SMARTboost learning for tabular data

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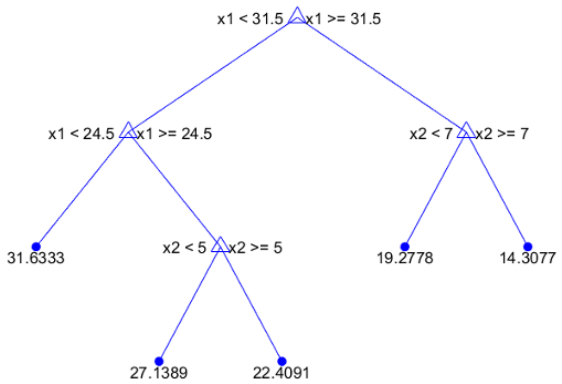
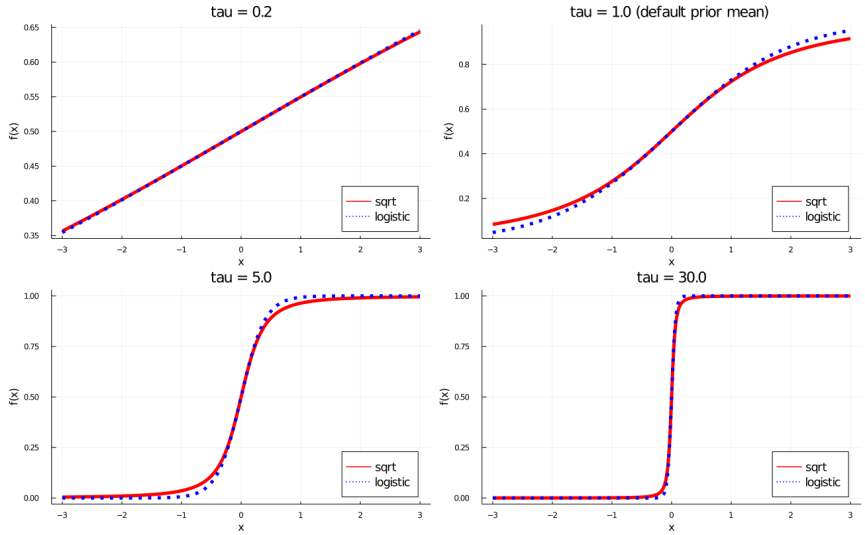
What is SMARTboost?

- Boosting not of standard regression trees, but of 'trees' with smooth threshold.
- Expected to be more accurate with continuous or mixed discrete-continuous features.
- Modeling choices and heuristics to reduce the high computing costs.
- Thoughtful default priors greatly reduce the need for CV.
- Priors also improve performance with small n and/or small SNR.
- Open source Julia code. R wrapper coming soon.

https://github.com/PaoloGiordani/SMARTboost.jl

Standard and Smooth Trees





Why SMARTboost?

Originally designed to be more effective than GBM for finance data, which are often:

1. Low SNR and panel data $\Rightarrow$ Low *effective* sample size.
2. Highly persistent and/or non-stationary features $\Rightarrow$ more frequent need to extrapolate.

A second paper will test on a broader range of ML datasets.

Why low effective sample size

- Panel data with substantial cross-correlation, e.g. equal weighted portfolio of SP500 stocks $\approx$ 5 uncorrelated stocks.
- Low SNR. e.g. $R^2 = 0.02\,(0.01)$ requires roughly 50 (100) times larger n than $R^2 = 0.5$ to have the same $var(f(x))$.
- $n = 500 \times 20 \times 12 = 120k$ could be $\approx n = 12$ at $R^2 = 0.5$.

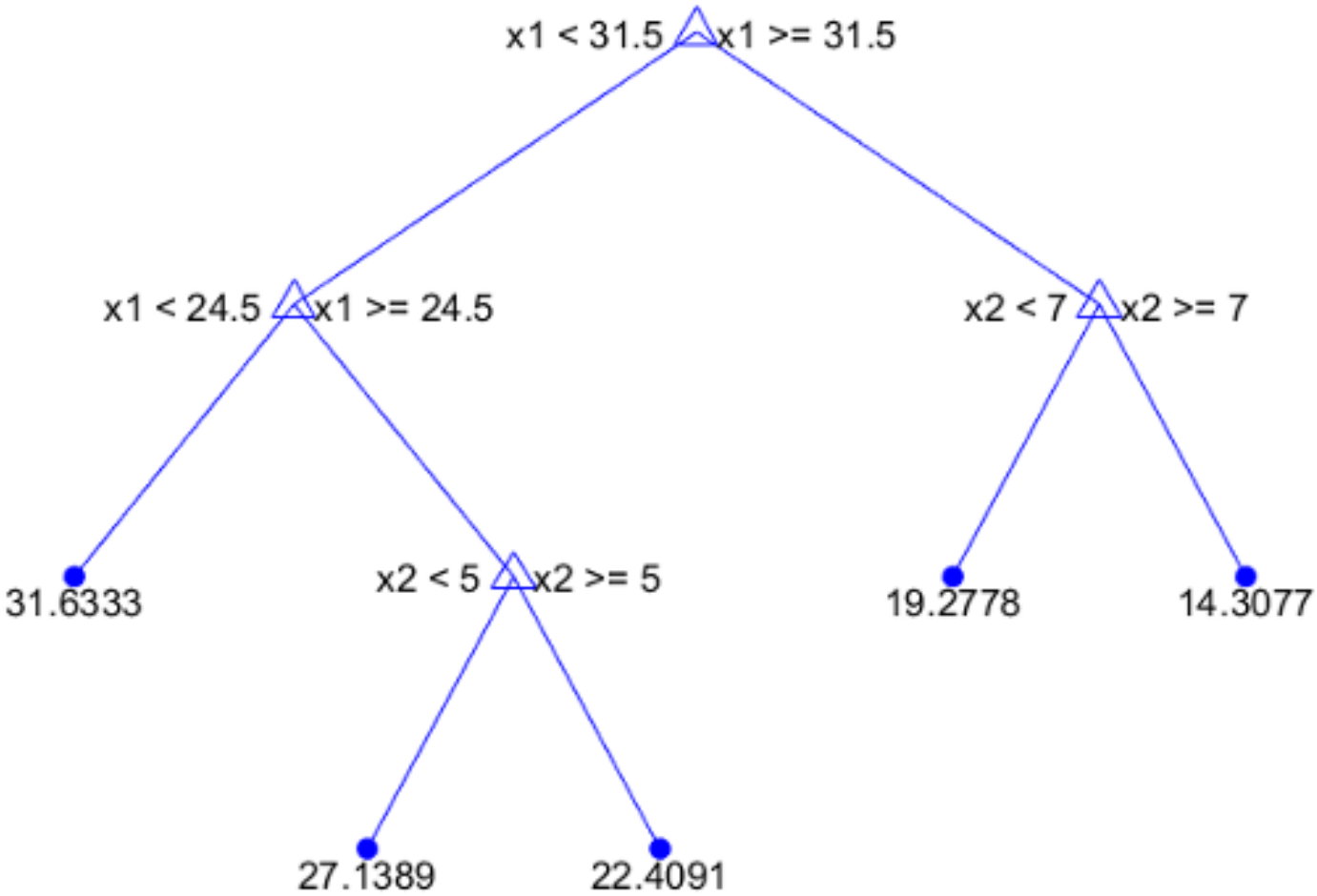
I want something that can do well at low SNR but also be able to recover very complex functions if n and/or SNR allow it.

Boosting Trees

"Boosting lives at the cutting edge of modern prediction methodology. They fit models of breathtaking complexity ... and are routinely used as prediction engines in a wide variety of industrial and scientific applications." Efron and Hastie (2016)

- Current default method for tabular data, particularly heterogeneous data. Unified methodology for regression and classification.
- Several open-source, multi-platform, industry-quality implementations: XGBoost (Chen and Guestrin 2016), LightGBM (Microsoft), CatBoost (Yandex).
- Fairly similar performance. I focus on the best-known, XGBoost. Used in many ML platforms: Google's AI Cloud, Amazon's Azure, Uber's Michelangelo.

A Simple Regression Tree (or Decision Tree)



Regression Trees

With a single tree:

$$E(y_i|x_i) = \sum_{m=1}^{M} \beta_m I(x_i \in R_m),$$

where the dummies $I(x_i \in R_m)$ are non-overlapping and the estimation of β_m is straightforward given $I(x_i \in R_m)$, which in turn depends on all parent split variables and split points. Full optimization impossible: heuristic greedy optimizers.

Boosting Trees for regression problems

- A single tree, however deep, fits and forecasts poorly. Ensembles of trees much more promising. Full optimization impossible. MCMC (BART) challenging.
- Boosting can be seen as a heuristic to fit an ensemble of B trees (or other base):

$$E(y|x) = \Sigma_{b=1}^{B} T_b(x; \theta_b)$$

- Recursively fits the residuals from the previous ensemble.

Boosting trees

1. Initialize $f_0(x_i) = 0$, $r_i = y_i$, *for* $i = 1, ..., n$. Then repeat step 2) B times.
2. Fit a single tree T_b to $r_{1:n}$. Update $\widehat{f}_b(x_i) = \widehat{f}_{b-1}(x_i) + \lambda T_b(x_i)$ and $r_i = y_i - \widehat{f}_b(x_i)$, where $0 < \lambda \leq 1$.

- Now world-class fit and predictions in many problems.

