Messy Data, Robust Inference?
Navigating Obstacles to Inference with `bigKRLS`

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Watch Live @ Noon Eastern

Overview

- **Part I**: Kernel Regularized Least Squares (KRLS)
  - What is it? Why use it?
  - Why optimize it?

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  - New Software Architecture
    - `bigmemory` for Size
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- **Discussion**: Data Science as Complexity vs. Interpretability

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- For Bayesian generalized version, Zhang, Dai & Jordan 2011

Some Details

We assume that the objective function $\mathbf{y} = \mathbf{f}(\mathbf{x})$ can be approximated by

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Let $\mathbf{c}^*$ be a vector of weights which reflects a squared L_2 penalty:

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Under assumptions (largely) analogous to classical regression, KRLS is unbiased and consistent (Hainmueller & Hazlett 2013).

"Actually" Marginal Effects

The marginal effects are:

$$\hat{\mathbf{\Delta}}_{\mathbf{N*P}} = [\hat{\delta}_{\mathbf{1}} \quad \hat{\delta}_{\mathbf{2}} \ldots \hat{\delta}_{\mathbf{P}}]$$

where, without loss of generality,

$$\hat{\delta}_{\mathbf{2}} = -\tfrac{2}{\sigma^2}(\mathbf{D_{(2)}} \cdot \mathbf{K}) * \hat{\mathbf{c}}^*$$

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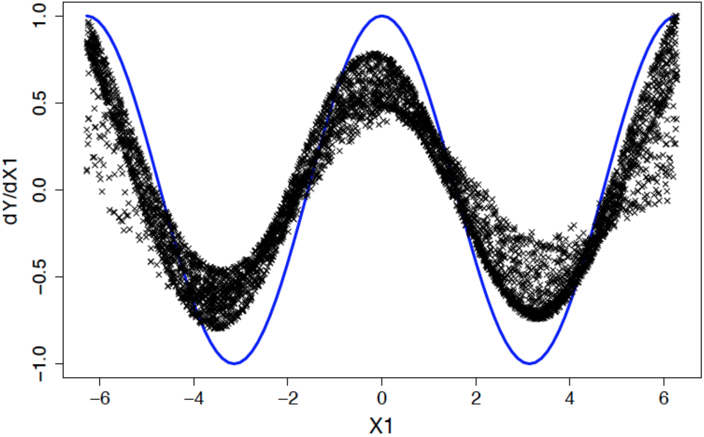
And the average marginal effects are the column means of $\hat{\mathbf{\Delta}}_{\mathbf{N*P}}$.

Quick Illustration...

```
library(bigKRLS)
N <- 5000
P <- 2
set.seed(11112016)
X <- matrix(runif(N * P, min = -2 * pi, max = 2 * pi),
    ncol = P)
y <- sin(X[, 1]) + X[, 2] + rnorm(N)
fit <- bigKRLS(y, X)
```

Marginal Effects of X1



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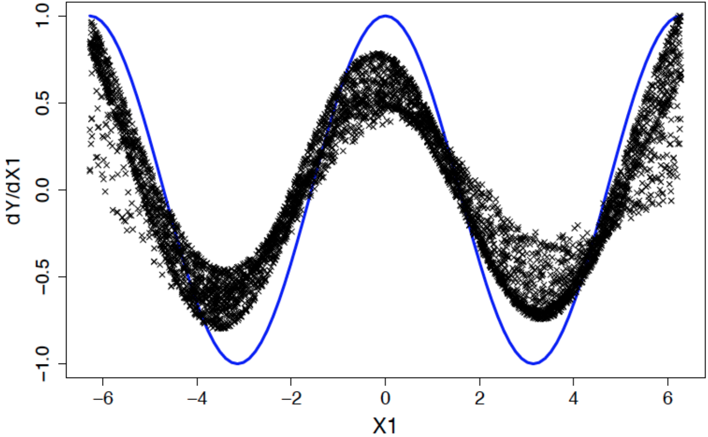


```r
mean((abs(fit$derivatives[,1]) < abs(cos(X[,1]))))
```

```
## [1] 0.8624
```

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5. Parallel Processing (*coming soon*). Most bigmemory calculations are best done on a single core but snow offers substantial speed gains for the derivatives.

