Bayesian Additive Regression Trees (BART)

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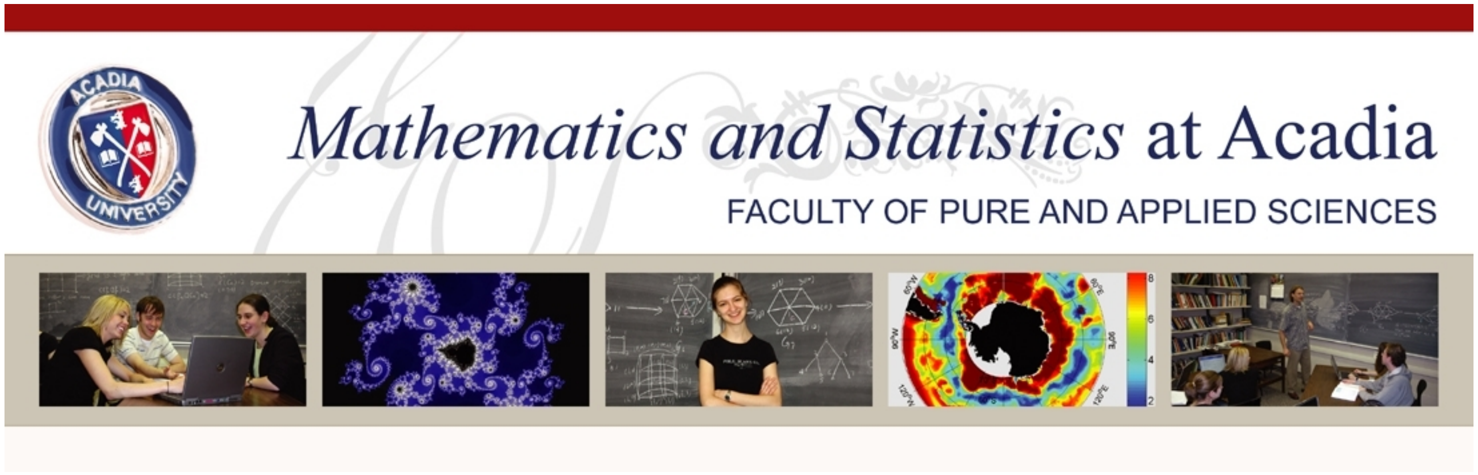
Software is available! Google "Hugh" and "Acadia".


Mathematics and Statistics at Acadia
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Outline:

1. Introduction to Ensemble models
2. A train/test bake-off comparison
3. BART: A Bayesian Ensemble
4. Examples and other cool stuff (fake & real examples, active learning)

Part 1: Introduction to Ensemble models

An Introduction to Ensembles:

- Basic problem: Function estimation with data
- Model is

$$y = f(x) + \text{noise}$$

  with
  - y a one dimensional variable
  - x a p-dimensional variable
  - Observed data are N pairs $(x_1, y_1), \ldots, (x_N, y_N)$.
  - $f(x)$ estimated using the observed data.
- Ensemble models assume that $f(x)$ is actually a sum of m (often many) functions:

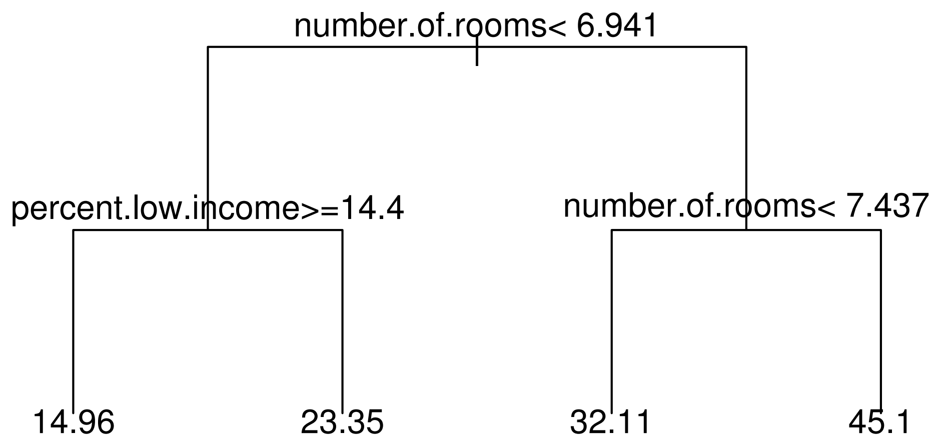
$$f(x) = g_1(x) + g_2(x) + \ldots + g_m(x)$$

  - Examples: Linear model, Generalized Additive Model, MARS, Neural net, ...
  - Original ensemble motivation: we get a better prediction by averaging a "committee" of individual models (g_i's).

An Introduction to Ensembles:

$$f(x) = g_1(x) + g_2(x) + \ldots + g_m(x)$$

- In principal, the individual g_i's could be any model.
- In practice, they're often **Trees**.



- Trees have several advantages:
  1. Selection of relevant X's.
  2. Able to represent interactions.
  3. Can handle missing values, categorical X's.

An Introduction to Ensembles:

$$f(x) = g_1(x) + g_2(x) + \ldots + g_m(x)$$

- Each tree g_i has parameters we must learn from the data:
  - Tree structure (topology and splitting rules): T_i
  - Predictions in terminal node: M_i (e.g. node constants $\mu_1, \mu_2, \ldots, \mu_b$ if there are b terminal nodes)

$$f(x) = g(x; T_1, M_1) + g(x; T_2, M_2) + \ldots + g(x; T_m, M_m)$$

- Simultaneous optimization of $T_1, ..., T_m, M_1, ..., M_m$ infeasible.

