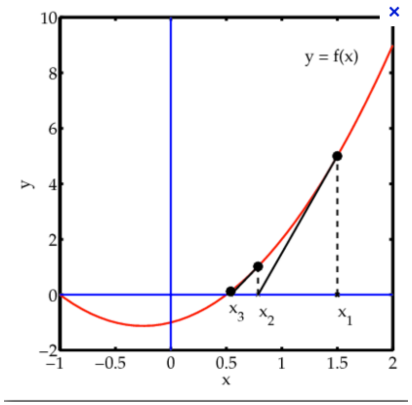
Committee Machines: Boosting Trees



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Outline

- Recap Adaboost
- Trees
- Boosting Trees
- Gradient Boosting motivation
- Steepest Descent
- Gradient Boosting algorithm
- Improving Gradient Boosting
- Interpretation (brief)
- Summary

AdaBoost.M1

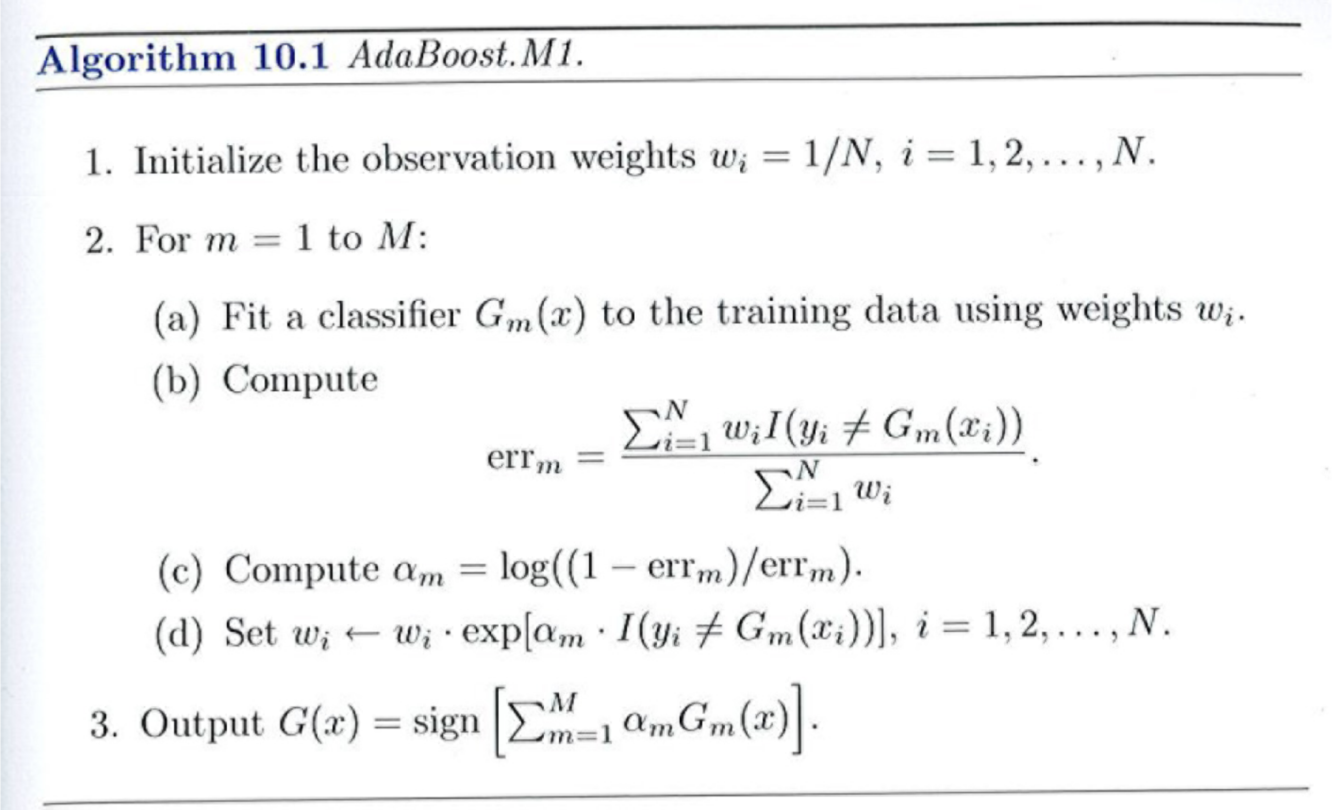
- At each boosting step, weights are applied $w_1, w_2, \ldots, w_N$, to each of the training observations (x_i, y_i), $i = 1, 2, \ldots, N$.

- At the initial step, $w_i = {}^1\!/\!_N$, $\forall i$.

- At each successive iteration, $m = 2, 3, \ldots, M$, the observation weights are individually modified and the classification algorithm is reapplied to the weighted observations.

- At step m, those observations that were misclassified by the classifier $G_{m-1}(x)$ induced at the previous step have their weights increased, whereas the weights are decreased for those that were classified correctly.

AdaBoost.M1



Algorithm 10.1 *AdaBoost.M1.*

```
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
        $$\mathrm{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
    (c) Compute $\alpha_m = \log((1 - \mathrm{err}_m)/\mathrm{err}_m)$.
    (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 $G(x) = \operatorname{sign}\left[\sum_{m=1}^{M} \alpha_m G_m(x)\right]$.
```

AdaBoost.M1 aka “Discrete Adaboost”, because returns a discrete class label.
Real AdaBoost – specifically for real valued predictions.
Others include: gentle adaboost, modest adaboost.