Example: “Get Out the Vote” Experiment

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Green et al ’09 also used this as an experimental benchmark for polynomial regression.

The Treatment

Dear Registered Voter:

WHAT IF YOUR NEIGHBORS KNEW WHETHER YOU VOTED?

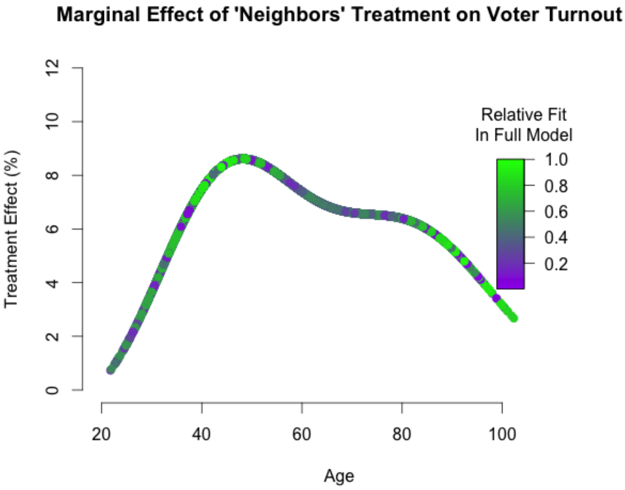
Why do so many people fail to vote? We've been talking about the problem for years, but it only seems to get worse. This year, we're taking a new approach. We're sending this mailing to you and your neighbors to publicize who does and does not vote.

The chart shows the names of some of your neighbors, showing which have voted in the past. After the August 8 election, we intend to mail an updated chart. You and your neighbors will all know who voted and who did not.

DO YOUR CIVIC DUTY — VOTE!

MAPLE DR	Aug 04	Nov 04	Aug 06
9995 JOSEPH JAMES SMITH	Voted	Voted	______
9995 JENNIFER KAY SMITH		Voted	______
9997 RICHARD B JACKSON		Voted	______
9999 KATHY MARIE JACKSON		Voted	______
9999 BRIAN JOSEPH JACKSON		Voted	______
9991 JENNIFER KAY THOMPSON		Voted	______
9991 BOB R THOMPSON		Voted	______
9993 BILL S SMITH			______
9989 WILLIAM LUKE CASPER		Voted	

Heterogeneous Treatment Effect



Analyzing Interactions

Do Americans prefer Donald Trump over Hillary Clinton?

- Data: Pew Research Center's January 2016 survey.
- DV: relative preference for Trump expressed as difference of two Likert responses:

$$\mathbf{y}_i \equiv \mathbf{Q22E}_i - \mathbf{Q22D}_i$$

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Note: costly under previous setup!

- Prohibitive given the number of categorical variables (state, race) and sample size

Trump vs. Hillary (Average Marginal Effects)

