Ensemble Methods (Part II)
Gradient Boosting

Schwartz

August 2, 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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  - 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 $f_k(\boldsymbol{x})$ be an estimator that predicts outcome Y based on features $\boldsymbol{x}$

  Define a new estimator

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  So W is a stump – a weak learner*
- W is fit to *improve* the available prediction of Y from $f_k(\boldsymbol{x})$
- 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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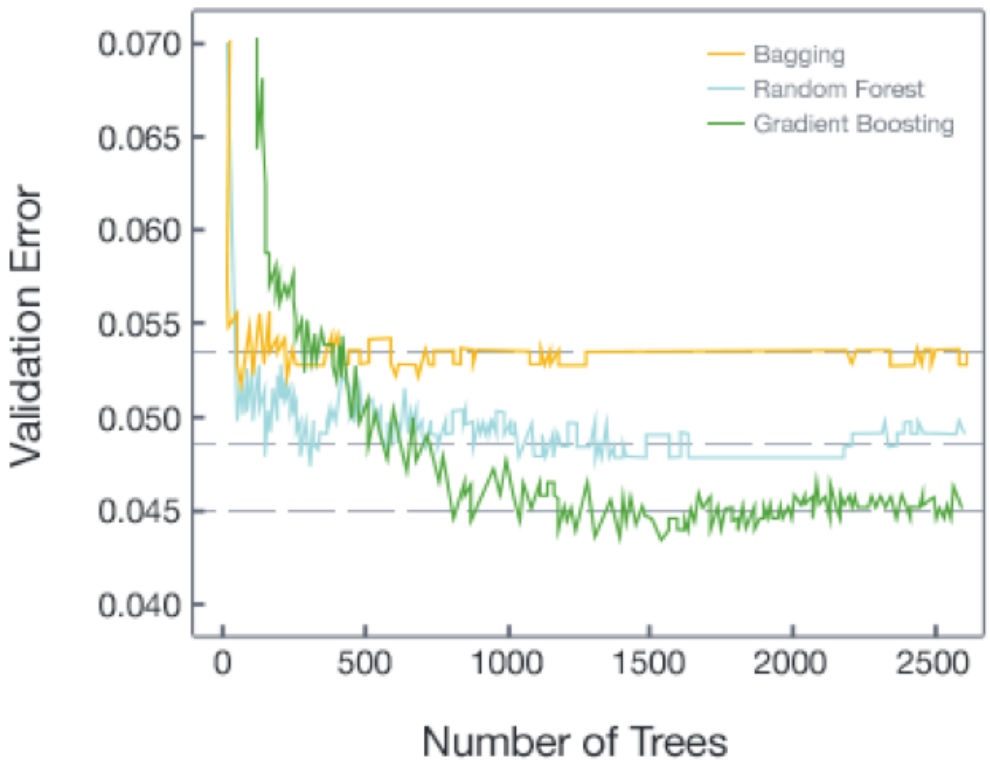

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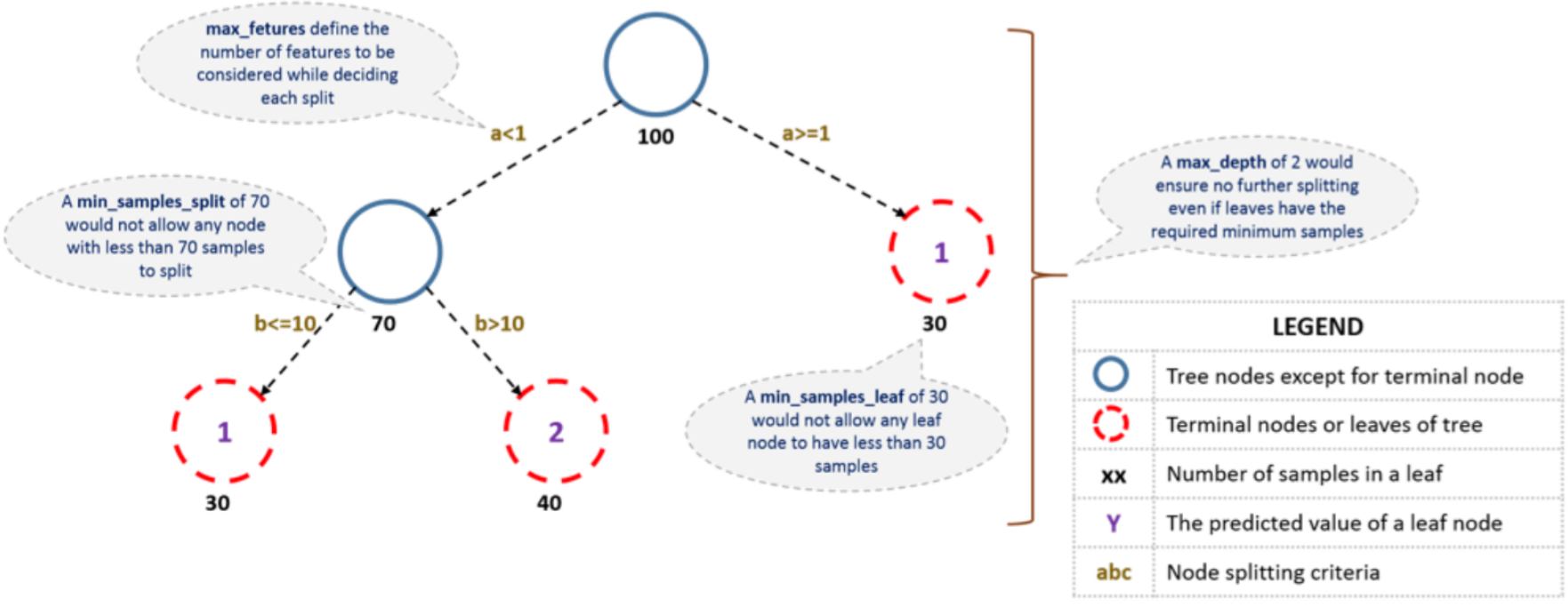

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```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.grid_search import GridSearchCV
param_grid = {'learning_rate': [0.001, 0.01, 0.1],
              'max_depth': [4, 6],
              'min_samples_leaf': [4, 8, 16],
           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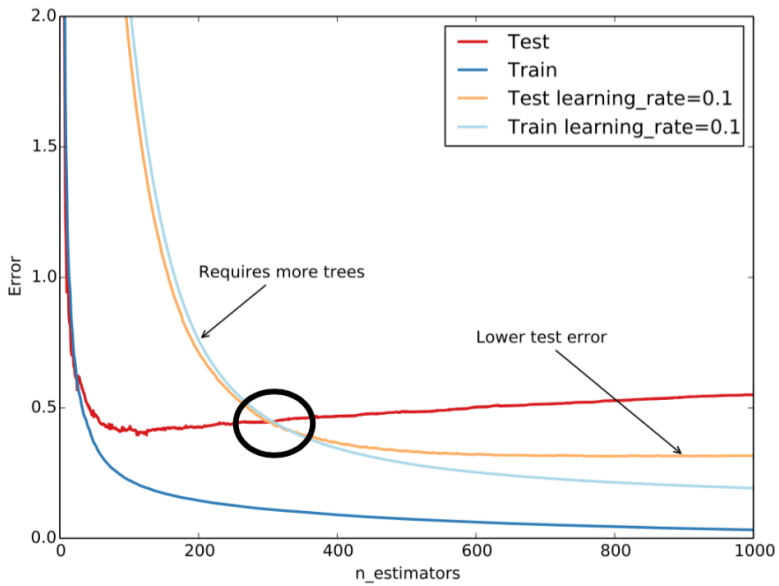