An Introduction to Ensembles:

Estimation: *"The algorithm is the model"* - Breiman, 2001

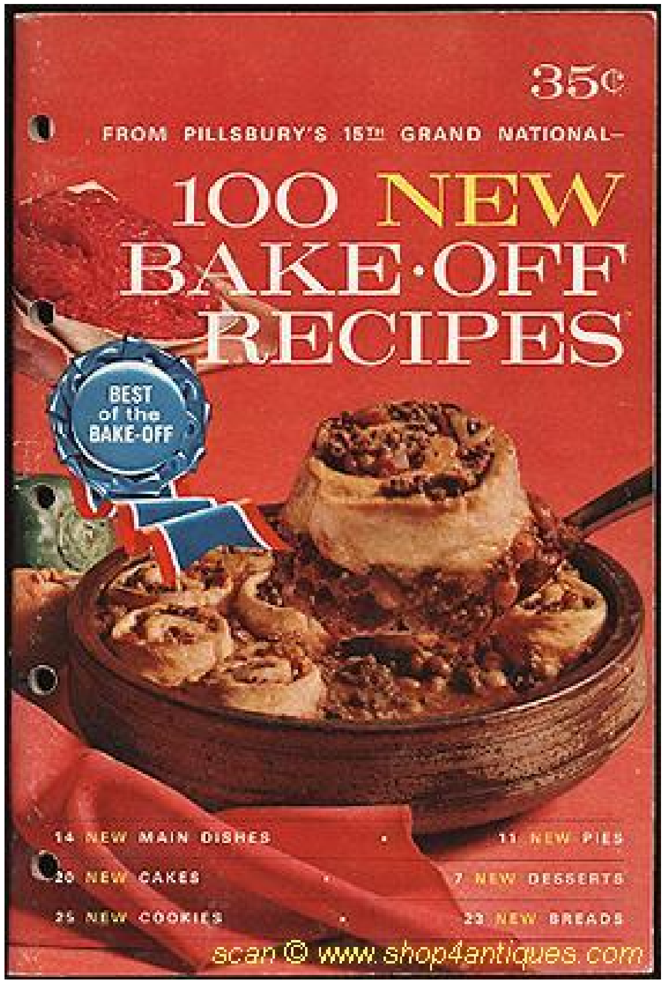
Several ways to estimate $T_1, ..., T_m, M_1, ..., M_m$:

- Bagging (Breiman 1996), Bayesian Tree models (Chipman, George, McCulloch 1998) and Random Forests (Breiman 2001):
  - Use randomized training (data resampling/stochastic search) to identify multiple trees that fit well.
  - Prediction is an average across individual tree predictions.
- Boosting (Freund and Schapire 1997, Friedman 2001)
  - has individual g_i that fit poorly (*weak learners*)
  - but they are chosen so that when combined they predict well.
- Both classes of models produce

$$f(x) = g(x; T_1, M_1) + g(x; T_2, M_2) + \ldots + g(x; T_m, M_m)$$

Part 2: Does it work?: A large empirical study

("Bake-Off", conducted for *Neural Information Processing Systems 2006)*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Experimental comparison: 6 learners $\times$ 42 datasets

- **Learners**:
  - Random Forests
  - Boosting (Friedman's gradient boosting machine)
  - BART-default - (Bayesian Additive Regression Trees)
  - BART-cv (BART, but treat prior parameters like tuning parameters via cross-validation)
  - Linear regression with lasso
  - Neural networks (single hidden layer)
- **Datasets:**
  - From Kim, Loh, Shih and Chaudhuri (2006)
  - Up to 65 predictors and 6806 observations
- **Details:**
  - Train on 5/6 of data, test on 1/6
  - Learners tuned via 5-fold CV within training set.
  - 20 Train/Test replications per dataset

Results: Root Mean Square Errors

Average test set RMSE across 42 datasets (after standardizing Y):

$$\text{RMSE} = \sqrt{\sum_{i=1}^{N} (Y_i - \hat{f}(x_i))^2 / N}$$

BART-CV:	0.5042
Boosting:	0.5089
BART:	0.5093
Random Forest:	0.5097
Neural Net:	0.5160
Lasso:	0.5896

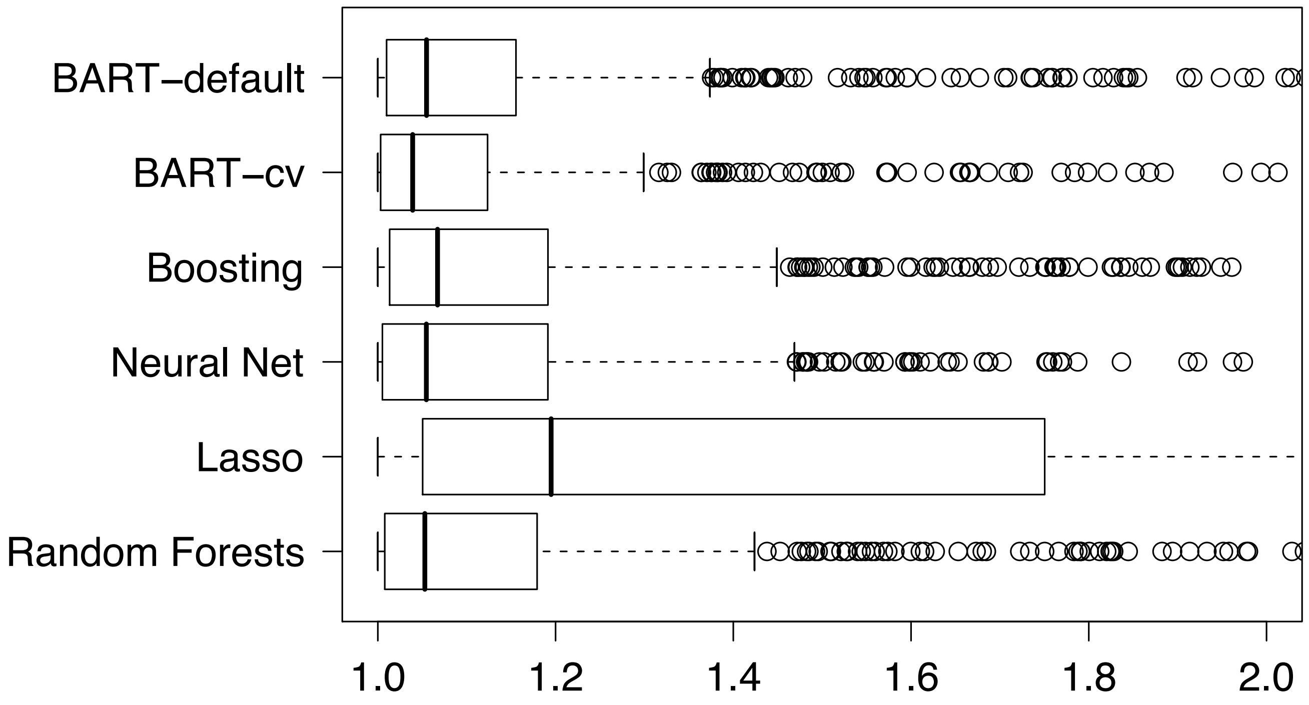
Some comments:

- BART does quite well
- Treating BART like a machine learner only gives a modest improvement.
- It's actually pretty surprising how close the different models are.

Results: Relative Root Mean Square Errors

"Relative" $\Rightarrow$ for each replicate on each data set, we identify best model, and all RMSEs are divided by the error of the best model.

