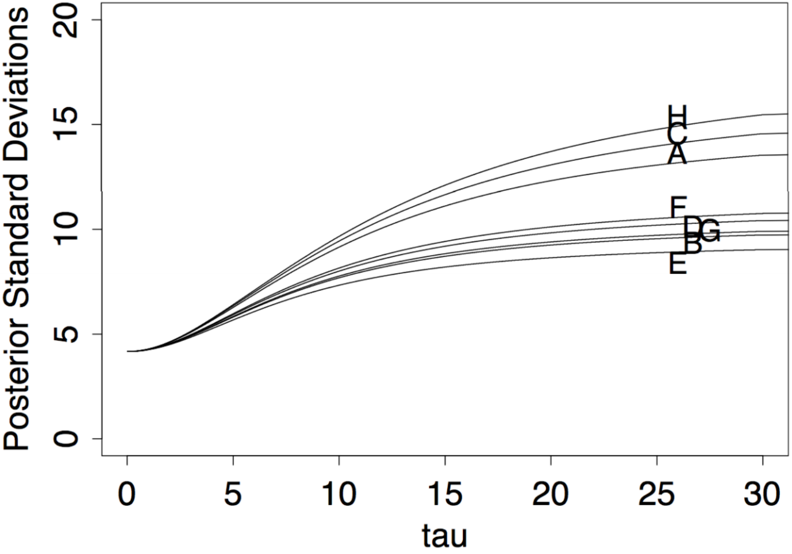
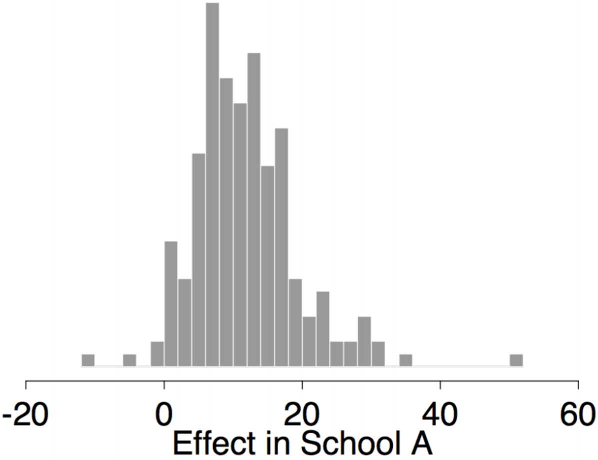

Estimated Treatment Effects
-5
0
5
10
15
20
25
30
A
G
H
B
D
F
C
E
0
5
10
15
20
25
30
tau

Results



Posterior Standard Deviations
0
5
10
15
20
tau
0
5
10
15
20
25
30
H
C
A
F
D
G
B
E

Results



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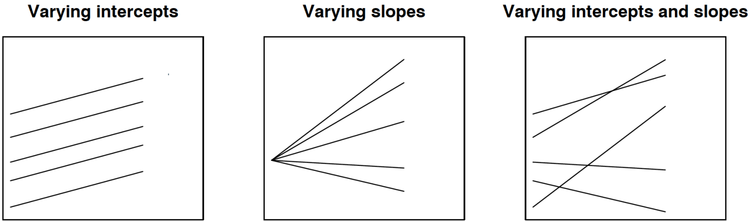
- Today we will consider the broader class of multilevel models
- Let's start with a simple structure: individuals within a group, individual level predictors only.
- We can think of three model variants:

$$\begin{aligned}
\text{varying-intercept model:} y_i &= a_{j[i]} + \beta x_i + \epsilon_i \\
\text{varying-slope model:} y_i &= \alpha + \beta_{j[i]} x_i + \epsilon_i \\
\text{varying intercept and slope model:} y_i &= a_{j[i]} + \beta_{j[i]} x_i + \epsilon_i
\end{aligned}$$

Varying Intercept and Slopes



Example Data

ID	dad age	mom race	informal support	city ID	city name	enforce intensity	benefit level	city indicators 1	2	⋯	20
1	19	hisp	1	1	Oakland	0.52	1.01	1	0	⋯	0
2	27	black	0	1	Oakland	0.52	1.01	1	0	⋯	0
3	26	black	1	1	Oakland	0.52	1.01	1	0	⋯	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮		⋮
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1366	21	black	1	20	Norfolk	−0.11	1.08	0	0	⋯	1
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An Example Multilevel Model for Fragile Families

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The multilevel estimate of α_j is a weighted average of the no-pooling estimate for the group and the regression prediction.

