# XGBoost (classification)

| Drug dosage | Drug usefulness |
|---|---|
| 5 | No |
| 8 | Yes |
| 11 | Yes |
| 18 | No |

Assuming that we have this very simple dataset

## Step 1: make the initial prediction

| Drug dosage | Drug usefulness |
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| 5 | No |
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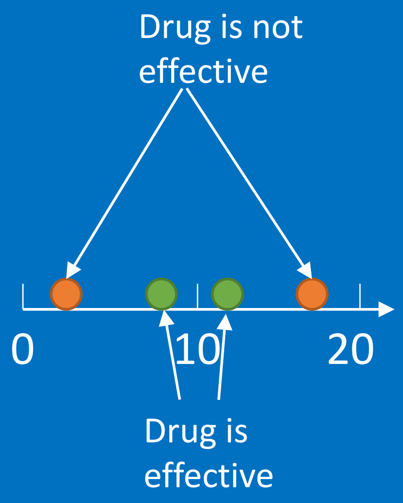
Plot it out, we have



Step 1: make the initial prediction

For example, the probability of the dosage is effective: 0.5

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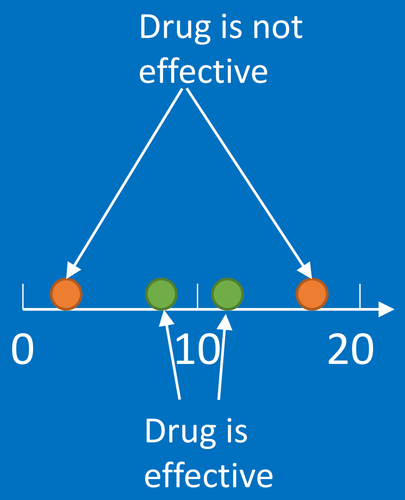

Step 1: make the initial prediction

For example, the probability of the dosage is effective: 0.5

In other words, does not matter how many dosages we take, the initial prediction for the usefulness for the drug is 50%

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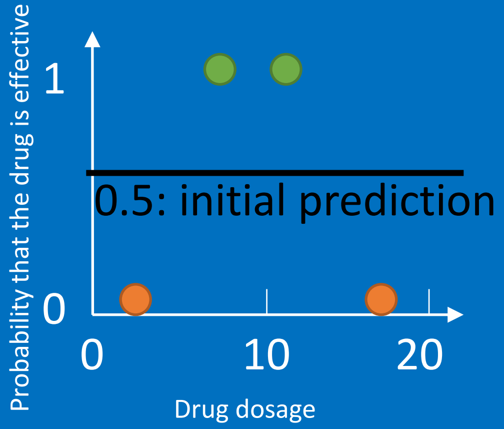

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For example, the probability of the dosage is effective: 0.5

Step 2: we get the residuals for all the samples

| Drug dosage | Drug usefulness | Residuals |
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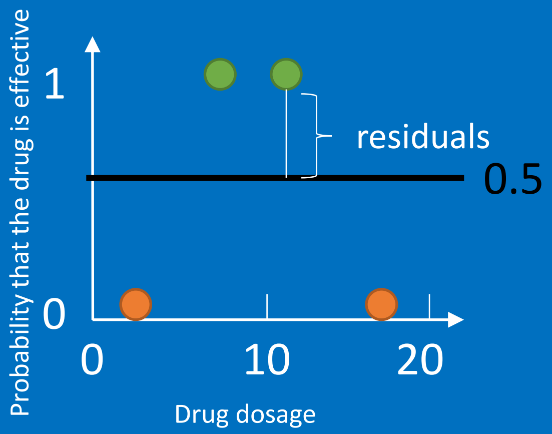

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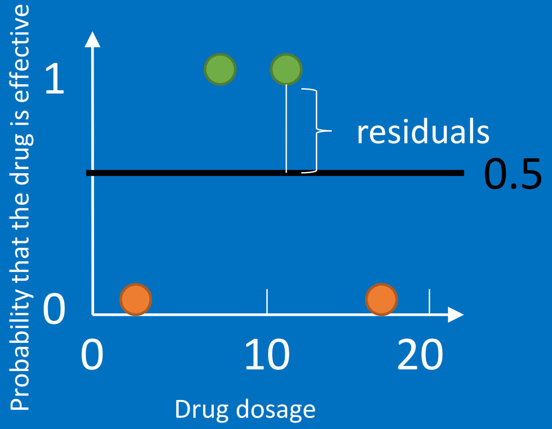

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3.1 All the tree starts from a leaf, with all the residuals

-0.5, 0.5, 0.5, -0.5

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Note that for regression:

$$Similarity\ score = \frac{(\sum residuals)^2}{number\ of\ residuals + \lambda}$$

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$$Similarity\ score = \frac{(\sum residuals)^2}{\sum previous\ prob_i \times (1 - previous\ prob_i) + \lambda}$$

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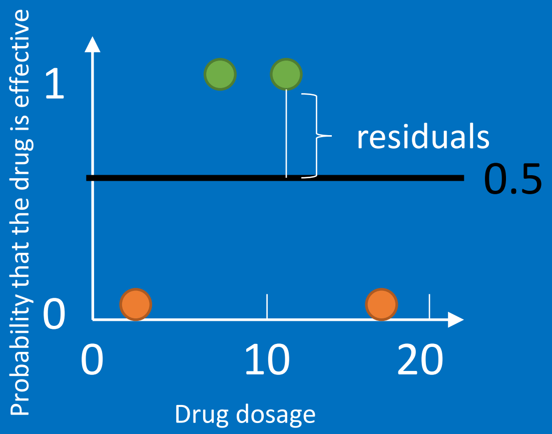

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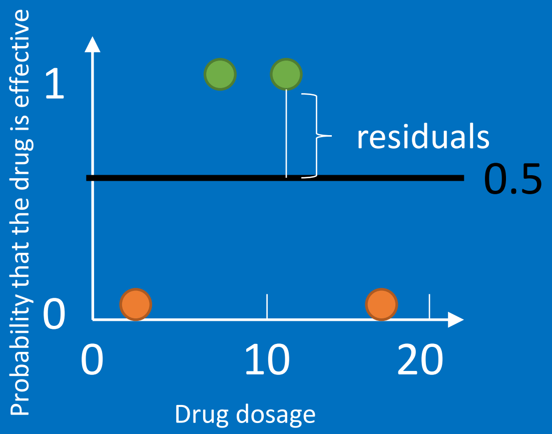

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For this case we have

$$Similarity\ score = \frac{(-0.5 + 0.5 + 0.5\ - 0.5)^2}{\sum previous\ prob_i \times (1 - previous\ prob_i) + \lambda} = 0$$