$\Rightarrow$ "1.0" is best, "2.0" is a RMSE twice as large as best model.



Results: Relative Root Mean Square Errors

- The other ensembles may be doing well for different reasons:
  - Boosting forces each learner to model different structure in the data
  - Random Forests use model averaging to reduce variability
- Neither ensemble gives any prediction inference.
  - This will be our goal: combine the strengths of boosting and random forests in a model that allows inference.
- Extra bonus(es):
  - Bayesian machinery largely removes need for tuning model parameters.
  - Pointwise uncertainty in predictions.
  - Uncertainty for the magnitude of the effect of a predictor.
  - Diagnostics for model checking.

Part 3: Bayesian Additive Regression Trees (BART)

- Ensembles as a statistical model.
- Prior specification
- MCMC estimation

Ensembles as a statistical model:
Bayesian Additive Regression Trees (BART)

Our data model is

$$Y = f(x) + \epsilon, \ \epsilon \sim N(0, \sigma^2)$$

or more specifically,

$$Y = g(x, T_1, M_1) + g(x, T_2, M_2) + \ldots + g(x, T_m, M_m) + \epsilon.$$

with the errors being iid Normal$(0, \sigma^2)$

The parameters we have to estimate are:

- m Trees $T_1, T_2, \ldots, T_m$.
- m sets of terminal node parameters $M_1, \ldots M_m$ (with b_j nodes in tree j).
- A single scale parameter σ for the residual variance.

Details:

1. Prior specification
2. MCMC sampling of the posterior

One important point. The model

$$Y = g(x, T_1, M_1) + g(x, T_2, M_2) + \ldots + g(x, T_m, M_m) + \epsilon.$$

is different from Bayesian model averaging of a single tree model.

We are obtaining a posterior for a "sum of m trees" model, with a joint posterior on m trees and m terminal node parameter vectors.

Prior specification:

Need to specify a prior on T's, M's, and σ.

- Assume prior structure:

$$p((T_1, M_1), (T_2, M_2), \ldots, (T_m, M_m), \sigma) \\ = p(T_1, T_2, \ldots, T_m)\, p(M_1, M_2, \ldots, M_m \,|\, T_1, T_2, \ldots, T_m)\, p(\sigma).$$

- Since the dimension of the M depends on the T, this conditional structure is essential.
- We simplify even further by imposing independence whenever possible.

$$p(T_1, T_2, \ldots, T_m) = \prod p(T_j)$$

$$p(M_1, M_2, \ldots, M_m \,|\, T_1, T_2, \ldots, T_m) = \prod p(M_j \,|\, T_j)$$

$$p(M_j \,|\, T_j) = \prod p(\mu_{i,j} \,|\, T_j)$$

Prior Specification:

Semi-automatic choices motivated by Empirical Bayes methods.

Basic ideas:

- T's: how big a tree is probable?
- σ: how much noise in the response?
- $M's$: How much can each individual tree contribute?
  Clever trick: Make this depend on the number of trees.
- Number of trees could be a parameter, but we fix it instead.

Prior Specification:

1. Residual variance σ^2:

   Prior for σ is simplest and most important.

   We use the standard conjugate prior:

$$\sigma^2 \sim \frac{\nu\,\lambda}{\chi^2_\nu}.$$

   - ν determines spread of the prior
   - λ determines location of the prior

   Instead of eliciting ν, λ directly we:

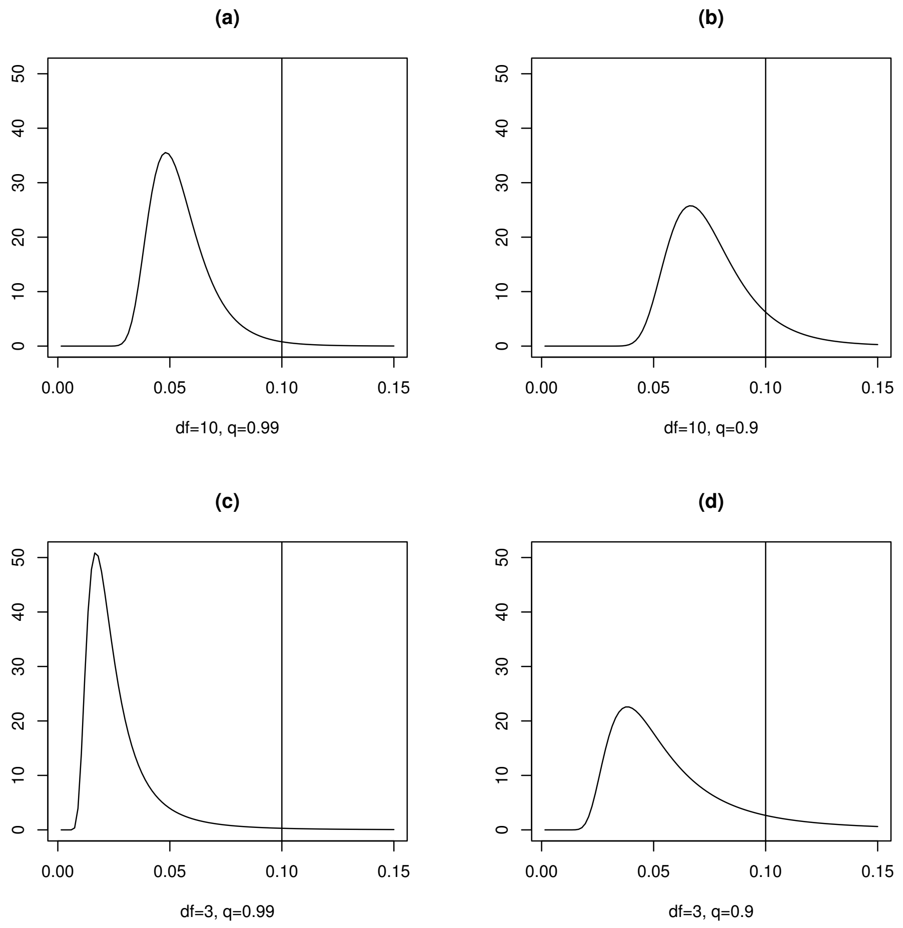
   (a) Guess at an upper quantile of σ, say 90% or 99%. Set this equal to least squares linear regression estimate of σ

   (b) Choose ν to give good spread of σ prior.

Prior Specification:

Vertical line indicates $\hat{\sigma}$, the rough estimate of σ from linear least squares model.

