Statistical Learning with Big Data

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Thanks to Rob Tibshirani for some slides

Some Take Home Messages

This talk is about supervised learning: building models from data that predict an outcome using a collection of input features.

- There are some powerful and exciting tools for making predictions from data.
- They are not magic! You should be skeptical. They require good data and proper internal validation.
- Human judgement and ingenuity are essential for their success.
- With big data
  - model fitting takes longer. This might test our patience for model evaluation and comparison.
  - difficult to look at the data; might be contaminated in parts.

  Careful subsampling can help with both of these.

Some Definitions

Machine Learning constructs algorithms that can learn from data.

Statistical Learning is a branch of applied statistics that emerged in response to machine learning, emphasizing statistical models and assessment of uncertainty.

Data Science is the extraction of knowledge from data, using ideas from mathematics, statistics, machine learning, computer science, engineering, ...

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Applied Statistics?

For Statisticians: 15 minutes of fame

2009 "I keep saying the sexy job in the next ten years will be statisticians. And I'm not kidding!" Hal Varian, Chief Economist Google

2012 "Data Scientist: The sexiest job of the 21st century." Harvard Business Review

Sexiest man alive?

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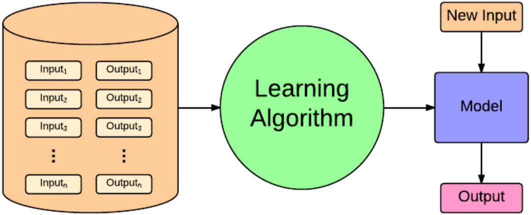
The Supervising Learning Paradigm



Training Data Fitting Prediction

Traditional statistics: domain experts work for 10 years to learn good features; they bring the statistician a small clean dataset

Today's approach: we start with a large dataset with many features, and use a machine learning algorithm to find the good ones. A huge change.

Internal Model Validation

- IMPORTANT! Don't trust me or anyone who says they have a wonderful machine learning algorithm, unless you see the results of a careful internal validation.
- Eg: divide data into two parts A and B. Run algorithm on part A and then test it on part B.
  Algorithm must not have seen any of the data in part B.
- If it works in part B, you have (some) confidence in it

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In God we trust. All others bring data.

Big data vary in *shape*. These call for different approaches.

Wide Data

Thousands / Millions of Variables

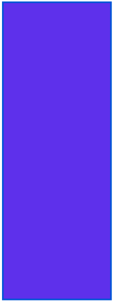
Hundreds of Samples

Screening and fdr,
Lasso, SVM, Stepwise

We have too many variables; prone to overfitting.

Need to remove variables, or regularize, or both.

Tall Data



Tens / Hundreds of Variables

Thousands / Millions of Samples

GLM, Random Forests,
Boosting, Deep Learning

Sometimes simple models (linear) don't suffice.

We have enough samples to fit nonlinear models with many interactions, and not too many variables.

Good automatic methods for doing this.

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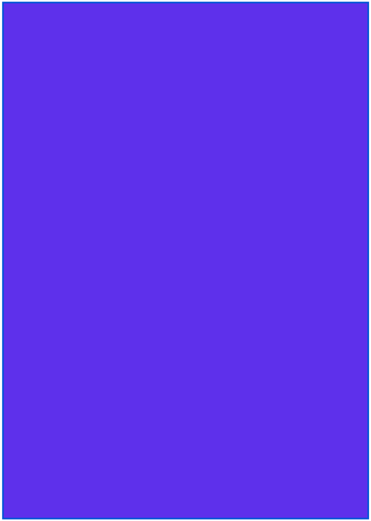
Tall and Wide Data



Thousands / Millions of Variables

Millions to Billions of Samples

Tricks of the Trade

Exploit sparsity

Random projections / hashing

Variable screening

Subsample rows

Divide and recombine

Case/ control sampling

MapReduce

ADMM (divide and conquer)

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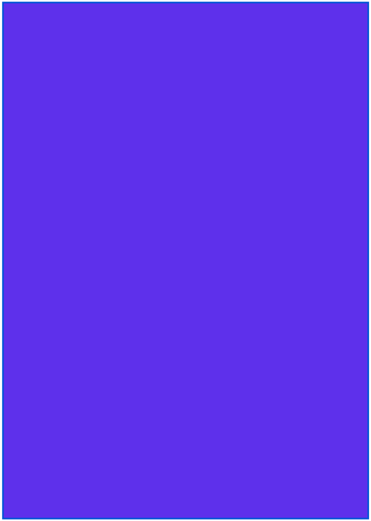

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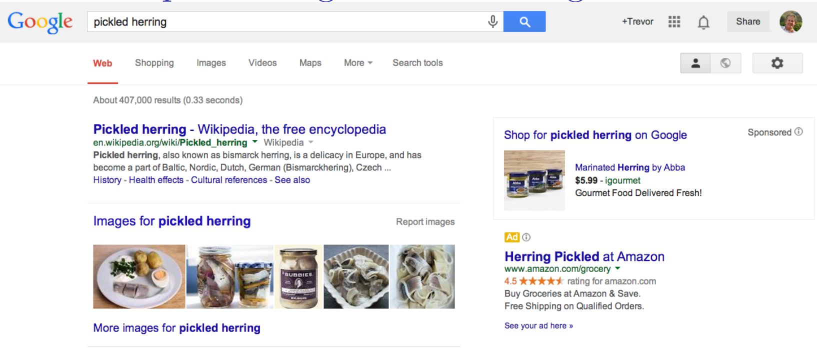
join Google

Examples of Big Data Learning Problems



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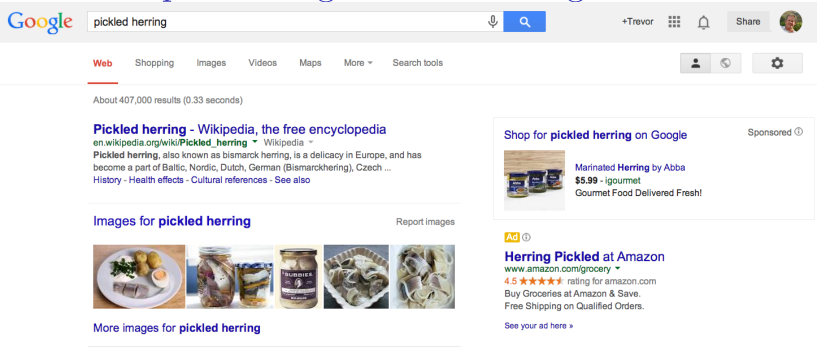
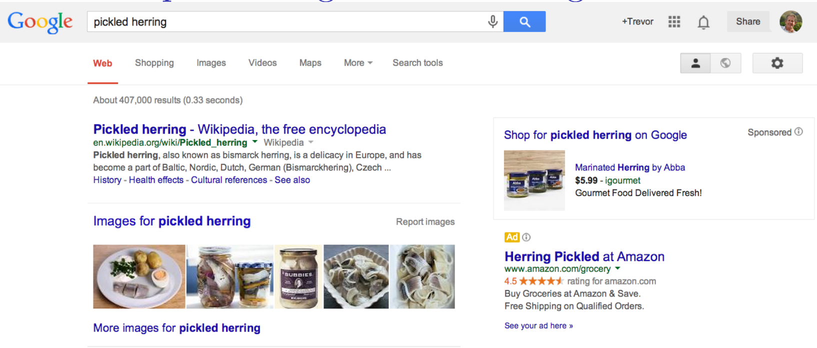


Click-through rate. Based on the search term, knowledge of this user (IPAddress), and the Webpage about to be served, what is the probability that each of the 30 candidate ads in an ad campaign would be clicked if placed in the right-hand panel.

Examples of Big Data Learning Problems



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Logistic regression with billions of training observations.

Each ad exchange does this, then bids on their top candidates, and if they win, serve the ad — all within 10ms!

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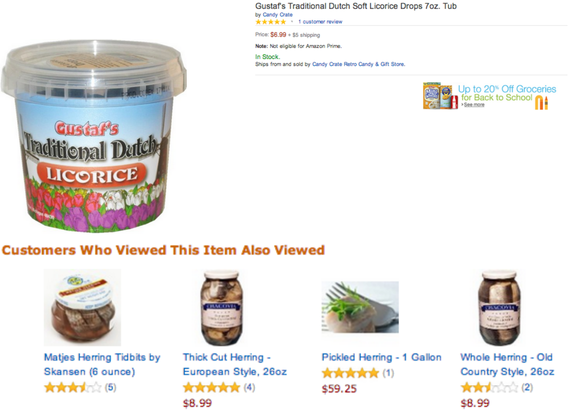

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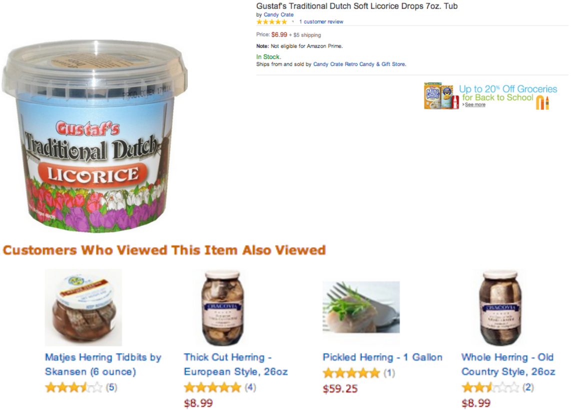

Recommender systems. Amazon online store, online DVD rentals, Kindle books, ...

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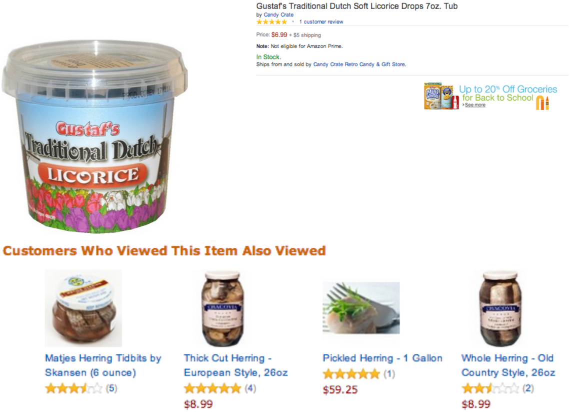

Recommender systems. Amazon online store, online DVD rentals, Kindle books, ...

Based on my past experiences, and those of others like me, what else would I chose?

Examples of Big Data Learning Problems

- Adverse drug interactions. US FDA (Food and Drug Administration) requires physicians to send in adverse drug reports, along with other patient information, including disease status and outcomes. Massive and messy data.

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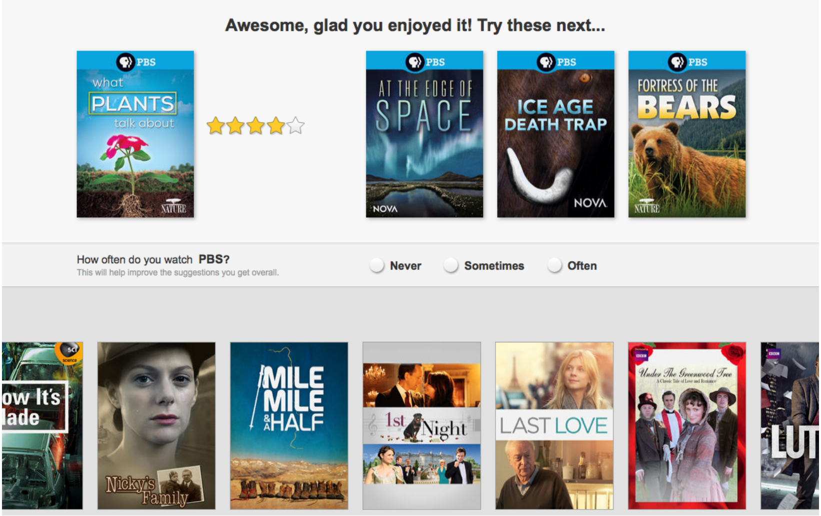
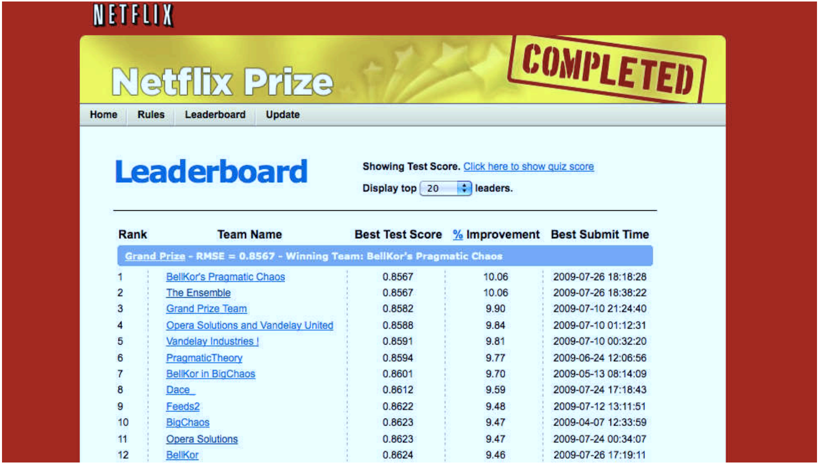
- Social networks. Based on who my friends are on Facebook or LinkedIn, make recommendations for who else I should invite. Predict which ads to show me.
  There are more than a billion Facebook members, and two orders of magnitude more connections. Knowledge about friends informs our knowledge about you. Graph modeling is a hot area of research. (e.g. Leskovec lab, Stanford CS.)

