Controlling for Monotonicity in Random Forest Regressors

Mark Seligman

Suiji

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- Arborist
- Training solution
- Simulated data
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- Conclusions, future work.

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Binary decision trees, briefly

- Prediction method posing series of T/F questions about data set.
  - I.e., questions about observations of given predictors.
- Answer determines which (of two) questions to pose next: branch.
  - E.g., $p <= 1.0?$: pose "left" question, else pose "right".
  - Here, "pose" can be thought of as branching.
- Different data traverse different paths through the tree.
- Terminal (or "leaf") node in path reports score for that path.
- Can build single tree and refine: "boosting".
- Can build "forest" of (typically) $100 - 1000$ trees.
  - Forest-wide score derived from aggregate of all trees' scores.

Random Forests, in a nutshell

- Trademarked by Leo Breiman (dec.) and Adele Cutler.
- Predicts an outcome vector, either numerical or categorical.
  - Regression forests train numerical-valued trees.
  - Classification forests train category-valued trees.
- Trains on design matrix of observations: columns of predictors.
  - Columns individually either numerical or categorical ("factors").
- Trees trained on randomly-selected ("bagged") set of matrix rows.
- Predictors sampled randomly throughout training
  - Separately chosen for each node: *mtry*.
- Validation on held-out subset: different for each tree.
- Independent prediction on separately-provided test sets.
- Focus here is on regression forests, numerical predictors.

Motivation

- Algorithm involves two levels of sampling.
  - Sampling original response to train individual tree.
  - Sampling predictors to split a node: *mtry*.
- Sampling helps reduce bias.
- But, also promotes variation among trees as estimators.
- Couple this with noise in the data itself:
  - Trees may predict values counter to knowledge or expectation.
- Is it possible to constrain training to expectation?
- Will show:
  - In the case of monotonicity: yes.
  - In fact, only a minor modification of existing algorithm.

Monotonicity

- Modeller may presume “hard” physical principle to hold.
  - E.g, signal intensity decreases with distance.
  - Predictive quality suspect if contradicted.
  - May wish to preclude from training.
- Might, alternatively, expect “soft” relationships to hold.
  - E.g., LGD increases with loan-to-value ratio.
  - Exceptions may or may not suggest poor predictive quality.
  - May wish to control in training.
- Monotonicity here either desirable or essential.
  - “Classical” RF appears not to offer constraining mechanism.

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Arborist

- General-purpose Random Forest (TM) implementation.
  - Regression, including quantiles.
  - Classification.
  - Numeric, factor predictors: no *a priori* limit on cardinality.
- Tunable to commodity hardware: e.g., multicore, GPU.
- Language-agnostic Core, with separate language "front ends".
  - **R** sets the standard.
  - **Python** under development.
  - Julia?
- Easily extended to support new features.
  - This talk emphasizes extensibility.

Arborist, cont.

- Currently in-memory only.
  - Out-of-core support planned.
- Scales well with sample count.
- Predictor scaling more nuanced:
  - Better scaling when predictor occupancy high:
  - i.e., *mtry* as a fraction of predictor count.
  - See Wright and Ziegler [to appear].
- Number two position on airline-data benchmark.

Rborist package, version 0.1-1, now on CRAN

- Repairs errors in separate prediction.
- Reduces memory footprint.
- Improves core occupancy during parallel execution.
- New features and improvements, including:
  - Quantile training now default.
  - Case weighting, with *auto* mode for unbalanced data.
  - *mtry* semantics now default for low-predictor regimes.
  - *preTrain* option caches state for iterative workflows.
  - Suports **forestFloor** feature-contribution package.
  - Supported by **Caret**.
  - Monotonic regression, the subject of this talk.

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- Infrastructural support for future releases: more later.

Training

- Helpful to think of individual tree nodes as sets of samples.
  - Begin by sampling original response vector, with or w/o replacement.
  - Root node "is" this sampled set of values.
  - Every node either splits into two successors or terminates.
  - Splitting effects a bipartition of a node's sample set.

