Boosting

Some figures in this presentation are taken from "The Elements of Statistical Learning" (Springer, 2009) with permission from the authors: Hastie, T; Tibshirani, R. & Friedman, J.;
Some figures are taken from Peter Prettenhofer's talk "Gradient Boosted Regression Trees in scikit-learn"

Overview

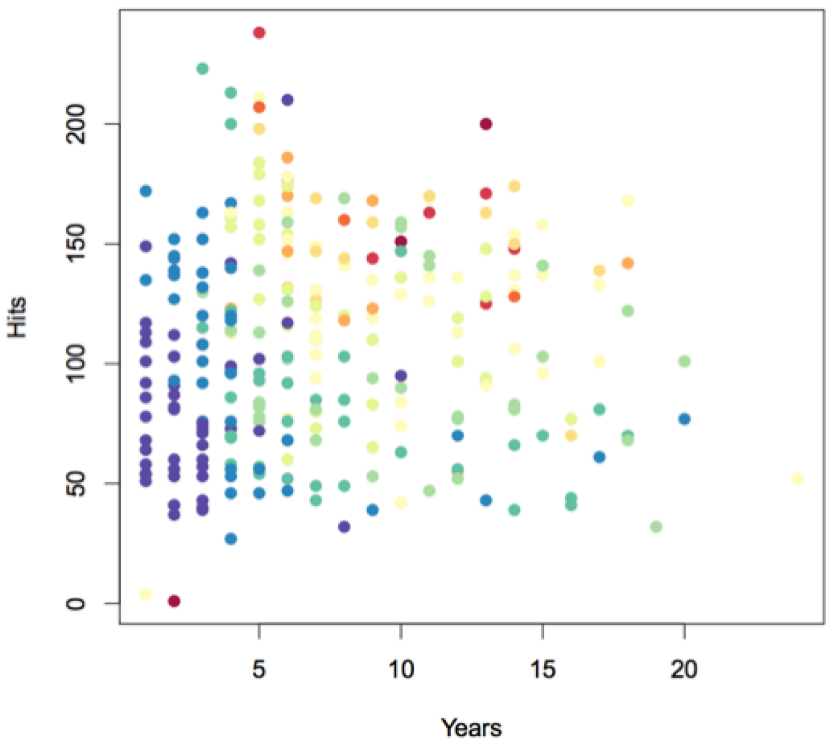
- Review of Decision Tree – Regression
- What is boosting?
- Boosting
  - AdaBoost
  - Gradient Boosted Regression Trees
- Gradient Boosted Regression Trees in sklearn
  - How to tune

- Discrete AdaBoost

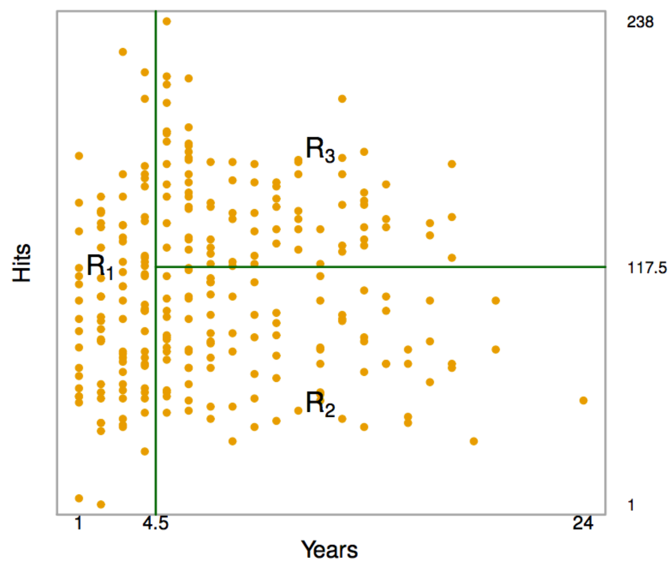
Decision Trees - Regression

Salaries color-coded from low to high

- Low salaries in blue, green
- High salaries in orange, red



Decision Trees – Regression



Consider sequence of trees indexed by tuning parameter α.

For each α, there is a corresponding subtree, **T**, such that the following is minimized:

$$\sum_{m=1}^{|T|} \sum_{i:\ x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|$$

where |T| is the number of terminal nodes

What is Boosting?

- Bagging – Bootstrap many trees, each tree independently grown, in an effort to decrease variance through averaging
- Random Forest – Similar idea, but take random subset of possible features at each split to "decorrelate the trees"

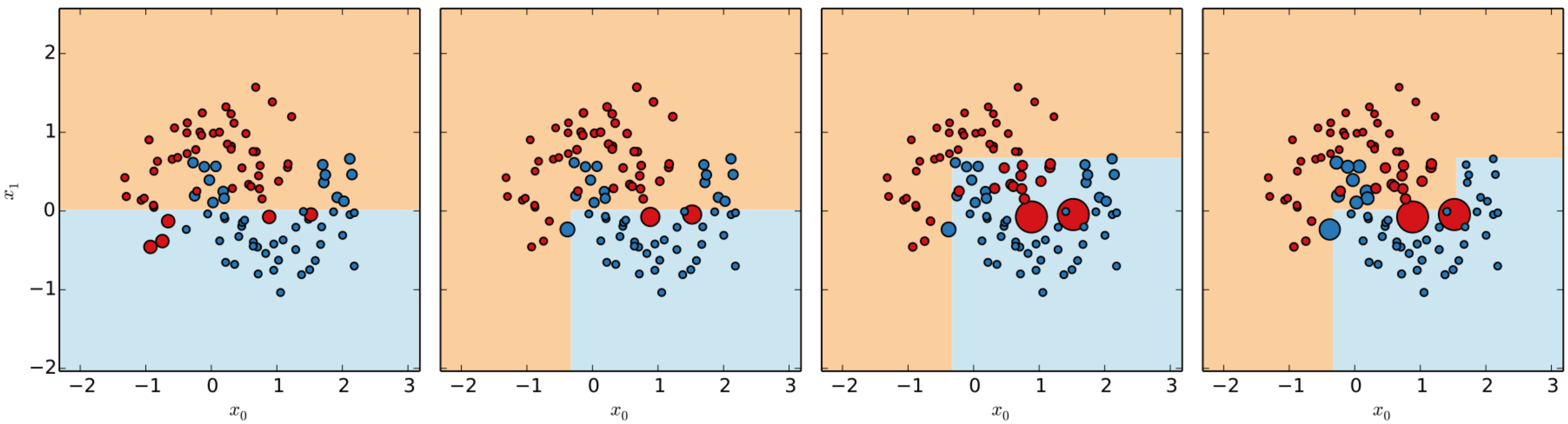
<u>What is Boosting?   Not at all like Bagging or Random Forest!</u>

- Idea: Combine set of "weak" learners to form strong learner
  - "weak" in that error rate only slightly better than random guessing
- How: Sequentially apply weak classification algorithm to modified versions of the data → sequence of weak classifiers
  - Each tree is grown using information from last tree

