Ensemble Methods (Part II)
Gradient Boosting

Schwartz

January 5, 2017

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%. "The Ensemble" tied the best score 19 minutes and 56 seconds later but got nothing. BellKor's solution hasn't been used in production as it is "too complicated". Today gradient boosting (usually in the form of XGBoost) satisfies itself with being the winningest algorithm in much smaller challenges such as Kaggle competitons.

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- *Critique* and *Sell* gradient boosting
  - As compared to other ensemble methods

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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

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

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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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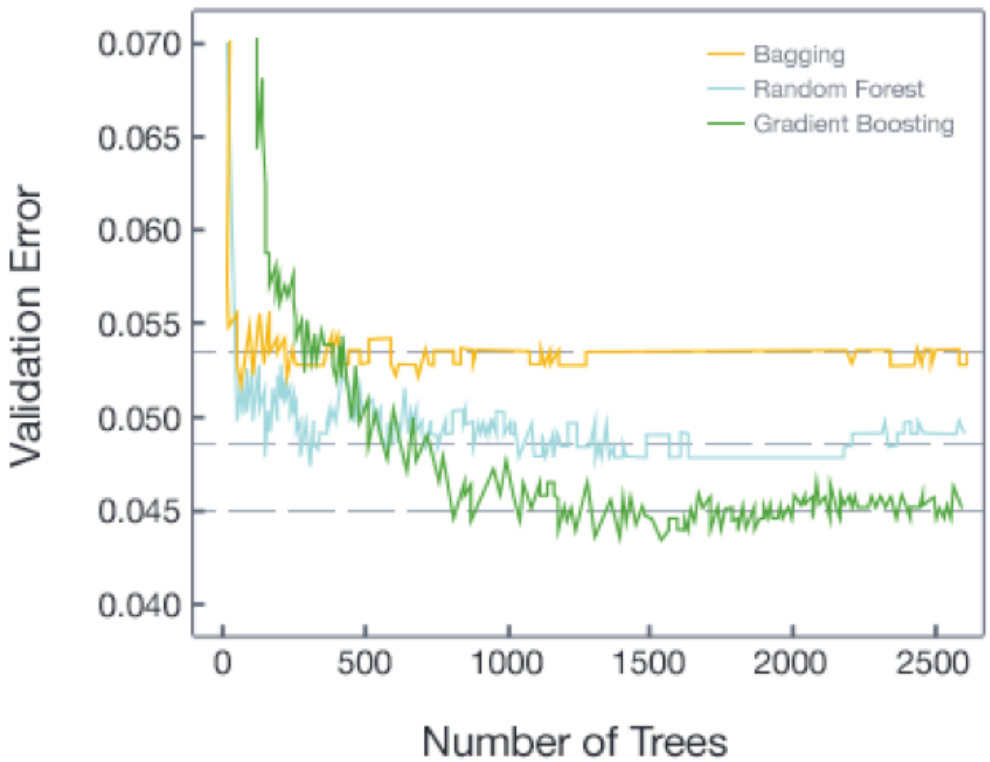

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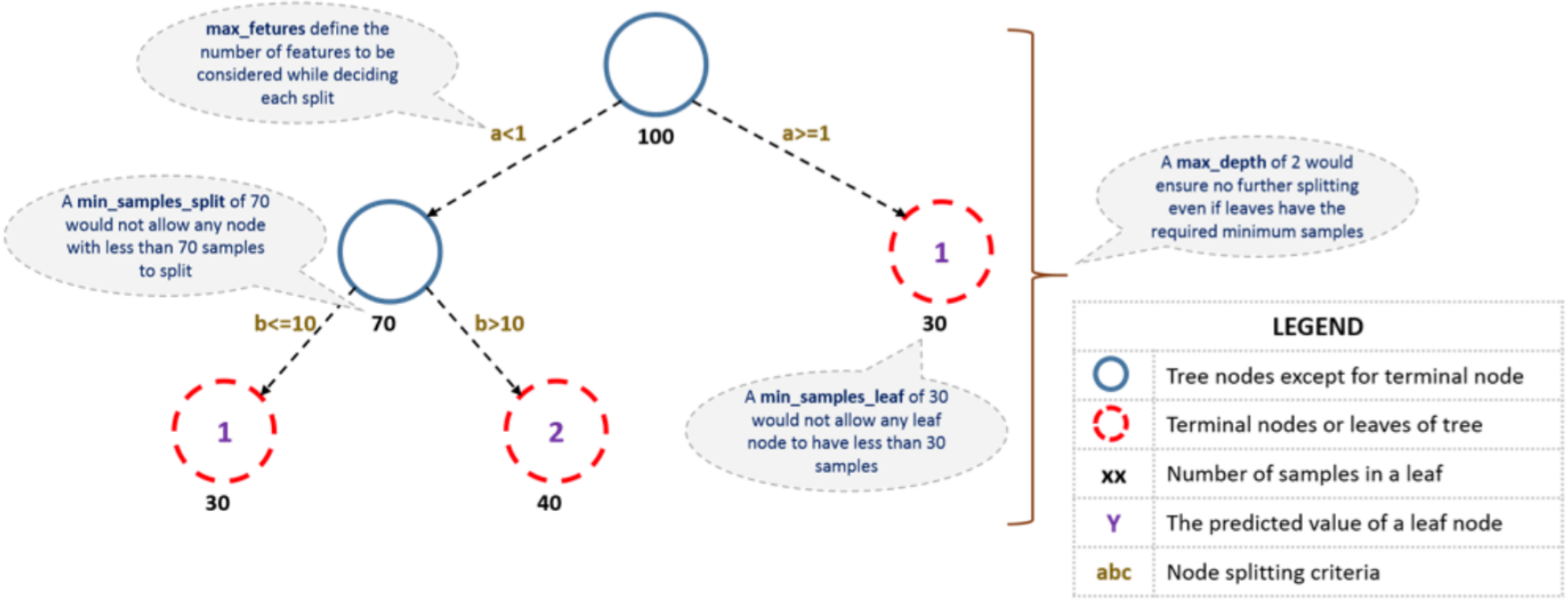

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```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.grid_search import GridSearchCV
param_grid = {'learning_rate': [0.001, 0.01, 0.1],
              'max_depth': [4, 6],
              'min_samples_leaf': [4, 8, 16],
              '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_
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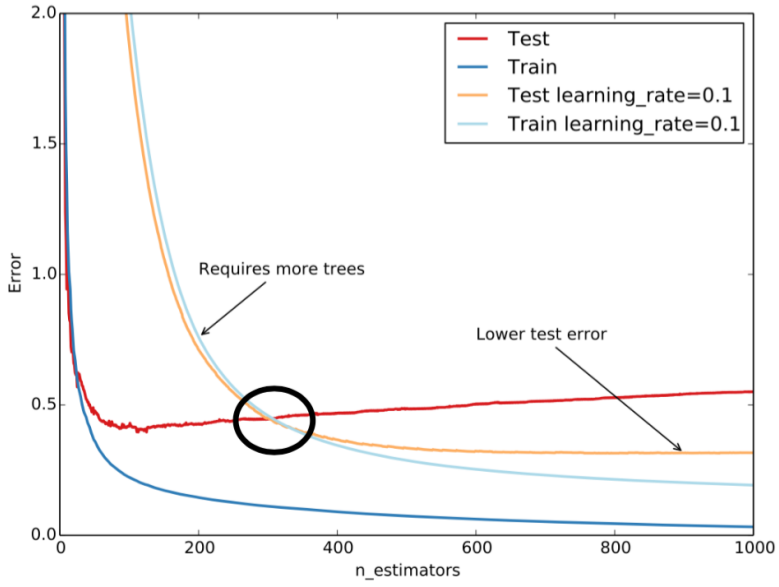