Trees

- Recall: Regression and classification trees partition the model space into disjoint regions: $R_1, R_2, \ldots, R_J$, which are represented as the terminal nodes of the tree.
- A constant γ_j is assigned to each region, such that,

$$x \in R_j \Rightarrow f(x) = \gamma_j.$$

- Thus, a tree can be formally expressed as:

$$T\left(x;\Theta\right) = \sum_{j=1}^{J} \gamma_j I\left(x \in R_j\right),$$

where $\Theta = \left\{R_j, \gamma_j\right\}_1^J$.

- Solution requires numerical optimization:

$$\Theta = \arg\min_{\Theta} \sum_{j=1}^{J} \sum_{x_i \in R_j} L\left(y_i, \gamma_j\right).$$

Trees

2-stage solution:

1. Find γ_j given R_j : trivial, $\hat{\gamma}_j = \bar{y}_j$ by the modeling assumptions.
2. Find R_j : more complicated, use greedy, top-down recursive partitioning algorithm.

Recall: in two dimensions, splitting half planes and enumerating all pairs of split variables and split points.

Boosting Trees

- The Boosted Tree:

$$f_M(x) = \sum_{m=1}^{N} T(x;\Theta_m),$$

Derived in a forward stagewise manner.

- At each step, the minimization problem is solved:

$$\hat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} L\left(y_i, f_{m-1}(x_i) + T(x_i;\Theta_m)\right),$$

over regions and constants $\hat{\Theta}_m = \left\{R_{jm}, \gamma_{jm}\right\}_1^{J_m}$ of the next tree, given the current model $f_{m-1}(x)$.

- As before, given the regions finding the optimal constants in each region is straightforward:

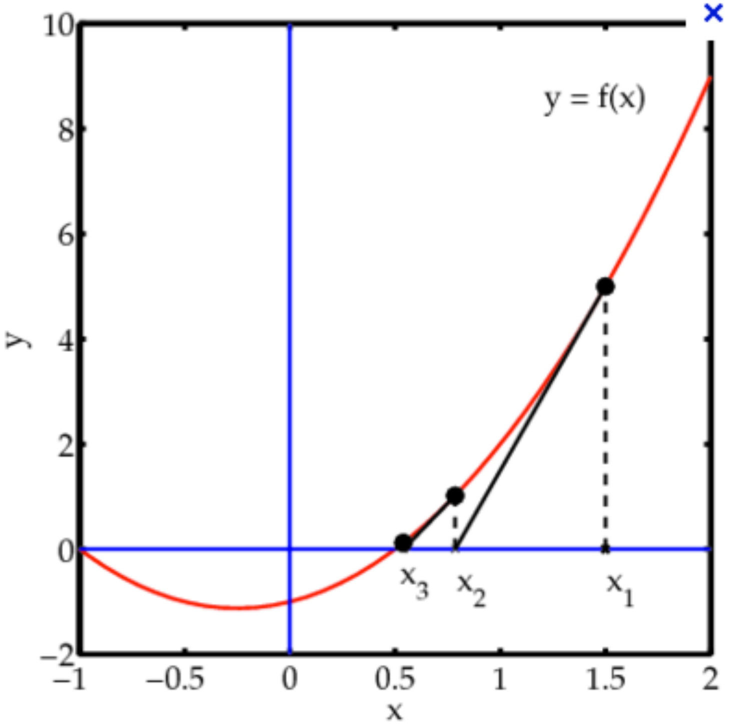
$$\hat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma_{jm}\right),$$

Gradient Boosting

- General boosting algorithm that works well with a variety of different loss functions.
- Gradient boosting builds additive tree models.
- Tree size is the parameter that determines the order of interaction.
- Gradient boosting inherits all the good features of trees (variable selection, missing data, and mixed predictors), and improves on the weak features, and ideally prediction performance.

Gradient Boosting

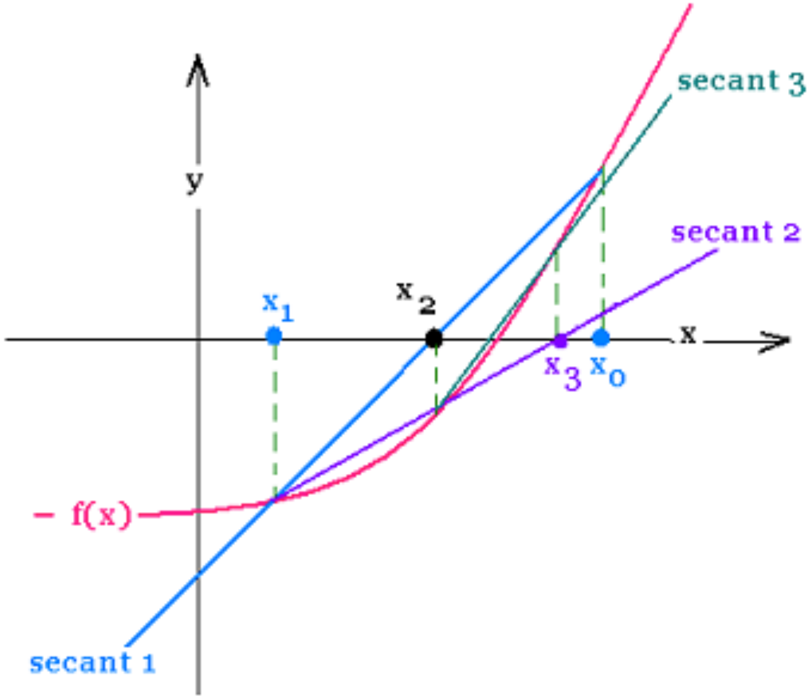
- Newton’s method – find a zero



Gradient Boosting

What if derivatives are unavailable?

- In many practical application $f'(x)$ is not given by a formula
- $f'(x)$ may not exist over the domain.
- Quasi-Newton methods – rely on $f(x)$ only, to approximate the solution. In the simplest case, the secant method.



Gradient Boosting

- Quasi-Newton's methods – find a minimum approximated by gradients.