Boosting

AdaBoost

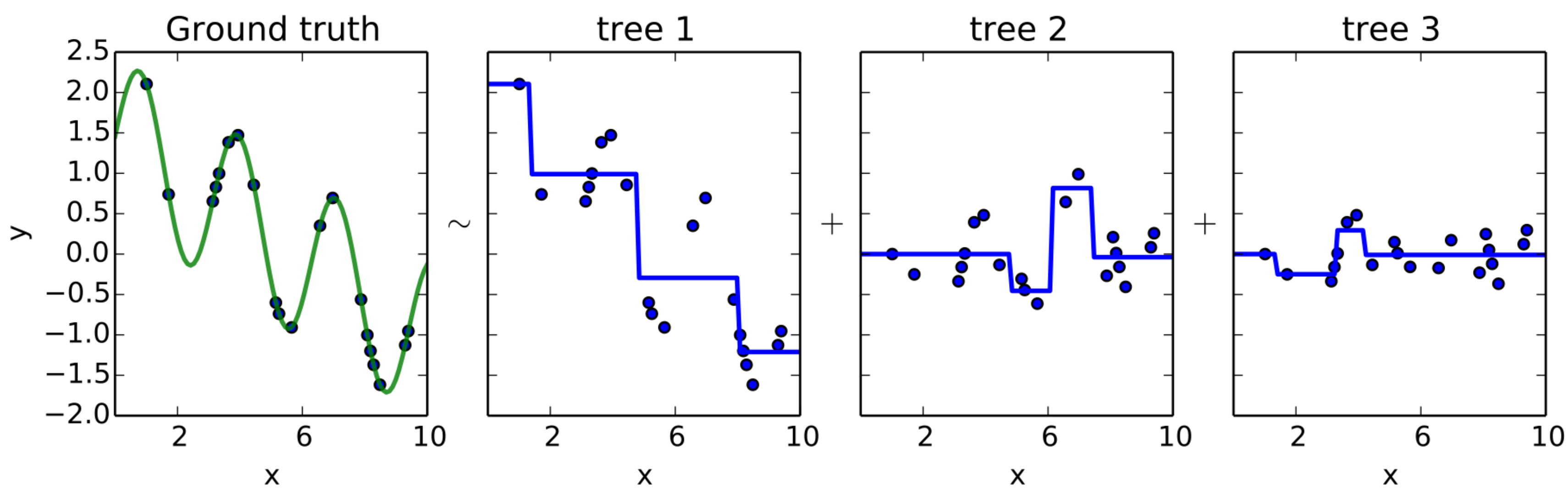
- Each tree is expert on attacking errors of predecessor
- Iteratively re-weights observations based on errors



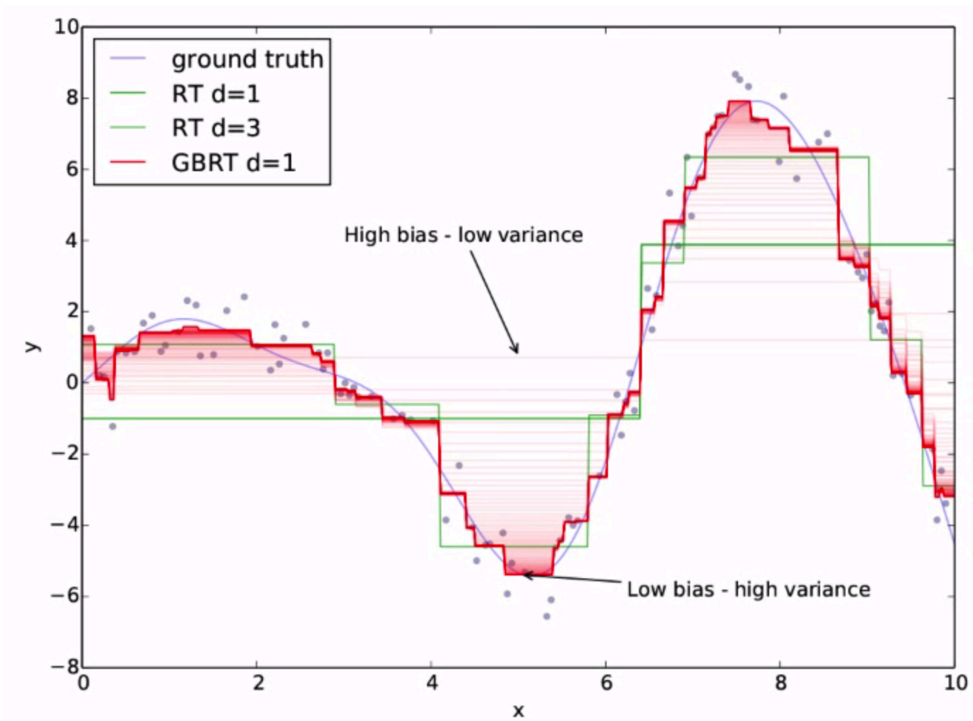
Boosting

Gradient Boosted Regression Trees

- Instead of fitting to reweighted training observations, fit residuals to of previous tree