	Est	SE	t value	p
Female*	-0.289	0.079	-3.665	< 0.001
Spanish Language Interview*	-0.745	0.173	-4.317	< 0.001
Liberalism	-0.477	0.031	-15.537	< 0.001
Approve Obama*	-2.045	0.090	-22.667	< 0.001
Follows Election	0.126	0.032	3.961	< 0.001
Age	-0.001	0.002	-0.821	0.412
Bachelors*	0.010	0.064	0.151	0.880
Associates*	0.014	0.102	0.141	0.888
Some Postgrad*	-0.288	0.200	-1.441	0.150
High School*	0.064	0.072	0.877	0.380
Postgrad*	-0.197	0.095	-2.061	0.039
Some College*	0.145	0.081	1.783	0.075
Refused*	0.813	0.369	2.201	0.028
Some High School*	-0.305	0.191	-1.594	0.111
No High School*	0.112	0.249	0.450	0.652
Population Density	-0.022	0.021	-1.039	0.299
Hispanic*	-0.207	0.142	-1.461	0.144
White*	0.164	0.120	1.368	0.171
Refused*	0.219	0.219	0.998	0.318
Hispanic Latino*	-0.452	0.169	-2.669	0.008
African American*	-0.425	0.144	-2.957	0.003
Native American*	0.294	0.232	1.270	0.204
Other*	-0.766	0.333	-2.298	0.022
Asian Or Asian American*	-0.398	0.190	-2.095	0.036
Pacific Islander Or Hawaiian*	0.342	0.363	0.942	0.346
Midwest*	-0.008	0.033	-0.233	0.816
South*	0.083	0.026	3.172	0.002
Northeast*	-0.078	0.035	-2.206	0.027
West*	-0.039	0.031	-1.253	0.210

$N = 2009$. * indicates binary variable for which first differences are computed (estimates for state and DC not shown); $R^2 = 0.676$.

Quick Overview of Trump vs. Hillary Results

The model fits the data quite well...

1. Even in January, long-term patterns are largely evident. Self-identified liberals, African Americans, Latinos, and women all favor Clinton, while whites (particularly in the South) tilt slightly towards Trump.

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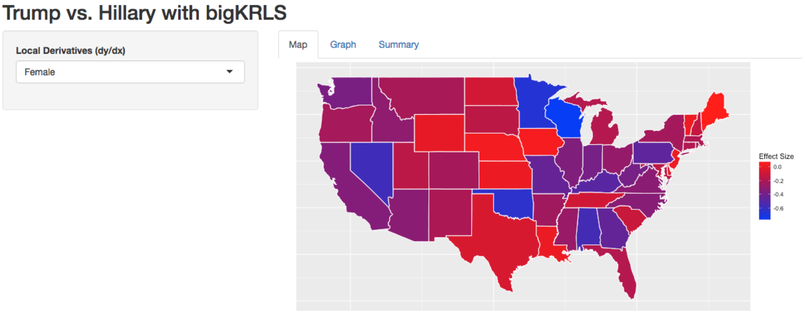
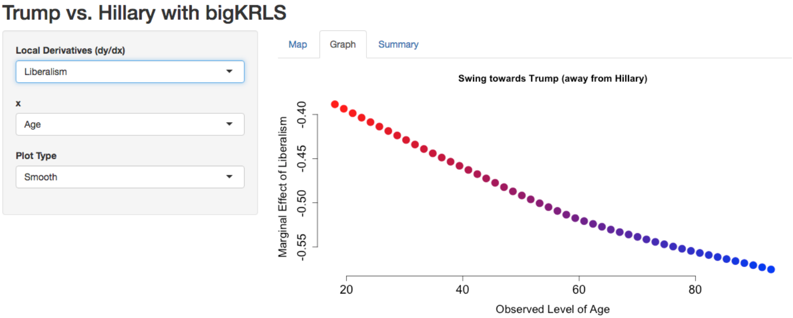
1. Even in January, long-term patterns are largely evident. Self-identified liberals, African Americans, Latinos, and women all favor Clinton, while whites (particularly in the South) tilt slightly towards Trump.
2. $R^2 \approx 0.68$.
3. Restricting the R^2 calculation to average marginal effects suggests that the model is (primarily) linear and additive, with $R^2_{AME} \approx 0.55$.
   - Or: average marginal effects provide approximately 80% of the explanatory power in the model.
   - R2AME now reported with summary(bigKRLS).

How Does the Effect of Gender Vary by State?