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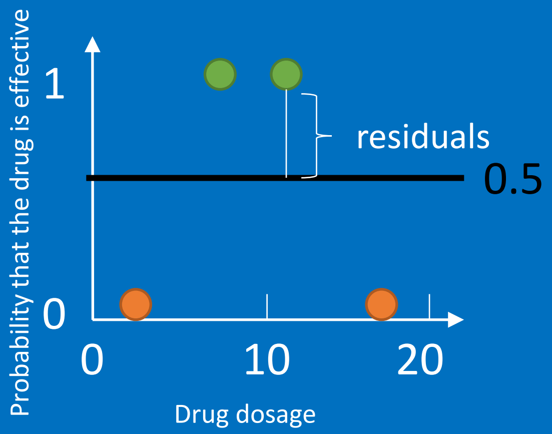

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3.3 Further split the tree

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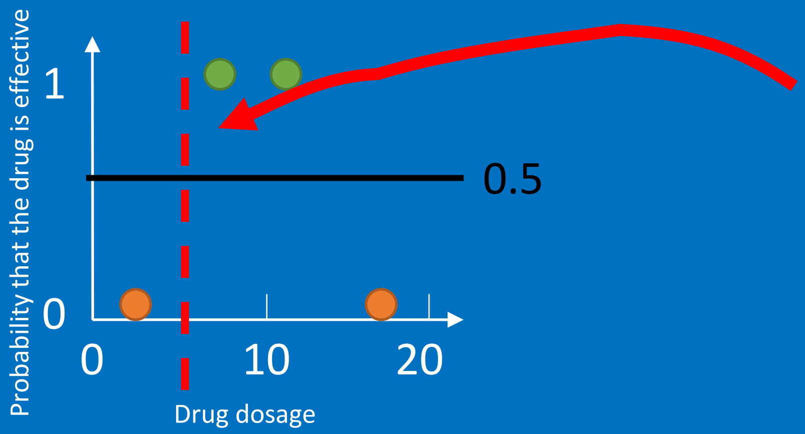

Similar to regression xgboost tree, we can start from the first data point, calculate the similarity score, and the gain. Then move to the next two points

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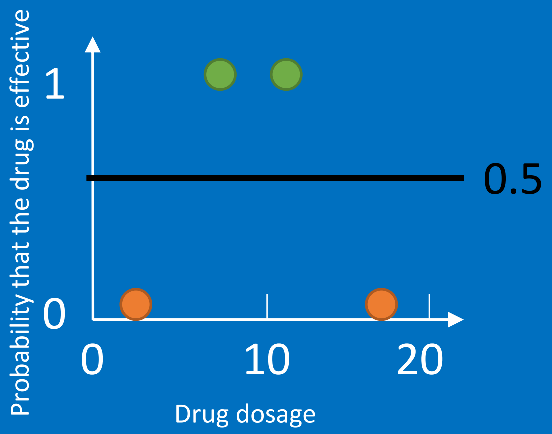

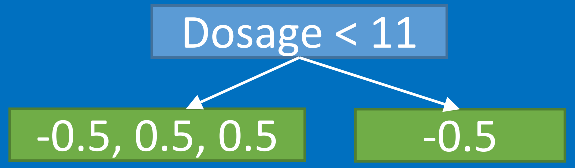

After gone through all the thresholds, we can tell that this tree gives the highest “Gain”

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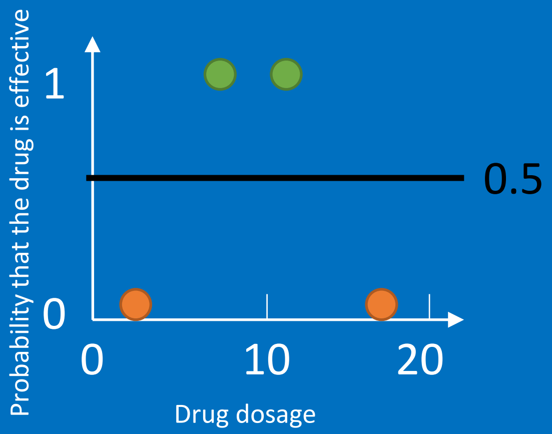

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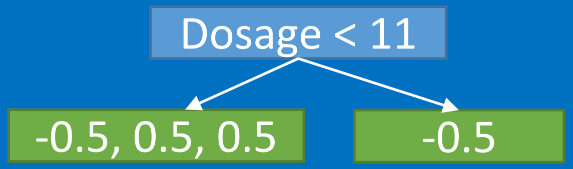
Dosage < 11

-0.5, 0.5, 0.5

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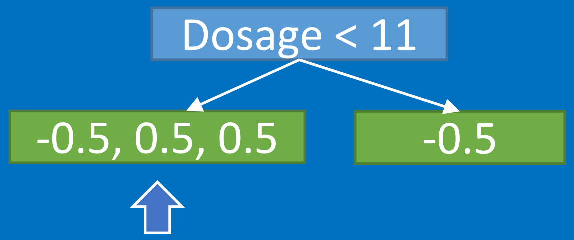

We can continue split these residuals (following the same method)…

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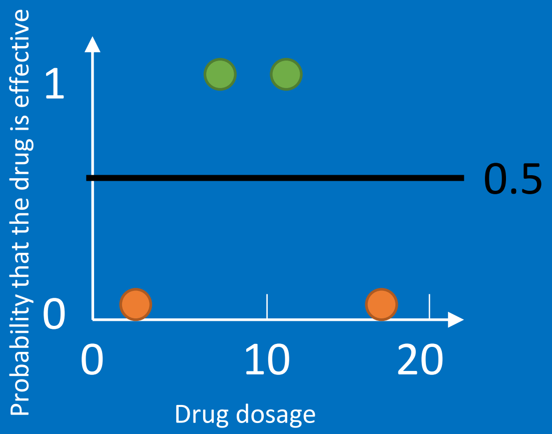

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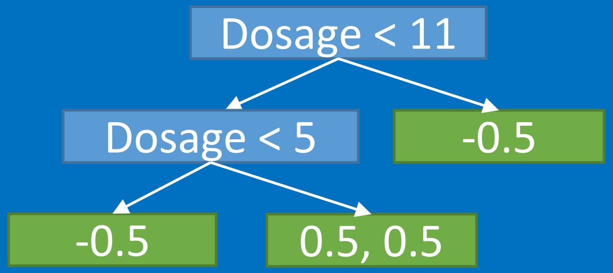

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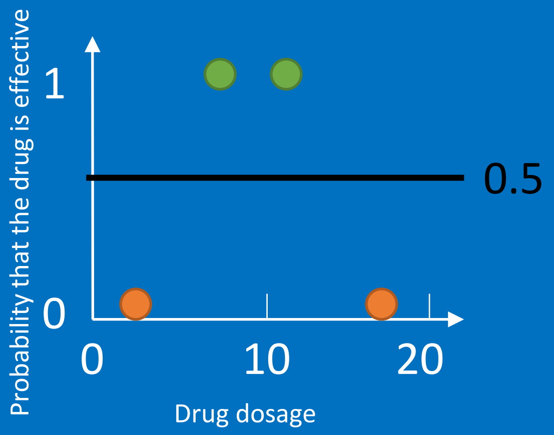