    Successor nodes are assigned complementary subsets.

    n samples: $\mathcal{O}(2^n)$ potential assignments.

    How an assignment is selected will be shown.
- Training splits the root set in this way until exhausted.
- The leaves of a trained tree together partition its root set.

Prediction

- Regression defines a leaf's score to be the mean of its sample values.
- Recall that prediction walks a data-dependent path down a tree.
  - The predicted value, then, is the score of the terminal leaf.
- A forest-wide prediction is the mean over all tree predictions.
- Quantile regression proceeds similarly.
  - Each leaf reports a collection of values, not just a mean.
  - The forest yields a collection of values, easily binned.
  - Quantiles can be inferred directly from the bins.

Regression: numeric splits

- Numeric splits involve a predictor and an order predicate on it.
  - E.g., predictor p with question "Is $p < 3.1$?"
  - Branching direction at prediction determined by predicate's value.
  - But how does training derive the predicate?
- Training evaluates trial predicates on the sample sets of a node.
- A trial optimal with respect to some metric is selected.
  - Over a random collection of predictors.
  - On all *conforming* bipartitions of the node's sample set.
- Numerical trial predicates, again, are order relationships.
  - Conforming bipartitions equivalent to cuts in ordered values.
  - For n samples, a predictor has at most $n - 1$ unique cuts.
  - For numeric regressors, then, splitting is $\mathcal{O}(n)$.

Constraining numeric splits: preview

- Node splitting involves both the sample set and its observations.
  - *Observation* ordering dictates the biparition.

    I.e., which samples map L/R.
  - *Sample* values yield information metric on the trial partition.

    Standard metric for numeric regressors is weighted sample variance.
- Rejection scheme: do not accept trials violating the constraint.
- Recall, subset assignments already in hand for each trial.
- Will show:
  - Straightfoward to derive successor contributions from the assignments.
  - In partiucalar, constraint reuses information already at hand.

In symbols

Denote the original response vector as $y = (y_0, y_1, y_2, \ldots, y_n)^T$.

Let T be a node with sample set $\mathcal{S}(T)$.

Denote the sample set cardinality by

$$t \equiv |\mathcal{S}(T)|.$$

Sample set cardinality is conserved by (left, right) trial successors L, R:

$$l \equiv |\mathcal{S}(L)|, \quad r \equiv |\mathcal{S}(R)|; \quad l + r = t$$

The *impurity* of T is a measure of variance (Ishwaran [2015]):

$$\mathcal{I}(T) \equiv \frac{1}{t} \sum_{i \in \mathcal{S}(T)} (y_i - \bar{y_T})^2$$

Optimality

Optimal trial pairs maximize weighted-variance impurity *difference*:

$$\mathcal{I}(T) - t^{-1}\left(l\mathcal{I}(L) + r\mathcal{I}(R)\right),$$

which can be shown to be equivalent to maximizing:

$$l^{-1}\left(\sum_{i\in L} y_i\right)^2 + r^{-1}\left(\sum_{i\in R} y_i\right)^2 \tag{1}$$

Recall that the respective left and right contributions are given by:

$$\bar{y_L} = l^{-1}\sum_{i\in L} y_i \quad \text{and} \quad \bar{y_R} = r^{-1}\sum_{i\in R} y_i. \tag{2}$$

Splitting, II

So monotonicity is enforced by maximizing (1), constraining for (2). Speed up by precomputing sum_T and accumulating sum_L:

$$\mathrm{sum}_T \equiv \sum_{i \in T} y_i, \quad \mathrm{sum}_L \equiv \sum_{i \in L} y_i. \tag{3}$$

For example, (1) then simplifies to:

$$l^{-1}\mathrm{sum}_L^2 + (t - l)^{-1}\left(\mathrm{sum}_T - \mathrm{sum}_L\right)^2$$

The nondecreasing constraint, for example, is:

$$\bar{y}_L \leq \bar{y}_R, \quad \text{or}$$

$$l^{-1}\mathrm{sum}_L \leq (t - l)^{-1}\left(\mathrm{sum}_T - \mathrm{sum}_L\right) \tag{4}$$

Putting it all together

- A node is split by visiting a random subcollection of the predictors.
- For each selected predictor, the sample set is visited in *predictor* order.
- Numerical regressors: conforming bipartitions based on order.
  - Conforming left/right trials are characterized by the cuts.
- Optimal trials maximize (3), i.e., “standard” RF behavior.
- Constrained trials satisfy (4).
- Optimal trials not meeting the constraint are rejected.