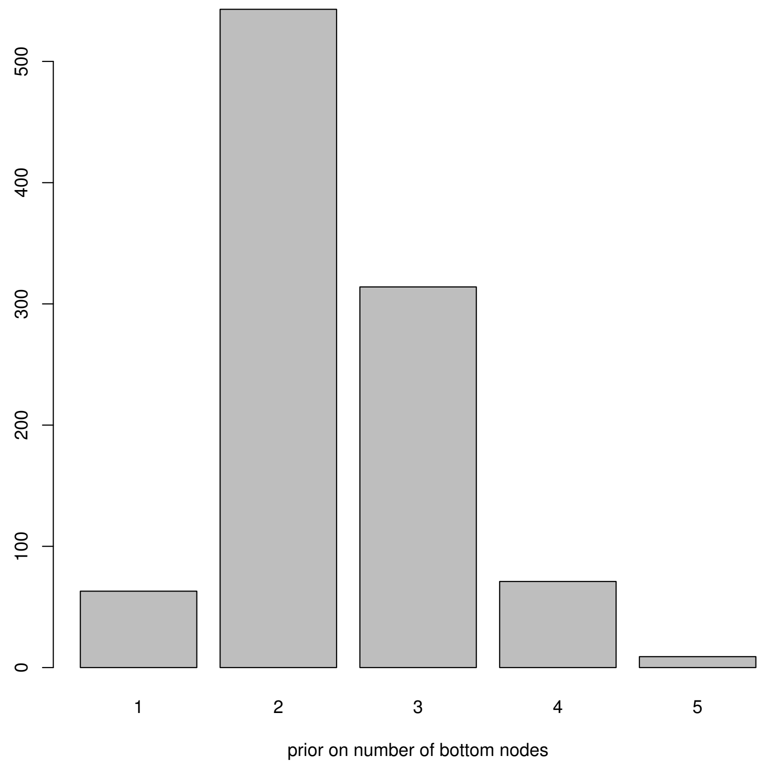
- Top: $\nu = 10$
- Bottom:$\nu = 3$
- Left: $\hat{\sigma}$ at 99th quantile.
- Right: $\hat{\sigma}$ at 90th quantile.



Prior Specification:

2. Prior on tree structure T:

- Basically a prior on tree size*.
- Actual prior used in examples later gives tree size prior in plot.
- NOTE that unlike Boosting, we don't fix tree depth. We put a prior on it and let the data determine tree depth.



- Tree size determines how many variables are used in each "weak learner" $g(x; T, M)$.

* Actually a distribution on whether you split, which variable you split on, and the splitting rule, for each node.

Prior Specification:

3. Terminal node parameters μ_i

- Suppose we have $m = 200$ trees.
- For any x, the prediction $f(x)$ will be a sum of 200 μ's, one from each tree.

$$\theta = E(Y|x) = f(x) = \sum_{i=1}^{200} \mu_i$$

$$\text{Var}(\theta) = \sum_{i=1}^{200} \text{Var}(\mu_i) = 200\text{Var}(\mu_i)$$

(assuming μ_i's independent given the trees)

- So, we can specify how much we expect the mean of y given x (i.e., θ) to vary, and take

$$\text{Var}(\mu_i) = \text{Var}(\theta)/200$$

$$\text{sd}(\mu_i) = \text{sd}(\theta)/\sqrt{200}$$

Prior Specification:

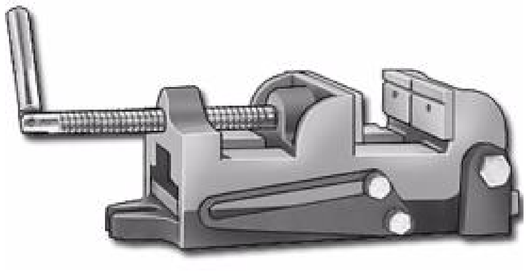
3. Terminal node parameters μ_i

- Assume μ_i is normally distributed, with mean 0, and standard deviation

$$\text{sd}(\mu_i) = \frac{\text{range(Y)}}{4\sqrt{200}}, \qquad \text{for 200 trees in sum}$$

  NOTE: The amount of shrinkage of the μ's *depends on the number of trees* (here $m = 200$).

- Each term g(x;T,M) will be "regularized" so it contributes only a small part of the overall fit.



So the model is adaptively regularized in several ways: Tree prior and terminal node prior.

MCMC Estimation:

Instead of explicitly maximizing the posterior, we simulate from it, via Markov chain Monte Carlo (MCMC).

In a nutshell:

Let $T_{(-j)}$ be all trees *except* T_j, define $M_{(-j)}$ similarly.
Repeat $k = 1, ..., 1000$ (say)

- Repeat $j = 1, ..., m$ times
  - Metropolis-Hastings step: Draw T_j conditional on $Y, T_{(-j)}, \sigma$
  - Draw M_j given $Y, T_1, \dots T_m, M_{(-j)}, \sigma$
- Draw σ given Y and all other parameters.

Note that the sample of T_j at step k is actually a modification of the T_j sample at step $k-1$.

MCMC Estimation:

Final prediction:

- Each sweep of algorithm yeilds a draw from the posterior of

$$f(x) = g(x, T_1, M_1) + g(x, T_2, M_2) + \ldots + g(x, T_m, M_m)$$

- Average the draws - gives the posterior average of $f(x)$.
- Uncertainty in $f(x)$ is also available, from the posterior distribution on $f(x)$.

Connections to other learning algorithms:

1. Bayesian Backfitting (Hastie and Tibshirani) is a similar MCMC approach.
2. Like Boosting, each of our "weak learners" $g(x; T_j, M_j)$ learns structure that the other weak learners do not capture.
3. Like Random Forests and Bagging, we model average over multiple draws of the sum of trees model.