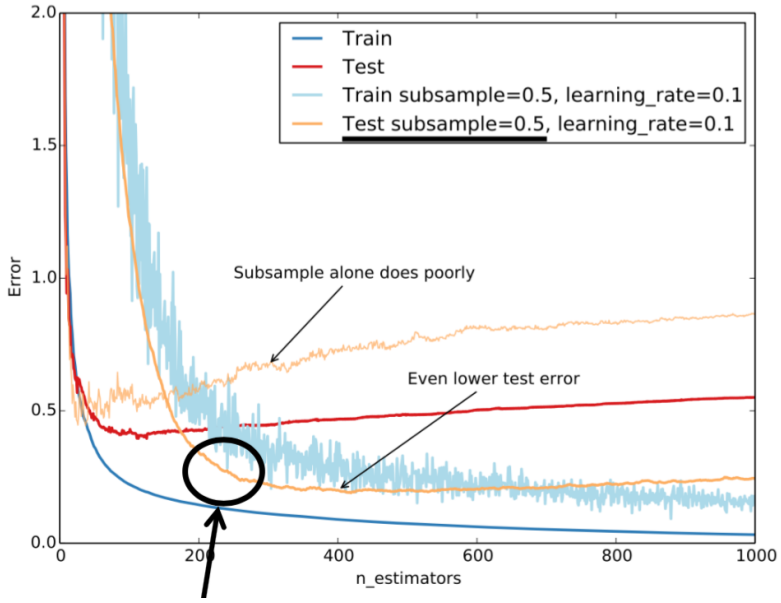

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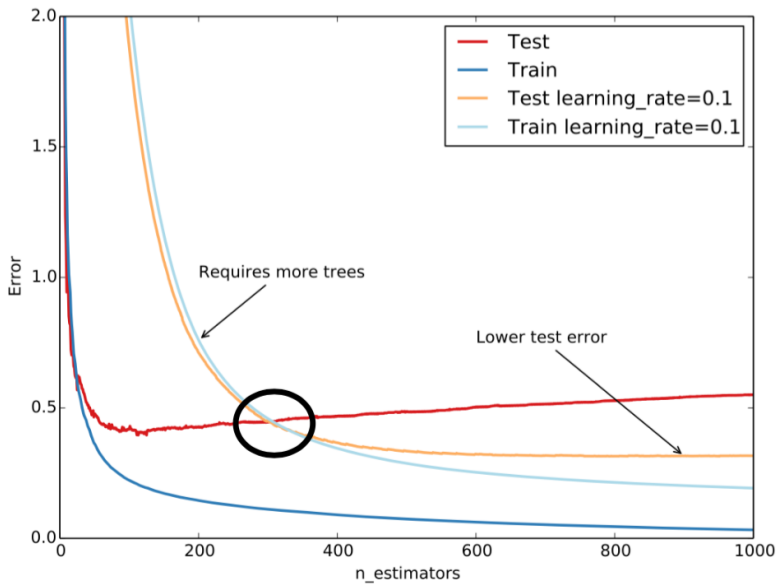
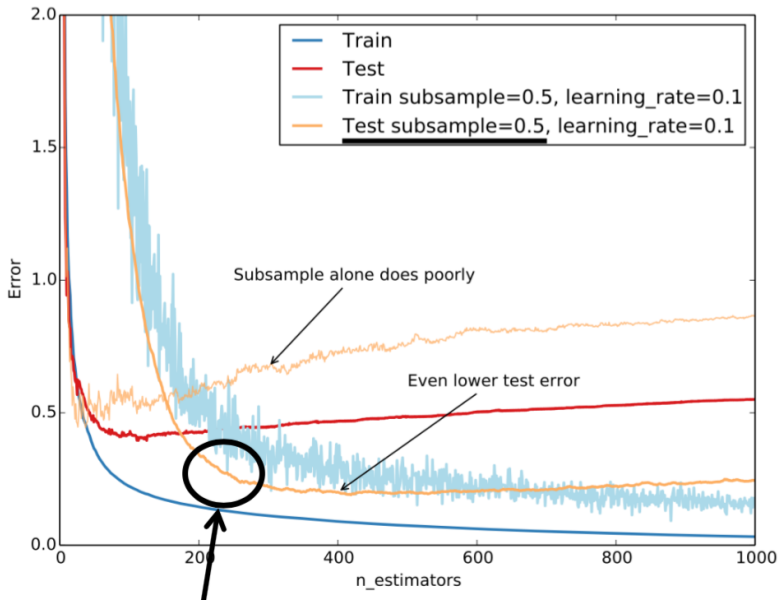
- Stochastic Gradient Boosting using subsamples also available
- Careful parameter tuning is necessary for good performance





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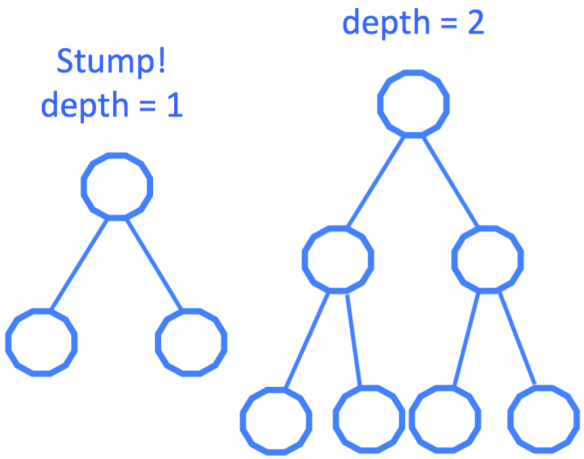
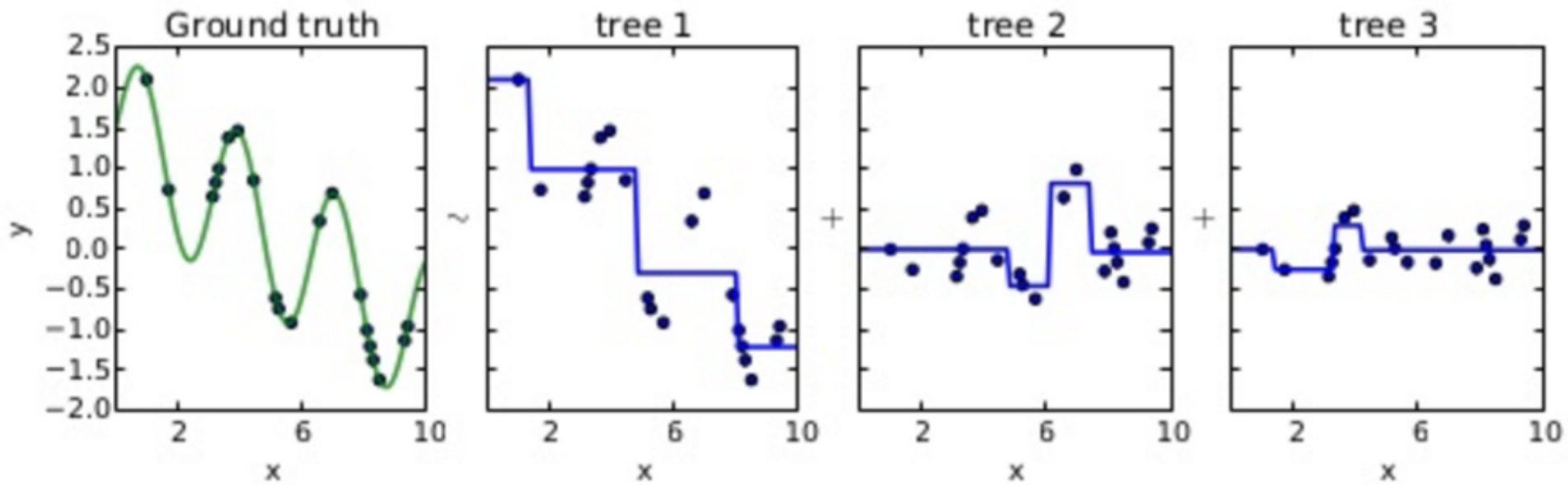
Why does this work better than Random Forests, etc.?

Fitting regressions on sequential residuals





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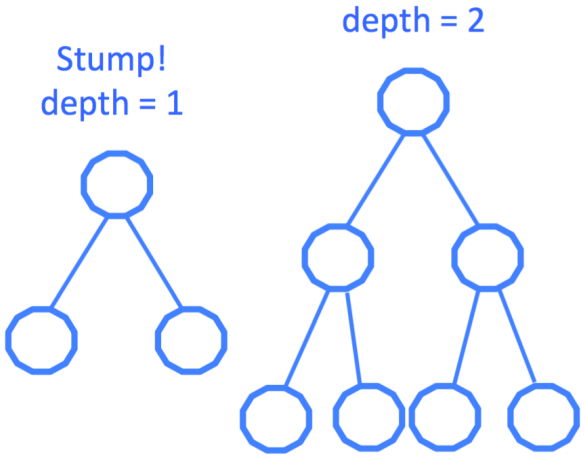

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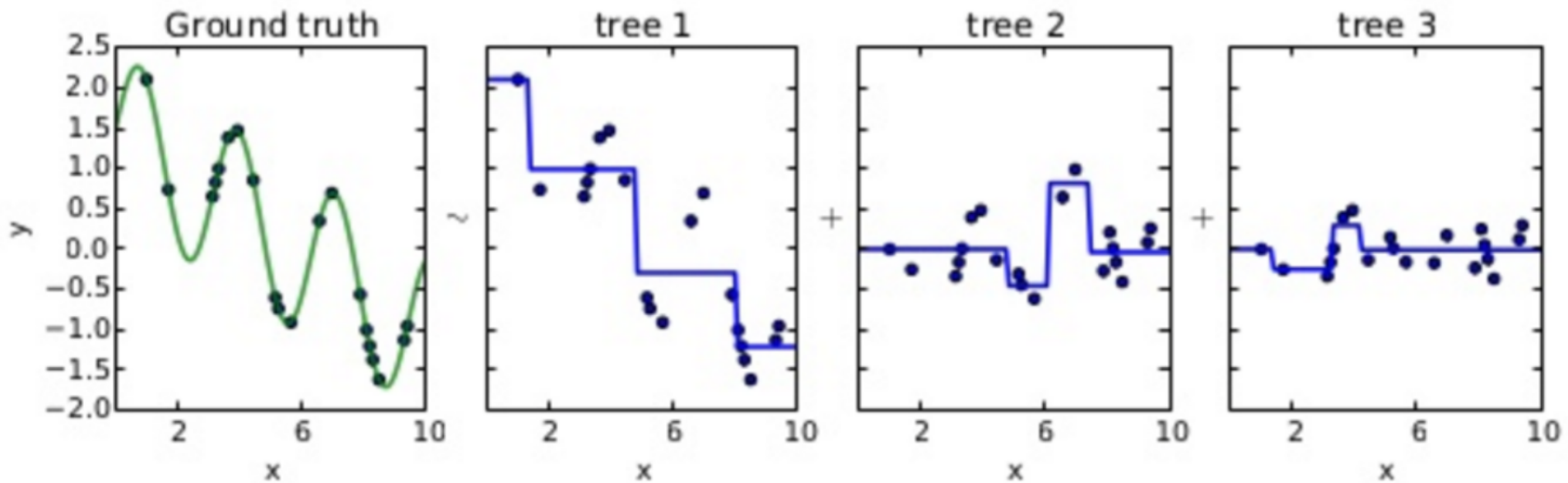