Boosting



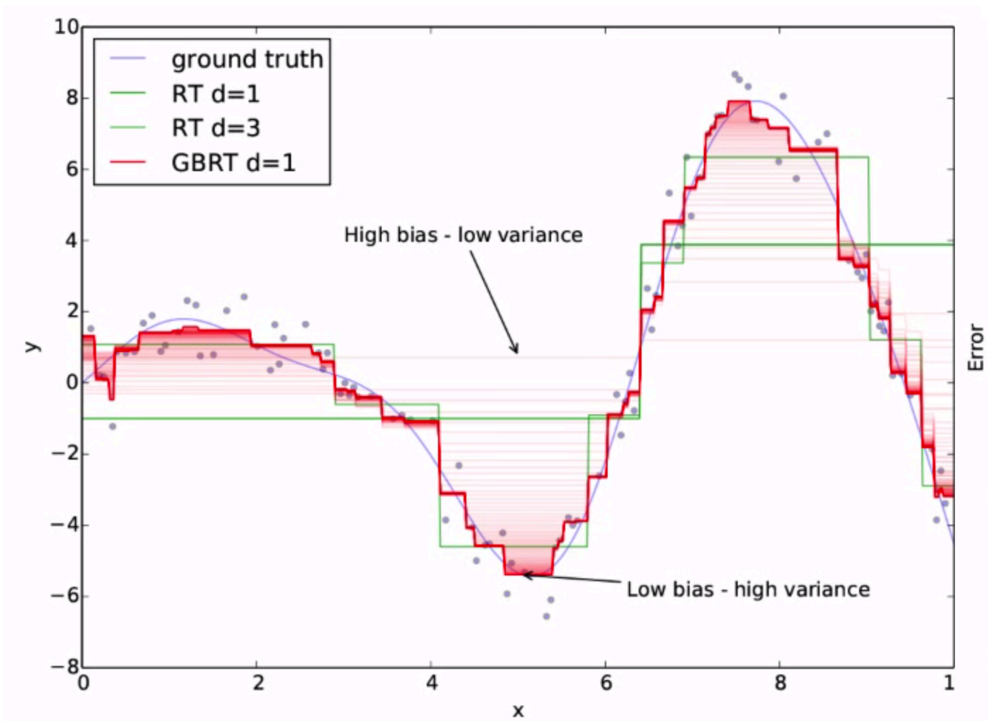
A single (boosted) tree,

→ High bias, Low variance

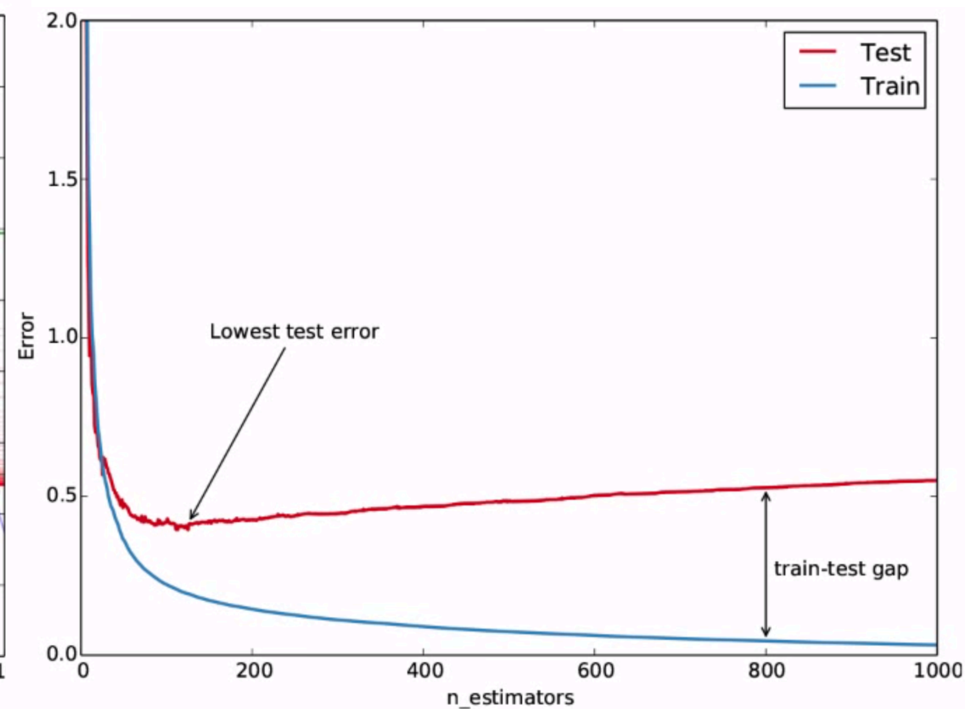
Many many (boosted) trees…

→ Low bias, High variance

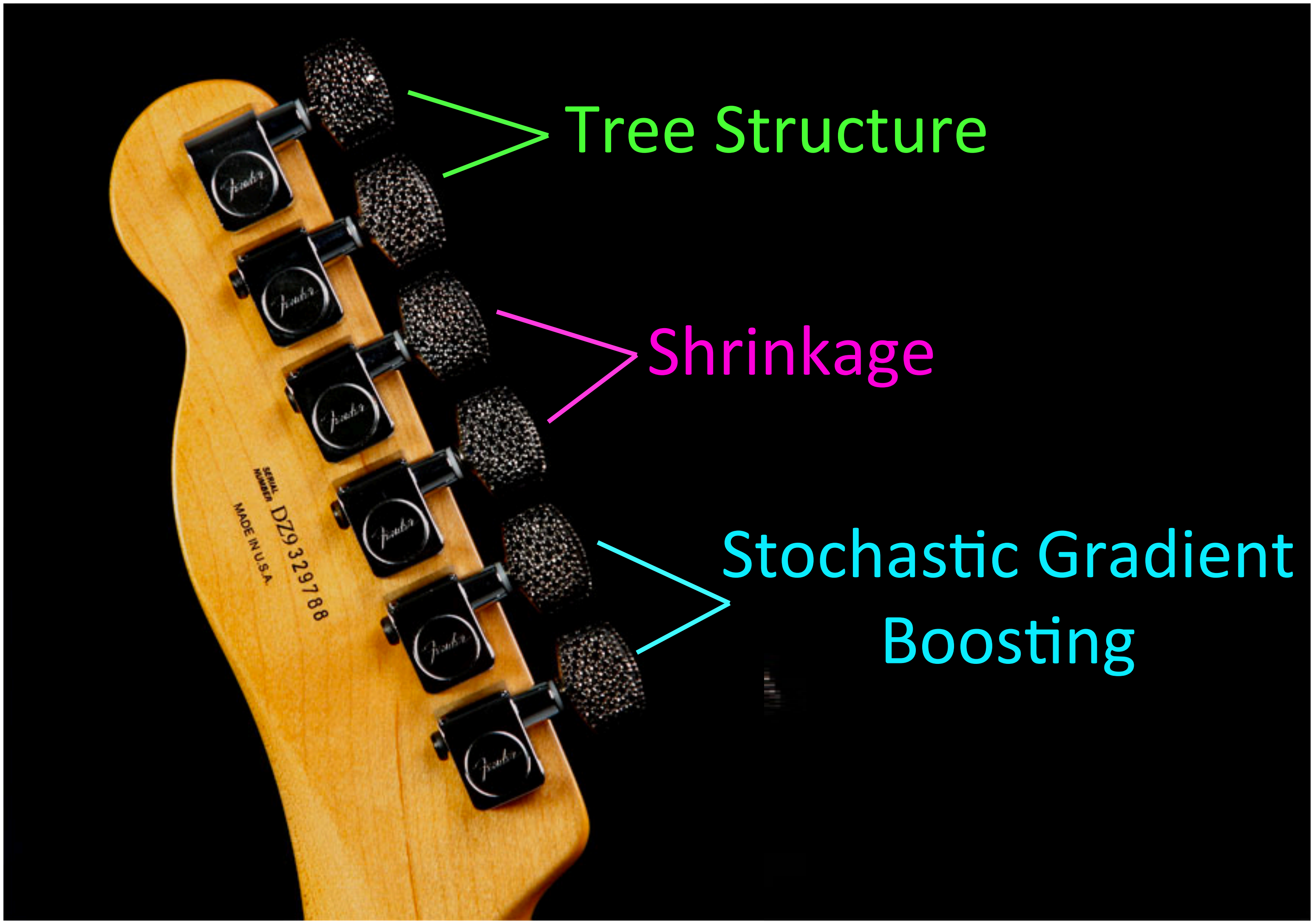
Boosting



As number of trees grows….