- Consider a general loss:

$$L(f) = \sum_{i=1}^{N} L\left(y_i, f\left(x_i\right)\right).$$

the goal is to minimize the loss with respect to ( ) .

Constrained to be the sum of trees

Gradient Boosting

- Let the values of the approximating function f at each of the data points x_i be denoted as:

$$\mathbf{f} = \{ f(x_1), f(x_2), \ldots, f(x_N) \}.$$

- The numerical optimization problem:

$$\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} L(\mathbf{f}).$$

where the “parameters” are $\hat{\mathbf{f}} \in \Re^N$.

- The solution can be expressed as a sum of component vectors:

$$\mathbf{f}_M = \sum_{m=0}^{M} \mathrm{h}_M, \quad \mathrm{h}_M \in \Re^N,$$

where $\mathbf{f}_0 = \mathbf{h}_0$ is an initial guess and each successive $\mathbf{f}_m$ is induced based on the current parameter vector $\mathbf{f}_{m-1}$.

Steepest Descent

- The solution is obtained via an iterative method, where the approximated function is updated repeatedly until convergence to the minimum. Updates are called “steps”.

- How long should we step toward the minimum? is not a trivial question.
- What direction should we step? is also not a trivial question.
- The method of steepest descent steps as far as possible in the steepest direction.
- The negated gradient is the steepest downhill direction.

Steepest Descent

- The steepest descent chooses $\mathbf{h}_m = -\rho_m g_m$ where ρ_m is a scalar and $\mathbf{g}_m \in \Re^N$ is the gradient of $L(\mathbf{f})$ evaluated at $\mathbf{f} = \mathbf{f}_{m-1}$.

- The components of the gradient are:

$$g_{im} = \left[\frac{\partial L\left(y_i, f\left(x_i\right)\right)}{\partial f\left(x_i\right)} \right]_{f\left(x_i\right) = f_{m-1}\left(x_i\right)}$$

  and the step length ρ_m is the solution to:

$$\rho_m = \arg\min_{\rho} L\left(\mathbf{f}_{m-1} - \rho_m g_m\right).$$

- The update: $\mathbf{f}_m = \mathbf{f}_{m-1} - \rho_m g_m$.

Gradient Boosting

- Steepest descent would be ideal if only concerned with minimizing the loss:

$$L(f) = \sum_{i=1}^{N} L\left(y_i, f(x_i)\right).$$

However, the gradient is only defined at training points x_i therefore, the approach may not be accurate to new data. The ultimate goal is to generalize $f_M(x)$ to new data.

- A resolution is to induce a tree $\left\{T(x_i;\Theta_m)\right\}$ as close as possible to the negative gradient,

$$\Theta_m = \arg\min_{\Theta} \sum_{i=1}^{N} \left(-g_{im} - T(x_i;\Theta)\right)^2$$

Note that the resulting regions will not be the same, but they will be close. The corresponding $\hat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma_{jm}\right),$

