Ensemble Methods (Part II) Gradient Boosting

Schwartz

September 12, 2016

The most powerful prediction algorithm on the planet

In “The BellKor Solution to the Netflix Grand Prize” Yehuda Koren reported on the use of gradient boosted decision trees (GBDT) in the top performing algorithm.

The Netflix Prize was an open competition for the best collaborative filtering algorithm to predict user ratings for films. The competition was open to anyone not connected with Netflix or a resident of Cuba, Iran, Syria, North Korea, Myanmar or Sudan. On 21 September 2009, the grand prize of $1,000,000 was given to the Pragmatic Chaos team which bested Netflix’s own prediction algorithm by 10.06%.

Netflix Prize COMPLETED

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Leaderboard

Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace	0.8612	9.59	2009-07-24 17:18:43

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- *Critique* and *Sell* gradient boosting

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Can many *sequential weak learners* be used to make a powerful prediction tool?

Do you think such an approach could suffer from overfitting?

Sequential Estimators Notation

- Let W be an untrained weak learner and $\phi_k(\boldsymbol{x})$ be an estimator that predicts outcome Y based on features $\boldsymbol{x}$

  Define a new estimator

  $$\phi_{k+1}(\boldsymbol{x}) = \phi_k(\boldsymbol{x}) + \alpha_k W(\boldsymbol{x}, \gamma_k)$$

  where W is trained on $\boldsymbol{x}$ "in the presence" of $\phi_k(\boldsymbol{x})$

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  So W is a stump – a weak learner*
- W is fit to *improve* the available prediction of Y from $\phi_k(\boldsymbol{x})$
- But the negligible impact of W^* will be further muted by α_k
- α_k **controls the learning rate of the boosting algorithm**

Compare and Contrast

(A) Tree
(B) Bagging
(C) Random Forests
(D) Sequential Weak Learners

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(A) Tree $\hat{f}^{(1)}(\boldsymbol{x})$

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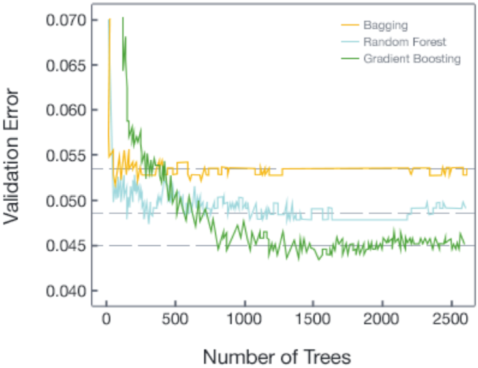
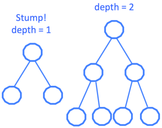


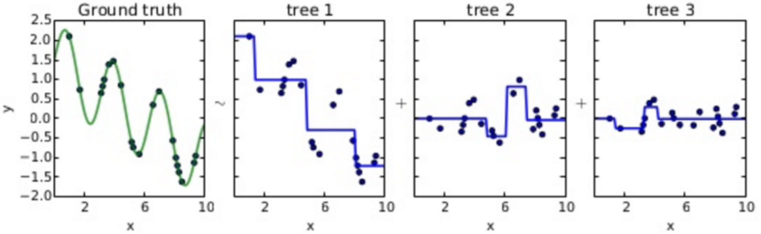
Fitting regressions on sequential residuals

- if we use squared error loss

$$L(Y_i, \phi_k(\boldsymbol{x}_i)) = \frac{1}{2}(Y_i - \phi_k(\boldsymbol{x}_i))^2$$

then the direction of the gradient is vector ϵ of residuals





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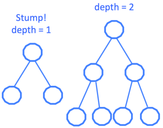

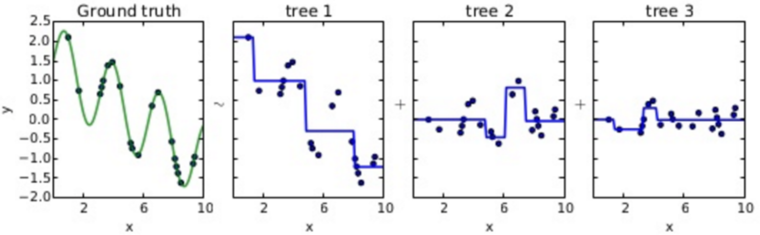

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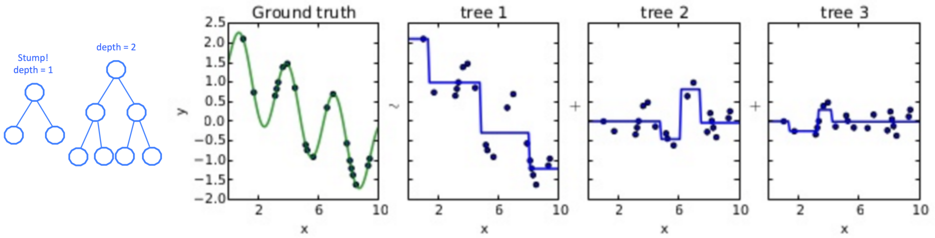