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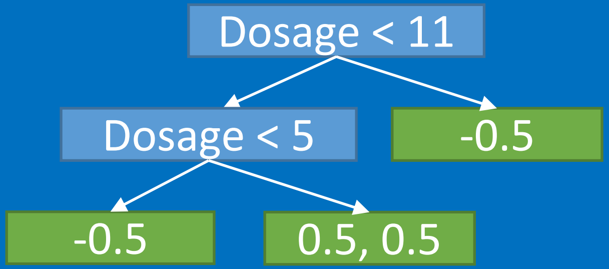

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Note that for a xgboost tree, there are two limitations we can implement:

- How many levels of the tree can grow (like any other tree methods)
- How many residuals in each leaf: this is defined as cover

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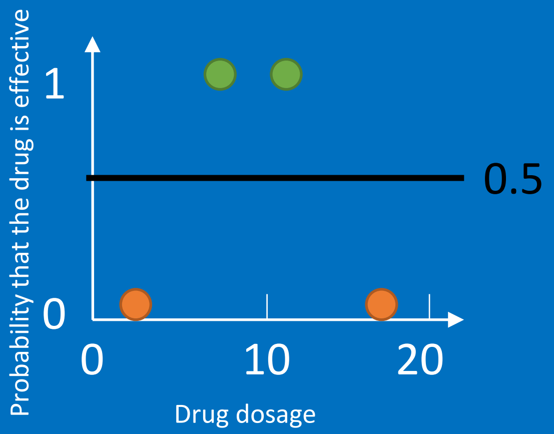

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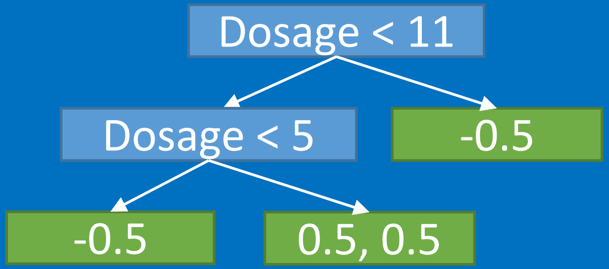

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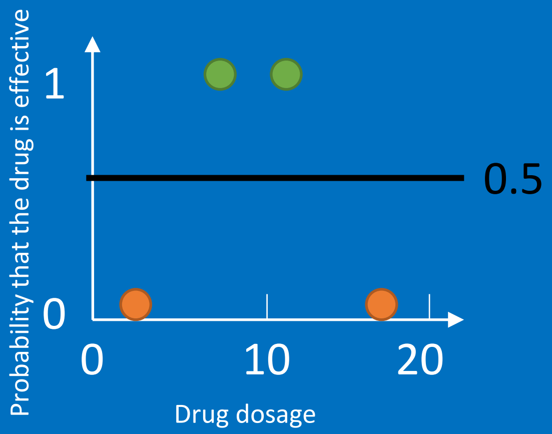

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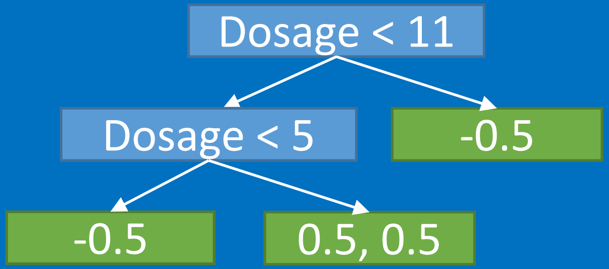
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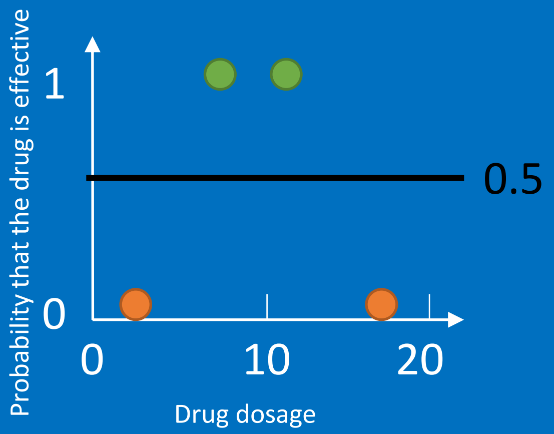

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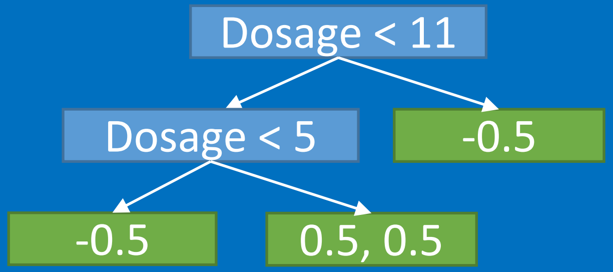

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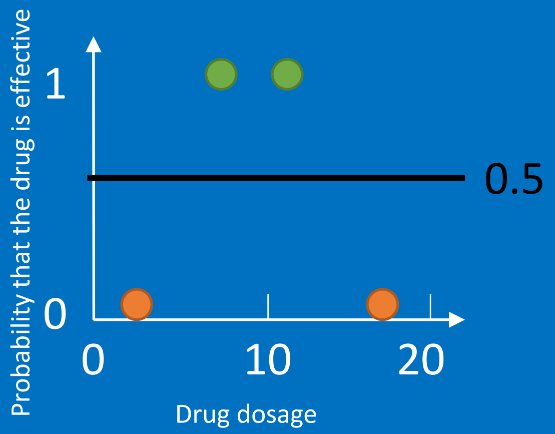

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For classification, it’s more complicated

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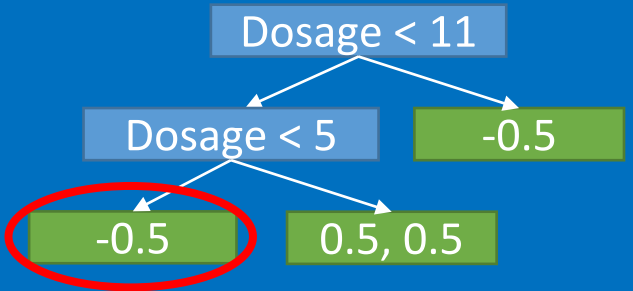

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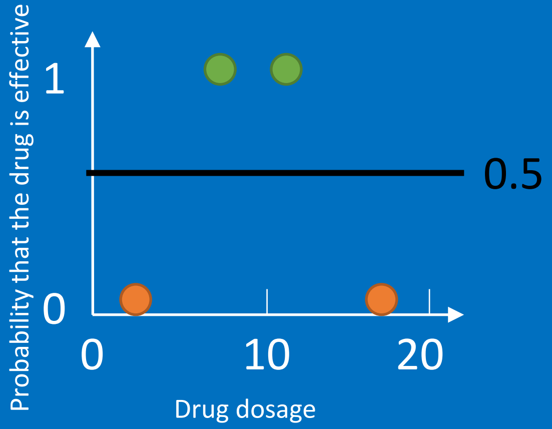