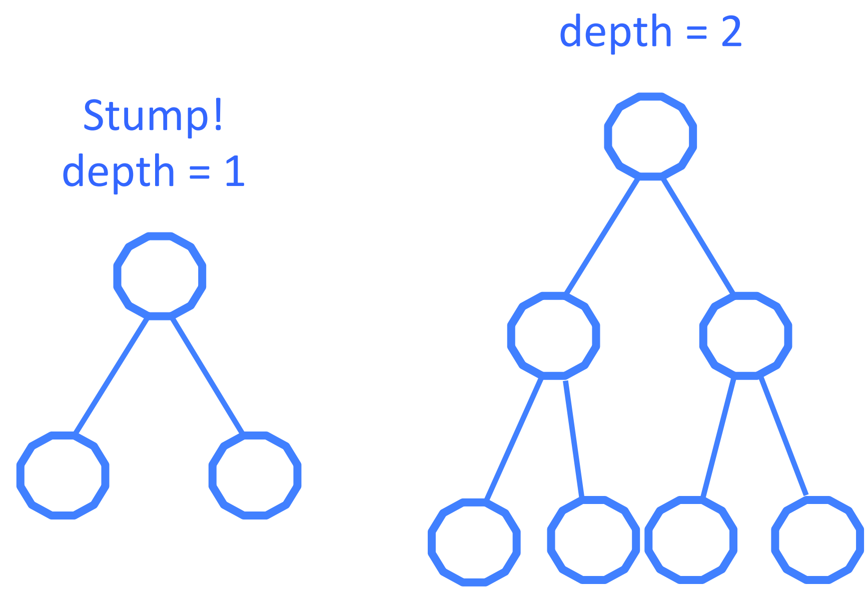
So you wanna boost some trees…



GBRT in sklearn

<u>Tree Structure</u>

- `max_depth`
  - controls degree of interactions
  - Ex. Latitude and Longitude
  - not often larger than 4 or 6

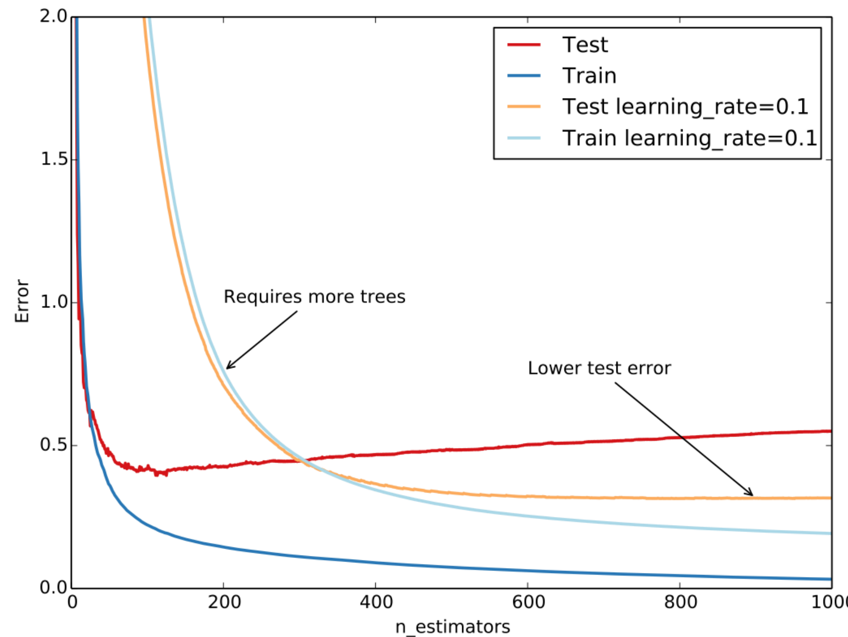


- `min_samples_per_leaf`
  - may not want terminal nodes with too few leaves

GBRT in sklearn

<u>Shrinkage</u>

- `n_estimators`
  - number of trees grown
- `learning_rate`
  - lower learning rate requires higher n_estimators



As the learning rate goes down, the number of trees needed goes up!

Learning rate is a very important tuning parameter.
Number of trees also needs to be tuned.

GBRT in sklearn

<u>Stochastic Gradient Boosting</u>

like in
Random Forests!

- `max_features`
  - random subsample of features
  - Especially good when you have lots of features

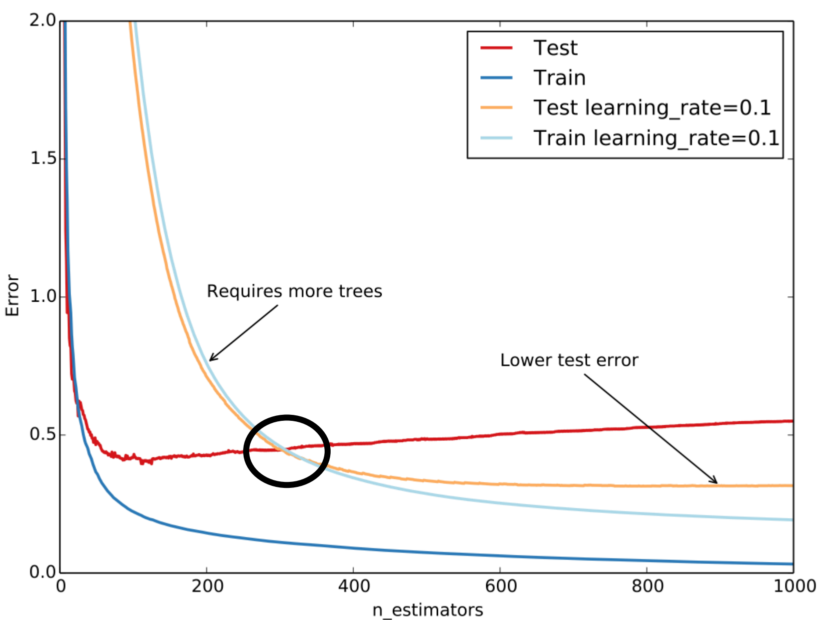
- `sub_sample`
  - random subset of the training set

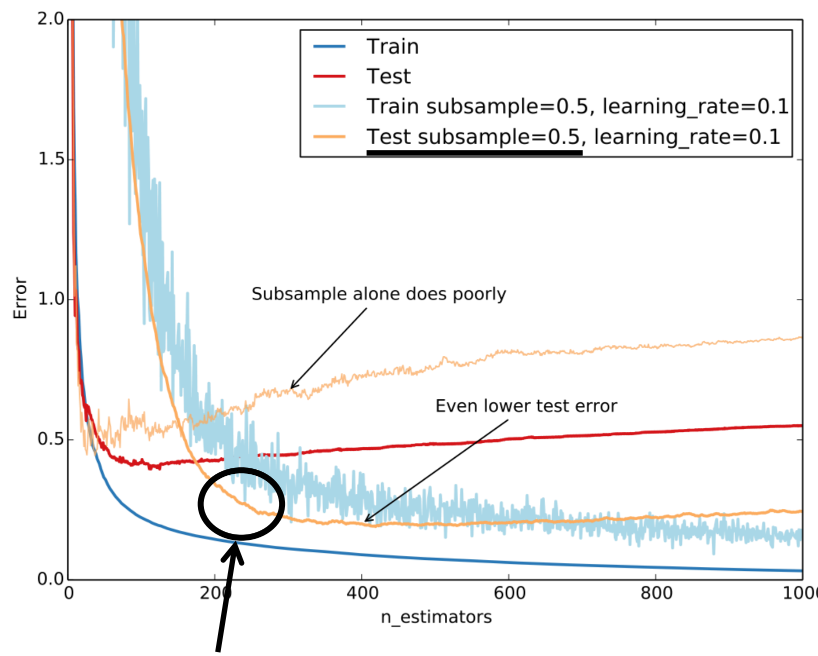
Both randomly sampling the features and randomly subseting the training set can lead to improved accuracy and reduced run-time

Pretty good deal!

