Statistical Methods in AI (CSE 471)
Ensemble Methods

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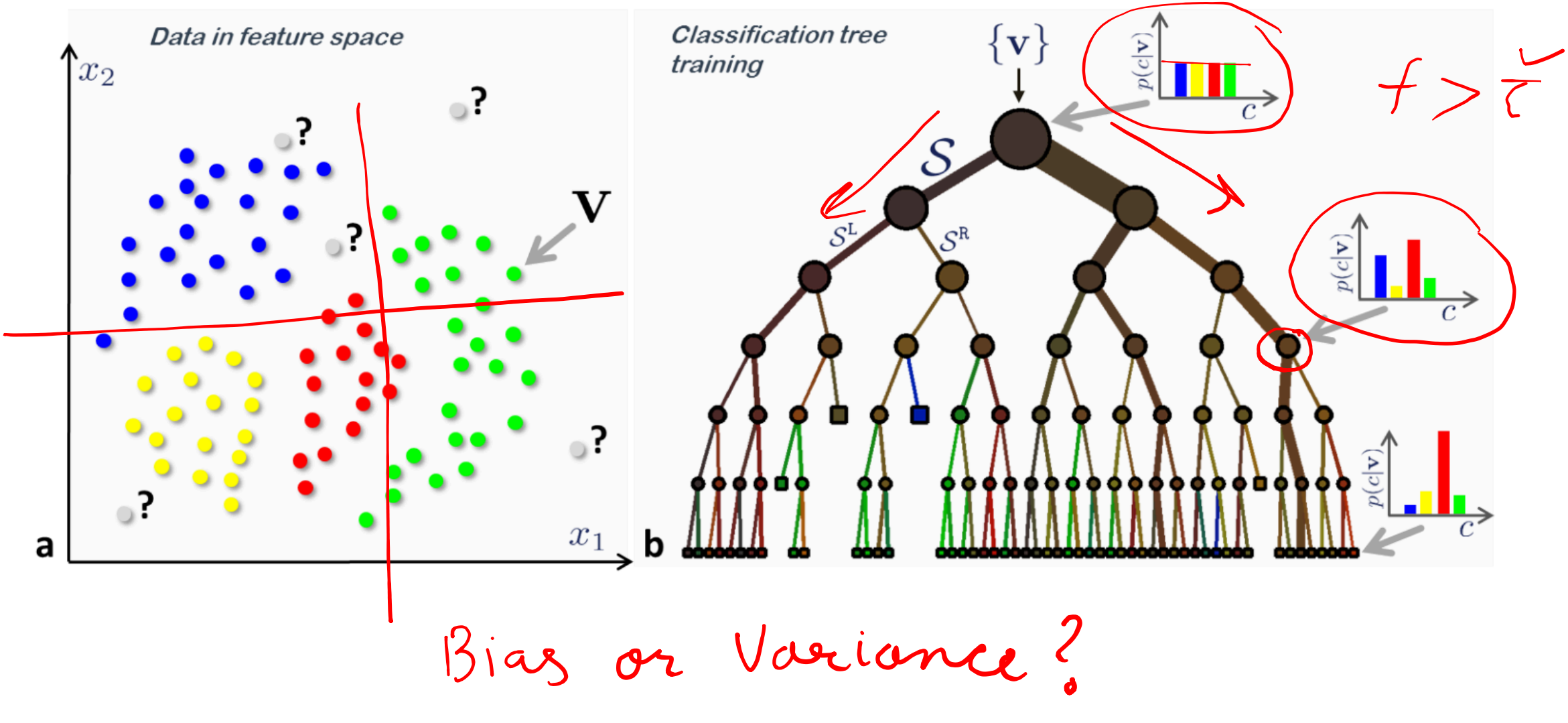
Many slides and figures from: Dr. Markus Kalisch ETH Zurich, Criminisi et al. Microsoft Research, StatQuest with Josh Starmer

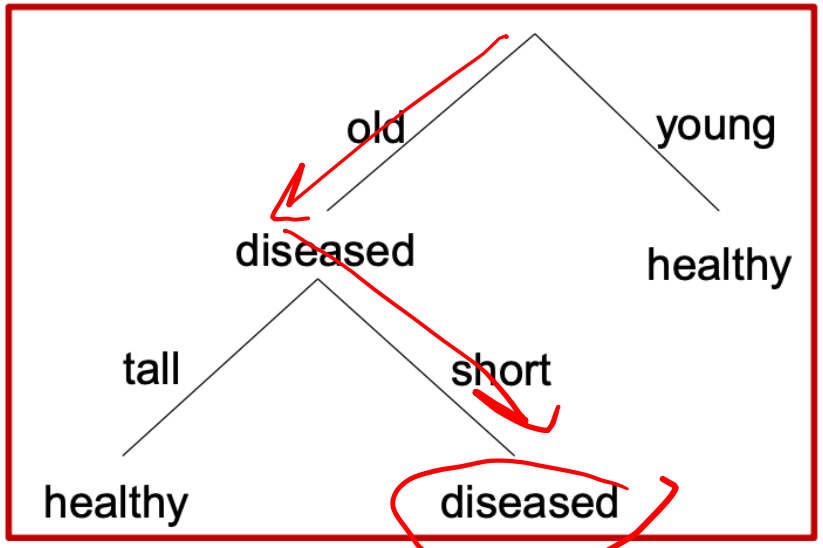
Single Tree



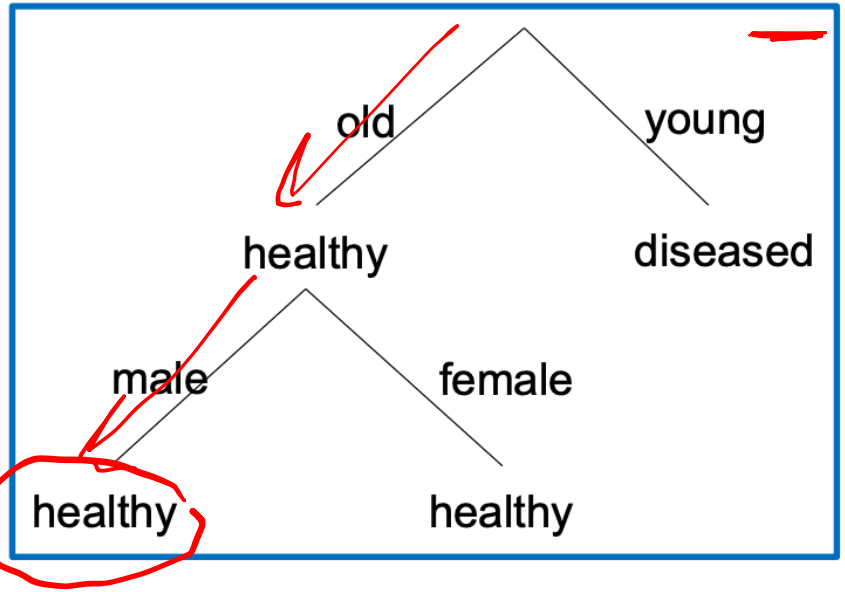
Bias or Variance?