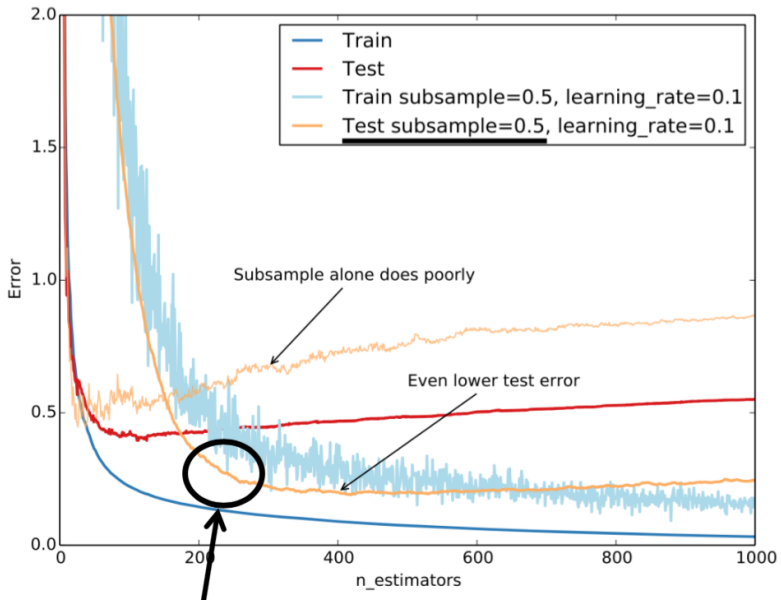

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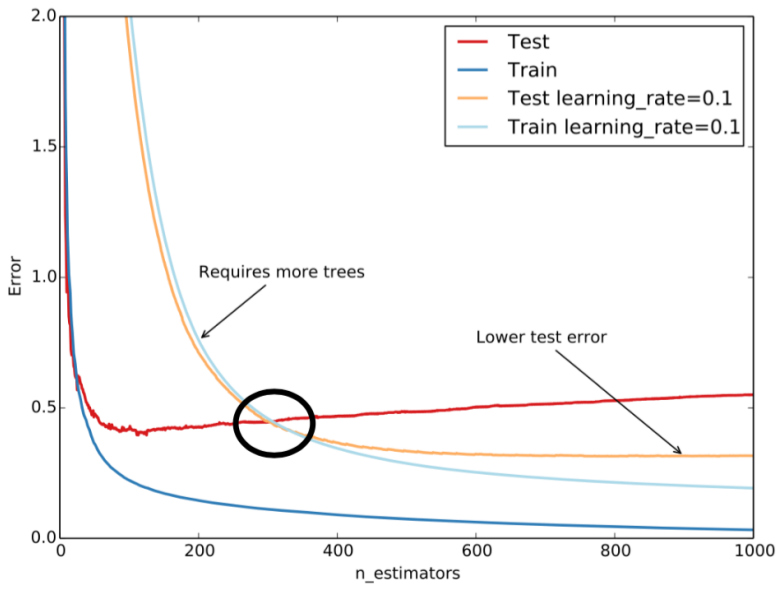
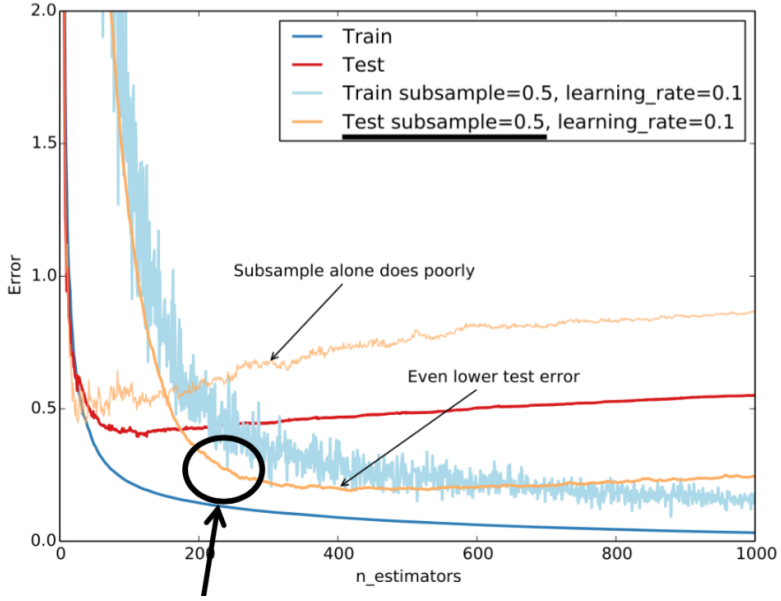
- Stochastic Gradient Boosting using subsamples also available
- Careful parameter tuning is necessary for good performance





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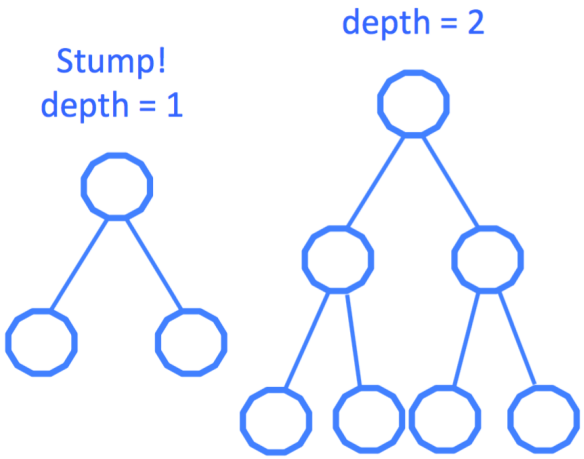
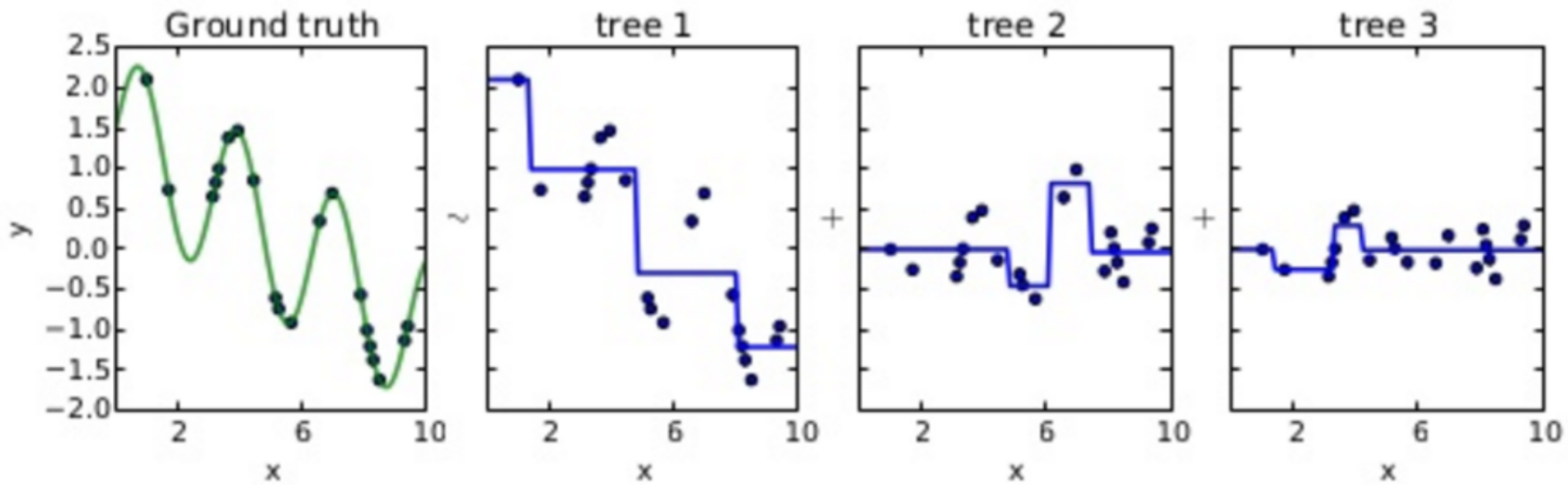
Why does this work better than Random Forests, etc.?

Fitting regressions on sequential residuals





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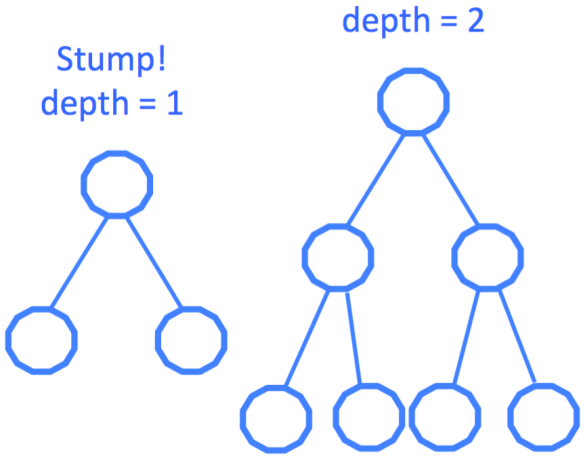

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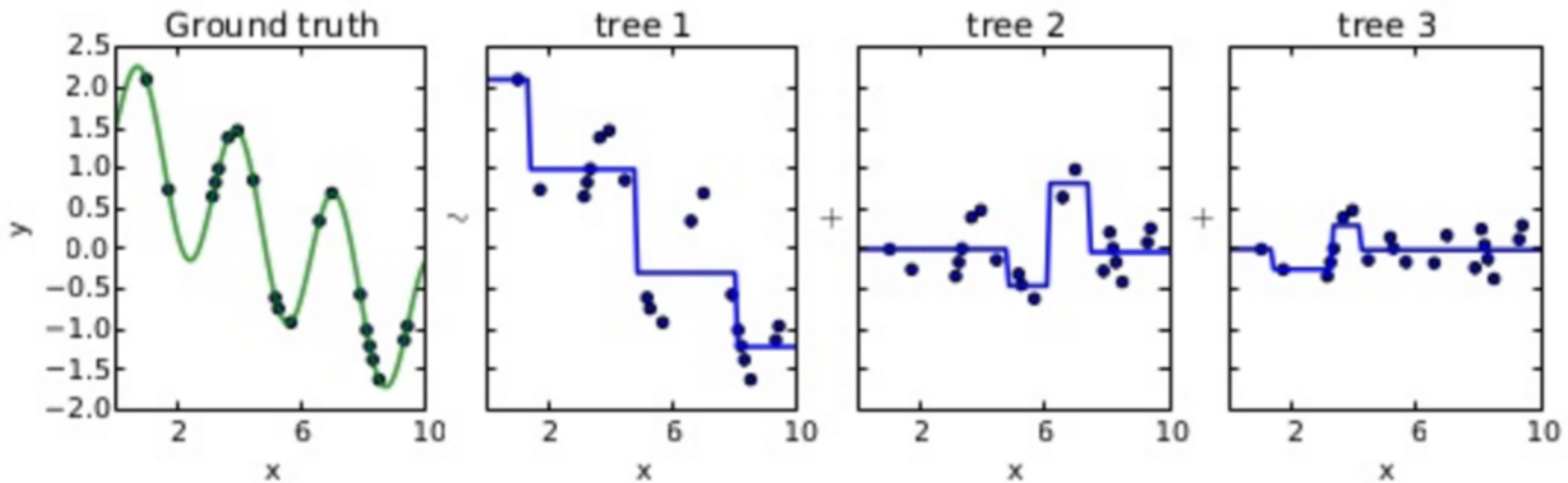

