DATA SCIENCE

DREAM JOB

Boosting Trees

One tree is not enough...

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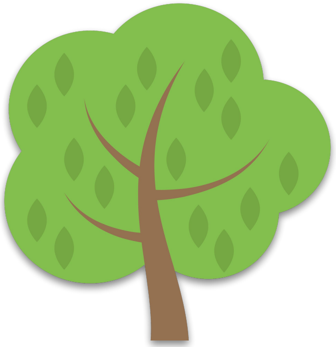
Introduction to Boosting



Goal: Convert weak learners → Strong Learner

❑ Combines simple models into one composite model

❑ **Composite Model = Simple Model (1) + Simple Model (2) + ...**

❑ Each simple model focuses on the errors of the previous one

❑ Each model is dependent upon the previous one

❑ Each model that is added tries to improve the overall performance of the ensemble

Gradient Boosting Strength/Weakness

Strengths: 💪

❑ Robust + Powerful

❑ Directly optimizes cost function

❑ Works for both regression/classification

❑ Can capture non-linear relationships

❑ Can capture various interactions in data

❑ Implicit variable selection (feature importance)

Weaknesses: 😫

❑ Requires careful tuning

❑ Prone to overfitting

❑ Several hyperparameters

Important Concepts / Terminologies

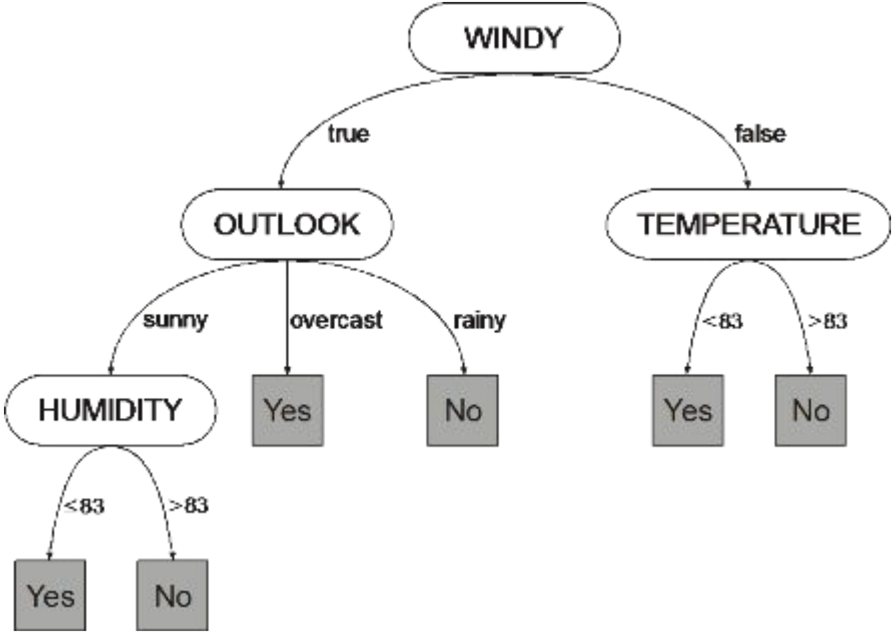
1. What is a Decision Tree?
2. What is an Ensemble?
3. What is an Additive Model?
4. What is a Residual/Error?
5. What is Gradient Descent? What is a Loss Function?

What is a Decision Tree?

Decision Trees look for the best split in your data and partitions it into sub-groups.

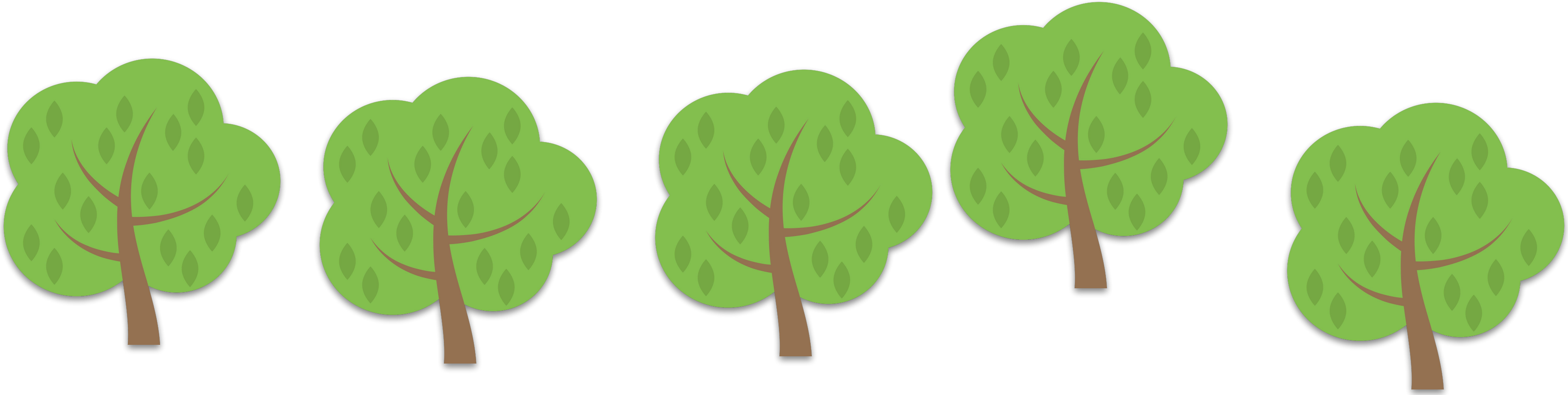
The importance of a feature is defined on top of the tree and is lowered as it goes down