The Netflix Recommender



The Netflix Prize — 2006–2009



Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace_	0.8612	9.59	2009-07-24 17:18:43
9	Feeds2	0.8622	9.48	2009-07-12 13:11:51
10	BigChaos	0.8623	9.47	2009-04-07 12:33:59
11	Opera Solutions	0.8623	9.47	2009-07-24 00:34:07
12	BellKor	0.8624	9.46	2009-07-26 17:19:11

41K teams participated! Competition ran for nearly 3 years. Winner "BellKor's Pragmatic Chaos", essentially tied with "The Ensemble".

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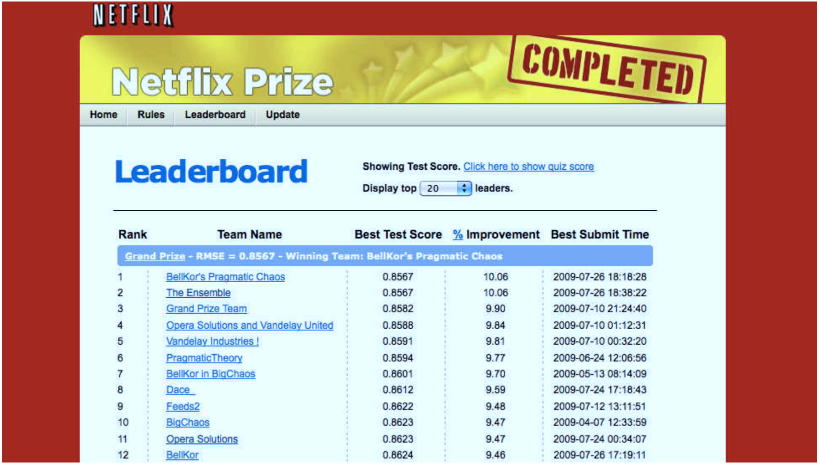

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The Netflix Data Set

	movie I	movie II	movie III	movie IV	$\cdots$
User A	1	?	5	4	$\cdots$
User B	?	2	3	?	$\cdots$
User C	4	1	2	?	$\cdots$
User D	?	5	1	3	$\cdots$
User E	1	2	?	?	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

- Training Data:
  $480K$ users, $18K$ movies,
  $100M$ ratings (1–5)
  (99% ratings missing)
- Goal:
  \$1M prize for 10% reduction in RMSE over Cinematch
- BellKor's Pragmatic Chaos declared winners on 9/21/2009

  Used ensemble of models, an important ingredient being low-rank factorization (SVD)

Strategies for modeling big data

Once the data have been cleaned and organized, we are often left with a massive matrix of observations.

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- If not sparse, use distributed, compressed databases. Many groups are developing fast algorithms and interfaces to these databases. For example `H2O` [CRAN] by H_2O interfaces from R to highly compressed versions of data, using Java-based implementations of many of the important modeling tools.

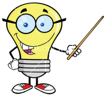
glmnet

Fit regularization paths for a variety of GLMs with lasso and elastic net penalties; e.g. logistic regression

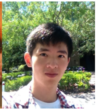
$$\log \frac{\Pr(Y = 1 \mid X = x)}{\Pr(Y = 0 \mid X = x)} = \beta_0 + \sum_{j=1}^{p} x_j \beta_j$$

- Lasso penalty [Tibshirani, 1996] induces *sparsity* in coefficients: $\sum_{j=1}^{p} |\beta_j| \leq s$. It shrinks them toward zero, and sets many to zero.
- Fit efficiently using coordinate descent. Handles sparse X naturally, and exploits sparsity of solutions, warms starts, variable screening, and includes methods for model selection using cross-validation.

`glmnet` team: TH, Jerome Friedman, Rob Tibshirani, Noah Simon, Junyang Qian.





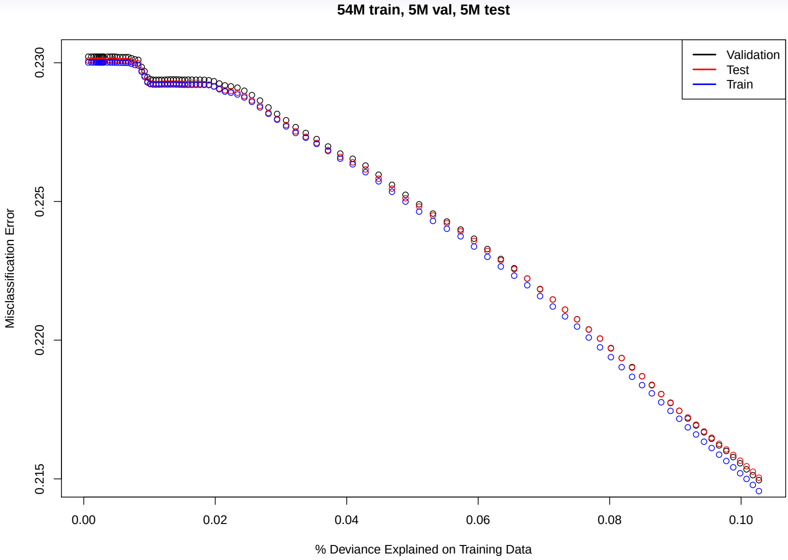


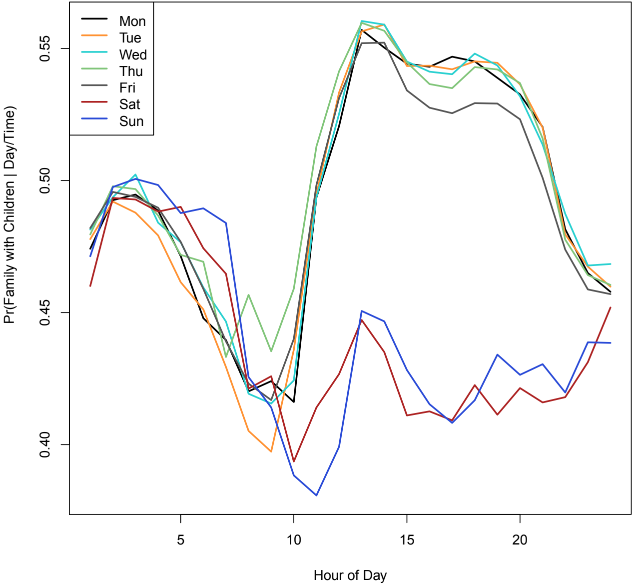
Example: Large Sparse Logistic Regression

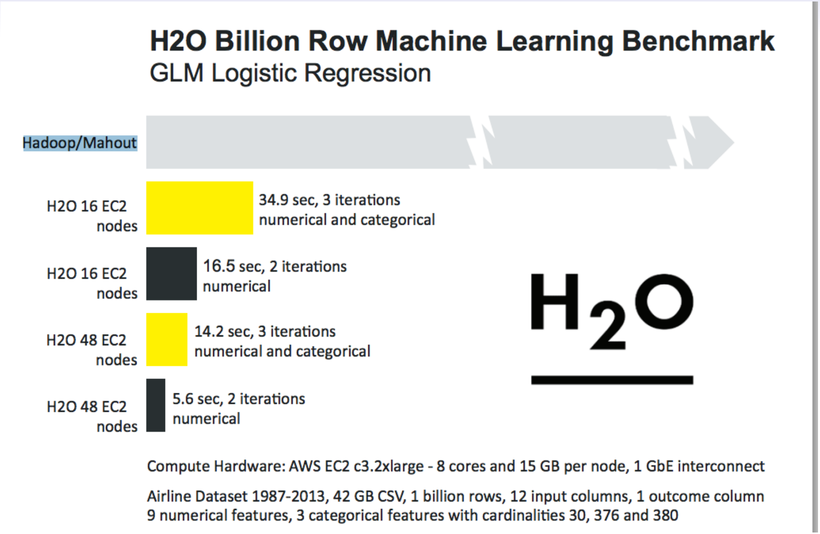
Quantcast is a digital marketing company.* Data are five-minute internet sessions. Binary target is type of family (≤ 2 adults vs adults plus children). 7 million features of session info (web page indicators and descriptors). Divided into training set (54M), validation (5M) and test (5M).

- All but 1.1M features could be screened because ≤ 3 nonzero values.
- Fit 100 models in 2 hours in R using `glmnet`.
- Richest model had 42K nonzero coefficients, and explained 10% deviance (like R-squared).

* TH on SAB


54M train, 5M val, 5M test
Misclassification Error
0.230
0.225
0.220
0.215
0.00
0.02
0.04
0.06
0.08
0.10
% Deviance Explained on Training Data
Validation
Test
Train


Mon
Tue
Wed
Thu
Fri
Sat
Sun
Pr(Family with Children | Day/Time)
0.40
0.45
0.50
0.55
5
10
15
20
Hour of Day


H2O Billion Row Machine Learning Benchmark
GLM Logistic Regression
Hadoop/Mahout
H2O 16 EC2 nodes
34.9 sec, 3 iterations
numerical and categorical
H2O 16 EC2 nodes
16.5 sec, 2 iterations
numerical
H2O 48 EC2 nodes
14.2 sec, 3 iterations
numerical and categorical
H2O 48 EC2 nodes
5.6 sec, 2 iterations
numerical
Compute Hardware: AWS EC2 c3.2xlarge - 8 cores and 15 GB per node, 1 GbE interconnect
Airline Dataset 1987-2013, 42 GB CSV, 1 billion rows, 12 input columns, 1 outcome column
9 numerical features, 3 categorical features with cardinalities 30, 376 and 380

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Will Fithian and TH (2014, Annals of Statistics) Local Case-Control Sampling: Efficient Subsampling in Imbalanced Data Sets

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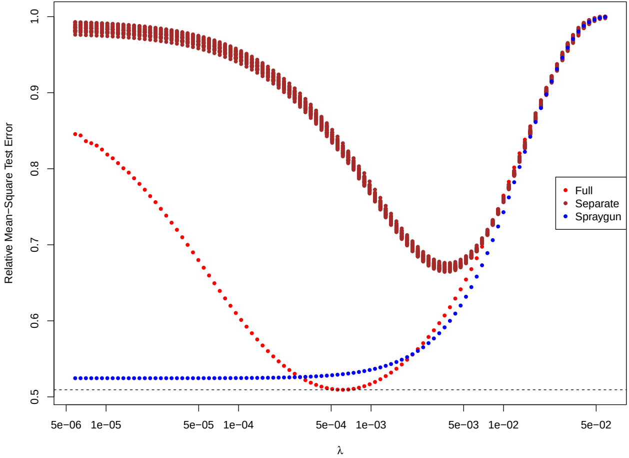
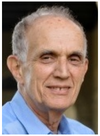
- Think out of the box! How much accuracy do you need? Timeliness can play a role, as well as the ability to explore different approaches. Explorations can be done on subsets of the data.

Thinking out the Box: Spraygun



Work with Brad Efron



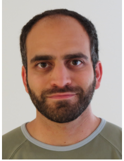
Beer ratings
1.4M ratings
0.75M vars
(sparse document features)

Lasso regression path: 70 mins.
Split data into 25 parts, distribute, and average: 30 secs.
In addition, free prediction standard errors and CV error.

