Ensembles

Following our Recipe for Machine Learning, we may try out several models before deciding on the final one.

Is a single "best" model really best ? Is there an alternative ?

By combining models with independent errors, we may be able to construct a combined model whose accuracy is better than the best individual model.

The combined models are called an *Ensemble*.

The individual models

- May be of different types:
    - Decision Tree, Logistic Regression, KNN
- May be of the *same* type, with different parameters/hyper-parameters:
    - Decision Trees of different depths or different features
    - Regression with polynomial features of different degrees

When the individual models are of the same type

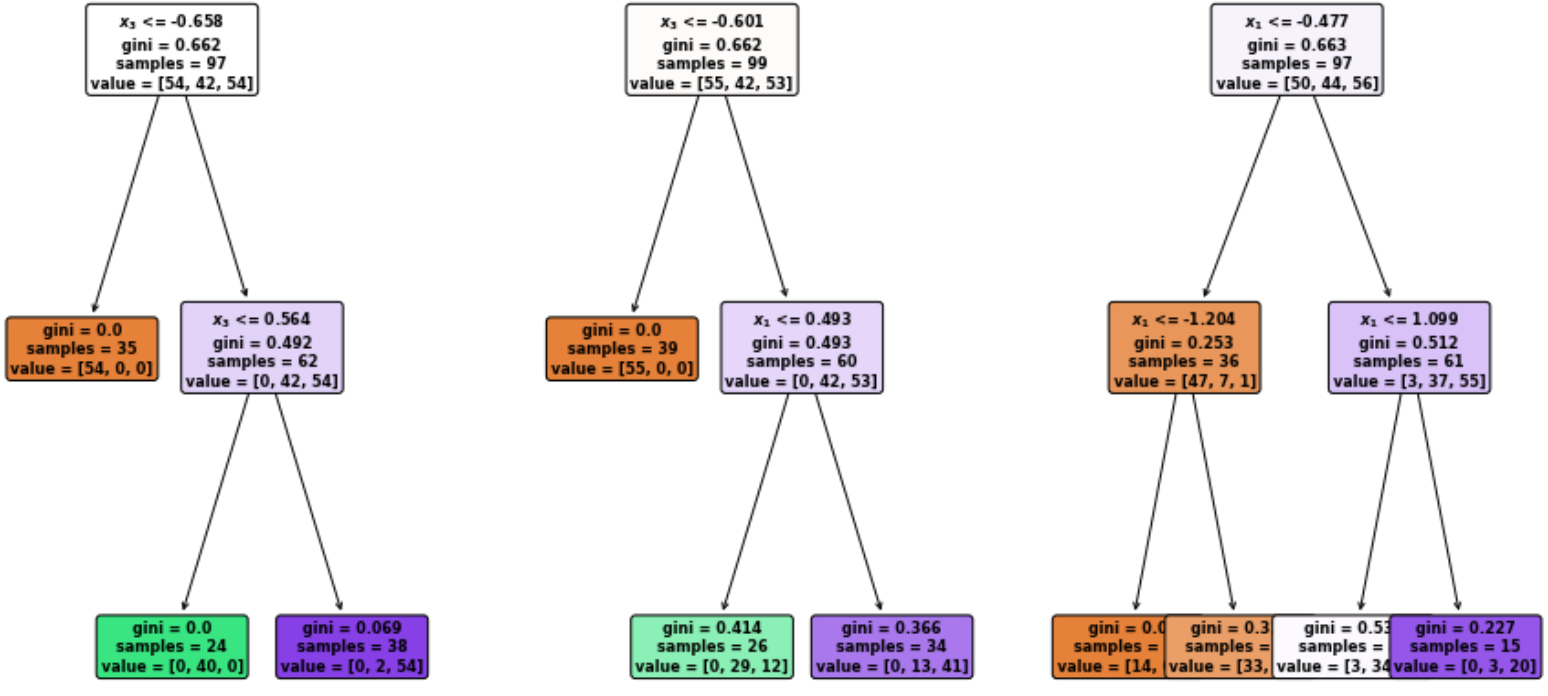
- Each individual models is trained on a *different* subset of the training examples
- This enables the individual models to produce different results
- Makes them more robust to outliers

We will shortly explain how the subsets are chosen.