Gradient Boosting

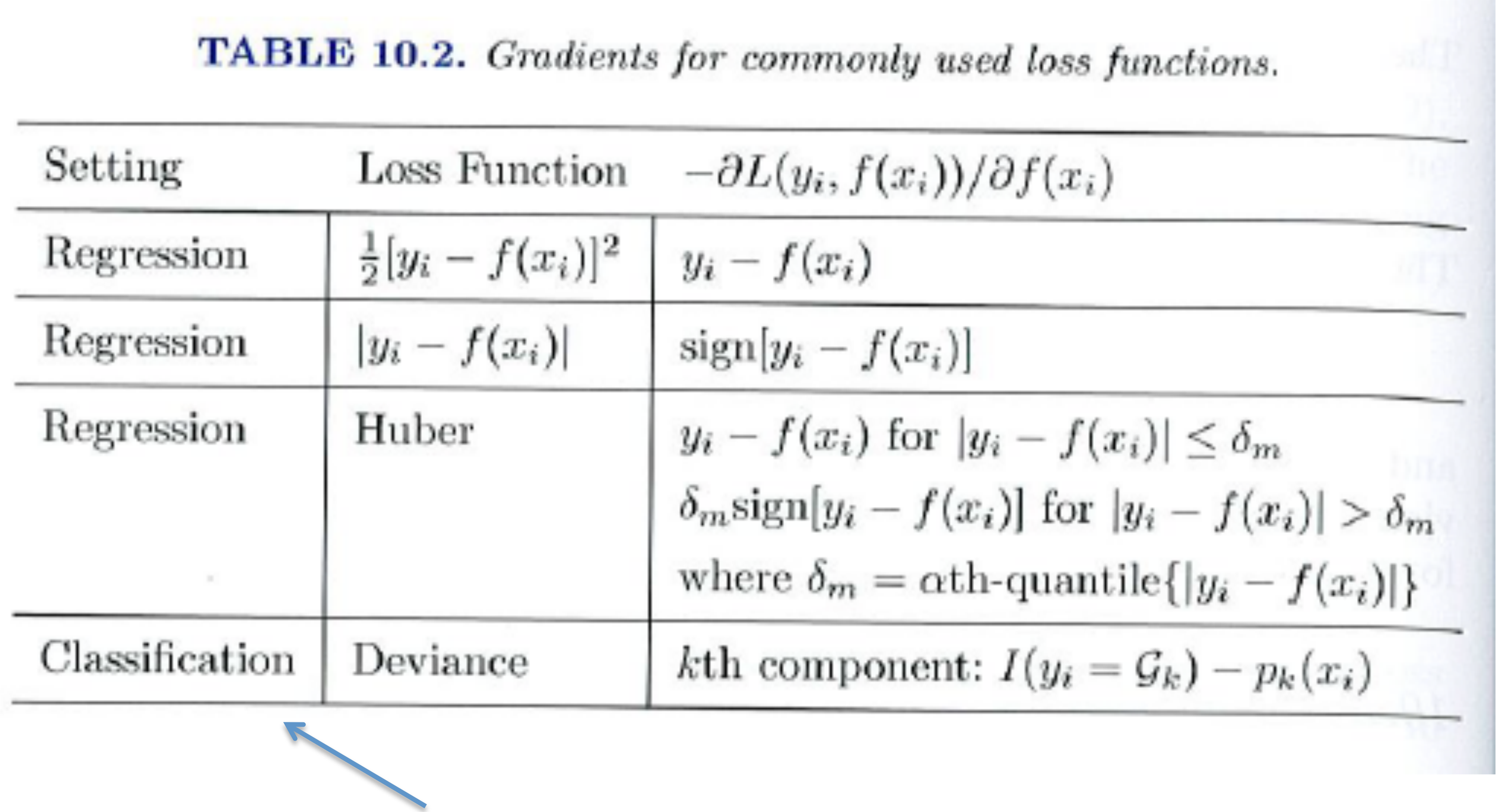
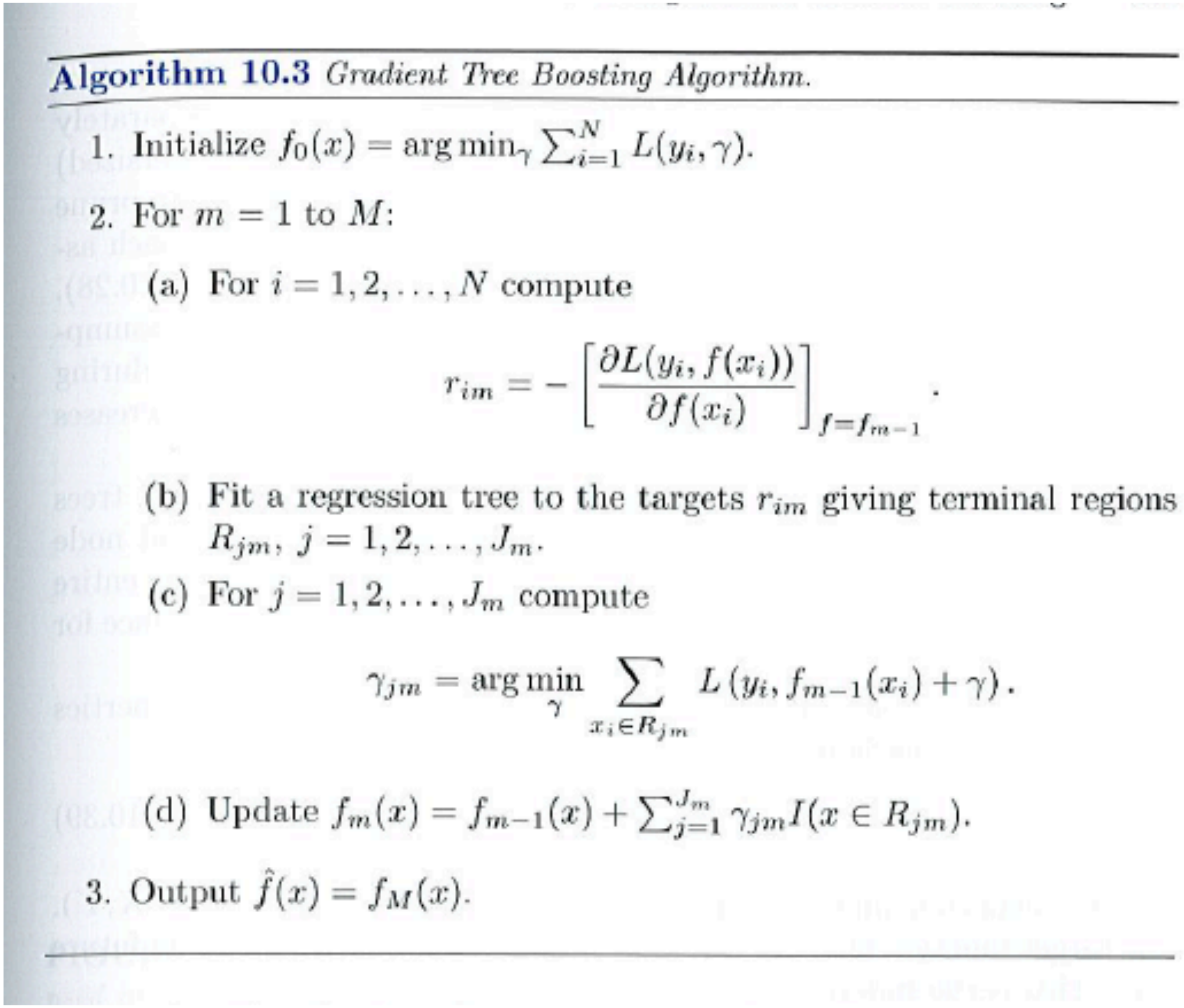


TABLE 10.2. *Gradients for commonly used loss functions.*

Setting	Loss Function	$-\partial L(y_i, f(x_i))/\partial f(x_i)$
Regression	$\frac{1}{2}[y_i - f(x_i)]^2$	$y_i - f(x_i)$
Regression	$\lvert y_i - f(x_i)\rvert$	$\text{sign}[y_i - f(x_i)]$
Regression	Huber	$y_i - f(x_i)$ for $\lvert y_i - f(x_i)\rvert \leq \delta_m$ $\delta_m \text{sign}[y_i - f(x_i)]$ for $\lvert y_i - f(x_i)\rvert > \delta_m$ where $\delta_m = \alpha\text{th-quantile}\{\lvert y_i - f(x_i)\rvert\}$
Classification	Deviance	kth component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$

K least squares trees are constructed at each iteration.
Each tree is fit to its corresponding gradient vector.
*Only one tree is needed for binary classification.