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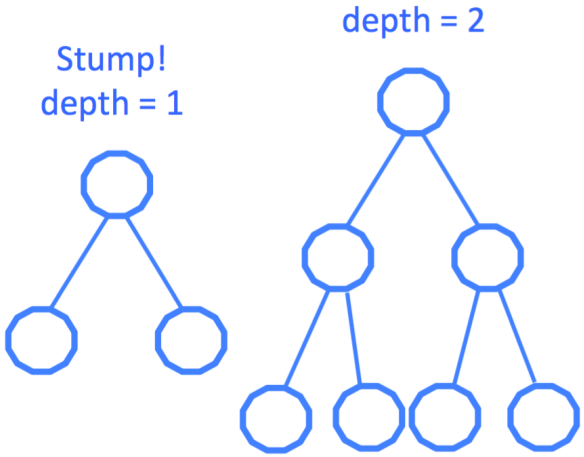

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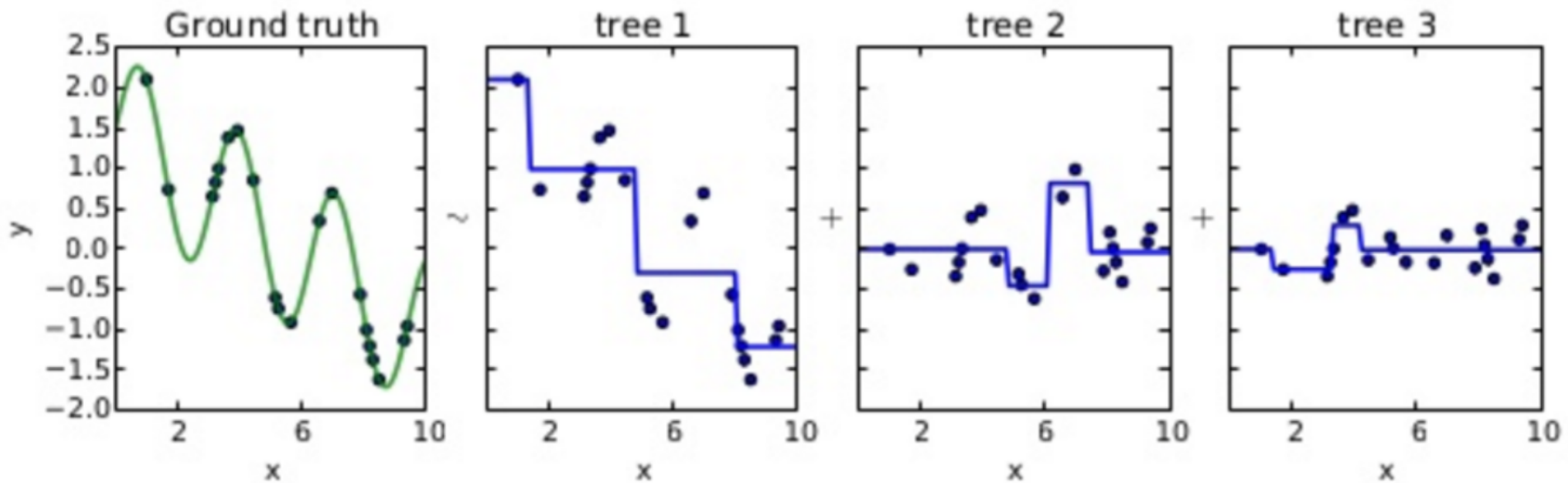

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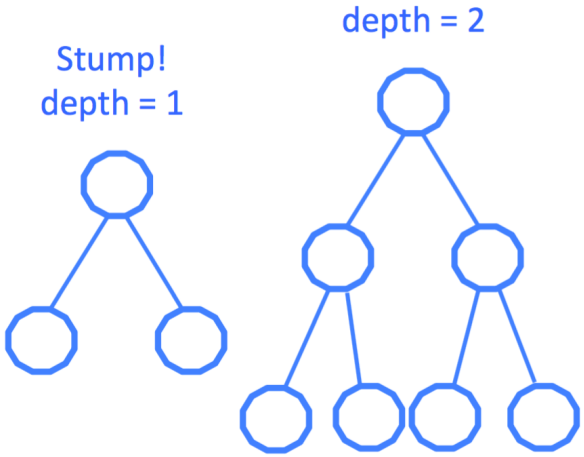

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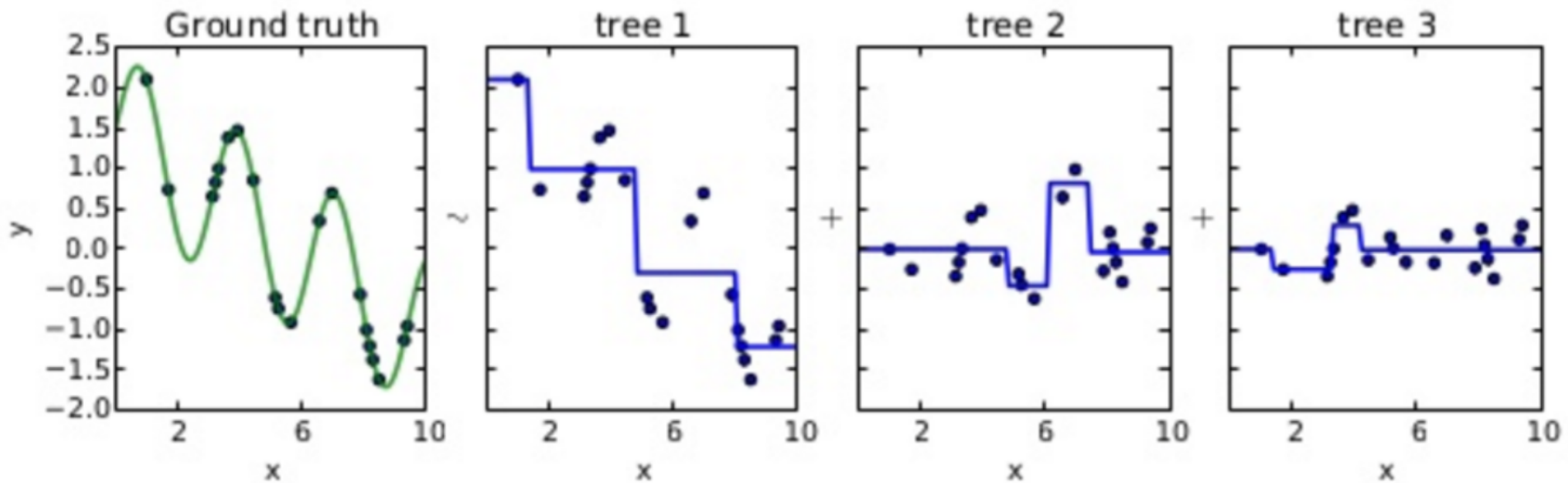

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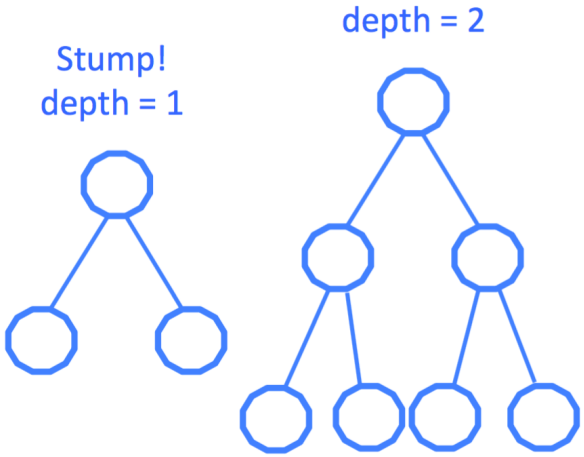