Here is an Ensemble of individual models of the same type: Decision Trees

In [7]:
```
fig_ens
```

Out[7]:



The individual models are usually quite simple and restricted.

- They are *weak learners*: accuracy only marginally better than chance
- But combine to create a *strong learner*.

If the prediction of an ensemble of M binary classifiers is based on a "majority vote"

- The prediction is incorrect only if $m' \geq \lceil M/2 \rceil$ classifiers are incorrect
- The probability of a particular set of m' models of equal accuracy A all being incorrect is $(1-A)^{m'}$
- There are
$$\begin{pmatrix} M \\ m' \end{pmatrix}$$
combinations of m' models
- So the probability of a correct ensemble prediction when m' classifiers are incorrect is
$$1 - \begin{pmatrix} M \\ m' \end{pmatrix} * (1-A)^{m'}$$
which tends to 1 as M increases.

The power of Ensembles comes via the size of M.

Ensembling is independent of the types of the individual models

- A meta-model that can combine many different types of individual models
- Under the assumption of **independent** errors
- Often applied in competitions

Ensemble prediction

Each individual model comes up with a prediction for the target $\hat{\mathbf{y}}^{(\mathbf{i})}$ of example i, given features $\mathbf{x}^{(\mathbf{i})}$.

Let $p^{(\mathbf{i})}_{(t),c}$

- Denote the probability predicted by the t^{th} individual classifier
- That target $\mathbf{y}^{(\mathbf{i})}$ is in category $c \in C$
- Given features $\mathbf{x}^{(\mathbf{i})}$

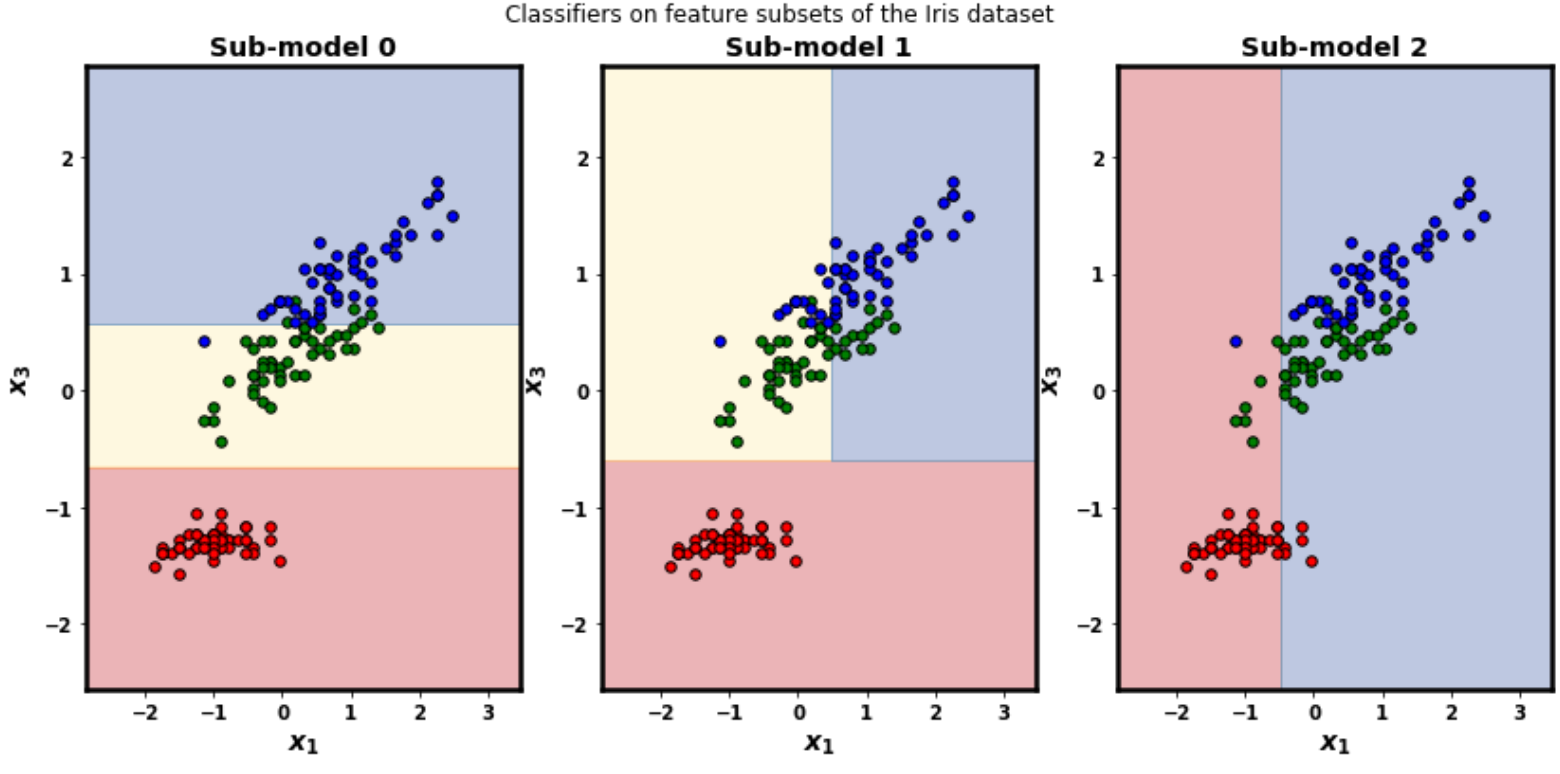
The class predicted by the ensemble is the one with highest average (across individual models) probability

