Ensemble Methods

Why Ensemble Methods ?

Kaggle

OSIC Pulmonary Fibrosis Progression Predict lung function decline Featured • 18 days to go • Code Competition • 1776 Teams	$55,000
RSNA-STR Pulmonary Embolism Detection Classify Pulmonary Embolism cases in chest CT scans Featured • a month to go • Code Competition • 118 Teams	$30,000
Lyft Motion Prediction for Autonomous Vehicles Build motion prediction models for self-driving vehicles Featured • 2 months to go • Code Competition • 405 Teams	$30,000
Mechanisms of Action (MoA) Prediction Can you improve the algorithm that classifies drugs based on their biological activity? Research • 2 months to go • Code Competition • 1325 Teams	$30,000
Google Landmark Recognition 2020 Label famous (and not-so-famous) landmarks in images Research • 11 days to go • Code Competition • 667 Teams	$25,000
OpenVaccine: COVID-19 mRNA Vaccine Degradation Prediction Urgent need to bring the COVID-19 vaccine to mass production Research • 17 days to go • 831 Teams	$25,000

Why Ensemble Methods ?

“This is how you win ML competitions: you take other peoples’ work and ensemble them together.” <u>Vitaly Kuznetsov</u> NIPS2014

	Competition	Solutions, interviews and articles
	2019 Data Science Bowl Uncover the factors to help measure how young children learn	Forum • 1st place (zr & oyx) • 2nd place (Fuson) Word2Vec features, • 3rd place (Limerobot) transformer • 4th place (Crystal cave miners) tfidf, rnn

5. Model

1. **Data augmentation** : The model is trained on the full data (full train history and test previous, improve + 0.002).
2. **Loss** : We use rmse loss for training, and weighted rmse loss for validate.
3. **Threshold** : Then use Opitmizer Rounder to optimize thresholds for weighted qwk.
4. **Ensemble** : We just try a simple blending method (0.8 * lightgbm + 0.2 * catboost, the private score is 0.570. Since the cv score is not improved, we do not select it for our final results.

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Modeling

- For the validation set, we resampled to ensure one sample per one user.
- StratifiedGroupKFold, 5-fold.
- RSA (5 random seed) of LGB, CB, and NN.

Post Processing

- Ensemble = 0.5 * LGB + 0.2 * CB + 0.3 * NN.
- Set the threshold to optimize cv qwk.

Why Ensemble Methods ?

Tree based models

Lightgbm,Xgb, Catboost. (will be soon)

Stack

0 level) NN folds in folds model (5 outer folds, 5 inner folds), lgbm, catboost.
1st level) MLP, Lightgbm.
2nd level) Ridge.
https://www.kaggle.com/c/data-science-bowl-2019/discussion/127312

	long-best-threshold-f1	short-best-threshold-f1
Bert-base	0.618	0.457
Bert-large	0.679	0.541
Albert-xxl	0.700	0.555
ensemble	0.731	0.582

Models

We trained CatBoost, LightGBM, and MLP models on different subsets of the data:

- 1 model per meter
- 1 model per site_id
- 1 model per (building_id, meter)

Why Ensemble Methods ?

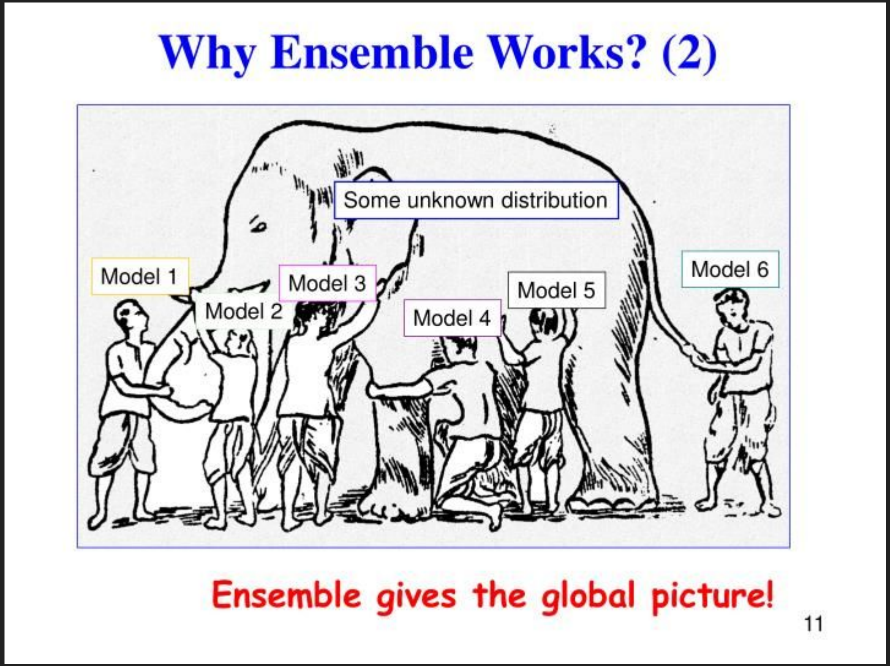
- Create a Baseline model.
- Works well for tabular data (pretty much any)
- Can Ensemble any model

Ensemble Methods ?

"Essentially, all models are wrong, but some are useful."

--- Box, George E. P.; Norman R. Draper (1987). Empirical Model-Building and Response Surfaces, p. 424, Wiley. ISBN 0471810339.

Ensemble Methods ?



The blind men and the elephant.

"Essentially, all models are wrong, but some are useful." and **their combination might be better**

Ensemble thought process

- Combine the predictions of many base estimators **that is combine many machine learning model prediction** **to improve the generalization and robustness of the model.**

Approaches :

