Boosting

Boosting

- We’ve learned about single Decision Trees and have seeked to improve upon them with Random Forest models.
- Let’s now explore another methodology of seeking to improve on the single decision tree, known as **boosting**.

Boosting

- Section Overview:
  - Boosting and Meta-Learning
  - AdaBoost (Adaptive Boosting) Theory
  - Example of AdaBoost
  - Gradient Boosting Theory
  - Example of Gradient Boosting

Boosting

- Related Reading:
    - ISLR: Section 8.2.3
- Relevant Wikipedia Articles:
- *wikipedia.org/wiki/Boosting_(machine_learning)*
- *wikipedia.org/wiki/AdaBoost*

Boosting

Motivation and History

Boosting

- The concept of **boosting** is not actually a machine learning algorithm, it is methodology *applied* to an existing machine learning algorithm, most commonly applied to the decision tree.
- Let's explore this idea of a meta-learning algorithm by reviewing a simple application and formula.

Boosting

- Main formula for boosting:

$$F_T(x) = \sum_{t=1}^{T} f_t(x)$$

Boosting

- Main formula for boosting:

$$F_T(x) = \sum_{t=1}^{T} \boxed{f_t(x)} \qquad \boxed{f_t(x) = \alpha_t h(x)}$$

Boosting

- Main formula for boosting:

$$F_T(x) = \sum_{t=1}^{T} \boxed{f_t(x)} \qquad \boxed{f_t(x) = \alpha_t h(x)}$$

- Implies that a combination of **estimators** with an applied **coefficient** could act as an effective **ensemble estimator**.

Boosting

- Main formula for boosting:

$$F_T(x) = \sum_{t=1}^{T} \boxed{f_t(x)} \qquad \boxed{f_t(x) = \alpha_t h(x)}$$

- Note **h(x)** can in theory be **any** machine learning algorithm (estimator/learner).

Boosting

- Main formula for boosting:

$$F_T(x) = \sum_{t=1}^{T} \boxed{f_t(x)} \qquad \boxed{f_t(x) = \alpha_t h(x)}$$

- Can an ensemble of **weak learners** (very simple models) be a **strong learner** when combined?

Boosting

- Main formula for boosting:

$$F_T(x) = \sum_{t=1}^{T} \boxed{f_t(x)} \qquad \boxed{f_t(x) = \alpha_t h(x)}$$

- For decision tree models, we can use simple trees in place of h(x) and combine them with the coefficients on each model.

Boosting

- The idea of **gradient boosting** originated from Leo Breiman when he observed that boosting can be interpreted as an optimization algorithm on a cost function in publications in the late 1990s.
- Later on Jerome H. Friedman and many others developed more explicit formulations of gradient boosting.

Boosting

- Also in the late 1990s Yoav Freund and Robert Schapire developed the AdaBoost (Adaptive Boosting) algorithm, which also combines weak learners in an ensemble to create a stronger model.

Boosting

- Let’s continue by focusing first on AdaBoost and building an understanding of how to combine weak learners to create a strong estimator.
- We will also explore why Decision Trees are so well suited for boosting.

AdaBoost

Intuition and Theory

Boosting

- AdaBoost (Adaptive Boosting) works by using an ensemble of **weak learners** and then combining them through the use of a weighted sum.
- Adaboost adapts by using previously created **weak learners** in order to adjust misclassified instances for the next created **weak learner.**

Boosting

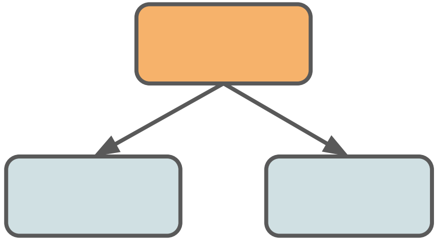
- What is a **weak learner**?

Boosting

- What is a **weak learner**?
  - A weak model is a model that is too simple to perform well on its own.

Boosting

- What is a **weak learner**?
  - A weak model is a model that is too simple to perform well on its own.
  - The weakest decision tree possible would be a **stump**, one node and two leaves!

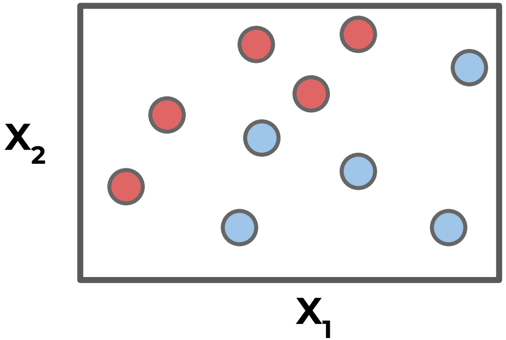


Boosting

- Unlike a single decision tree which fits to all the data at once (*fitting the data hard*), AdaBoost aggregates multiple weak learners, allowing the overall **ensemble** model to *learn slowly* from the features.
- Let's first understand how this works from a data perspective!

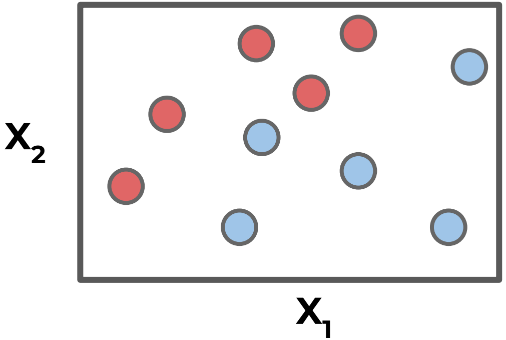
Boosting

- Imagine a classification task:



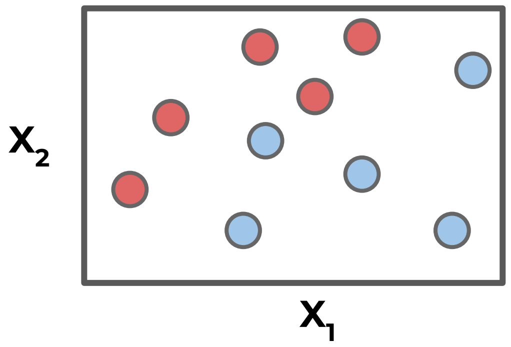
Boosting

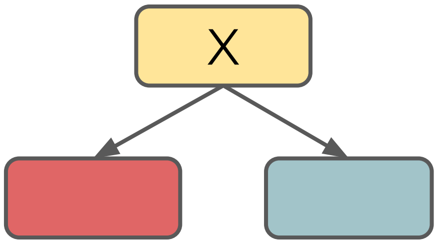
- What would a stump classification look like?



Boosting

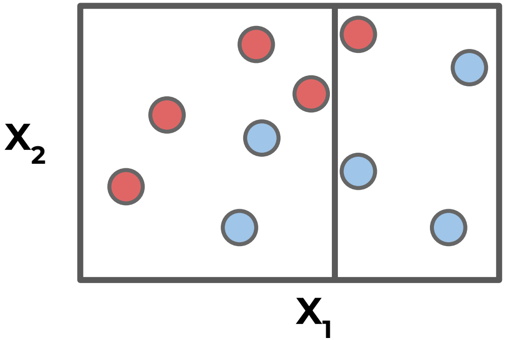
- What would a stump classification look like?

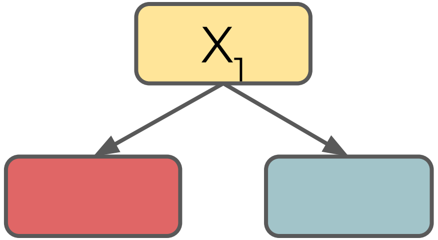




Boosting

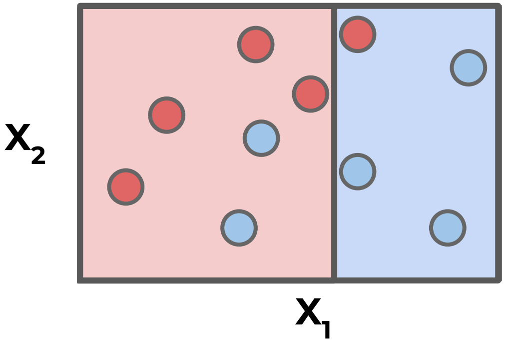
- What would a stump classification look like?

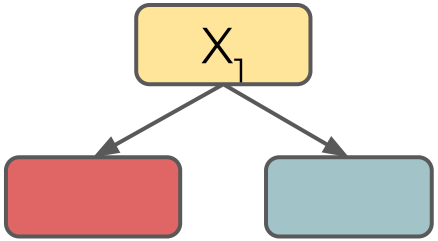




Boosting

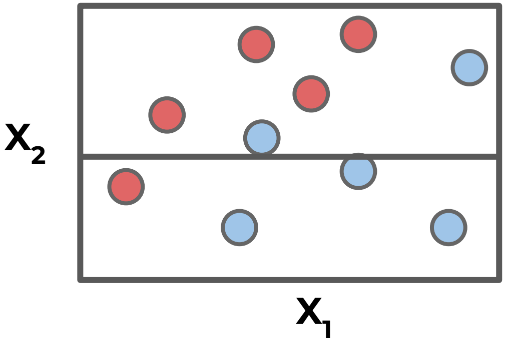
- What would a stump classification look like?