GBRT in sklearn

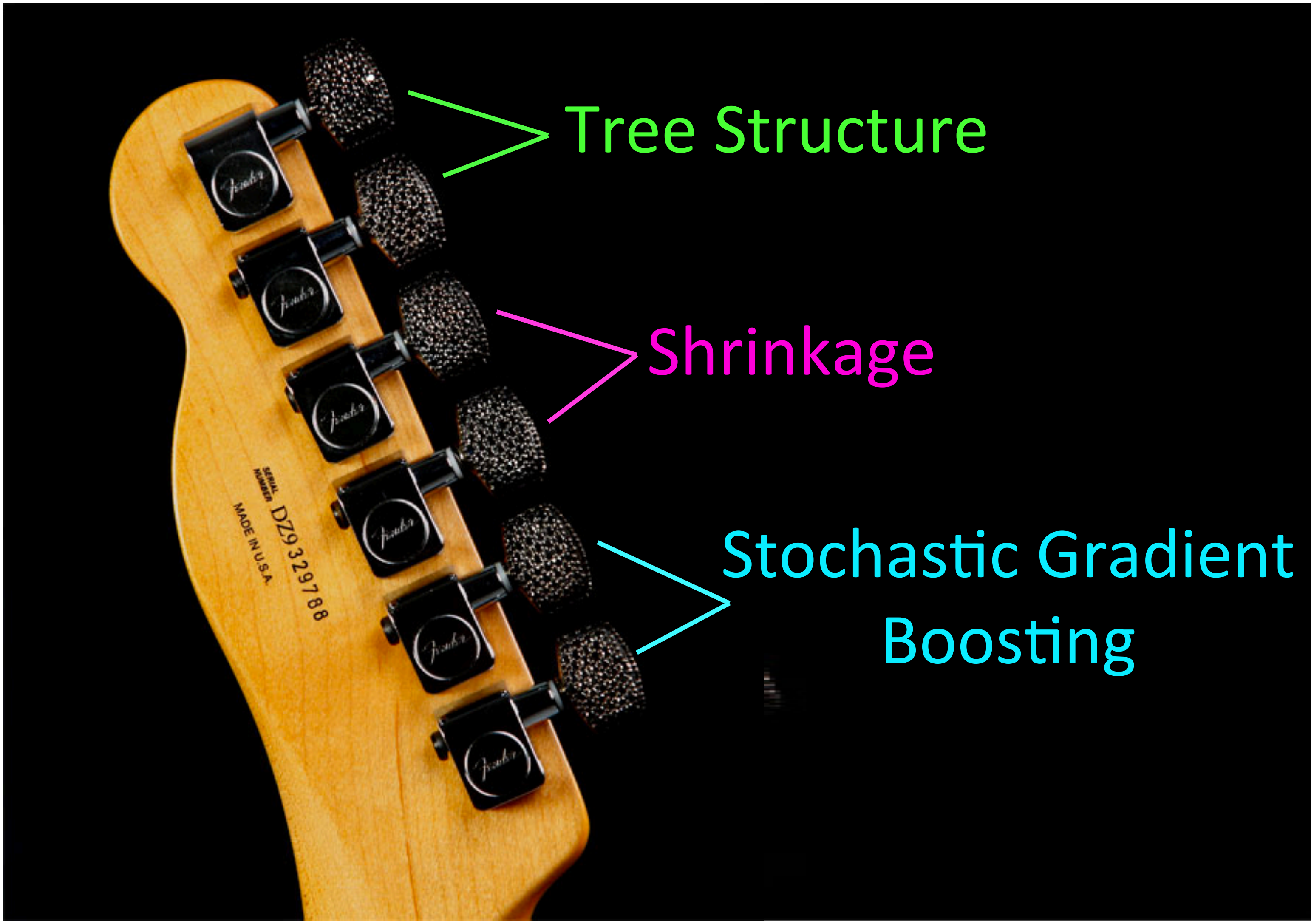
Stochastic Gradient Boosting can **improve accuracy** and **reduce runtime!**





Lower test error!
Fewer trees to get there!

Gee that was a lot of knobs…



GBRT in sklearn

Tuning – a good starting setup

(1) Set `n_estimators` high as possible

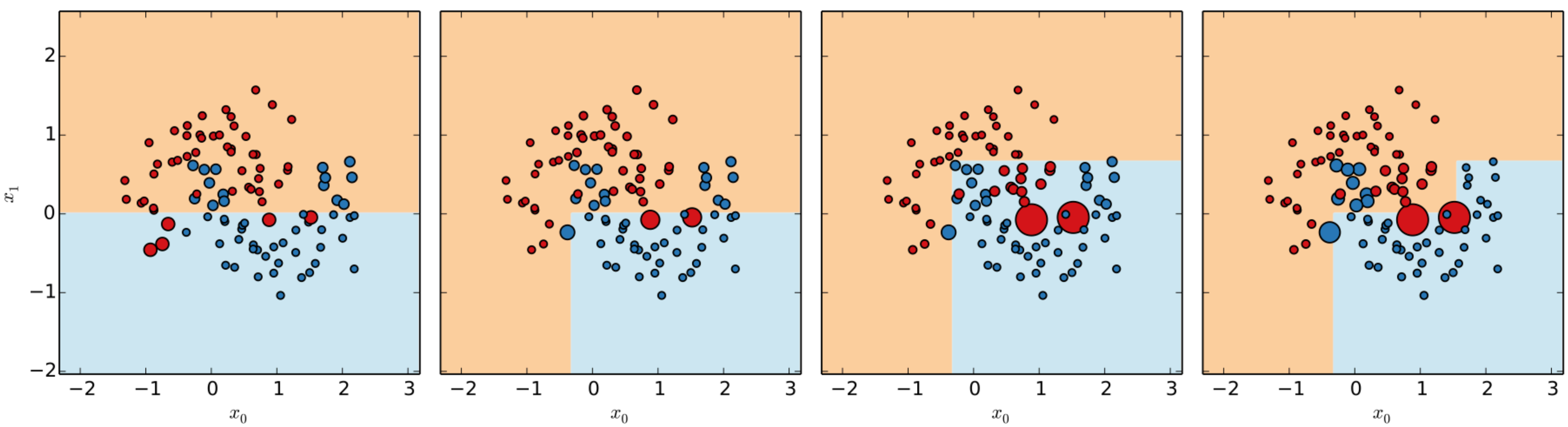
(2) Tune hyperparameters together via grid search

```
from sklearn.grid_search import GridSearchCV
param_grid = {'learning_rate': [0.1, 0.05, 0.02, 0.01],
              'max_depth': [4, 6],
              'min_samples_leaf': [3, 5, 9, 17],
              'max_features': [1.0, 0.3, 0.1]}
est = GradientBoostingRegressor(n_estimators=3000)
gs_cv = GridSearchCV(est, param_grid).fit(X, y)
# best hyperparameter setting
gs_cv.best_params_
```