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For example, the cover for this leaf is

$$cover = 0.5 \times (1 - 0.5) = 0.25$$

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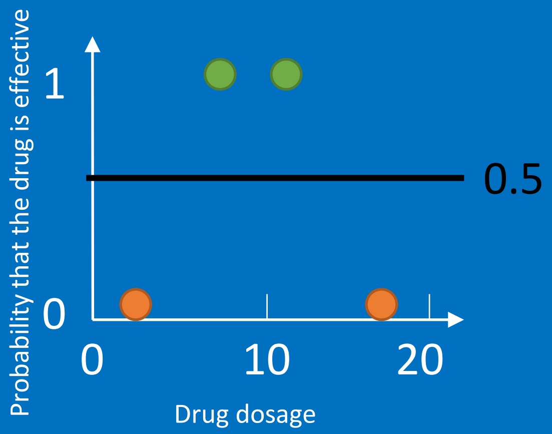

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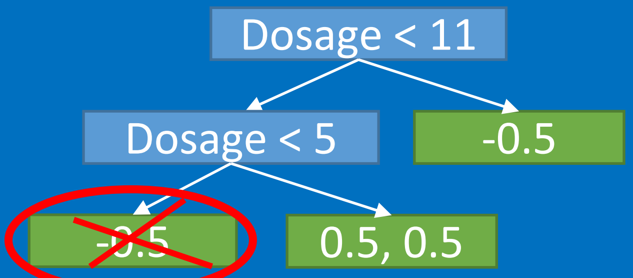

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For example, the cover for this leaf is

$$cover = 0.5 \times (1 - 0.5) = 0.25$$

So this leaf will be removed

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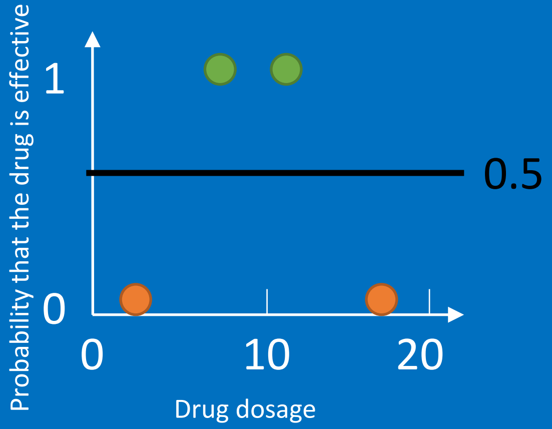

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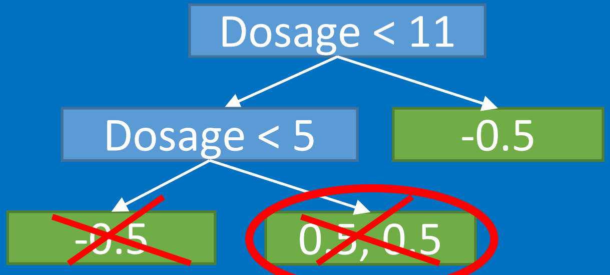

Dosage < 11

Dosage < 5

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~~-0.5~~

~~0.5, 0.5~~

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For classification, it's more complicated

For example, the cover for this leaf is

$$cover = 0.5 \times (1 - 0.5) + 0.5 \times (1 - 0.5) = 0.5$$

So this leaf will be removed, too

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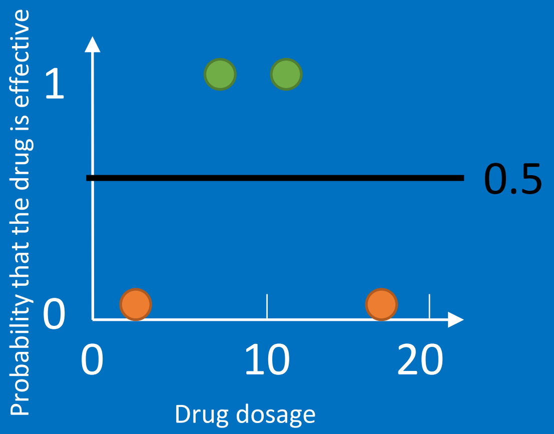

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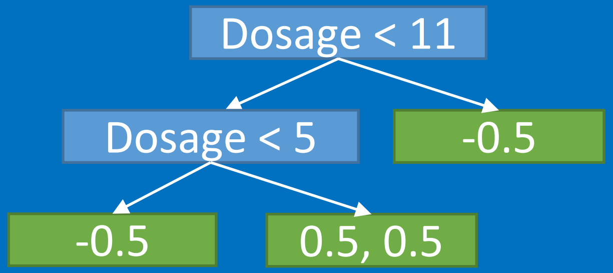

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So as you can see, by default, too many leaf will be removed in this example, if we use the default cover. In order to make this example working, let's just set cover=0

In some packages, cover is called min_child_weight

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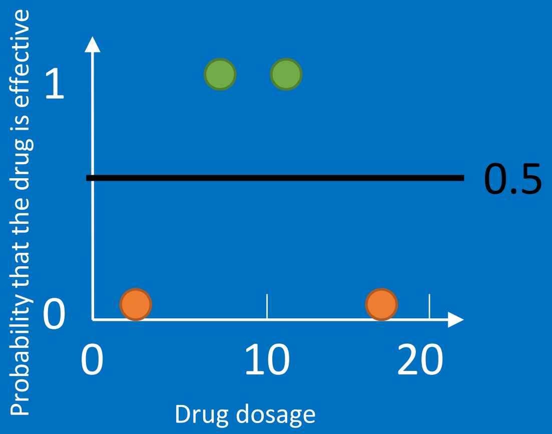

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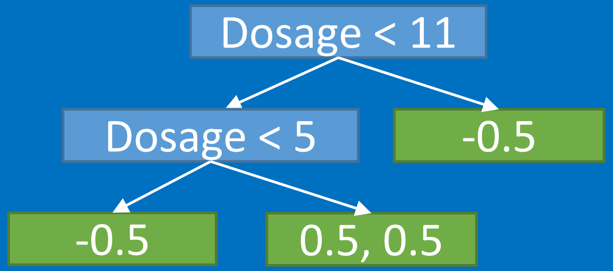
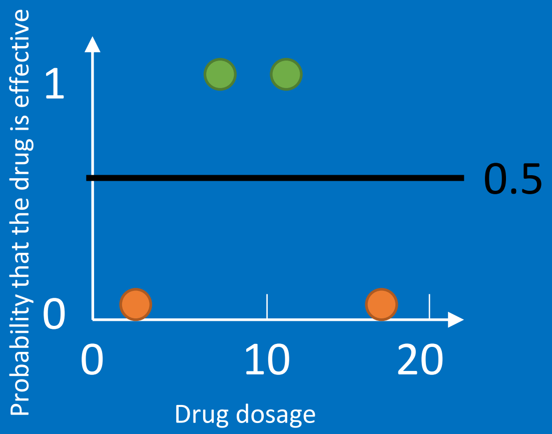