The Effect of Liberalism by Age

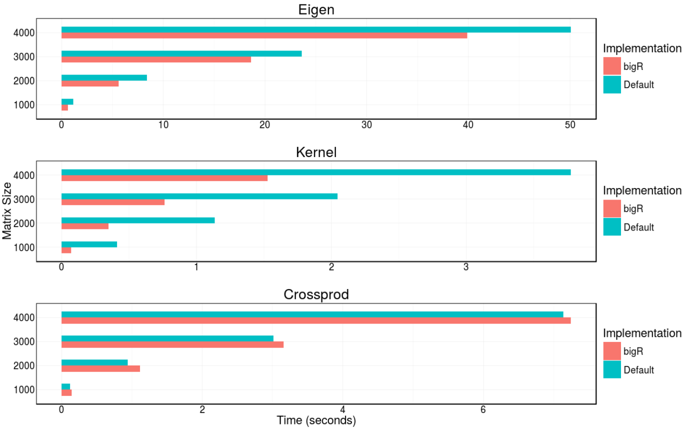


Complexity

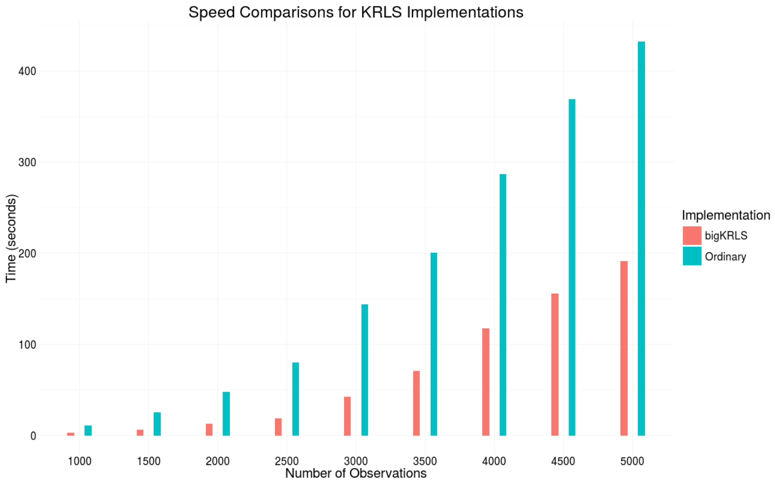
	Major Steps	Runtime	Memory
(1)	Standardize $\mathbf{X}_{\mathrm{N*P}}$, $\mathbf{y}$	—	—
(2)	Calculate kernel $\mathbf{K}_{N\times N}$	$O(N^2)$	$O(N^2)$
(3)	Eigendecompose $\mathbf{KE} = \mathbf{Ev}$	$O(N^3)$	$O(N^2)$
(4)	Regularization parameter λ	$O(N^3)$	—
(5)	Estimate weights $\hat{\mathbf{c}} = \mathbf{f}(\lambda, \mathbf{y}, \mathbf{E}, \mathbf{v})$	$O(N^3)$	—
(6)	Fit values $\hat{\mathbf{y}} = \mathbf{K}\hat{\mathbf{c}}$	—	—
(7)	Estimate local derivatives, $\hat{\mathbf{\Delta}}_{\mathbf{N*P}} = [\hat{\delta}_1 \quad \hat{\delta}_2 \ldots \hat{\delta}_{\mathbf{P}}]$	$O(PN^3)$	$O(N^2)$

Letting i, j index observations and $p = 1, 2, \ldots P$ index x variables. Steps 4-6 are followed by uncertainty estimates.