$$\hat{\mathbf{y}}^{(\mathbf{i})} = \underset{c}{\operatorname{argmax}} \sum_{t=1}^{M} p^{(\mathbf{i})}_{(t),c}$$

Returning to the Ensemble of Decision Trees example, we can plot the decision boundary of each individual model

In [8]:
```
fig_submodels
```

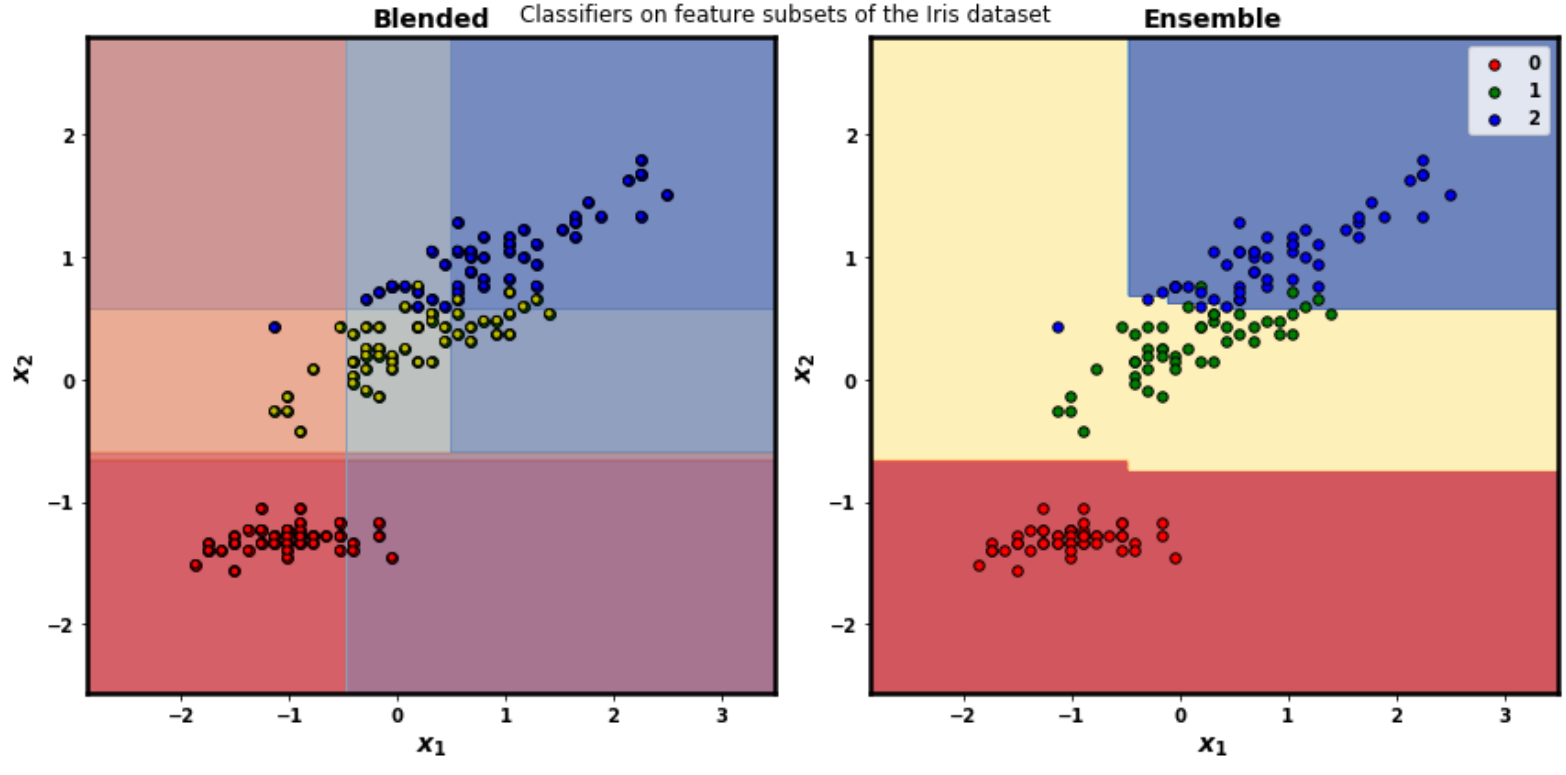
Out[8]:



By superimposing these boundaries on top of one another, we can visualize the "vote"

In [9]:
```
fig_sum
```

Out[9]:



- The left plot is the super-position
- The right plot is the final boundary of the ensemble

You can see that the combination of the weak learners does a pretty good job !

Bagging, Bootstrapping

One way to construct multiple weak learners of the *same* type of model

- Is to train each individual model on a *restricted* set of training examples

Because each individual model is trained on different examples, the predictions made by each are hopefully somewhat independent.

Given the full set of training examples

$$\langle \mathbf{X}, \mathbf{y} \rangle = [\mathbf{x^{(i)}}, \mathbf{y^{(i)}} | 1 \leq i \leq m]$$

we construct a restricted set of examples

$$\langle \mathbf{X}_{(t)}, \mathbf{y}_{(t)} \rangle$$

on which to train the t^{th} individual model

The restricted set is constructed by

- Selecting m examples at random from $\langle \mathbf{X}, \mathbf{y} \rangle$
- *With replacement*
- So it is possible for an example i' to appear more than once in $\langle \mathbf{X}_{(t)}, \mathbf{y}_{(t)} \rangle$

This process is called *bootstrapping* and results in

- $\langle \mathbf{X}_{(t)}, \mathbf{y}_{(t)} \rangle$
  $= [\mathbf{x}^{(i')}, \mathbf{y}^{(i')} | i' \in \{i_1, \ldots, i_m\}]$
- Where $i'_1, \ldots, i'_m$ are the indices of the m chosen examples

If each of the m examples in $\langle \mathbf{X}, \mathbf{y} \rangle$ is chosen with equal probability $\frac{1}{m}$