Gradient Boosting (MART)



Algorithm 10.3 *Gradient Tree Boosting Algorithm.*

```
1. Initialize $f_0(x) = \arg\min_\gamma \sum_{i=1}^{N} L(y_i, \gamma)$.
2. For $m = 1$ to $M$:
   (a) For $i = 1, 2, \ldots, N$ compute
       $r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}$.
   (b) Fit a regression tree to the targets $r_{im}$ giving terminal regions
       $R_{jm},\ j = 1, 2, \ldots, J_m$.
   (c) For $j = 1, 2, \ldots, J_m$ compute
       $\gamma_{jm} = \arg\min_{\gamma} \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma\right)$.
   (d) Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.
3. Output $\hat{f}(x) = f_M(x)$.
```

Tree Size

- Tree size – one approach, decide independently. Does not work well in practice for the boosting.
- Alternative strategy: require all of the trees to be the same size $J_m = J, \ \forall m$, where J_m is a j-terminal node tree.
- *J* is a meta-parameter.

What is the effect of different size J?

Tree Size

- Interaction level is limited to tree size and this constraint carries over to boosted tree.

  Example:

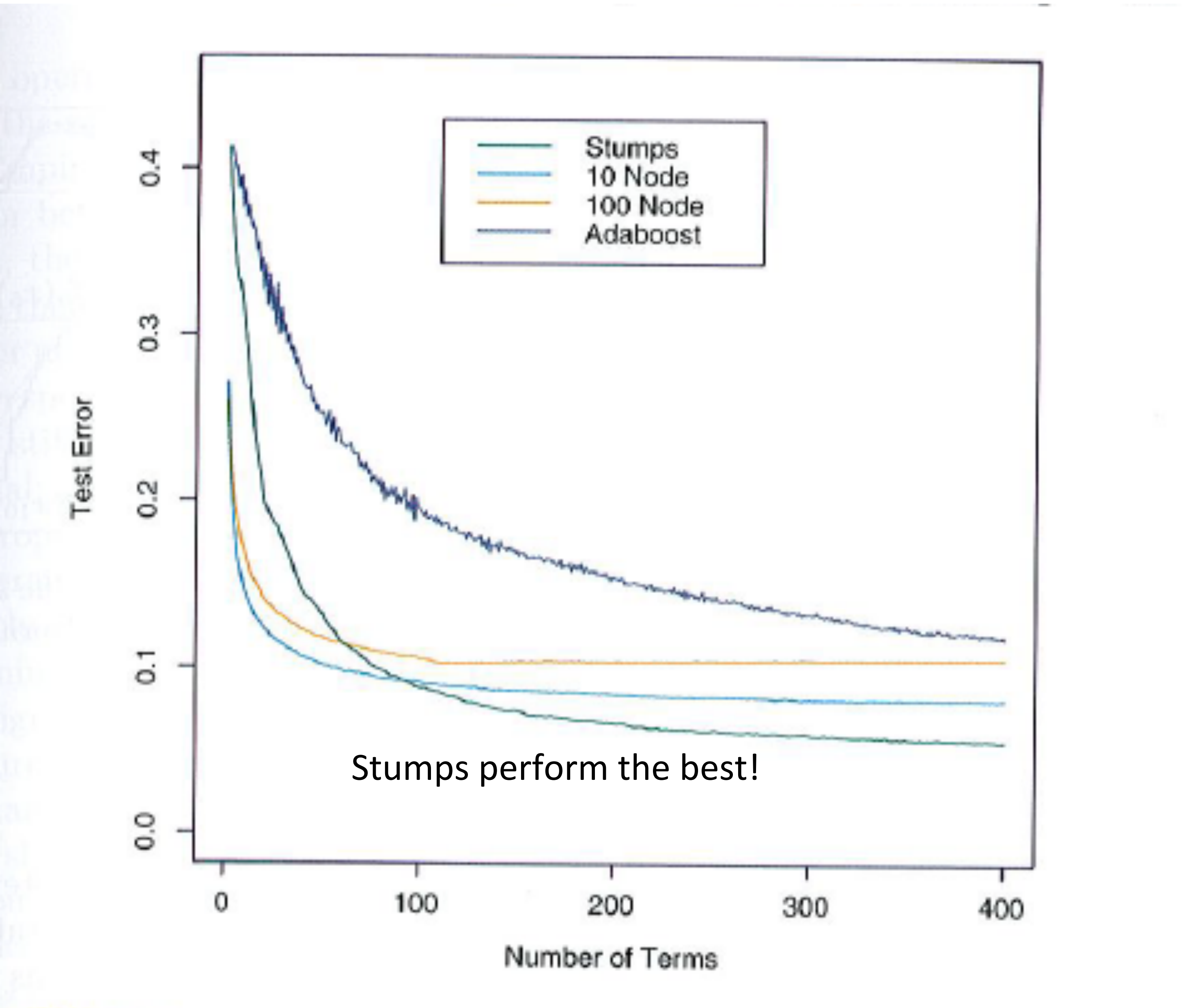
  J = 2 ~ produces a boosted model with only main effects.

  J = 3 ~ 2 variable interactions permitted.

- The value of J should reflect knowledge about the number of interactions (usually unknown, but most often low).

  Rule of thumb: J=2 too small, J>10 too big, between 4 and 10 is good.