Predicting the Pathogenicity of Missense Variants

Goal: prioritize list of candidate genes for prostate cancer

Joint work with Epidemiology colleagues Weiva Sieh, Joe Rothstein, Nilah Monnier Ioannidis, and Alice Whittemore

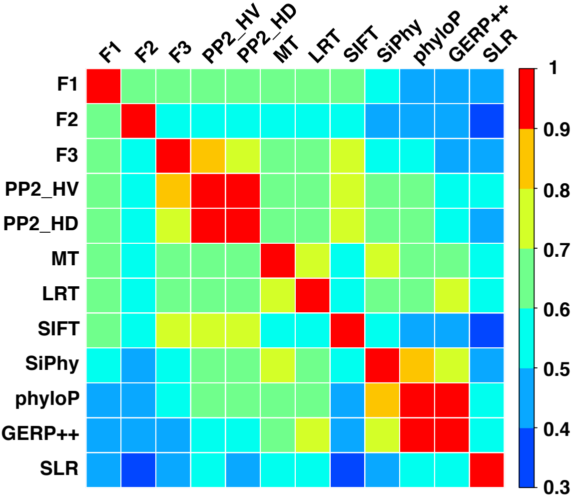
   

Approach

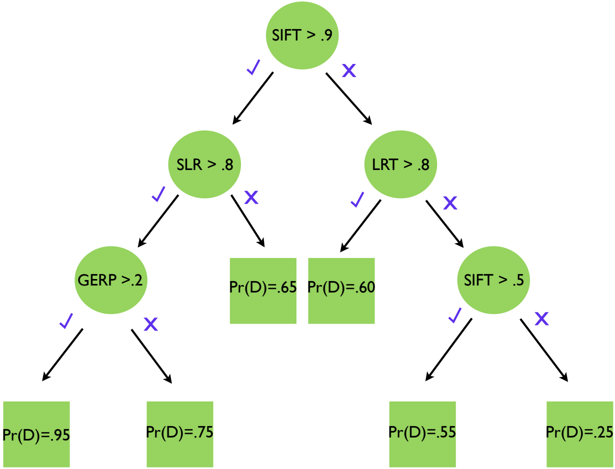
- A number of existing scores for disease status do not always agree (e.g SIFT, Polyphen).
- Idea is to use a Random Forest algorithm to integrate these scores into a single consensus score for predicting disease.
- We will use existing functional prediction scores, conservation scores, etc as features — 12 features in all.
- Data acquired through SwissVar. 52K variants classified as

  disease — 21K variants
  neutral — 31K variants

Correlation of Features

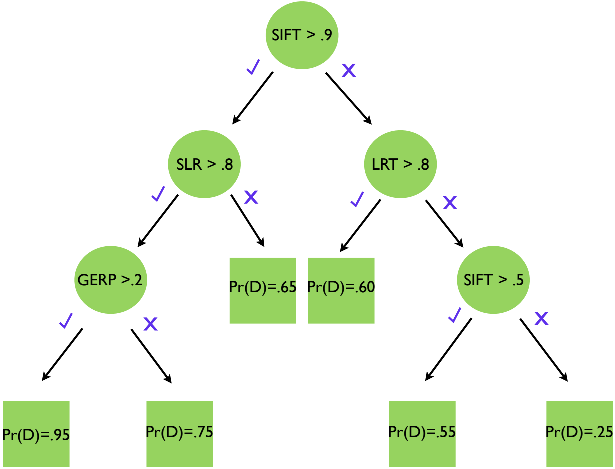


Decision Trees



Trees use the features to create subgroups in the data to refine the estimate of disease.

Decision Trees



Trees use the features to create subgroups in the data to refine the estimate of disease. Shallow trees are too coarse/inaccurate.

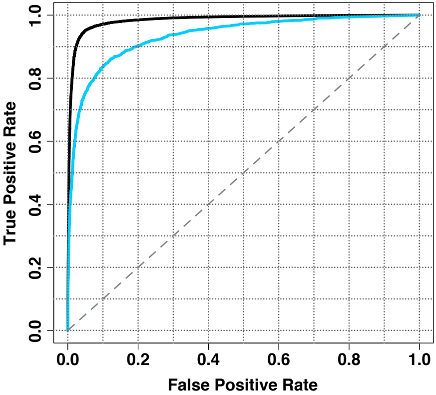
Random Forests

Leo Breiman (1928–2005)

- Deep trees (fine subgroups) are more accurate, but very noisy.
- Idea: fit many (1000s) different and very-deep trees, and average their predictions to reduce the noise.
- How to get different trees?
  - Grow trees to bootstrap subsampled versions of the data.
  - Randomly ignore variables as candidates for splits.

Random Forests are very effective and give accurate predictions. They are automatic, and give good CV estimates of prediction error (for free!). R package `RandomForest`.

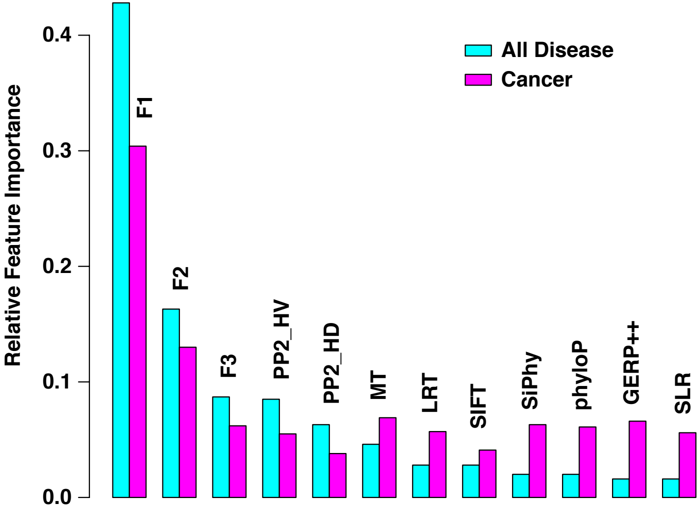
Results for Random Forests



Performance evaluated using OOB (out-of-bag) predictions for:

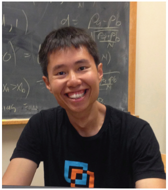
- All disease vs neutral variants (AUC 0.984)
- Cancer vs neutral variants (AUC 0.935)

Feature Importance



Two New Methods

Glinternet



With past PhD student Michael Lim (JCGS 2014).
Main effect + two-factor interaction models selected using the *group lasso*.

Gamsel

With past Ph.D student Alexandra Chouldechova, using *overlap group lasso*.
Automatic, *sticky* selection between zero, linear or nonlinear terms in GAMs:

$$\eta(x) = \sum_{j=1}^{p} f_j(x_j)$$

Glinternet

Example: GWAS with $p = 27K$ Snps , each a 3-level factor, and a binary response, $N = 3500$.

- Let X_j be $N \times 3$ indicator matrix for each Snp, and $X_{j:k} = X_j \star X_k$ be the $N \times 9$ *interaction* matrix.
- We fit model

$$\log \frac{\Pr(Y=1|X)}{\Pr(Y=0|X)} = \alpha + \sum_{j=1}^{p} X_j \beta_j + \sum_{j<k} X_{j:k}\theta_{j:k}$$

- note: $X_{j:k}$ encodes main effects and interactions.
- Maximize group-lasso penalized likelihood:

$$\ell(\mathbf{y}, \mathbf{p}) - \lambda \left[\sum_{j=1}^{p} \|\beta_j\|_2 + \sum_{j<k} \|\theta_{j:k}\|_2 \right]$$

- Solutions map to traditional hierarchical main-effects/interactions model (with effects summing to zero).

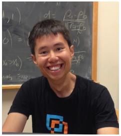
GLINTERNET (continued)

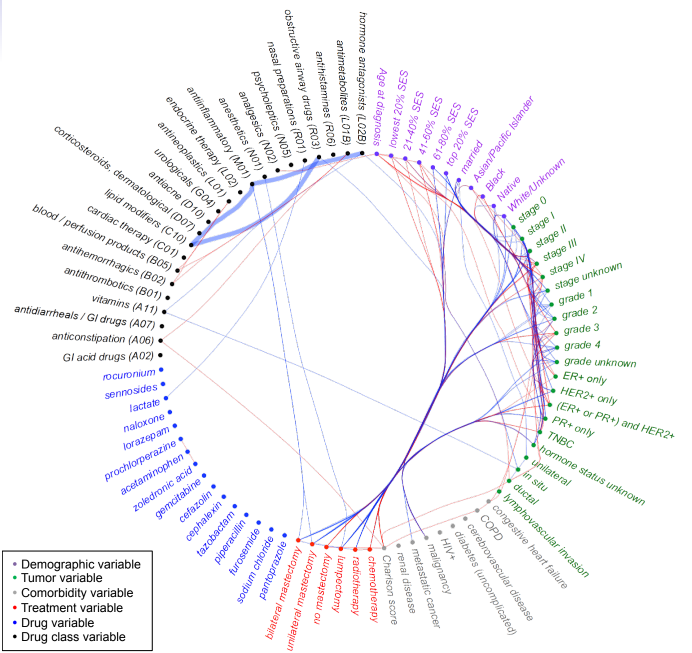
- Strong rules for feature filtering essential here — parallel and distributed computing useful too. GWAS search space of 729M interactions!
- Formulated for all types of interactions, not just categorical variables.
- GLINTERNET very fast — two-orders of magnitude faster than competition, with similar performance.

Example: Mining Electronic Health Records for Synergistic Drug Combinations

Using Oncoshare database (EHR from Stanford Hospital and Palo Alto Medical Foundation) looked for synergistic effects between 296 drugs in treatment of 9,945 breast cancer patients.

Used GLINTERNET to discover three potential synergies.
Joint work with Yen Low, Michael Lim, TH, Nigam Shah and others.

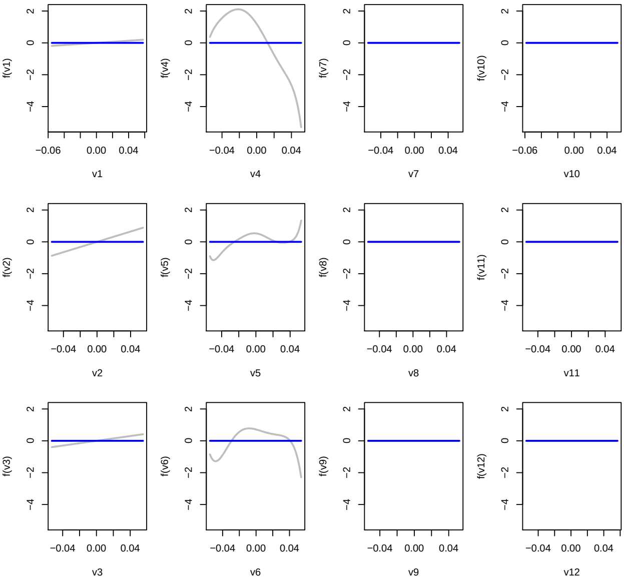

hormone antagonists (L02B)
antimetabolites (L01B)
antihistamines (R06)
obstructive airway drugs (R03)
nasal preparations (R01)
psycholeptics (N05)
analgesics (N02)
anesthetics (N01)
antiinflammatory (M01)
endocrine therapy (L02)
antineoplastics (L01)
urologicals (G04)
antiacne (D10)
corticosteroids, dermatological (D07)
lipid modifiers (C10)
cardiac therapy (C01)
blood / perfusion products (B05)
antihemorrhagics (B02)
antithrombotics (B01)
vitamins (A11)
antidiarrheals / GI drugs (A07)
anticonstipation (A06)
GI acid drugs (A02)
rocuronium
sennosides
lactate
naloxone
lorazepam
prochlorperazine
acetaminophen
zoledronic acid
gemcitabine
cefazolin
cephalexin
tazobactam
piperacillin
furosemide
sodium chloride
pantoprazole
bilateral mastectomy
unilateral mastectomy
no mastectomy
lumpectomy
radiotherapy
chemotherapy
Charlson score
renal disease
metastatic cancer
malignancy
HIV+
diabetes (uncomplicated)
cerebrovascular disease
COPD
congestive heart failure
lymphovascular invasion
ductal
in situ
unilateral
hormone status unknown
TNBC
PR+ only
(ER+ or PR+) and HER2+
HER2+ only
ER+ only
grade unknown
grade 4
grade 3
grade 2
grade 1
stage unknown
stage IV
stage III
stage II
stage I
stage 0
White/Unknown
Native
Black
Asian/Pacific Islander
married
top 20% SES
61-80% SES
41-60% SES
21-40% SES
lowest 20% SES
Age at diagnosis
Demographic variable
Tumor variable
Comorbidity variable
Treatment variable
Drug variable
Drug class variable