1. Different training sets.
2. Different feature sampling.
3. Different algorithms.
4. Different hyperparameters.

CLEVER
AGGREGATION

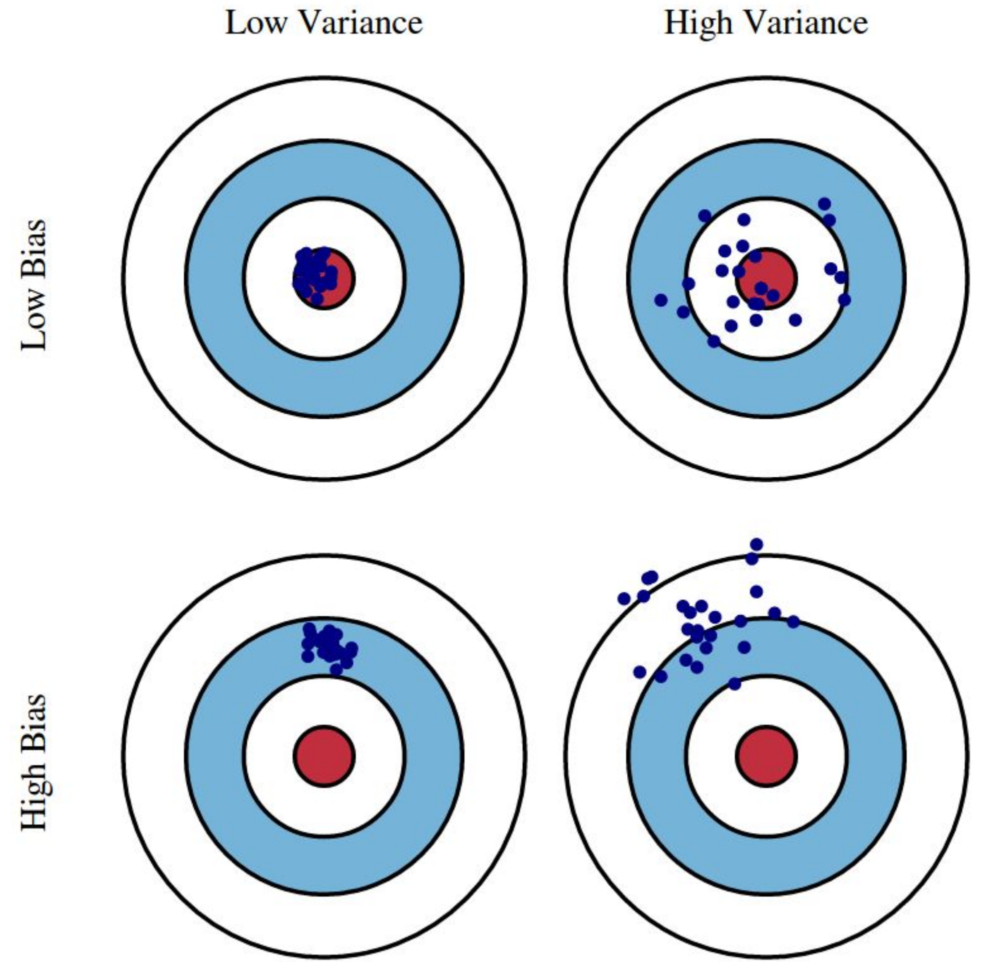
Ensemble thought process

- Combine the predictions of many base estimators **that is combine many machine learning model prediction** **to improve the generalization and robustness of the model.**

Types :

1. Averaging
2. Boosting
3. Voting
4. Stacking

CLEVER AGGREGATION

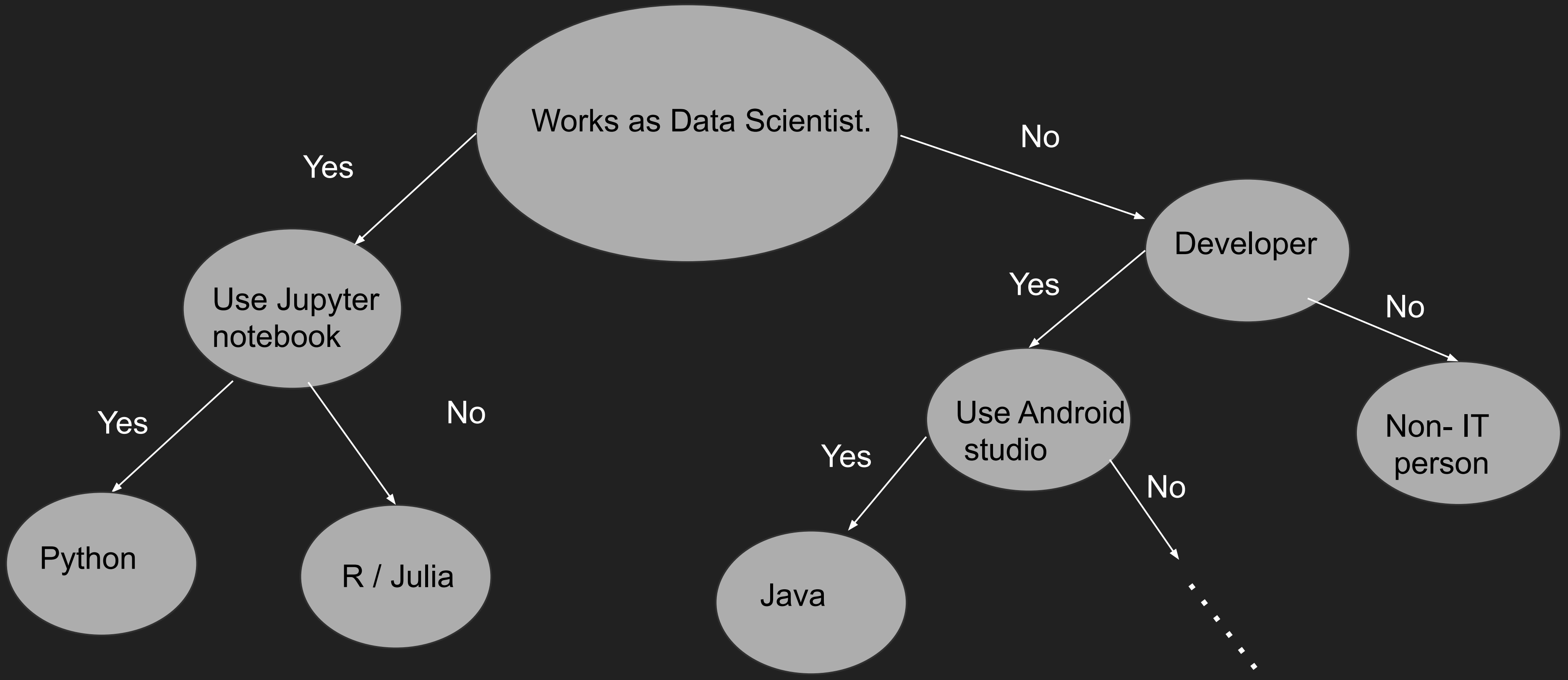

Low Variance
High Variance
Low Bias
High Bias

Ensemble thought process

- Combine the predictions of many base estimators **that is combine many machine learning model prediction** **to improve the generalization and robustness of the model.**

1. Averaging :

   Build different models **independently** and **average** their prediction to **reduce variance.**


Works as Data Scientist.
Yes
No
Use Jupyter notebook
Developer
Yes
No
Yes
No
Python
R / Julia
Use Android studio
Non- IT person
Yes
No
Java
......

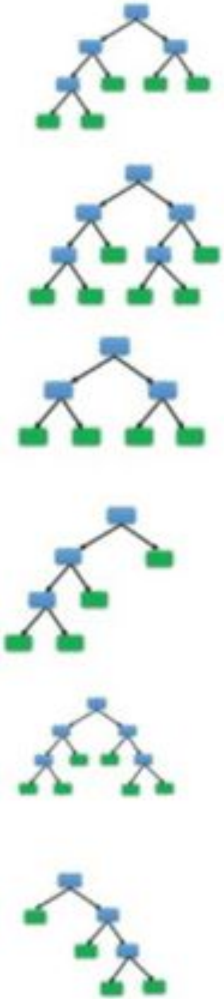
Random Forest

Random Forest :

1. Ensemble of Decision trees :

    a. Create different overfitted decision tree classifiers **using bootstrap aggregation.**

    b. While constructing each decision tree ; randomly choose k features among d.