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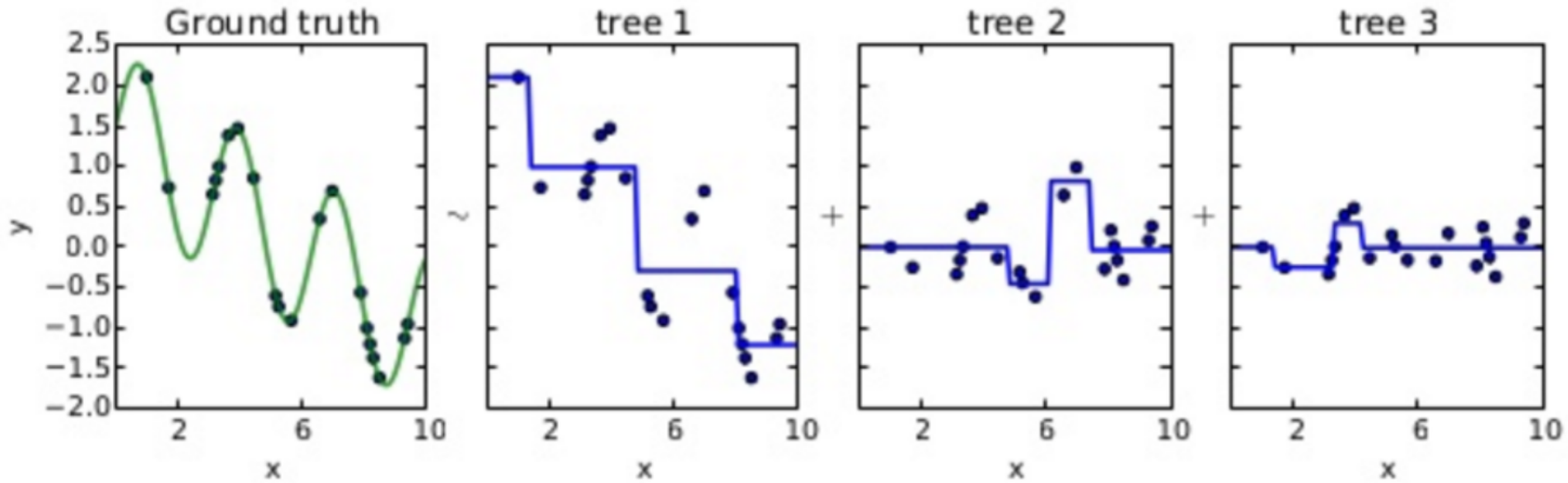

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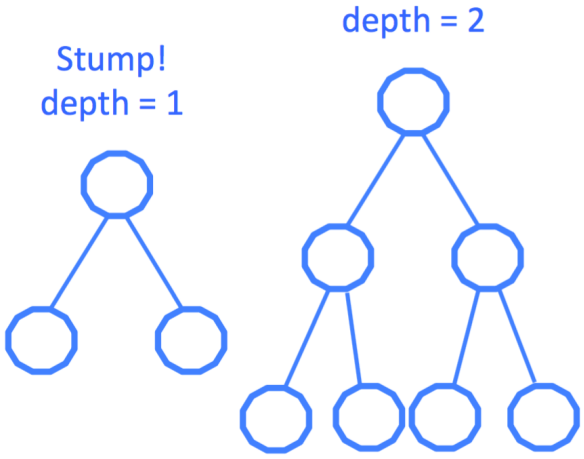

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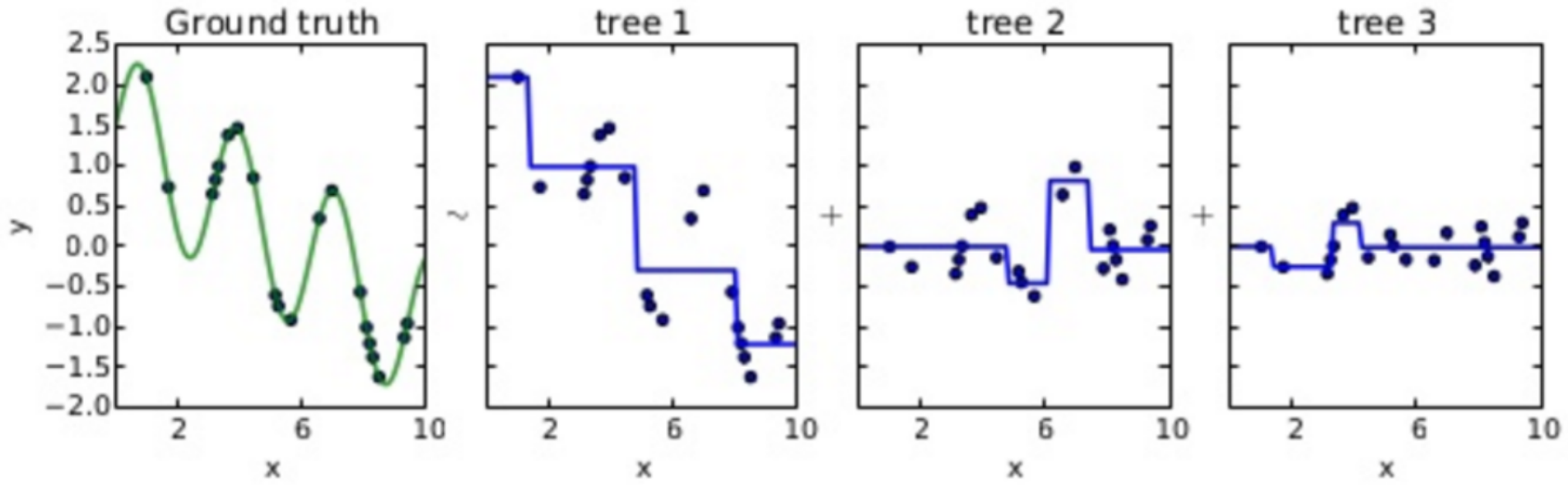

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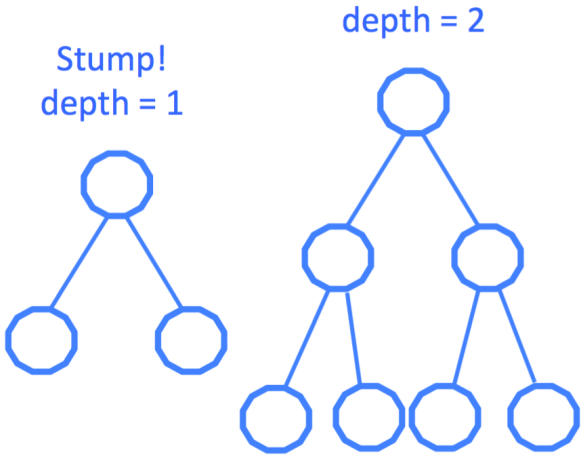

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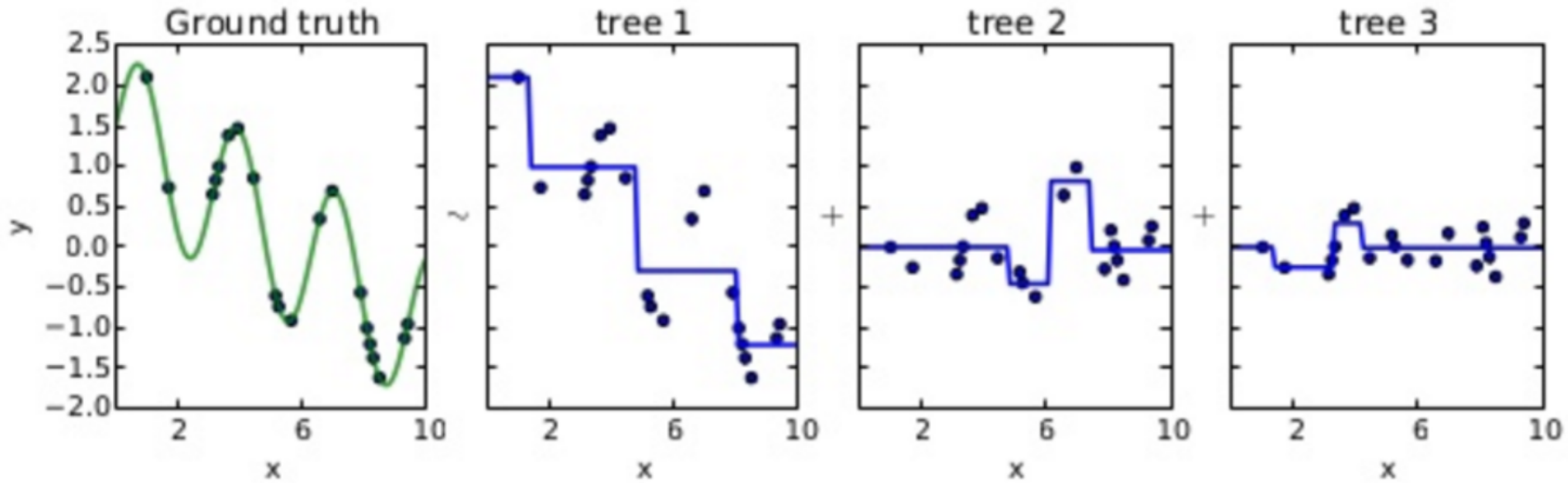
3. Return the boosted model $\hat{f}(x_i) = \sum_{k=1}^{m} \alpha_k f^{(k)}(x_i)$