GAMSEL: Generalized Additive Model Selection

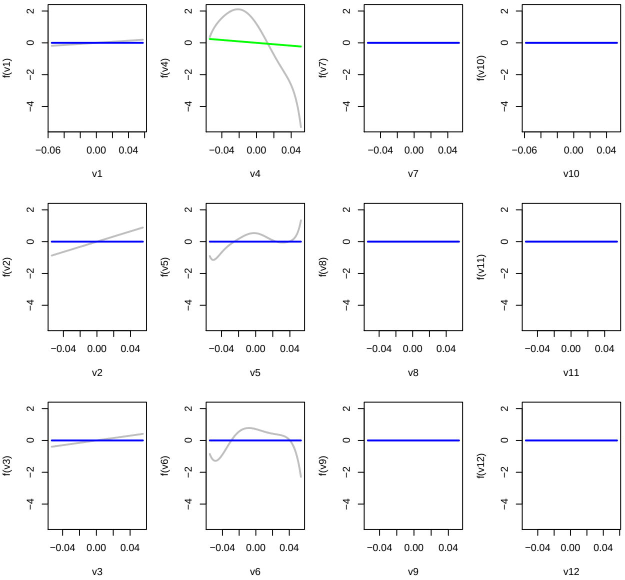
$$
\begin{aligned}
\frac{1}{2}\left\| y - \sum_{j=1}^{p} \alpha_j x_j - \sum_{j=1}^{p} U_j \beta_j \right\|^2 \quad &+ \quad \lambda \sum_{j=1}^{p} \left\{ (1-\gamma)|\alpha_j| + \gamma \|\beta_j\|_{D_j^*} \right\} \\
&+ \quad \frac{1}{2} \sum_{j=1}^{p} \psi_j \|\beta_j\|_{D_j}^2
\end{aligned}
$$

- $U_j = [x_j \; p_1(x_j) \; \cdots \; p_k(x_j)]$ where the p_i are orthogonal Demmler-Reinsch spline basis functions of increasing degree.
- $D_j = \mathrm{diag}(d_{j0}, d_{j1}, \ldots, d_{jk})$ diagonal penalty matrix with $0 = d_{j0} < d_{j1} \leq d_{j2} \leq \cdots \leq d_{jk}$, and $D_j^* = D_j$ but with $d_{j0} = d_{j1}$.