(3) Set `n_estimators` even higher while tuning `learning_rate`

AdaBoost

- Each tree is expert on attacking errors of predecessor
- Iteratively re-weights observations based on errors



Discrete AdaBoost

- One of the most popular boosting algorithms
  - also known as AdaBoost.M1,Freund & Schapire (1997)

Y: {-1, 1}

G(X): classifier producing predictions taking two values {-1, 1}

Error rate on the training set:

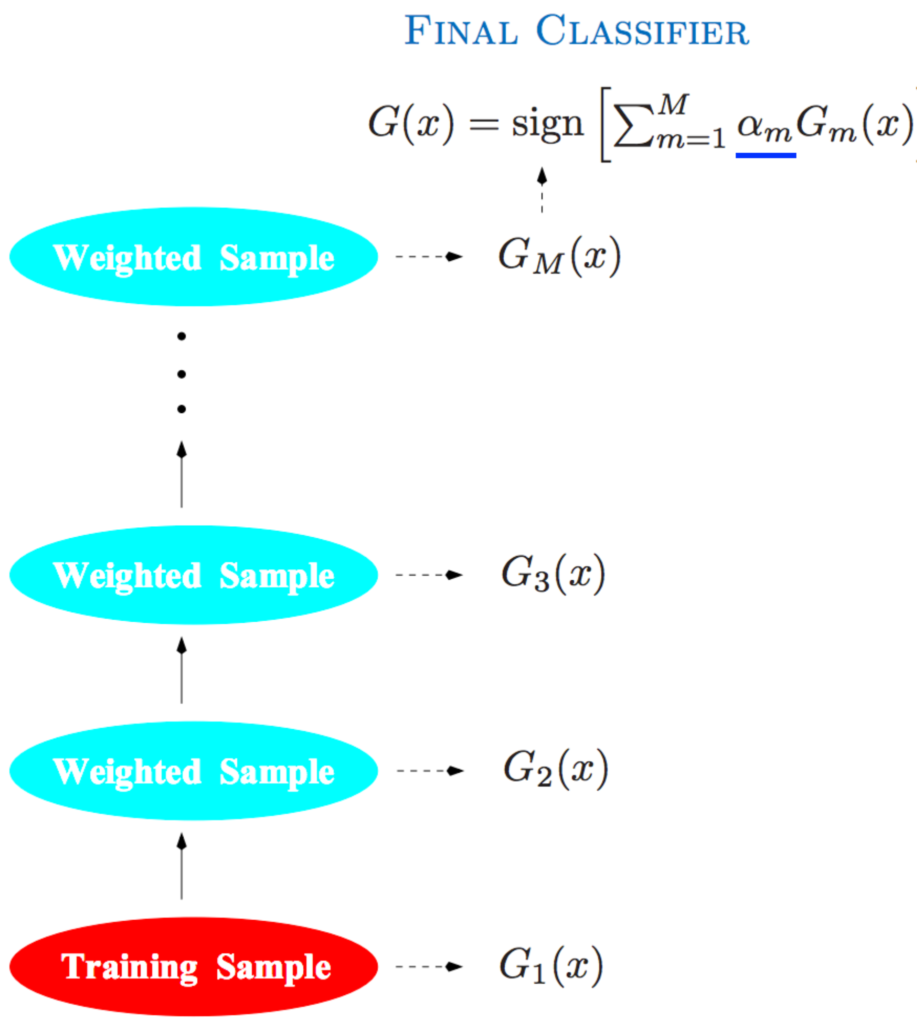
$$\boxed{\overline{\text{err}} = \frac{1}{N}\sum_{i=1}^{N} I(y_i \neq G(x_i))}$$

<u>Discrete AdaBoost</u>

$G_i(x)$ weak classifiers

$G(x)$ strong learner

Note only $G_1(x)$ fit on training



Discrete AdaBoost

1. Initialize the observation weights $w_i = 1/N,\ i = 1, 2, \ldots, N$.
2. For $m = 1$ to M:
   (a) Fit a classifier $G_m(x)$ to the training data using weights w_i.
   (b) Compute
   $$\text{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
   (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
   (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))],\ i = 1, 2, \ldots, N$.
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.

1. Initialize the observation weights $w_i = 1/N$, $i = 1, 2, \ldots, N$.
2. For $m = 1$ to M:
   (a) Fit a classifier $G_m(x)$ to the training data using weights w_i.
   (b) Compute
   $$\text{err}_m = \frac{\sum_{i=1}^N w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^N w_i}.$$
   (c) Compute $\alpha_m = \log((1 - \text{err}_m)/\text{err}_m)$.
   (d) Set $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(x_i))]$, $i = 1, 2, \ldots, N$.
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^M \alpha_m G_m(x)\right]$.

- For first weak classifier, $G_1(x)$, just use training data
- For subsequent weak classifier, same classification algorithm but modify weights
  - If previously misclassified, scale by $e^{\wedge}(\alpha_m)$
  - else, w_i same
- Final strong classifier G(x) determined by weighted majority votes
  - $\alpha_1, \ldots \alpha_M$ as weight of votes
  - The smaller the error of the weak classifier, the greater the weight

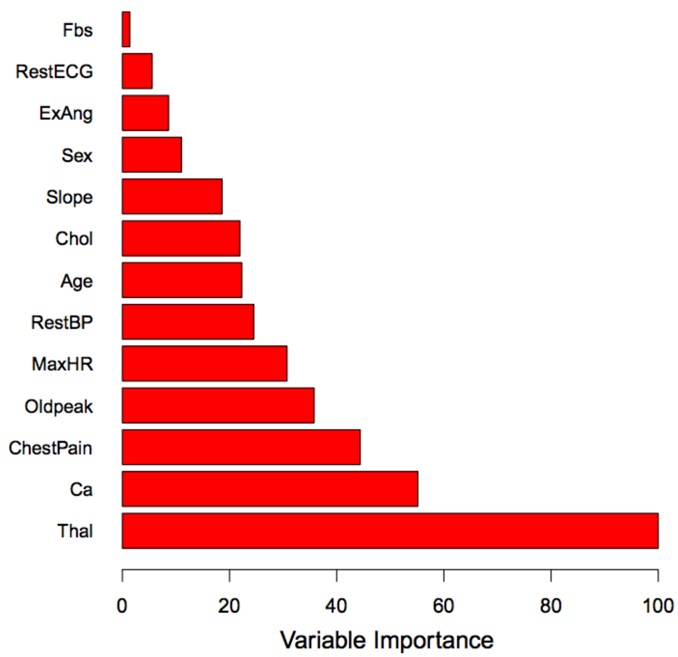
Observe that…

- $\alpha_1, \ldots, \alpha_M$ give higher influence to more accurate classifiers
- At each step m, observations previously misclassified by $G_{m-1}(x)$ have their weights increased

  → Each successive classifier forced to concentrate on training observations previously missed

Bagging/RF/Boosting
Variable Importance

- For bagged/RF regression trees, we record the total amount that the RSS is decreased due to splits over a given predictor, averaged over all B trees. A large value indicates an important predictor.
- Similarly, for bagged/RF classification trees, we add up the total amount that the Gini index is decreased by splits over a given predictor, averaged over all B trees.