- The probability of a particular example i **not** being in $\langle \mathbf{X}_{(t)}, \mathbf{y}_{(t)} \rangle$ is

$$(1 - \frac{1}{m})^m$$

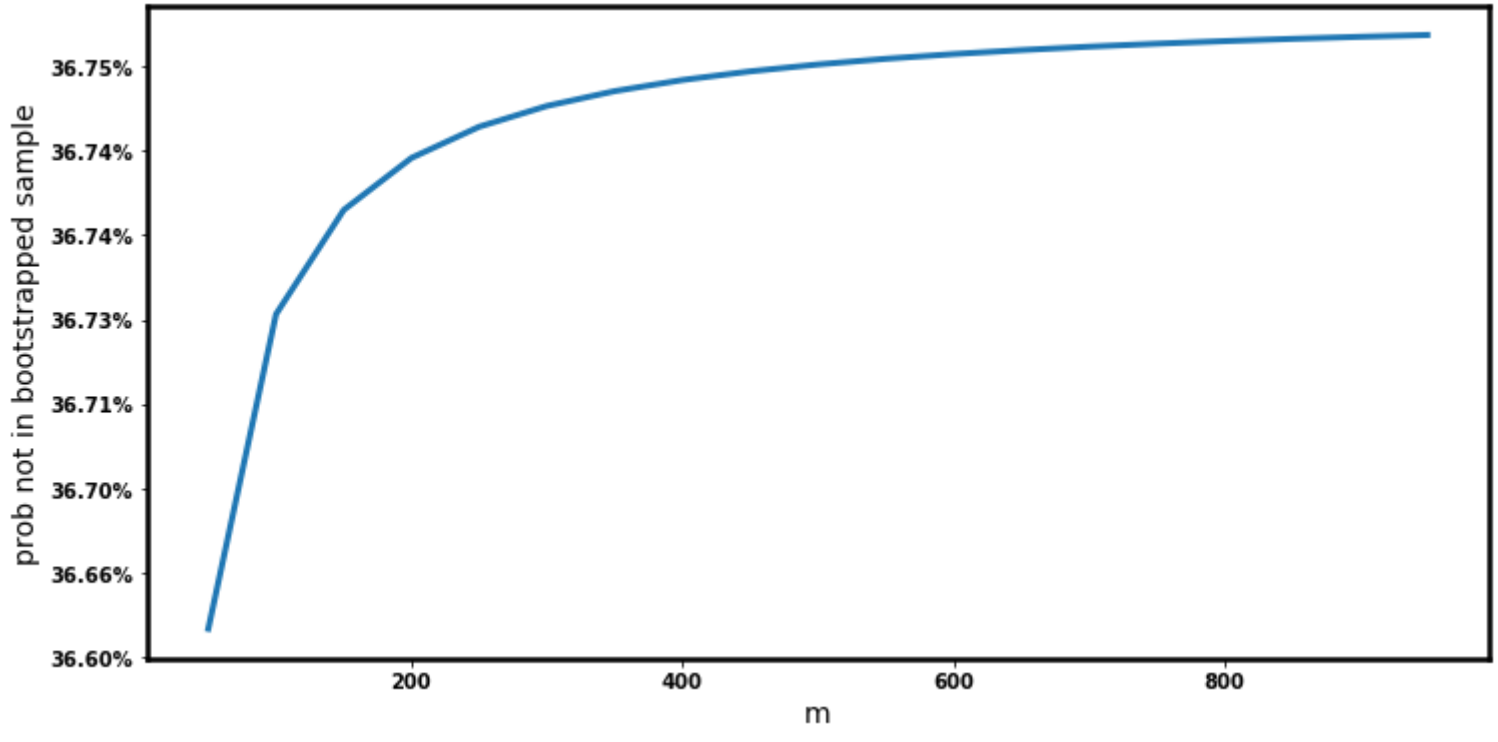
In [10]:

```
m = np.arange(50, 1000, 50)
p = (1 - 1/m)**m


fig, ax = plt.subplots(1,1, figsize=(12,6))
_= ax.plot(m, p)
_= ax.set_xlabel("m")
_= ax.set_ylabel("prob not in bootstrapped sample")
_= ax.set_yticklabels( [ "{:.2%}".format(y) for y in p])
plt.close(fig)
```

In [11]:
```
fig
```

Out[11]:



Thus about 63% of the examples in the bootstrapped set are duplicates.

The weak learner can't overfit to any example that is not in its training set.