Tree Size



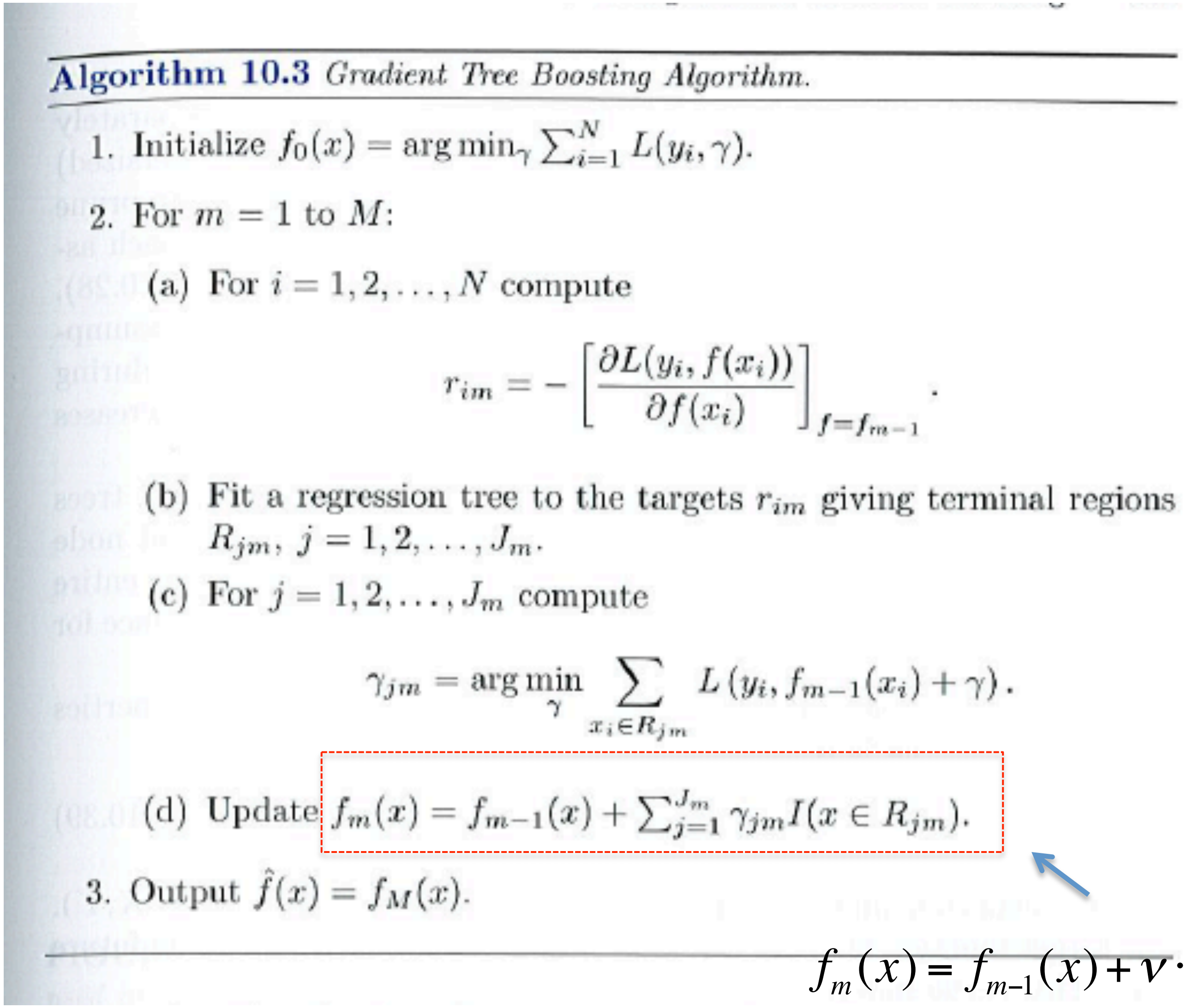
Stumps perform the best!

Shrinkage

- The second consideration, how many trees to include in the boosting.
- Same issues wrt overfitting.
- Strategy: model prediction risk (error) on a validation sample.

  Find the M^* that minimizes the predicted risk.

Shrinkage



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    (d) Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.
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```

$$f_m(x) = f_{m-1}(x) + \nu \cdot \sum_{j=1}^{J} \gamma_{jm} I\left(x \in R_{jm}\right)$$

Shrinkage

$$f_m(x) = f_{m-1}(x) + \nu \cdot \sum_{j=1}^{J} \gamma_{jm} I\left(x \in R_{jm}\right)$$

- Now we have another complexity parameter that also controls prediction risk.
- Inverse relationship between ν and M.
- Empirically, it has been shown that smaller values of ν favor better test error and require corresponding larger values of M.