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regMono option

- Vector of probabilities, with sign.
- Length $==$ $\#$ predictors.
- Default is 0 for all predictors, if not passed.
- Values are probabilities, p, with sign indicating direction.
  - $p > 0$: nondecreasing.
  - $p == 0$: no constraint.
  - $p < 0$: nonincreasing.
  - $|p| \in [0, 1]$: reject with probability p.
- Will complain if:
  - Classification.
  - Vector length does not match predictor count.
  - Nonzero entries for factors.
  - $p \notin [-1, 1]$.

Usage

```
# Width == predictor count.
constraint <- rep(0.0, ncol(x))

# Predictor 5 rejects nondecreasing paths a.s.:
constraint[5] <- -1.0

# Predictor 2 rejects increasing paths with
# probability 0.7:
constraint[2] <- 0.7

rb <- Rborist(x, y, regMono = constraint)
```

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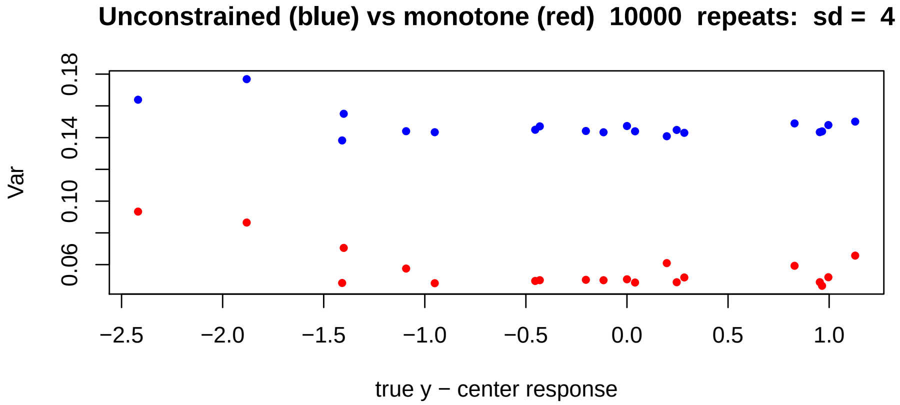
Strategy

Select several linear and quadratic transformations.
Choose several different dimensions, n.
Choose several magnitudes of noise jitter.
Apply $10,000$ times per selected transformation:

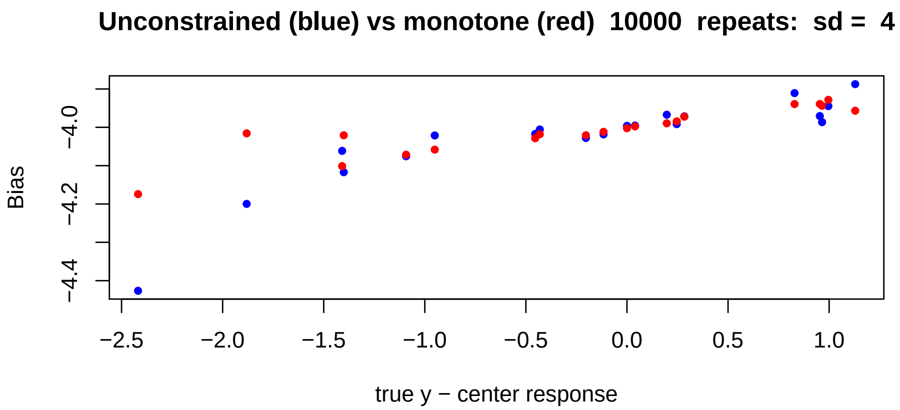
- Sample points in $[0,1]^n$ uniformly.
- Apply selected transformation.
- Jitter with Gaussian noise, selected variance.
- Train on resulting data set, with and w/o constraint.
  - Constraint parameter always 1.0, for simplicity.
- Separate prediction at 20 predetermined points.