1. **Root Node:** It represents entire population or sample and this further gets divided into two or more homogeneous sets.
2. **Splitting:** It is a process of dividing a node into two or more sub-nodes.
3. **Decision Node:** When a sub-node splits into further sub-nodes, then it is called decision node.
4. **Leaf/Terminal Node:** Nodes do not split is called Leaf or Terminal node.

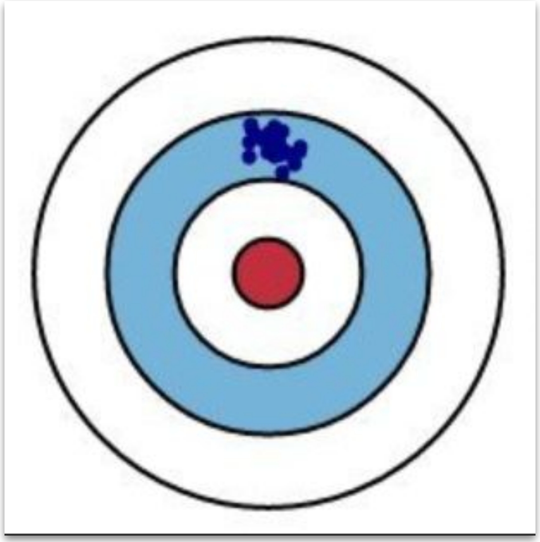


What is an Ensemble?

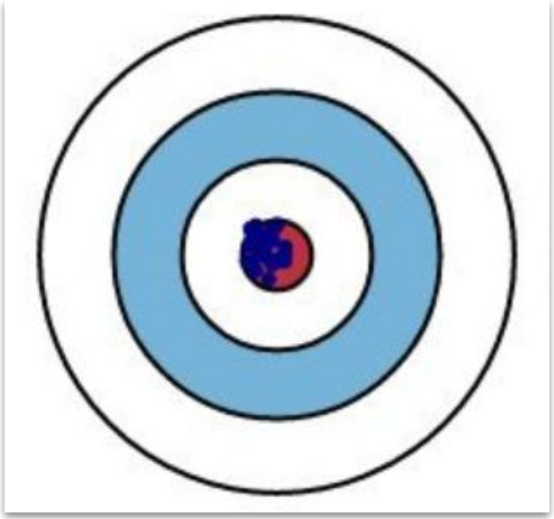
- It’s a ***collection*** of predictors that comes together to make a final prediction
- Ensembles learn many weak classifiers that are good at different parts of the input space.
- Helps reduce bias and variance error
- **Two Types**: Boosting & Bagging