Step 4: Prune the tree (like the xgboost for regression)

| Drug dosage | Drug usefulness | Residuals |
|---|---|---|
| 5 | No | -0.5 |
| 8 | Yes | 0.5 |
| 11 | Yes | 0.5 |
| 18 | No | -0.5 |

Plot it out, we have



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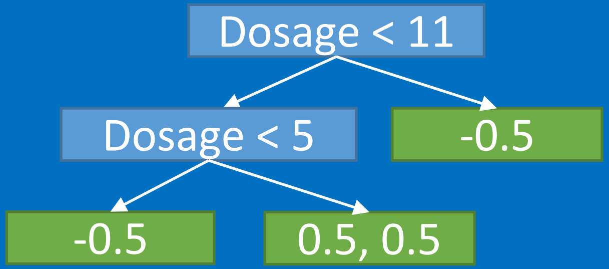

Step 4: Prune the tree (like the xgboost for regression)

Step 5: Determine the output value

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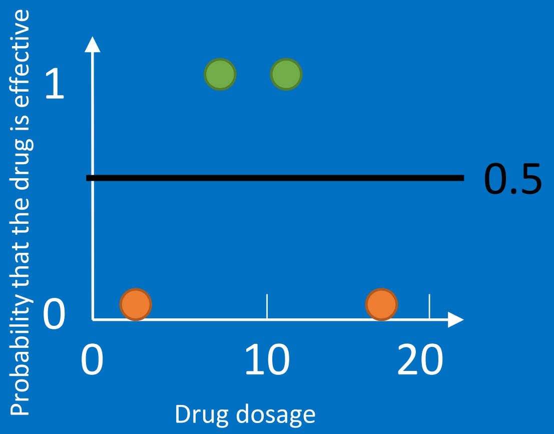

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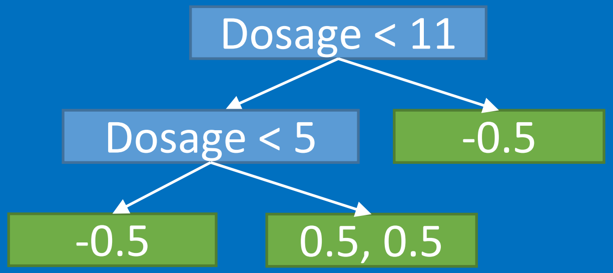

Step 4: Prune the tree (like the xgboost for regression)

Step 5: Determine the output value

Note that for regression xgboost:

$$output = \frac{sum\ of\ residuals}{number\ of\ residuals + \lambda}$$

$$output = \frac{\sum residuals}{\sum previous\ prob_i \times (1 - previous\ prob_i) + \lambda}$$

| Drug dosage | Drug usefulness | Residuals |
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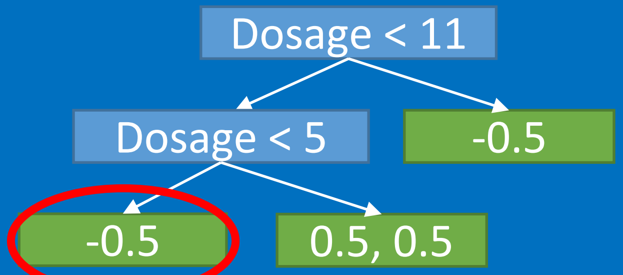

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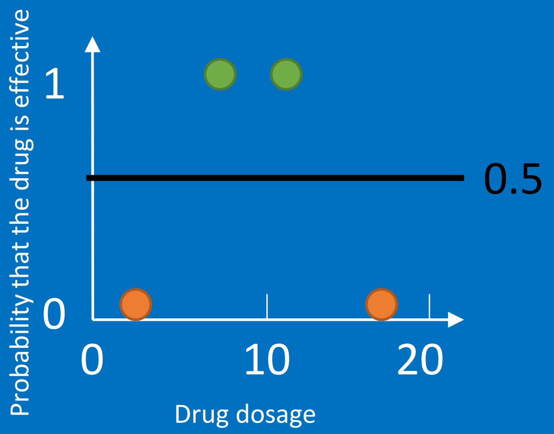

Step 4: Prune the tree (like the xgboost for regression)

Step 5: Determine the output value

$$output = \frac{\sum residuals}{\sum previous\ prob_i \times (1 - previous\ prob_i) + \lambda}$$

So for this leaf, we have (assuming lambda=0):

$$output = \frac{-0.5}{0.5 \times (1 - 0.5) + 0} = -2$$

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|---|---|---|
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| 11 | Yes | 0.5 |
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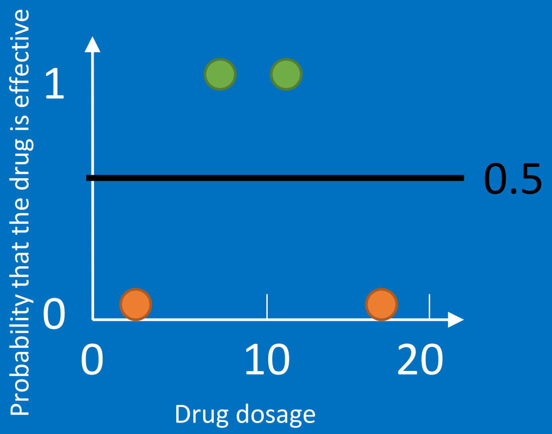

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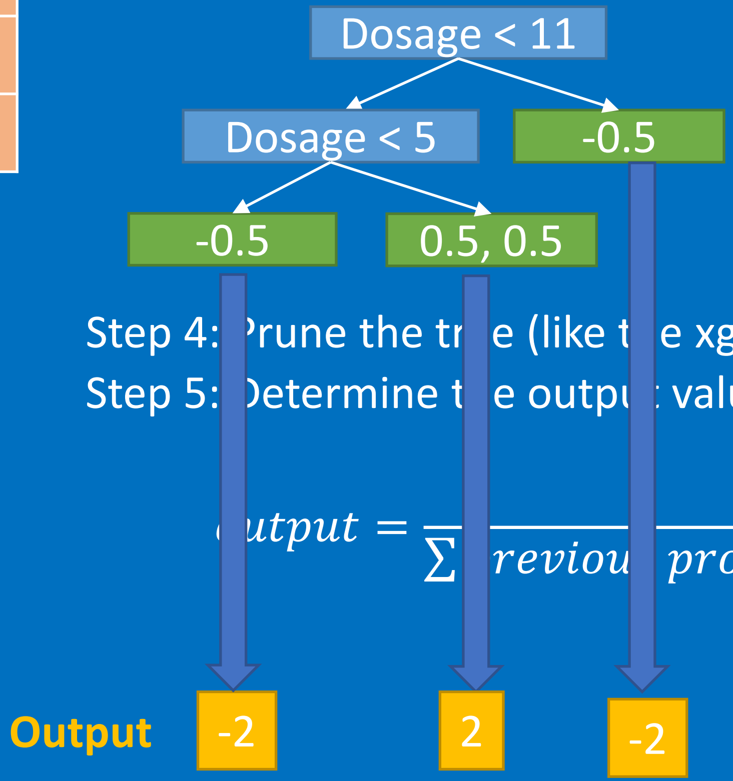