Biases should be low in either case, unless constraints detrimental.
Variances are the quantities of interest.

Variance vs. distance from response center.
Transformation: $y = 0.1 + 2.5x_1 + 2.5x_2$

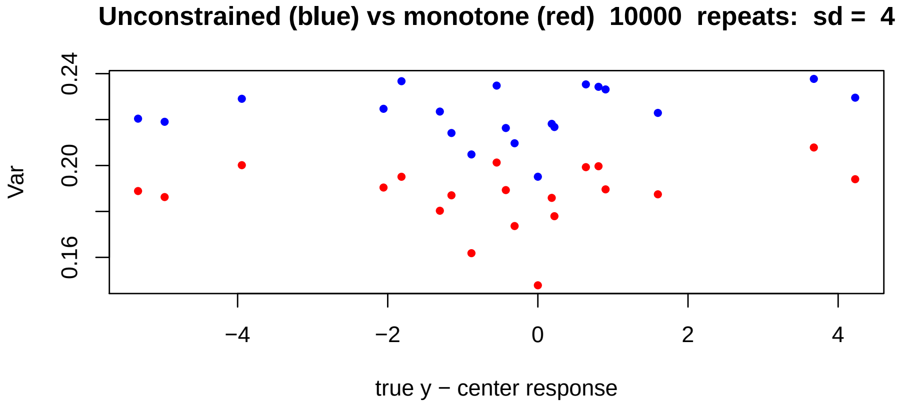


Bias vs. distance from response center.
Transformation: $y = 0.1 + 2.5x_1 + 2.5x_2$



Variance vs. distance from response center.

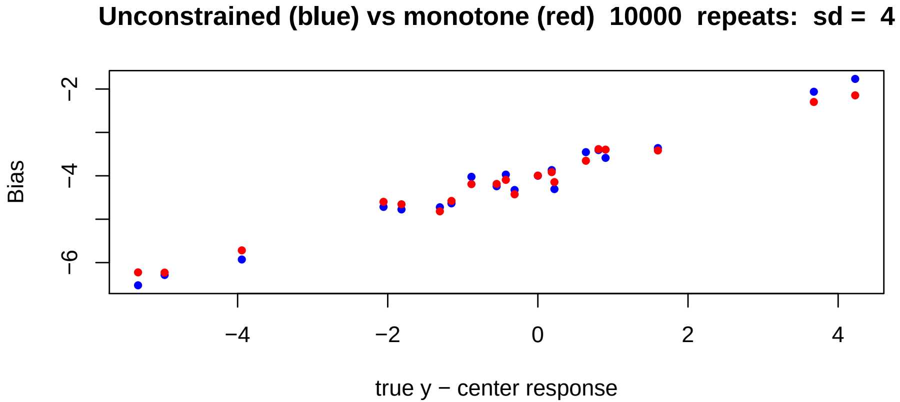
Transformation: $y =$
$0.1+0.3x_1+0.8x_2+1.2x_3+1.6x_4+2.2x_5+2.7x_6+3.1x_7+3.5x_8+3.8x_9+4.2x_{10}$