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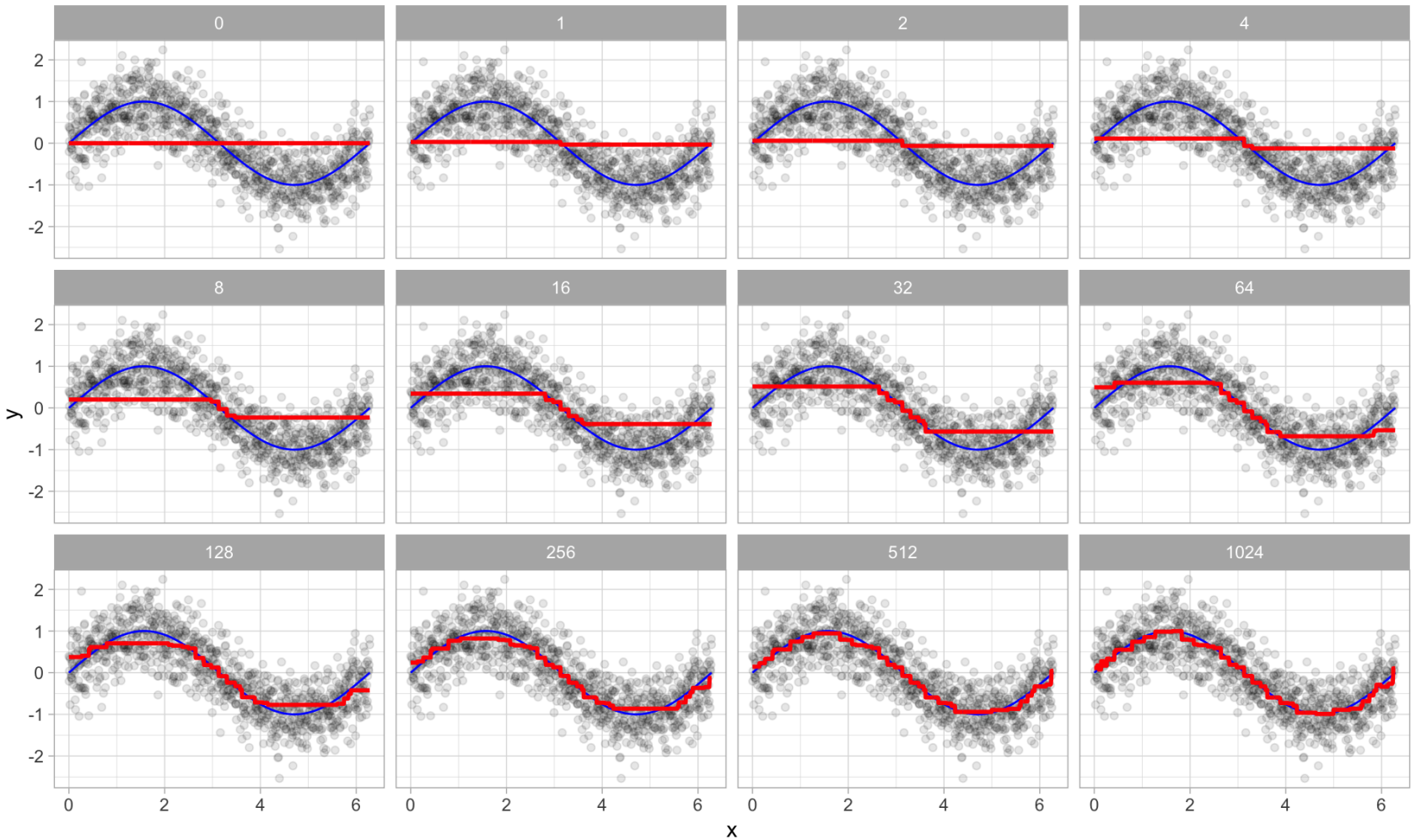
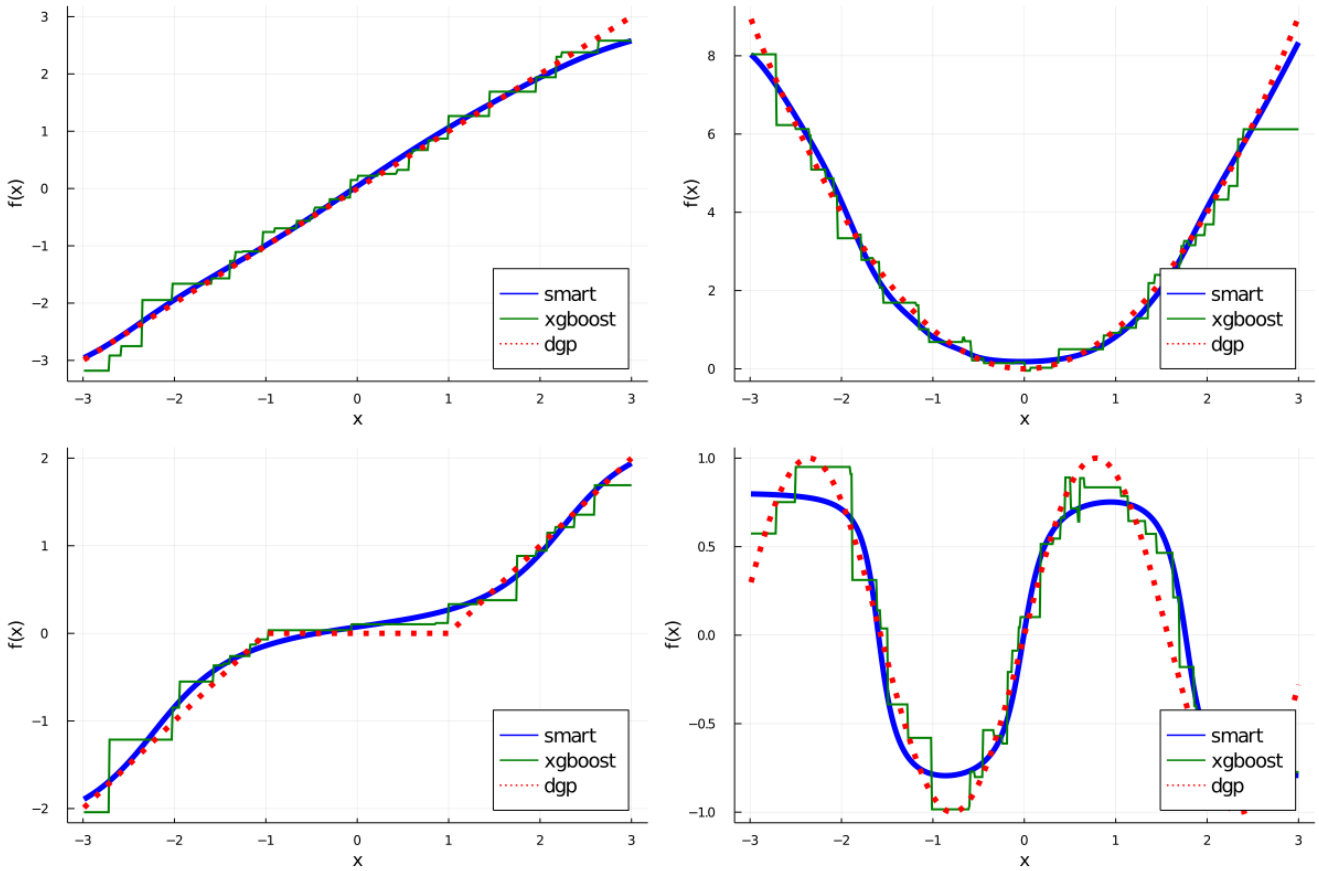
Boosting in action



"Why Does XGBoost Win Every Forecasting Competition?"

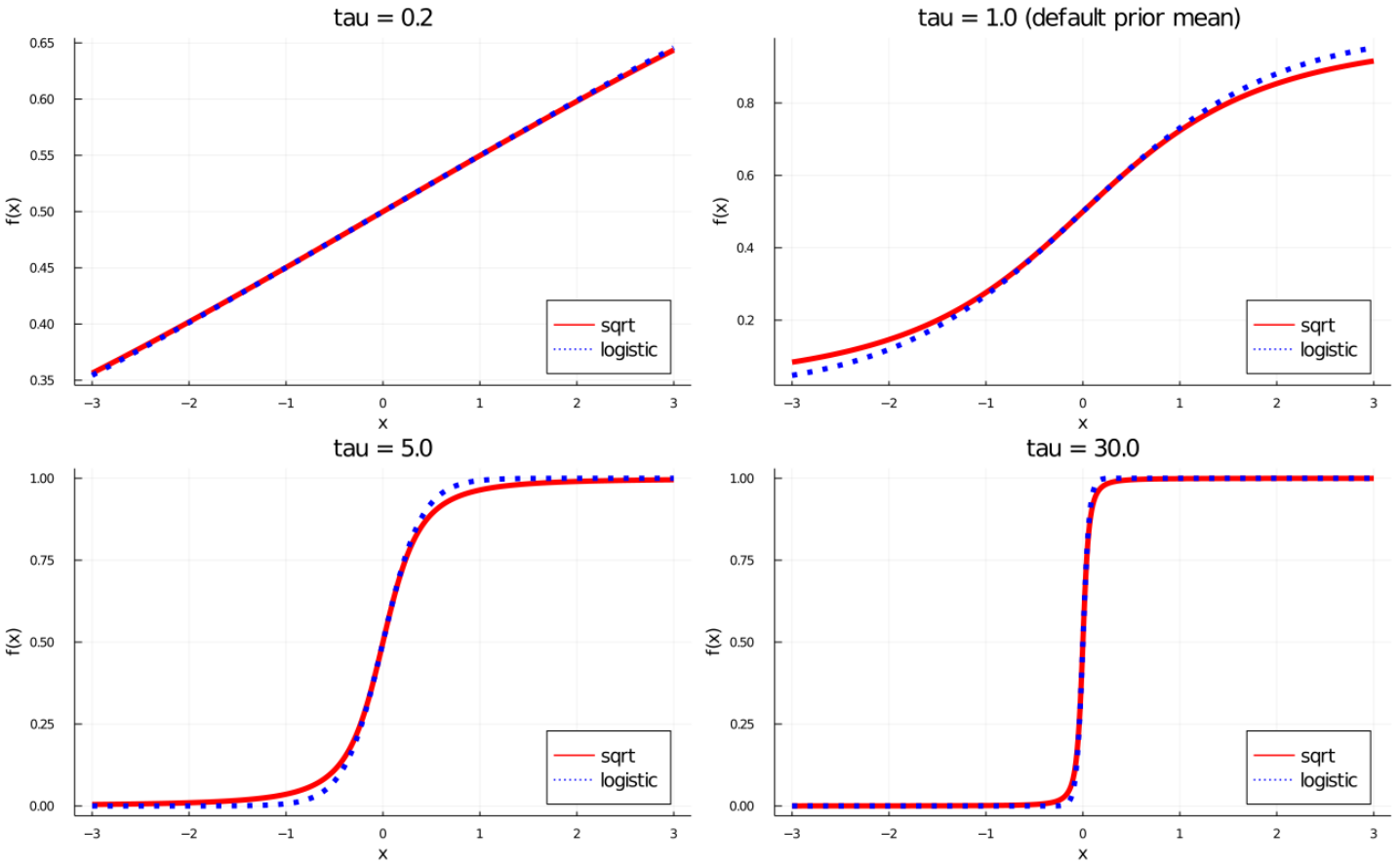
Understandable with binary features. Otherwise surprising that step functions should do so well ...



XGBoost wins forecasting competitions because ...

- Can capture additive nonlinearities and interaction effects in high dimensions (large p), with any combination of continuous and discrete variables.
- Automatic feature selection.
- Robust to leverage points, and messy, noisy, highly non-Gaussian features. Little affected by feature transformation.
- Model complexity is determined automatically by pseudo-out-of-sample fit.

Smooth Trees



Why aren't smooth trees used?