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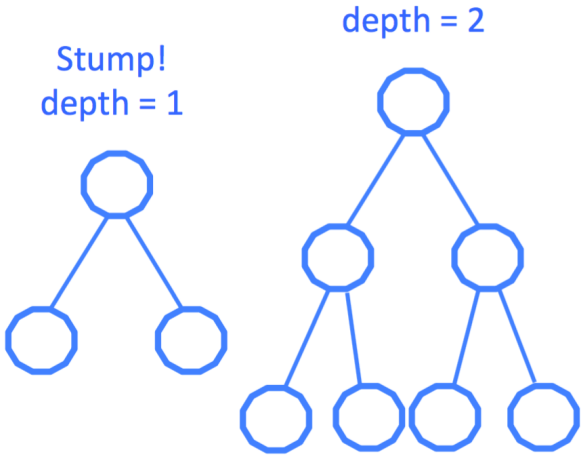

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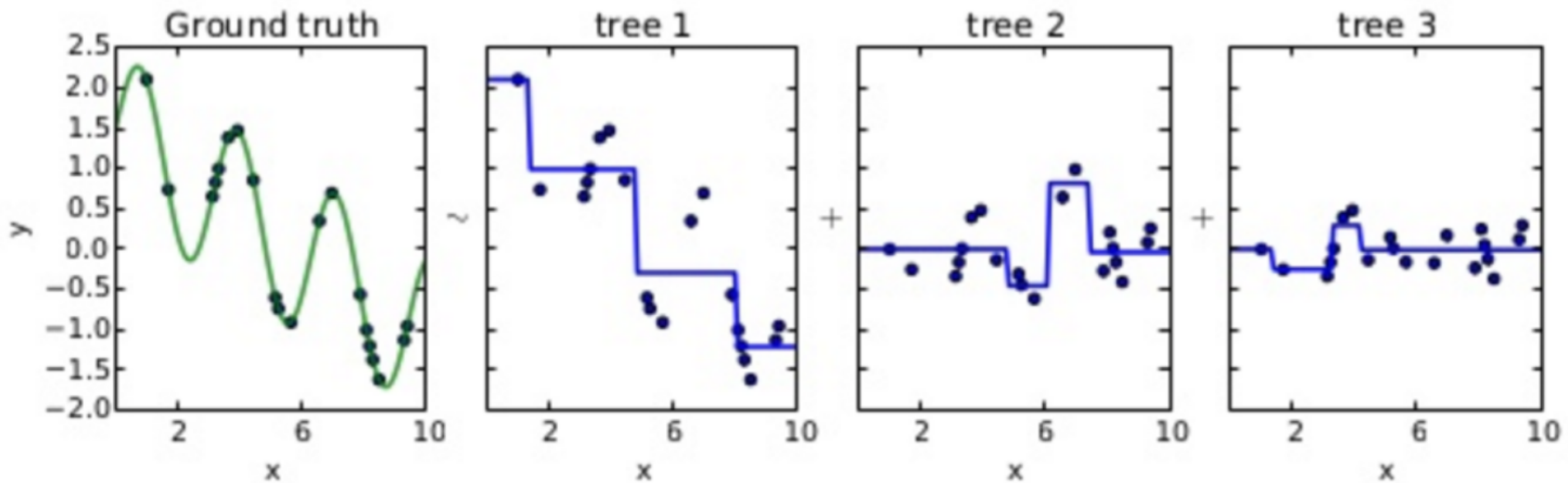

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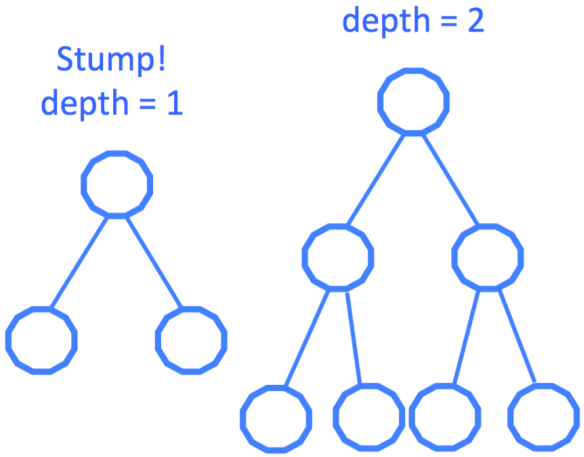

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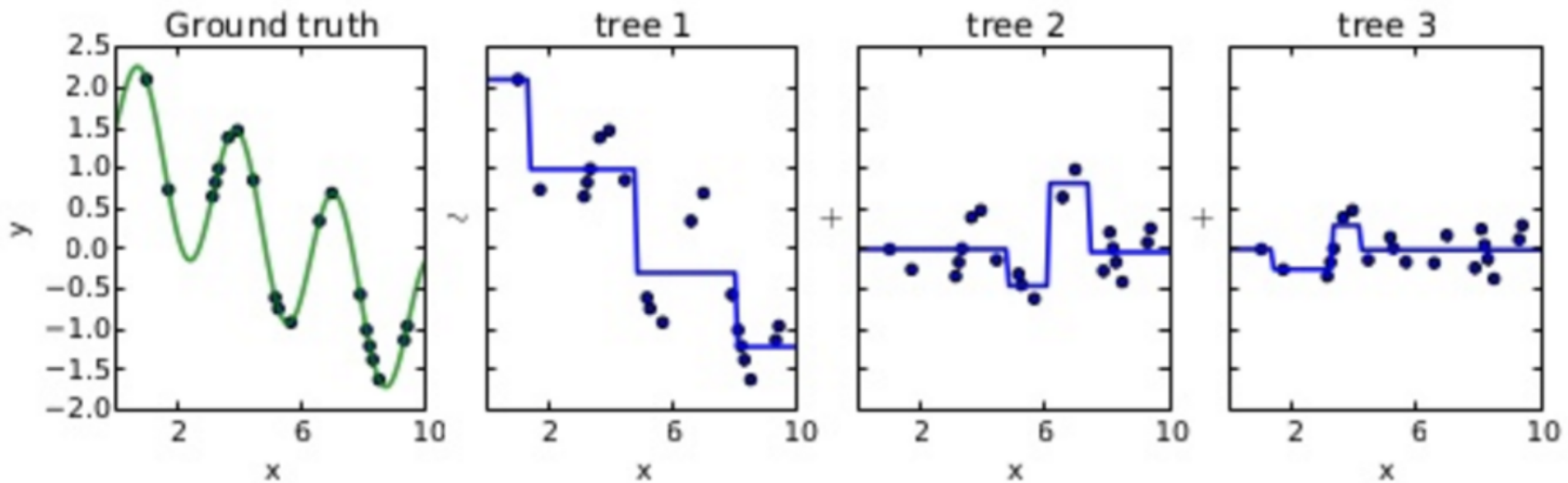

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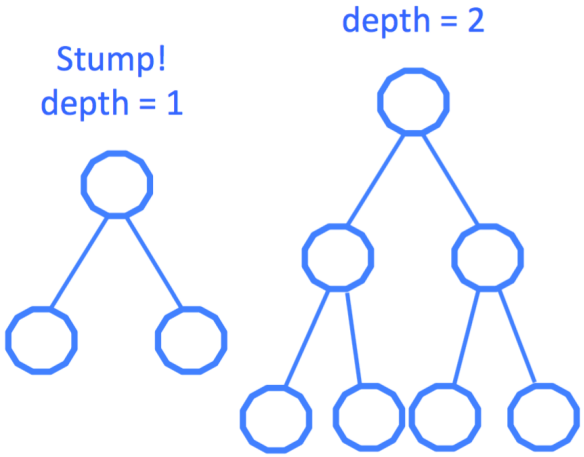