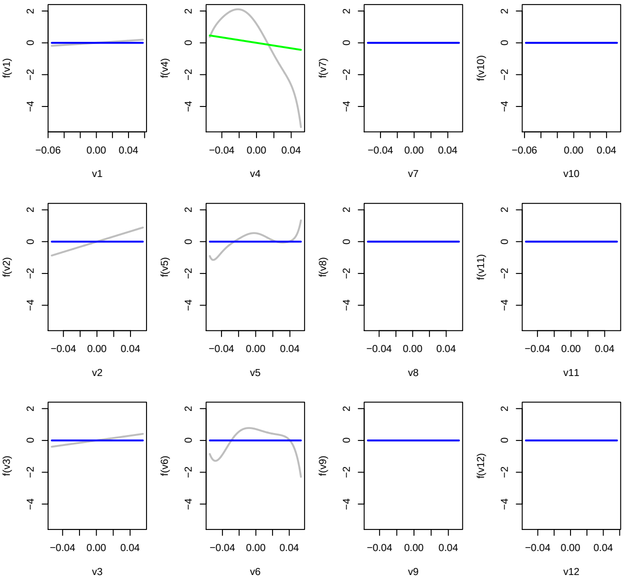
Step= 1   lambda = 125.43



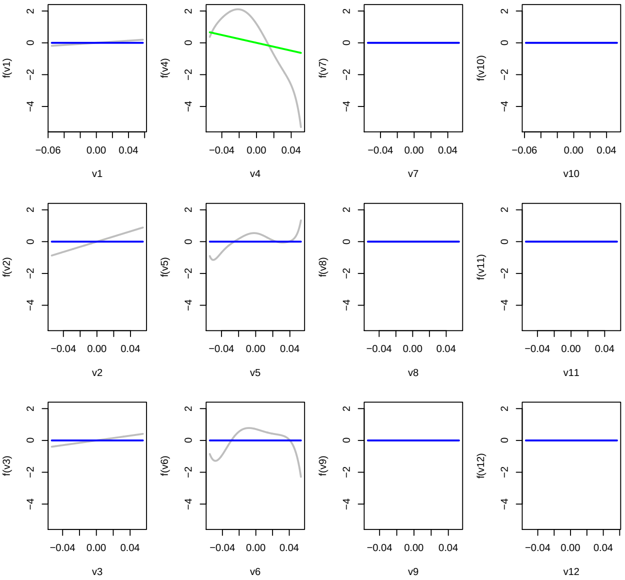
Step= 2   lambda = 114.18



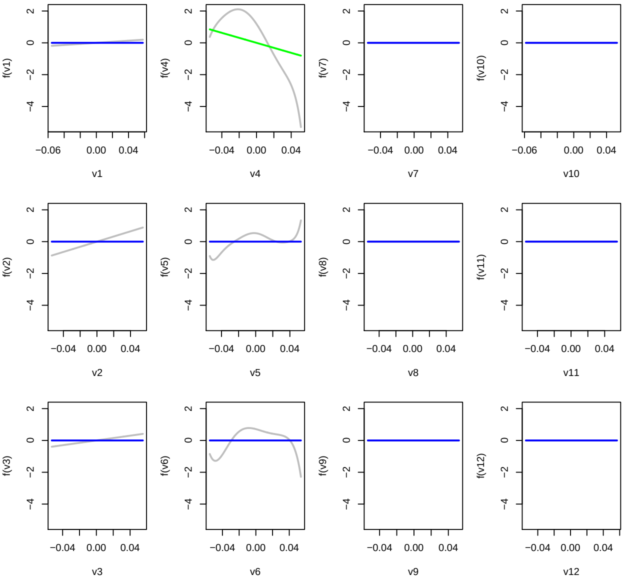
Step= 3   lambda = 103.94



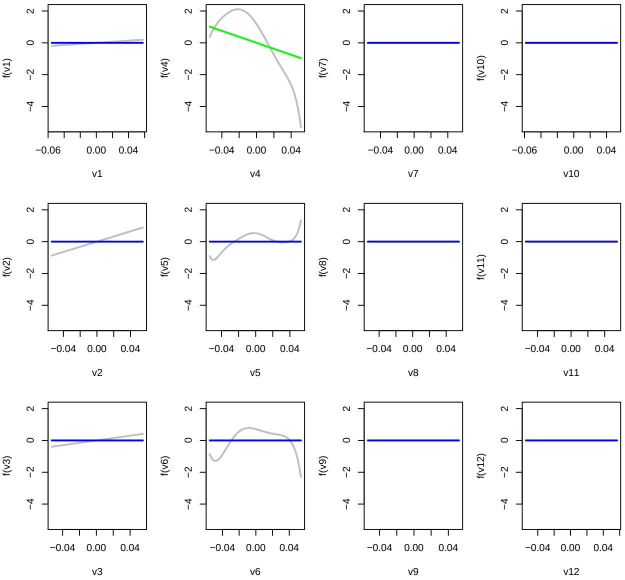
Step= 4   lambda = 94.61



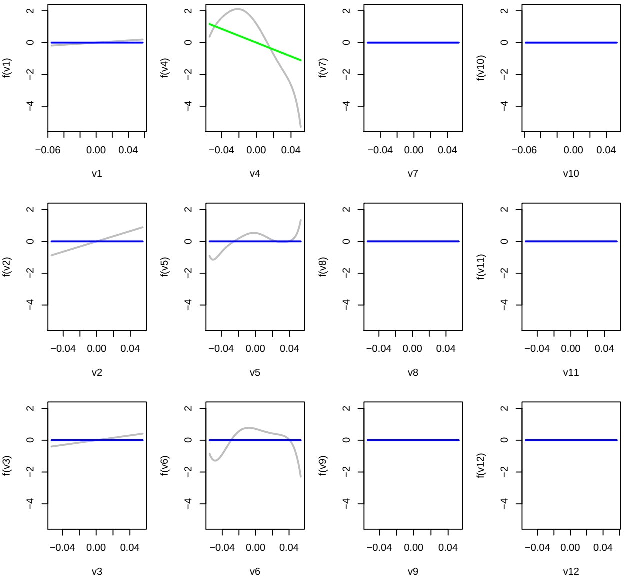
Step= 5   lambda = 86.13



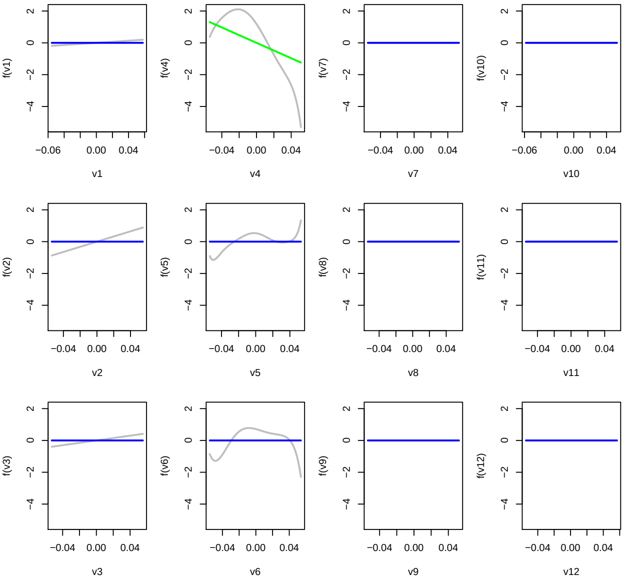
Step= 6   lambda = 78.4



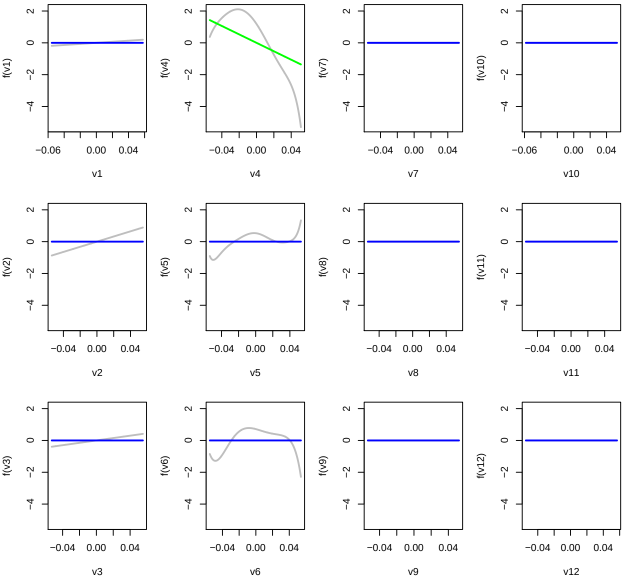
Step= 7   lambda = 71.37



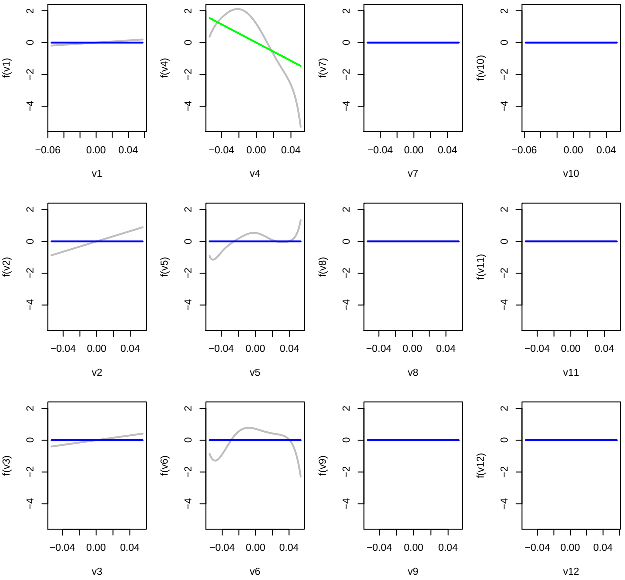
Step= 8   lambda = 64.97



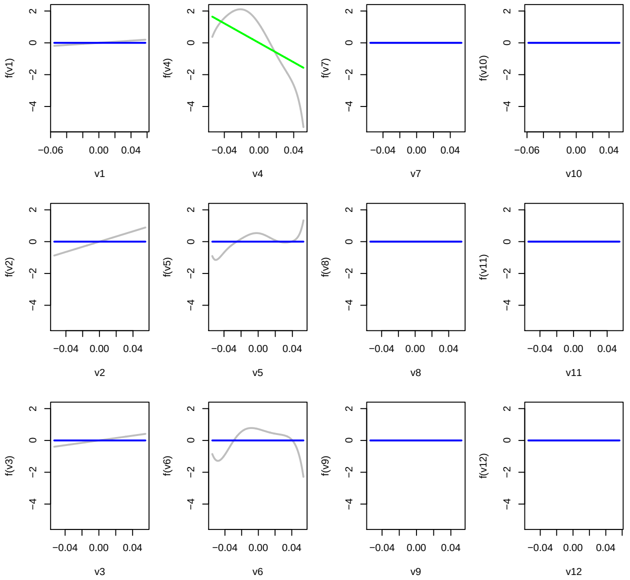
Step= 9 lambda = 59.14



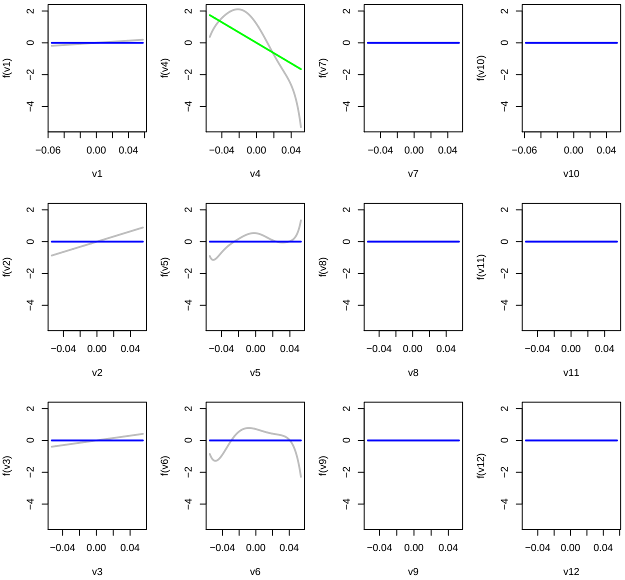
Step= 10   lambda = 53.83



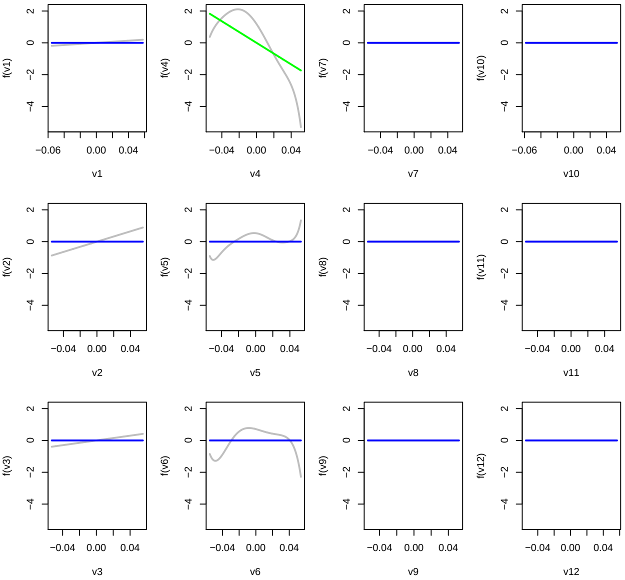
Step= 11   lambda = 49.01



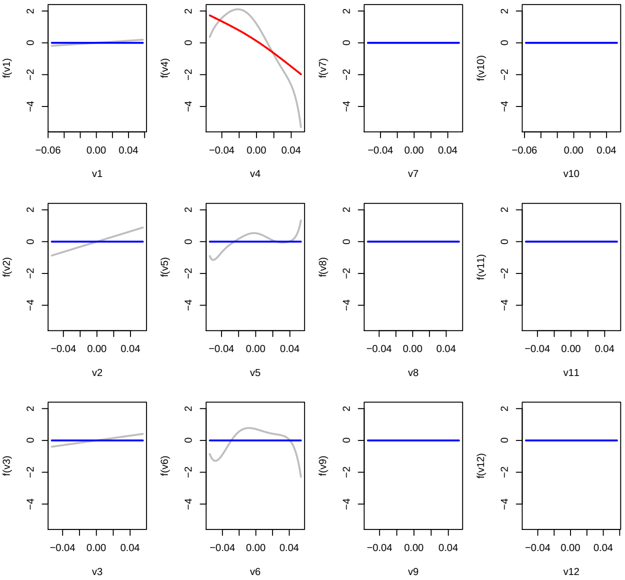
Step= 12   lambda = 44.61



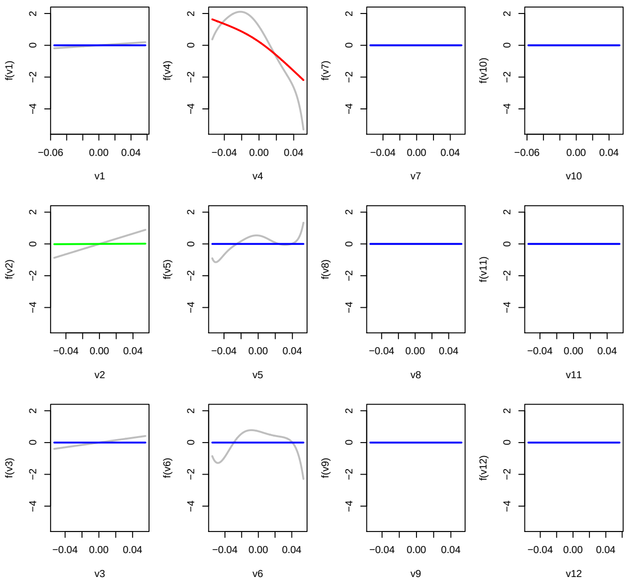
Step= 13   lambda = 40.61



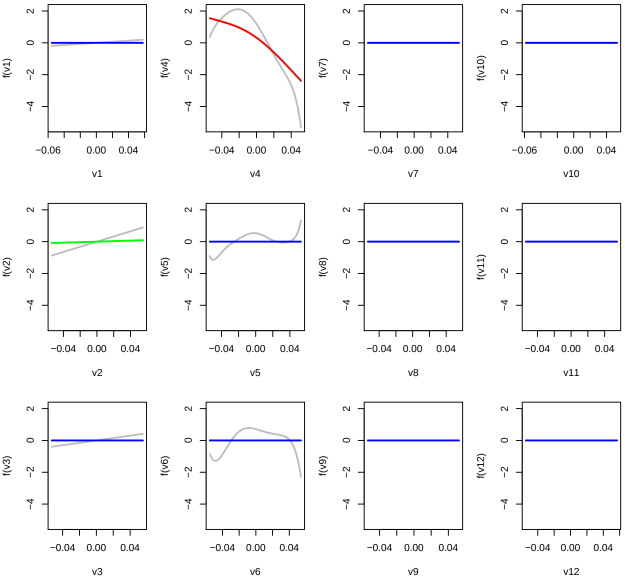
Step= 14   lambda = 36.97



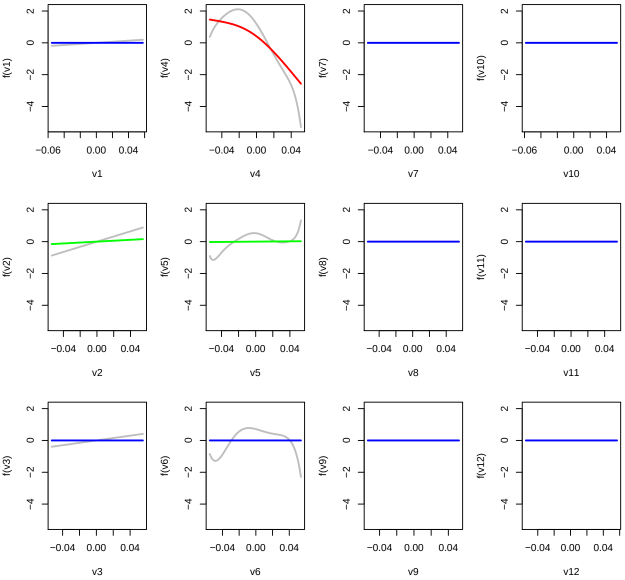