- The idea of a Fuzzy Tree goes back to Chang and Pavlidis (1977) and Jang (1994). Olaru and Wehenkel (2003), De Rosa and Medeiros (2008).
- Linero and Yang (2018) fully Bayesian (MCMC) estimation of an ensemble of probabilistic trees.
- More flexible. Should perform better in many instances. Yet never used.
- Computations are several orders of magnitude slower. Current solutions not practical.

Why are smooth trees so slow?

A single smooth tree can be written as

$$\boldsymbol{y} \sim N(\mathbf{G}\beta, \sigma^2\mathbf{I}), \tag{1}$$

where *at every node*, we need to: a) build the *full* $\boldsymbol{G(\iota, \tau, \mu)}$, which is $(n, 2^{depth})$, b) compute the *full* matrix $\mathbf{G'G}$.
Boosting calls for evaluating a split at every quantile of every feature, and now also to optimize over the smoothness parameter τ.

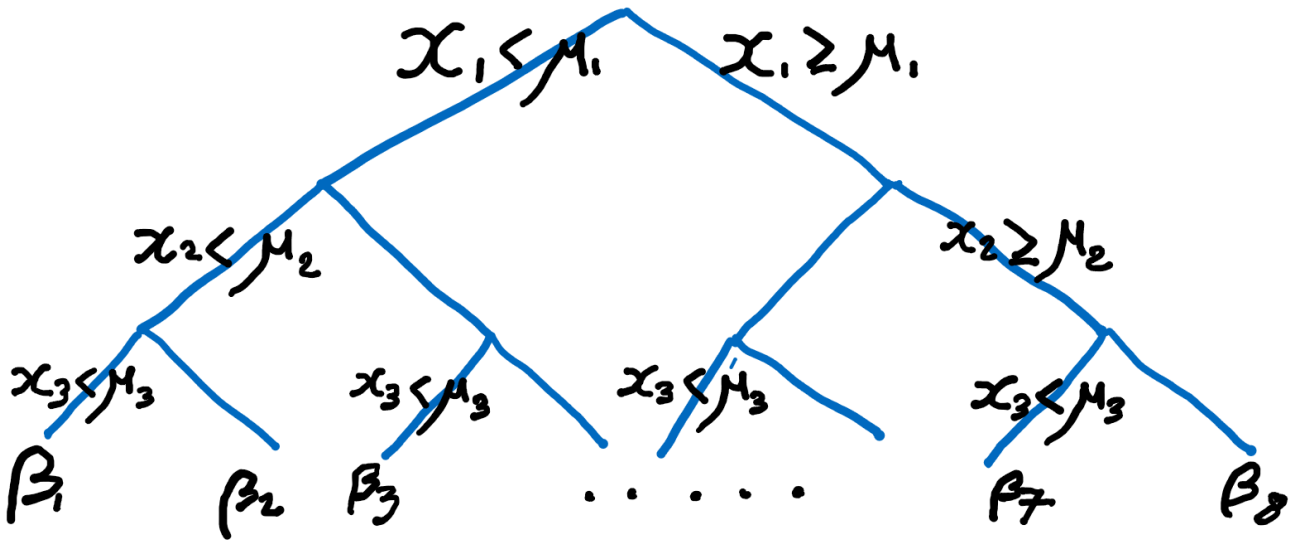
SMARTboost

1. A different base (Symmetric Trees) is roughly 10-20 times faster and often fits better, particularly at low SNR.
2. A set of algorithms and short-cuts to further increase speed with no or minimal loss of fit.
3. A set of Bayesian priors (MAP inference) to reduce the need for cv and hence computing time, and improve performance for low signal-to-noise.

Resulting in great performance even with low SNR and for many DGPs, and feasible for 'large' n (in the millions).

Symmetric trees

A Symmetric Tree (or Oblivious Tree) restricts the splitting variable and point to be the same for all nodes at a given depth. For standard trees, fitting is not any faster. Implemented in CatBoost because forecasting is faster, and at least as good on average. For smooth trees of depth 4 (5), it is 8 (17) times faster.



Symmetry is restrictive for one tree, but not for an ensemble of trees

- Imposing symmetry is restrictive for a single tree, but not for a tree ensemble $E(y|x) = \Sigma_{b=1}^{B} T_b(x; \theta_b)$, where it acts more like a prior/penalization.
- Ensembles of symmetric trees can approximate ensembles of (shallow) standard trees arbitrarily well asymptotically, because:

1. A shallow non-symmetric (standard) tree can be represented as a deeper symmetric tree.
2. A non-symmetric (standard) tree can be represented as a small collection of symmetric trees.

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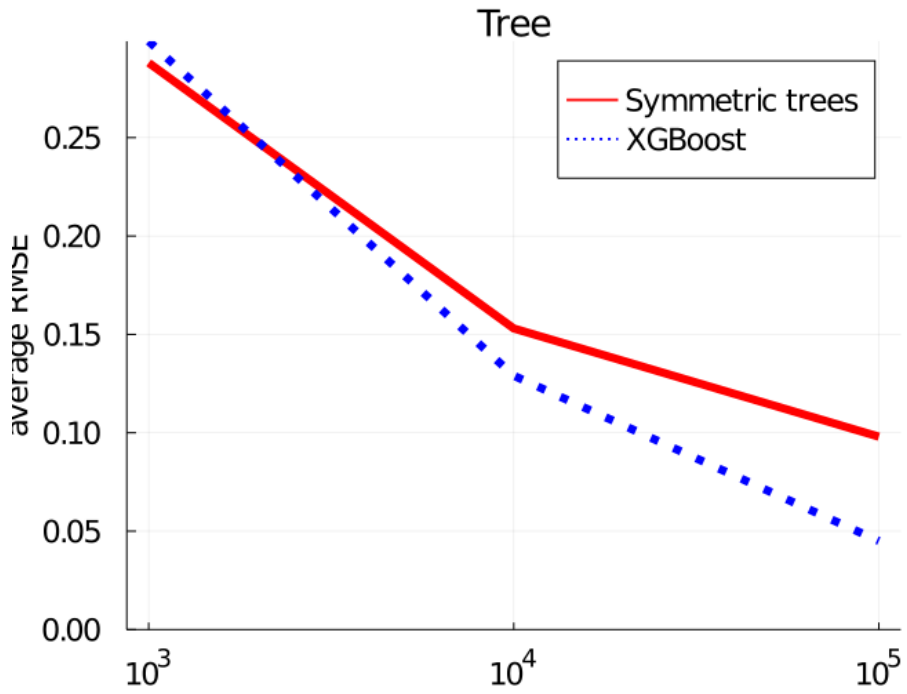
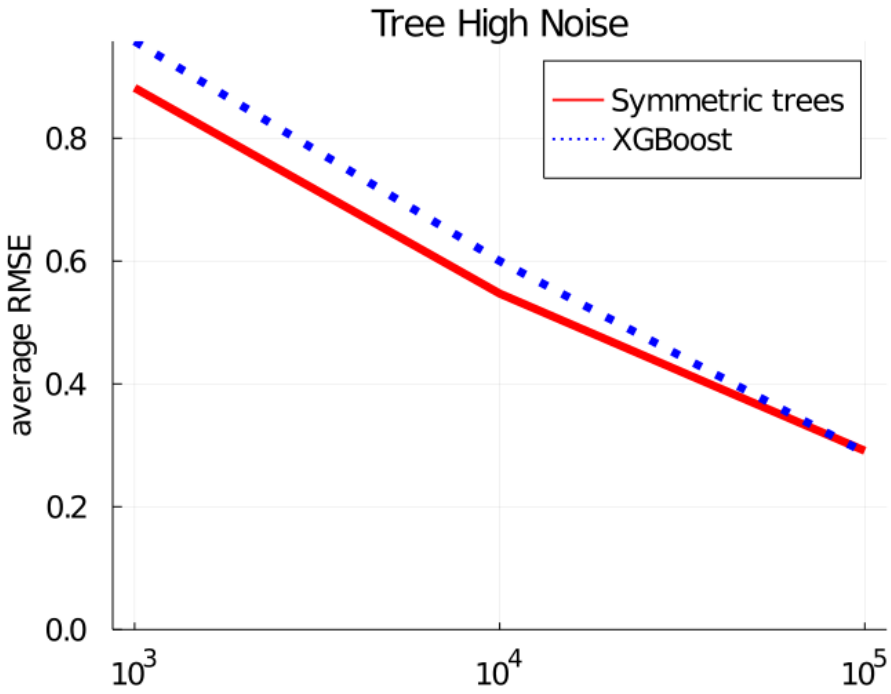
Symmetric trees outperform for low n and/or low SNR

DGP is a tree with no symmetry (all splits on different features, split points and coefficients random).





Speeding up smooth trees

1. Symmetric trees are 8 (17) times faster at depth $= 4$ (5).
2. Two phases: i) faster feature selection, with a very rough optimization, ii) refine optimization only for the selected feature. 3-5 times faster.
3. Refinement: univariate optimization of μ on a grid of τ. Very robust and can be parallelized.
4. Square root sigmoid instead of exponential (10 times faster).

50-100 times faster. Still 10-30 times slower than XGBoost for $10k \leq n \leq 1m$.