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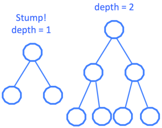

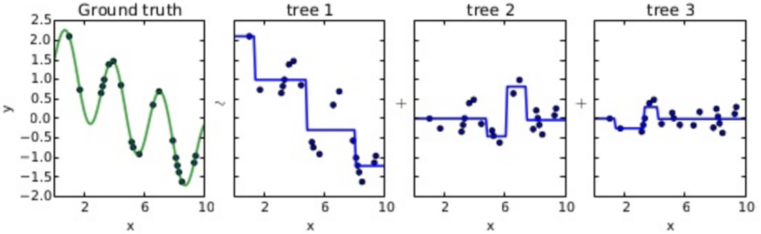

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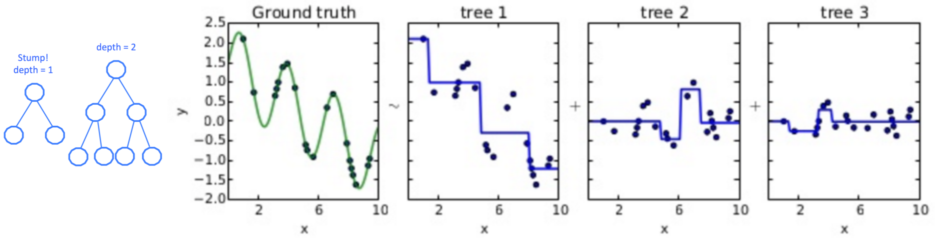

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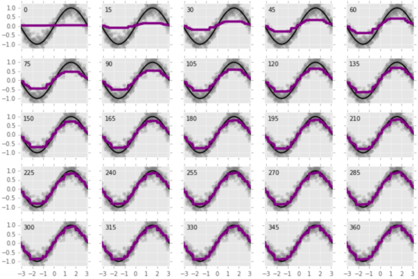

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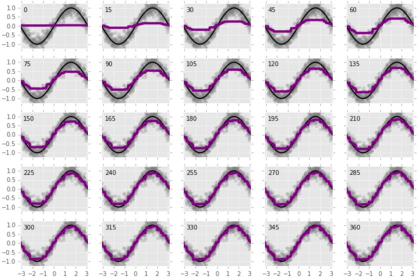

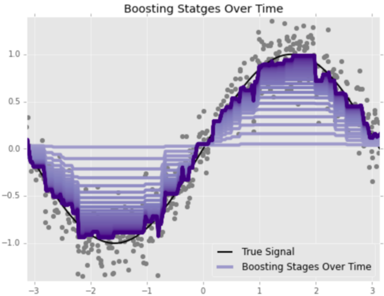

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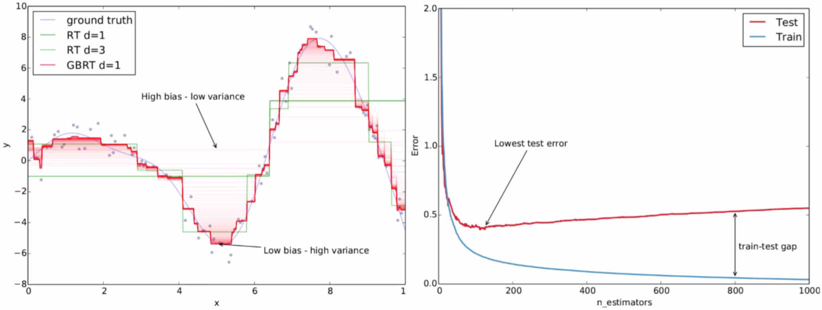

https://www.r-bloggers.com/an-attempt-to-understand-boosting-algorithms/

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gives the instantaneous Δ in $L(Y_i, \hat{Y}_i)$ at $\hat{Y}_i \longrightarrow \hat{Y}_i + \epsilon$

I.e., it tells how the loss function changes as $\hat{Y}_i$ increases

(this is a very simple idea with somewhat complex notation)