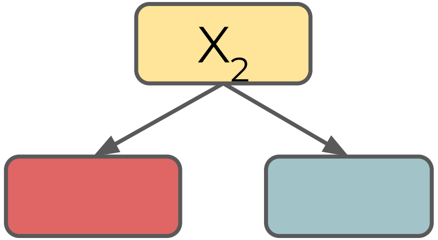




Boosting

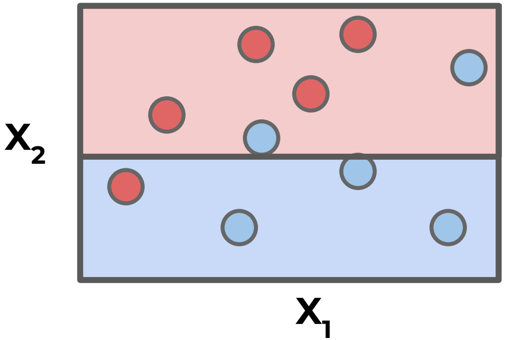
- What would a stump classification look like?

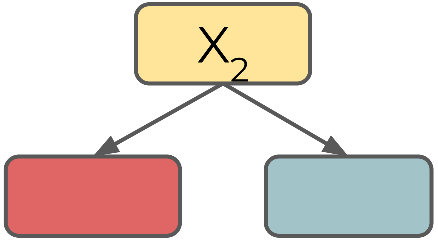




Boosting

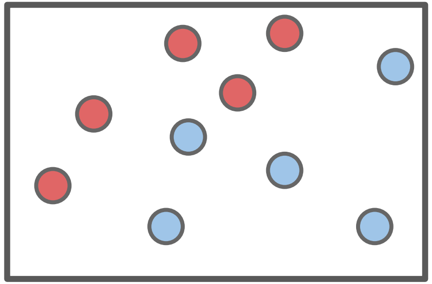
- What would a stump classification look like?





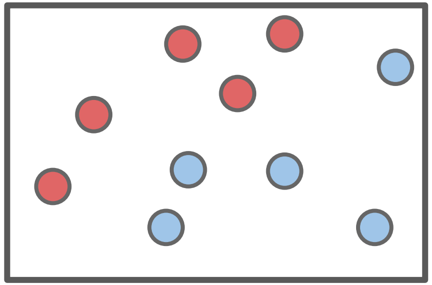
Boosting

- How can we combine stumps? How to improve performance with an ensemble?



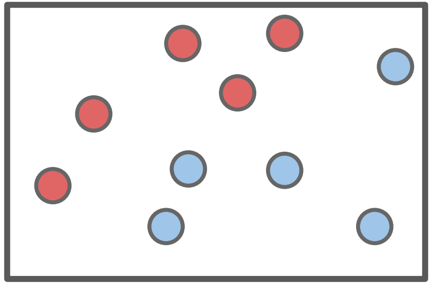
Boosting

- AdaBoost Process:



Boosting

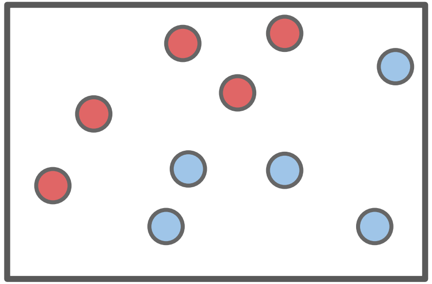
- AdaBoost Process:



- Main Formulas
- Algorithmic Steps
- Visual Walkthrough of Algorithm

Boosting

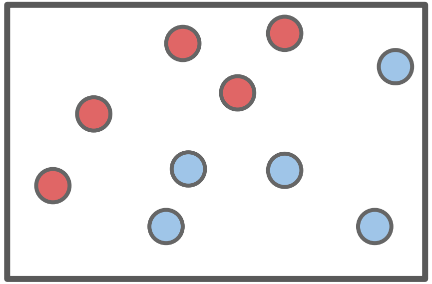
- AdaBoost Process: Main Formulas



$$F_T(x) = \sum_{t=1}^{T} f_t(x)$$

Boosting

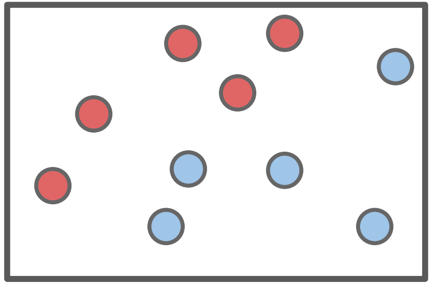
- AdaBoost Process:



$$F_T(x) = \sum_{t=1}^{T} \boxed{f_t(x)} \qquad \boxed{f_t(x) = \alpha_t h(x)}$$

Boosting

- AdaBoost Process:

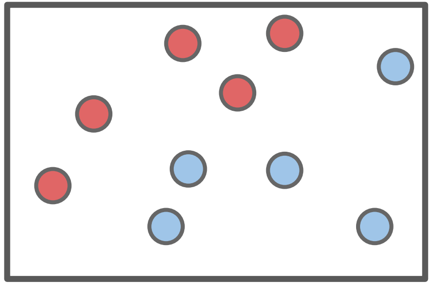


$$F_T(x) = \sum_{t=1}^{T} f_t(x)$$

$$f_t(x) = \boxed{\alpha_t} h(x)$$

Boosting

- AdaBoost Process:



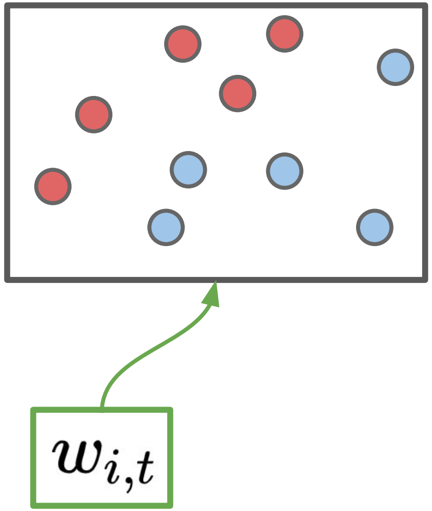
$$F_T(x) = \sum_{t=1}^{T} f_t(x)$$

$$f_t(x) = \boxed{\alpha_t} h(x)$$

$$E_t = \sum_i E[F_{t-1}(x_i) + \boxed{\alpha_t} h(x_i)]$$

Boosting

- AdaBoost Process:



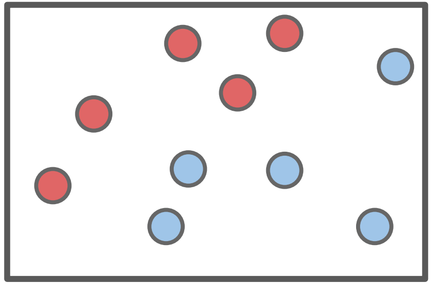
$$F_T(x) = \sum_{t=1}^{T} f_t(x)$$

$$f_t(x) = \alpha_t h(x)$$

$$E_t = \sum_{i} E[F_{t-1}(x_i) + \alpha_t h(x_i)]$$

Boosting

- AdaBoost Process: Algorithm Steps

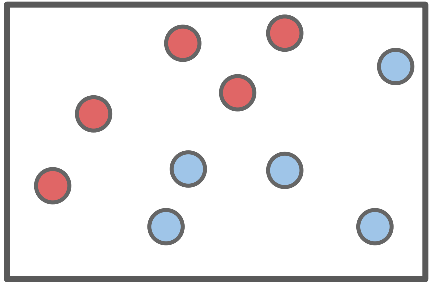


With:

- Samples $x_1 \ldots x_n$
- Desired outputs $y_1 \ldots y_n, y \in \{-1, 1\}$
- Initial weights $w_{1,1} \ldots w_{n,1}$ set to $\frac{1}{n}$
- Error function $E(f(x), y, i) = e^{-y_i f(x_i)}$
- Weak learners $h: x \rightarrow \{-1, 1\}$

Boosting

- AdaBoost Process:

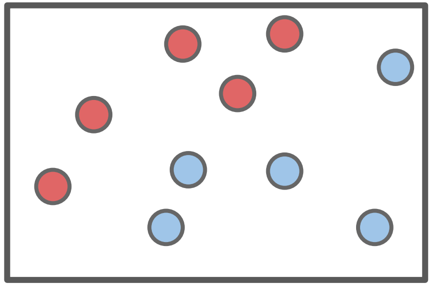


For t in $1 \ldots T$:

- Choose $h_t(x)$:
  - Find weak learner $h_t(x)$ that minimizes ϵ_t, the weighted sum error for misclassified points $\epsilon_t = \sum_{\substack{i=1 \\ h_t(x_i) \neq y_i}}^{n} w_{i,t}$
  - Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$

Boosting

- AdaBoost Process:

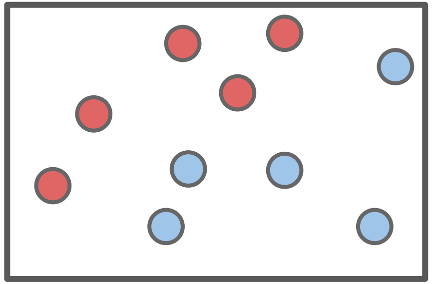


For t in $1 \ldots T$:

- Add to ensemble:
  - $F_t(x) = F_{t-1}(x) + \alpha_t h_t(x)$
- Update weights:
  - $w_{i,t+1} = w_{i,t} e^{-y_i \alpha_t h_t(x_i)}$ for i in $1 \ldots n$
  - Renormalize $w_{i,t+1}$ such that $\sum_i w_{i,t+1} = 1$

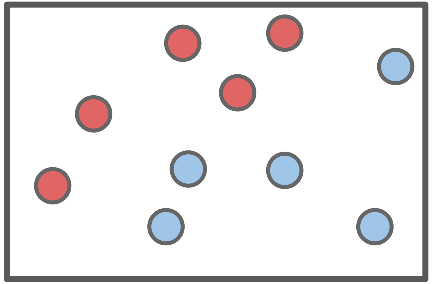
Boosting

- AdaBoost Process: Visual Walkthrough



Boosting

- AdaBoost Process: Visual Walkthrough

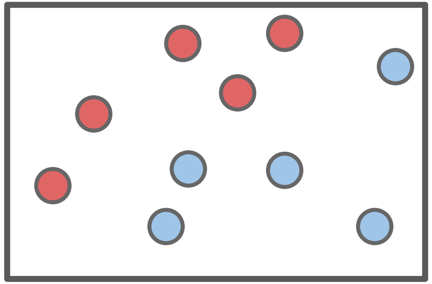


With:

- Samples $x_1 \ldots x_n$
- Desired outputs $y_1 \ldots y_n, y \in \{-1, 1\}$
- Initial weights $w_{1,1} \ldots w_{n,1}$ set to $\frac{1}{n}$
- Error function $E(f(x), y, i) = e^{-y_i f(x_i)}$
- Weak learners $h\colon x \to \{-1, 1\}$

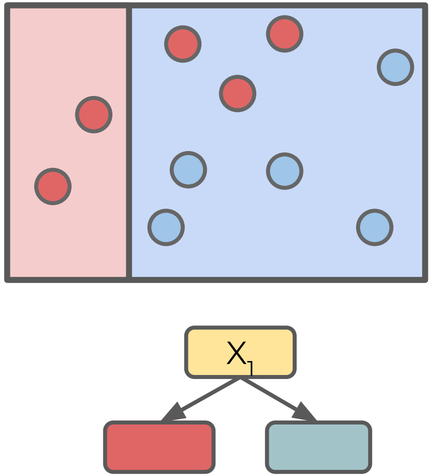
Boosting

- AdaBoost Process: Visual Walkthrough



Boosting

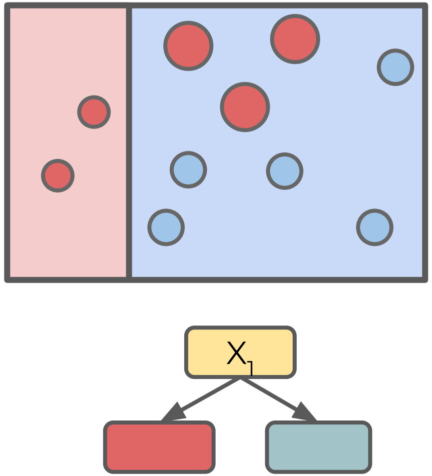
- AdaBoost Process:



- Choose $h_t(x)$:
  - Find weak learner $h_t(x)$ that minimizes ϵ_t, the weighted sum error for misclassified points $\epsilon_t = \sum_{\substack{i=1 \\ h_t(x_i) \neq y_i}}^{n} w_{i,t}$

Boosting

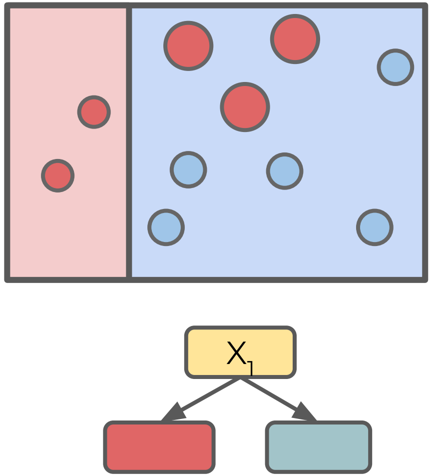
- AdaBoost Process:



- Choose $h_t(x)$:
  - Find weak learner $h_t(x)$ that minimizes ϵ_t, the weighted sum error for misclassified points $\epsilon_t = \sum_{\substack{i=1 \\ h_t(x_i) \neq y_i}}^{n} w_{i,t}$

Boosting

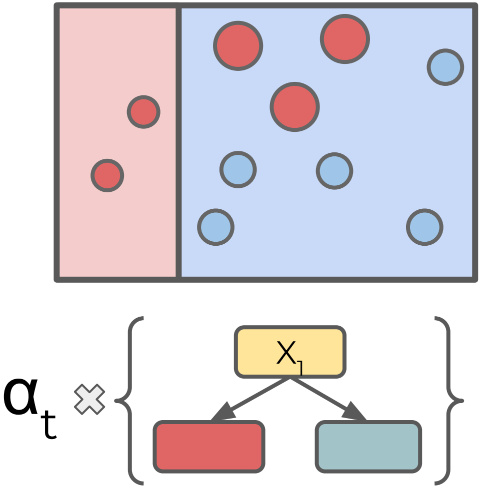
- AdaBoost Process:



- Choose $h_t(x)$:
  - Find weak learner $h_t(x)$ that minimizes ϵ_t, the weighted sum error for misclassified points $\epsilon_t = \sum_{\substack{i=1 \\ h_t(x_i) \neq y_i}}^{n} w_{i,t}$
  - Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$

Boosting

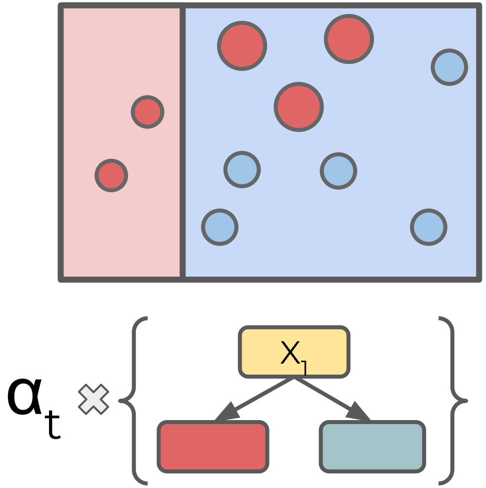
- AdaBoost Process:



- Choose $h_t(x)$:
  - Find weak learner $h_t(x)$ that minimizes ϵ_t, the weighted sum error for misclassified points $\epsilon_t = \sum_{\substack{i=1 \\ h_t(x_i) \neq y_i}}^{n} w_{i,t}$
  - Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$

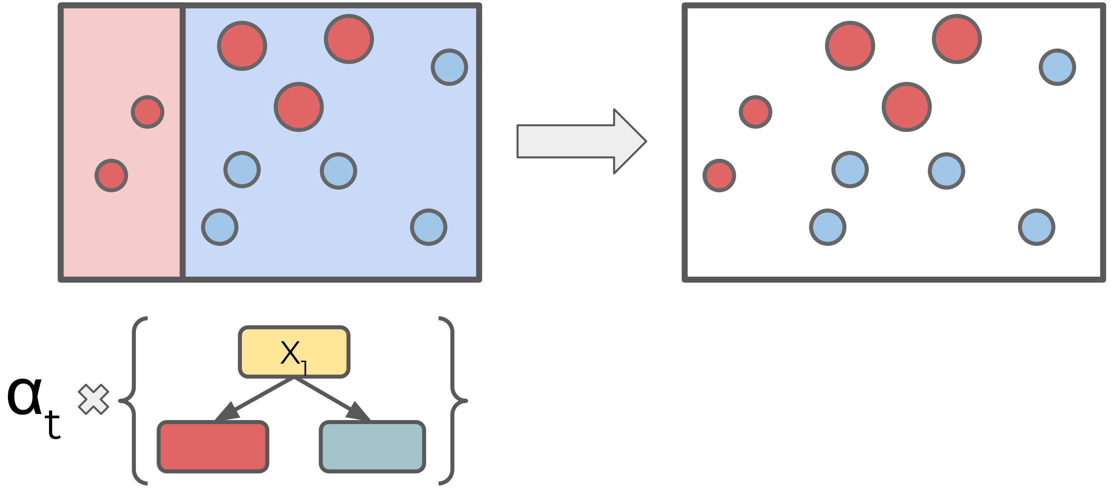
Boosting

- AdaBoost Process:



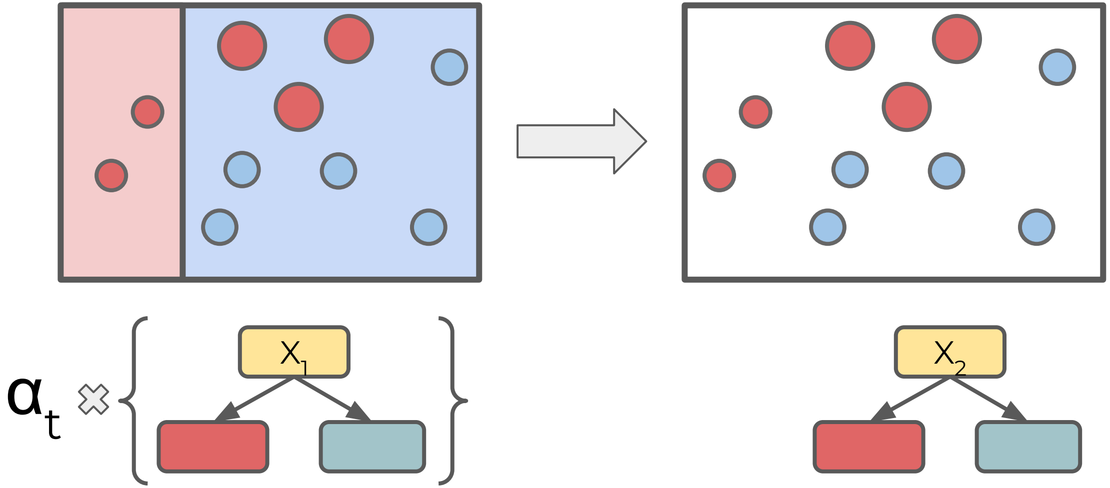
Boosting

- AdaBoost Process:



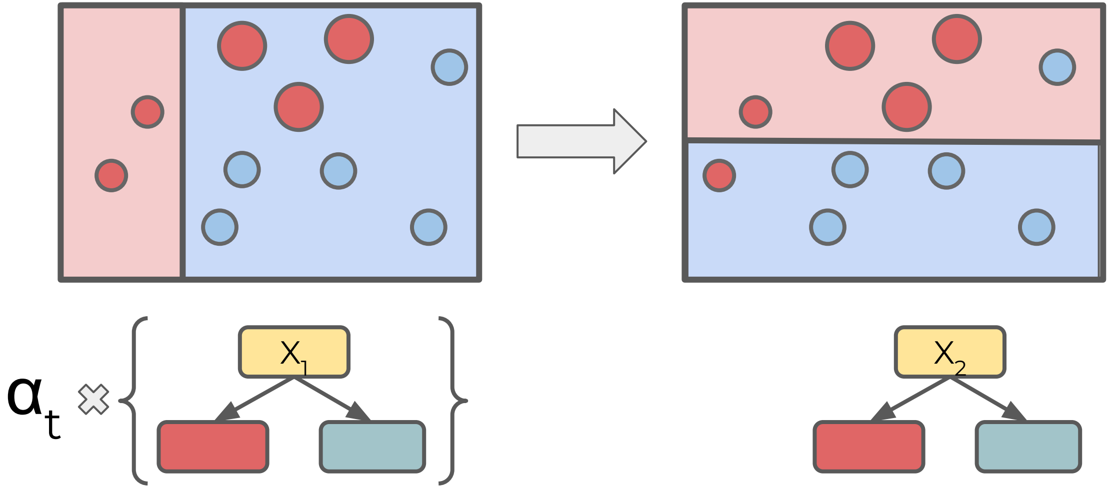
Boosting

- AdaBoost Process:



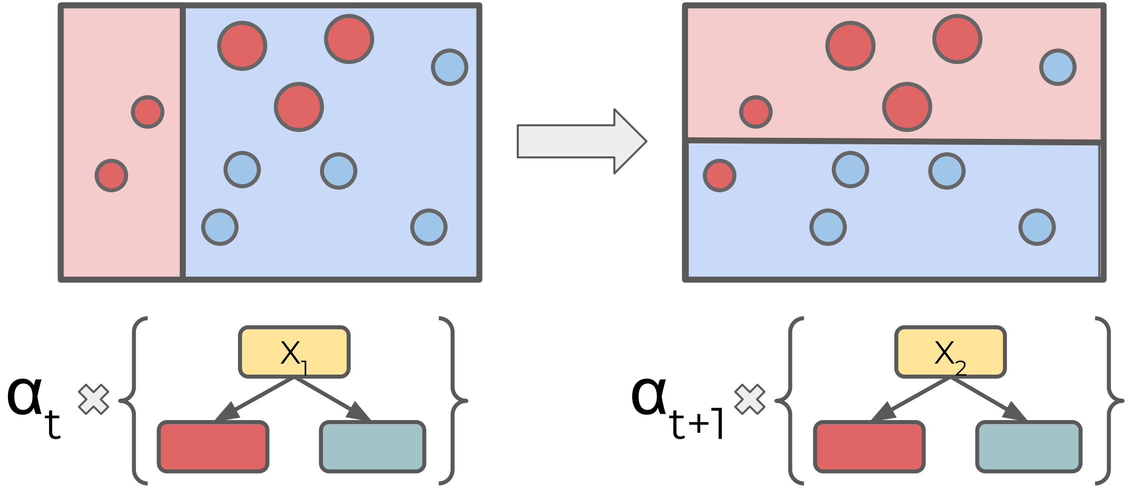
Boosting

- AdaBoost Process:



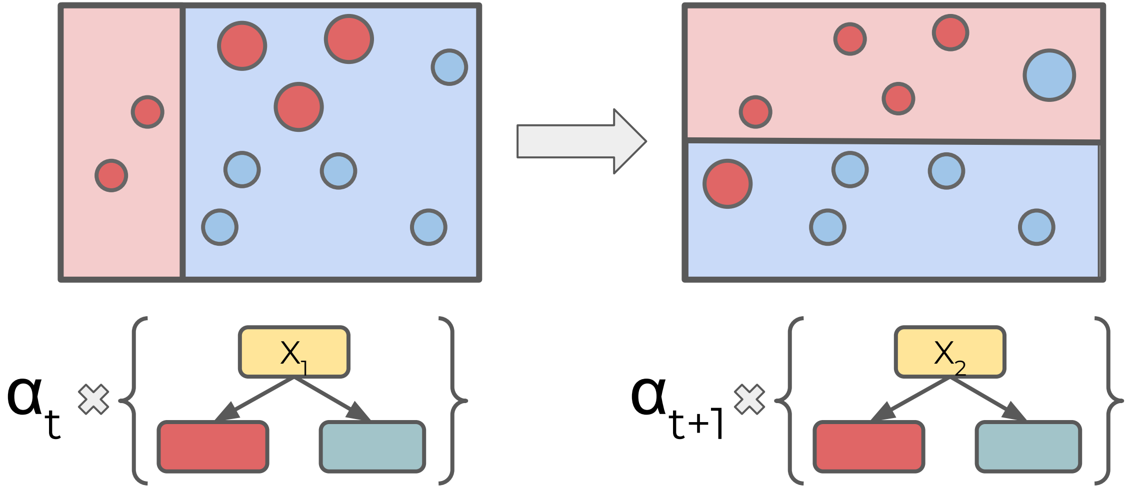
Boosting

- AdaBoost Process:



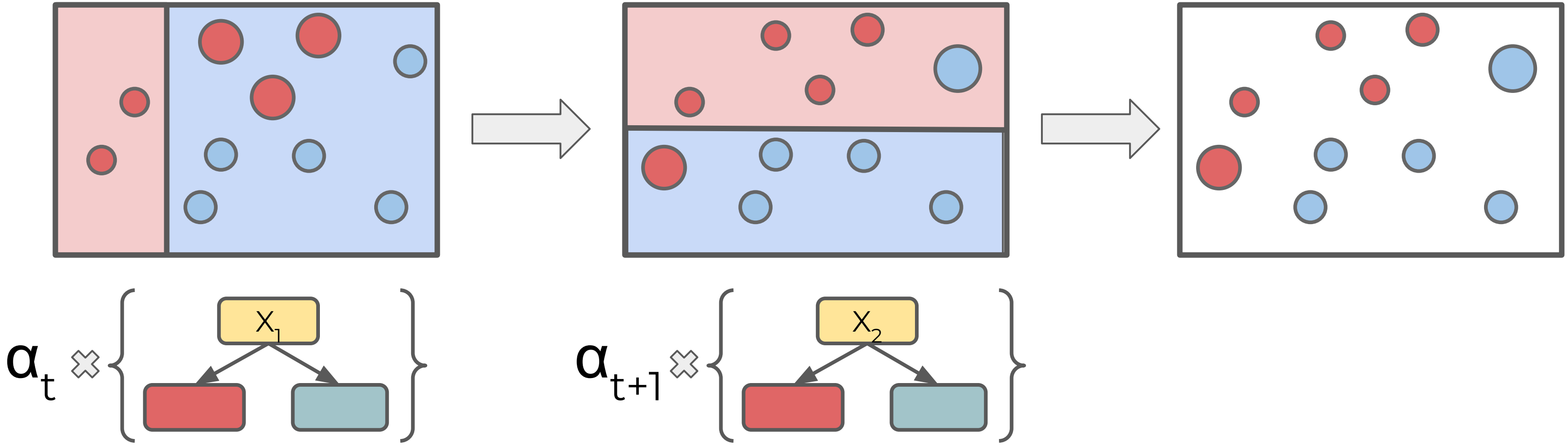
Boosting

- AdaBoost Process:



Boosting

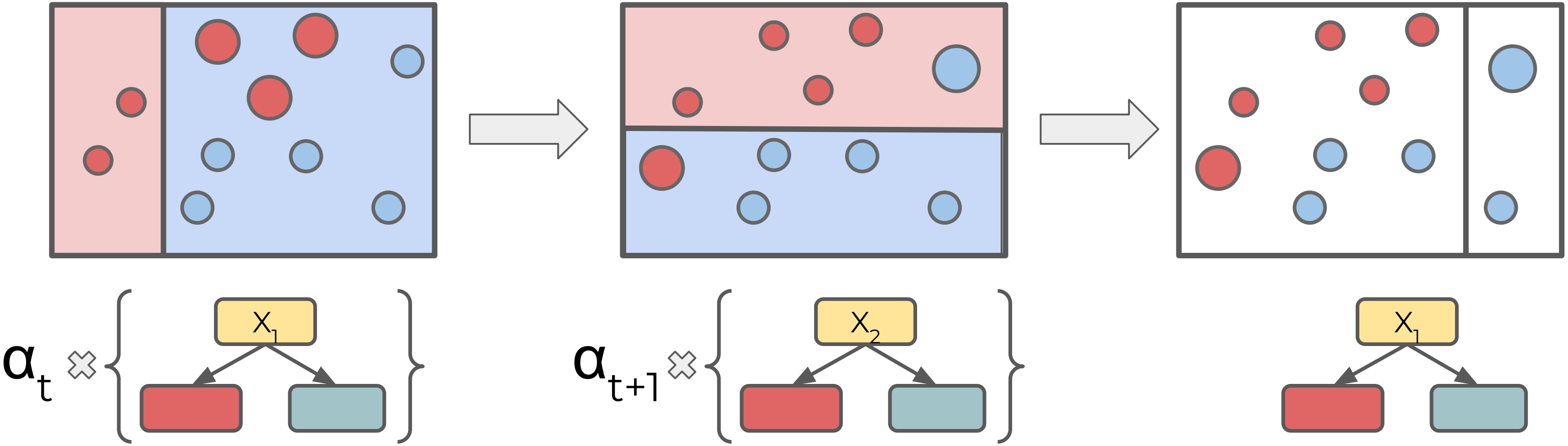
- AdaBoost Process:



$\alpha_t \times \{\ \}$ $\alpha_{t+1} \times \{\ \}$

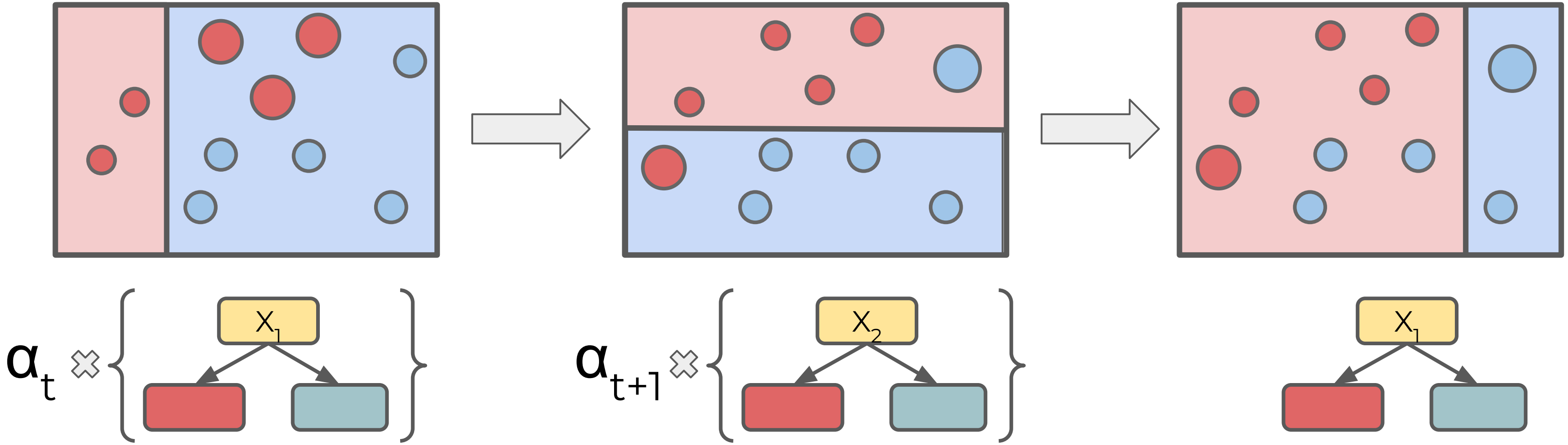
Boosting

- AdaBoost Process:



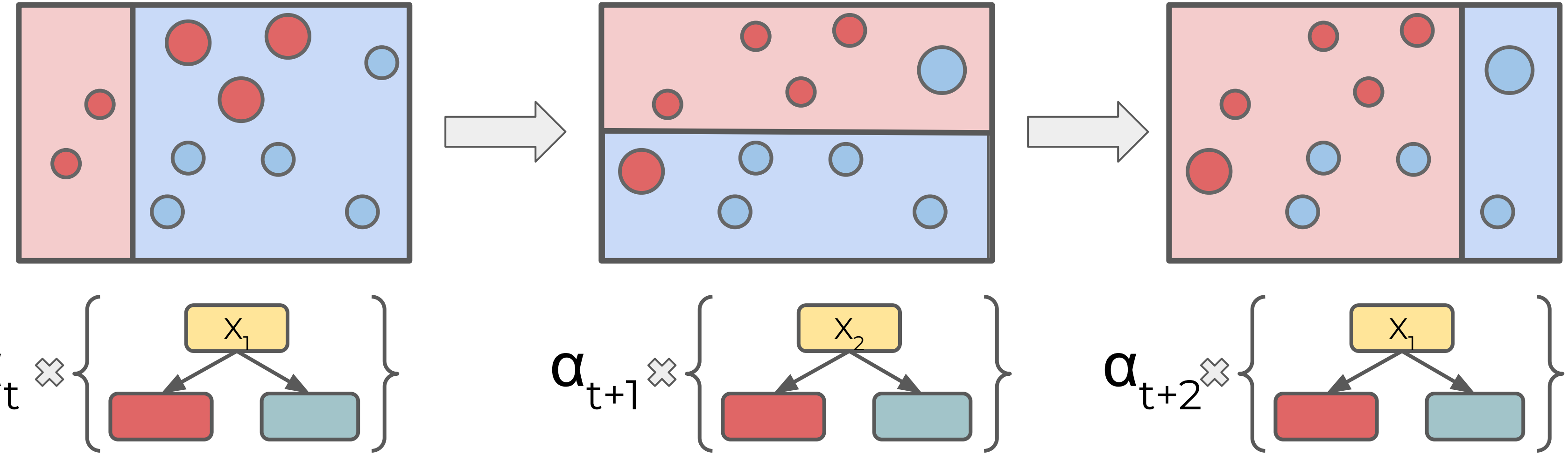
Boosting

- AdaBoost Process:



Boosting

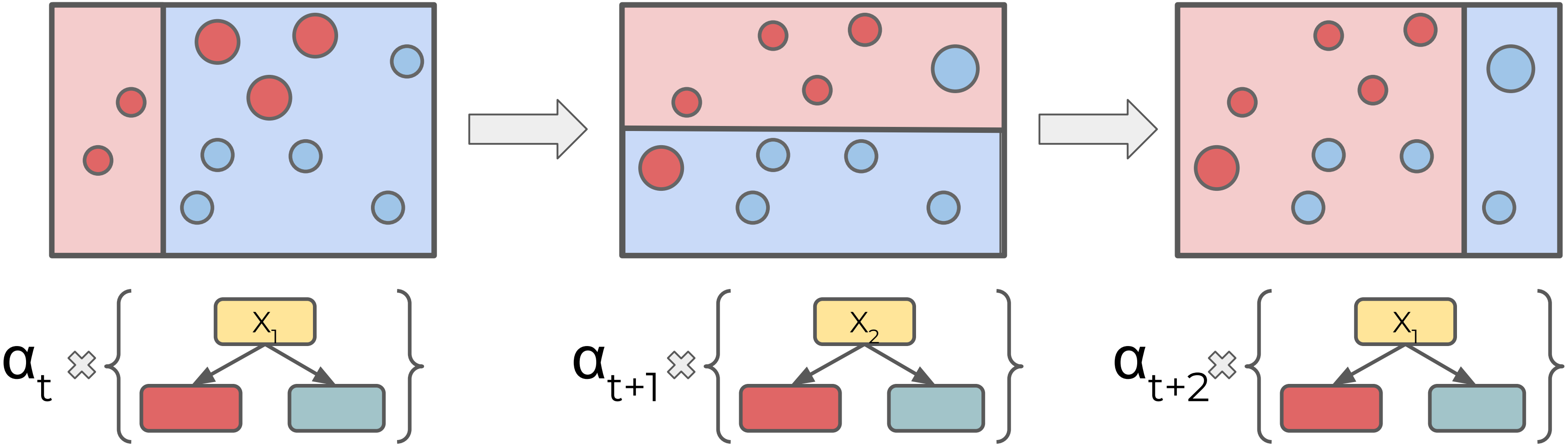
- AdaBoost Process:



$\alpha_t \times$ $\alpha_{t+1} \times$ $\alpha_{t+2} \times$

Boosting

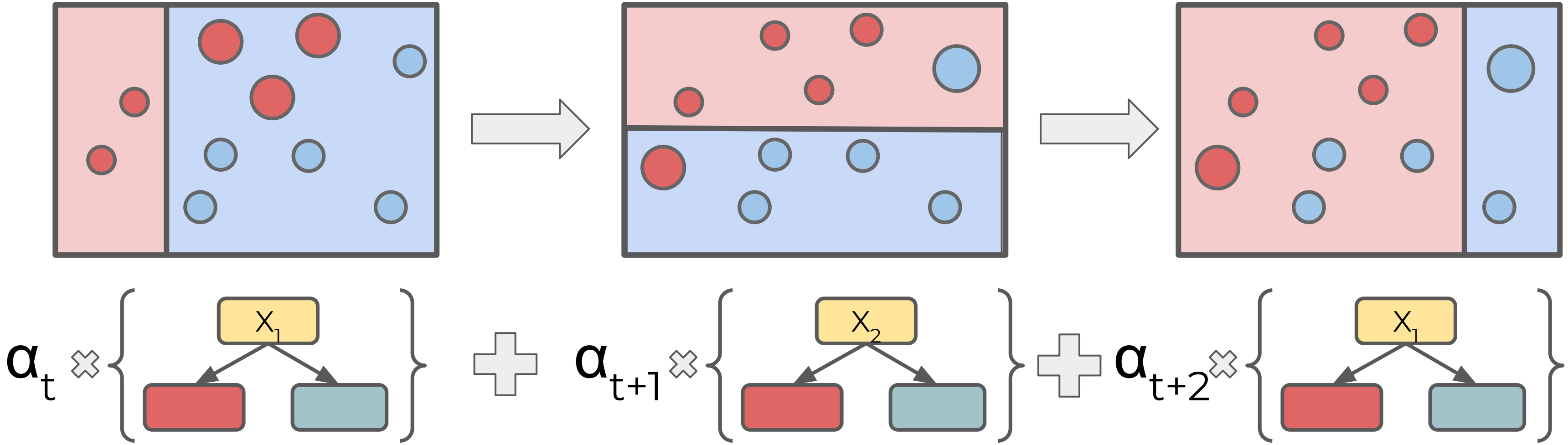
- AdaBoost Process:



$$F_T(x) = \sum_{t=1}^{T} f_t(x) \qquad f_t(x) = \alpha_t h(x)$$

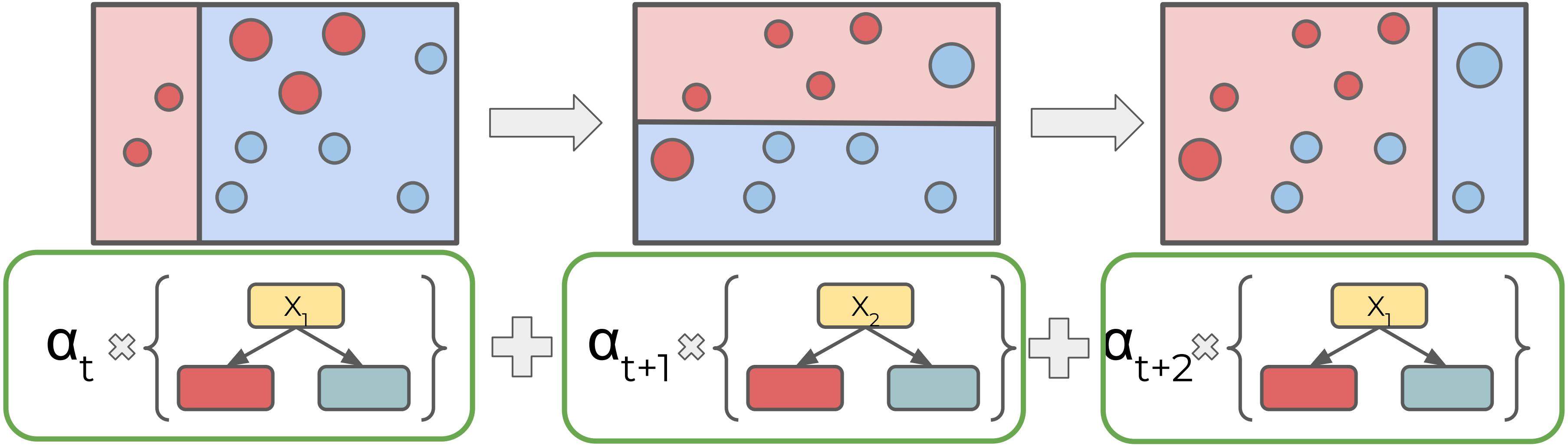
Boosting

- AdaBoost Process:



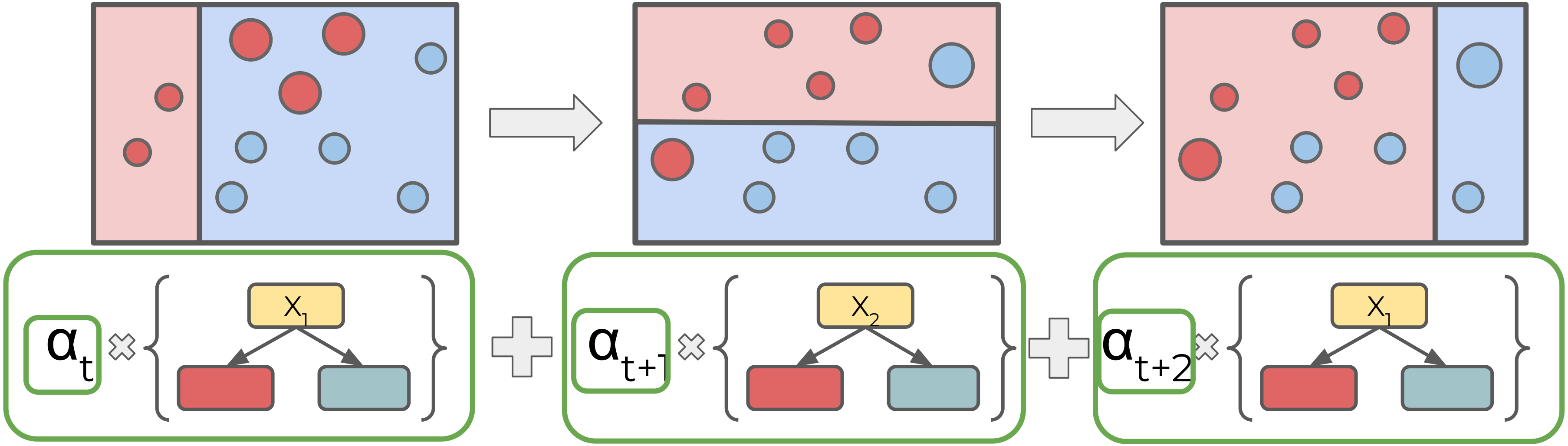
Boosting

- AdaBoost Process:



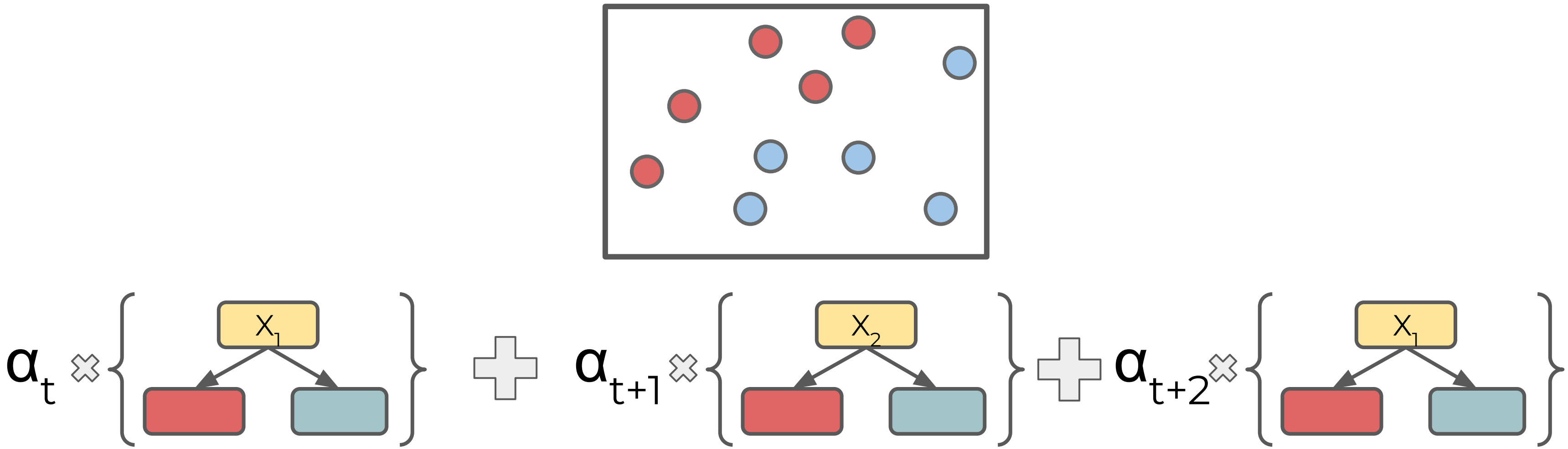
Boosting

- AdaBoost Process:



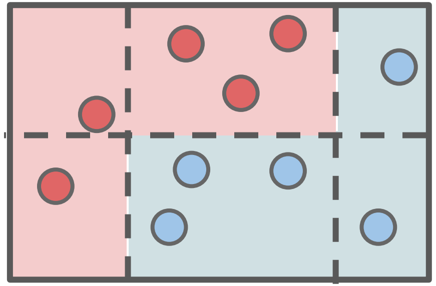
Boosting

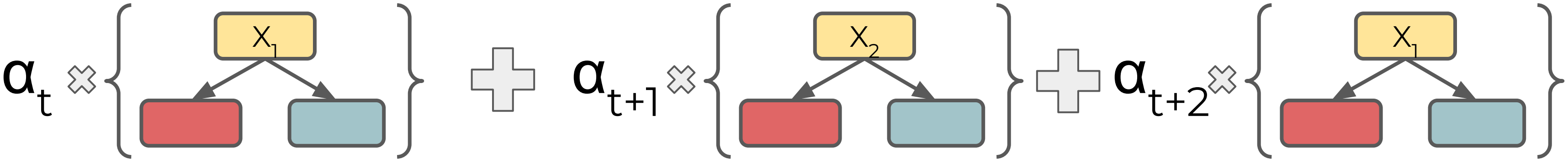
- AdaBoost Process:



Boosting

- AdaBoost Process:





Boosting

- AdaBoost uses an ensemble of **weak learners** that learn slowly in series.
- Certain weak learners have more “say” in the final output than others due to the multiplied alpha parameter.
- Each subsequent **t** weak learner is built using a reweighted data set from the **t-1** weak learner.

Boosting

- Intuition of Adaptive Boosting:
  - Each stump essentially represents the strength of a feature to predict.
  - Building these stumps in series and adding in the alpha parameter allows us to intelligently combine the importance of each feature together.

Boosting

- Notes on Adaptive Boosting:
  - Unlike Random Forest, it is possible to overfit with AdaBoost, however it takes many trees to do this.
  - Usually error has already stabilized way before enough trees are added to cause overfitting.

Gradient Boosting

Theory and Intuition

Boosting

- Gradient Boosting is a very similar idea to AdaBoost, where weak learners are created in series in order to produce a strong ensemble model.
- Gradient Boosting makes use of the residual error for learning.

Boosting

- Gradient Boosting vs. Adaboost:
  - Larger Trees allowed in Gradient Boosting.
  - Learning Rate coefficient same for all weak learners.
  - Gradual series learning is based on training on the **residuals** of the previous model.

Boosting

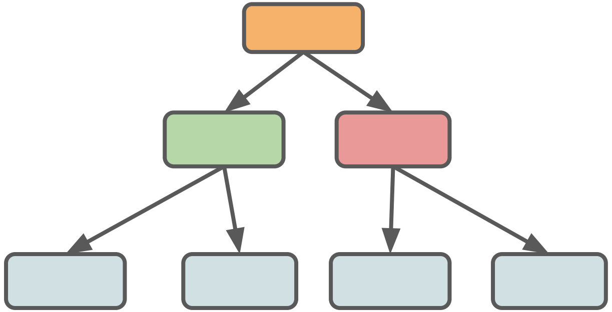
- Gradient Boosting Regression Example

Area m^2	Bedrooms	Bathrooms	Price
200	3	2	$500,000
190	2	1	$462,000
230	3	3	$565,000

Boosting

- Train a decision tree on data

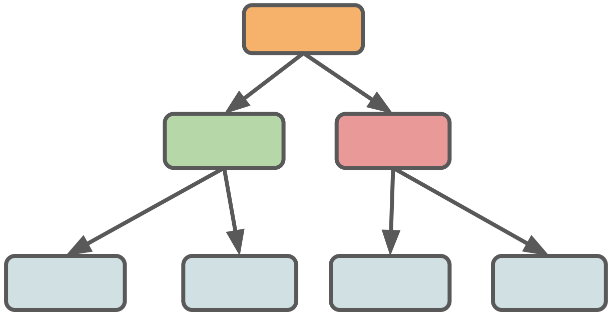
Area m^2	Bedrooms	Bathrooms	Price
200	3	2	$500,000
190	2	1	$462,000
230	3	3	$565,000



Boosting

- Note - not just a stump!

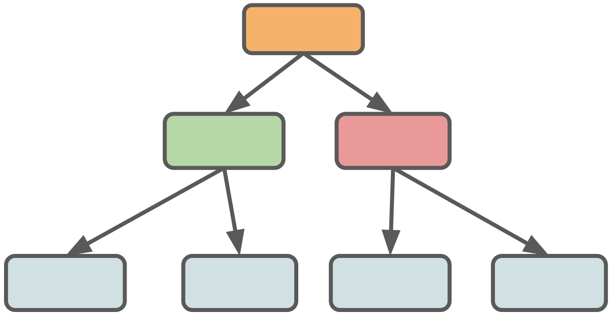
Area m^2	Bedrooms	Bathrooms	Price
200	3	2	$500,000
190	2	1	$462,000
230	3	3	$565,000



Boosting

- Get predicted **ŷ** value

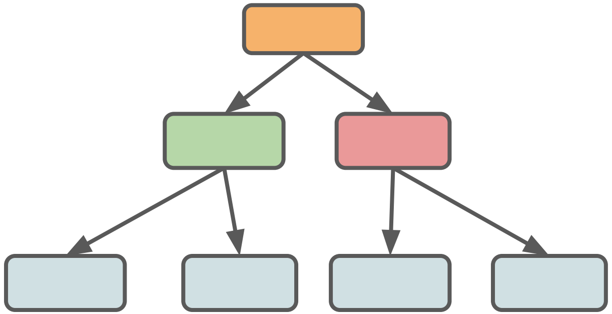
Area m^2	Bedrooms	Bathrooms	Price
200	3	2	$500,000
190	2	1	$462,000
230	3	3	$565,000



Boosting

- Get predicted ŷ value

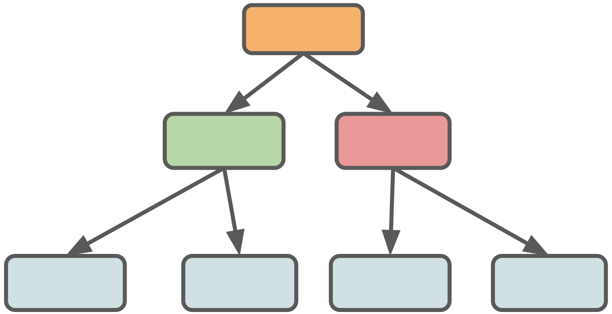
Area m^2	Bedrooms	Bathrooms	y
200	3	2	$500,000
190	2	1	$462,000
230	3	3	$565,000



Boosting

- Get predicted **ŷ** value

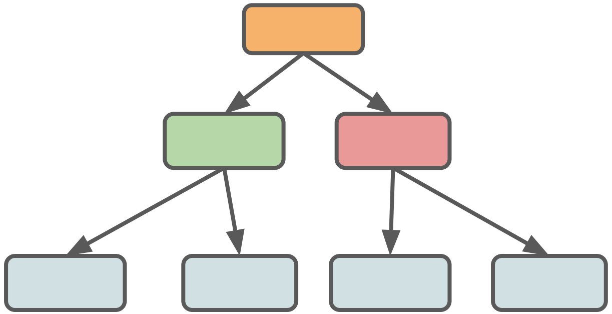
y	ŷ
$500,000	$509,000
$462,000	$509,000
$565,000	$509,000



Boosting

- Calculate residual: $\mathbf{e = y - \hat{y}}$

y	ŷ	e
$500,000	$509,000	-$9,000
$462,000	$509,000	-$47,000
$565,000	$509,000	$56,000