Intuition of Random Forest

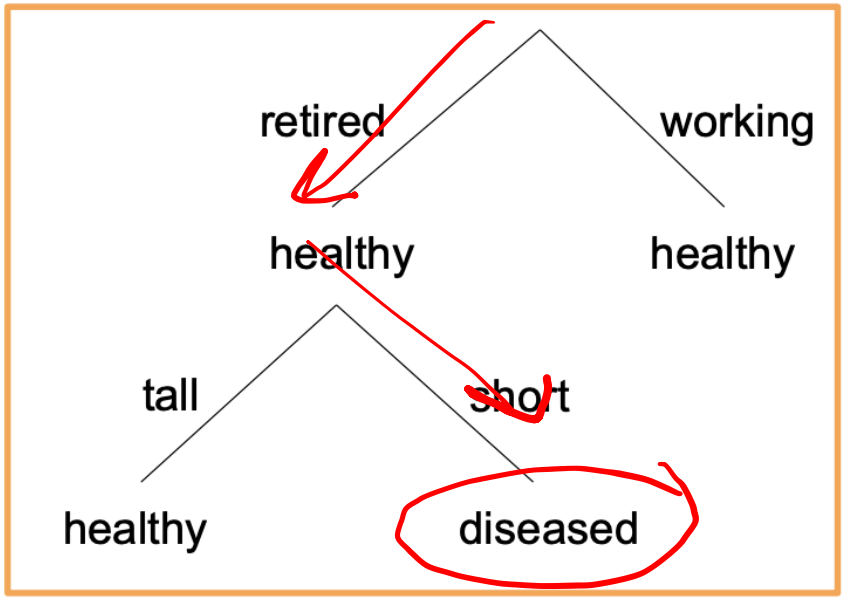
Tree 1



Tree 2



Tree 3



New sample:

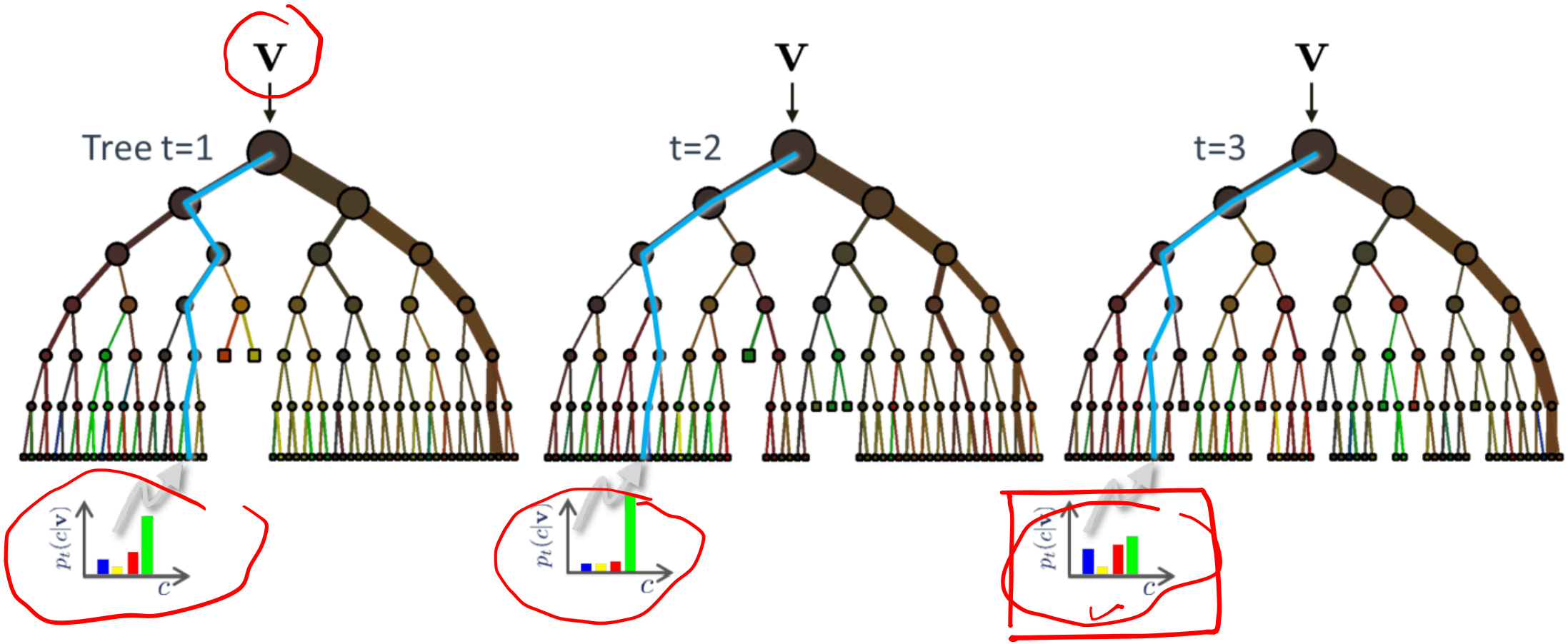
old, retired, male, short

Tree predictions:

diseased, healthy, diseased

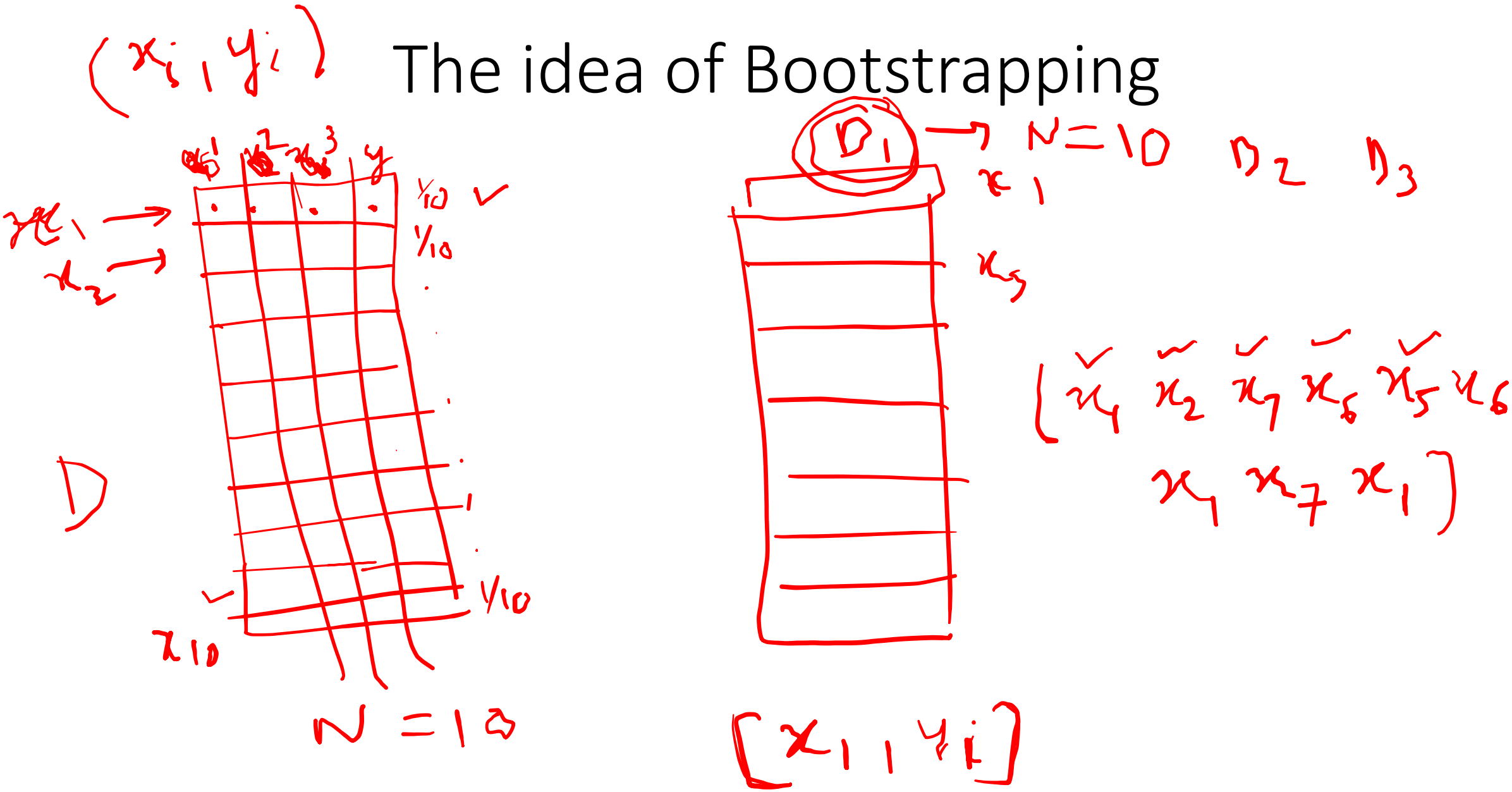
Majority rule:

diseased



$$p(c|\mathbf{v}) = \frac{1}{T}\sum_{t}^{T} p_t(c|\mathbf{v}).$$

The idea of Bootstrapping



Bootstrap aggregating = Bagging

- Generate many training sets by sampling with replacement from the given training data
- Given the original data of n points, we generate B number of training sets, each of size n' , by randomly sampling from the given dataset
- We learn model on each of the B training sets
- Final error could be average of errors of all the models