Part 4: Examples with Data (Simulated, Boston, Active Learning)

Simulated example: Friedman (1991)

$$y = f(x) + \epsilon, \qquad \epsilon \sim N(0,1)$$

where

$$f(x) = 10\sin(\pi x_1 x_2) + 20(x_3 - .5)^2 + 10x_4 + 5x_5 + 0x_6 + ... + 0x_{10}$$

(10 x's but only the first 5 matter)

$N = 100$ observations

BART settings:

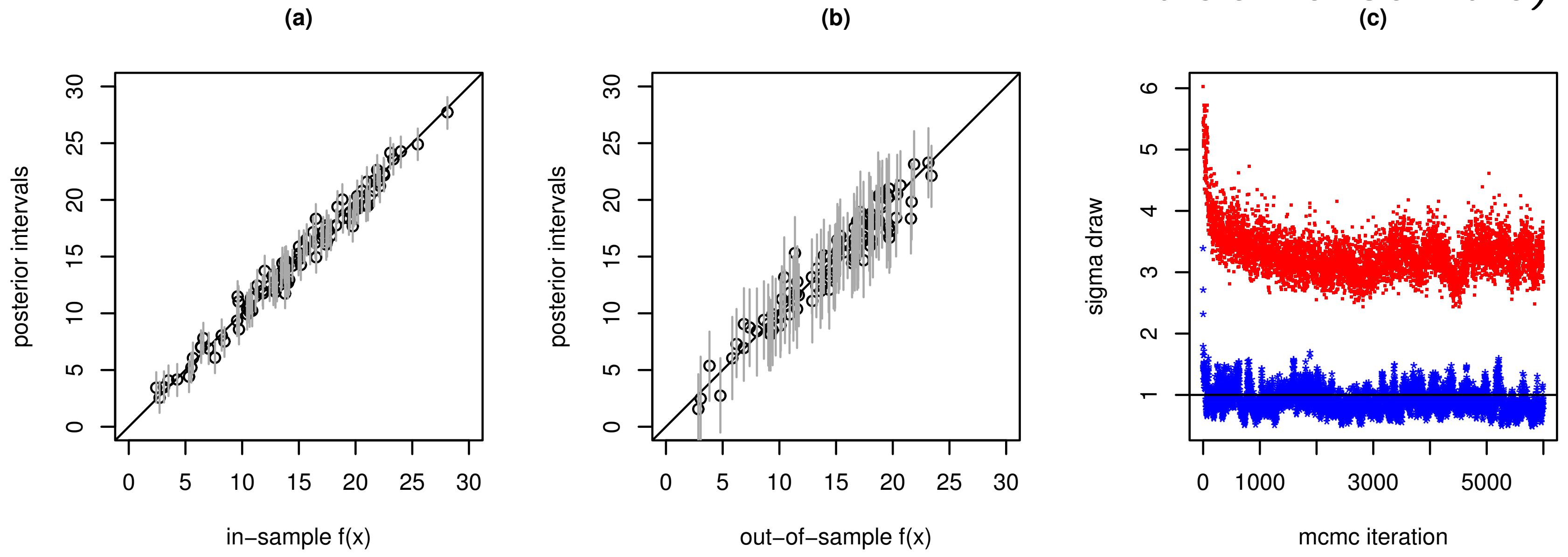
- $m = 100$ trees
- σ prior uses $\hat{\sigma}$ from linear least squares regression as 90th quantile, $\nu = 3$.
- Tree prior puts most probability on 2, 3 terminal nodes.
- Automatic choice of $M = \{\mu_j\}$ prior just discussed.

Simulated example:

Training sample predictions

Test sample predictions

posterior for σ (red= 1 tree, blue=ensemble)



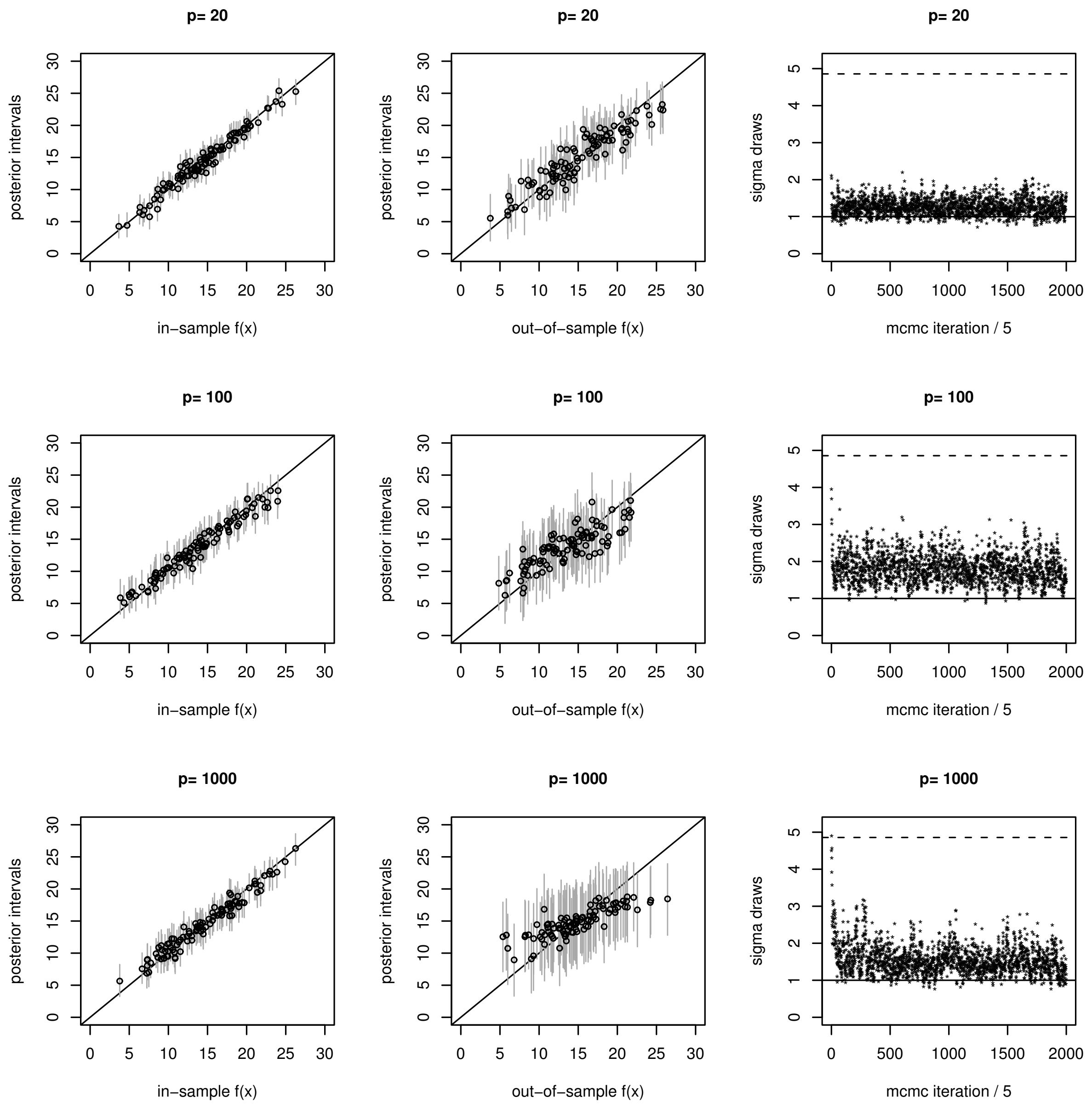
- Chain converges quickly and mixes well.
- Note that the model is not identifiable, but we are really only interested in identifiability of predictions.