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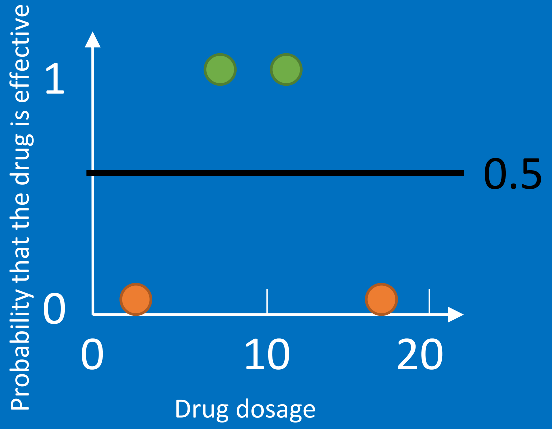

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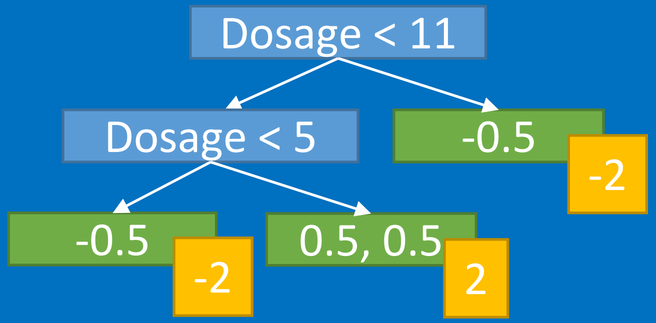

So the first tree is completed

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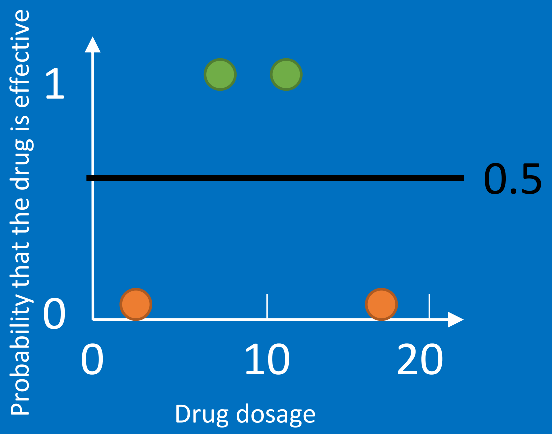

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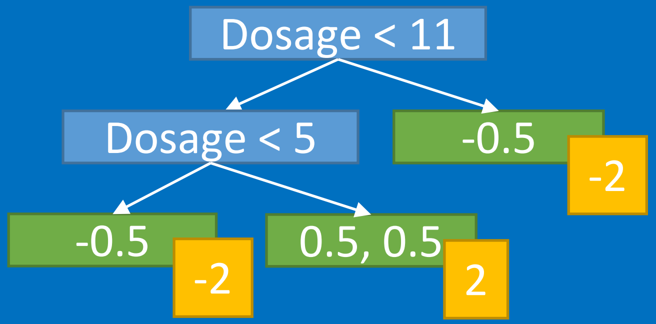

So the first tree is completed

Step 6: Start making predictions

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| 8 | Yes | 0.5 |
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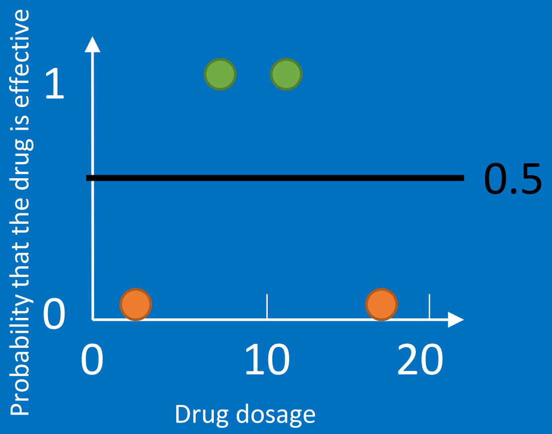

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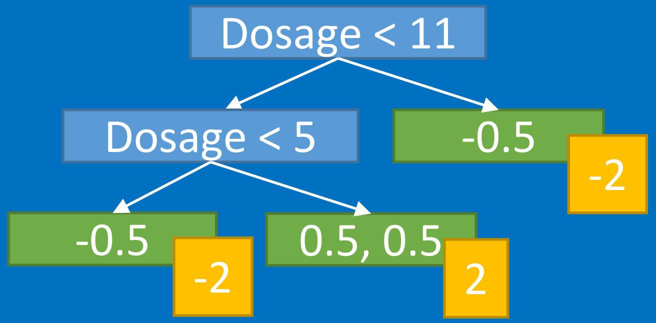

So the first tree is completed

Step 6: Start making predictions

6.1: first we need to convert the previous prob to log(odds)

The equation is $\log(odds) = \log(\frac{p}{1-p})$

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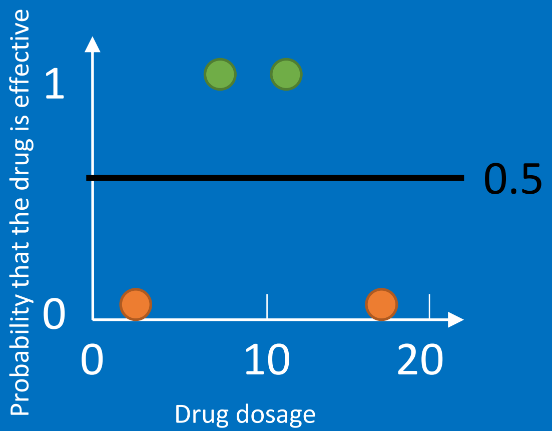

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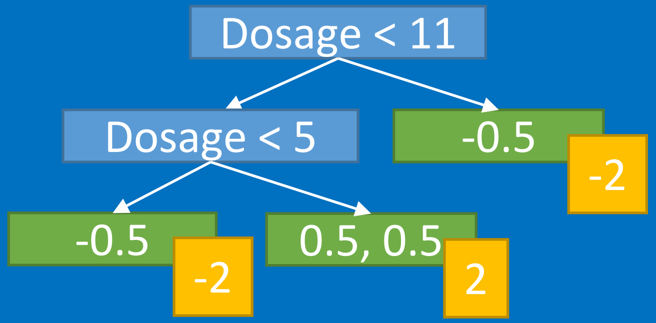

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Step 6: Start making predictions

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The equation is $\log(odds) = \log(\frac{p}{1-p})$

The previous probability is 0.5, so log(odds) = 0

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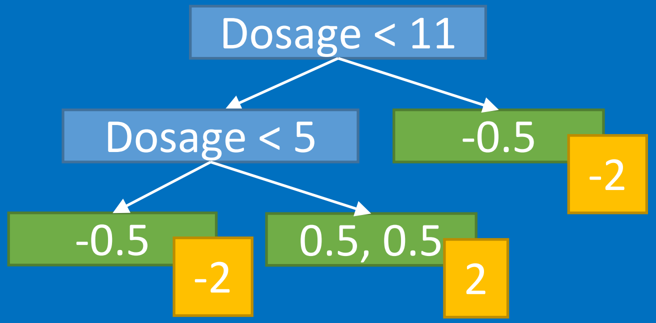