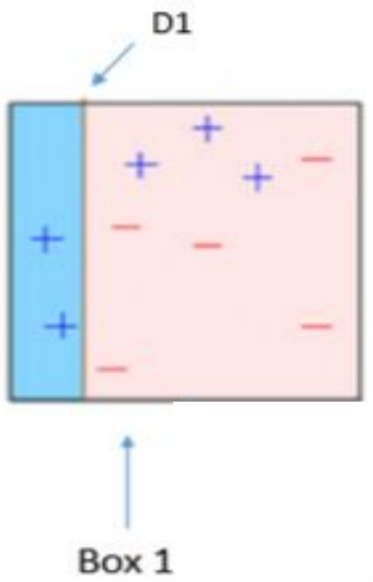
Random Forest in Action!!!

Boosting

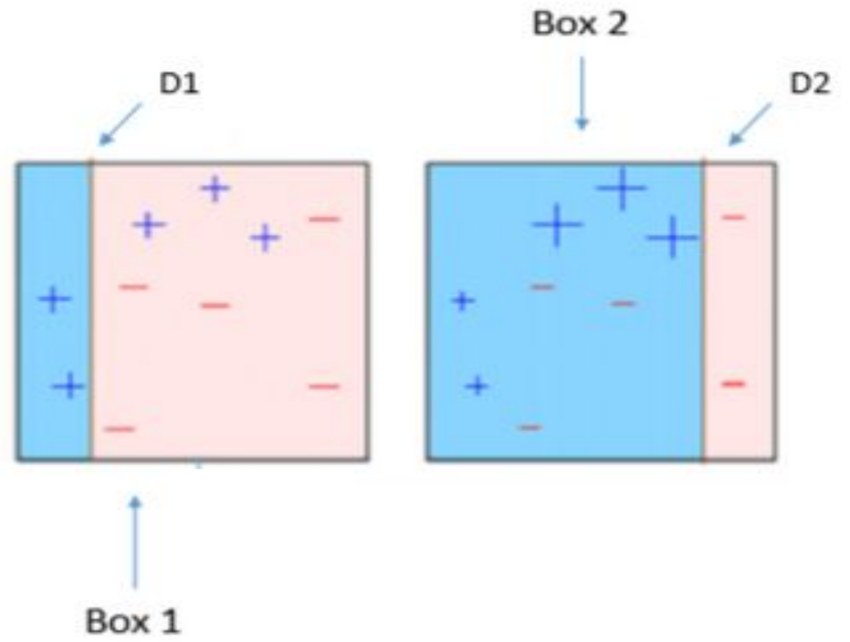
Build different models sequentially and by combining them try to reduce the bias.

- Weighted Boosting
- Gradient based Boosting.

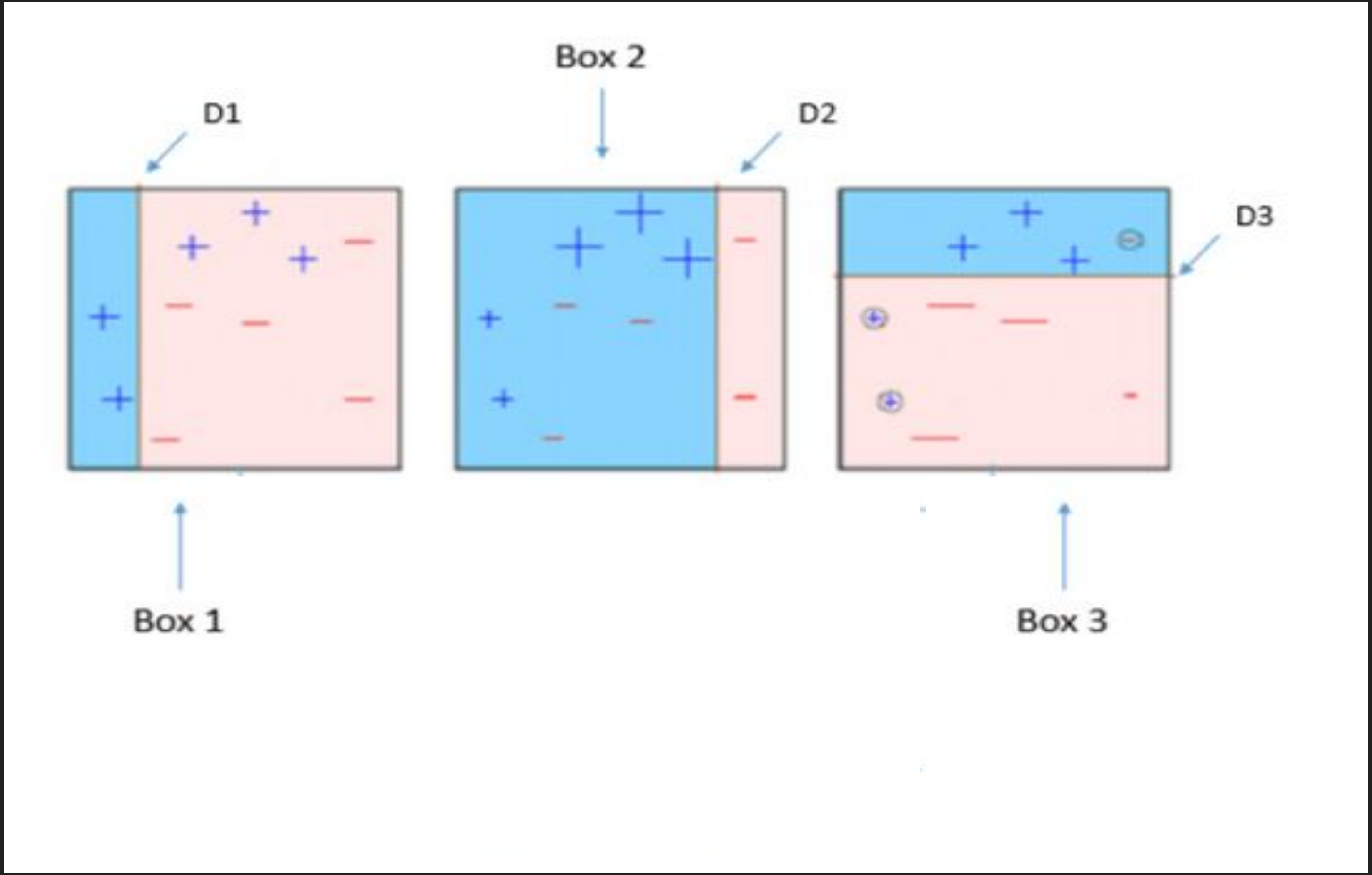
Weighted Boosting (AdaBoost)