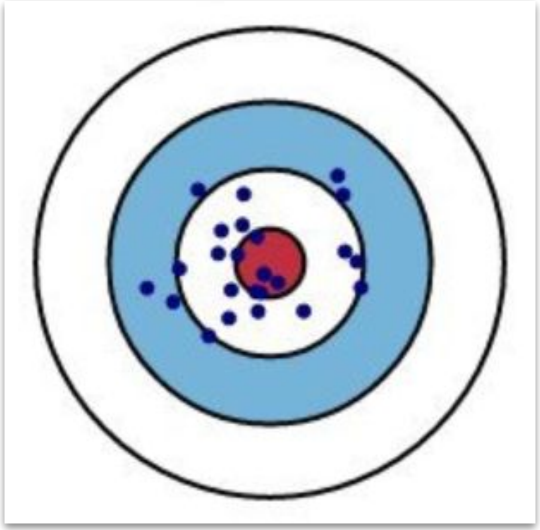
Bias Variance Tradeoff



High Bias



Low Bias & Low Variance



High Variance

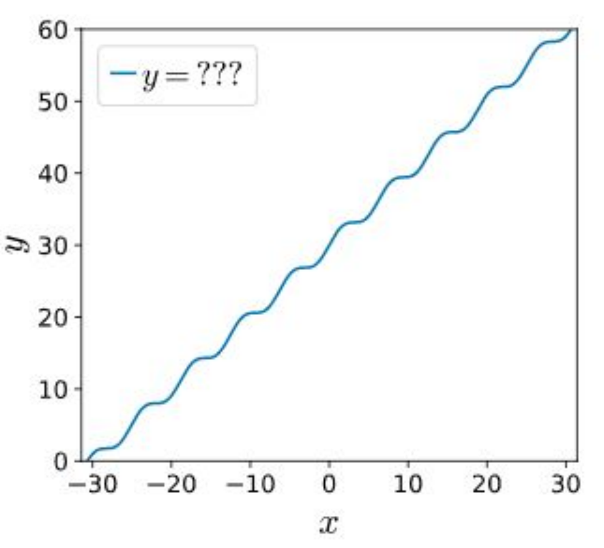
What is an Additive Model?

❑ **Big Idea:** Add a bunch of simple functions (models) to create a more complex function

❑ Boosting is an Additive Model

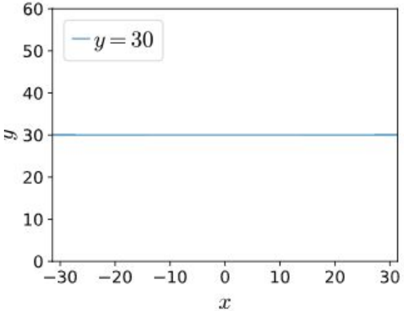
❑ Foundation of boosting algorithm

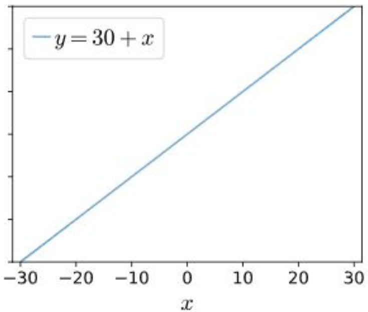
❑ F(x) = f1(x) + f2(x) + f3(x)

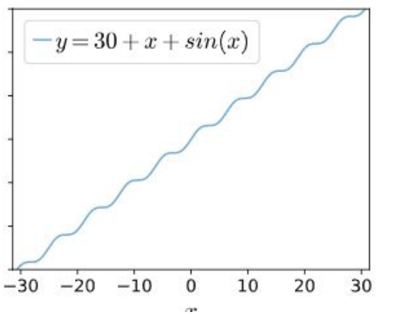


What function is this??

Model_1 + Model_2 + Model_3





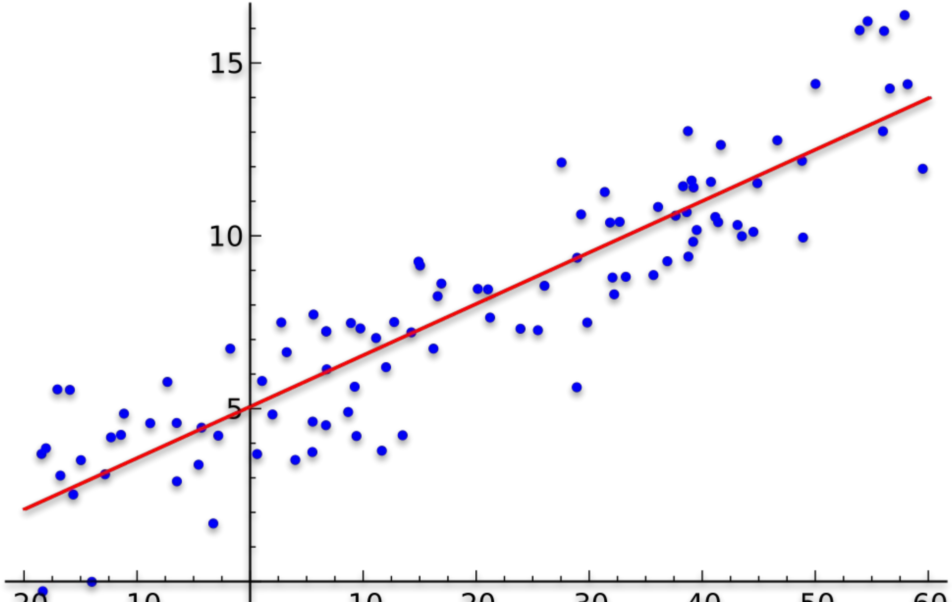


What is a Residual?