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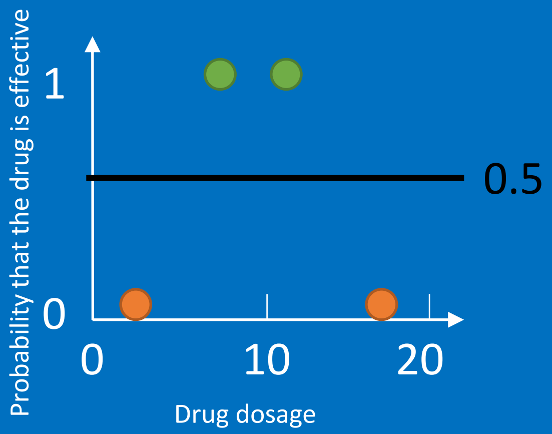
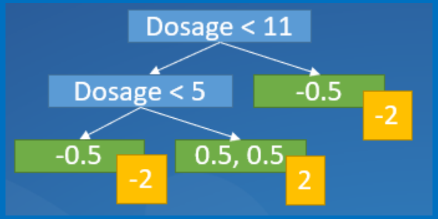


Step 6: Start making predictions

6.1: first we need to convert the previous prob to log(odds)=0

6.2: making prediction with

0.5 log(odds)=0 + 0.3 X



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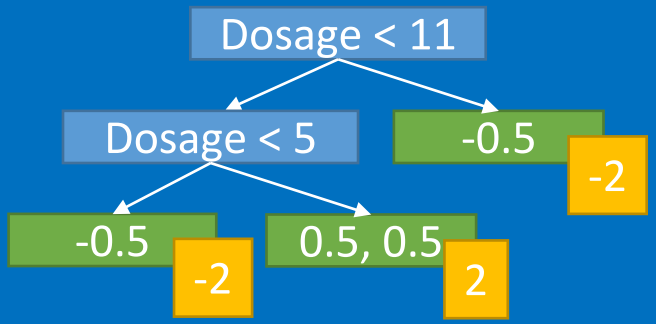

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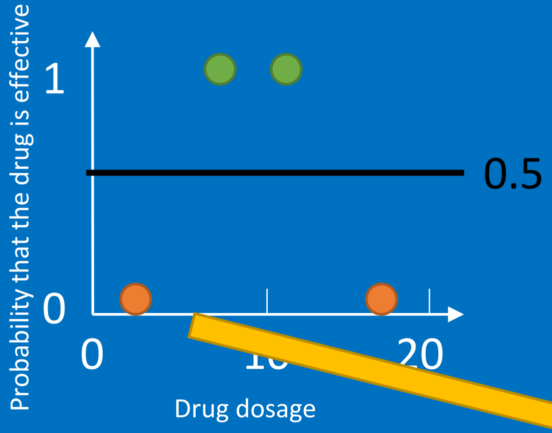

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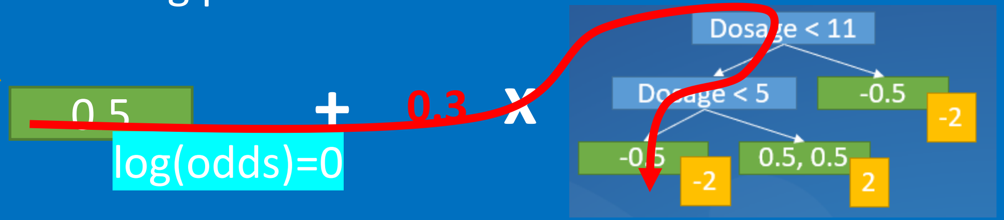

For example, for the first sample, we can have the log(odds) prediction as 0+0.3x(-2)=-0.6

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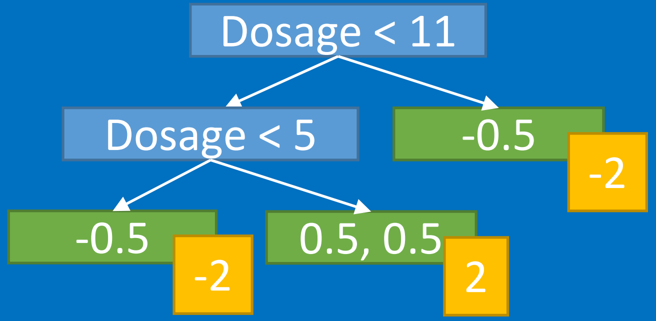

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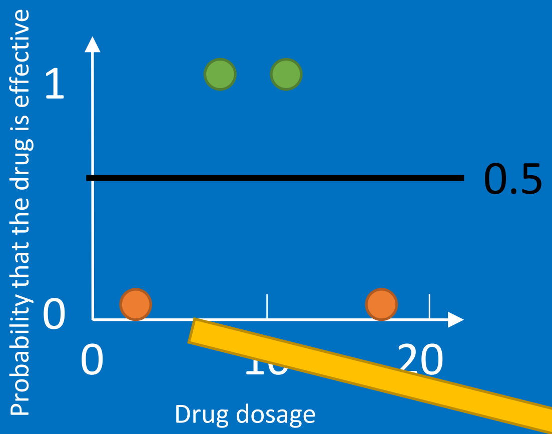

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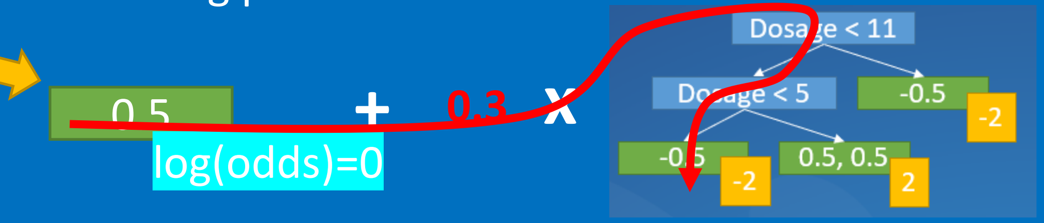