The process of

- Bootstrapping restricted training examples
- Training individual models on the bootstrapped examples
- Aggregating model predictions into a single prediction

is called *bagging* and each individual training set is called a bag

Bagging has a nice side-effect

- About 37% of the full set of examples are not present in a given bag
- Called *out of bag*

The out of bag examples thus can be used to test out of sample prediction !

Random Forests

A Random Forest

- Is a collection of Decision Trees
- Of restricted power (weak learners)
- Created by Bagging

The learners are made weak by

- Training on a bootstrapped subset
- By limiting the depth of the Decision Tree
- By limiting the choice of feature on which to split a node
    - To a random subset of all features

The result is that the individual models (Decision Trees) are relatively independent.

Boosting

There is another approach to creating ensembles of weak learners.

The method is called *boosting*

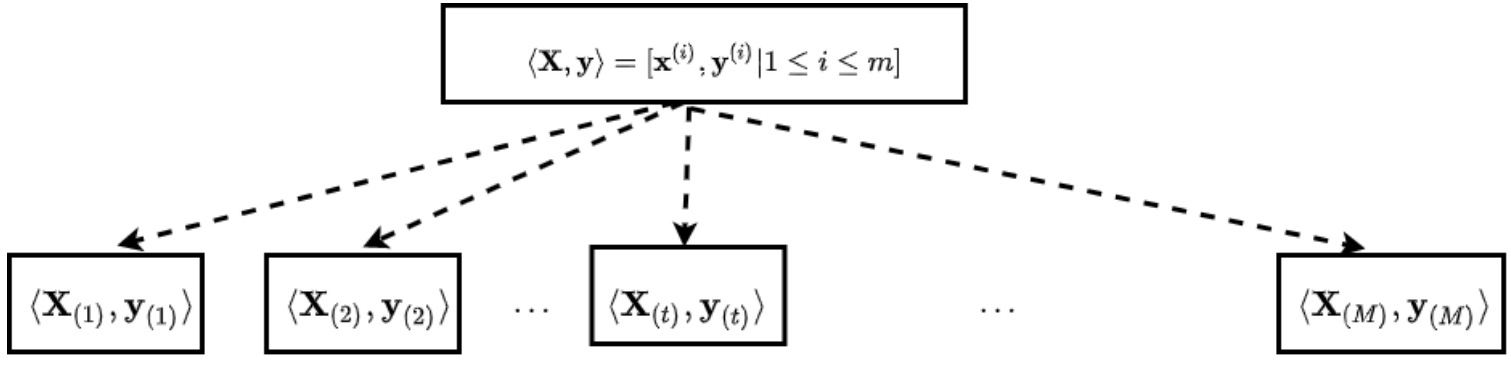
- Rather than create weak learners independently, i.e., a *set*
- Boosting creates a *sequence* of weak learners: $M_{(0)}, M_{(1)}, \ldots, M_{(M)}$
- Where the $(t+1)^{th}$ individual model in the sequence
- Focuses on correctly predicting those examples *incorrectly* predicted by the t^{th} individual model

Notation

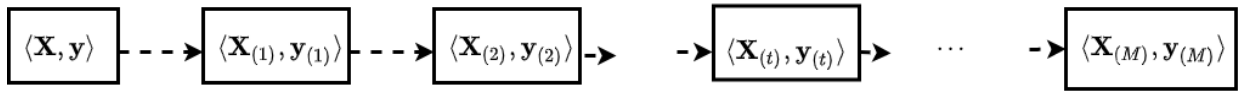
We will be dealing with many sequences. We use subscripts in parentheses to index elements of a sequence.

$$M_{(0)}, M_{(1)}, \ldots, M_{(M)}$$

Bagging


$\langle \mathbf{X}, \mathbf{y} \rangle = [\mathbf{x}^{(i)}, \mathbf{y}^{(i)} | 1 \leq i \leq m]$
$\langle \mathbf{X}_{(1)}, \mathbf{y}_{(1)} \rangle$
$\langle \mathbf{X}_{(2)}, \mathbf{y}_{(2)} \rangle$
$\cdots$
$\langle \mathbf{X}_{(t)}, \mathbf{y}_{(t)} \rangle$
$\cdots$
$\langle \mathbf{X}_{(M)}, \mathbf{y}_{(M)} \rangle$