SMARTboost prior on β (regularization) requires no cv

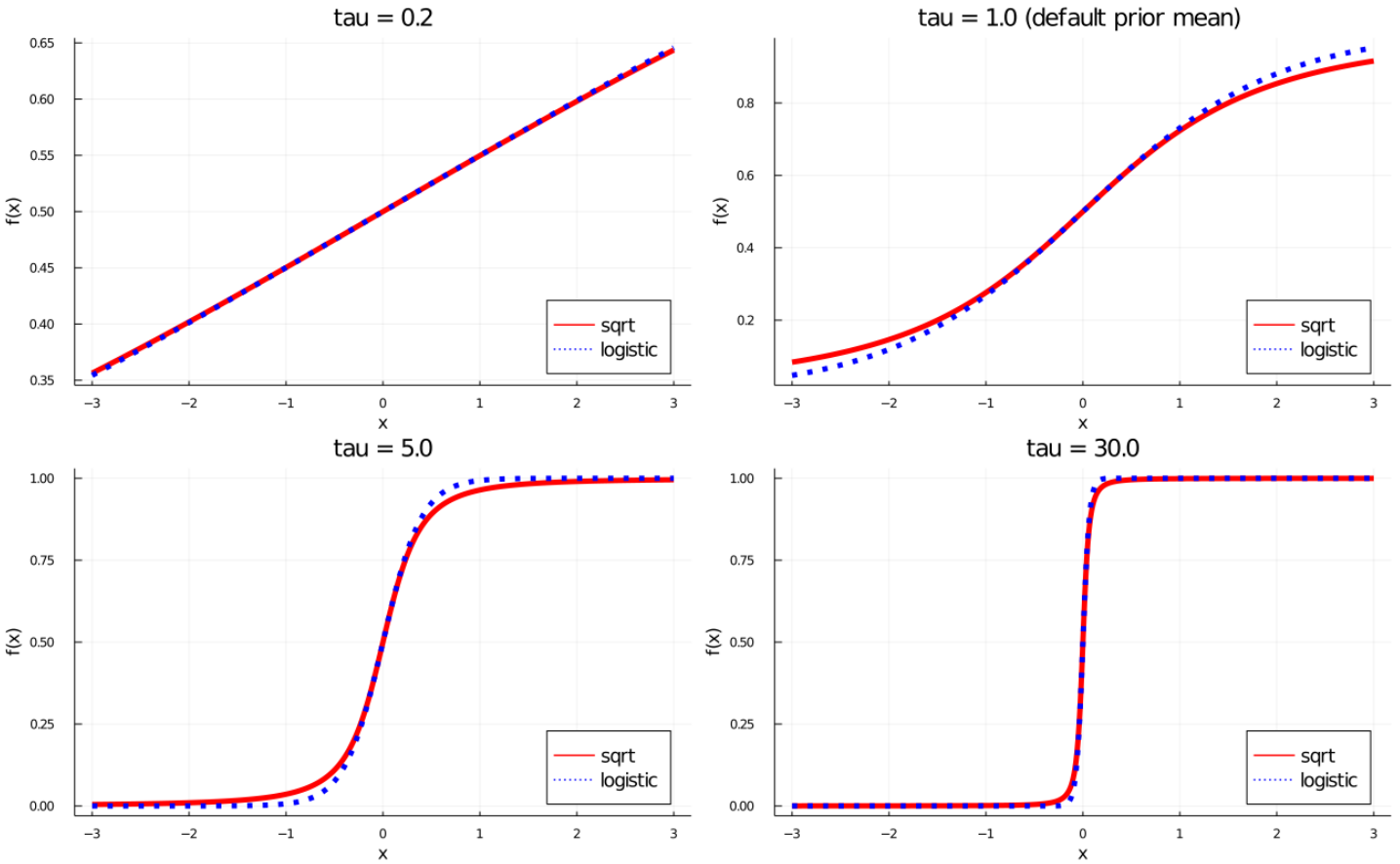
Instead of regularization in the form $\eta\beta'\beta$, prior on β formulated in terms of R^2 of the entire tree (automatically calibrated on the first tree)

$$\beta \sim N(\mathbf{0}, \mathbf{P}_\beta^{-1})$$

$$\mathbf{P}_\beta = \left(\frac{\mathrm{trace}(\mathbf{G'G})/\mathrm{n}}{\mathrm{var}(\mathbf{r}) \times \mathrm{R}_\mathrm{p}^2} \right) \times \mathbf{I},$$

adapts automatically to SNR, depth, and smoothness. 'Coherent' prior: β drawn from the prior imply $\boldsymbol{G}\beta$ that, given $\boldsymbol{r}$ and $\boldsymbol{G}$, result in $E(R^2) = R_p^2$).

Default prior centered on very smooth f(x)



SMARTboost prior encourages smoothness without imposing it

Default prior centered on near-linearity, informative but not dogmatic:

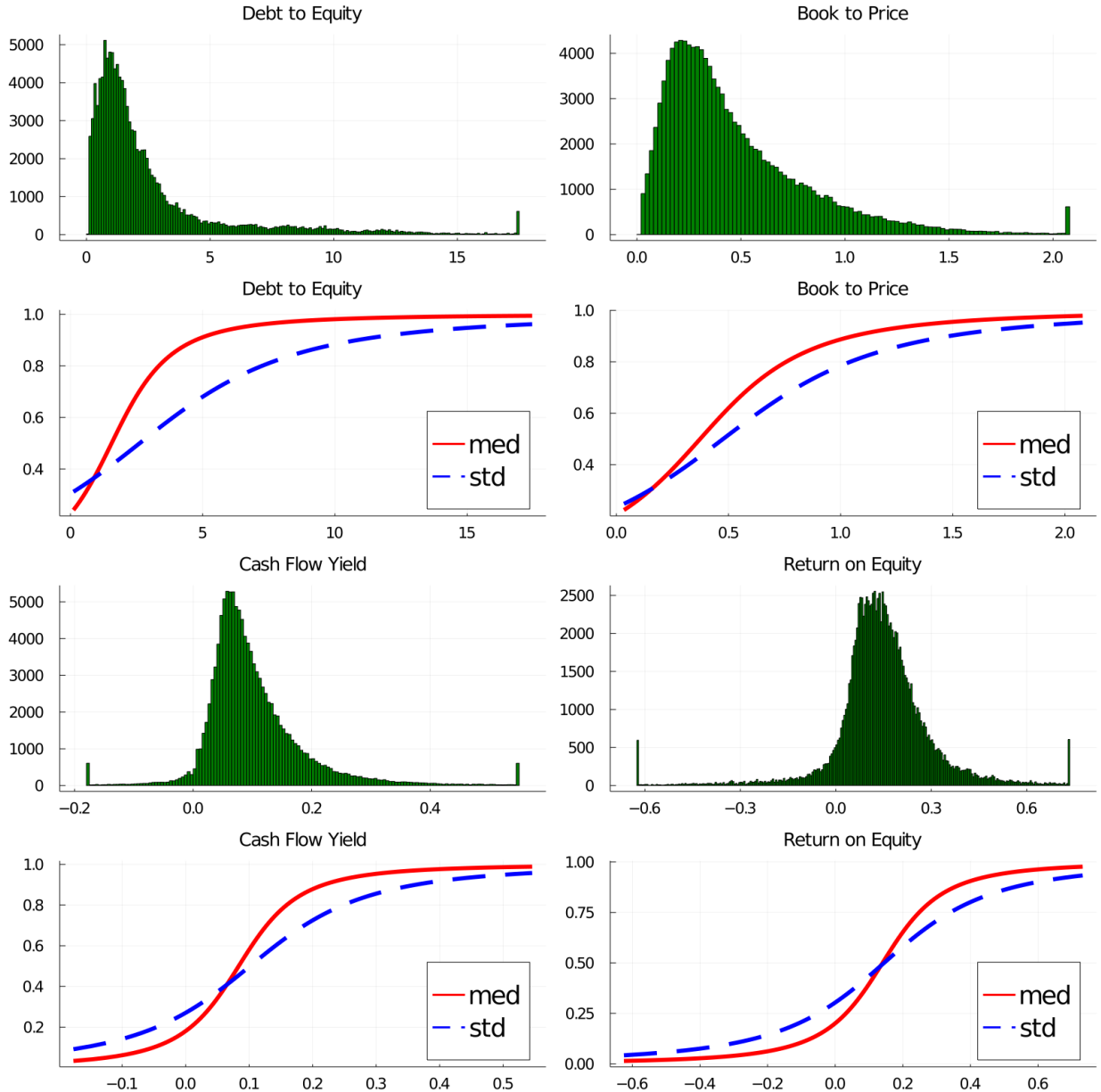
$$\log(\tau) \sim t(0, 1/d, 5), \tag{2}$$

where we scale each continuous feature as

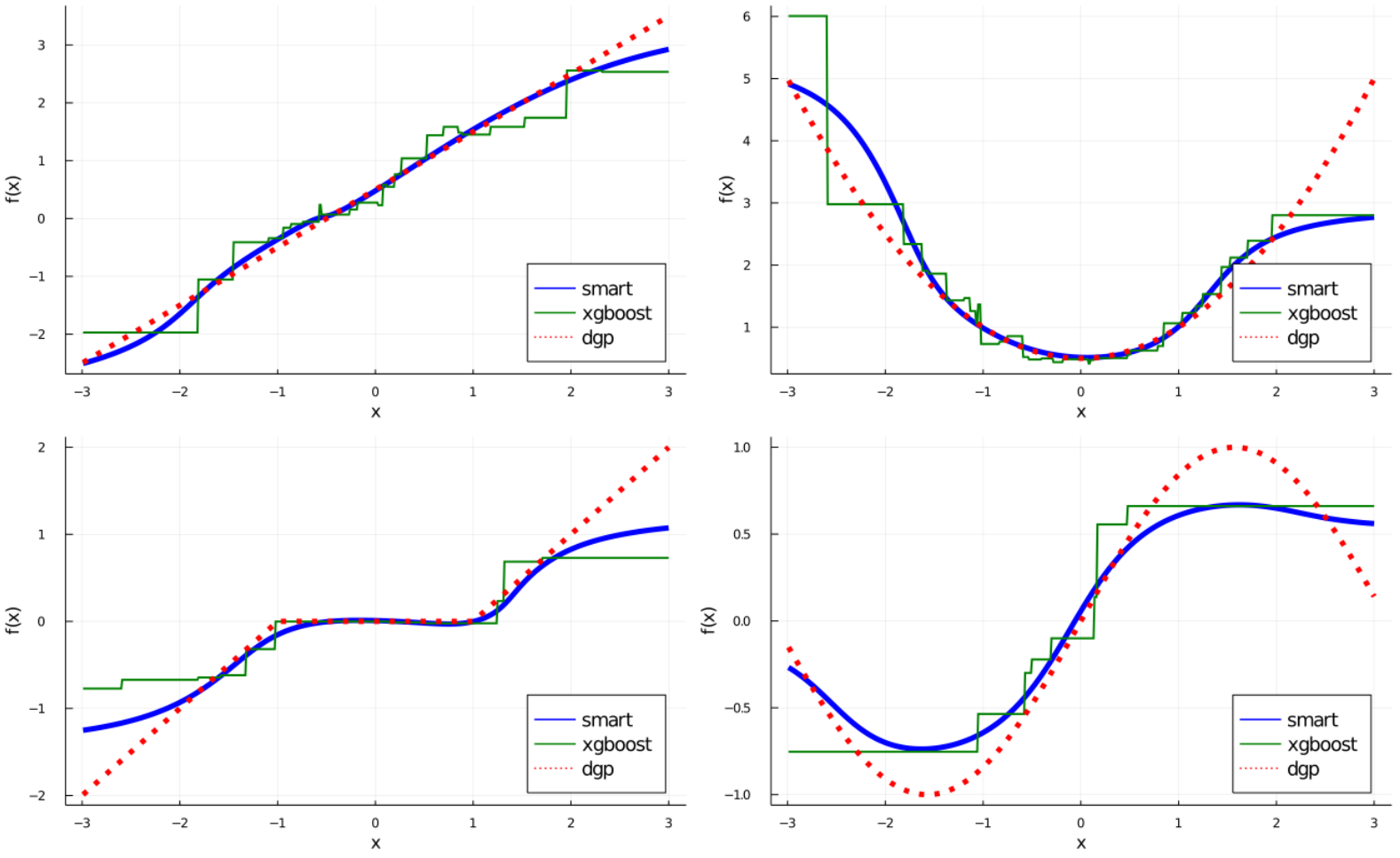
$$x \leftarrow \frac{x - median(x)}{1.42 \times median\left(|x - median(x)|\right)}. \tag{3}$$

to suggest that near linear functions are less likely for highly skewed and leptokurtic features.