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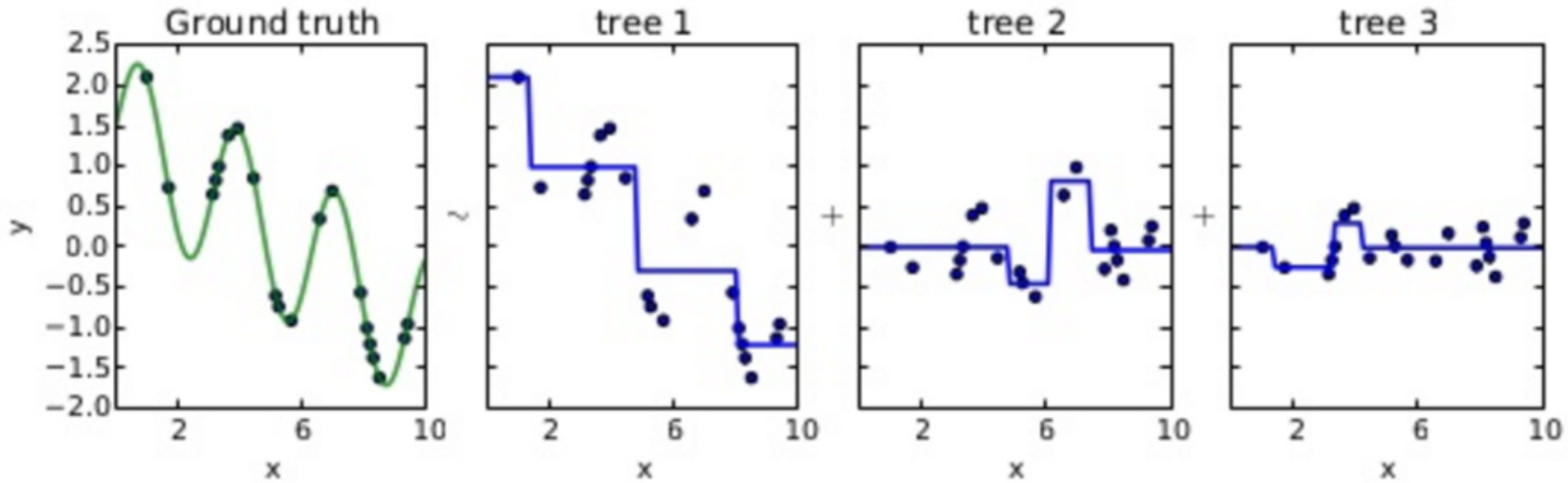

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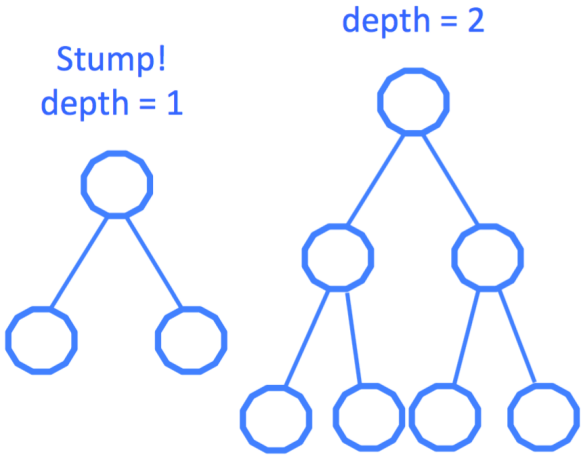

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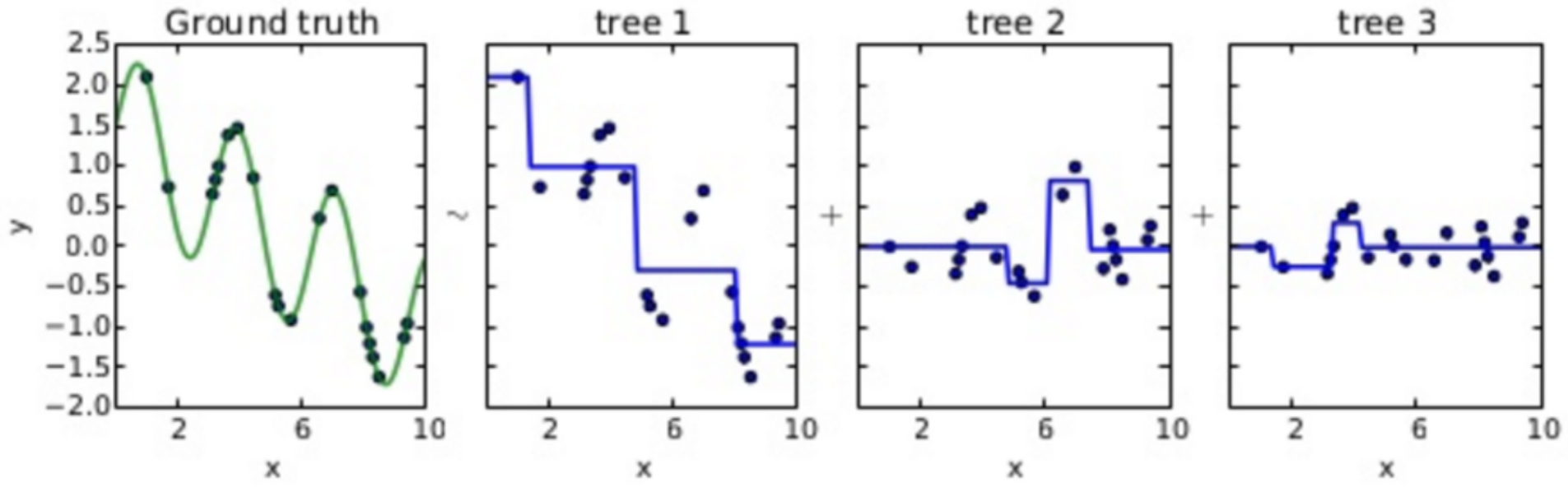

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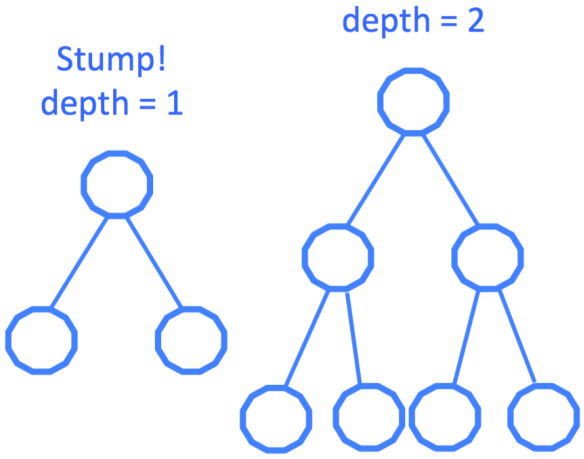

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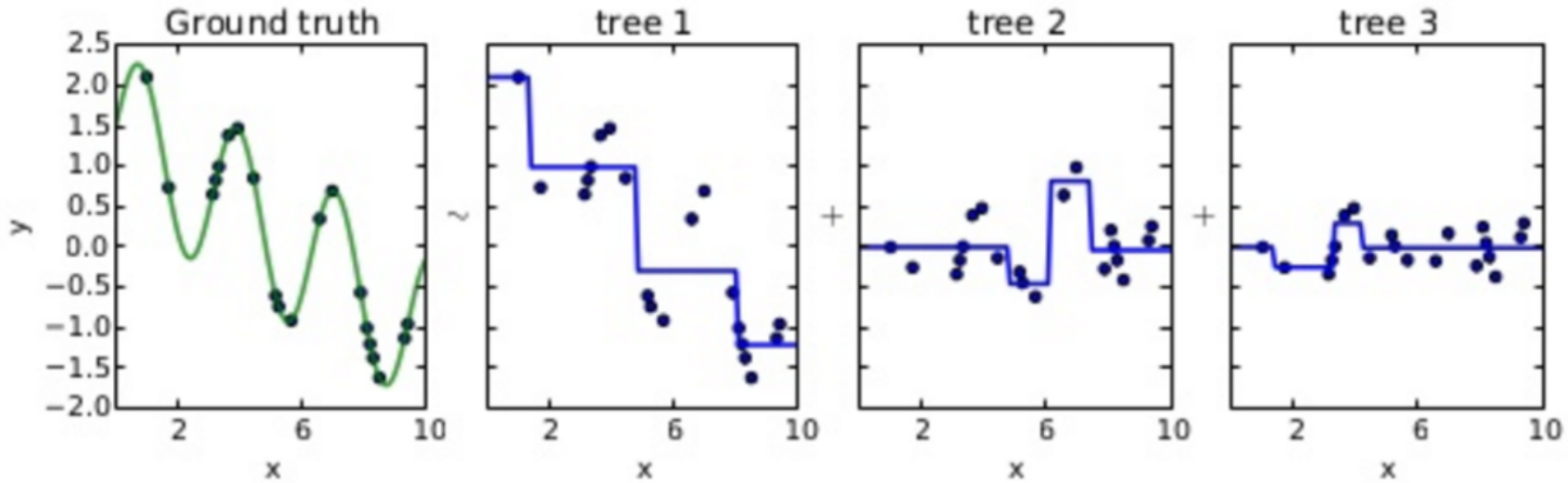
3. Return the boosted model $\hat{f}(x_i) = \sum_{k=1}^{m} \alpha_k f^{(k)}(x_i)$