Simulated example:

$p = 20$ dimensions

$p = 100$ dimensions

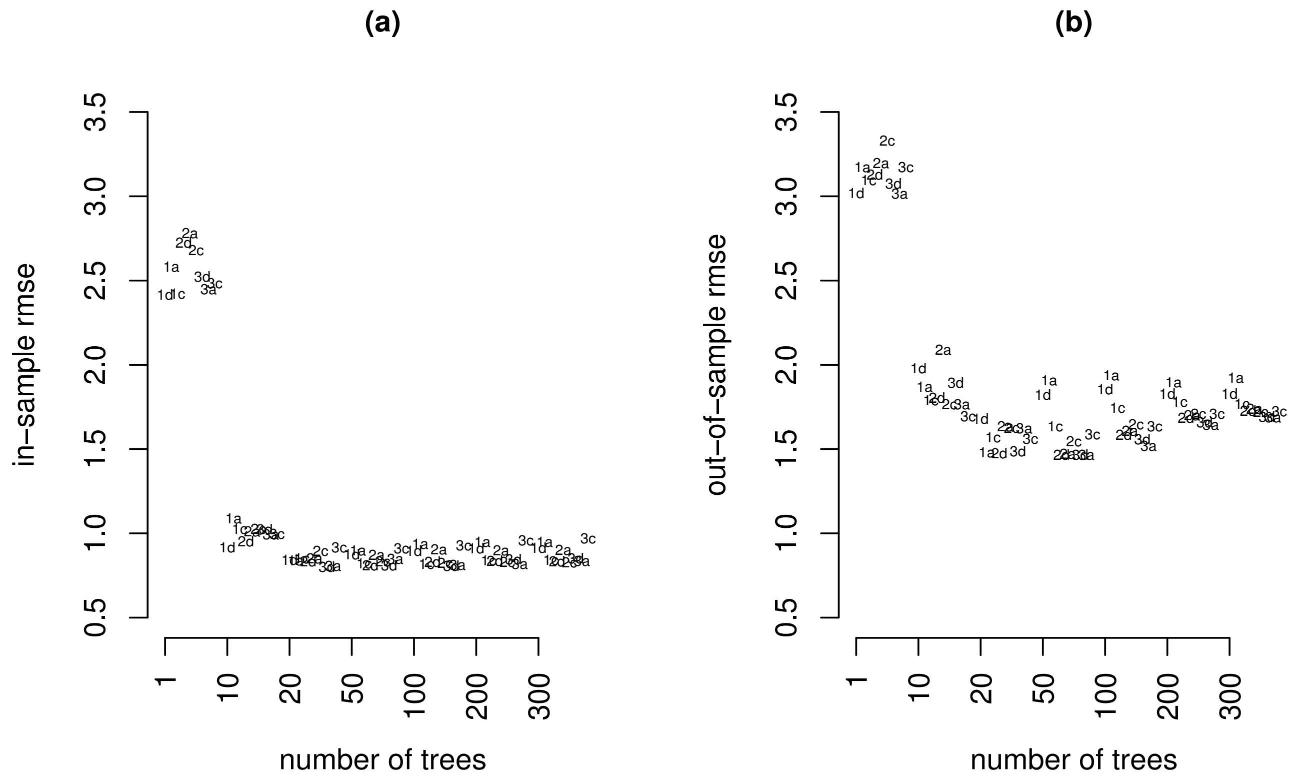
$p = 1000$ dimensions



Simulated example:

Previous page: BART capable of extracting low-dimensional signal with many x's. (Even $n \ll p$, i.e. $n = 100$ observations in $p = 1000$ dimensions!)

Also reasonable robustness to prior settings:



Training Results   Test Results

Additional Goodies: The Boston Housing Example

- Goal: Predict neighbourhood house price using demographic variables.
- Data:
  - y=log median house price in the region (the response)
  - X is 13 predictors, measuring pollution, crime, house sizes, commute distance, racial diversity, tax rates, etc.
- Common "benchmark" problem.

Additional Goodies: The Boston Housing Example

Posterior distribution on the number of terminal nodes of the 200 trees (actually a draw from the posterior).

Number nodes	1	2	3	4	5	6
Relative freq (%)	3.5	54.5	32.5	8.5	0.5	0.5

This can be interesting because

- a 1-node tree doesn't contribute to the model
- a 2 node tree is a main effect for one variable
- a 3 node tree is a two-way interaction
- ... etc.

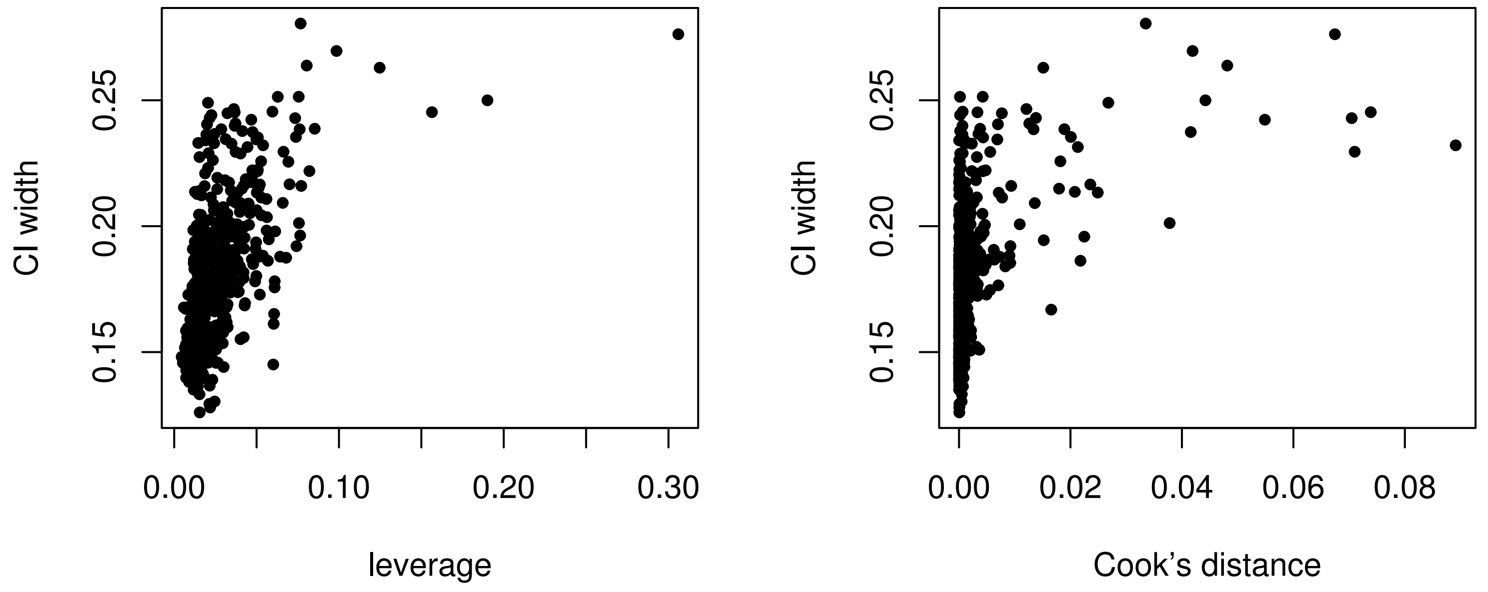
In this case, there seems to be mostly main effects and some two-way interactions.