Gradient Decent

- But if we have partial derivatives we can use gradient decent

$$\nabla_{\hat{\boldsymbol{Y}}} L(\boldsymbol{Y}, \hat{\boldsymbol{Y}}) = \begin{bmatrix} \frac{\partial L(Y_1, \hat{Y}_1)}{\partial \hat{Y}_1} \\ \frac{\partial L(Y_2, \hat{Y}_2)}{\partial \hat{Y}_2} \\ \vdots \\ \frac{\partial L(Y_i, \hat{Y}_i)}{\partial \hat{Y}_i} \\ \vdots \\ \frac{\partial L(Y_n, \hat{Y}_i)}{\partial \hat{Y}_n} \end{bmatrix}$$

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to move in the direction of greatest decrease in loss

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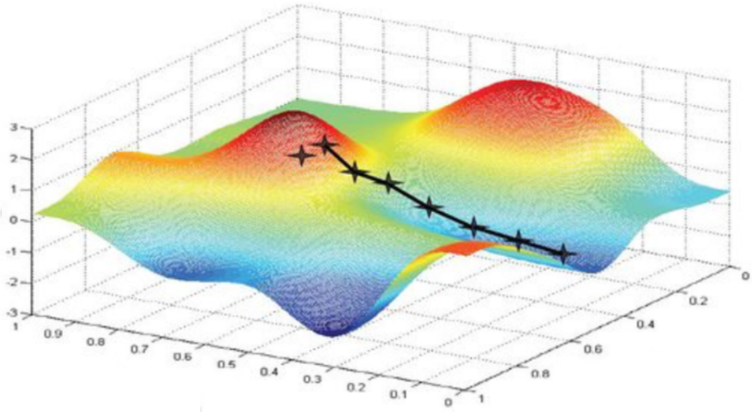

The direction of maximal increase is the the gradient of a function

(The negative of the gradient is the direction of maximal decrease)

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- But $\hat{\boldsymbol{Y}} = \{\hat{Y}_1, \hat{Y}_2, \cdots \hat{Y}_n\}$ so we compromise between all Δ_i^k

$$\hat{W}(\cdot, \gamma_k) = \underset{W(\cdot,\gamma_k)}{\operatorname{argmin}} \sum_{i=1}^{n} D(\Delta_i^k, W(\boldsymbol{x}_i, \gamma_k))$$

and set

$$\phi_{k+1}(\boldsymbol{x}) = \phi_k(\boldsymbol{x}) + \alpha_k \hat{W}(\boldsymbol{x}, \gamma_k)$$

where $\hat{W}(\cdot, \gamma_k)$ is a *weak learner* boosted at *learning rate* α_k

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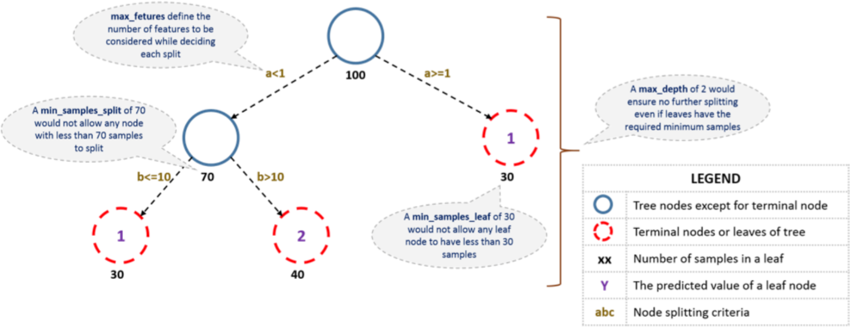

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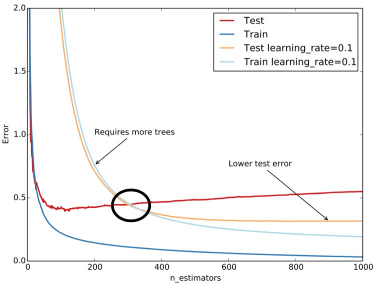
- Nonetheless, number of leaves, depth, minimum split size, minimum leaf, size, and restricted features* can be tuned...
- The learning rate/number of trees α/m needs to be tuned

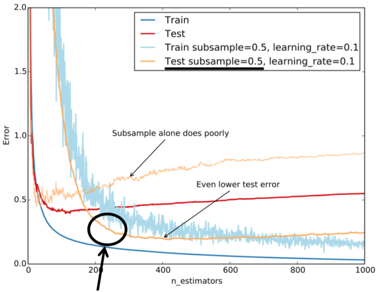
```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.grid_search import GridSearchCV
param_grid = {'learning_rate': [0.001, 0.01, 0.1],
              'max_depth': [4, 6],
              'min_samples_leaf': [4, 8, 16],
              'max_features': [0.75, 0.9, 1]}
model = GradientBoostingRegressor(n_estimators=3000)
gs_cv = GridSearchCV(model, param_grid).fit(X, y)

gs_cv.best_params_, gs_cv.best_score_, gs_cv.best_estimator_
```