Step= 15   lambda = 33.65



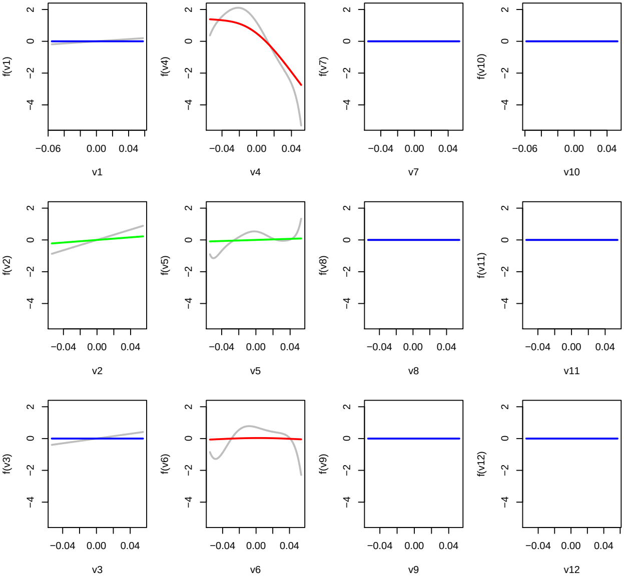
Step= 16   lambda = 30.63



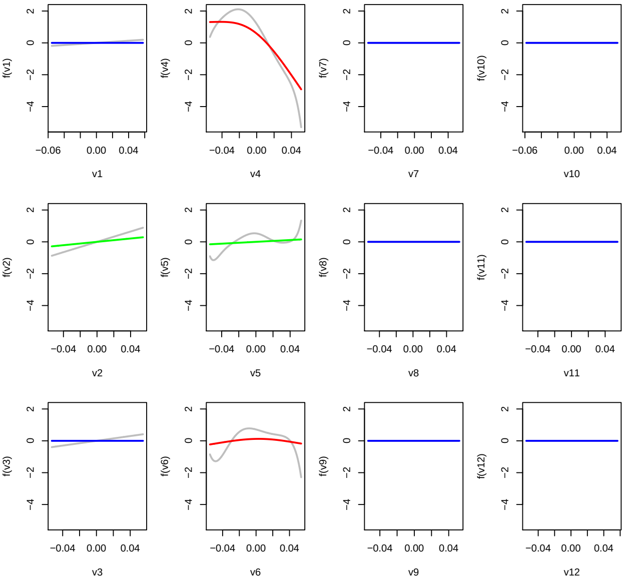
Step= 17   lambda = 27.88



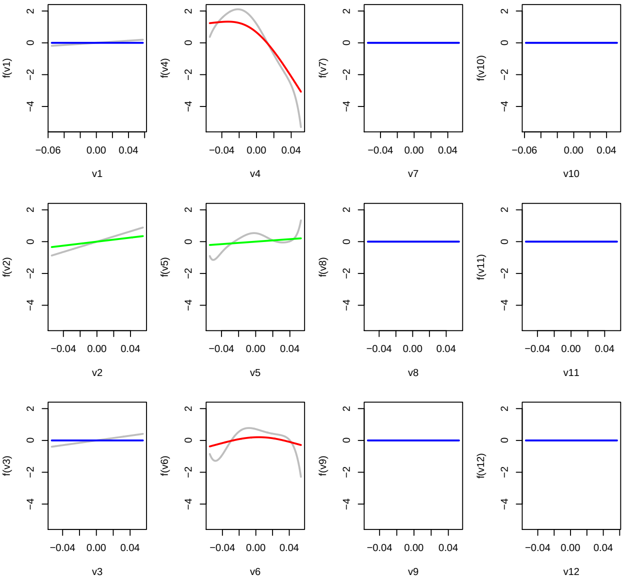
Step= 18   lambda = 25.38



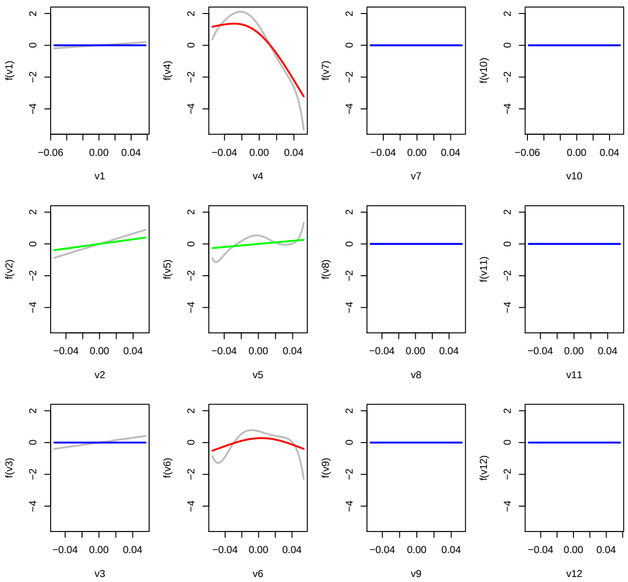
Step= 19   lambda = 23.11



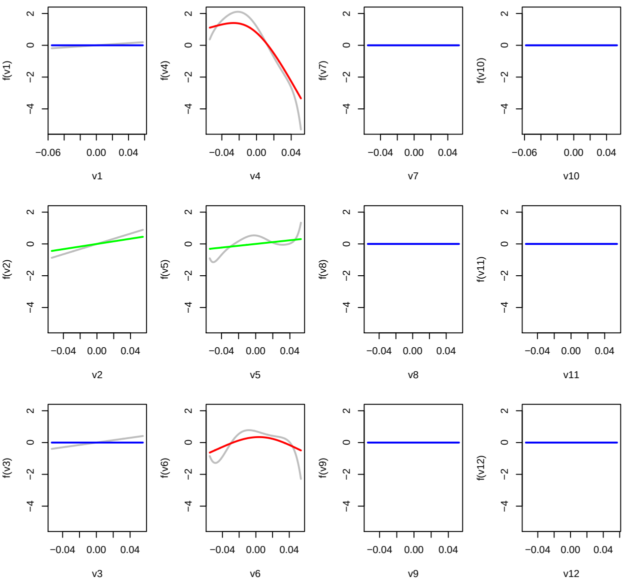
Step= 20   lambda = 21.03



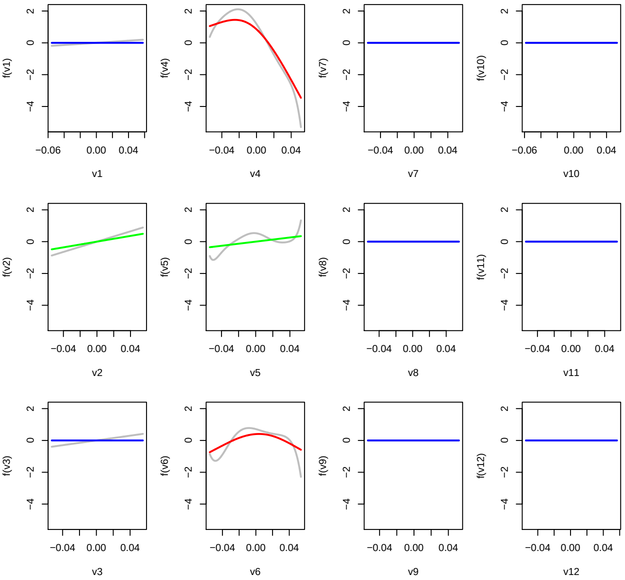
Step= 21   lambda = 19.15



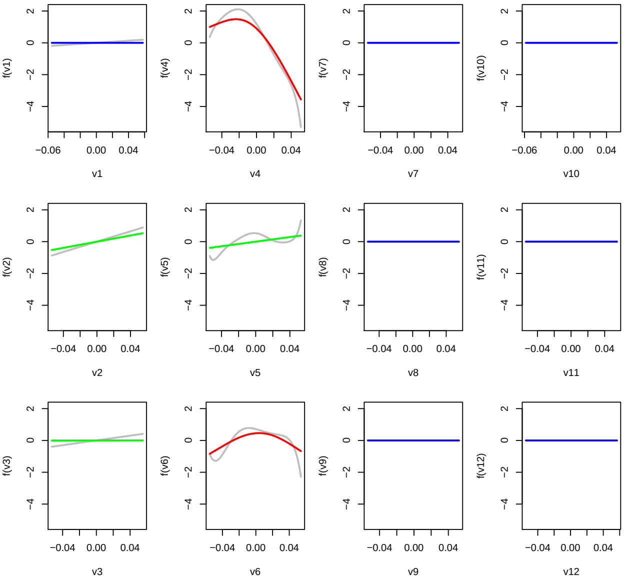
Step= 22   lambda = 17.43



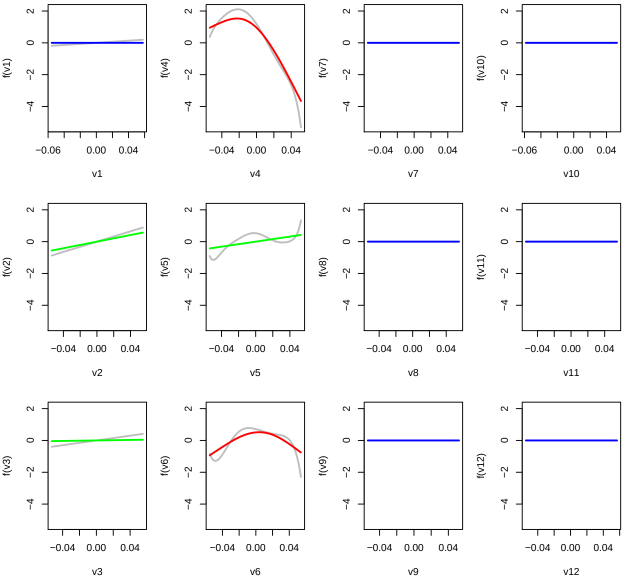
Step= 23   lambda = 15.87



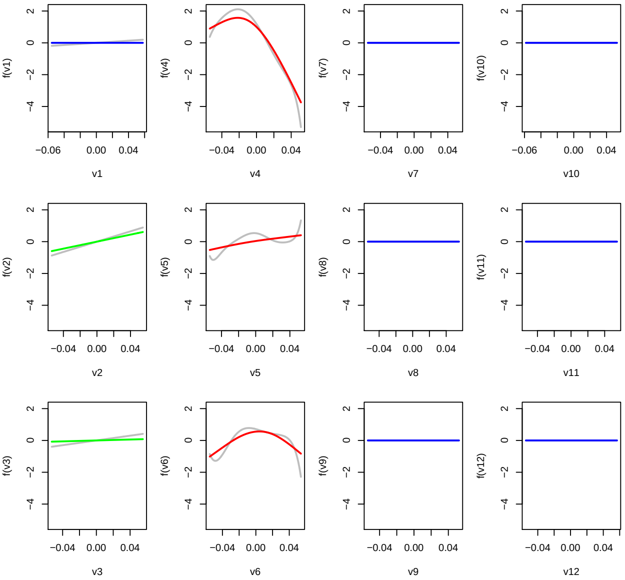
Step= 24   lambda = 14.44

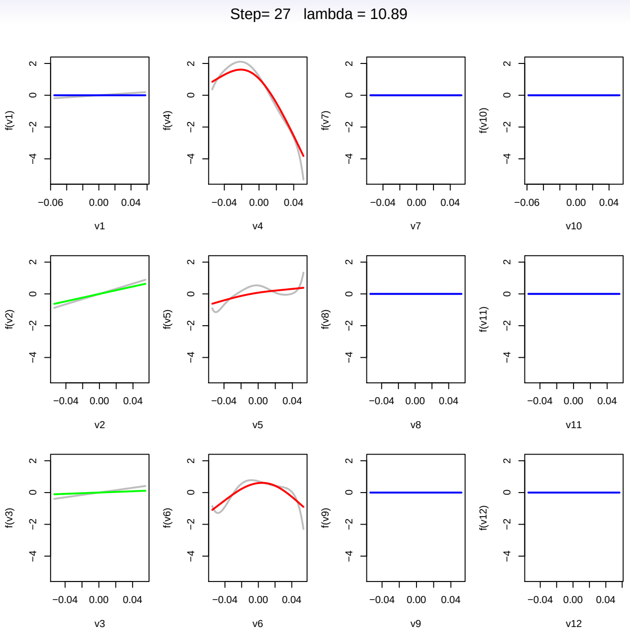


Step= 25   lambda = 13.15

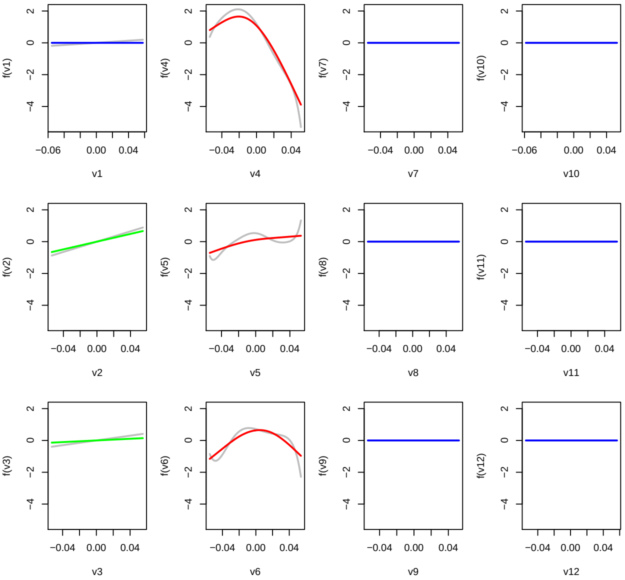


Step= 26   lambda = 11.97

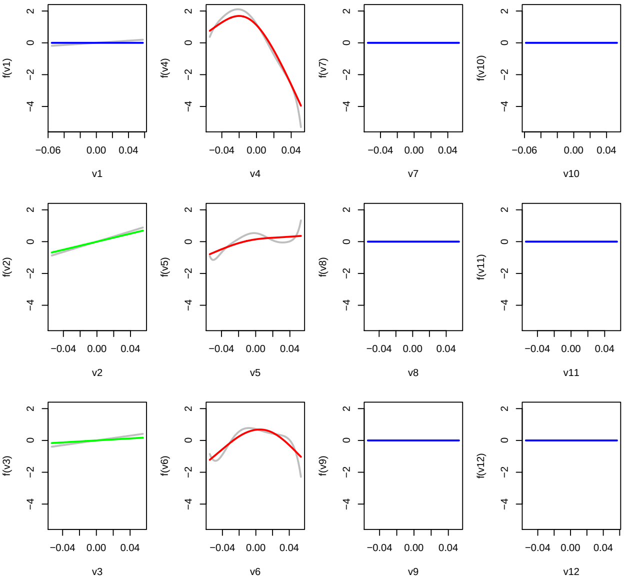



Step= 27 lambda = 10.89
f(v1)
v1
f(v4)
v4
f(v7)
v7
f(v10)
v10
f(v2)
v2
f(v5)
v5
f(v8)
v8
f(v11)
v11
f(v3)
v3
f(v6)
v6
f(v9)
v9
f(v12)
v12