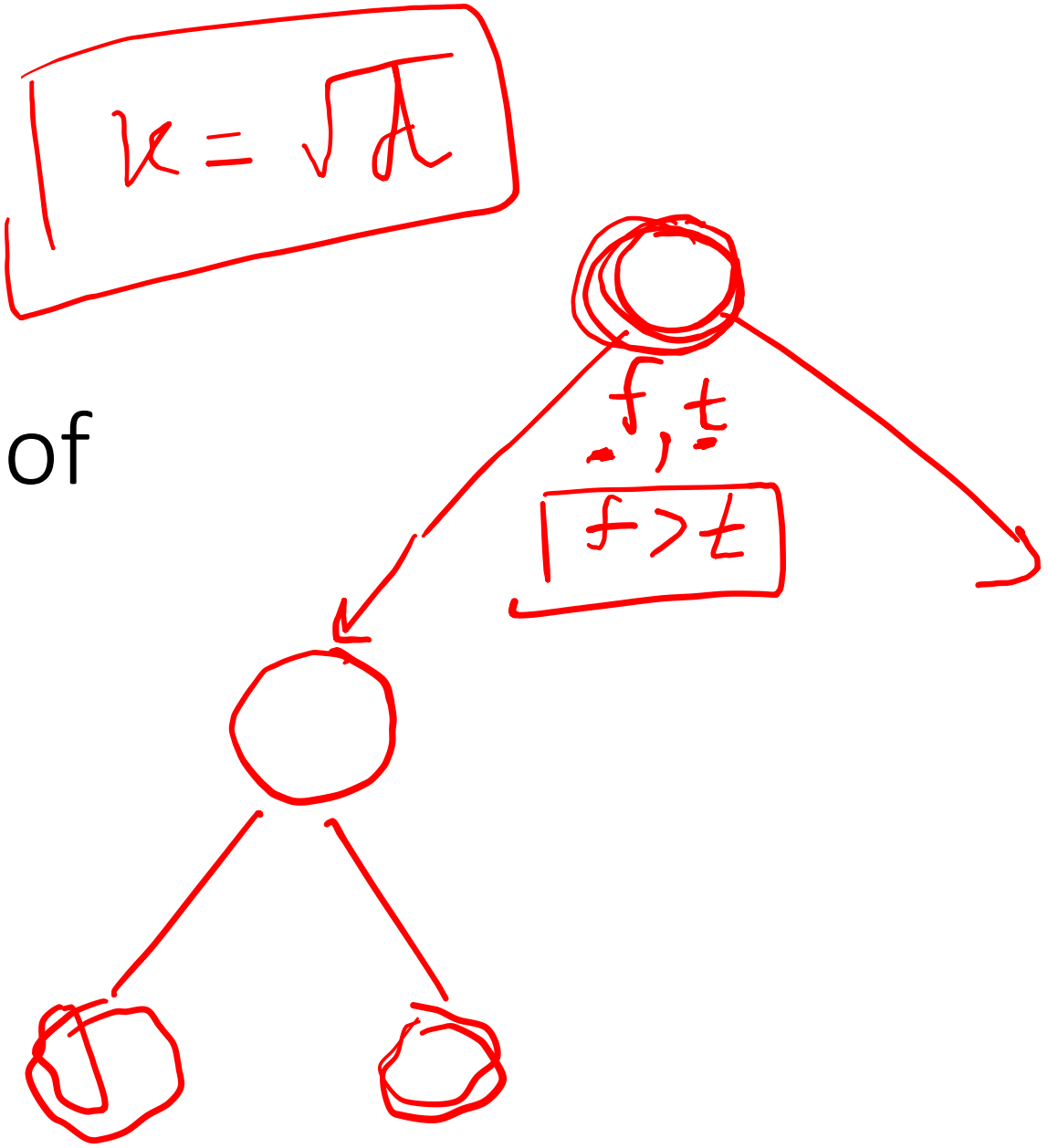
$h_1 \rightarrow B_1$

$h_2 \rightarrow D_2$

$$y_i = \frac{1}{M} \sum_{i=1}^{M} h_i(x_i)$$

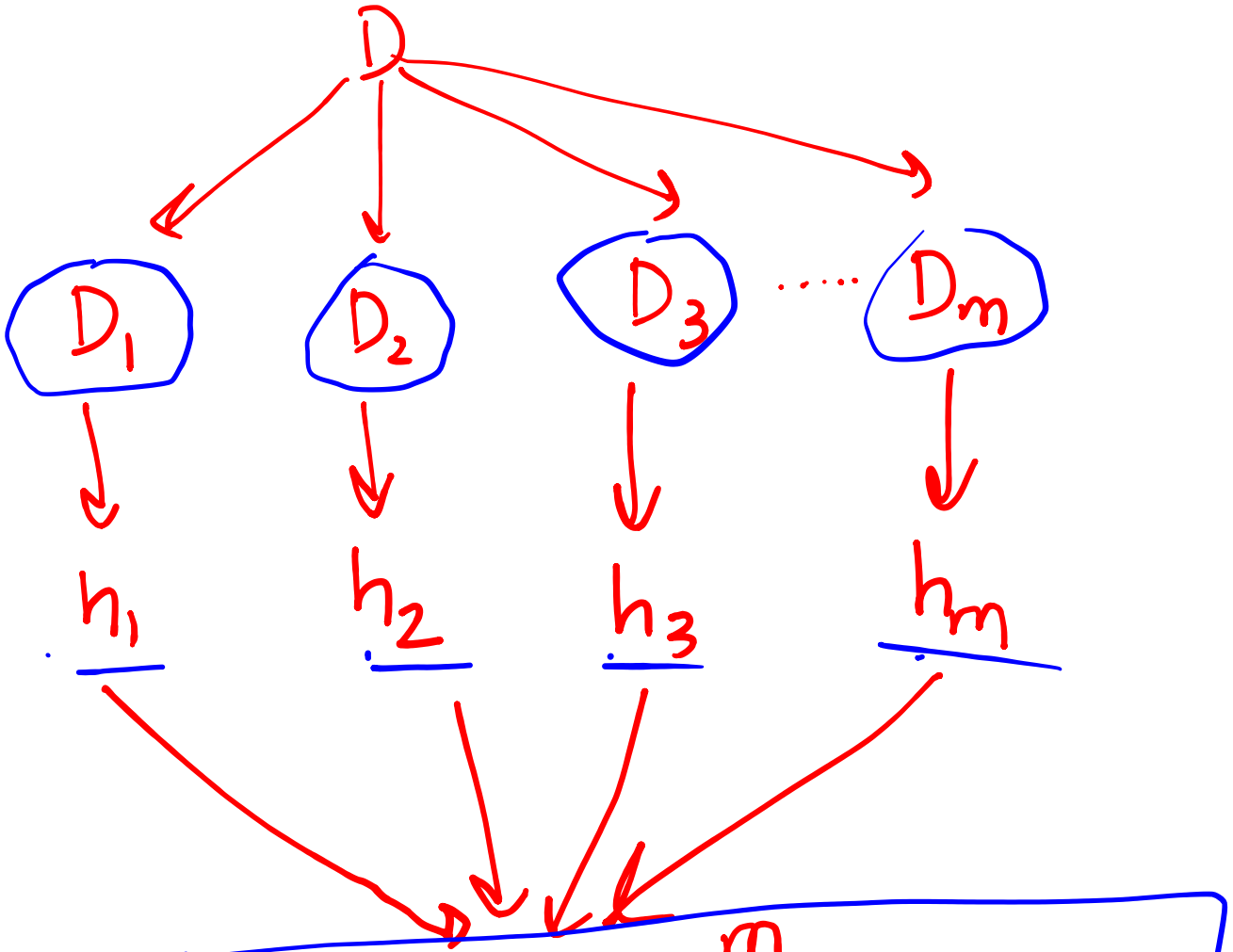
$\{-1, 1\}$

The idea of random variable selection

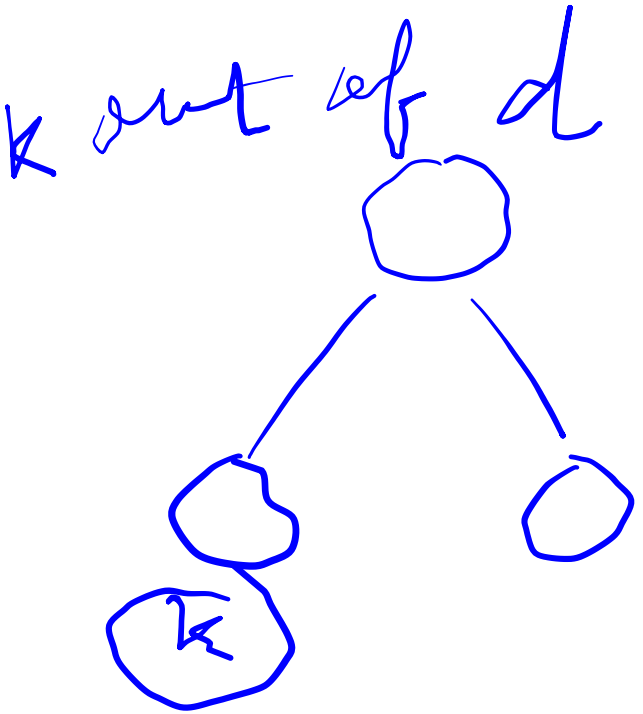


$k \ll d$

m | F x
- R | W
- B_a | A_g
S | T x



$$h(x) = \frac{1}{m} \sum_{j=1}^{m} h_j(x)$$



The Random Forest Algorithm

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

To make a prediction at a new point x:

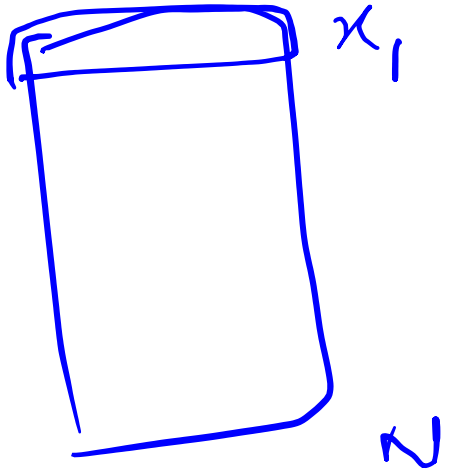
Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

Differences to standard tree

- Train each tree on bootstrap resample of data
  (Bootstrap resample of data set with N samples:
  Make new data set by drawing **with replacement** N samples; i.e., some samples will probably occur multiple times in new data set)
- For each split, consider only m randomly selected variables
- Don’t prune
- Fit B trees in such a way and use average or majority voting to aggregate results