Gradient Boosting *Tuning*

Gradient Boosting is typically applied using trees

- Shallow trees (stumps?) provide weak learners/reduce tuning
- Nonetheless, number of leaves, depth, minimum split size, minimum leaf, size, and restricted features* can be tuned...
- The learning rate/number of trees α/m needs to be tuned
- Stochastic Gradient Boosting using subsamples also available





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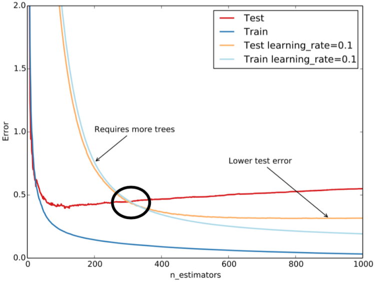

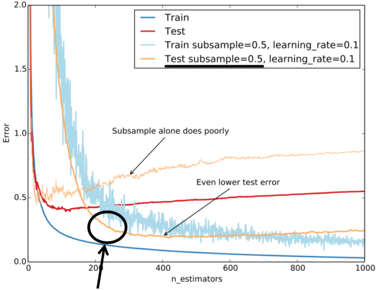

Buy or Sell Gradient Boosting?

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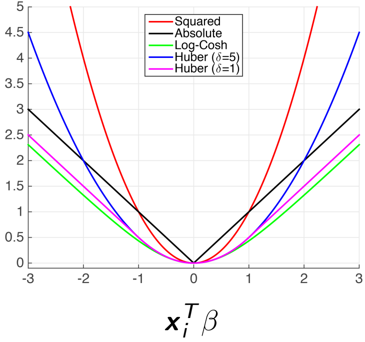
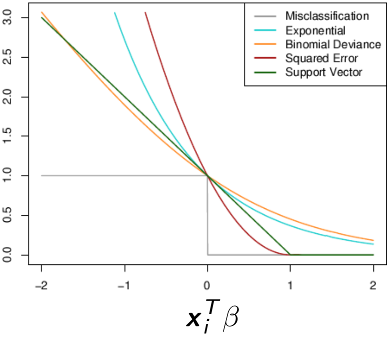
Why does this work better than Random Forests, etc.?

More loss functions

<u>Regression</u>		
Squared Loss	$\frac{1}{2}(y_i - \boldsymbol{x}_i^T\beta)^2$	
Absolute Loss	$\lvert Y_i - \boldsymbol{x}_i^T\beta\rvert$	
<u>Classification</u>		
Log Loss	$1 - \frac{1}{1+e^{-\boldsymbol{x}_i^T\beta}}$	(Bernoulli Deviance/Logistic Reg.)
Exponential Loss	$\exp(-y_i \cdot \boldsymbol{x}_i^T\beta)$	(Ada Boost)





AdaBoost (Adaptive Boosting)

$Y \in \{-1, 1\}$

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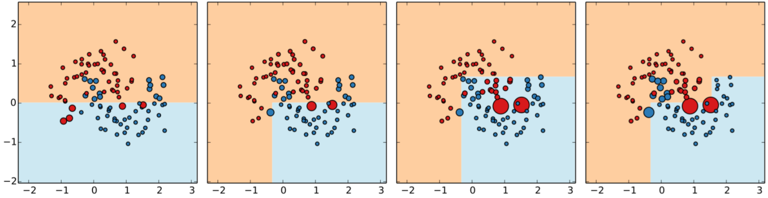

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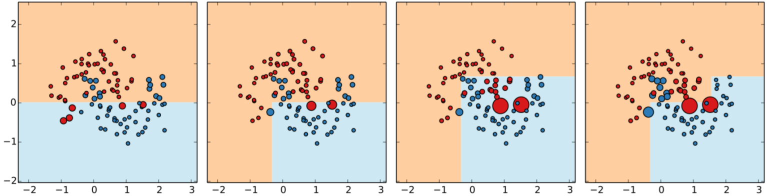

*Sean Sall's slides have an appendix showing that AdaBoost is exponential loss

XGBoost (eXtreme Gradient Boosting)

- Faster/More Efficient
- Features are binned into percentiles for splitting (smaller search space)
- Handles missing data
- Handles mixed data types
- Allows for out-of-core computation
- Builds in smart memory management
- Install using pip – it has an sklearn interface