Speed Tests of Key Functions: HH's KRLS vs. bigKRLS



bigKRLS, with & without “big R” + Rcpp



First Differences

For each binary variable b, we calculate first differences $\hat{\delta}_{\mathbf{b}}$:

$$\begin{aligned}\hat{\delta}_{\mathbf{b}} &= \hat{\mathbf{y}}_{\{1\}} - \hat{\mathbf{y}}_{\{0\}} \\ &= \left(\mathbf{K}_{\{1\}} - \mathbf{K}_{\{0\}}\right) * \hat{\mathbf{c}} *\end{aligned}$$

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\end{aligned}
$$

Existing Algorithm

1. Construct two copies of $\mathbf{X}$ as $\mathbf{X}^{(0)}$ and $\mathbf{X}^{(1)}$; assign $\mathbf{X}_{\mathbf{b}}^{(0)} = \mathbf{0}$ and $\mathbf{X}_{\mathbf{b}}^{(1)} = \mathbf{1}$.
2. Compute $\mathbf{X}_{new} = [\mathbf{X}_{obs} \,|\, \mathbf{X}_{\mathbf{b}}^{(0)} \,|\, \mathbf{X}_{\mathbf{b}}^{(1)}]$.
   - Note $9N^2$ memory footprint!
3. Let $\mathbf{K}_{new} = [\mathbf{K}_{\{1\}} \,|\, \mathbf{K}_{\{0\}}]'$

Boolean Counterfactual Similarity

$$
\begin{aligned}
\mathbf{K_{i,j}} &= e^{-||\mathbf{x_i}-\mathbf{x_j}||^2/\sigma^2} \\
&= e^{[(\mathbf{x_{i,1}}-\mathbf{x_{j,1}})^2+(\mathbf{x_{i,2}}-\mathbf{x_{j,2}})^2+\ldots+(\mathbf{x_{i,b}}-\mathbf{x_{j,b}})^2+\ldots]} \\
&= e^{(\mathbf{x_{i,b}}-\mathbf{x_{j,b}})^2/\sigma^2} e^{[(\mathbf{x_{i,1}}-\mathbf{x_{j,1}})^2+(\mathbf{x_{i,2}}-\mathbf{x_{j,2}})^2+\ldots]} \\
&= e^{(\mathbf{x_{i,b}}-\mathbf{x_{j,b}})^2/\sigma^2} \mathbf{K^*_{i,j}} \\
&= \phi \mathbf{K^*_{i,j}}
\end{aligned}
$$

Boolean Counterfactual Similarity

$\mathbf{X}_{i,b}$	$\mathbf{X}_{j,b}$	$\mathbf{K}_{i,j}$	$\mathbf{K}_{\{1\},j}$	$\mathbf{K}_{\{0\},j}$	$\mathbf{K}_{\{1\},j} - \mathbf{K}_{\{0\},j}$
1	1	$\mathbf{K}^*_{i,j}$	$\mathbf{K}^*_{i,j}$	$\phi\mathbf{K}^*_{i,j}$	$(1-\phi) * \mathbf{K}_{i,j}$
1	0	$\phi\mathbf{K}^*_{i,j}$	$\phi\mathbf{K}^*_{i,j}$	$\mathbf{K}^*_{i,j}$	$\frac{(\phi-1)}{\phi} * \mathbf{K}_{i,j}$
0	1	$\phi\mathbf{K}^*_{i,j}$	$\mathbf{K}^*_{i,j}$	$\phi\mathbf{K}^*_{i,j}$	$\frac{(1-\phi)}{\phi} * \mathbf{K}_{i,j}$
0	0	$\mathbf{K}^*_{i,j}$	$\phi\mathbf{K}^*_{i,j}$	$\mathbf{K}^*_{i,j}$	$(\phi-1) * \mathbf{K}_{i,j}$