The idea of Out of bag error

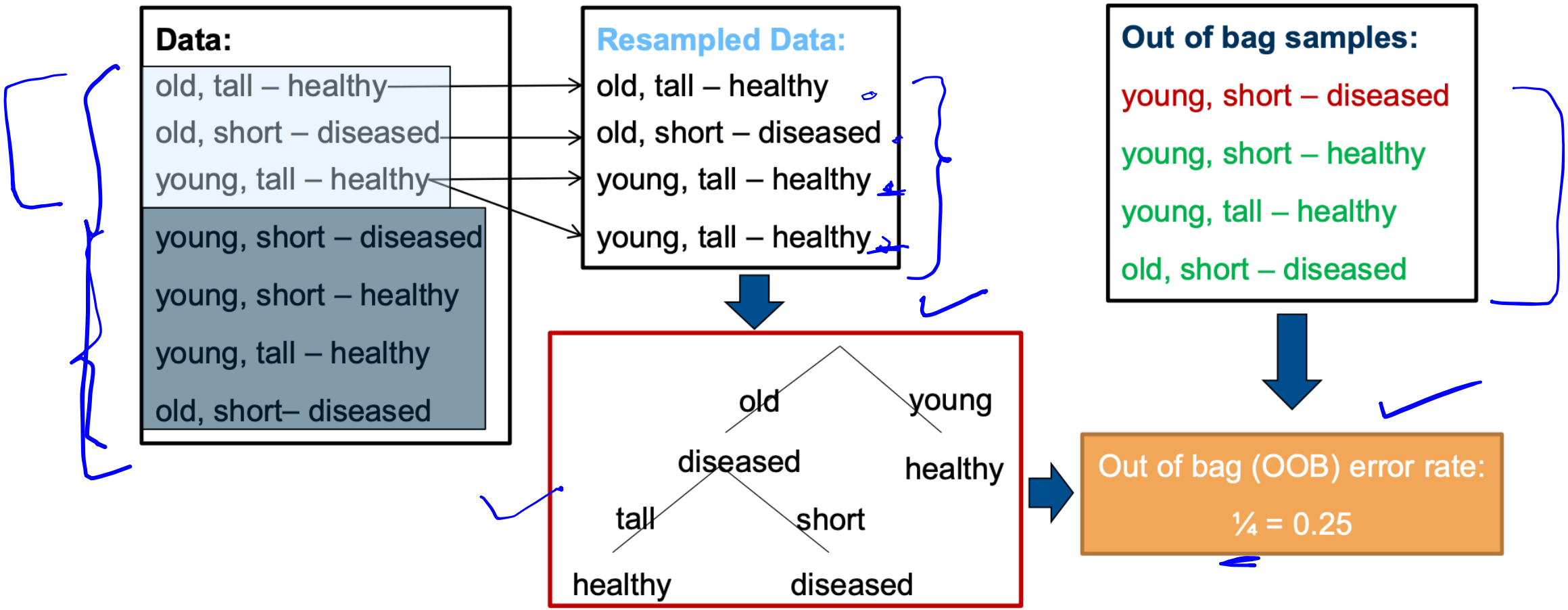


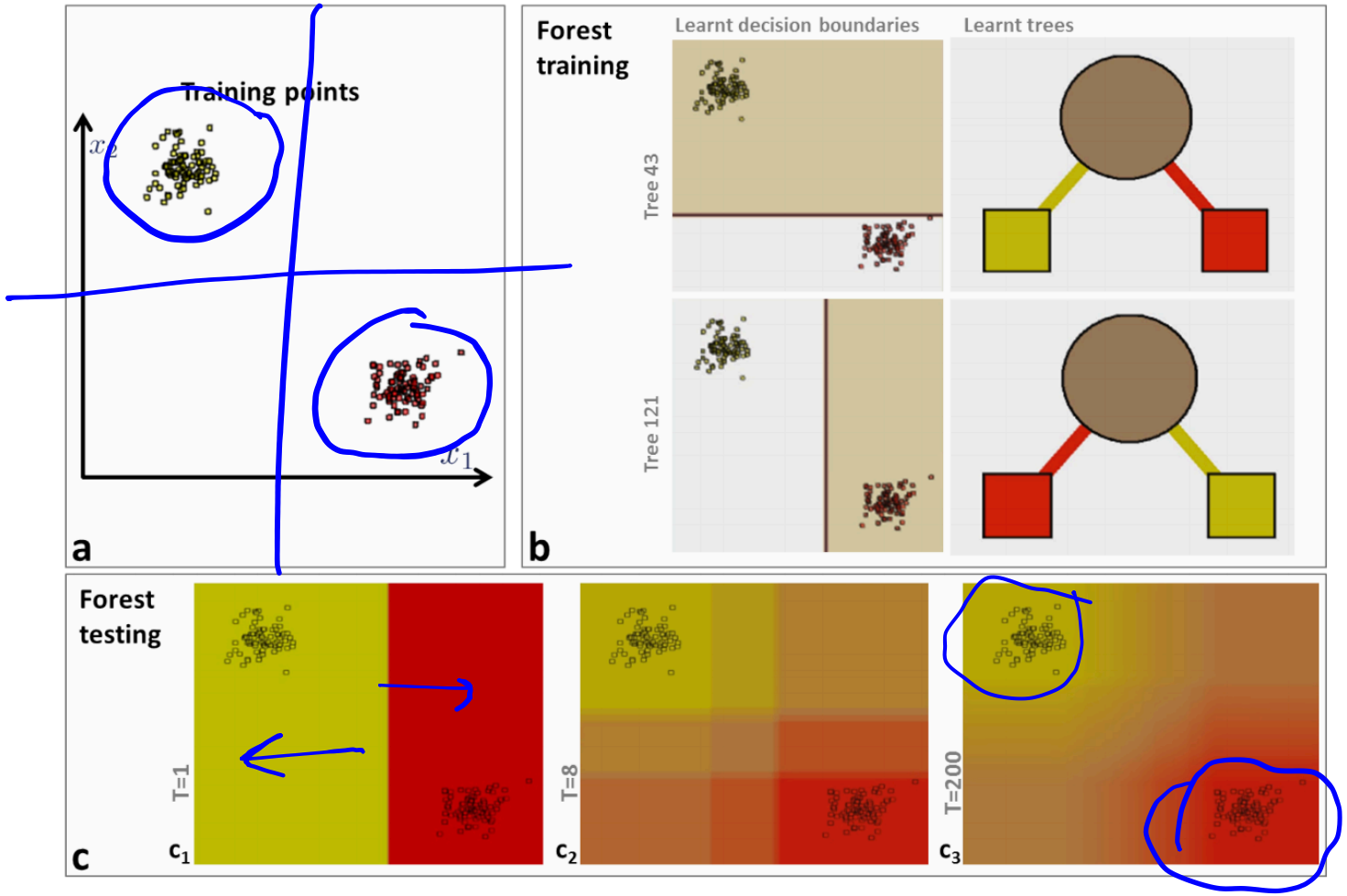
B_1 B_2 B_3 -- . . B_4 - - . . B_M

T_1 T_2 T_3 T_4 T_M

Estimating generalization error: Out-of bag (OOB) error

- Similar to leave-one-out cross-validation, but almost without any additional computational burden
- OOB error is a random number, since based on random resamples of the data