Boosting


$\langle \mathbf{X}, \mathbf{y} \rangle$
$\langle \mathbf{X}_{(1)}, \mathbf{y}_{(1)} \rangle$
$\langle \mathbf{X}_{(2)}, \mathbf{y}_{(2)} \rangle$
$\langle \mathbf{X}_{(t)}, \mathbf{y}_{(t)} \rangle$
$\cdots$
$\langle \mathbf{X}_{(M)}, \mathbf{y}_{(M)} \rangle$

How do we get an individual model to focus on some particular examples ?

- By assigning each example a weight
- Increasing the probability that more heavily weighted examples are included in the training examples for the model

Let $\text{say}_{(t)}^{\textbf{(i)}}$ denote the weight assigned to example i in the training set for the t^{th} individual model

The "say" is adjusted from the t^{th} model to the $(t+1)^{th}$ individual model

$$\text{If example } i \text{ is incorrectly predicted in model } t: \quad \text{say}_{(t+1)}^{\textbf{(i)}} > \text{say}_{(t)}^{\textbf{(i)}}$$

$$\text{If example } i \text{ is correctly predicted in model } t: \quad \text{say}_{(t+1)}^{\textbf{(i)}} < \text{say}_{(t)}^{\textbf{(i)}}$$

When bootstrapping, rather than drawing examples with equal probability

- Draw examples for model $(t+1)$ in proportion to it's $\mathbf{say}^{(\mathbf{i})}_{(t+1)}$
- So examples that were "problematic" in model t are over-represented in training model $(t+1)$

- Boosting creates a collection of "specialists" (focus on hard to predict examples)
- Bagging creates a collection of "generalists", each a little better than random

AdaBoost

AdaBoost is a particular model that uses boosting

- The individual models are Decision Trees
    - Usually depth 1; "stumps"
- There is an "importance" associated with each individual model
- Models with higher weight have a greater impact on ensemble prediction

Let

$$\text{importance}_{(t)}$$

denote the weight of the t^{th} individual model in the sequence.

- $\text{importance}_{(t)}$ is determined by the Performance Metric (e.g., Accuracy) of individual model t
- The class predicted by the ensemble is the one with highest *importance-weighted* average (across individual models) probability

$$\hat{\mathbf{y}}^{(\mathbf{i})} = \underset{c}{\text{argmax}} \sum_{t=1}^{M} (p_{(t),c}^{(\mathbf{i})} * \text{importance}_{(t)})$$

Thus, models that are more successful have greater weight.

Gradient Boosting

Gradient Boosting is a "more mathematical" (less operational) approach to boosting

- A Loss Function is defined
- That measures the Loss $\mathcal{L}_{(t)}$ of the ensemble consisting of the first t models in the sequence
- Computes the gradient of the Loss $\mathcal{L}_{(t)}$
- Adds model $(t+1)$ to explicitly reduce the loss by moving in the direction of the gradient

$$\mathcal{L}_{(t+1)} < \mathcal{L}_{(t)}$$

We illustrate Gradient Boosting with a Regression task: predict continuous $\hat{\mathbf{y}}$

- We will produce a sequence of models $M_{(0)}, M_{(1)}, \ldots, M_{(M)}$

We have not specified the functional form of the models M_t

- It will typically be something like a Decision Tree and *not* Linear Regression

Model t will have

- Target denoted by $e_{(t)}$
- Predictions denoted by $\hat{e}_{(t)}$
- We define $\hat{e}_{(0)} = \bar{\mathbf{y}}$
    - where $\bar{\mathbf{y}}$ is the mean (over the m examples in training) of the target

$$\bar{\mathbf{y}} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{y^{(i)}}$$

The prediction of the *ensemble* (rather than individual models) consisting of the first t models is

$$\hat{\mathbf{y}}_{(t)} = \sum_{t'=0}^{t} \alpha * \hat{e}_{(t)}$$

That is: the *ensemble prediction* is the weighted sum of the *predictions of the individual models*.