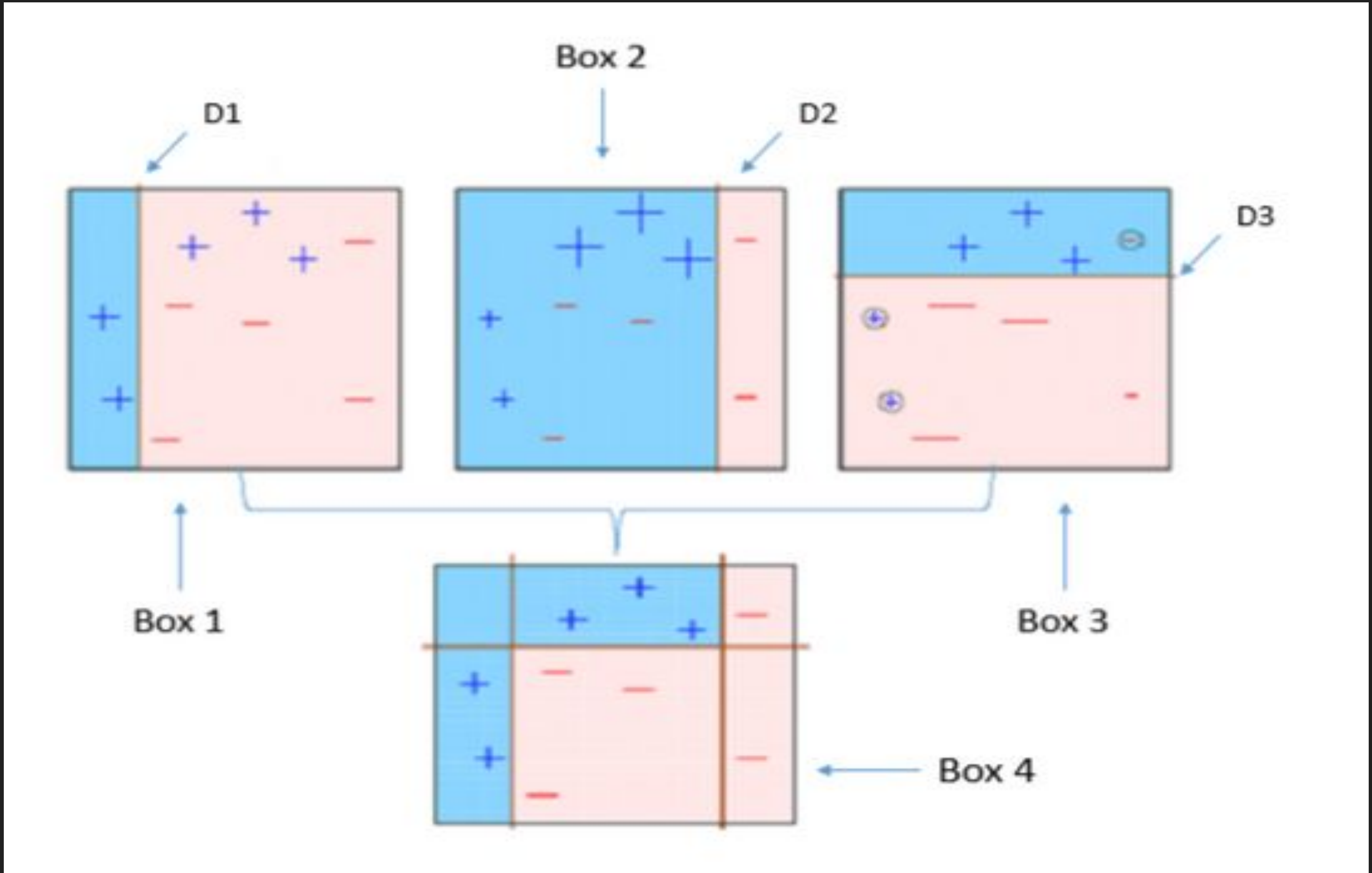
Weighted Boosting (AdaBoost)



Weighted Boosting (AdaBoost)



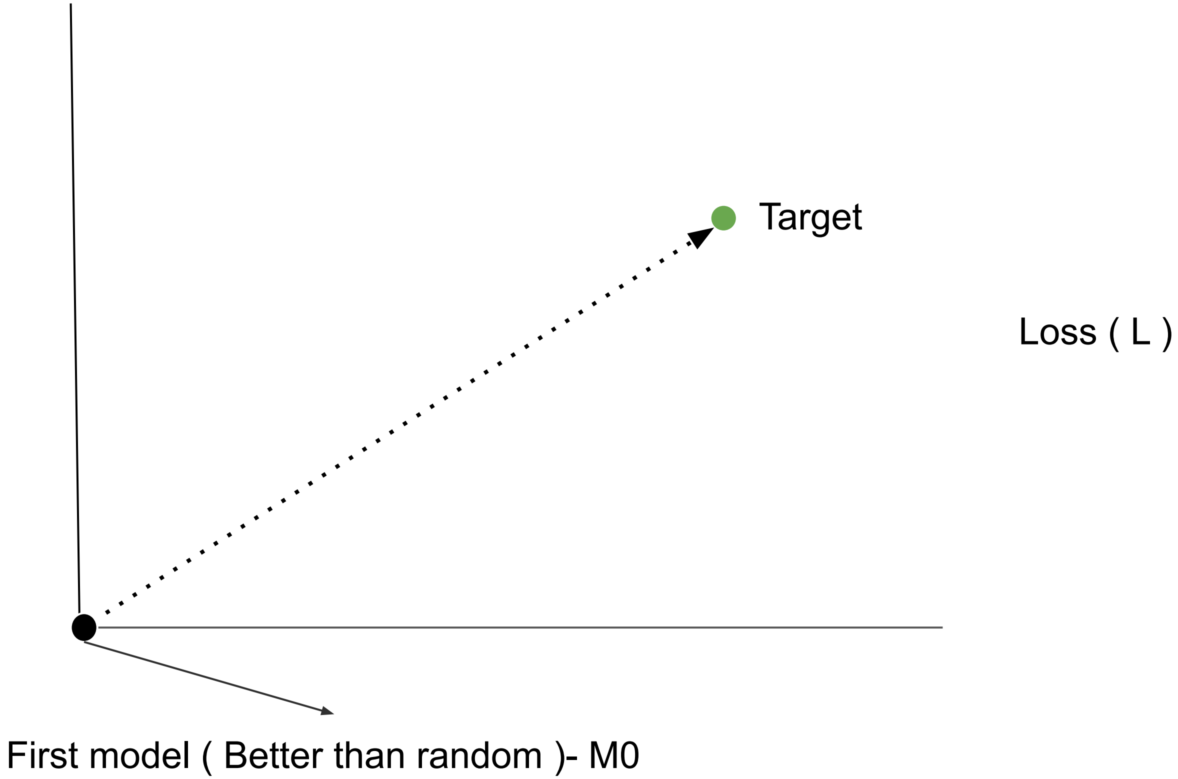
Weighted Boosting (AdaBoost)