Linearity less likely a-priori if features are highly non-Gaussian



SMARTboost univariate examples



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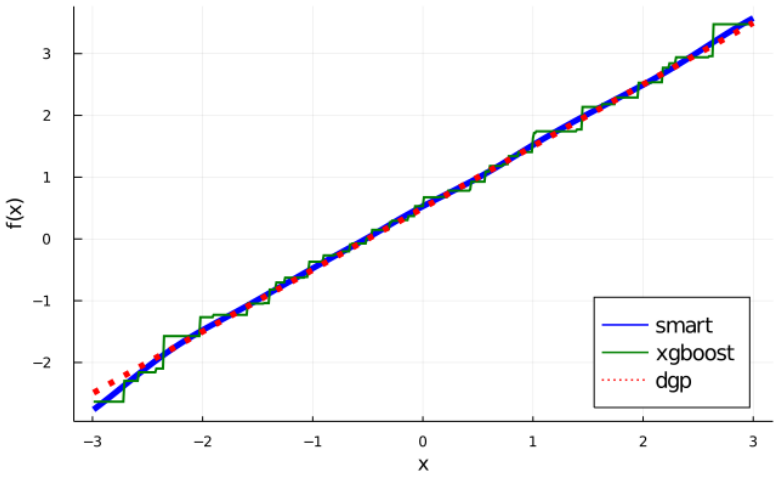
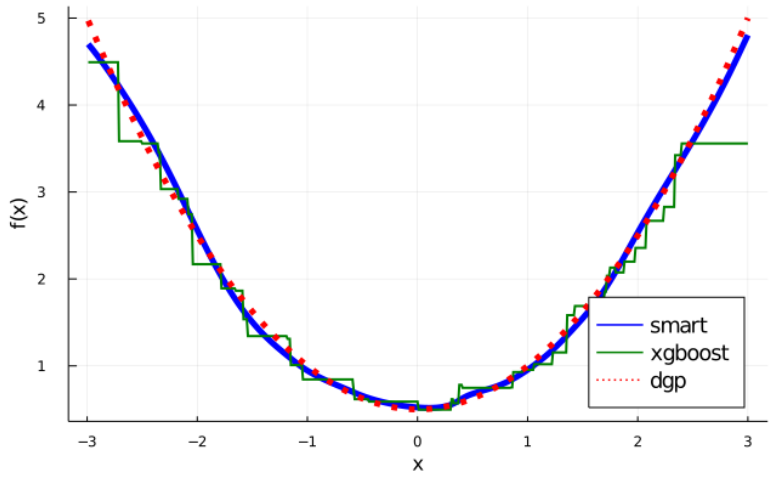
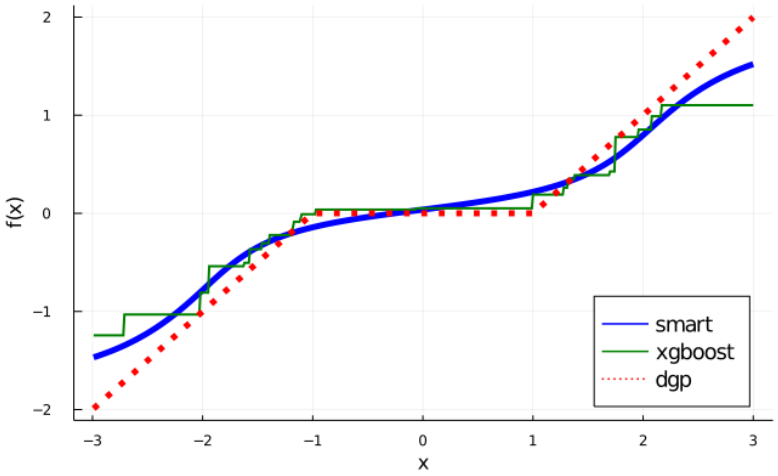
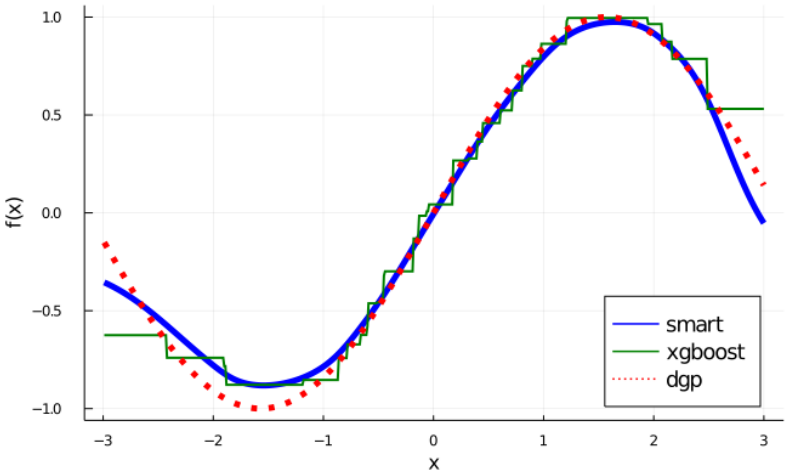
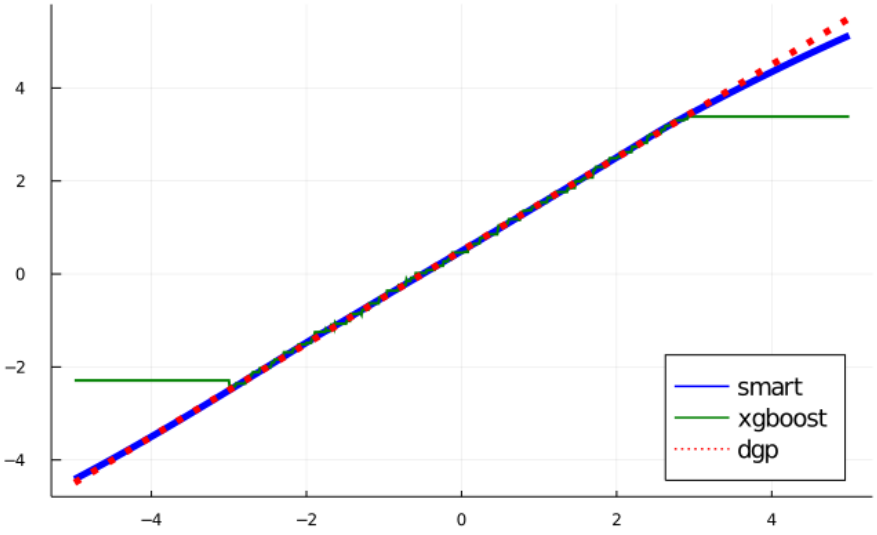


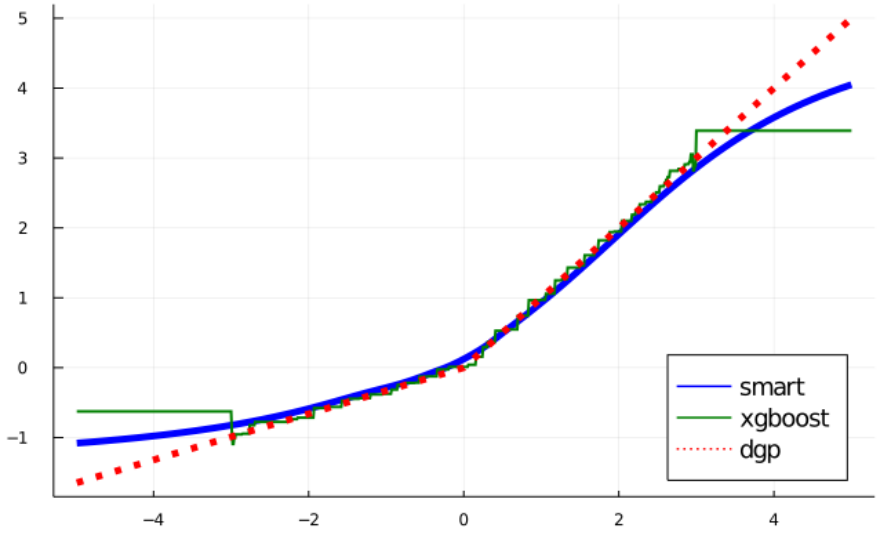


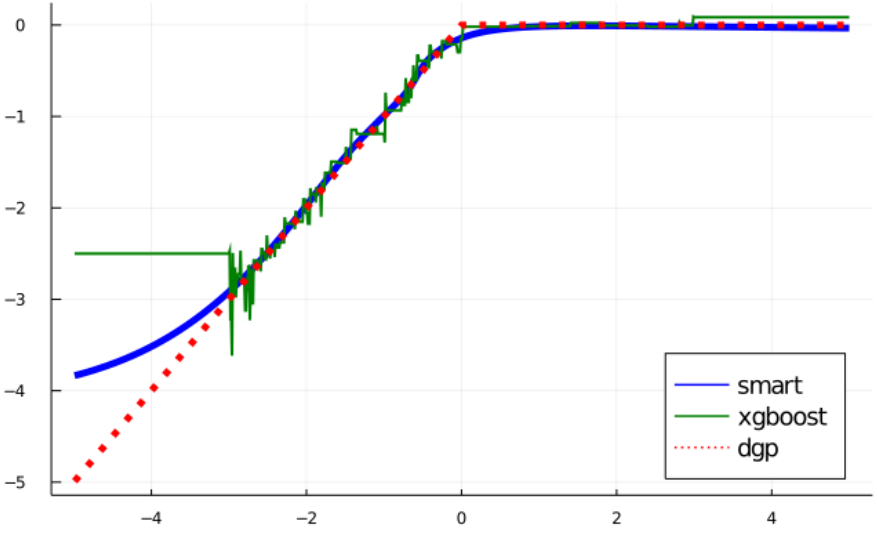


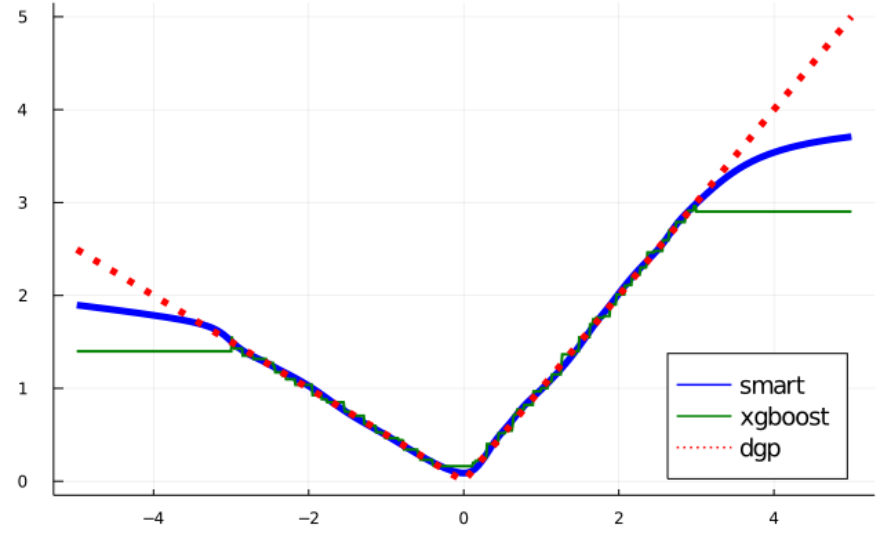


More intuitive extrapolation









Default CV settings assume a time series or panel structure

- The most common, default CV settings in ML are not appropriate for time series and panels.
- The default in SMARTboost is Purged CV (Purged CV of De Prado), adapted to panels.
- Cross-correlation and auto-correlation of panel data taken into account in setting default priors.