- ❏ **Residual** = Actual - Predicted

- ❏ Also known as the **errors**

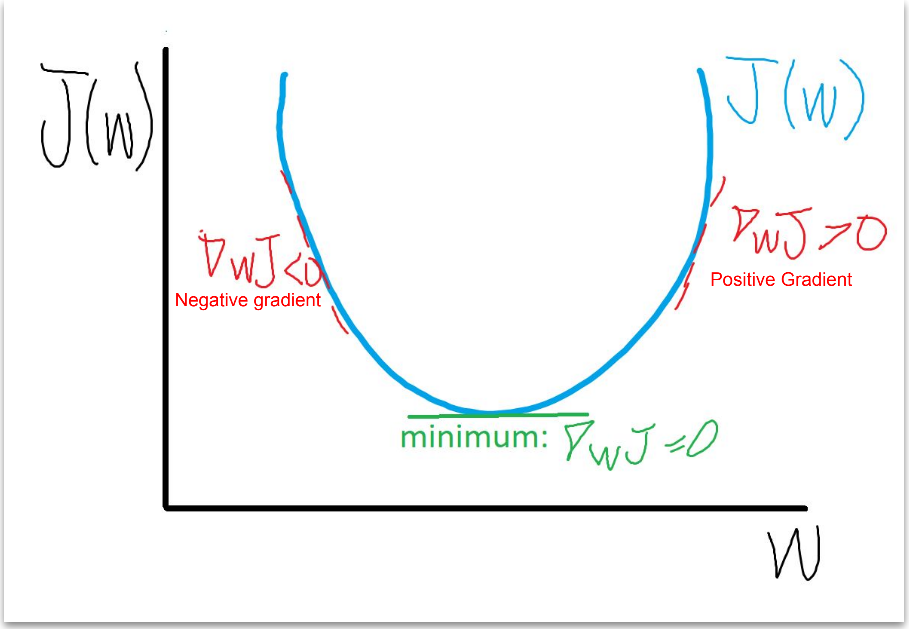
- ❏ Tells you how far off you are from the actual value



Source: https://upload.wikimedia.org/wikipedia/commons/thumb/3/3a/Linear_regression.svg/1000px-Linear_regression.svg.png

What is Gradient Descent?
What is a Loss Function?

Goal of Gradient Descent: Find optimal weight that minimizes the loss function



$$Loss = MSE = \sum (y_i - y_i^p)^2$$

where, y_i = ith target value, y_i^p = ith prediction, $L(y_i, y_i^p)$ is Loss function

Types of Boosting Methods

1. AdaBoost 🌳
2. Gradient Boosting 🌳
3. XGBoost 🌳
4. LightGBM 🌳
5. CatBoost 🌳

AdaBoost vs Gradient Boosting

They differ on **how they create the weak learners** during the additive stages.

- ❏ In each stage, the learner will try to **fix** the **“weaknesses”** of the previous learner.
- ❏ Gradient Boosting uses **different** training samples at each stage
- ❏ AdaBoost uses the **same** training samples at each stage

Gradient Boosting

“Weaknesses” = “Residuals”

AdaBoost

“Weaknesses” = “High-weight data points”

- ❏ These **“weaknesses”** tell us how to improve our model

AdaBoost

General idea is to have each learner concentrate on instances that are difficult to correctly classify