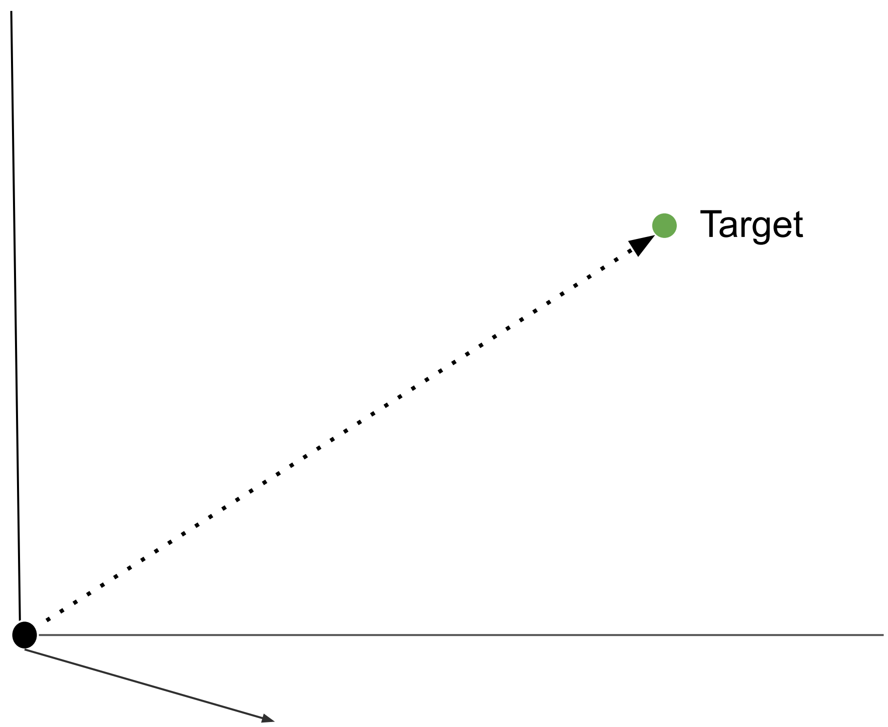


Boosting

Gradient Based Boosting (Gradient Boosting / Xgboost)

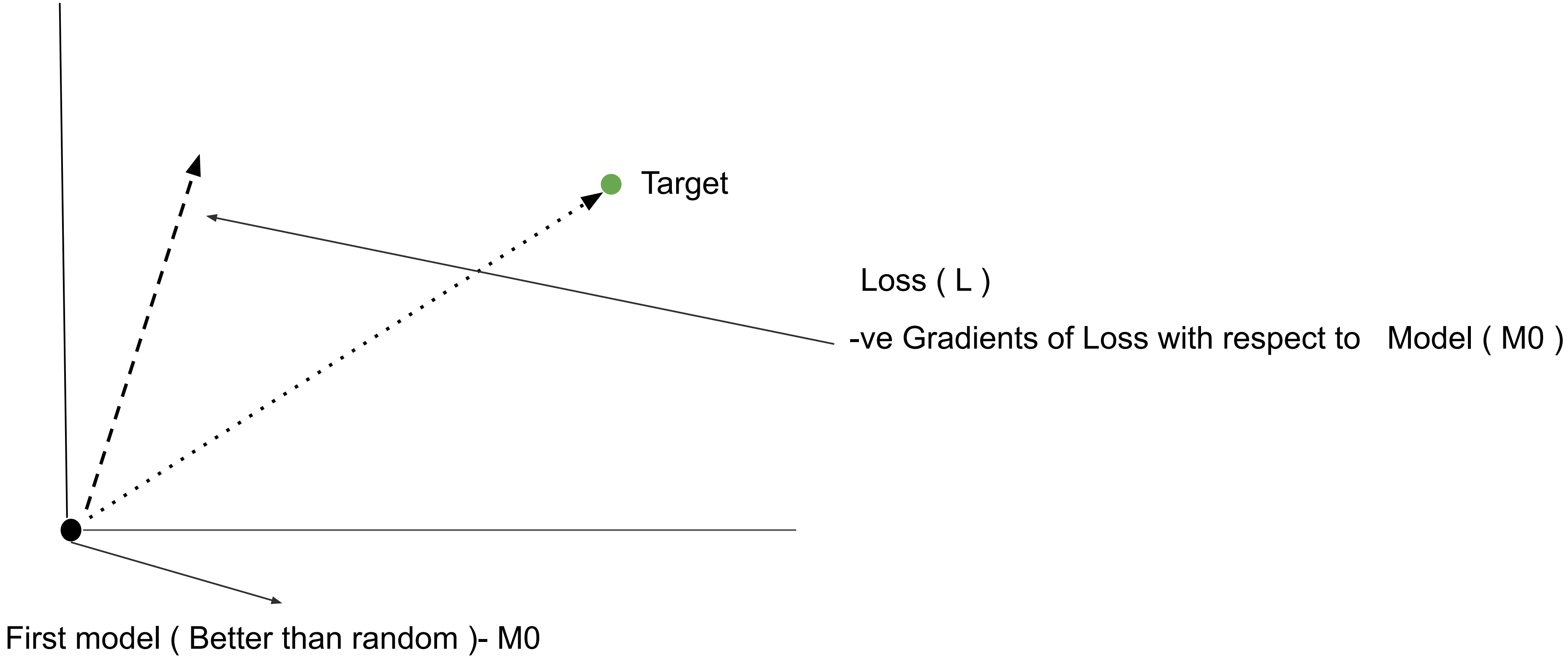
Every model should be better than random guess