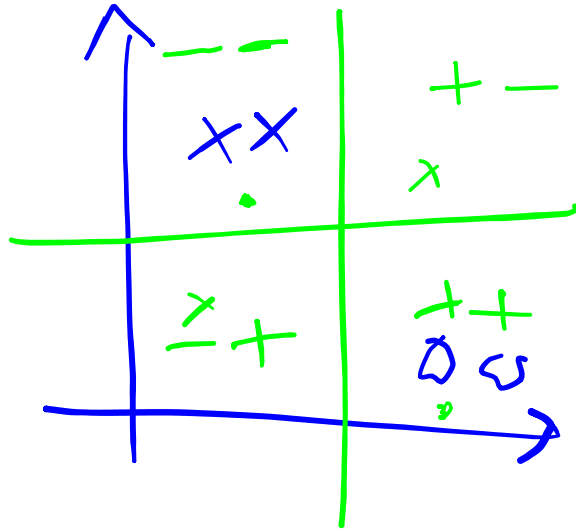
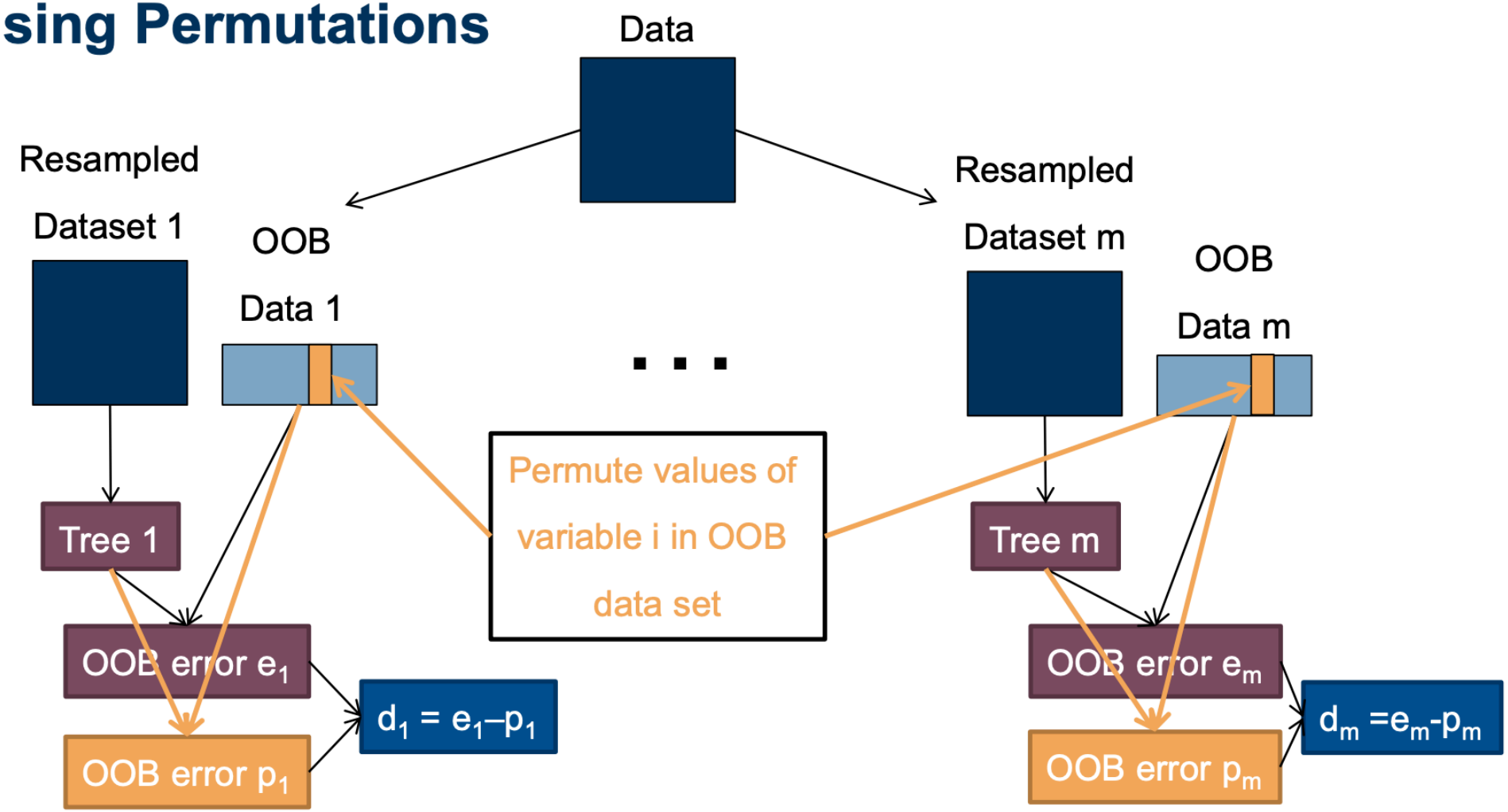


Fig. 3.3: **A first classification forest and the effect of forest size T.** **(a)** Training points belonging to two classes. **(b)** Different training trees produce different partitions and thus different leaf predictors. The colour of tree nodes and edges indicates the class probability of training points going through them. **(c)** In testing, increasing the forest size T produces smoother class posteriors. All experiments were run with $D = 2$ and axis-aligned weak learners. See text for details.

One feature selection

https://blog.datadive.net/selecting-good-features-part-iii-random-forests/

Variable Importance for variable i using Permutations



$$\bar{d} = \frac{1}{m}\sum_{i=1}^{m} d_i$$

$$s_d^2 = \frac{1}{m-1}\sum_{i=1}^{m}(d_i - \bar{d})^2$$

$$v_i = \frac{\bar{d}}{s_d}$$

Trees vs. Random Forest

+ Trees yield insight into decision rules
+ Rather fast
+ Easy to tune parameters

- Prediction of trees tend to have a high variance

+ RF as smaller prediction variance and therefore usually a better general performance
+ Easy to tune parameters

- Rather slow
- “Black Box”: Rather hard to get insights into decision rules

More reasons, why RF's are cool

- Works out of the box [: no feature scaling
  : categorical data]