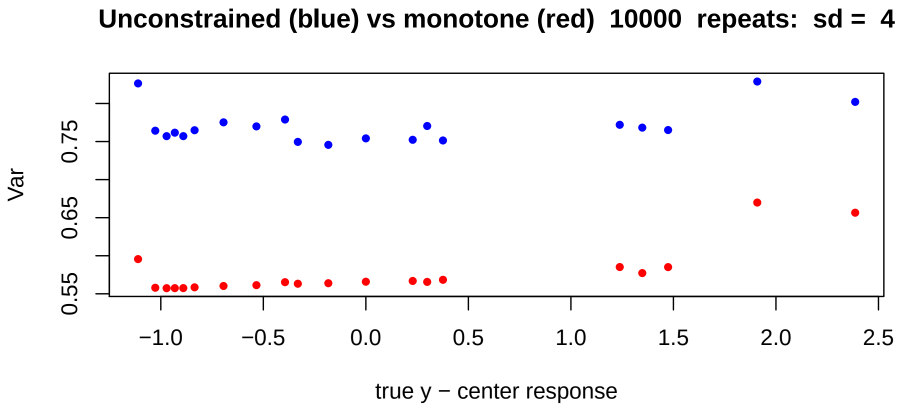
Bias vs. distance from response center.

Transformation: $y =$

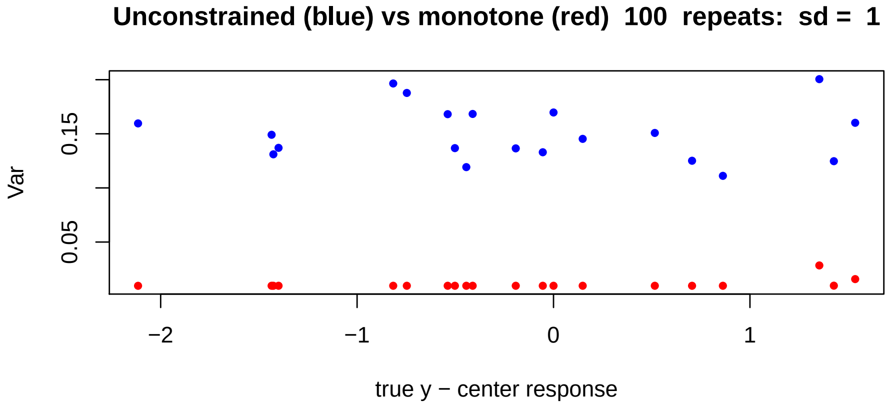
$0.1+0.3x_1+0.8x_2+1.2x_3+1.6x_4+2.2x_5+2.7x_6+3.1x_7+3.5x_8+3.8x_9+4.2x_{10}$



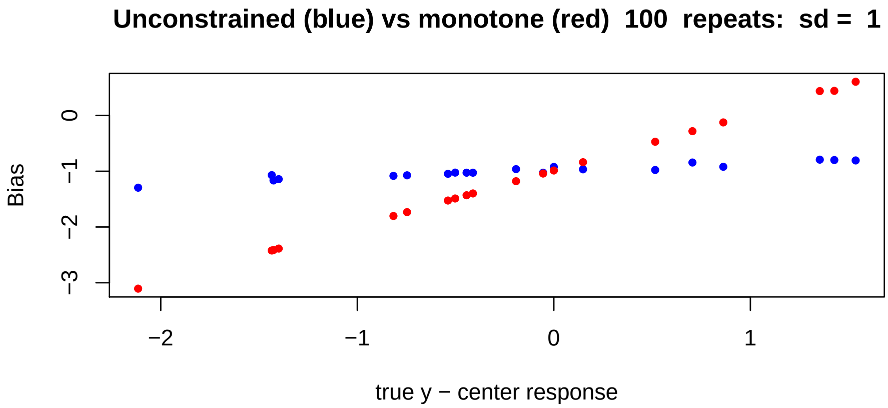
Variance vs. distance from response center.
Transformation: $y = 0.1 + 2.5x_1^2 + 2.5x_2^2$



Variance vs. distance from response center.
Transformation: $y = 0.1 - 2.5x_1 - 2.5x_2$



Bias vs. distance from response center.
Transformation: $y = 0.1 - 2.5x_1 - 2.5x_2$



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Boston housing data

Well-known benchmark appearing in ML repositories: Lichman [2013].

Data gleaned from census reports from greater Boston area.

13 demographic and spatial covariates..

Median housing prices of 506 census tracts.

Originally studied by Harrison and Rubinfeld [1978].