Variable importance plot for the `Heart` data

Partial Dependence Plots

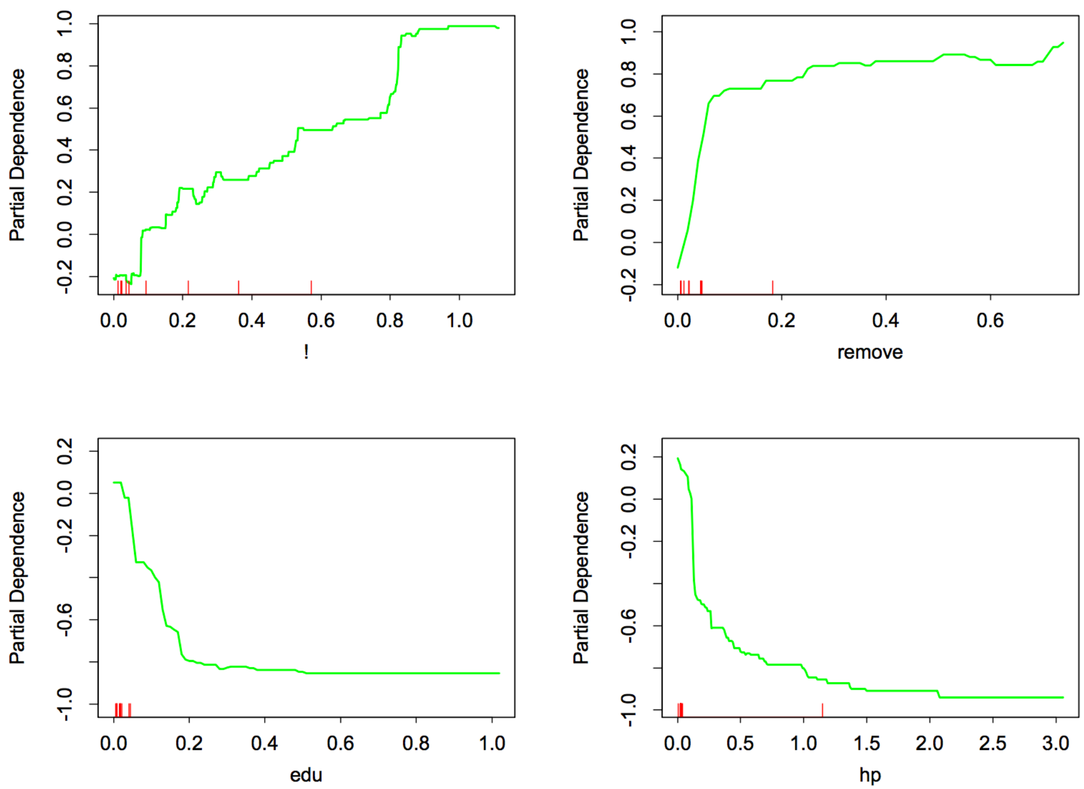


FIGURE 10.7. *Partial dependence of log-odds of* `spam` *on four important predictors. The red ticks at the base of the plots are deciles of the input variable.*

Partial dependence plots show dependence between target function (in this case, proportion of spam as represented by the log-odds), marginalizing over the values of all other features.

Partial Dependence Plots (2 var)

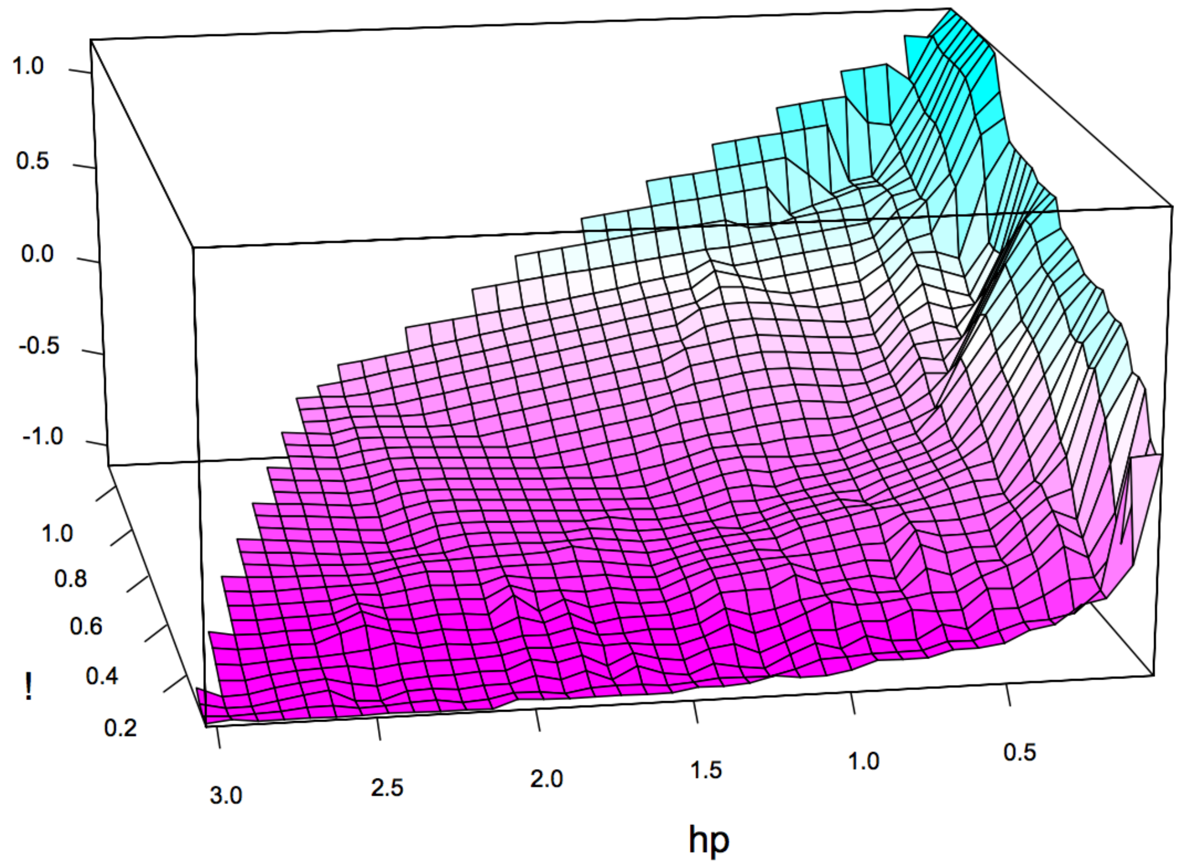


FIGURE 10.8. *Partial dependence of the log-odds of* `spam` *vs.* `email` *as a function of joint frequencies of* `hp` *and the character* `!`.