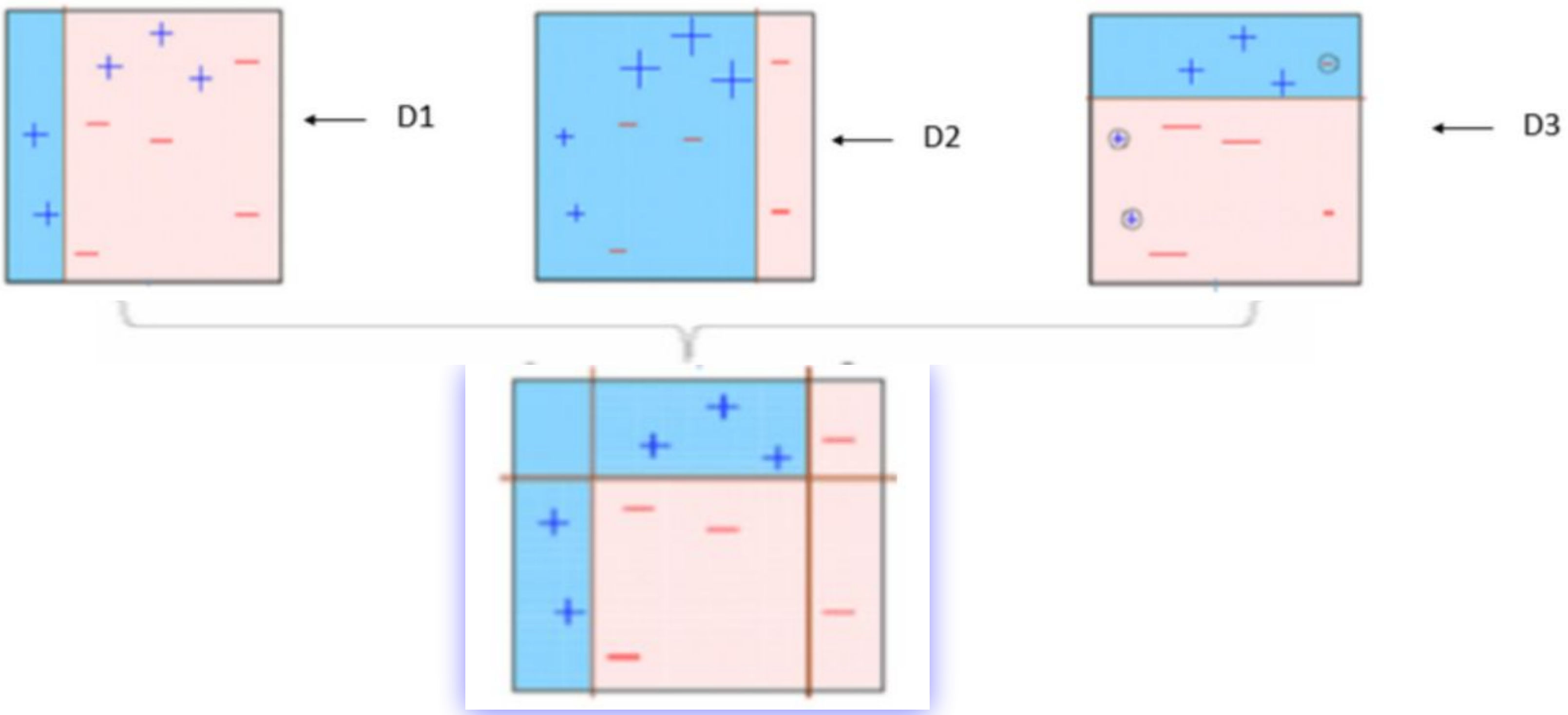
❑ A model is fitted in a **forward stage-wise** fashion

❑ Increases the weights of the wrongly predicted instances

❑ Decreases the weights of the correctly predicted instances

❑ Weak learner focuses more on the difficult instances (errors) from the previous learner

AdaBoost Example



D1 + D2 + D3
(Ensemble)

Gradient Boosting

- ❑ Intuitively, Gradient Boosting is a **residual fitting method**
- ❑ A model is fitted in a **forward stage-wise** fashion
- ❑ Focuses on learning the remaining errors (aka **error fitting**)
- ❑ Can utilize other loss functions

3 Parts of Gradient Boosting

1. A **loss function** to be optimized
2. A **weak learner** to make predictions
3. An **additive model** to add weak learners to minimize loss function

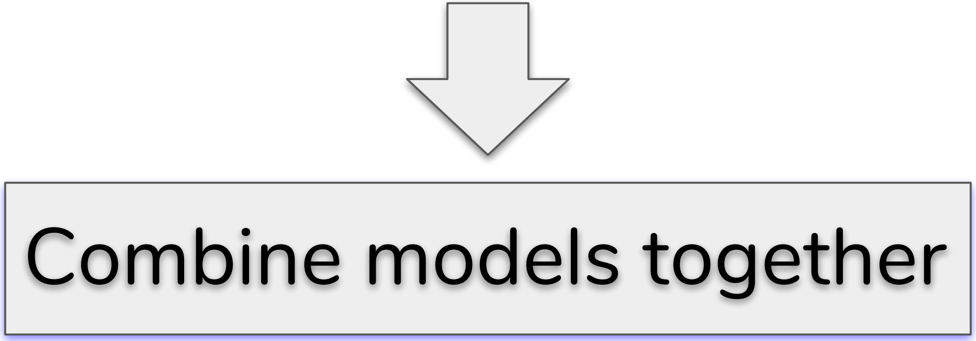
❑ Loss function must be differentiable (e.g. MSE, MAE, LogLoss)