(still a somewhat dodgy way to measure interaction order)

Additional Goodies: The Boston Housing Example

Relation to model diagnostics

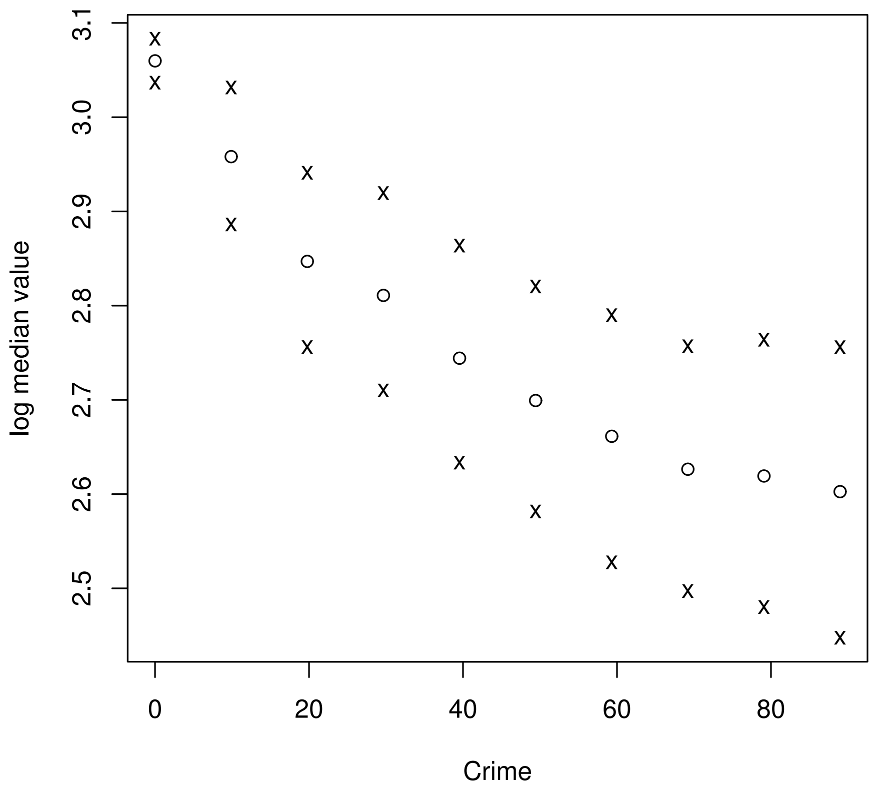
- Consider predicting y. For each point, plot the posterior interval width against traditional regression diagnostics (left: leverage, right: Cook's distance).
- Influential points tend to have larger posterior intervals.
- Posterior gives information about influential points.



Additional Goodies: The Boston Housing Example

Partial Dependence Plots

- Want to measure the effect of one or two x's on $f(x)$.
- Basically we margin over the other variables (Friedman 2001).
- Full posterior inference for such a plot is straightforward.
- Example: `crime rate`



- Almost all crime rates are in the 0-5 range.
- Bounds widen as we have less data (high crime rate).

And Now for Something Completely Different....

Active Learning

Active Learning

The game we play:

- Same "regression" scenario as before: predict Y using X.
- The difference is that **we can sequentially choose the x's at which we measure Y**.
- That is, we assume that all potential x's are known, and we need to choose which ones we measure Y at.
- By "actively learning" (ie sequentially gathering data) we hope to build a better model with less data.
- This is essentially experimental design.
- Much of the theory for design applies to linear models, here we show how adaptive models can be used for sequential design.

Active Learning

Sketch of the active learning algorithm:

1. Select an initial design (i.e., initial set of observations) X_0 with n_0 points via some criterion.
2. Obtain response values Y_0 for data.
3. Build a model using data $D_0 = (X_0, Y_0)$.
4. Repeat $j = 1, ..., n$:
   (a) For each potential design point $x_i \in$ candidate set C, calculate the design criterion
   (b) Select point x_{i^*} with best design criterion yielding design $X_j = (X_{j-1}, x_{i^*})^T$.
   (c) Measure response at X_j, giving $Y_j = (Y_{j-1}, y_{i^*})^T$
   (d) Build model M_j using $D_j = (X_j, Y_j)$.

Note:

- At the end of this algorithm, we will have n_0+n observations.
- Details on calculation in 4(a) on subsequent pages.

Active Learning

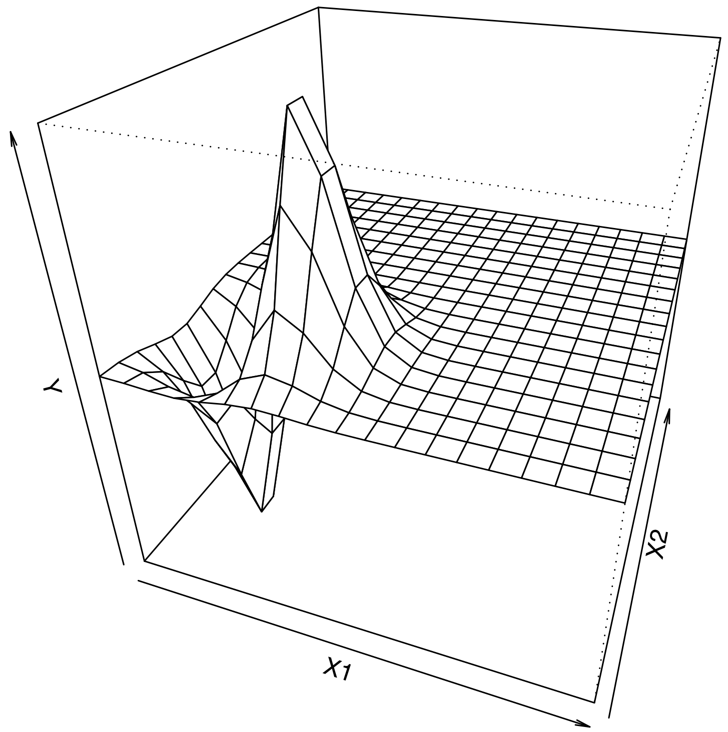
Two possible design criteria:

1. Maximize variance of predicted response ("ALM" - MacKay (1992))
   (*where do I know the least about Y?*).
2. Maximize expected reduction in variance of predicted response, averaged over a candidate set C ("ALC" - Cohn (1996))
   (*what data point will improve my model's predictions most?*)

We'll use # 1 here

2-D example (Gramacy and Lee 2006)

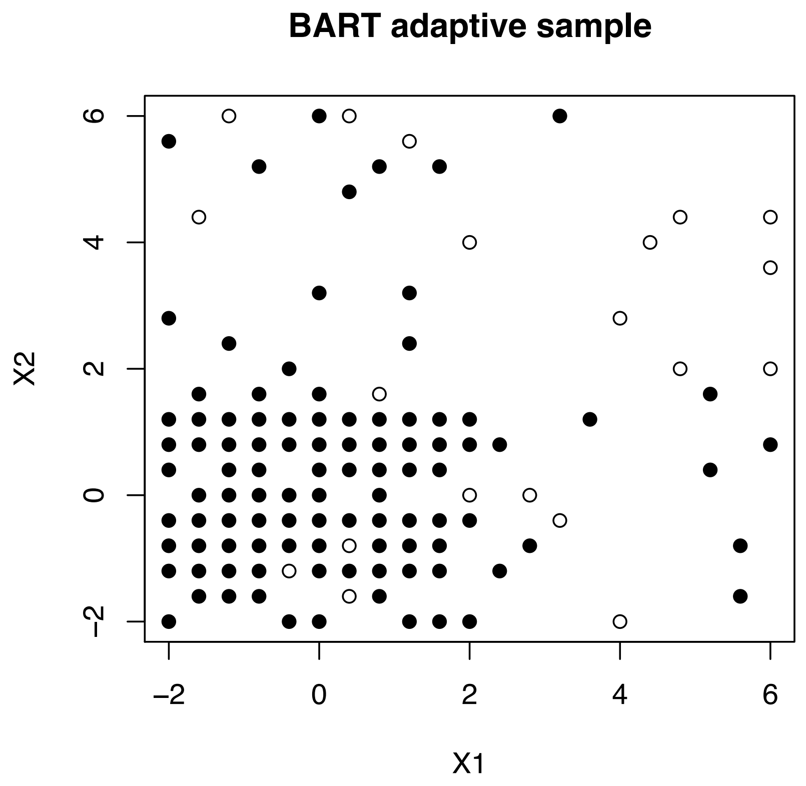
- Two predictors
- Function (right) nearly constant in 75% of input space
- Initial SRS of 20 observations, followed by adaptive sampling of 100 observations.
- All observations on a 21×21 grid.

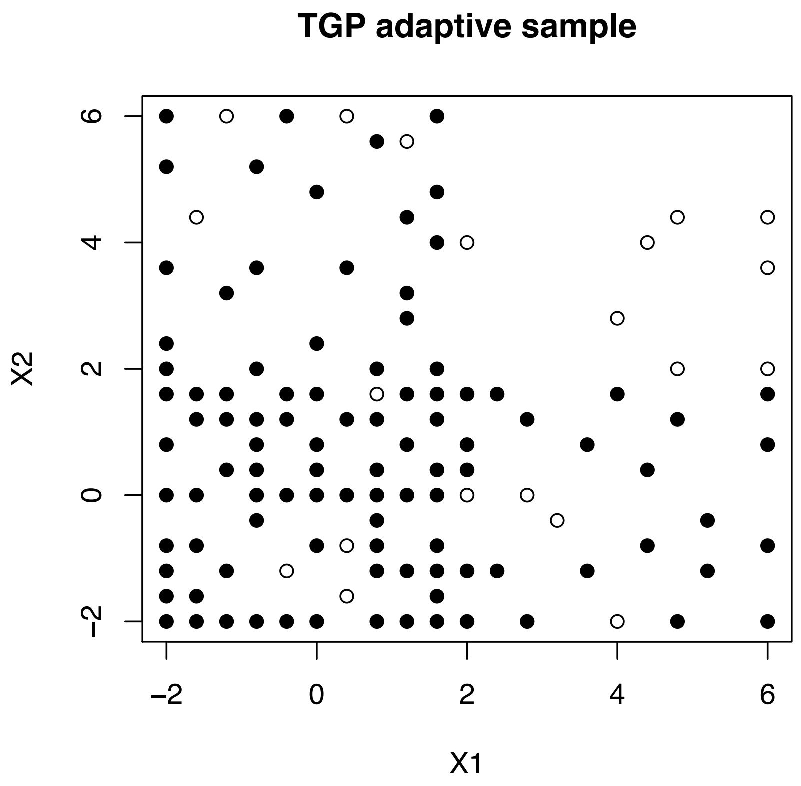


We'll make comparisons with Gramacy and Lee's "Treed Gaussian Processes" (TGP)

2-D example (Gramacy and Lee 2006)

Points sampled by BART and TGP:





Test-set MSE's (right) indicate

- Both select good samples
- TGP fits better (smooth)

MSE	Model	
	TGP	BART
SRS sample	3.66	15.96
BART sample	0.35	2.84
TGP sample	0.40	2.93

Active Learning

- This may look like a dead heat, but ...
  - BART scales well to large n and large p.
  - Ability of BART to discard irrelevant variables may be handy.
  - BART can handle categorical X's

Summary and future work:

1. It is possible to have a flexible predictive model, but still use it to make statistical inferences.
   - There is some computational cost.
   - Some derivations of models necessary.
   - But it's worth it: Cross-validation not necessary.
2. Extension to classification: 2-class problem is immediate: view binary outcome as corresponding to a latent continuous variable.
3. We plan to do extension to exponential family (similarities with Hastie and Tibshirani's Bayesian Backfitting).
4. Because we have a probability model, we can build in many interesting features. (e.g., different response data types, hi-erarchical models, outliers, modelling of σ as well as μ,...)