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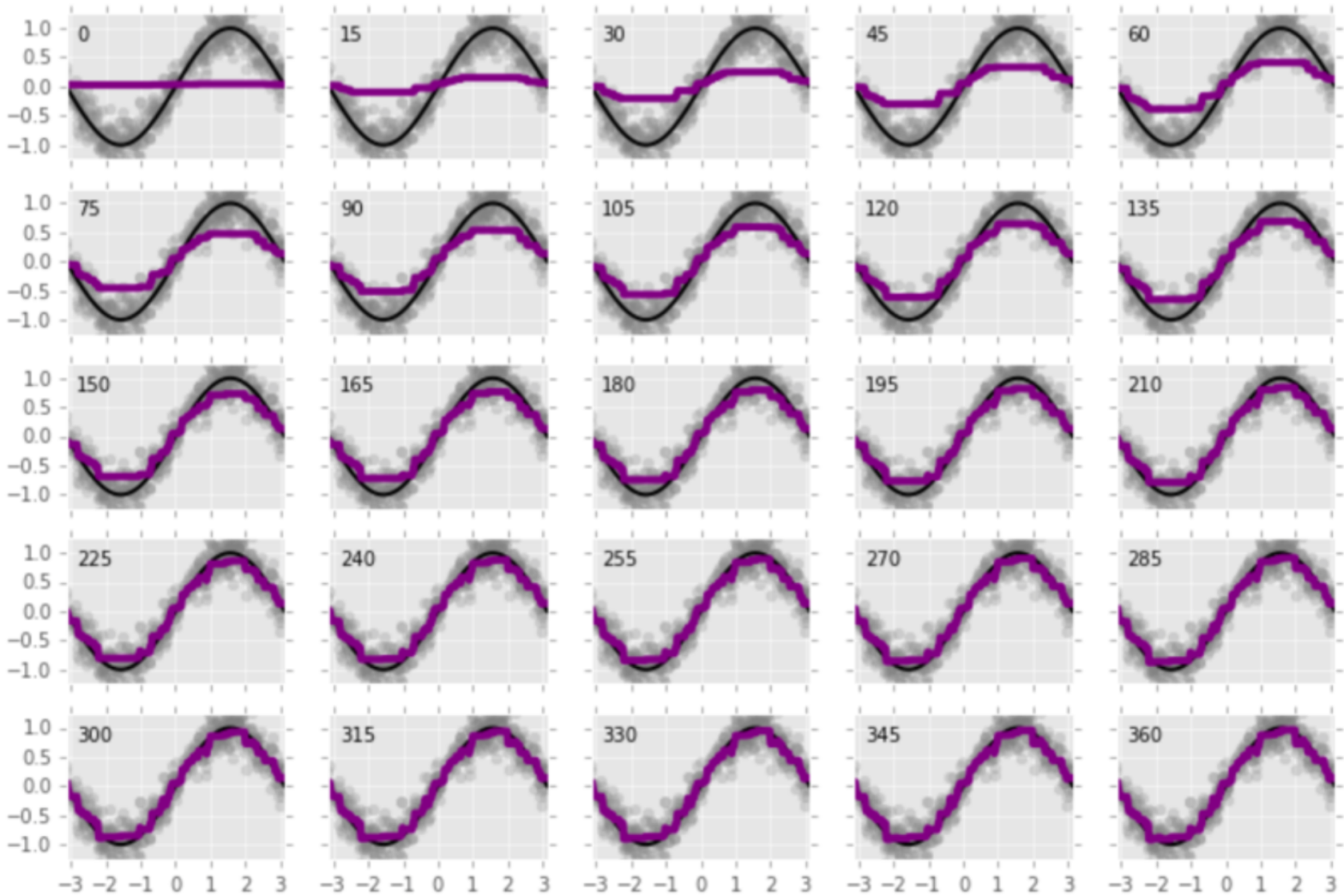

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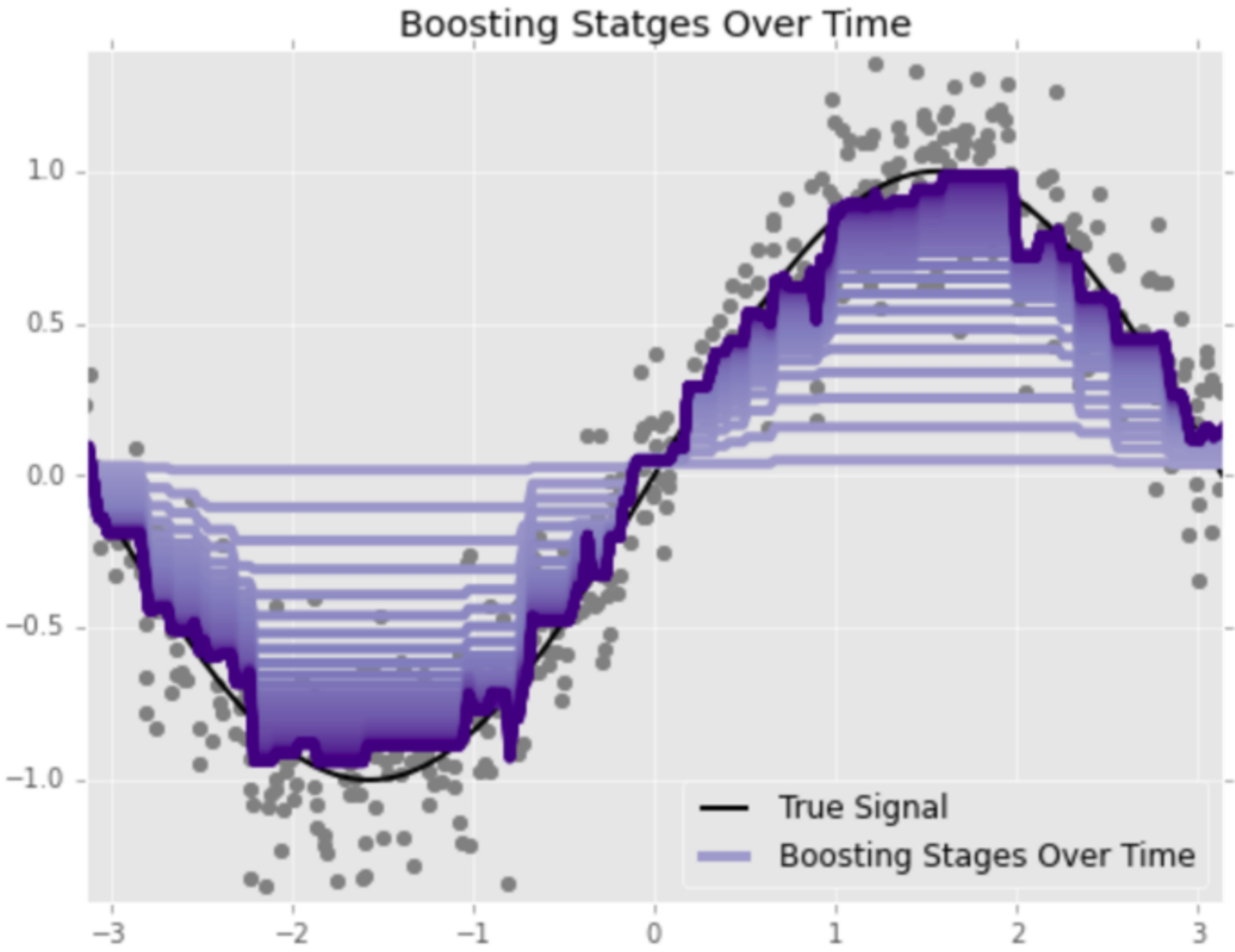

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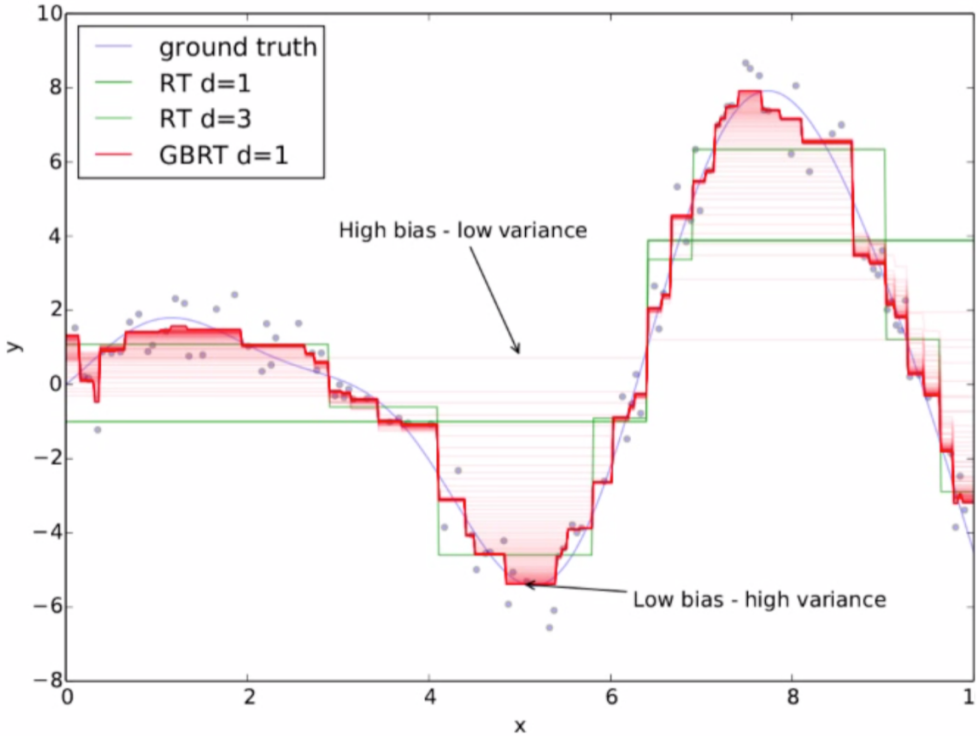