SMARTboost outperforms in a large number of settings familiar to econometrics and ML

Linear:

$$f(x) = 2x_1 + 1.5x_2 + x_3 + 0.5x_4,$$

Friedman:

$$f(x) = 10sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5,$$

Threshold Friedman:

$$f_1(x) = 10sin(\pi x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5$$
$$f_2(x) = 2sin(\pi x_2) + 10(x_3 - 0.5)^2 + 20x_4 + 10x_5$$
$$f(x) = f_1(x)I(x_1 < 0) + f_2(x)I(x_1 \geq 0).$$

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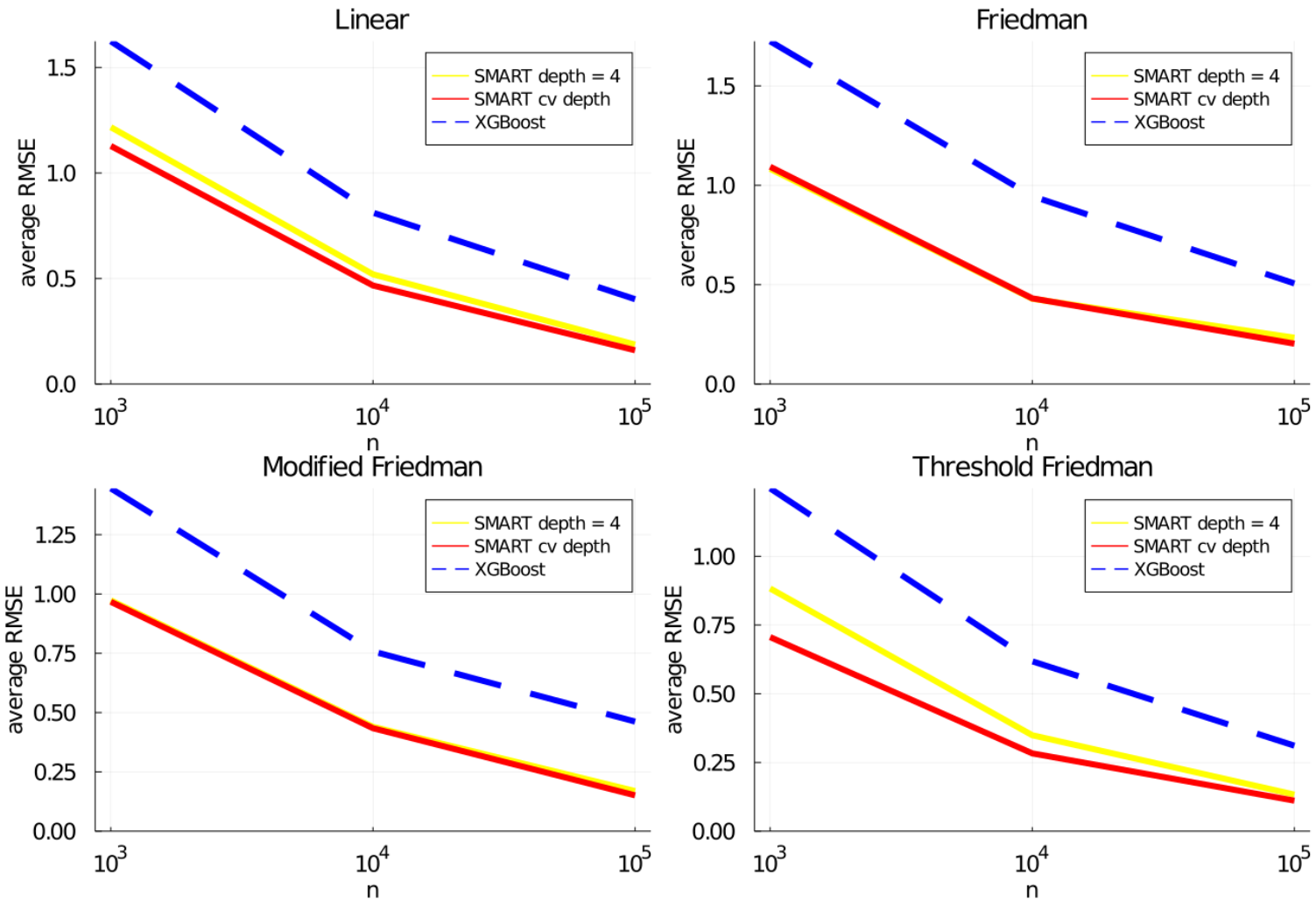

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Linear and non-linear factor models:

$$y \sim N\left(\overline{x}_1 + (\overline{x}_2 + 1)I(\overline{x}_2 < -1) + (\overline{x}_2 - 1)I(\overline{x}_2 > 1) + \overline{x}_3 I(\overline{x}_3 > 0), 1\right),$$

where $\overline{x}_i = mean(\mathbf{x_i})$, $\boldsymbol{x}_i$ is a ten-dimensional vector of multivariate N(0,1), and all cross-correlations 0.5.

Neural network:

$$\begin{aligned} z_1 = x_1 + x_2 + x_3,\ f_1 = z_1 I(z_1 > 0) \\ z_2 = x_4 + x_5 + x_6,\ f_2 = (z_2 - 1)I(z_2 > 1) \\ z_3 = x_7 + x_8 + x_9,\ f_3 = -z_3 I(z_3 > 0) \\ z_4 = 1.5 f_1 + f_2 + 0.5 f_3 \\ y \sim N\left(z_4 I(z_4 > 0), 1.0\right). \end{aligned}$$

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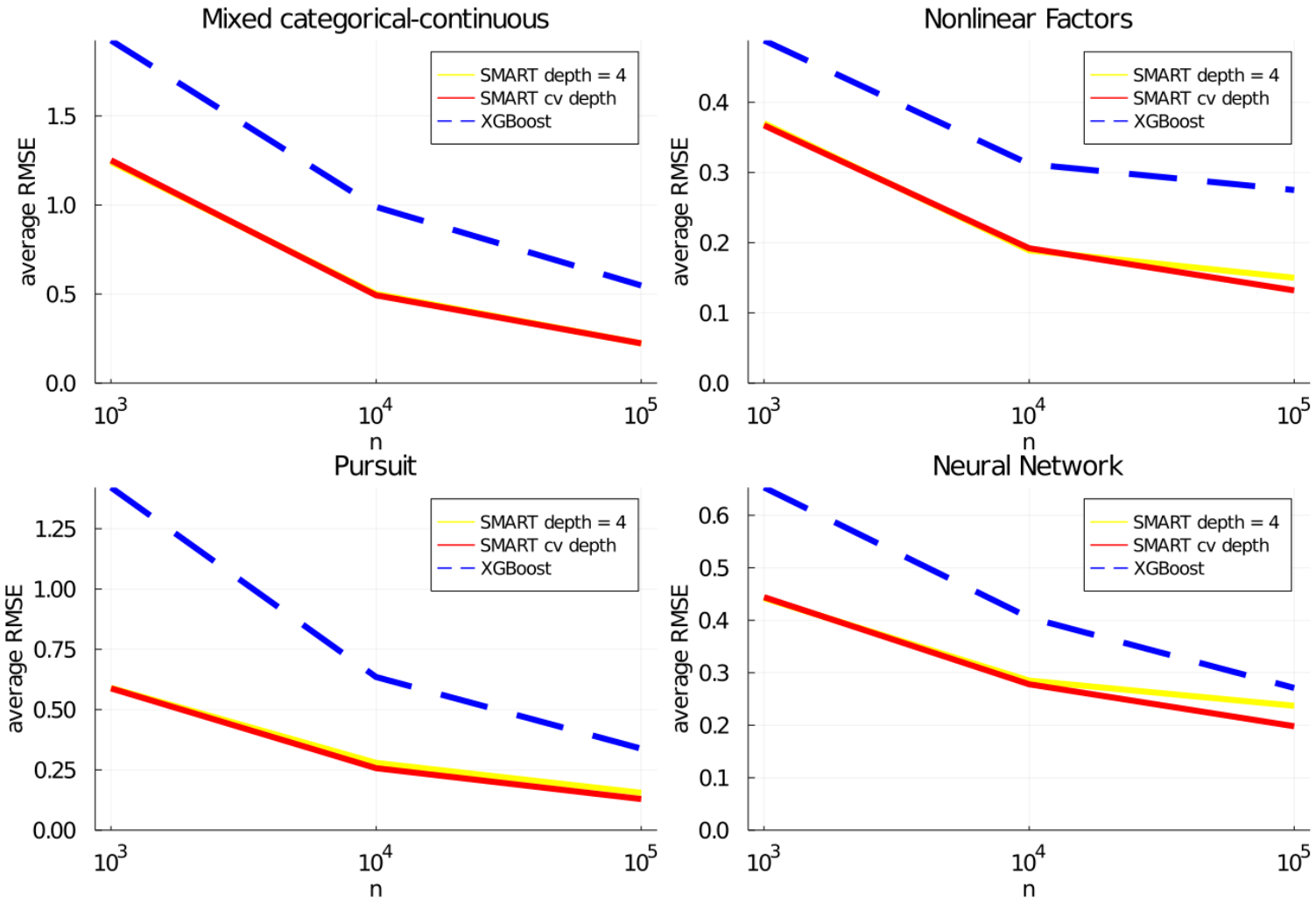