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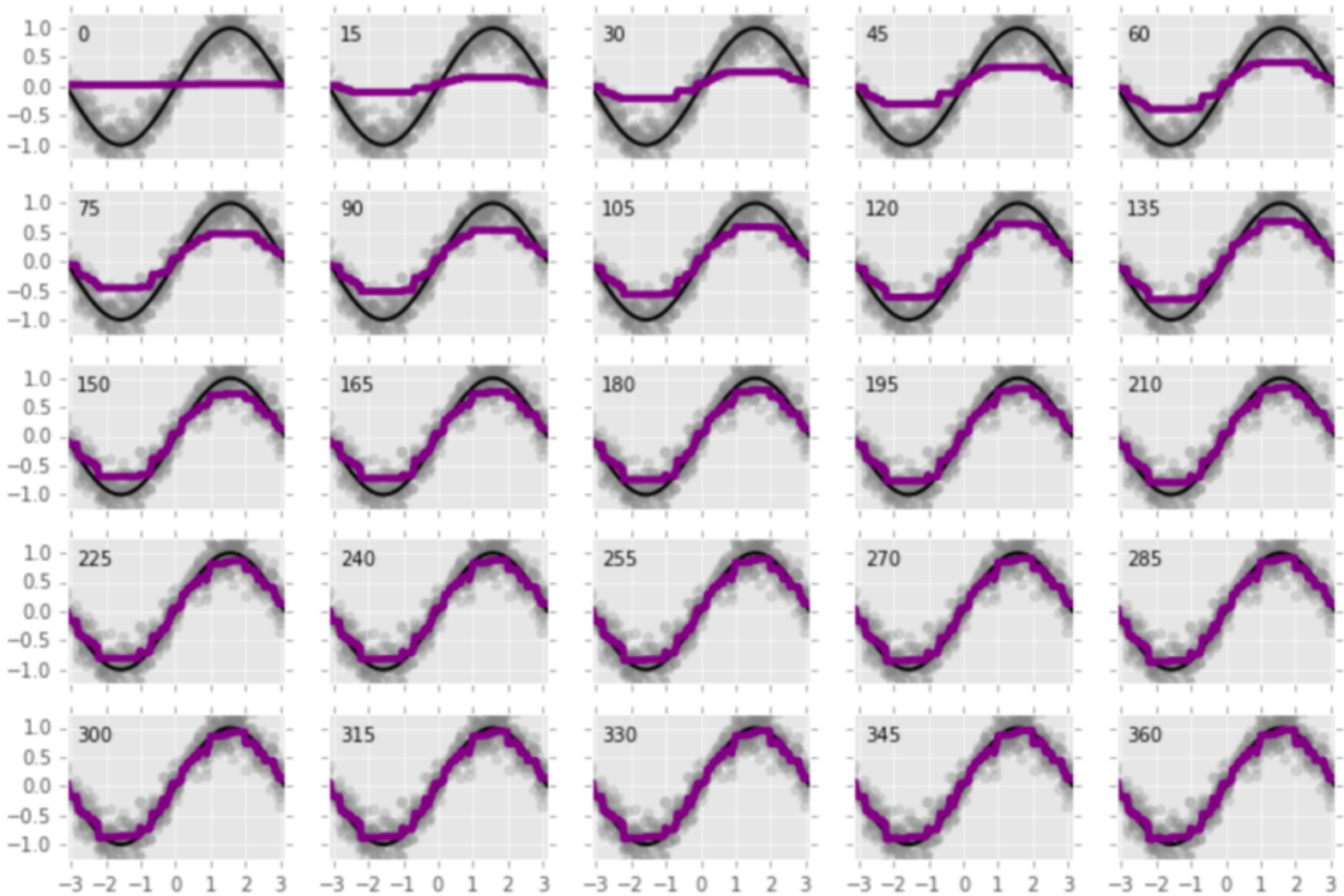

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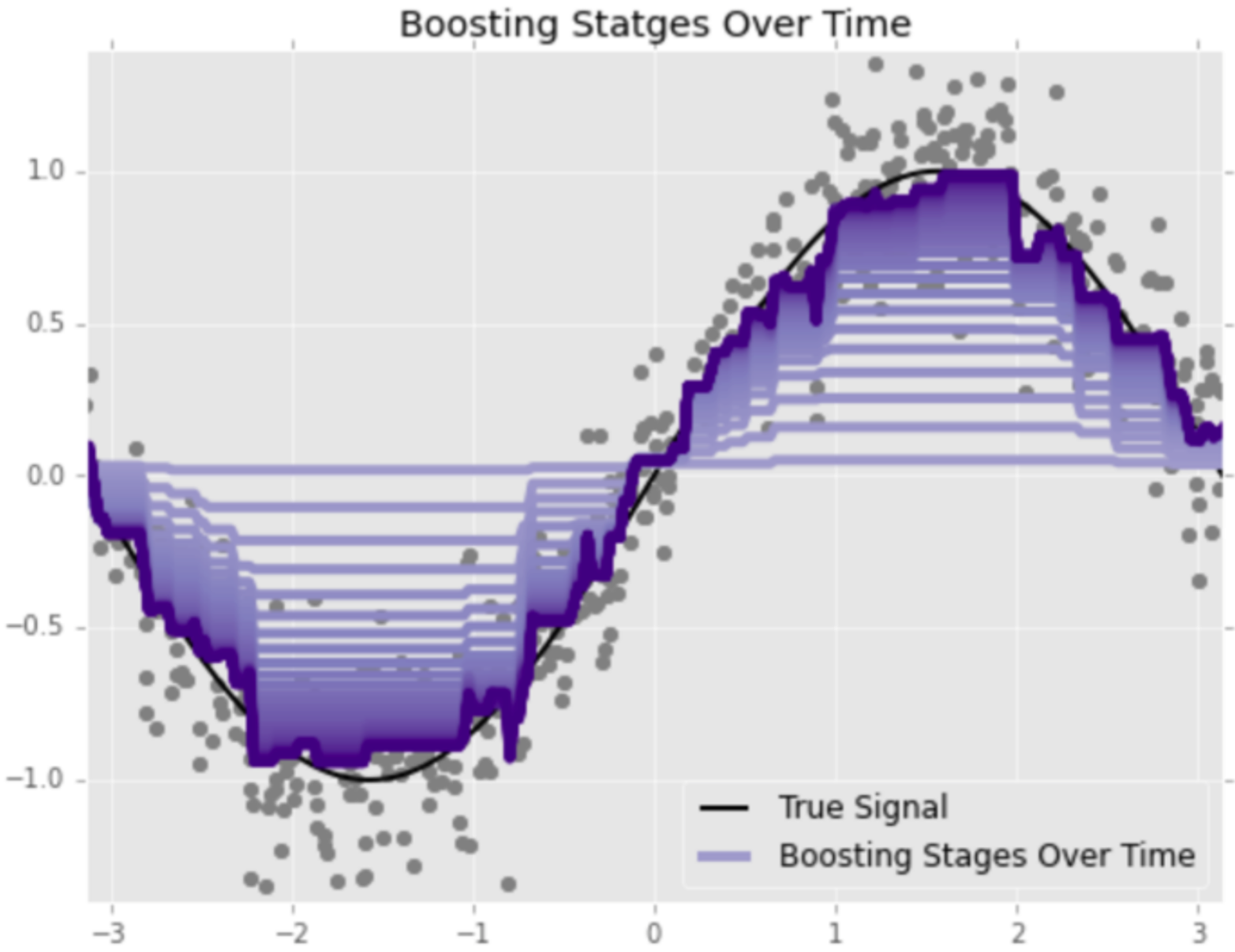

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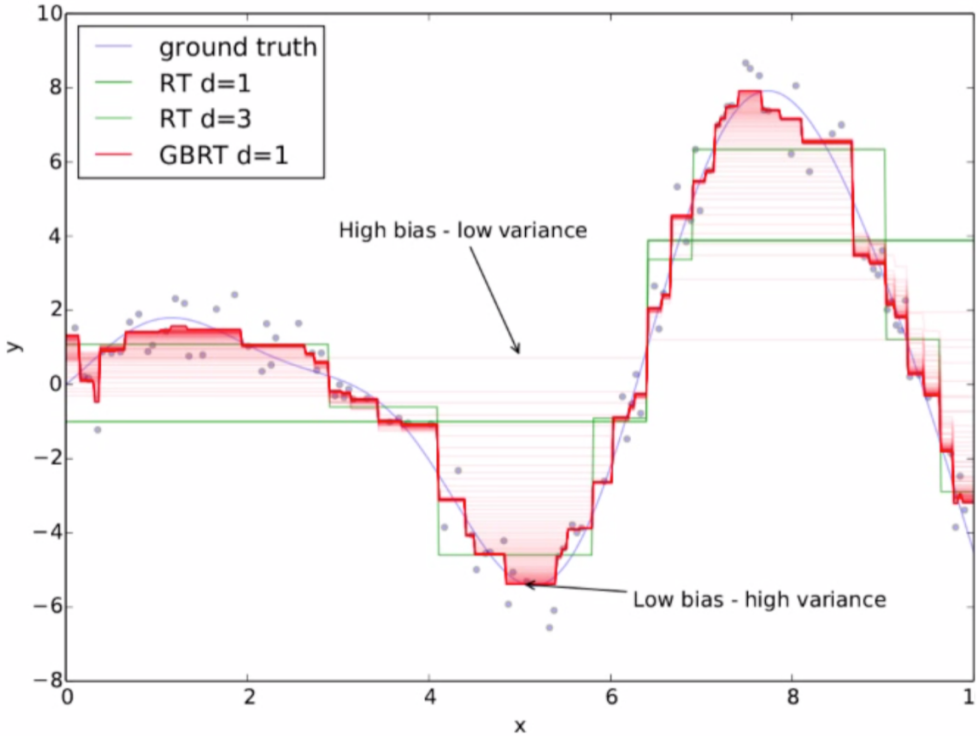