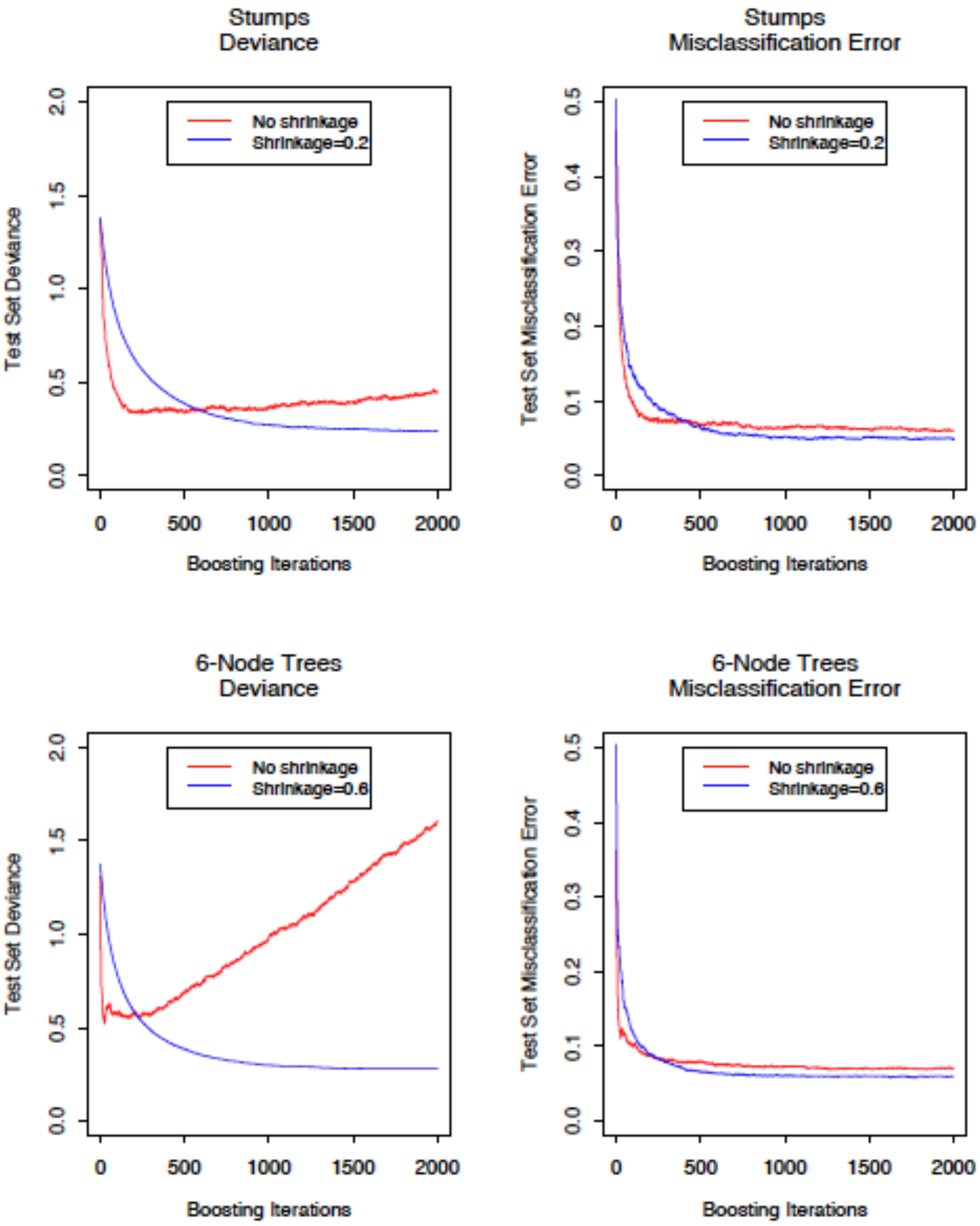
Another possibility…. Subsampling.