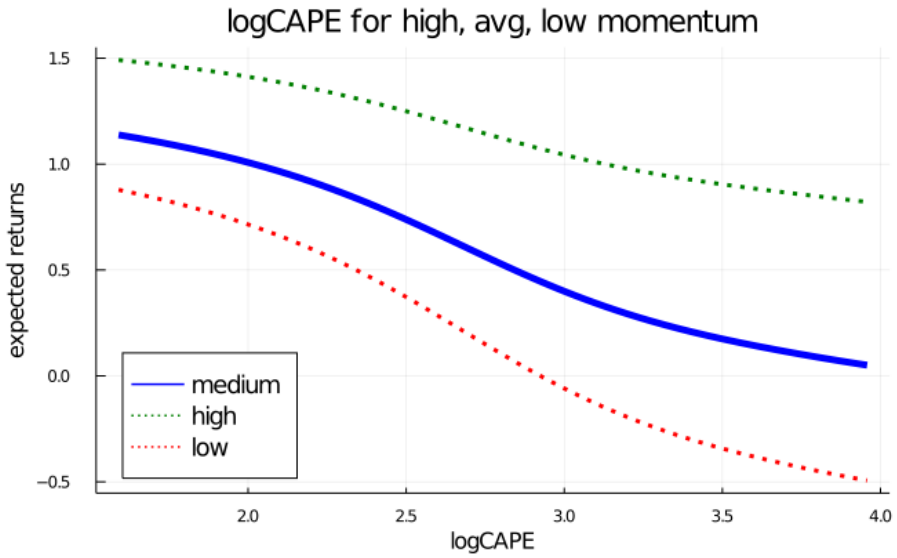
Global Equity Indexes

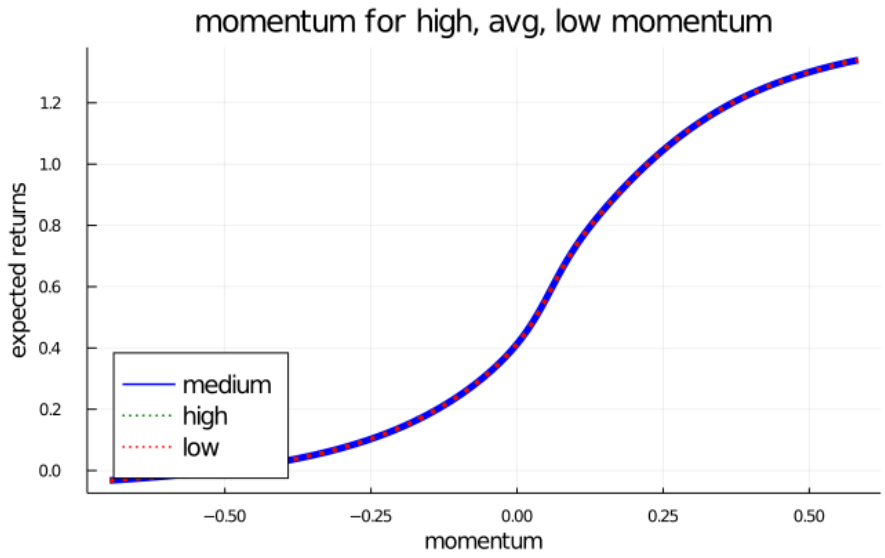
- Monthly total returns of global equity indexes. n = 13k.
- Low n, low SNR, few well-behaved variables: XGBoost does poorly, SMARTboost well, OLS can do well but is sensitive to data-transformation (showing OLS best results here).
- It's all in the interaction: SMARTboost performance drops if depth = 1 is forced.

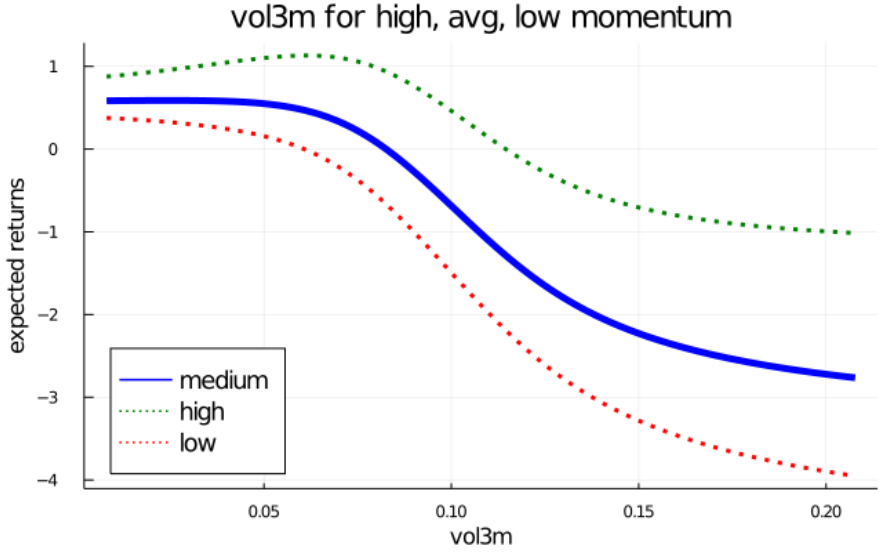
oos R^2 in %	log returns	returns
SMART depth = 4	2.16	1.86
SMART depth CV	2.15	1.57
XGBoost	0.84	0.21
OLS	1.16	0.48

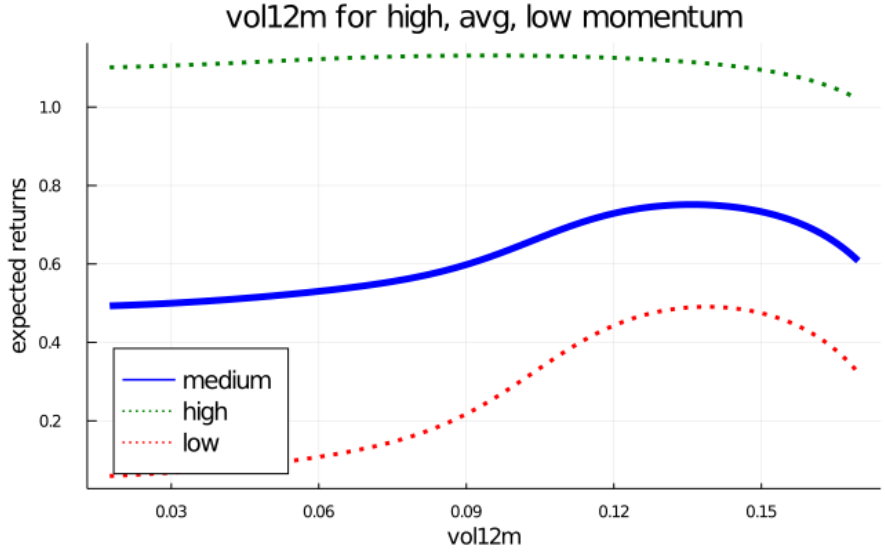
Table: Cross-validated out-of-sample R^2 in % on global equity indexes