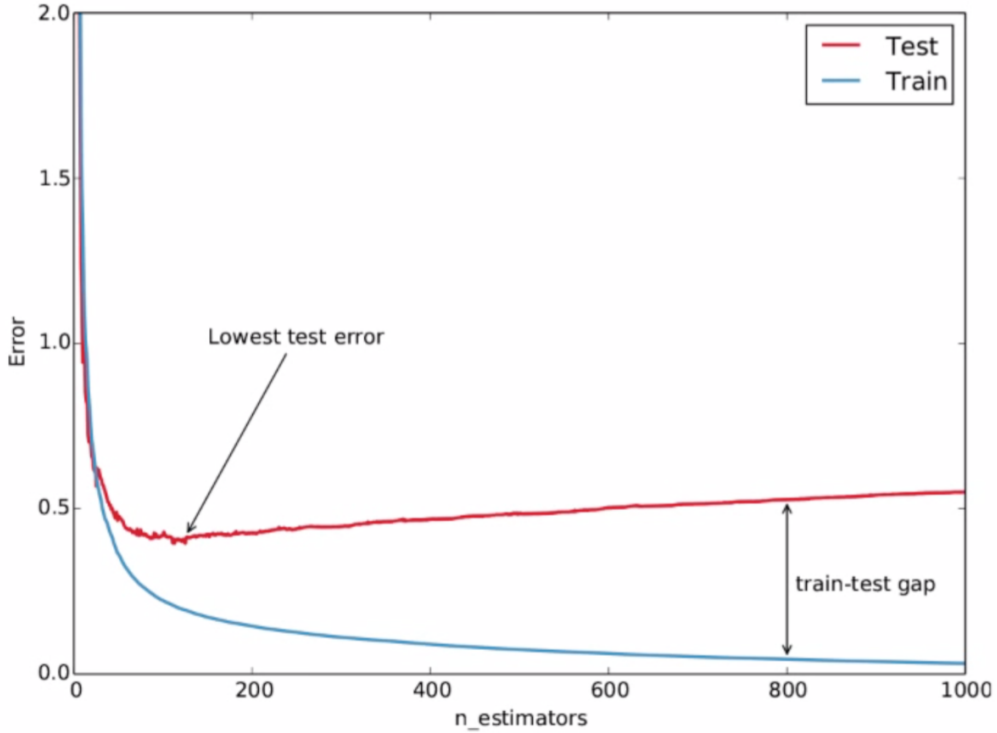

https://www.r-bloggers.com/an-attempt-to-understand-boosting-algorithms/

Loss Functions

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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 descent

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

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

to move in the direction of greatest decrease in loss

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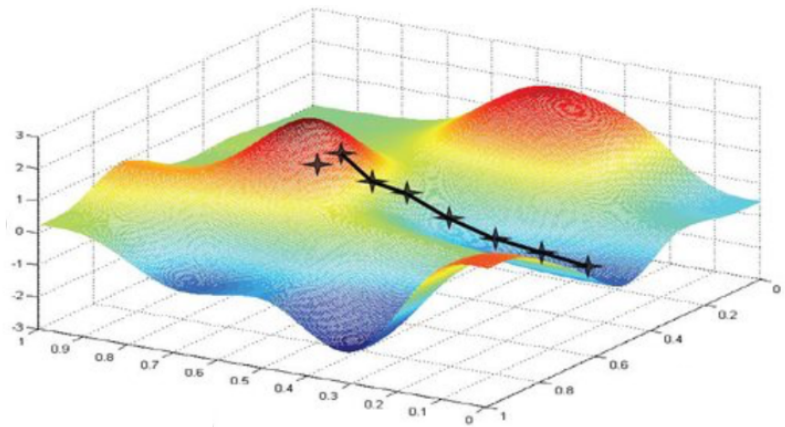

The direction of maximal increase is the the gradient of a function

(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

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

  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

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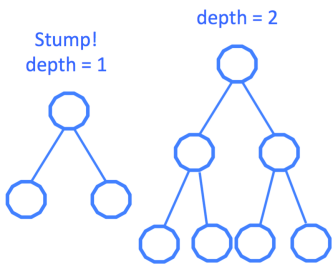

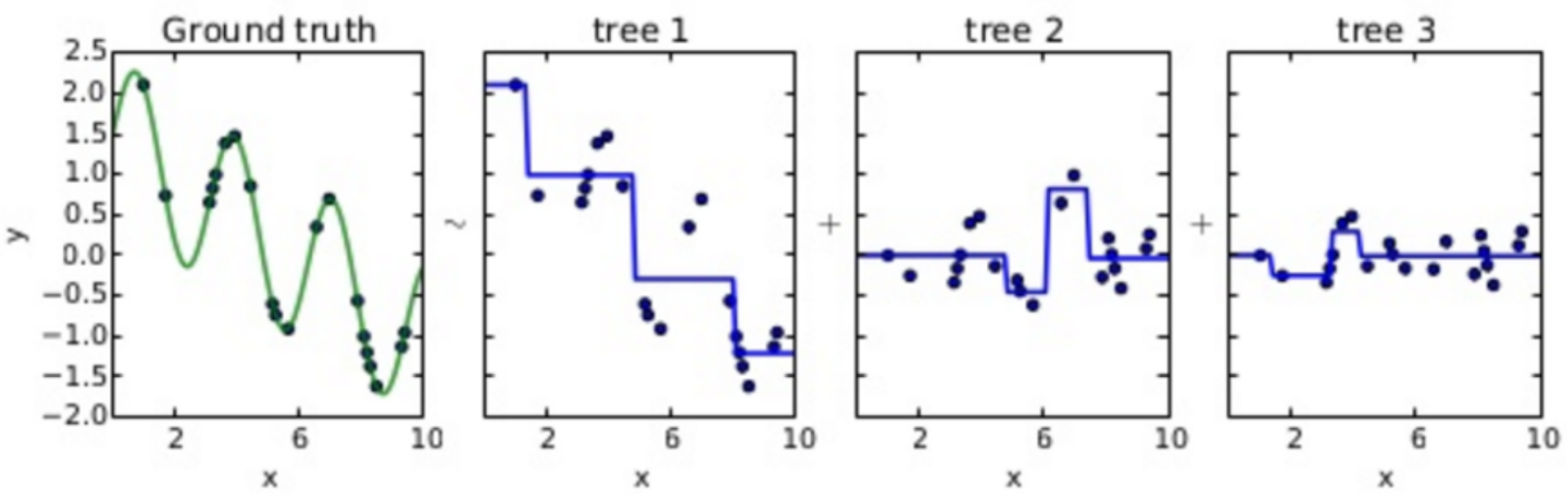

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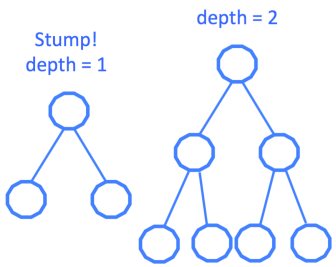

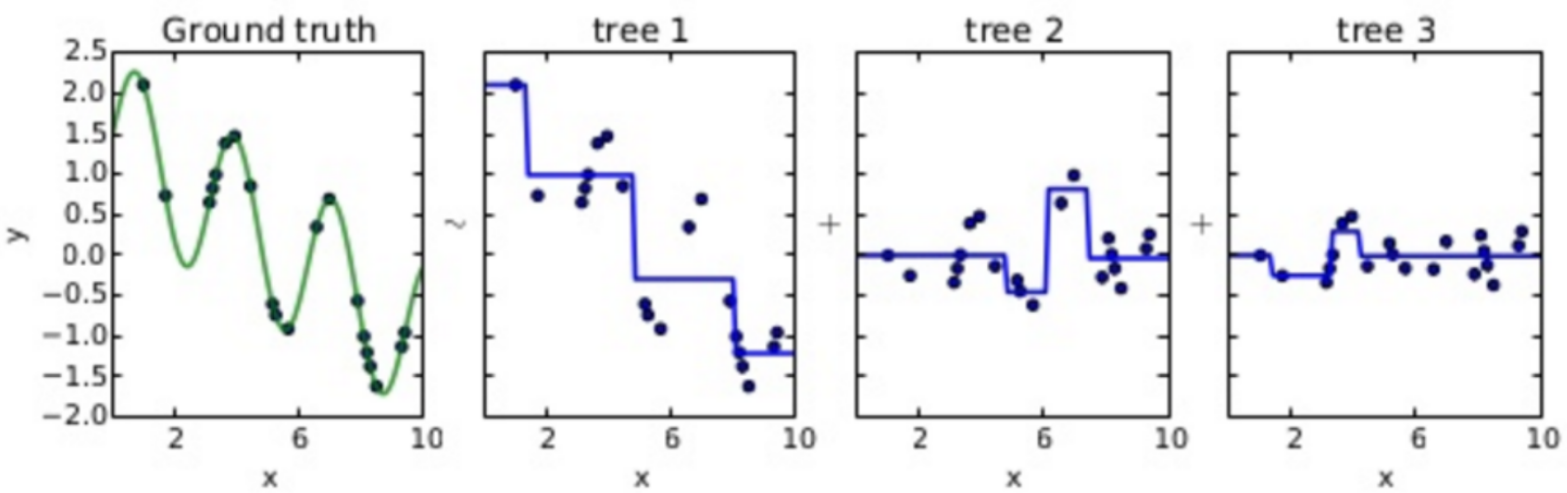

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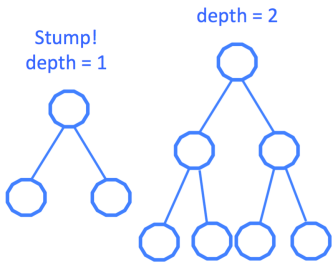