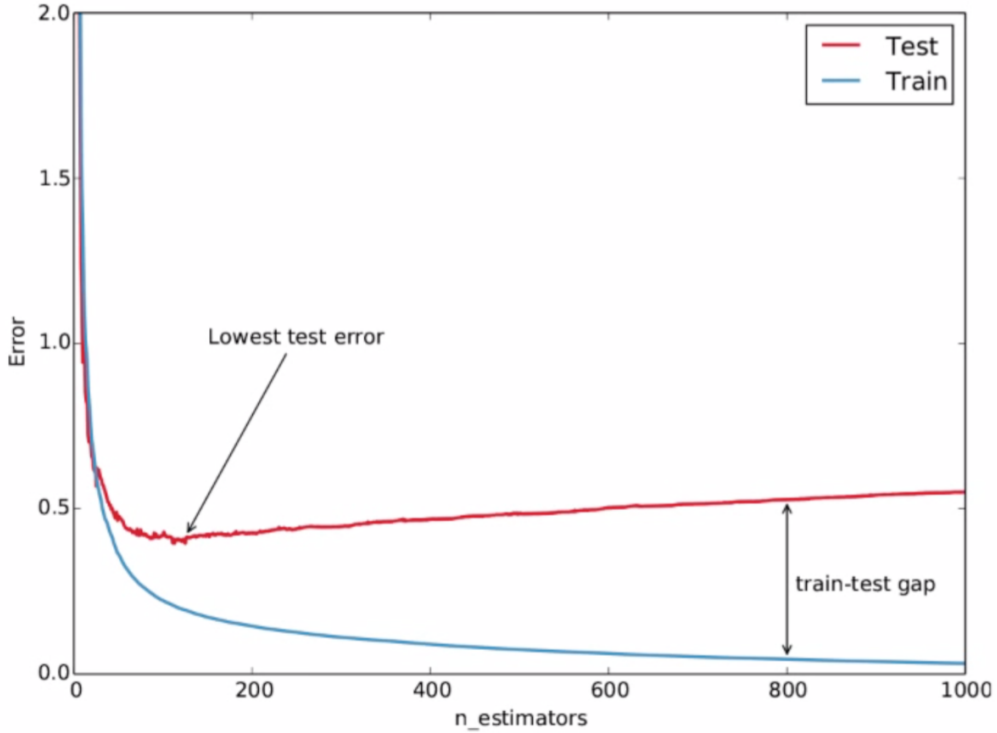

https://www.r-bloggers.com/an-attempt-to-understand-boosting-algorithms/

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- The gradient of the loss function with respect to $\hat{Y}_i$

$$\frac{\partial L(Y_i, \hat{Y}_i)}{\partial \hat{Y}_i}$$

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

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- The gradient of the loss function with respect to $\hat{Y}_i$

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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

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

to move in the direction of greatest decrease in loss

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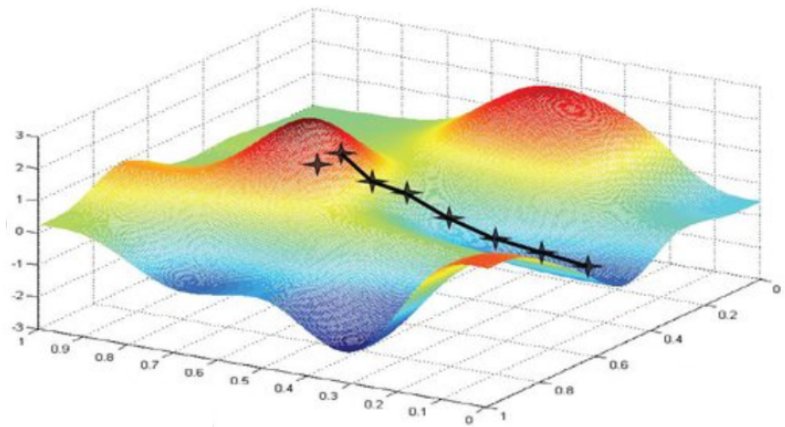

The direction of maximal increase is the the gradient of a function

(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

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

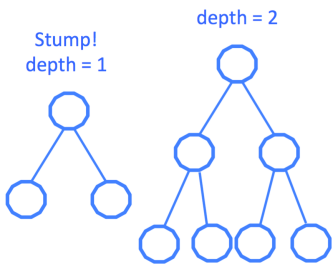
  where $\hat{W}(\cdot, \gamma_k)$ is a *weak learner* boosted at *learning rate* α_k

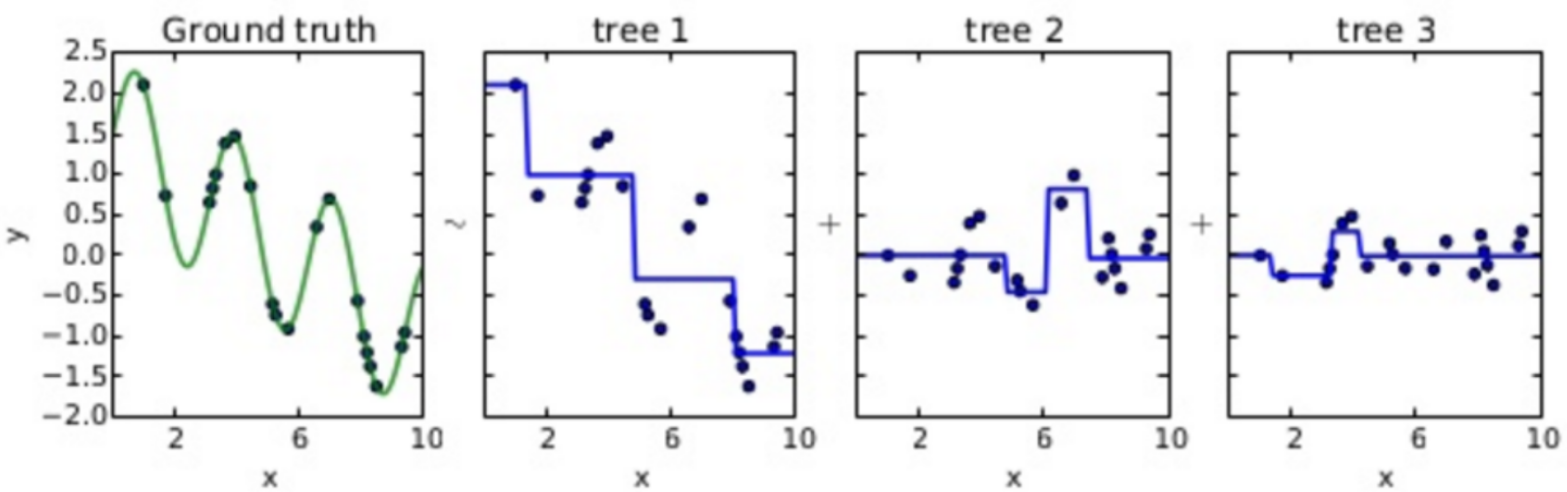
Fitting regressions on sequential residuals

- 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_i of residuals





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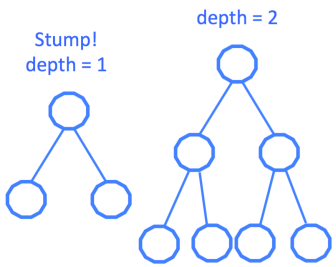