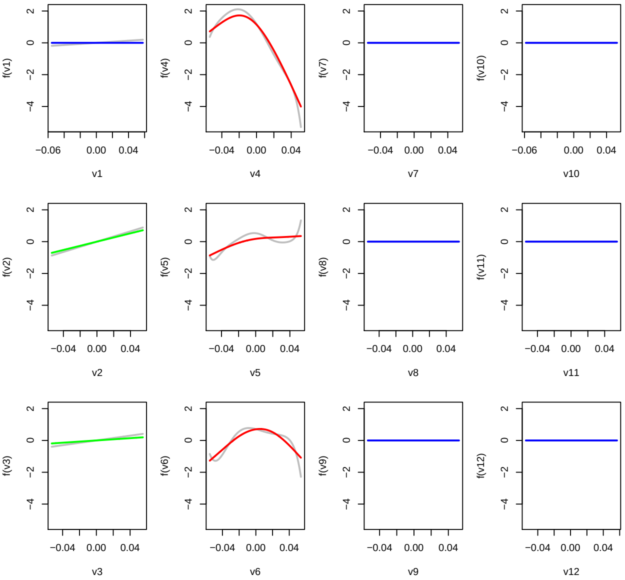
Step= 28   lambda = 9.92



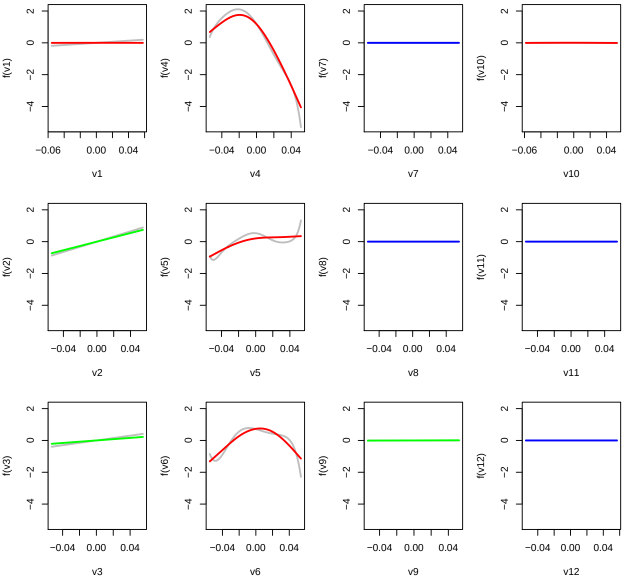
Step= 29   lambda = 9.03



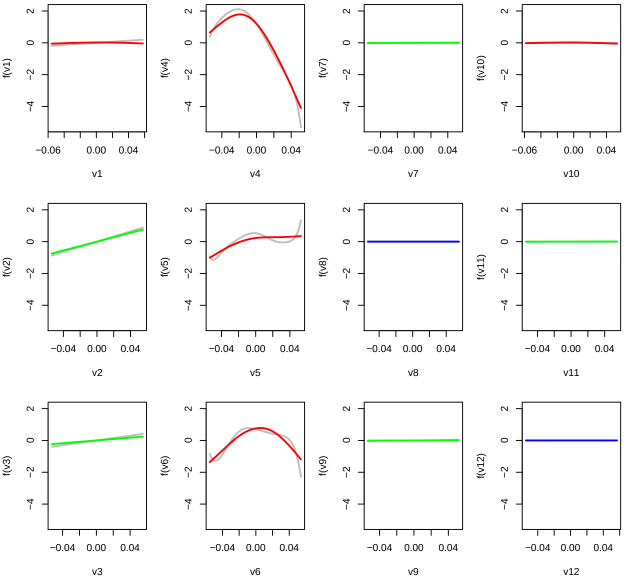
Step= 30   lambda = 8.22



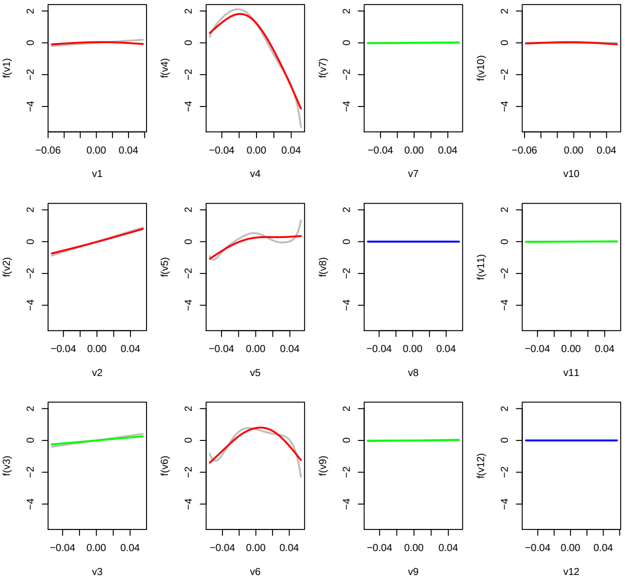
Step= 31   lambda = 7.48



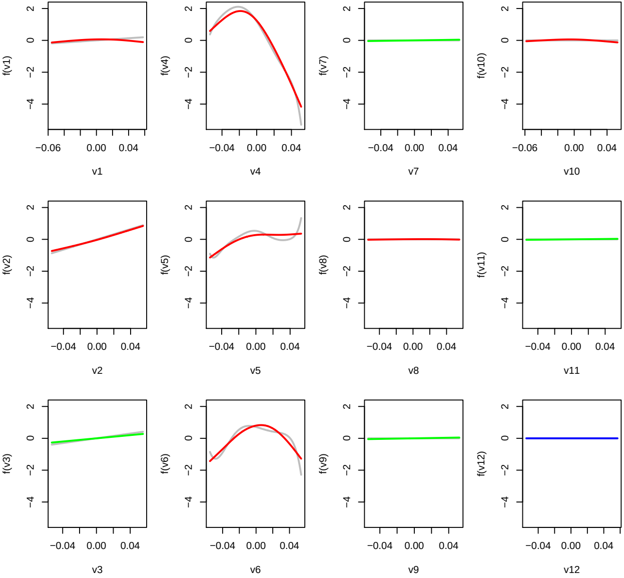
Step= 32   lambda = 6.81



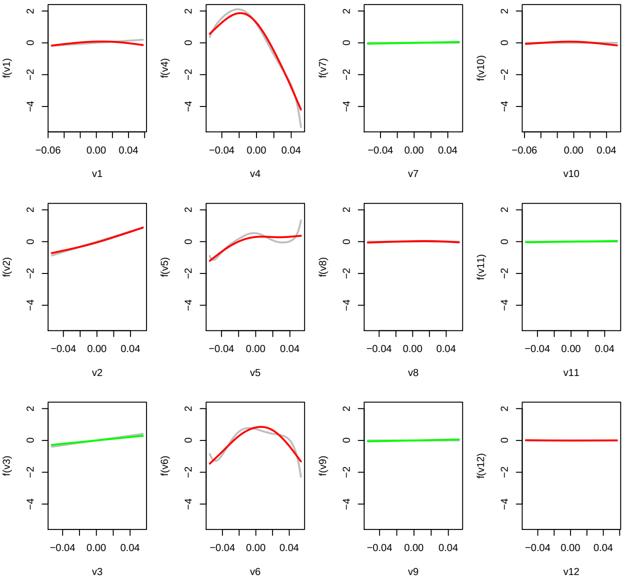
Step= 33   lambda = 6.2



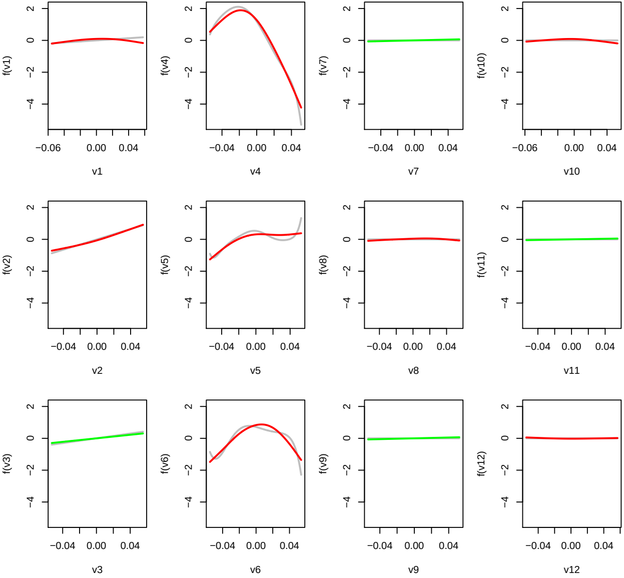
Step= 34   lambda = 5.64



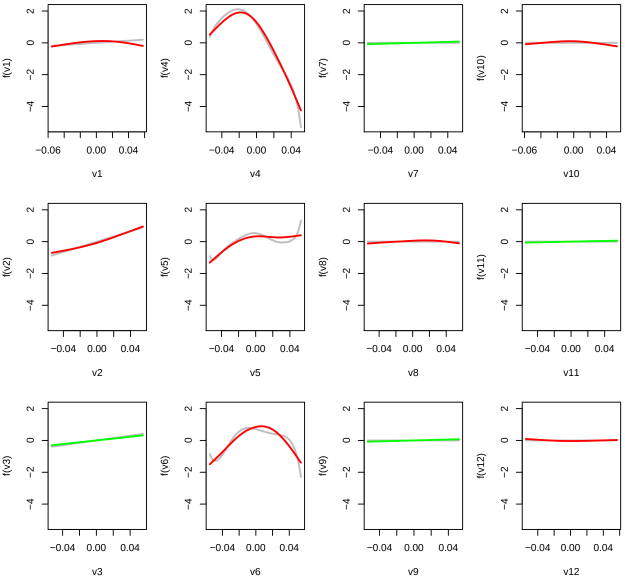
Step= 35   lambda = 5.14



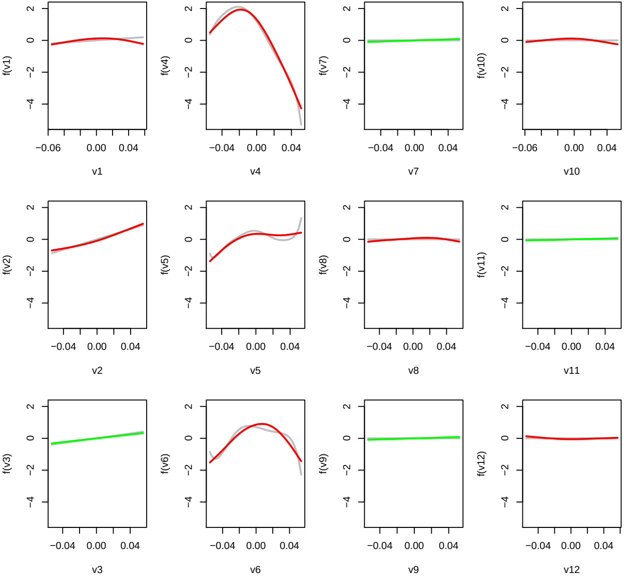
Step= 36   lambda = 4.68



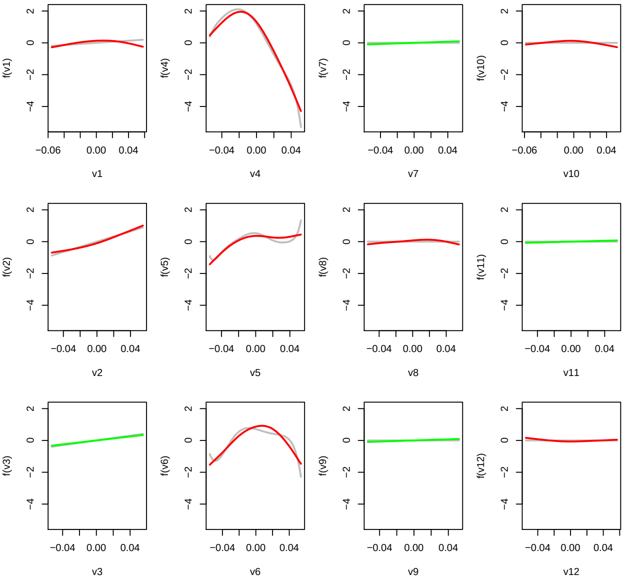
Step= 37   lambda = 4.26



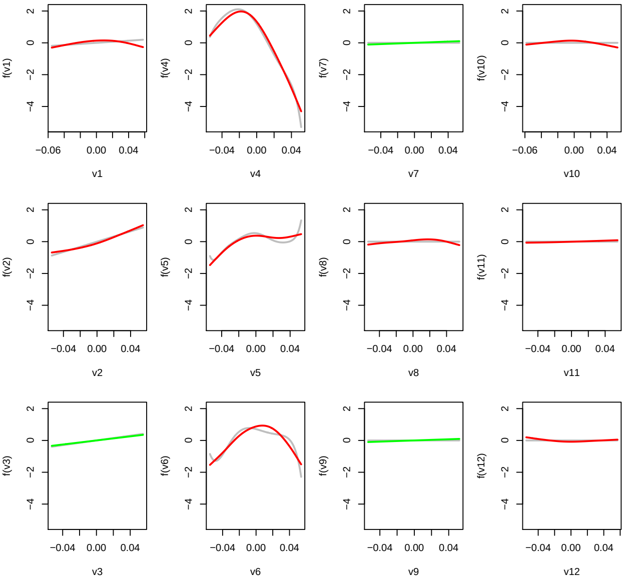
Step= 38   lambda = 3.87



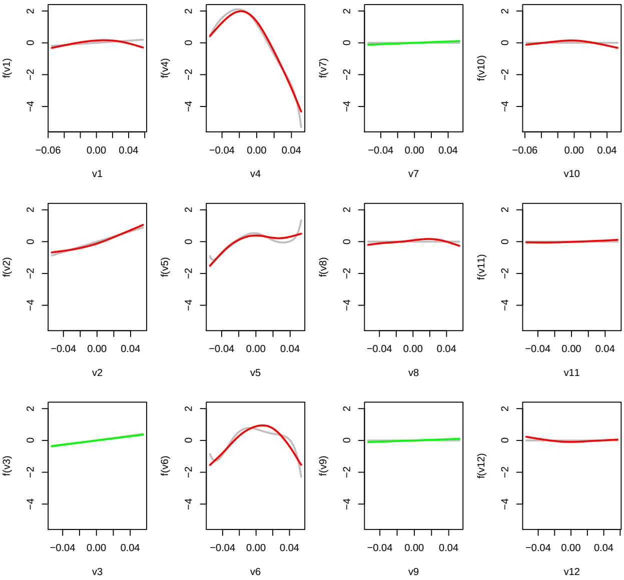
Step= 39   lambda = 3.53



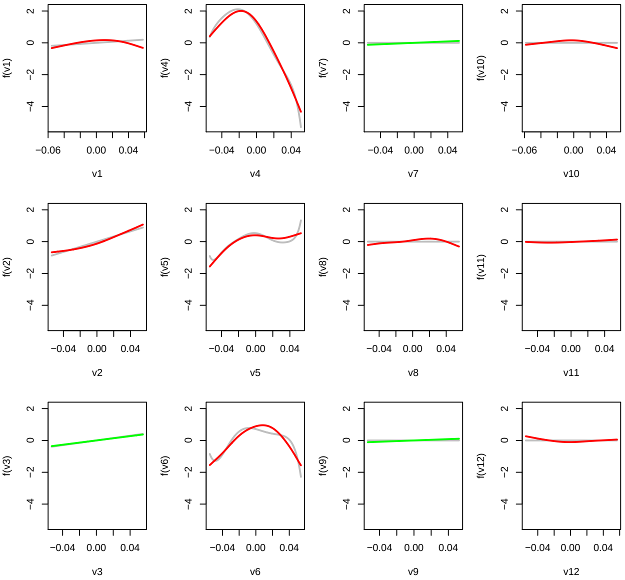
Step= 40   lambda = 3.21



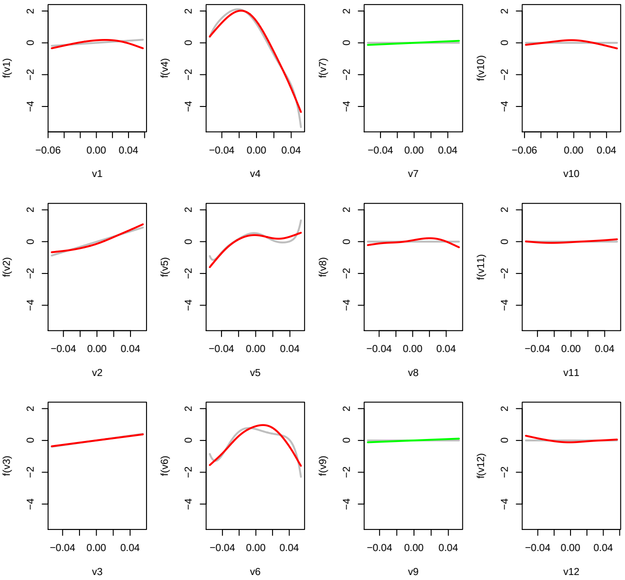
Step= 41   lambda = 2.92



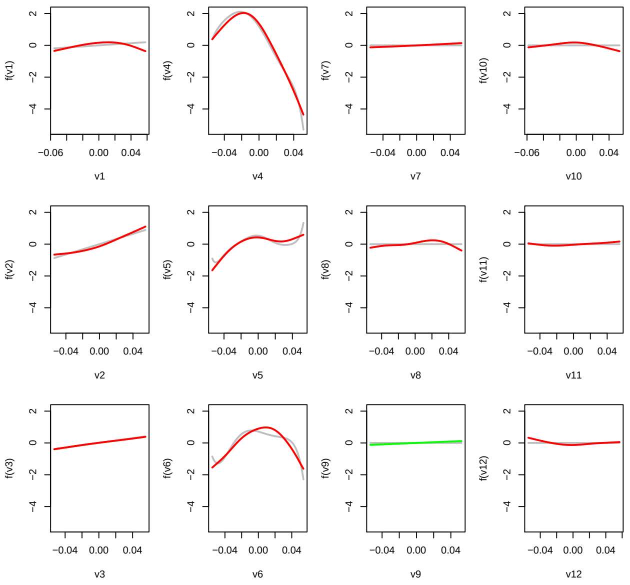
Step= 42   lambda = 2.66



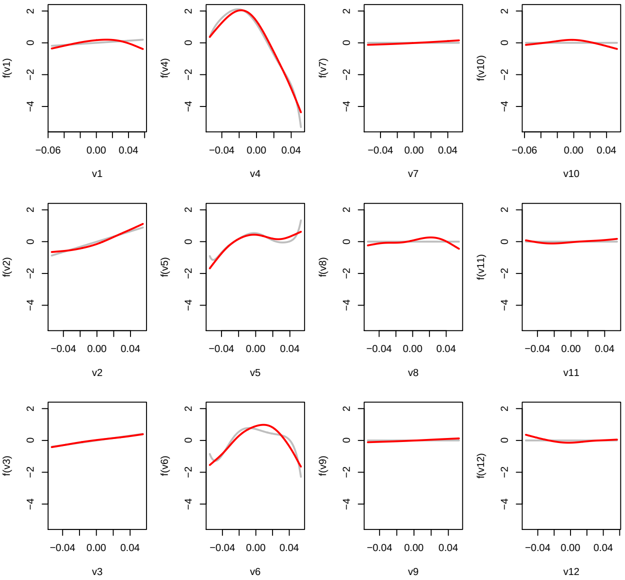
Step= 43   lambda = 2.42