Deviance

Misclassification Rate

Stumps

6 Node Tree



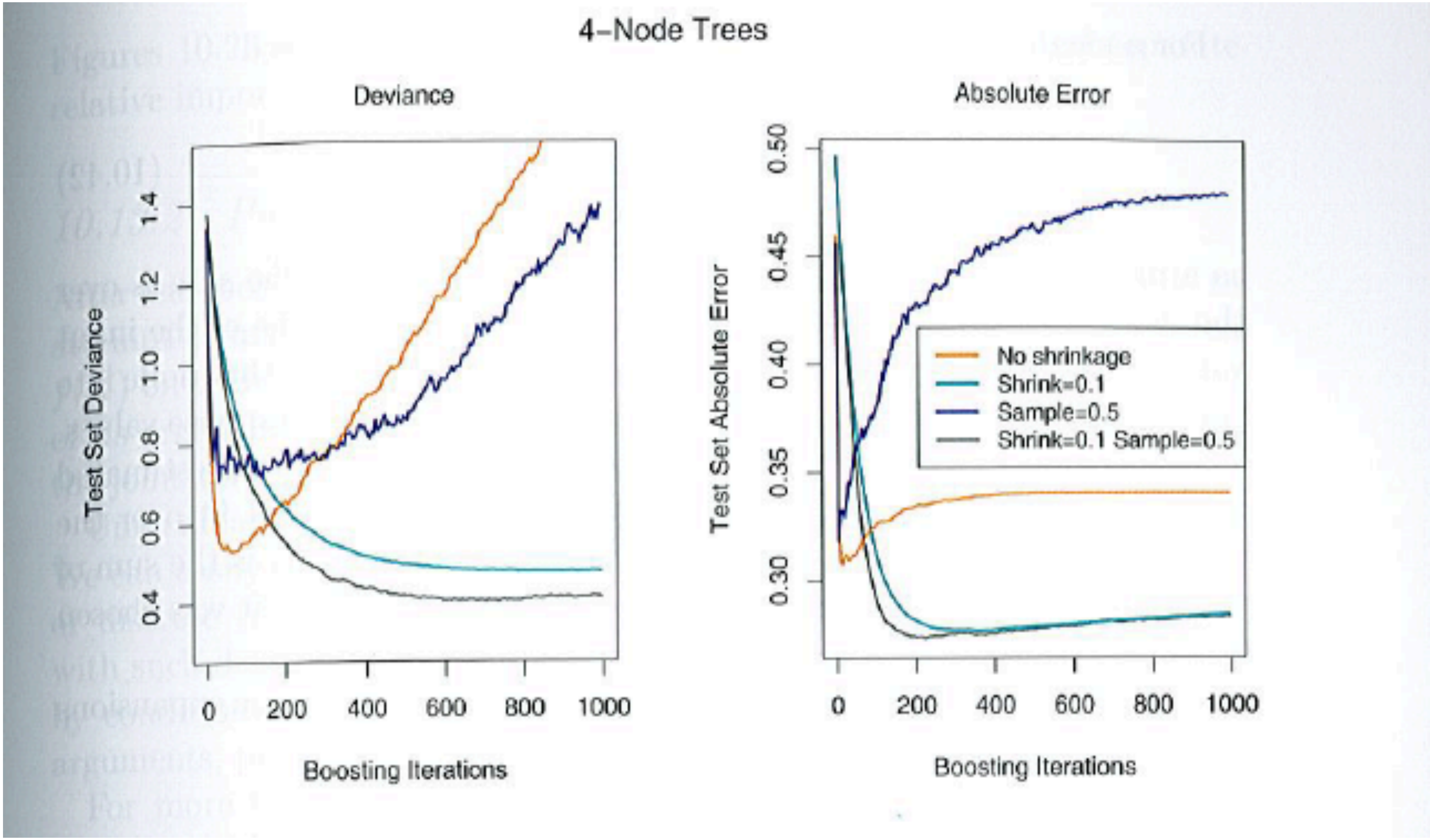
Red: Shrinkage
Blue: No Shrinkage

Number of Trees

Stochastic Gradient Boosting ~ at each iteration, we sample a fraction of the training data η without replacement. Grow the next tree using the subsample.

- Reduction in computation
- Often produces a more accurate model when used with shrinkage.
- We are up to four complexity parameters: $J, M, \nu,$ and η.

Number of Trees



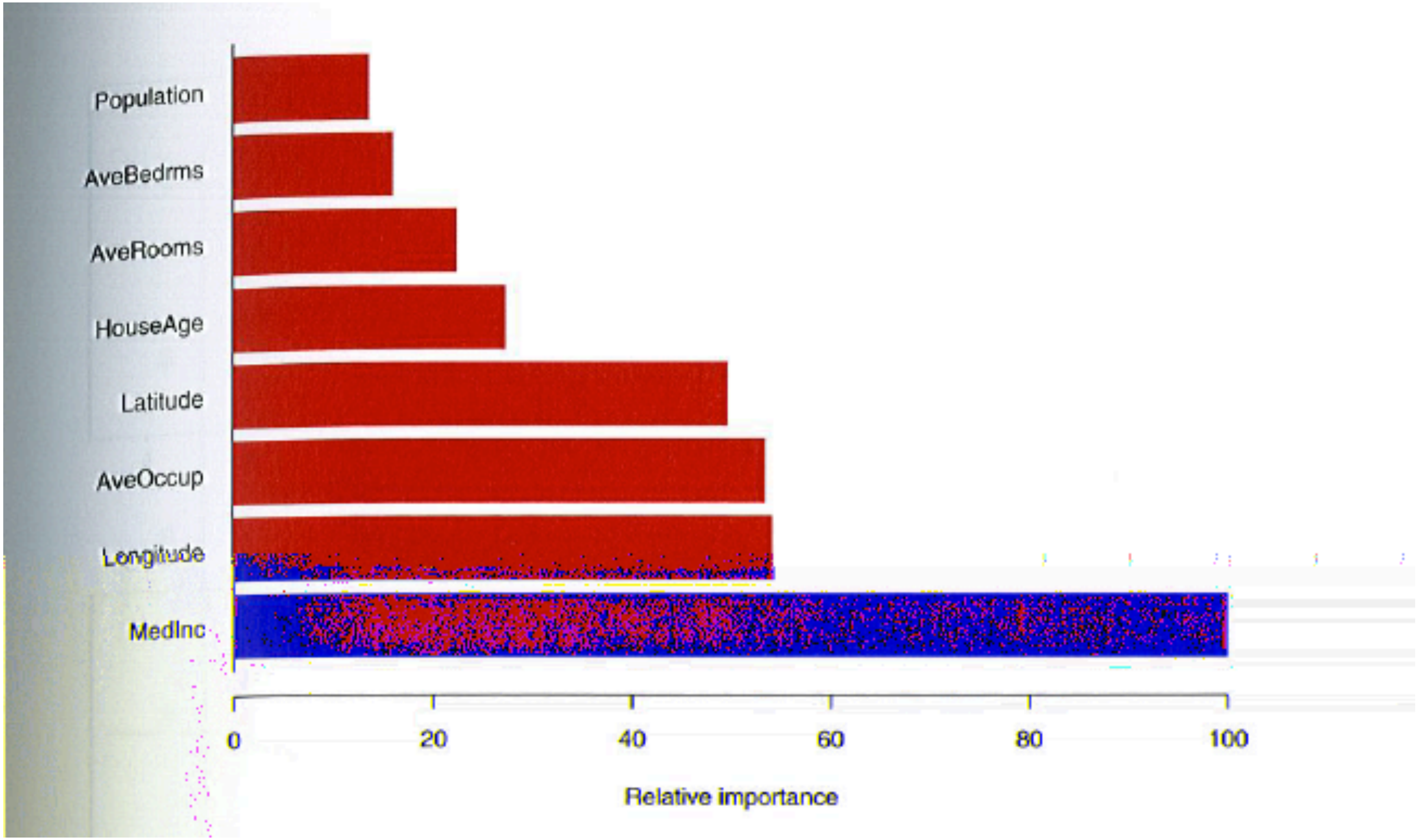
Interpretation

- Interpretation is lost with boosting.
- We need to rely on alternative metrics to reveal the model structure.

Relative Importance of a Predictor variable.

- Often many nuisance predictors which cloud model interpretation.
- Important to understand how important a variable is in predicting response, and dividing classes.

Relative Importance



Summary

- Boosting trees is complicated.
- Steepest descent a good idea… but prone to being too "greedy" by nature of the step.
- Gradient boosting a "less greedy" alternative.
- Main idea: fit trees to "residuals" defined as gradient function evaluations. Update functional approximation in an iterative manner. (Quasi-Newton like).
- Several improvements can be made to gradient boosting, including: subsampling, and shrinkage.
- Lots of parameters have to be set: number of trees, depth, subsampling, and shrinkage!

But….. It really works!