❑ Weak learners are usually decision trees

❑ An additive model is a model of many other learners

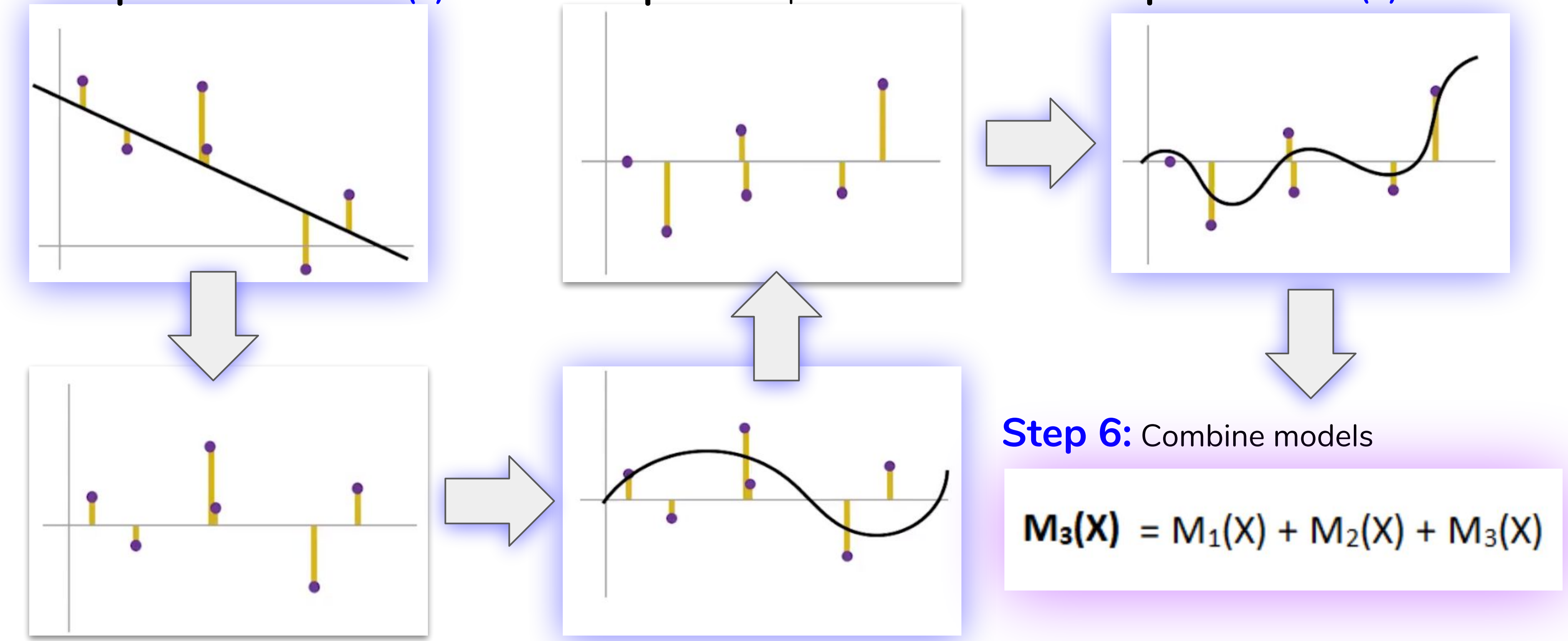
3 Steps of Gradient Boosting

1. You fit a model
2. You compute the errors or residuals
3. You fit another model to the residuals



Combine models together

Gradient Boosting Example



Step 1: Fit base **Model (1)**

Step 2: Compute residuals

Step 3: Fit **Model (2)** on residuals

Step 4: Compute residuals

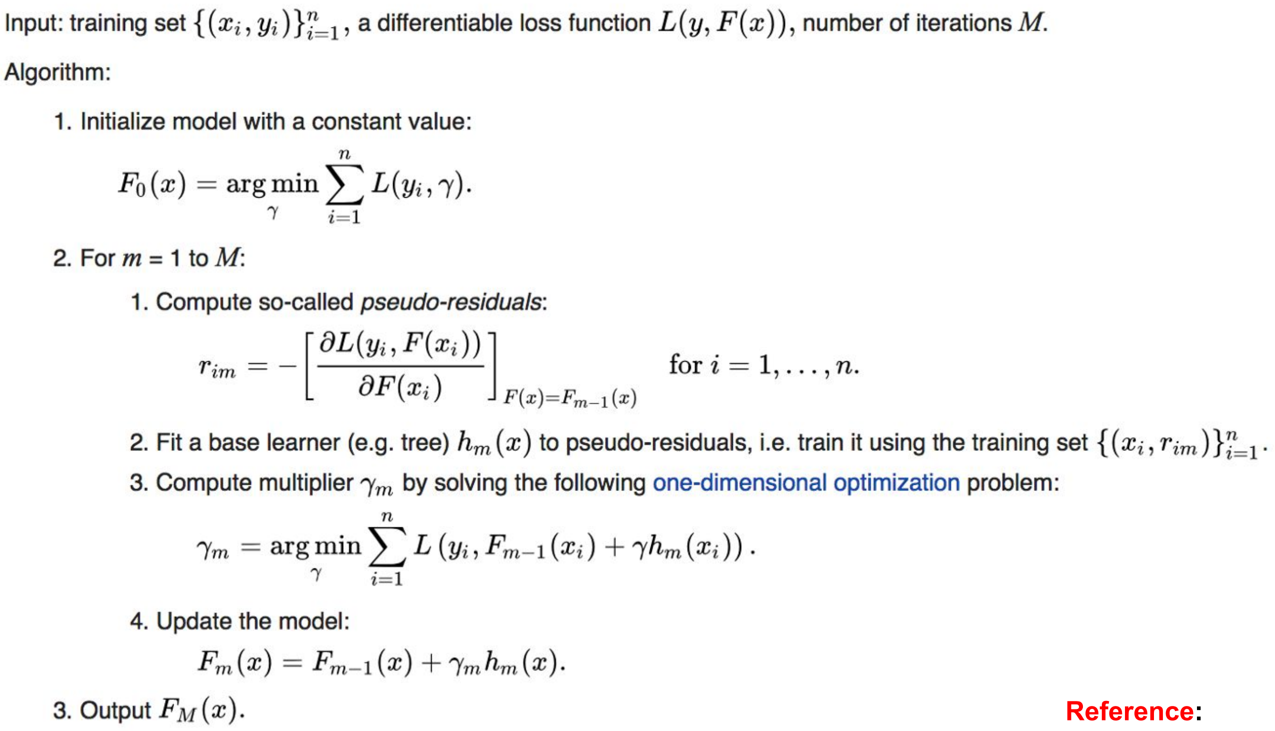
Step 5: Fit **Model (3)** on residuals

Step 6: Combine models

$$\mathbf{M_3(X)} = M_1(X) + M_2(X) + M_3(X)$$

Gradient Boosting Algorithm

From Wikipedia:



Input: training set $\{(x_i, y_i)\}_{i=1}^{n}$, a differentiable loss function $L(y, F(x))$, number of iterations M.

Algorithm:

1. Initialize model with a constant value:

   $$F_0(x) = \underset{\gamma}{\arg\min} \sum_{i=1}^{n} L(y_i, \gamma).$$