Target
Loss (L)
First model (Better than random)- M0

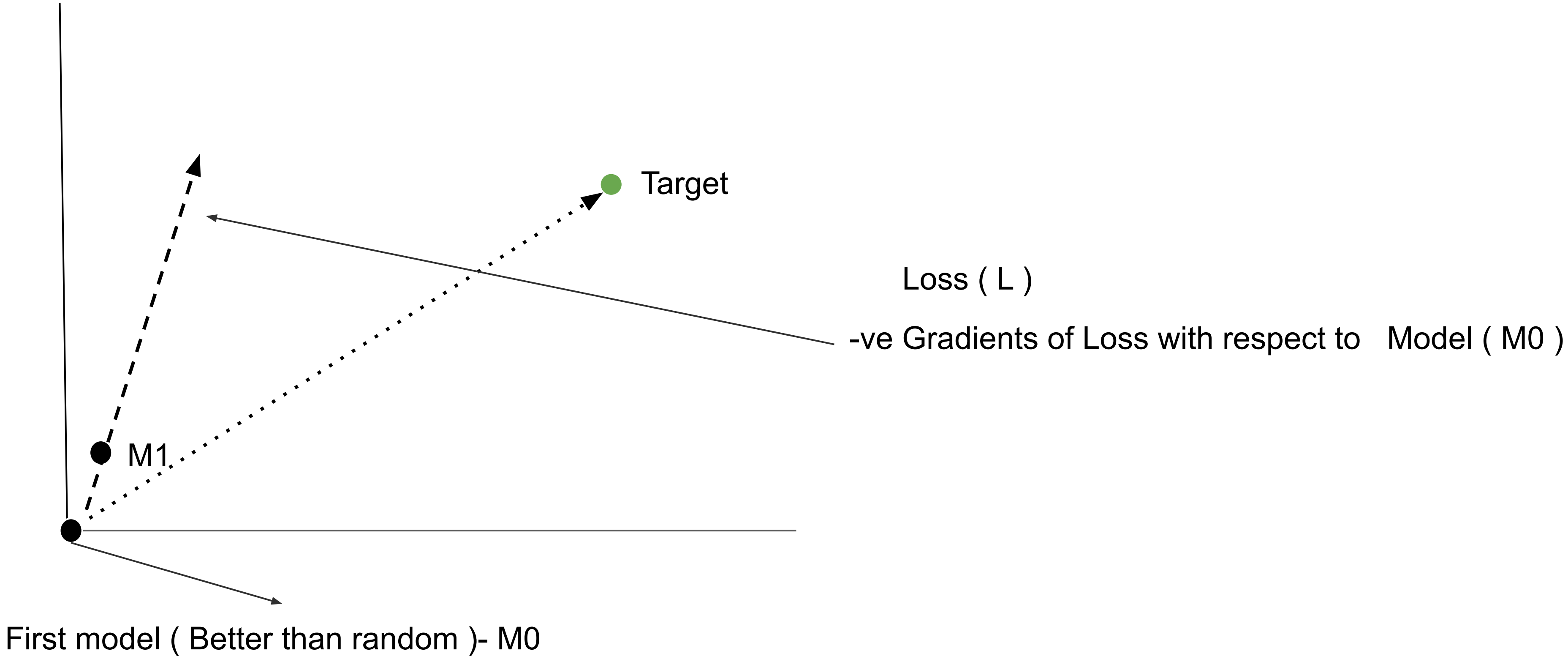


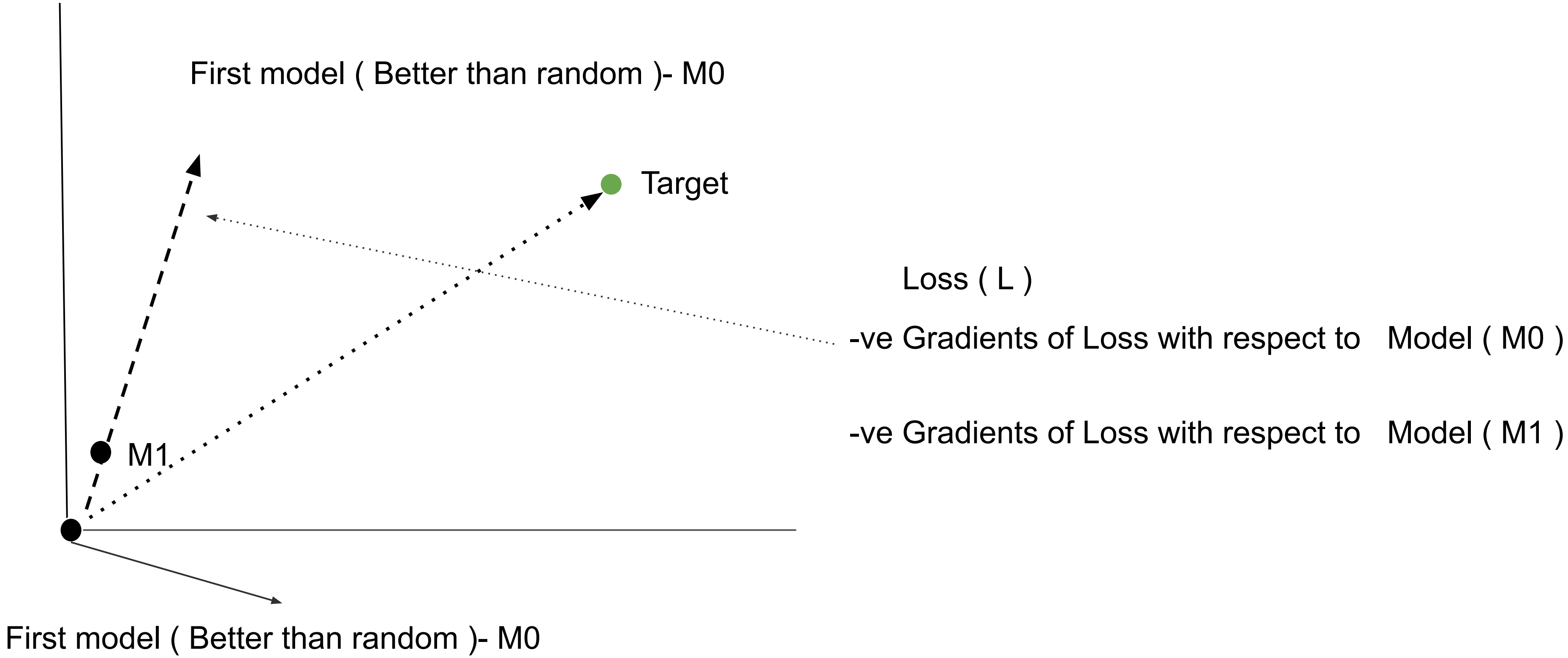
Loss (L)