Boosting

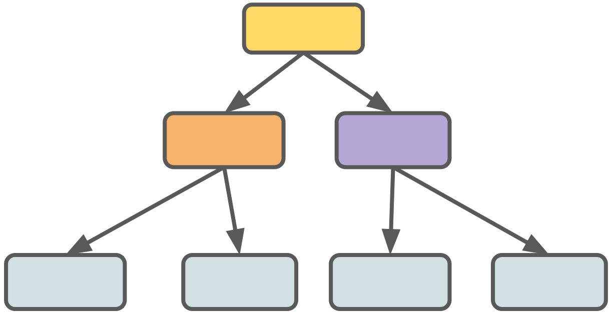
- Create new model to predict the **error**

y	ŷ	e
$500,000	$509,000	-$9,000
$462,000	$509,000	-$47,000
$565,000	$509,000	$56,000

Boosting

- Create new model to predict the **error**

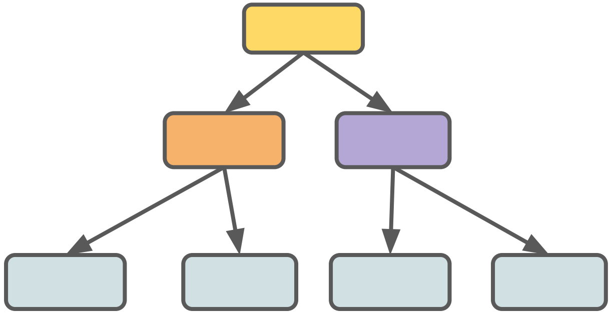
y	ŷ	e
$500,000	$509,000	-$9,000
$462,000	$509,000	-$47,000
$565,000	$509,000	$56,000



Boosting

- Create new model to predict the **error**

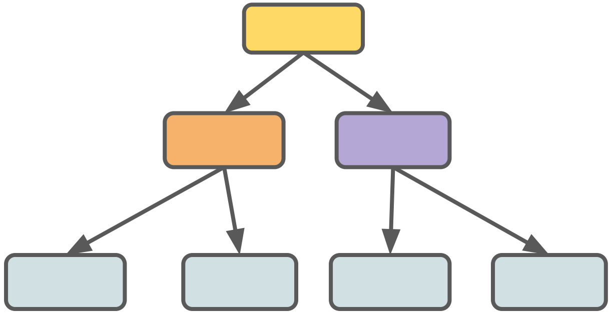
y	ŷ	e	f1
$500,000	$509,000	-$9,000	-$8,000
$462,000	$509,000	-$47,000	-$50,000
$565,000	$509,000	$56,000	$50,000



Boosting

- Create new model to predict the **error**

y	ŷ	e	f1
$500,000	$509,000	-$9,000	-$8,000
$462,000	$509,000	-$47,000	-$50,000
$565,000	$509,000	$56,000	$50,000



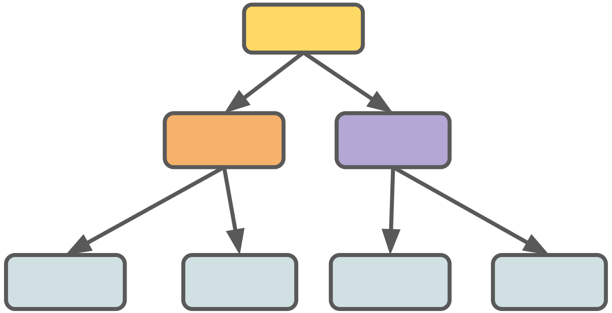
Area m^2	Bedrooms	Bathrooms
200	3	2
190	2	1
230	3	3

Boosting

- Create new model to predict the **error**

y	ŷ	e	f1
$500,000	$509,000	-$9,000	-$8,000
$462,000	$509,000	-$47,000	-$50,000
$565,000	$509,000	$56,000	$50,000

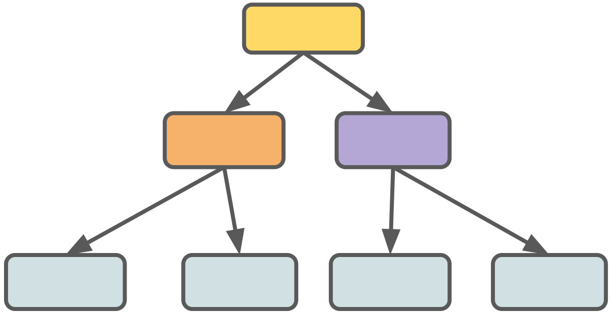
Area m^2	Bedrooms	Bathrooms
200	3	2
190	2	1
230	3	3



Boosting

- Update prediction using **error prediction**

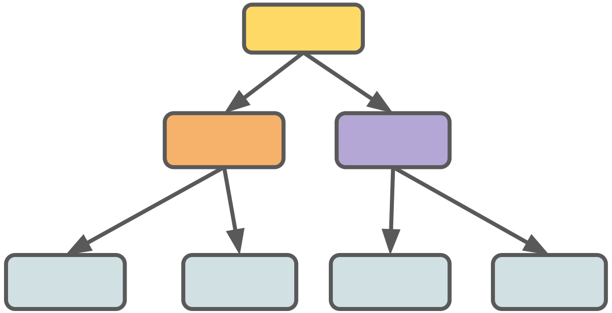
y	ŷ	e	f1
$500,000	$509,000	-$9,000	-$8,000
$462,000	$509,000	-$47,000	-$50,000
$565,000	$509,000	$56,000	$50,000



Boosting

- Update prediction using **error prediction**

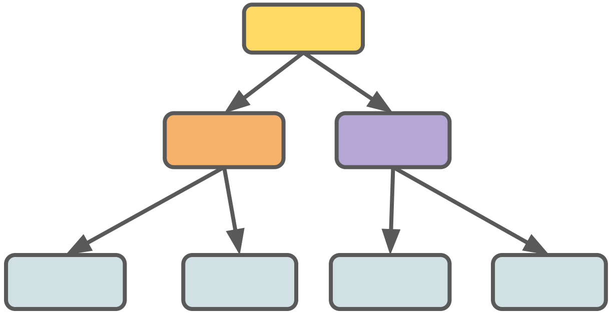
y	ŷ	e	f1	F1 = ŷ + f1
$500,000	$509,000	-$9,000	-$8,000	
$462,000	$509,000	-$47,000	-$50,000	
$565,000	$509,000	$56,000	$50,000	



Boosting

- Update prediction using **error prediction**

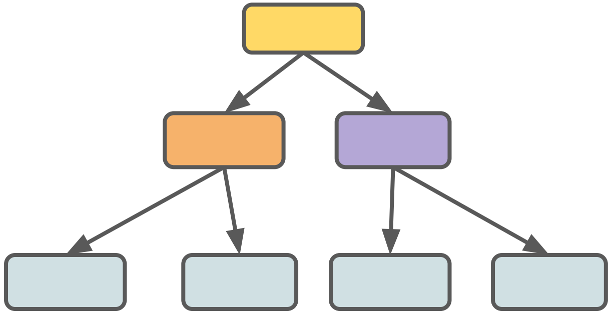
y	ŷ	e	f1	F1 = ŷ + f1
$500,000	$509,000	-$9,000	-$8,000	$501,000
$462,000	$509,000	-$47,000	-$50,000	$459,000
$565,000	$509,000	$56,000	$50,000	$559,000



Boosting

- We can continue this process in series

y	ŷ	e	f1	F1 = ŷ + f1
$500,000	$509,000	-$9,000	-$8,000	$501,000
$462,000	$509,000	-$47,000	-$50,000	$459,000
$565,000	$509,000	$56,000	$50,000	$559,000



Boosting

- Gradient Boosting Process

$$F_m = F_{m-1} + f_m$$

Boosting

- Gradient Boosting Process

$$F_m = F_{m-1} + f_m$$

$$F_m = F_{m-1} + (\text{learning rate} * f_m)$$

Boosting

- Gradient Boosting Process
  - Create initial model: f_0
  - Train another model on error
    - $e = y - f_0$
  - Create new prediction
    - $F_1 = f_0 + \eta f_1$
  - Repeat as needed
    - $F_m = f_{m-1} + \eta f_m$

Boosting

- Note, for classification we can use the logit as an error metric:

$$\hat{y} = \log\left(\frac{\hat{p}}{1-\hat{p}}\right) \qquad \hat{p} = \frac{1}{1+e^{-\hat{y}}}$$

Boosting

- Note, the learning rate is the same for each new model in the series, it is **not** unique to each subsequent model (unlike AdaBoost's alpha coefficient).
- Gradient Boosting is fairly robust to overfitting, allowing for the number of estimators to be set high be default (~100).

Boosting

- Gradient Boosting Intuition
  - We optimize the series of trees by learning on the residuals, forcing subsequent trees to attempt to correct for the error in the previous trees.

Boosting

- Gradient Boosting Intuition
  - The trade-off is training time.
  - A learning rate is between 0-1, which means a very low value would mean each subsequent tree has little “say”, meaning more trees need to be created, causing a longer computational training time.