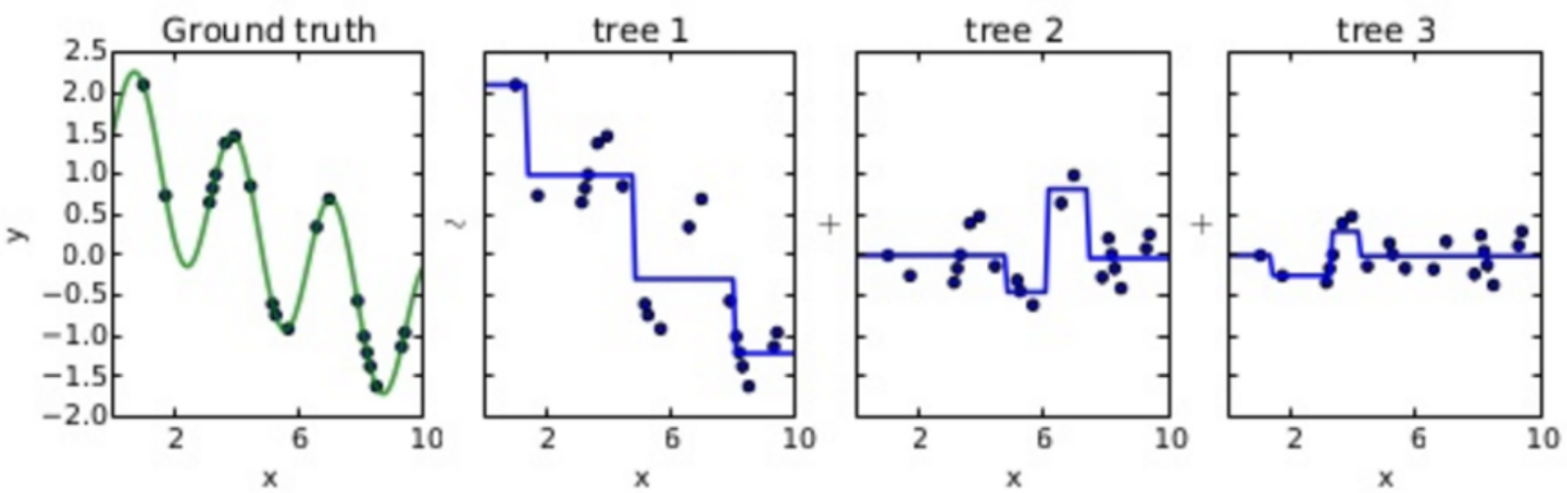

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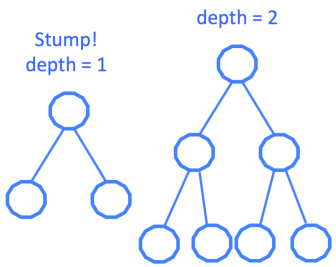

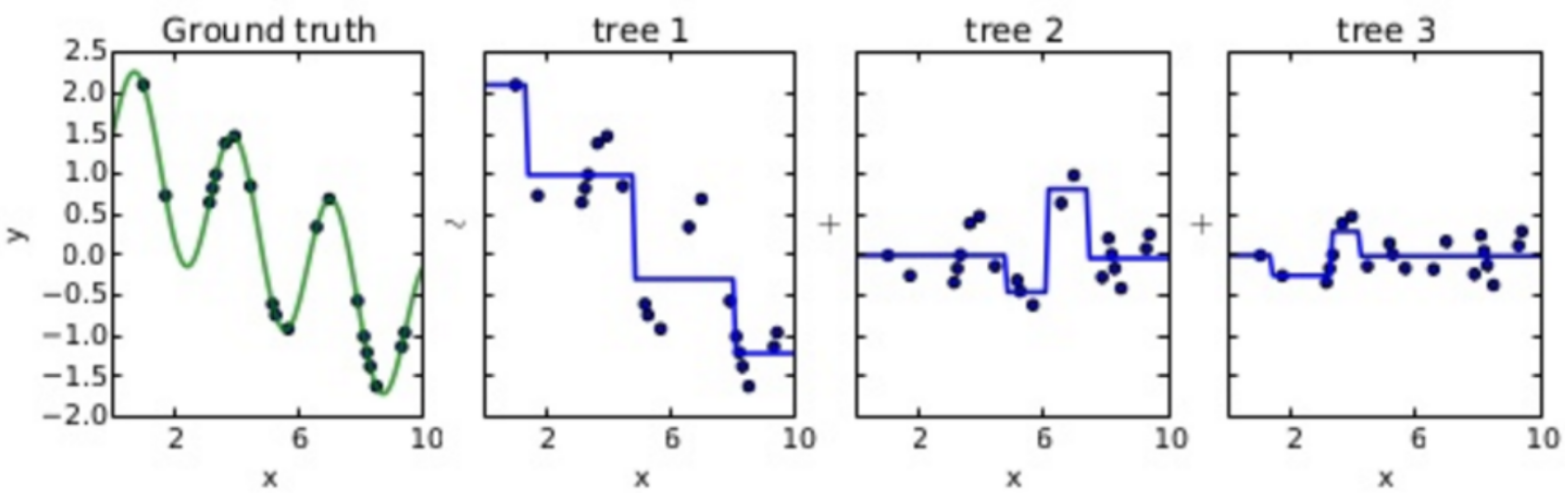

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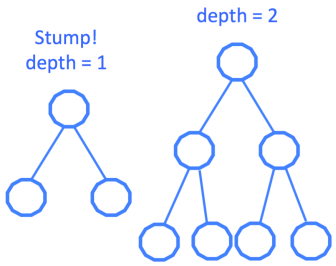

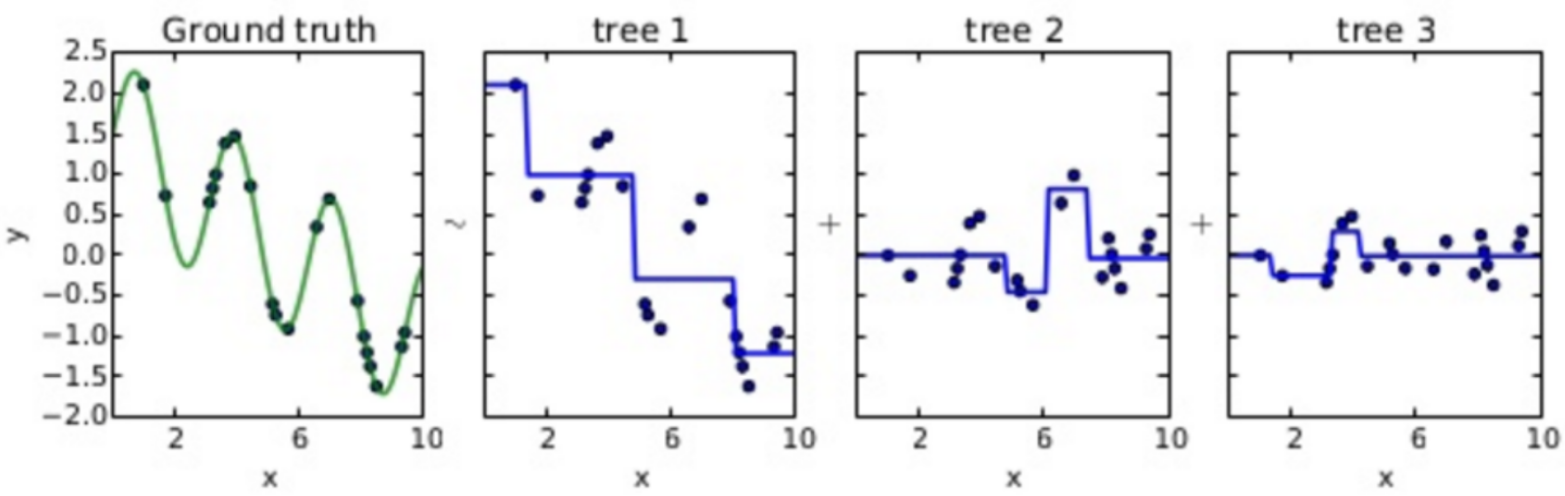

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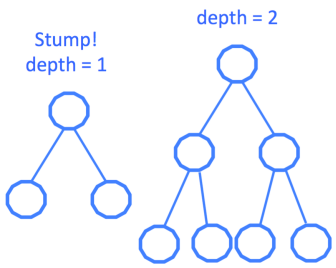