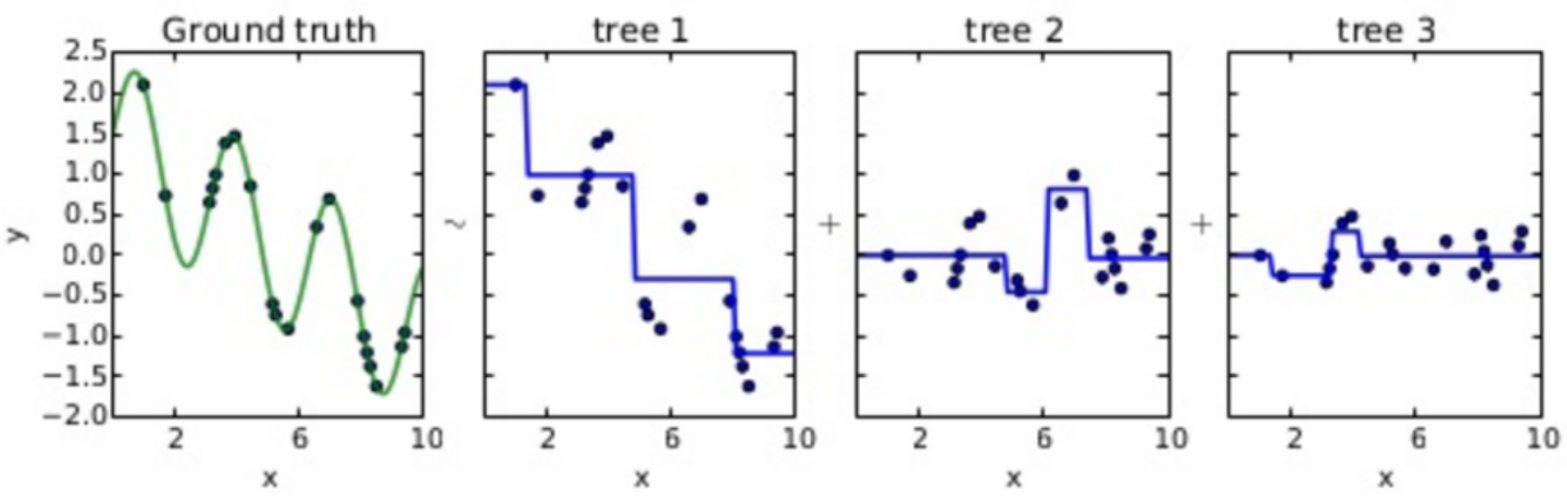

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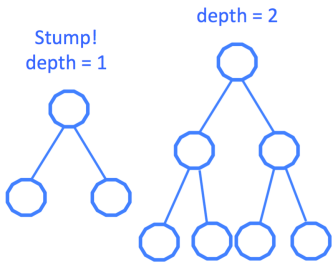

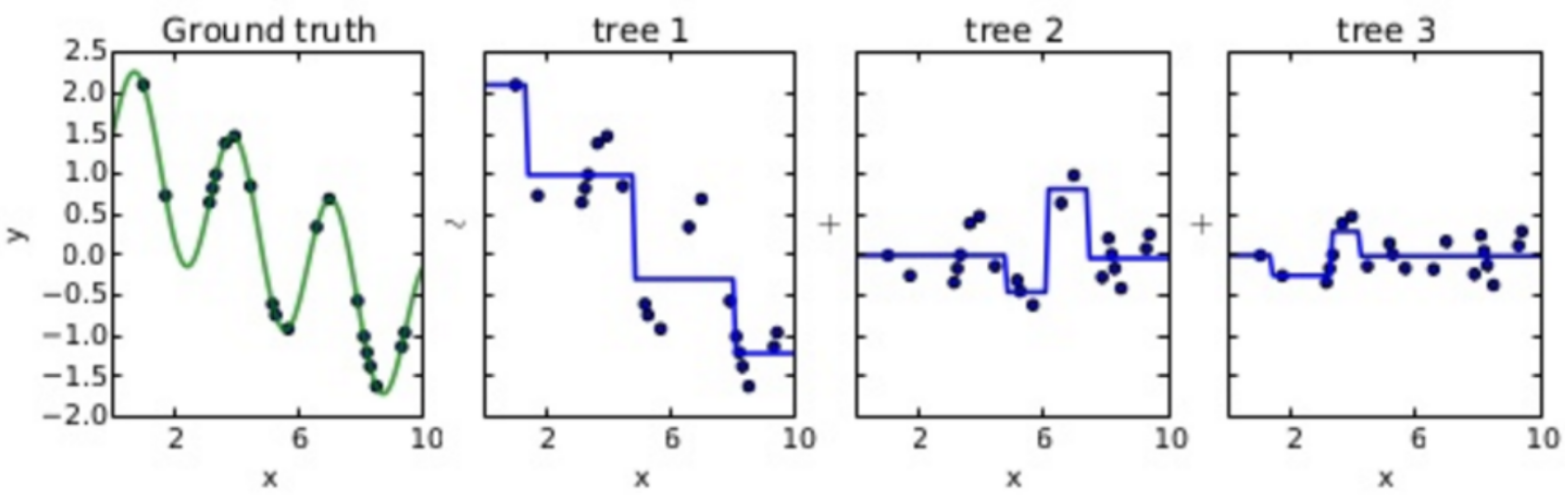

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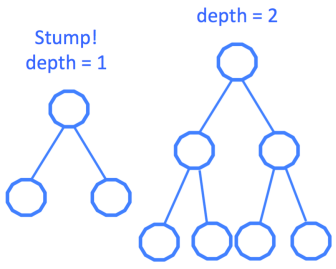

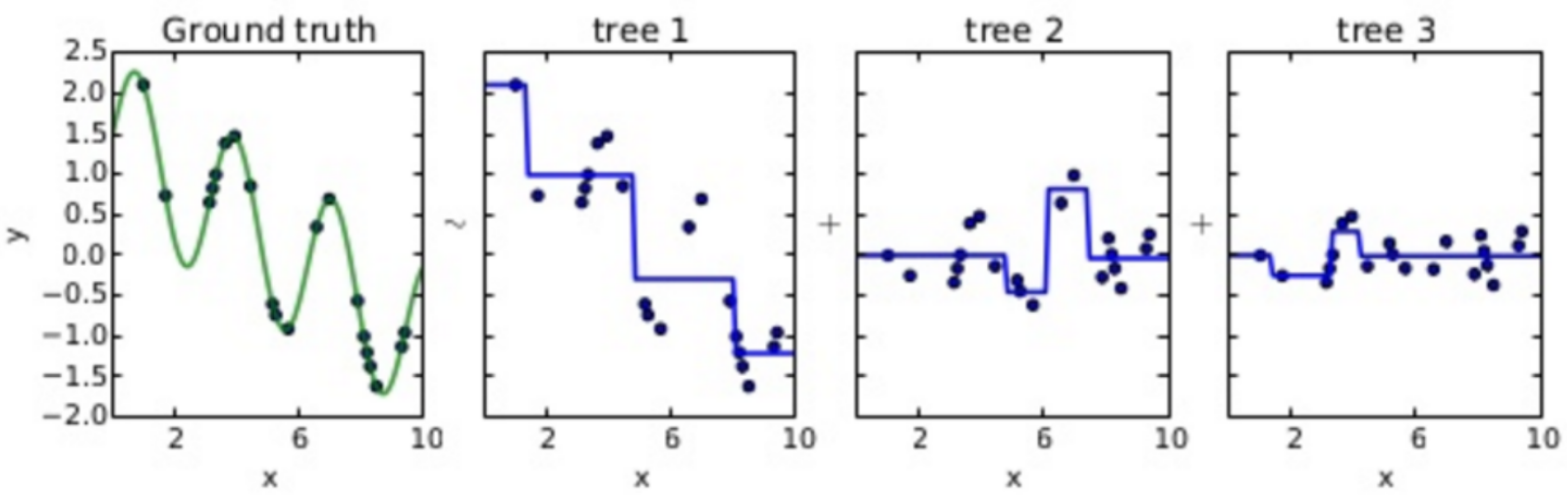

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  - we only move to $f_k(\boldsymbol{x}) + \alpha_k \hat{W}(\boldsymbol{x}, \gamma_k)$ at learning rate α_k

Some loss functions

Regression

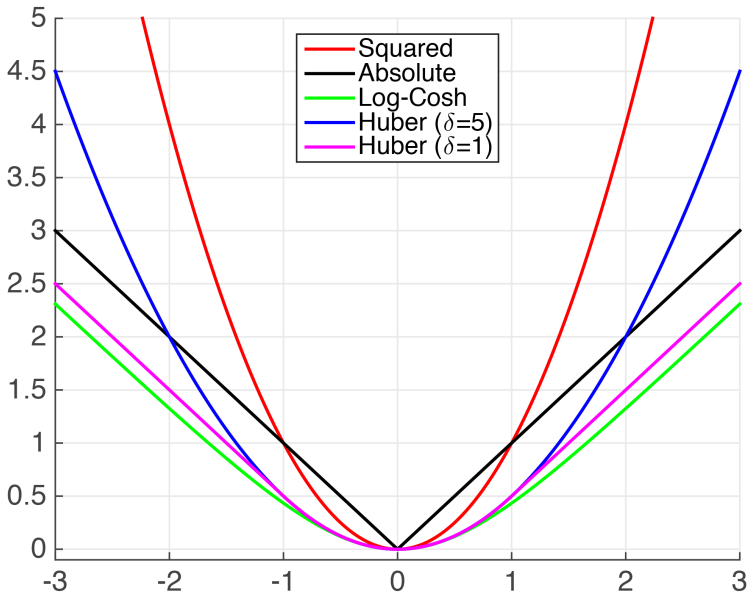
Squared Loss $\frac{1}{2}(Y_i - \boldsymbol{x}_i^T\beta)^2$