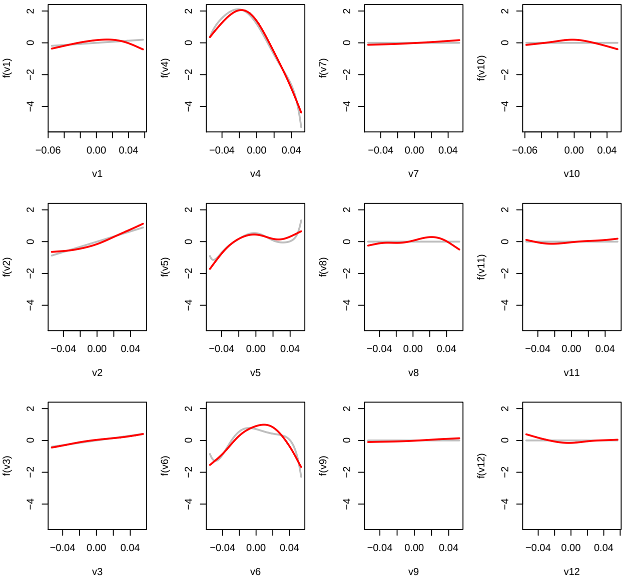
Step= 44   lambda = 2.2



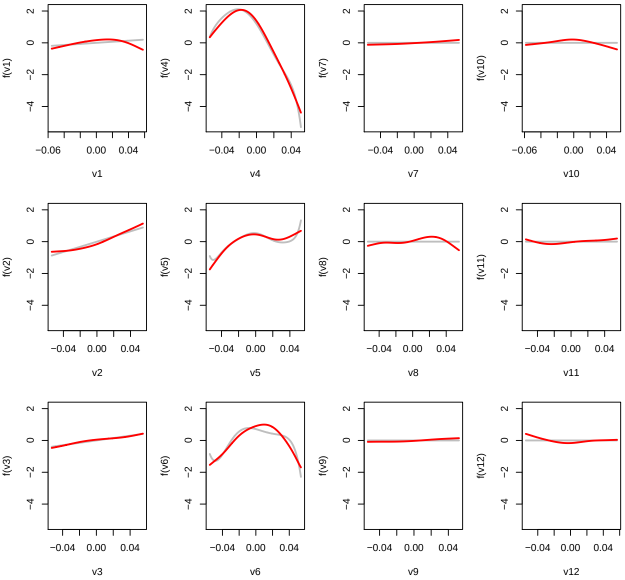
Step= 45   lambda = 2.01



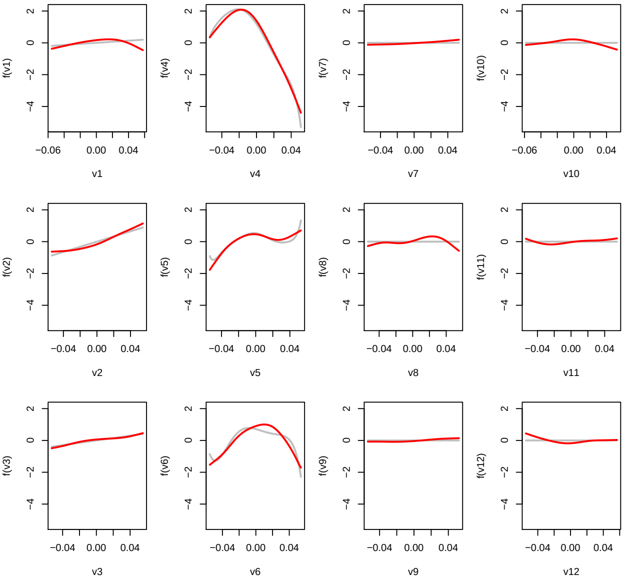
Step= 46   lambda = 1.83



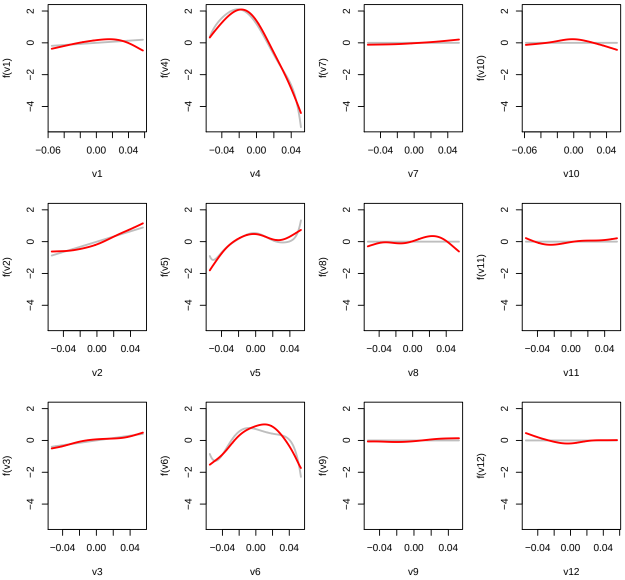
Step= 47   lambda = 1.66



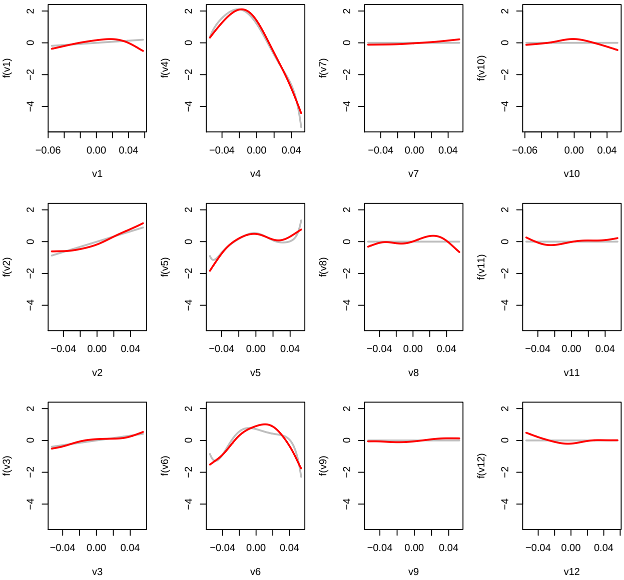
Step= 48   lambda = 1.51



Step= 49 lambda = 1.38



Step= 50   lambda = 1.25



useR! 2016

All the tools I described are implemented in R, which is wonderful free software that gets increasingly more powerful as it interfaces with other systems. R can be found on CRAN: `http://cran.us.r-project.org`

27–30 June 2016, R user conference at Stanford!

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$\cdots$ and now for some cheap marketing …

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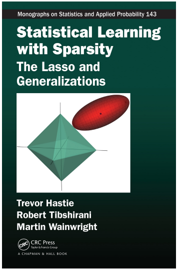

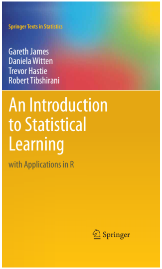

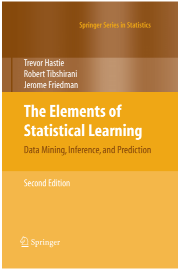

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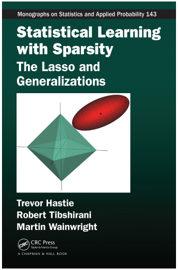

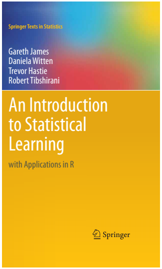

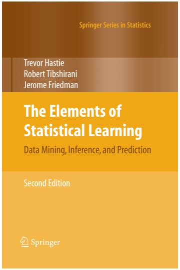

Thank you!