Questions

- Describe the following tuning parameters for gradient boosting
  - `max_depth`
  - `learning_rate` and `n_estimators`
  - `max_features` and `sub_sample`

- In gradient boosted trees,
  - How do the trees relate to one another?
    - Relate to preceding tree, talk about residuals

Appendix

Boosting Algorithm for Regression Trees

1. Set $\hat{f}(x) = 0$ and $\underline{r_i = y_i}$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   2.1 Fit a tree $\hat{f}^b$ with d splits ($d + 1$ terminal nodes) to the training data (X, r).
   2.2 Update $\hat{f}$ by adding in a shrunken version of the new tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) \underline{+ \lambda \hat{f}^b(x)}.$$
   2.3 Update the residuals,
   $$r_i \leftarrow r_i \underline{- \lambda \hat{f}^b(x_i)}.$$
3. Output the boosted model,
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$$

Simplified version. Easier to understand for building intuition.

Details on GBRT, see page 361
http://web.stanford.edu/~hastie/local.ftp/Springer/OLD/ESLII_print4.pdf

AdaBoost is not black magic

- But there is quite a bit of math and underpinning concepts to go through to really understand it.
  http://web.stanford.edu/~hastie/local.ftp/Springer/OLD/ESLII_print4.pdf - Page 341-346

Very very roughly,

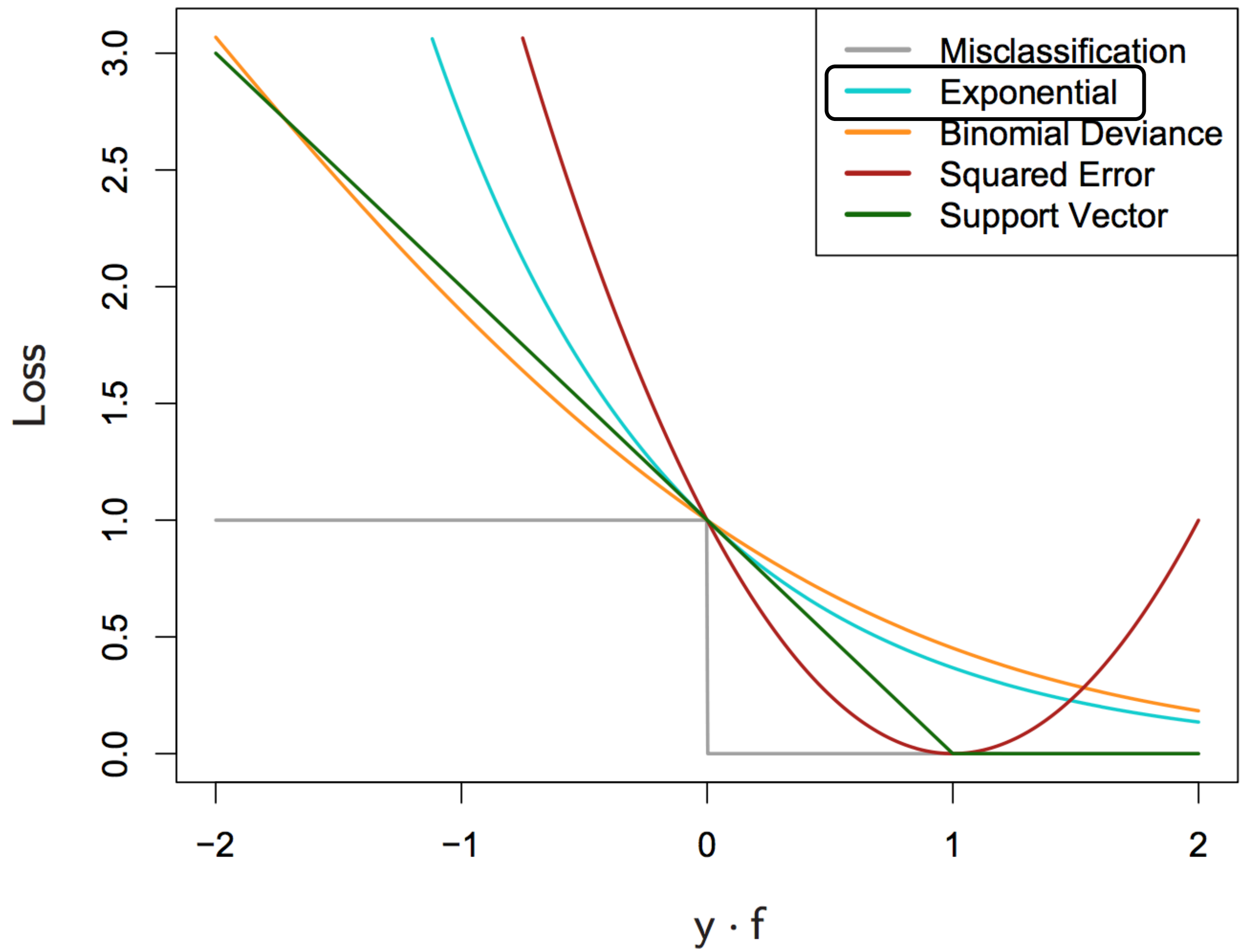
- It is a version of Forward Stagewise Additive Modeling, which adds new basis functions without adjusting previous parameters and coefficients.
  - This contrasts with gradient boosting, see pg 342 vs. pg 361 in link above
  - AdaBoost uses Exponential Loss $L(y, f(x)) = \exp(-y\, f(x))$.
    - It can be shown that to minimize this loss, at each iteration, we can reweight our observations $w_i^{(m+1)} = w_i^{(m)} \cdot e^{\alpha_m I(y_i \neq G_m(x_i))} \cdot e^{-\beta_m}$
  - Use exponential loss because of computational advantage; could consider others.
- Can be shown that the additive expansion in AdaBoost is estimating

$$f^*(x) = \arg\min_{f(x)} \mathrm{E}_{Y|x}(e^{-Yf(x)}) = \frac{1}{2}\log\frac{\Pr(Y=1|x)}{\Pr(Y=-1|x)}$$

which justifies taking the sign as classification rule for final classifier

$$G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$$

Comparison of Loss Functions for Classification



Comparison of Loss Functions for Regression