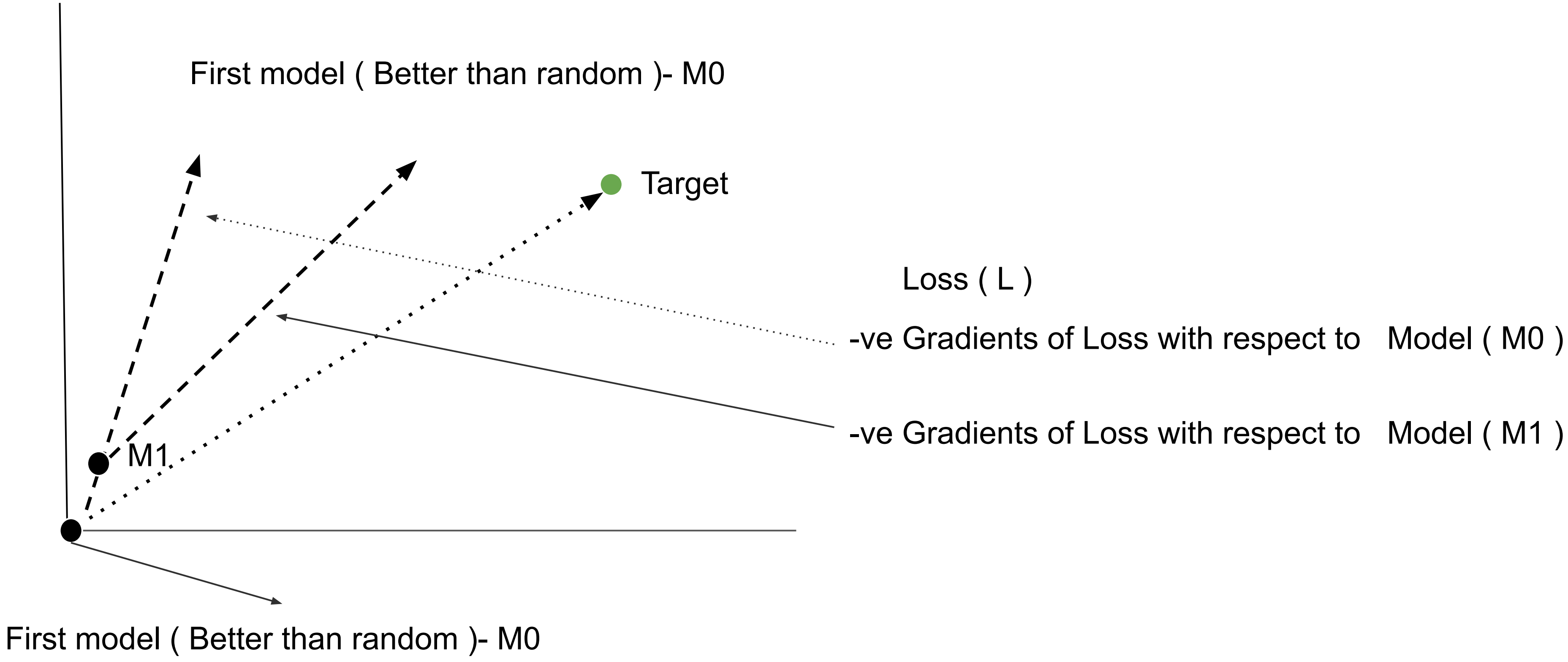
-ve Gradients of Loss with respect to   Model (M0)

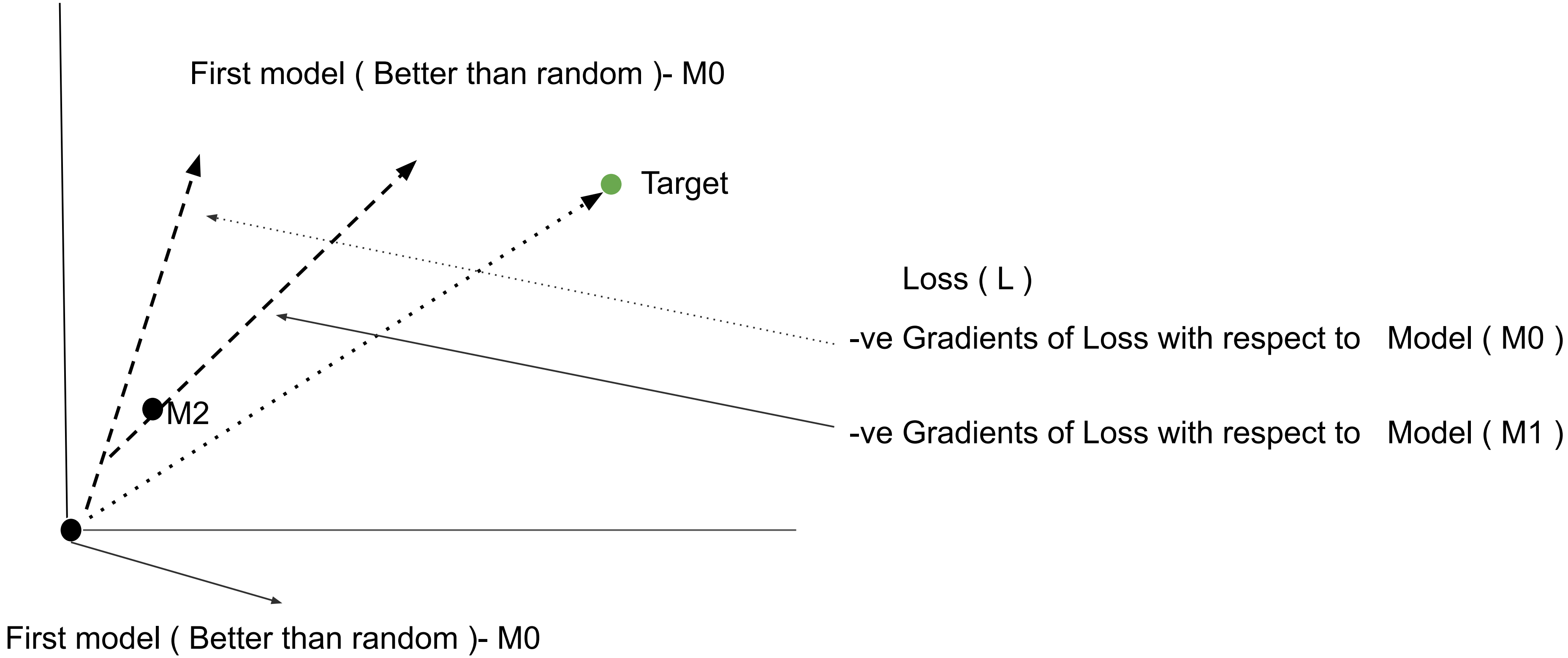


Target
Loss (L)
-ve Gradients of Loss with respect to   Model (M0)
First model (Better than random)- M0


Target
Loss (L)
-ve Gradients of Loss with respect to Model (M0)
M1
First model (Better than random)- M0


First model (Better than random)- M0
Target
Loss (L)
-ve Gradients of Loss with respect to Model (M0)
-ve Gradients of Loss with respect to Model (M1)
M1
First model (Better than random)- M0


First model (Better than random)- M0
Target
Loss (L)
-ve Gradients of Loss with respect to Model (M0)
-ve Gradients of Loss with respect to Model (M1)
M1
First model (Better than random)- M0