Then we need to convert log(odds) back to probability as:

$$p = \frac{e^{\log(odds)}}{1 + e^{\log(odds)}}$$

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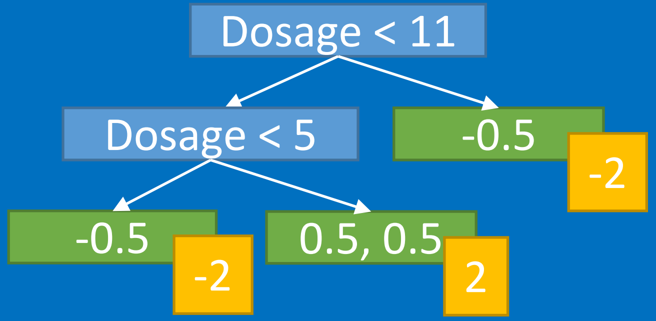
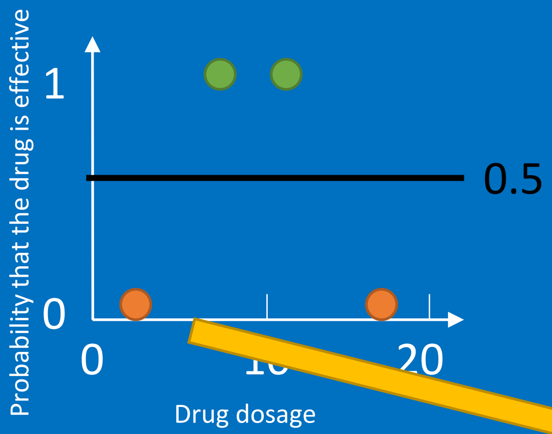


So the first tree is completed

So for the first sample, the prediction of probability is

$$p = \frac{e^{\log(odds)}}{1+e^{\log(odds)}} = \frac{e^{-0.6}}{1+e^{-0.6}} = 0.35$$

Plot it out, we have



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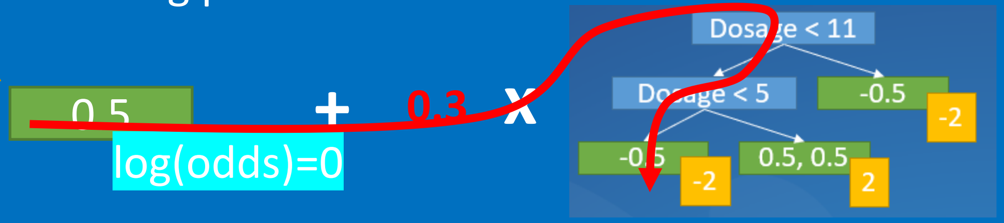

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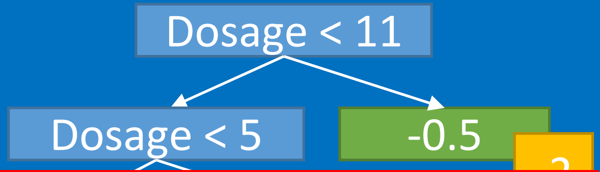

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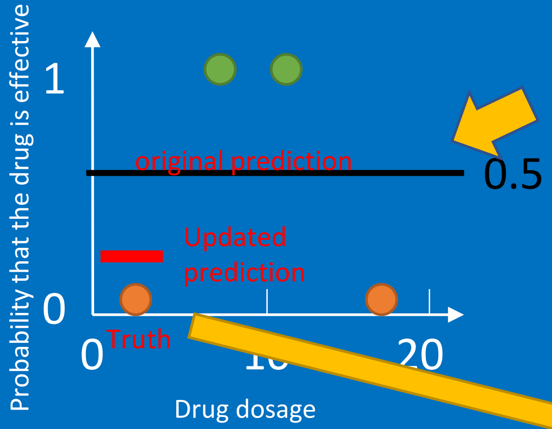

The original prediction is 0.5, and the new prediction is 0.35 (get reduced from the original), and it is getting closer to the truth

So for the first sample, the prediction of probability is

$$p = \frac{e^{\log(odds)}}{1 + e^{\log(odds)}} = \frac{e^{-0.6}}{1 + e^{-0.6}} = 0.35$$

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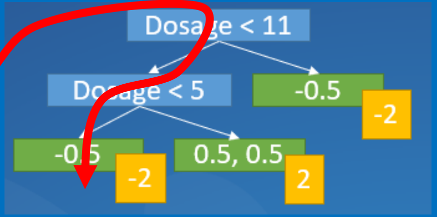
6.2: making prediction with

0.5 log(odds)=0 + 0.3 x



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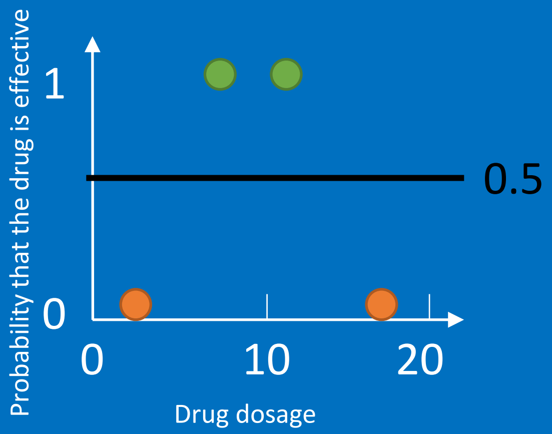

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Step 6: Start making predictions

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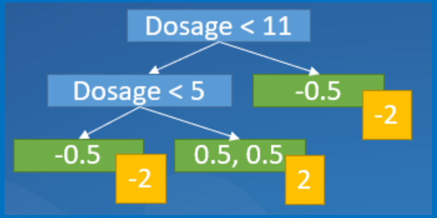
6.2: making prediction with

0.5 log(odds) + 0.3 X



We repeat the process from Step 1 to Step 6 but with updated prediction, every time we get reduced residuals, until the residuals do not change much anymore …

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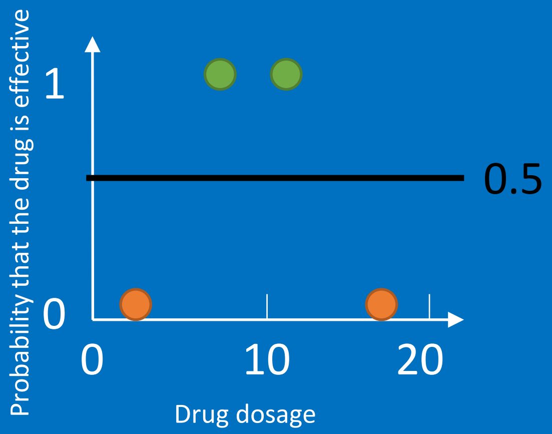

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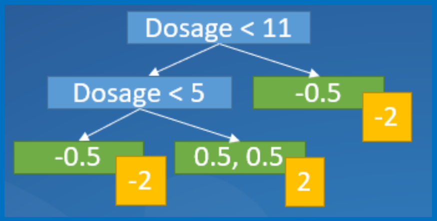

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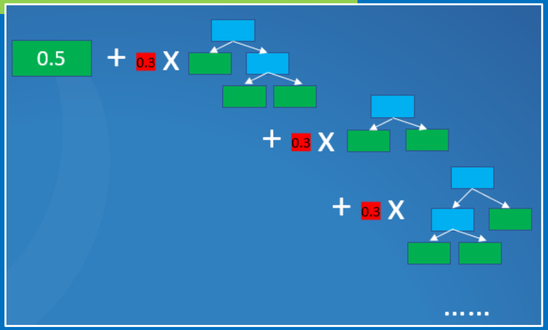
So the final xgboost tree for classification will be something like this:



0.5
+ 0.3 X
+ 0.3 X
+ 0.3 X
……