- Unlike AdaBoost: the weights for each model are identical (α)

Loss function

The Loss function for the ensemble consisting of the first t models will be the MSE:

$$\mathcal{L}_{(t)} = \frac{1}{m} \sum_{i=1}^{m} (\mathbf{y^{(i)}} - \mathbf{\hat{y}}_{(t)}^{\mathbf{(i)}})^2$$

The ensemble prediction $\hat{\mathbf{y}}_{(t)}$ differs from the regression target $\mathbf{y}$ by

$$\mathbf{y} - \hat{\mathbf{y}}_{(t)} = \mathbf{e}_{(t+1)}$$

We therefore set the target for model $(t+1)$

- To be $\mathbf{e}_{(t+1)}$
- Which is the *residual* (error) of the target with respect to the ensemble prediction up to step t

In other words: model $(t+1)$ is tasked with predicting the residual remaining after the ensemble prediction of the first t individual models.

To be clear, let's suppose the $M_{(t)}$ are Decision Trees.

- Each tree $M_{(t)}$ is constructed from *scratch*
  - It does not "extend" tree $M_{(t-1)}$
- It's thus possible that two trees in the sequence have the same test
- Each tree $M_{(t)}$ has a different target
  - The target for $M_{(t)}$ is the remaining error between target $\mathbf{y}$ and the prediction of the ensemble prefix of length $(t-1)$

- Because we defined $\mathbf{e}_{(0)} = \bar{\mathbf{y}}$
    - $\mathbf{e}_{(1)} = \mathbf{y} - \bar{\mathbf{y}}$
- So model $M_{(1)}$ is trying to predict the residual with respect to a simpler model (one that always predicts $\bar{\mathbf{y}}$)
- The ensemble of length 1 predicts

$$\bar{\mathbf{y}} + \hat{e}_{(1)}$$

Each model t in the sequence attempts to reduce the residual left over from the ensemble prediction of the prefix of length $(t-1)$.

Where are the gradients in Gradient Boosting ?

Consider the derivative of the Loss function (MSE) with respect to the ensemble prediction

$$
\begin{aligned}
\frac{\partial \mathcal{L}_{(t)}}{\partial \hat{\mathbf{y}}_t} &= \frac{\partial \frac{1}{m} \sum_{i=1}^{m} (\mathbf{y^{(i)}} - \hat{\mathbf{y}}_{(t)})^{\mathbf{(i)}})^2}{\partial \hat{\mathbf{y}}_t} \\
&= \frac{2}{m}(\mathbf{y^{(i)}} - \hat{\mathbf{y}}_{(t)}^{\mathbf{(i)}}) * -1 && \text{chain rule} \\
&= -\frac{2}{m}\mathbf{e}_{(t+1)} && \text{definition of } \mathbf{e}_{(t+1)}
\end{aligned}
$$

That is: the gradient is proportional to the residual of the target with respect to the the prediction of the ensemble consisting of the first t models

You shouldn't be surprised to see the residual in the gradient; this is just a fact of the MSE

- It's derivative is closely related to the residual
- One can argue that the MSE was *chosen* exactly because of this property

So the ensemble of $(t+1)$ models can decrease the loss compared to the ensemble with t models

$$\mathcal{L}_{(t+1)} < \mathcal{L}_{(t)}$$

by making $\hat{\mathbf{y}}_{(t+1)}$ equal to $\hat{\mathbf{y}}_{(t)}$ plus the approximation of the residual.

This process of

- Minimizing a Loss function
- By incrementally updating predictions
    - In the direction (opposite direction really, because gradient is negative) the gradient is called *Gradient Descent*.

Gradient Descent

- Will be our prime method of solving optimization problems, such as training models (minimizing Loss)
- Is a key component of Deep Learning

We will explore Gradient Descent in a subsequent module.

Aside

Even though AdaBoost was created prior to Gradient Boosting

- It can be shown to be equivalent to Gradient Boosting when the Loss function is Exponential Loss.

In [12]:
```
print("Done")
```

```
Done
```