2. For *m* = 1 to M:
   1. Compute so-called *pseudo-residuals*:

      $$r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, \ldots, n.$$

   2. Fit a base learner (e.g. tree) $h_m(x)$ to pseudo-residuals, i.e. train it using the training set $\{(x_i, r_{im})\}_{i=1}^{n}$.
   3. Compute multiplier γ_m by solving the following one-dimensional optimization problem:

      $$\gamma_m = \underset{\gamma}{\arg\min} \sum_{i=1}^{n} L\left(y_i, F_{m-1}(x_i) + \gamma h_m(x_i)\right).$$

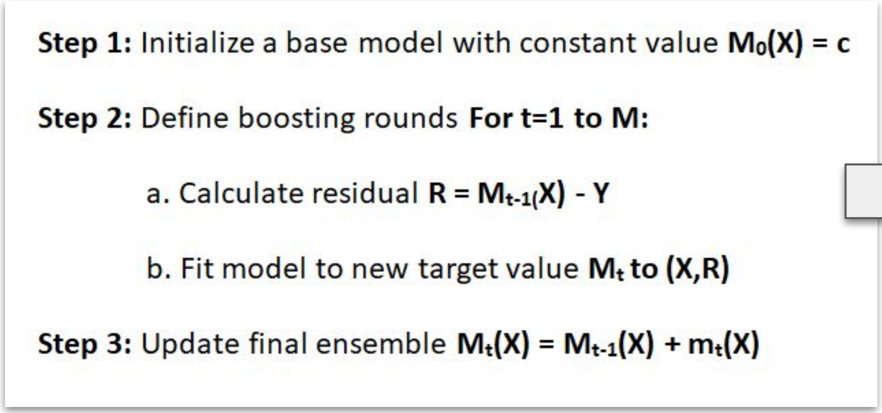
   4. Update the model:

      $$F_m(x) = F_{m-1}(x) + \gamma_m h_m(x).$$

3. Output $F_M(x)$.

Reference:
https://en.wikipedia.org/wiki/Gradient_boosting#Algorithm

Gradient Boosting Algorithm Simplified



Step 1: Initialize a base model with constant value $\mathbf{M_0(X) = c}$

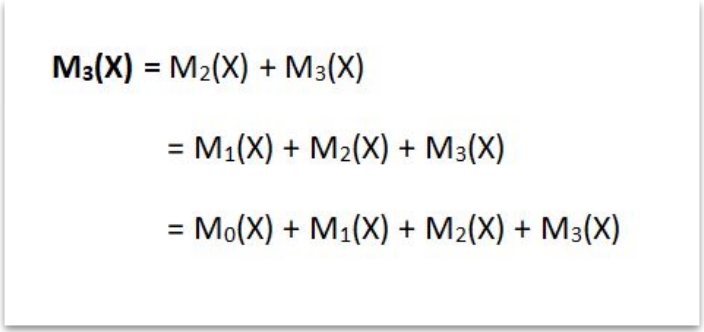
Step 2: Define boosting rounds **For t=1 to M:**