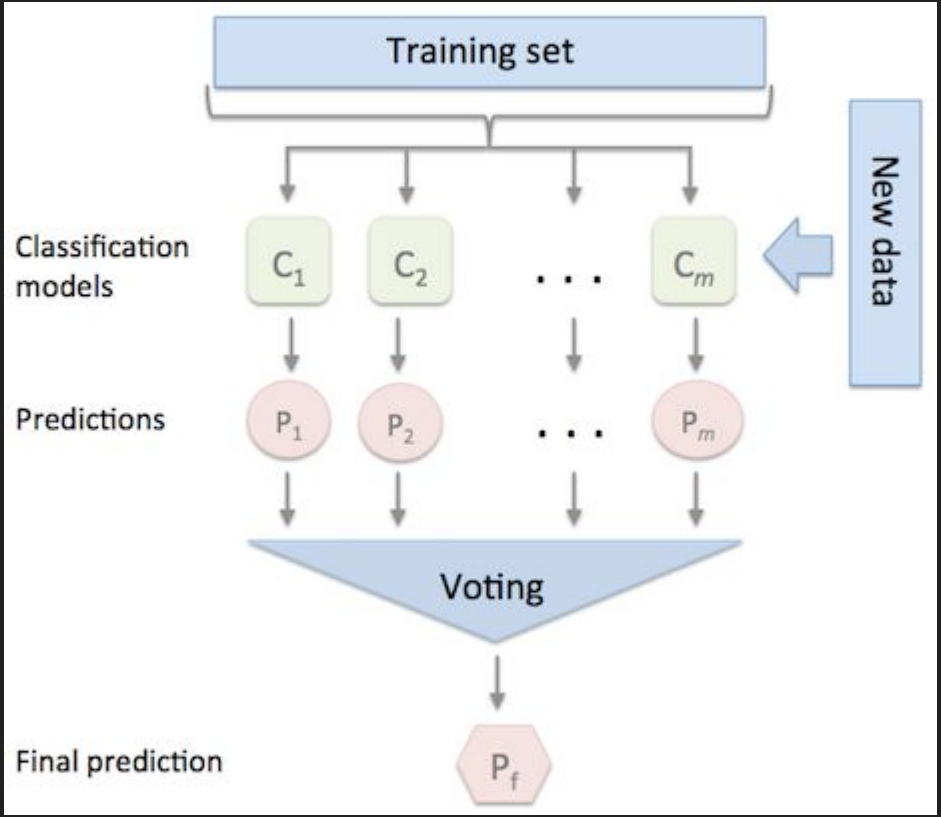

First model (Better than random)- M0
Target
Loss (L)
-ve Gradients of Loss with respect to Model (M0)
M2
-ve Gradients of Loss with respect to Model (M1)
First model (Better than random)- M0

Voting

- Use different classifiers ; and use the majority vote or soft vote to combine.

To ensemble equally well performing model to balance out their individual weakness.

Voting


Training set
New data
Classification models
C_1
C_2
. . .
C_m
Predictions
P_1
P_2
. . .
P_m
Voting
Final prediction
P_f

Voting

Hard Voting : The majority (mode) of the class label is predicted.

Soft Voting : The argmax() of the sum of predicted probabilities is predicted.

Soft Voting and Hard Voting

Classifier 1 predicts class A

Classifier 2 predicts class B

Classifier 3 predicts class B

Final Prediction is
B

Classifier 1 predicts class A with probability 99%

Classifier 2 predicts class A with probability 49%

Classifier 3 predicts class A with probability 49%

(99 + 49 + 49) / 3 = 65.67%

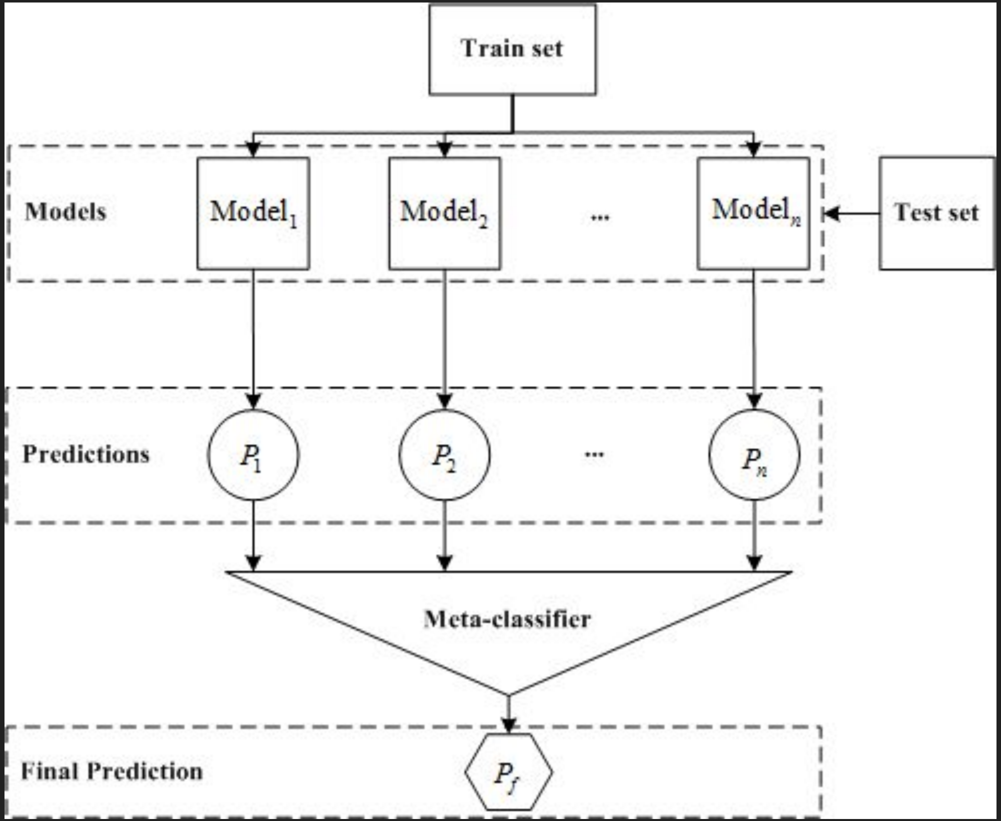
(1 + 51 + 51) / 3 = 34%

Final Prediction is A

Stacking

- To use the outputs of different algorithm as the input feature for the meta-classifier (Final Classifier)

Stacking



Train set
Models
$Model_1$
$Model_2$
...
$Model_n$
Test set
Predictions
P_1
P_2
...
P_n
Meta-classifier
Final Prediction
P_f

Advantages of Ensemble

1. Robustness
2. Good Generalization performance.
3. Parallelization

Disadvantages of Ensemble

1. Human readability / explainability is not good.
2. Takes a lot of time to train.
3. Time - effort off trade off to make accuracy may not make sense.

Resources :

- Kaggle Discussion forum
- Coursera (How to Win kaggle Competitions)
- Book (Ensemble methods , Foundations and Algorithms)
- Practice