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

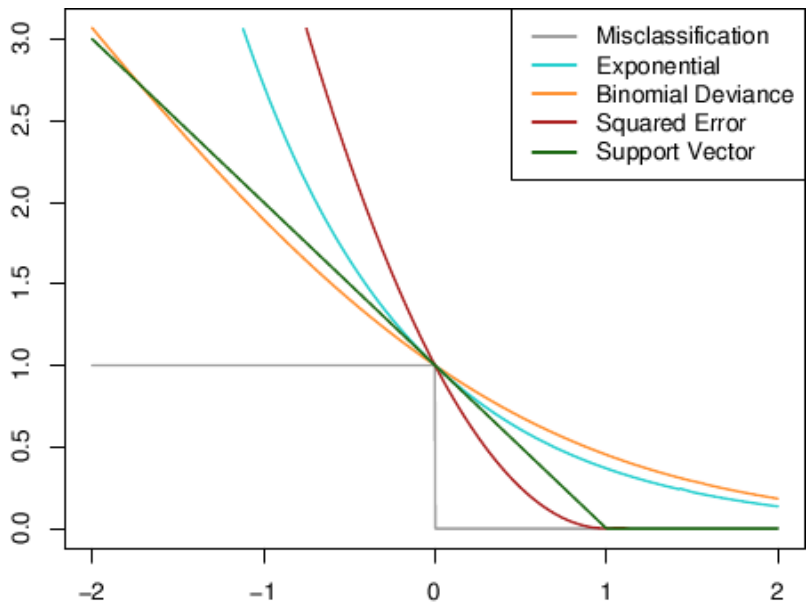
Classification {-1, 1}

Log Loss $\frac{1}{ln2} ln(1 + e^{-Y_i/\left(1+e^{-\boldsymbol{x}_i^T\beta}\right)})$ (Logistic Reg.)

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



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



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

Gradient Boosting VS Gradient Descent

$$\frac{\partial L(Y_i, \hat{Y}_i = \boldsymbol{x}_i^T \boldsymbol{\beta})}{\partial \hat{Y}_i} \text{ VS } \frac{\partial L(Y_i, \hat{Y}_i = \boldsymbol{x}_i^T \boldsymbol{\beta})}{\beta_j}$$

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$Y \in \{-1, 1\}$ $W(\cdot, \gamma_k)$ is a "weak learner"

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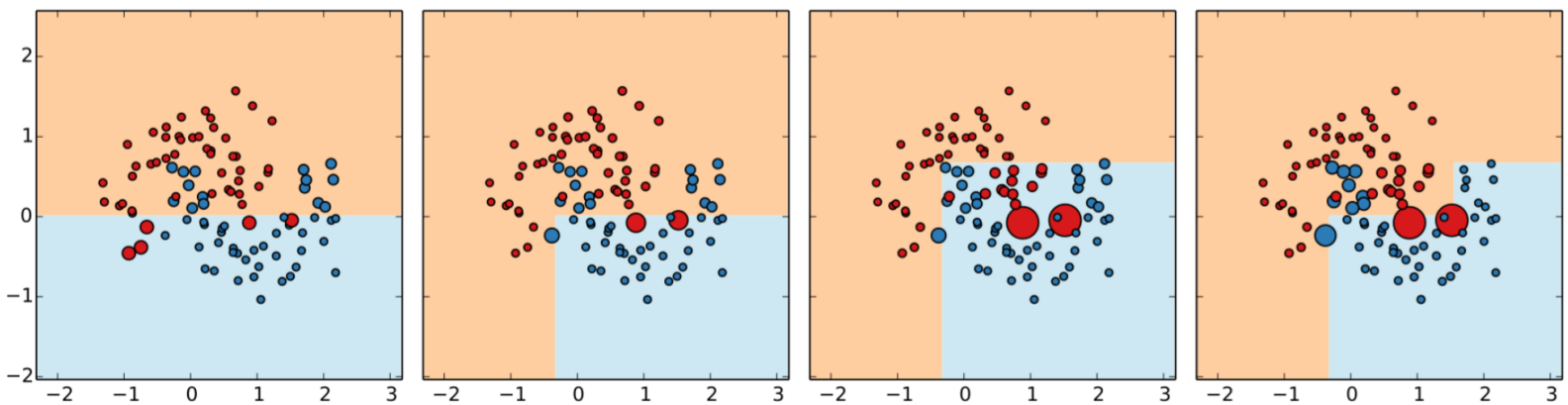

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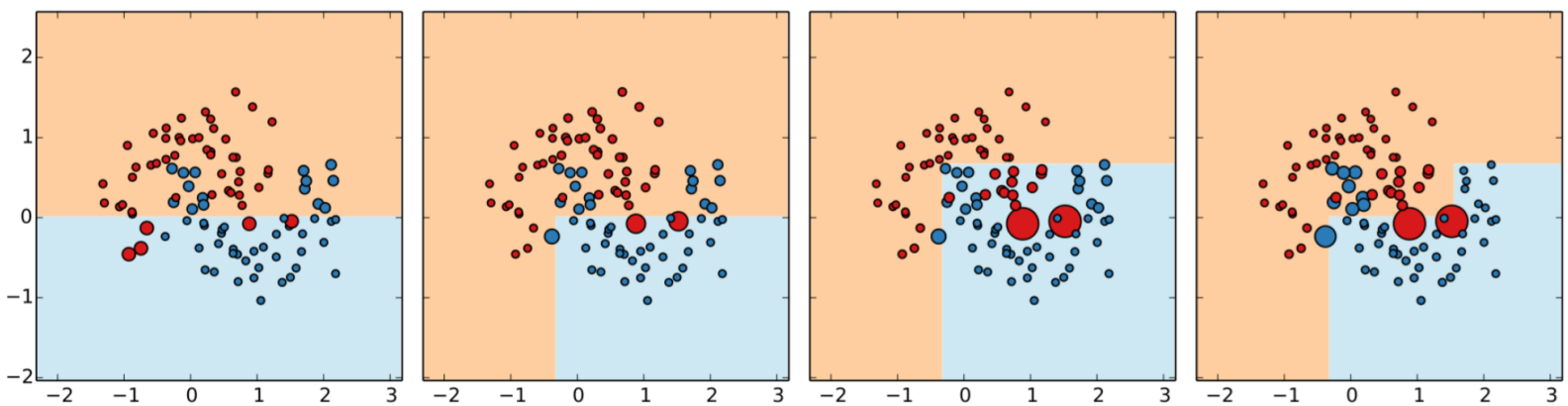

*Sean Sall's slides have an appendix showing that AdaBoost is exponential loss

XGBoost (eXtreme Gradient Boosting)

- Percentiles binned features: faster/more efficient splitting
- Handles missing data
- Smart memory management/out-of-core computation
  (i.e., data too big to fit into memory)

`http://xgboost.readthedocs.io`

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

New Segment: "Scott's Sage Words of Wizdum"

- If your "in sample" prediction error matches your "out of sample" prediction error, your model is generalizing well out of sample.
- Otherwise, you're overfitting.
- This is checked with K-folds cross-validation.
- If you're generalizing well out of sample, then you might as well use all your data for your final fit.
- If you're not then generalizing well out of sample (or even if you are) you can get a feel for the types of errors you'll make (based on your prediction performance from K-folds); you can aggregate your fits across the K-folds somehow and expect that sort of error.
- Aggregating and using all your data when you know you're overfitting means you know you have overfitting issues (and kind of know what they are based on k-folds) but you're happy to use all your data and risk even further overfitting anyway. LOO cross validation might be a reasonable way to assess what your actual errors would be under the "full data usage" approach.

- Random Forests *can* overfit; but not because you add more trees; rather, because the trees can be very complex (though this can be tuned) and therefore fit idiosyncrasies of the data (even in spite of the bootstrapping – i.e., the idiosyncrasies that still show through in the bootstrapping).
- Random Forests just don't overfit as a result of adding more predictors (i.e., trees).
- OOB and training error *are not* the same thing; yes, OOB tells you how you generalize *within your training set*, but that doesn't matter if your test set has associations that are not reflected in the training set.
- This is of course also the same risk in K-folds... but, as with OOB, one hopes such problems aren't present
- Or, all of these methods can overfit (find spurious associations or chase outliers) in sample. OOB doesn't save you from that. And of course OOB is not apples to apples across methodologies.

- Random forests are built in a very structured, data partitioning manner that can have some intrinsic bias, actually. Because boosting moves so slowly, sequentially rather than instantaneously partitioning the data, it can remove that bias. And while too many trees can cause boosting to be a high variance (overfitting prone) model, boosting moves so slowly that actually it is not so responsive to outlier data points until deep into the process.

- all of these methods can overfit in sample but still potentially improve in out of sample performance over models that are capturing more "generalizable", but coarser, associations.
- Inference here may not be key for prediction then, unless of course extrapolations are needed and work under the simpler model
- Inference is needed when you don't have the ability to perform predictive testing