a. Calculate residual $\mathbf{R = M_{t-1(}X) - Y}$

b. Fit model to new target value **$\mathbf{M_t}$ to (X,R)**

Step 3: Update final ensemble $\mathbf{M_t(X) = M_{t-1}(X) + m_t(X)}$

Final Ensemble



$\mathbf{M_3(X)} = M_2(X) + M_3(X)$

$= M_1(X) + M_2(X) + M_3(X)$

$= M_0(X) + M_1(X) + M_2(X) + M_3(X)$

GRADIENT BOOSTING

$$\hat{y}[i] = \hat{y}[i] + \underline{\text{alpha f}[i]}$$

GRADIENT DESCENT

$$\theta = \theta - \eta * \underline{\nabla_\theta J(\theta)}$$

The updates to reduce error

Cost Function (MSE)

$$J(.) = \sum (y[i] - \hat{y}[i])^2$$

$$\Downarrow$$

Gradient of Cost Function

“Residuals”

$$\nabla J(y, \hat{y}) = (y[i]-\hat{y}[i])$$

★ By taking the **derivative of our cost function** J(.) w.r.t. y_hat , then we simply get the **residual**

How is Gradient Boosting Related to Gradient Descent?

❏ **Gradient Boosting**: Learning from the **residuals** nudges us to the right direction towards the **true y**

❏ **Gradient Descent**: Following the **negative gradient** of the loss function nudges us to the right direction towards the **true y**

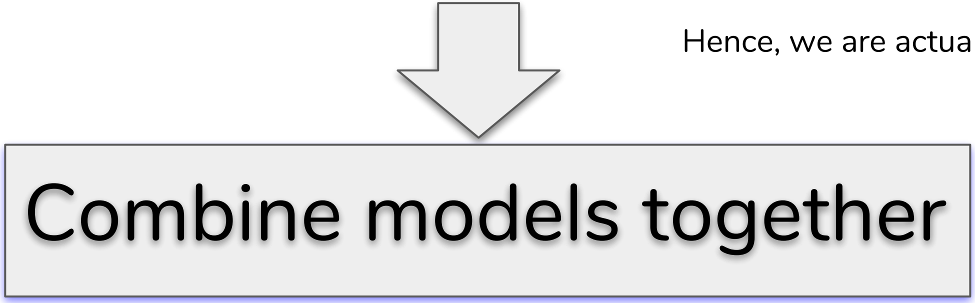
❏ So by following the **residuals/errors** in Gradient Boosting we are indirectly following the **negative gradient** of the loss function.

3 Steps of Gradient Boosting (AGAIN)

Residual ⇔ Negative Gradient

1. You fit a model
2. You compute errors on residuals ⇔ You compute errors on negative gradient
3. Fit model to residuals ⇔ Fit model to negative gradients

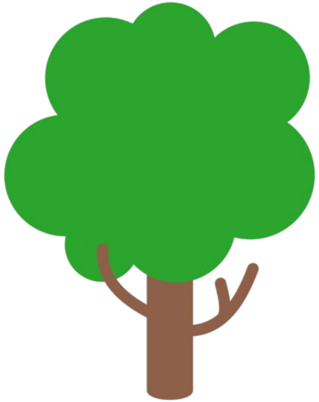
Update model based on residual ⇔ Update model based on negative gradient



Combine models together

Hence, we are actually **updating** our model **using gradient descent!**

Summary



Ensemble methods:

❏ Combine multiple models to make a “better” one
❏ Each model is going to learn something the others can’t
❏ Wisdom of the crowd

Boosting method:

❏ Combine “weak” learners → “strong” learner
❏ Each additive model focuses on the “weaknesses” of the previous one
❏ The “weaknesses” tells us how to improve our model
❏ Sum of predictions makes it more accurate and complex
❏ It learns sequentially

Sources & Reference

Decision Tree Diagram:

https://www.google.com/url?sa=i&source=images&cd=&cad=rja&uact=8&ved=2ahUKEwisjsSkn6zfAhUIFnwKHXcEA5kQjRx6BAgBEAU&url=https%3A%2F%2Fen.wikipedia.org%2Fwiki%2FFile%3ADecision_tree_for_playing_outside.png&psig=AOvVaw37_R5dcmt9hVaNU1hj31mG&ust=1545320944074870

Bias/Variance Diagram: https://qph.fs.quoracdn.net/main-qimg-a55358a5a12b02c3f71010c965a2c4dc

AdaBoost Diagram: https://slideplayer.com/slide/9092209/27/images/19/Algorithm+Adaboost+-+Example.jpg