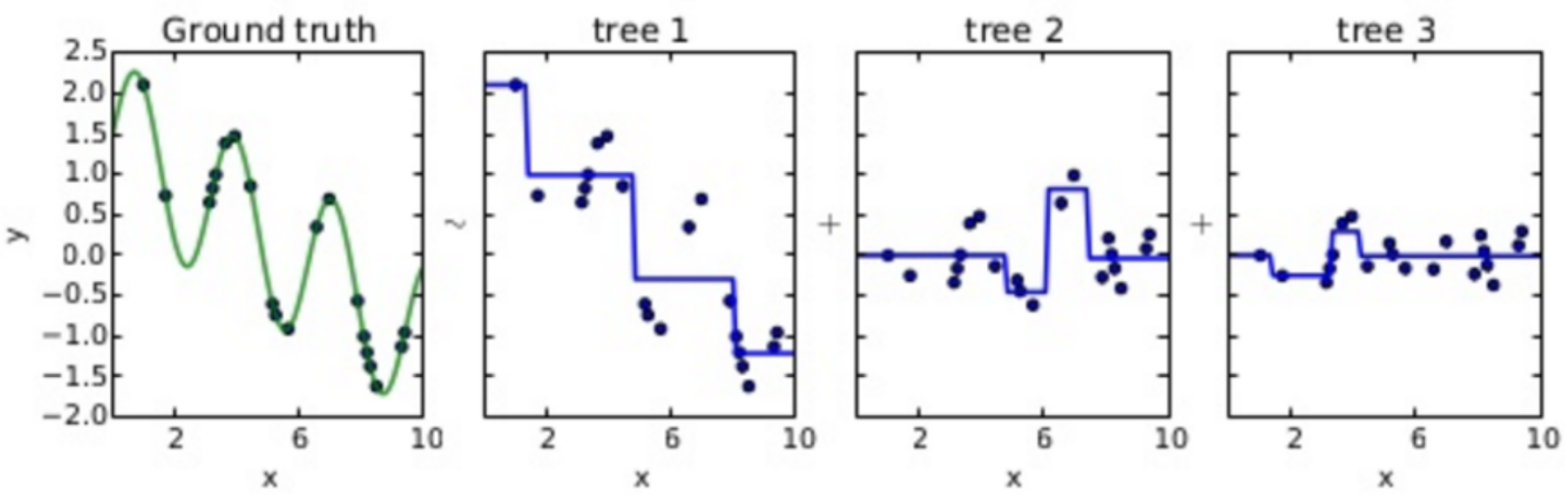

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Some loss functions

Regression

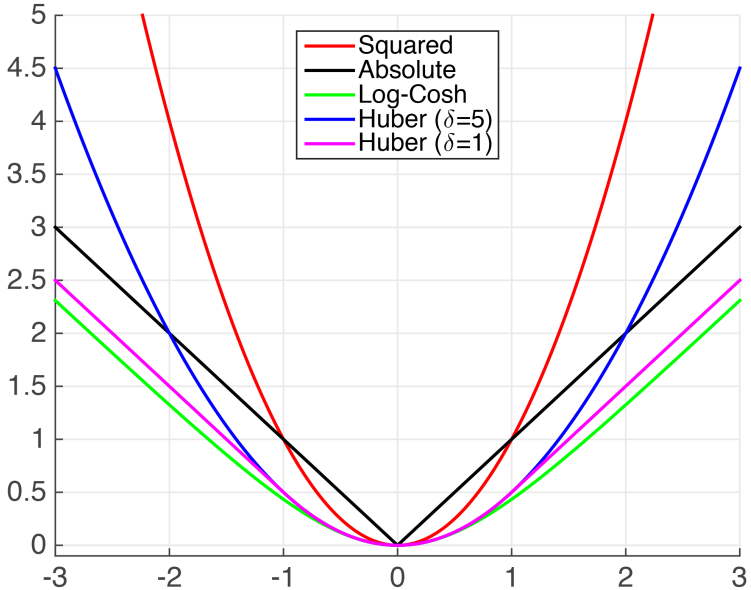
Squared Loss $\frac{1}{2}(y_i - \boldsymbol{x}_i^T\beta)^2$

Absolute Loss $|Y_i - \boldsymbol{x}_i^T\beta|$

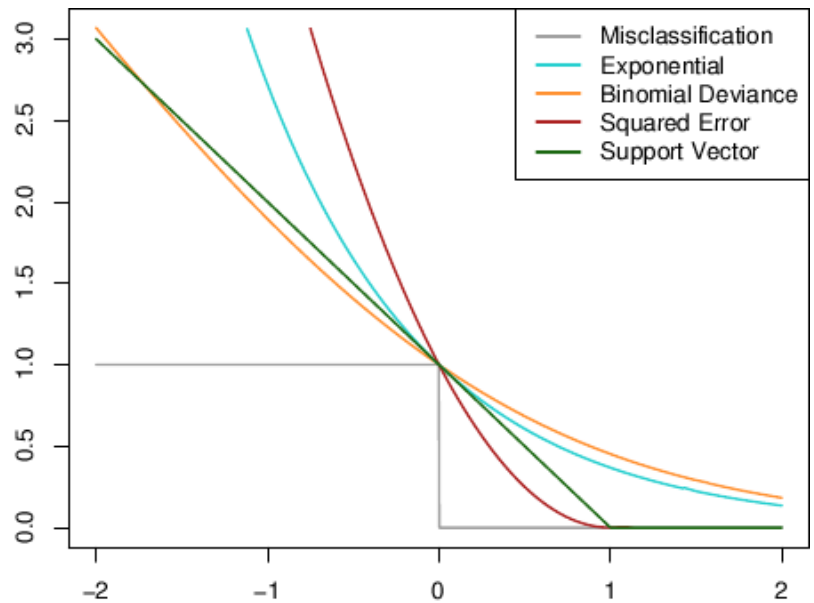
Classification

Log Loss $1 - \frac{1}{1+e^{-x_i^T\beta}}$ (Bernoulli Deviance/Logistic Reg.)

Exponential Loss $\exp(-y_i \cdot \boldsymbol{x}_i^T\beta)$ (Ada Boost)



$\boldsymbol{x}_i^T\beta$



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AdaBoost (Adaptive Boosting)

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

1. Set weights $w_i^{(1)} = \frac{1}{n}$

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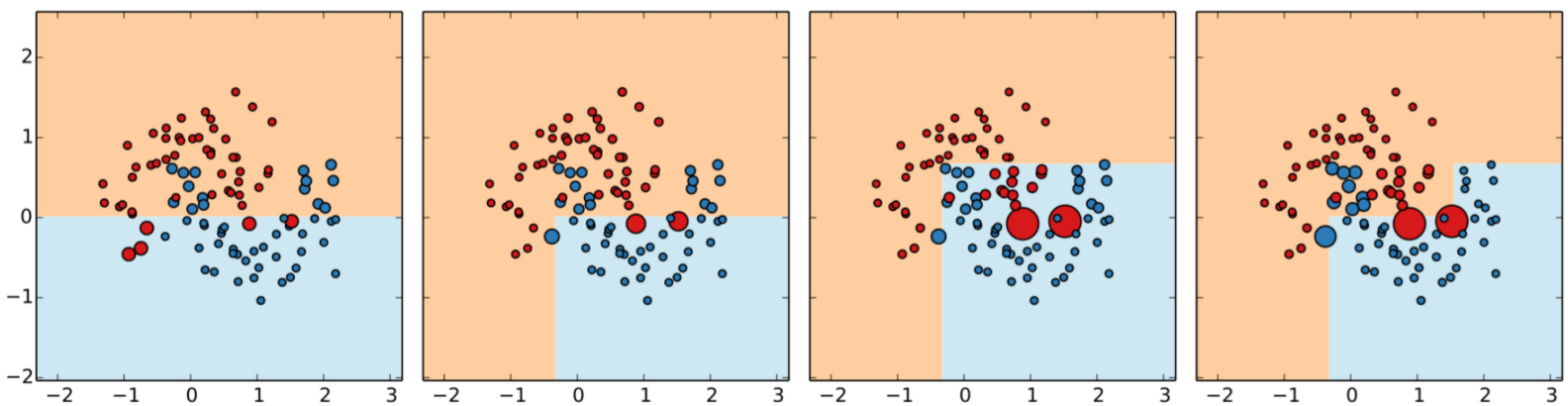

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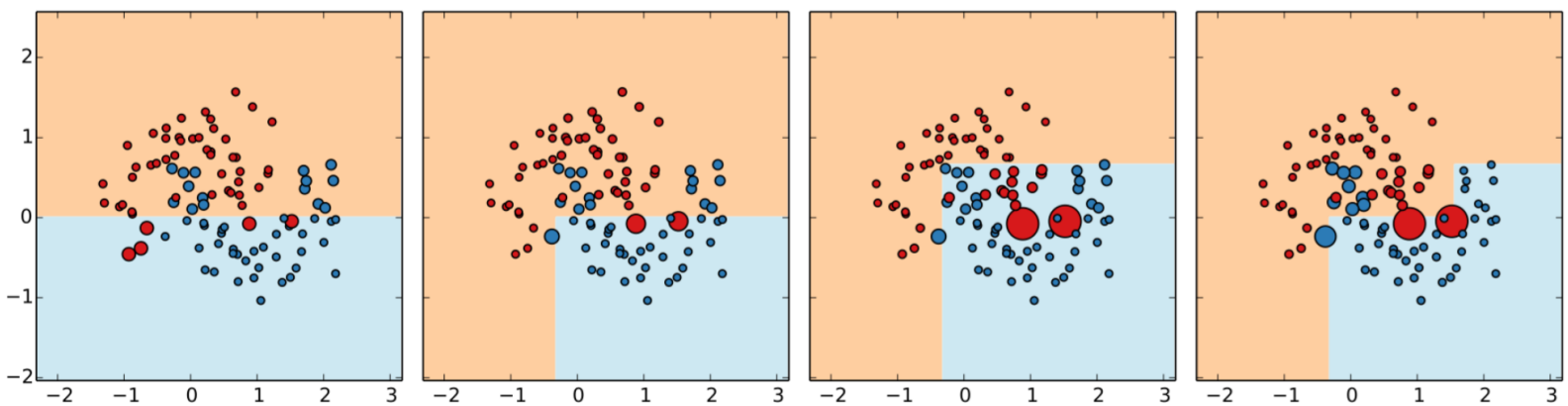

*Sean Sall's slides have an appendix showing that AdaBoost is exponential loss

XGBoost (eXtreme Gradient Boosting)

- Percentiles binned features: faster/more efficient splitting
- Handles missing data
- Smart memory management/out-of-core computation

`http://xgboost.readthedocs.io`

- Knobs
- Get Started (Python Install)
- Packages $>$ Python $>$ Python API Reference
  - Core Data Structure
  - Learning API
  - Scikit-Learn API