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We can extend this framework to settings which are not cleanly nested such as longitudinal data.

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person		parents smoke?		wave 1		wave 2		⋯
ID	sex	mom	dad	age	smokes?	age	smokes?	
1	f	Y	Y	15:0	N	15:6	N	⋯
2	f	N	N	14:7	N	15:1	N	⋯
3	m	Y	N	15:1	N	15:7	Y	⋯
4	f	N	N	15:3	N	15:9	N	⋯
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋱

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⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋱

$$\Pr(y_i = 1) = \text{logit}^{-1}(\beta_0 + \beta_1 \text{psmoke}_j + \beta_2 \text{female}_j + \beta_3 t + \beta_4(\text{female}_j)t + \alpha_j)$$

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- Perspectives and estimation in econometrics

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When should we bother?
Roughly speaking when the number of groups is > 5 with decent amounts of variation between groups and/or small group sizes.

Different Ways of Writing the Same Model

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  $y_i = X_i\beta + \epsilon^{\text{all}}_i, \epsilon^{\text{all}}_i \sim N(0, \Sigma)$ where Σ is structured in a particular way.
- Generally I find it easier to think about the intercepts as latent variables, but the error formulation is more intuitive to some people.

Varying Slopes

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Varying slopes are essentially the same but we now allow slope coefficients to vary, possibly via group level predictors

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$$
\begin{aligned}
y_a &= \alpha_{j[i]} + \beta_{j[i]} x_i + \epsilon_i \\
\alpha_j &= \gamma_0^{\alpha} + \gamma_1^{\alpha} u_j + \eta_j^{\alpha} \\
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We can re-express this as a regression with interactions:

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y_i = \left[\gamma_0^\alpha + \gamma_1^\alpha u_{j[i]} + \eta_{j[i]}^\alpha\right] + \left[\gamma_0^\beta + \gamma_1^\beta u_{j[i]} + \eta_{j[i]}^\beta\right] x_i + \epsilon_i
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Treating $u_{j[i]}$ as an individual level predictor, we can see that this is a model with interactions between x and all the group indicators, and between x and between u and x.

Centering

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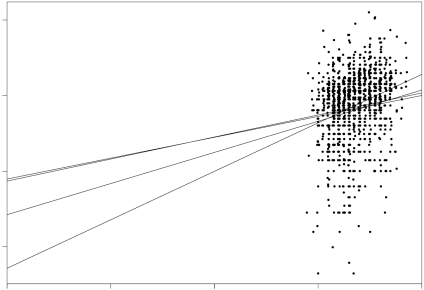
Centering can have large impacts on speed of convergence in estimation but also interpretation. The intuition for interpretation differences follows from the analog to interactions.



Distributions for Slope Models

The strong correlation between the slope and the intercept needs to be included in our model .

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Gelman recommends a scaled inverse-Wishart distribution which we won't discuss now. See Gelman and Hill (2007) Chapter 13 for more.

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- Different types of smoothing can be imposed when groups are ordered either temporally, spatially or both
- Many large classes of models are simply special cases of the hierarchical models considered here
- The downside is that things get complicated quickly- which is why focused treatments of these specialized cases are important!

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- Let's focus on two alternatives in `R` which are both important in their own right: `lmer` in `lme4` and `rstanarm`
- Stan is a cross-platform probabilistic programming language. It can be used to expand to almost any model you can dream of.

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- ~~When in doubt~~ Always check your models!
- Read Chapter 21: "Understanding and summarizing the fitted models" in Gelman and Hill (2007)
- Gelman and Hill (2007) is great, but the computation has modernized a bit (due to Gelman's own work!) and you should use Stan for computation over the book recommended BUGS.