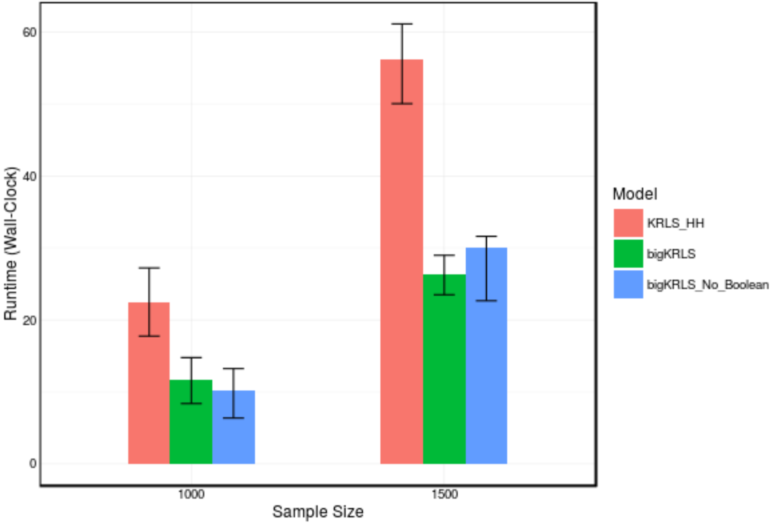
Tackling the Variance Estimator

$$(\mathbf{K}_{new}\hat{\mathbf{V}}_{\mathbf{c}^*})\mathbf{K}'_{\mathbf{new}} = \left[\mathbf{K}_{\{1\}}\mathbf{K}_{\{0\}}\right]\hat{\mathbf{V}}_{\mathbf{c}^*}\left[\begin{array}{c}\mathbf{K}'_{\{1\}}\\ \mathbf{K}'_{\{0\}}\end{array}\right]$$

$$= \begin{bmatrix}\mathbf{K}_{\{1\}}\hat{\mathbf{V}}_{\mathbf{c}^*}\mathbf{K}'_{\{\mathbf{1}\}} & \mathbf{K}_{\{1\}}\hat{\mathbf{V}}_{\mathbf{c}^*}\mathbf{K}'_{\{\mathbf{1}\}}\\ \mathbf{K}_{\{1\}}\hat{\mathbf{V}}_{\mathbf{c}^*}\mathbf{K}'_{\{\mathbf{0}\}} & \mathbf{K}_{\{0\}}\hat{\mathbf{V}}_{\mathbf{c}^*}\mathbf{K}'_{\{\mathbf{0}\}}\end{bmatrix}$$

...which allows us to factor out each individual submatrix.

Preliminary Tests of the “Boolean” Estimator



Discussion

Complexity, Interpretability, Scalability – Impossible Trilemma?

Computational Complexity Frontier

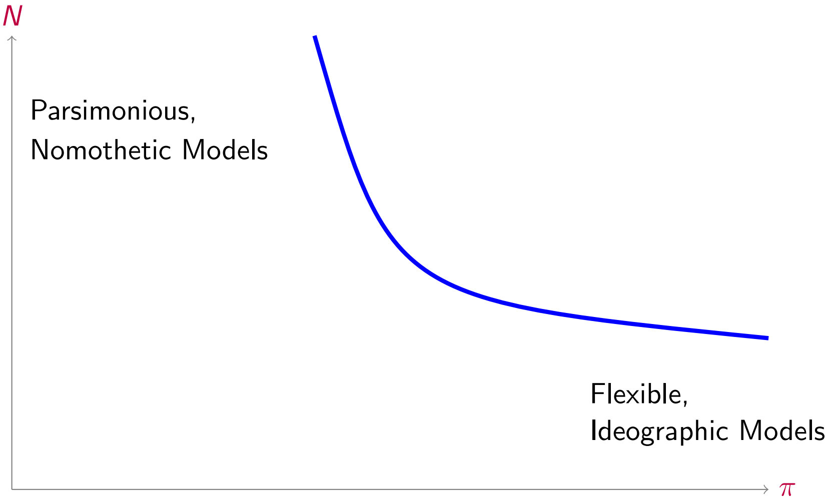


Figure: Scalability as Constraint

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- `bigKRLS` attempts to ease some of these constraints
- Directions for Future Work:
  - Integration of Data Reduction Options
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  - *robustness*
  - *predictive accuracy*
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Thanks!!

`bigKRLS` available at https://github.com/rdrr1990/bigKRLS

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