Exploring interactions and the fragility of high valuations

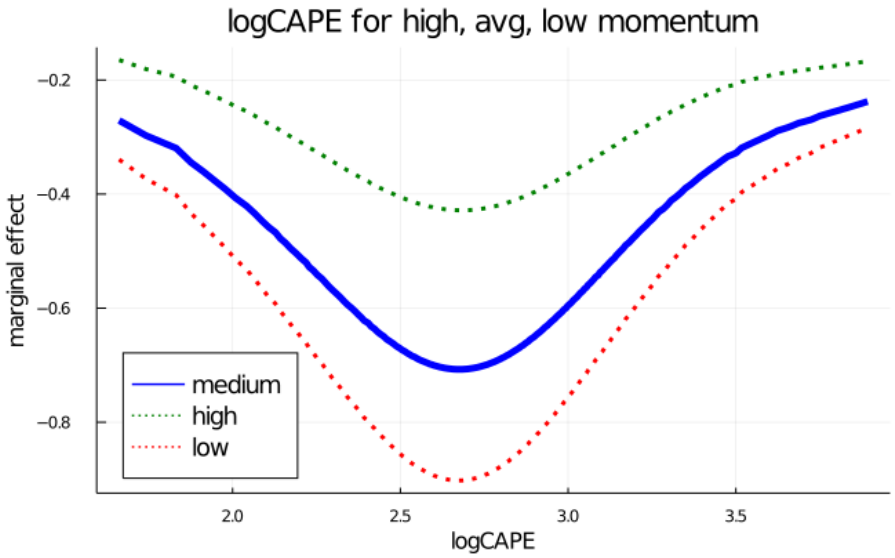


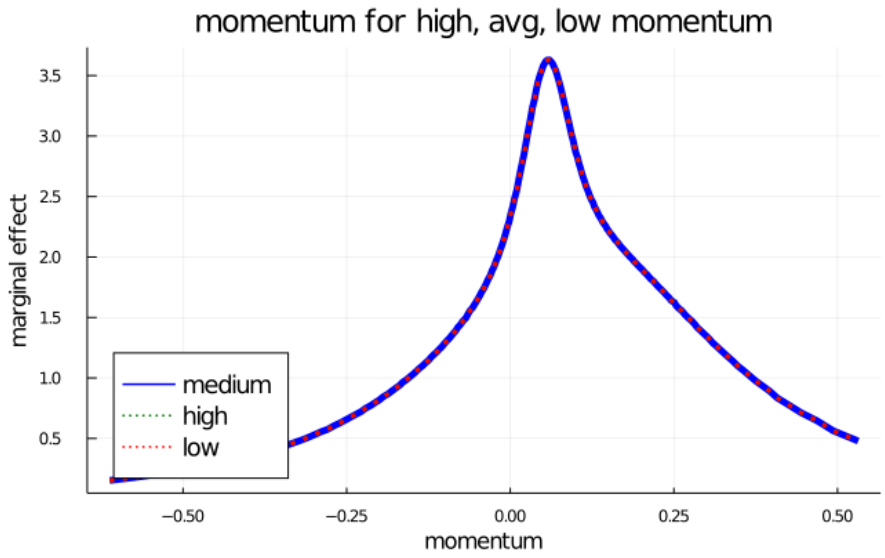


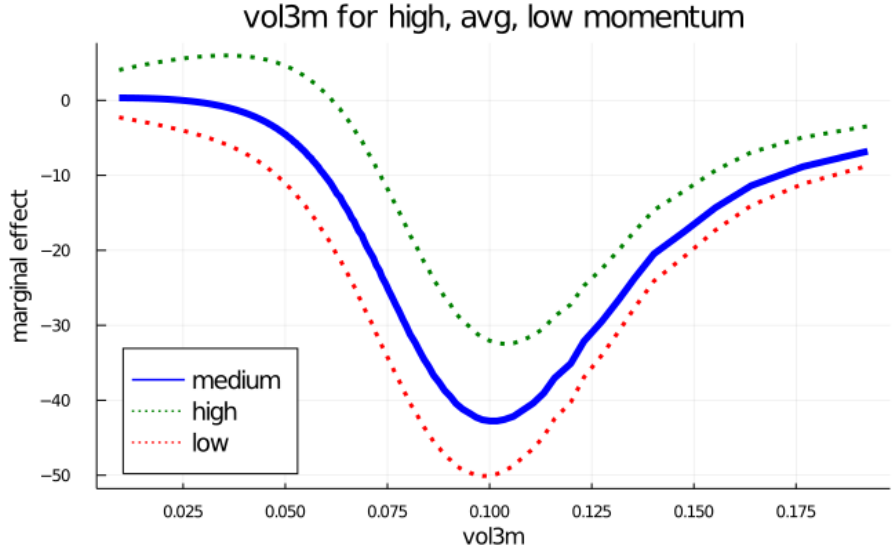


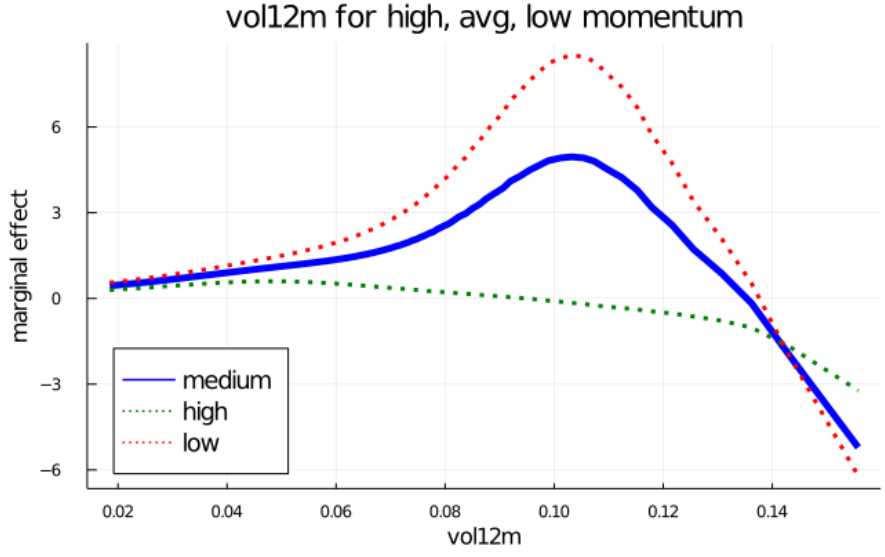


Marginal effects

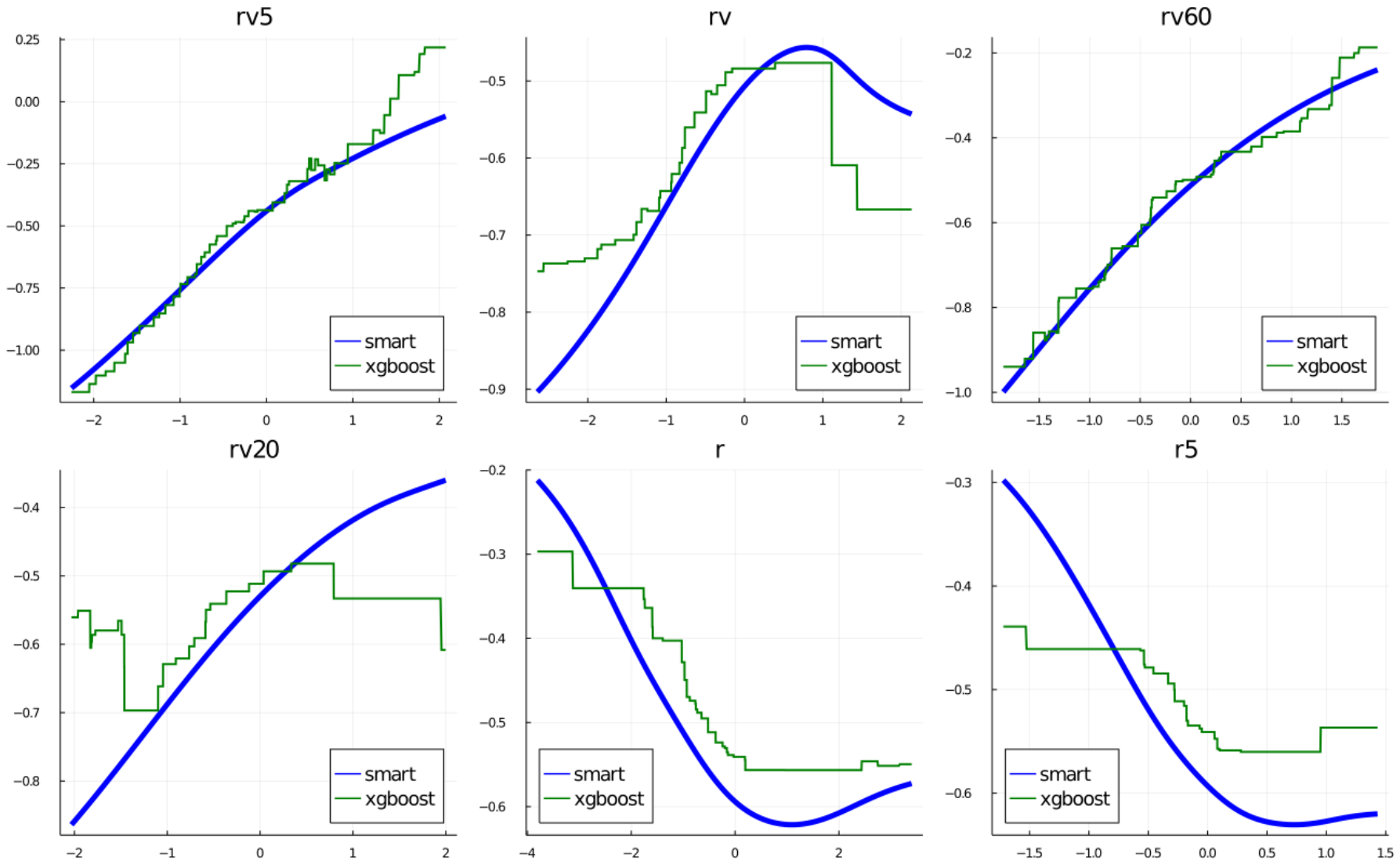








Realized Volatility in Equity Indexes

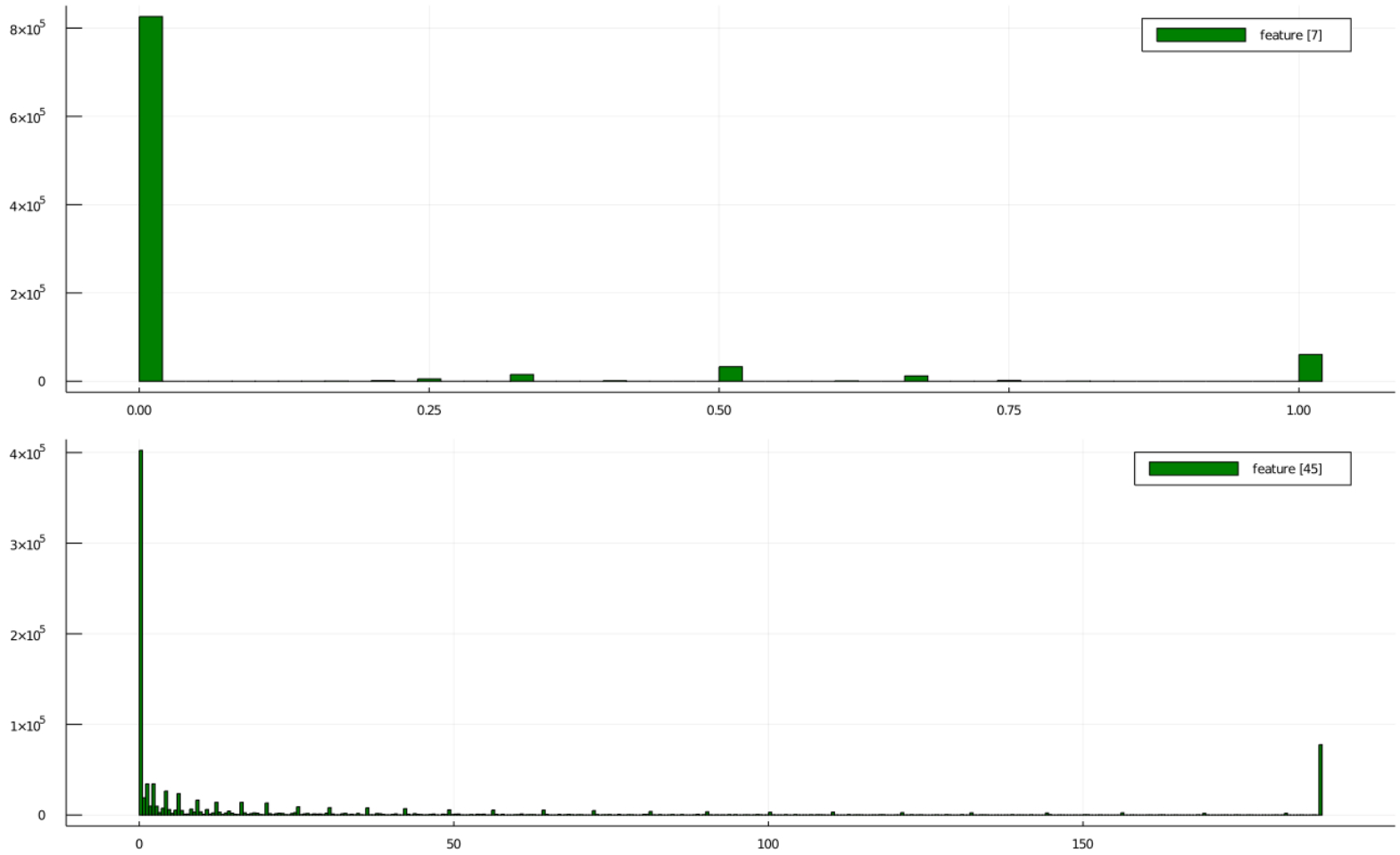


Some limitations of SMARTboost

- Computationally inefficient for sparse features.
- Unlike XGBoost, cannot deal with missing values automatically.
- Truly large datasets will be challenging.
- In small samples, reasonably insensitive but not invariant to monotonic transformations of the features.

When is SMARTboost unlikely to beat other GBM?

Preliminary and vague but intuitive: when most relevant features have non-continuous distributions. Example from the Microsoft dataset:



What next?

- General log-likelihood/loss function.
- ML applications, including large n and p: when is it more accurate than XGBoost and CatBoost? When more accurate than NN?
- Improve software.