Covariate descriptions

Covariate	Description
crim	local per-capita crime rate
zn	proportion of residential land zoned over 25,000 sq.ft
indus	proportion of town area with non-retail business
chas	adjacency to Charles river: binary encoding
nox	concentration of NO in parts-per-10-million
rm	average number of rooms
age	proportion owner-occupied units built pre-1940
dis	weighted mean distances to nearby employment centers
rad	index of accessibility to radial highways
tax	full-value property-tax rate per $10,000
pratio	pupil-teacher ratio by town
black	weighting of local proportion of African-Americans
lstat	% population deemed "lower status"

Correlation with price

Covariate	Correlation
lstat	-0.7376627
ptratio	-0.5077867
indus	-0.4837252
tax	-0.4685359
nox	-0.4273208
crim	-0.3883046
rad	-0.3816262
age	-0.3769546
chas	0.1752602
dis	0.2499287
black	0.3334608
zn	0.3604453
rm	0.6953599

Constraints

Highest correlate: concentration of “low status” residents.

- Look for decreasing trend.

Room count also has high correlation.

- Look for increasing trend.

Crime, far from highest, might also contribute monotonically.

- Look for decreasing trend.

Hold-out experiments

- Repeat on all combinations of the three covariates:
- Apply 500 times, with and without constraint.

  Train with random 20% of samples held out.

  Predict held-out samples using trained forest.
- Compare MSE of predictions.

  One-sided Wilcoxon paired test.

  H_0 : unconstrained MSE $\geq$ constrained.

Boston: results

Constraint	p-value
- crim	0.2392
+ rm	8.389e-14
- lstat	0.3015
- crim + rm	0.3.517e-09
+ rm - lstat	1.489e-10
- crim - lstat	0.9554
- crim + rm - lstat	1.559e-10

- Only # rooms clearly benefits alone from monotone constraint.
  - Yet low-status covariate is more highly correlated.
  - Low status, in particular, may be effect rather than cause.
- Other two do benefit, but only in combination with # rooms.

Stochastic control

- Also examined effect of probability threshold.
- Same scheme as above.
- Following table considers room count alone:

Rooms constraint: probability	p-value
0.2	0.1485
0.4	0.001191
0.6	4.743e-09
0.8	6.732e-11
1.0	8.389e-14

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Conclusions

- Monotonic constraints are straightforward to implement in RF.
- Can reduce variance when *a priori* evidence suggests their use.
- Can improve predictive quality in some cases.
- Correlation is not necessarily a guide to employing them.

Constraint-based regression

- Monotonic regression should extend to other tree-based approaches.
  - CART
  - PRIM
  - Gradient boosting.
- Note: **GBM** package offers a monotone option. (Scooped?)
- May extend to shape-based regression.
  - Rejection scheme, while simple, is a blunt instrument.
  - May benefit from utilizing *distribution* of sampled values.
  - Inference on convexity, for example.
  - Computationally more expensive, but software changes strictly local.

Rborist: nearer term

- Greedy restaging replaced by "patient" scheme.
  - Improves performance at medium/low predictor occupancy.
- Sparse data representations.
  - Infrastructural changes mostly complete.
- Specialized GPU version.
  - On-coprocessor restaging.
    - Experimental package completed.
    - High break-even point: $> 50,000$ rows.
    - Communication costs dominate.
  - On-coprocessor restaging + splitting.
    - Little/no communication cost.
    - Regression under development.
    - Factors a little tricky, especially at high cardinality.
    - Binary classification to follow, or accompany.
    - Full classification further out.

Rborist, longer term

- Cluster implementations.
  - Infrastucture in place to train tree blocks independently.
  - Head node / work node model.
  - MPI or Spark/Hadoop hooks still needed.
- Out-of-memory support.
  - General attack mapped out.
  - Combination of tiling and streaming approaches.
- Near-memory computing (much longer term).
  - Exciting features anticipated from 3D memory cubes.
  - In-memory transformations, such as sorting.
  - Could greatly diminish some key performance bottlenecks.

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