- Only two main hyperparameters
  i.e. K and m

$K = \sqrt{d}$

$m \rightarrow$ as much as we can afford

Boosting

The idea of probabilistic sampling

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	1/8
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	1/8
No	Yes	156	No	1/8
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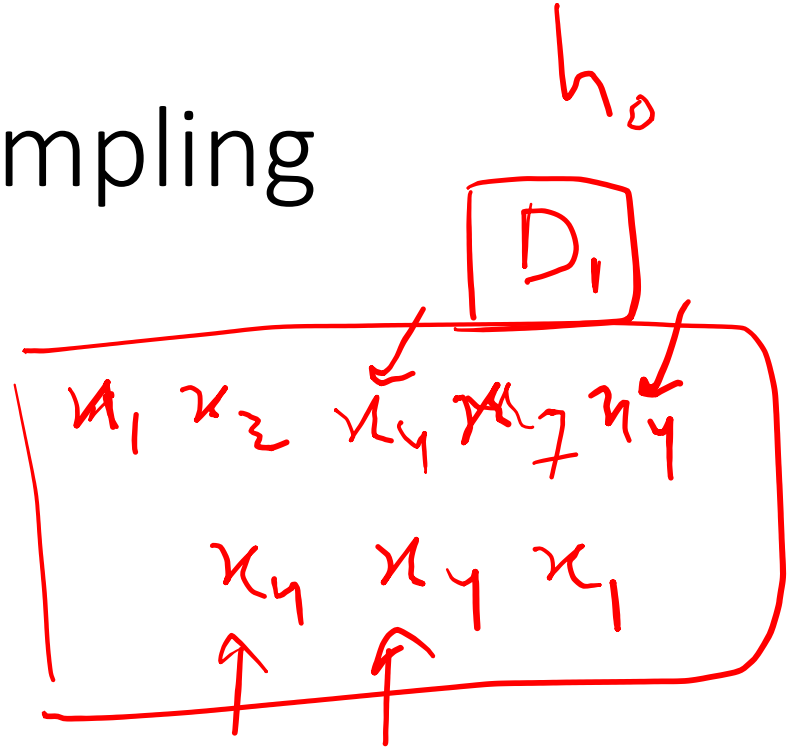
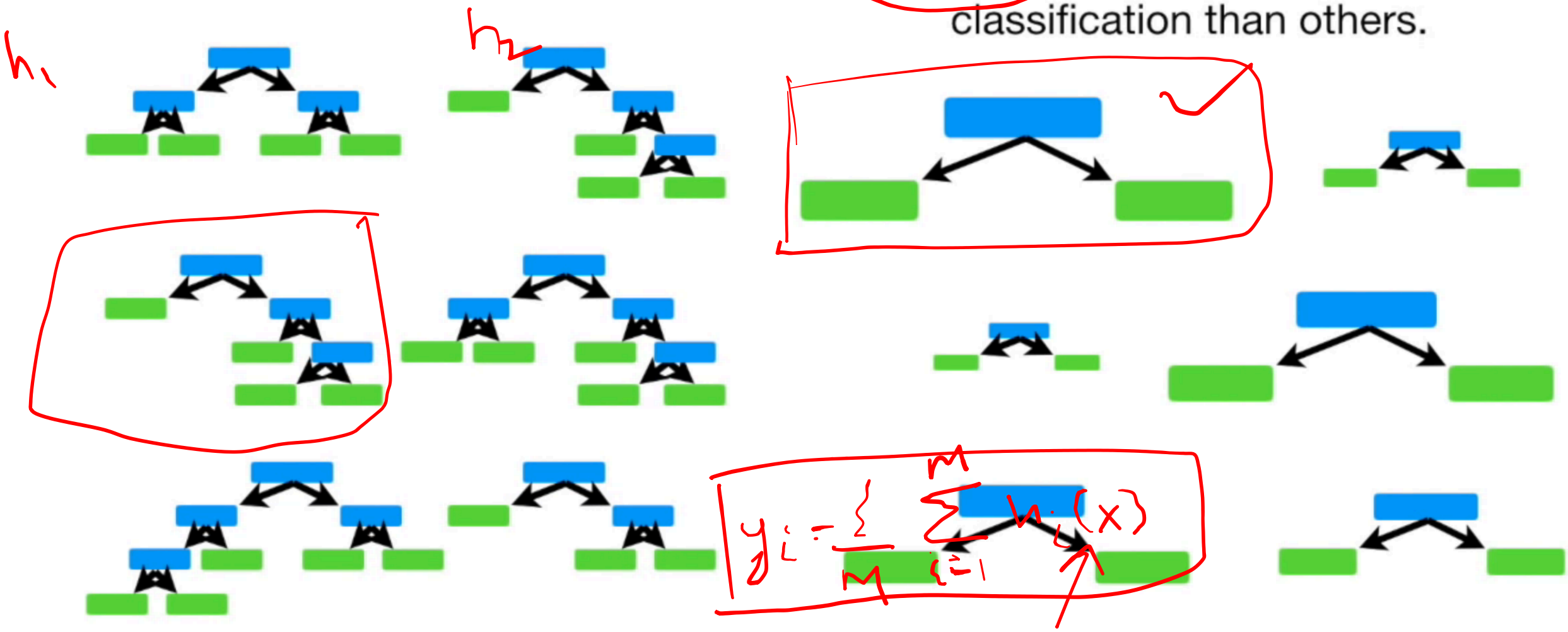
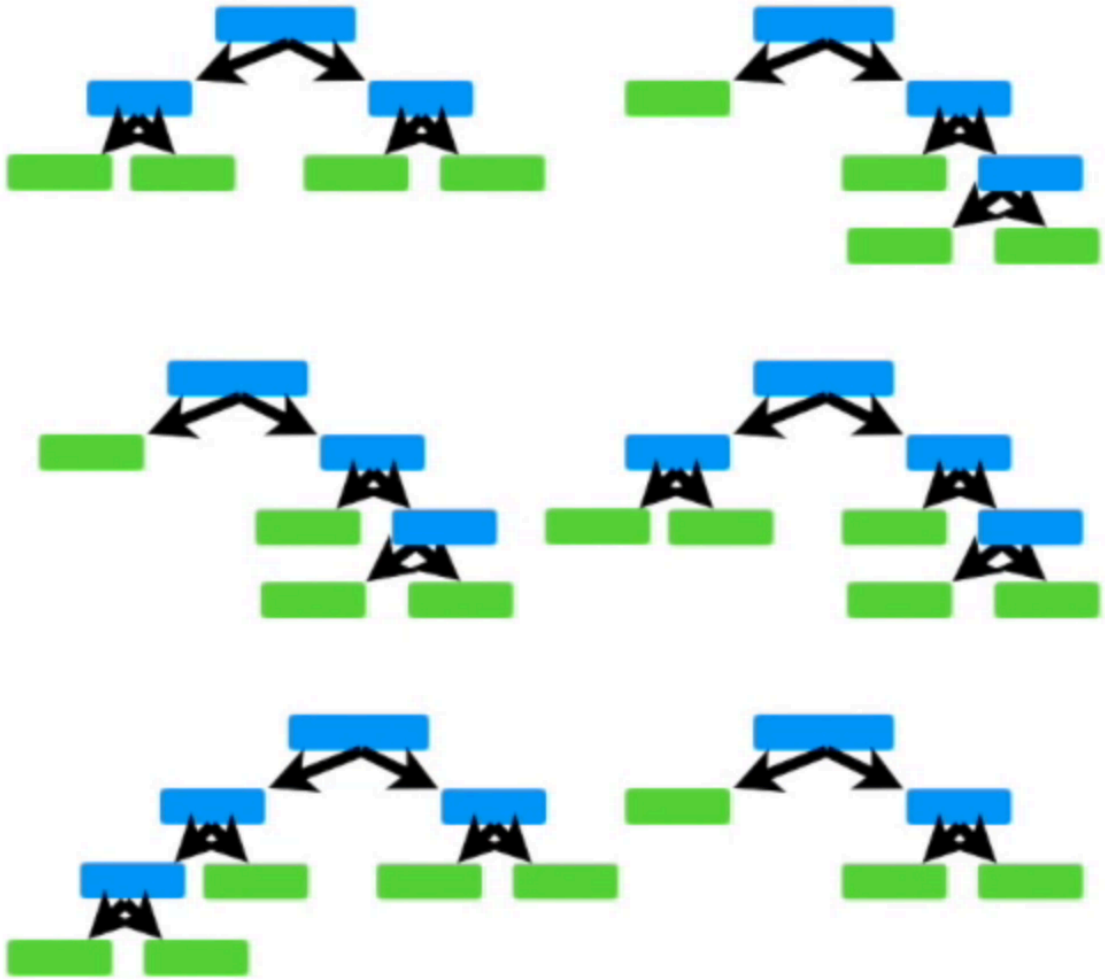


In a **Random Forest**, each tree has an equal vote on the final classification.

In contrast, in a **Forest of Stumps** made with **AdaBoost**, some stumps get more say in the final classification than others.

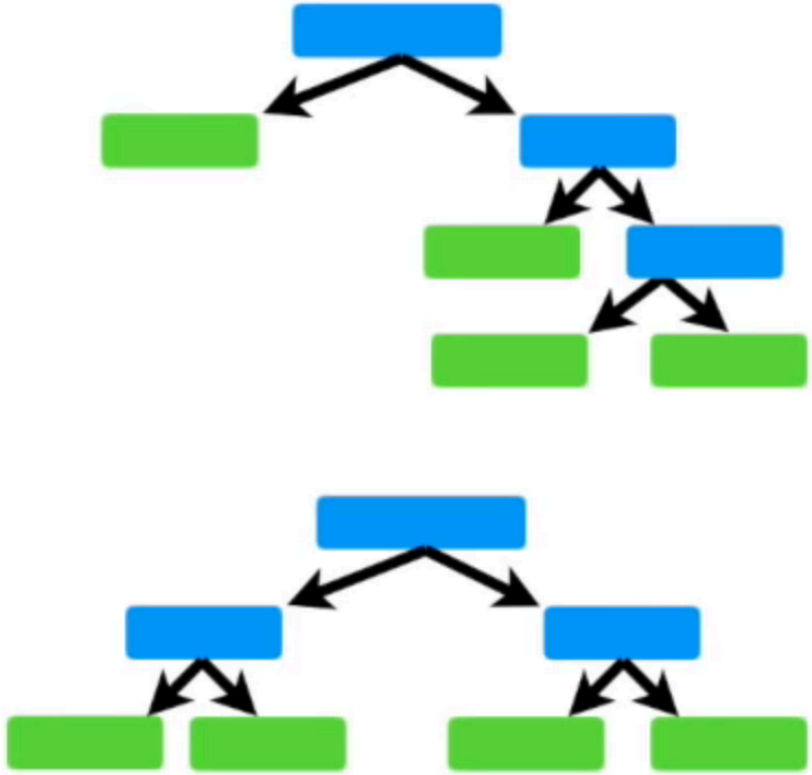


Lastly, in a **Random Forest**, each decision tree is made independently of the others.

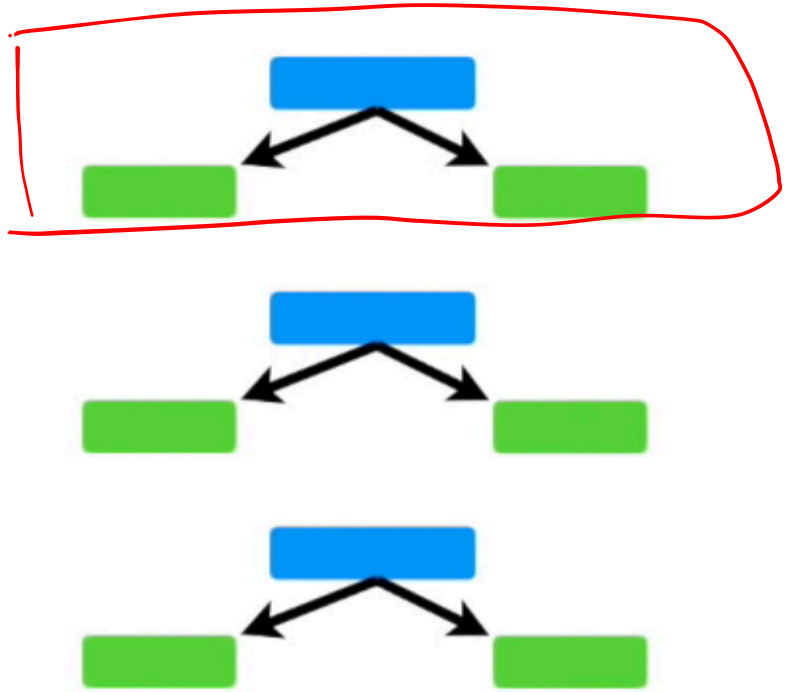


In contrast, in a **Forest of Stumps** made with **AdaBoost**, order is important.

In a **Random Forest**, each time you make a tree, you make a full sized tree.



In contrast, in a **Forest of Trees** made with **AdaBoost**, the trees are usually just a **node** and two **leaves**.



Adaboost

- In Adaboost we assign (non-negative) weights to points in the data set, which are then normalised so that they sum to one
- Iteratively learn new classifier
- In each iteration, we generate a training set by sampling from the data using the weights
- After learning the current classifier, we increase the (relative) weights of the data points which are misclassified by the current classifier
- The final classifier is the weighted majority voting by all classifiers

Adaboost

- Let $\{(X_1, y_1),\ldots,(X_n,y_n)\}$ be the data. We take y_i in $\{-1, +1\}$
- Let $w_i(k)$ denote the weight for the ith data point at kth iteration
- Let h_k be the classifier learnt at kth iteration, we take $h_k(X)$ in $\{-1,+1\}$
- We assume error rate of each classifier on its training data is less than 0.5

Adaboost algorithm

1. Initialize: $w_i(1) = 1/n$
2. For m =1:M do
   A. Generate a training set by sampling with $\{w_i(m)\}$
   B. Learn classifier h_m using the training set
   C. Let

$$\xi_m = \sum_{i=1}^{n} w_i(m) I_{[y_i \neq h_m(X_i)]}$$

We assume it be less than 0.5

   D. Set

$$\alpha_m = \ln\left(\frac{1-\xi_m}{\xi_m}\right) \qquad \alpha_m > 0$$

   E. Update Weights

$$w_i'(m+1) = w_i(m) exp(\alpha_m I_{[y_i \neq h_m(X_i)]})$$

$$= w_i(m) \cdot exp(-\alpha_m \cdot y_i \cdot h(x_i))$$

$$w_i(m+1) = \frac{w'(m+1)}{\sum_i w'(m+1)}$$

Adaboost algorithm

3. Final classifier

$$h(X) = sgn(\sum_{m=1}^{M} \alpha_m h_m(X))$$

Lets take an example

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
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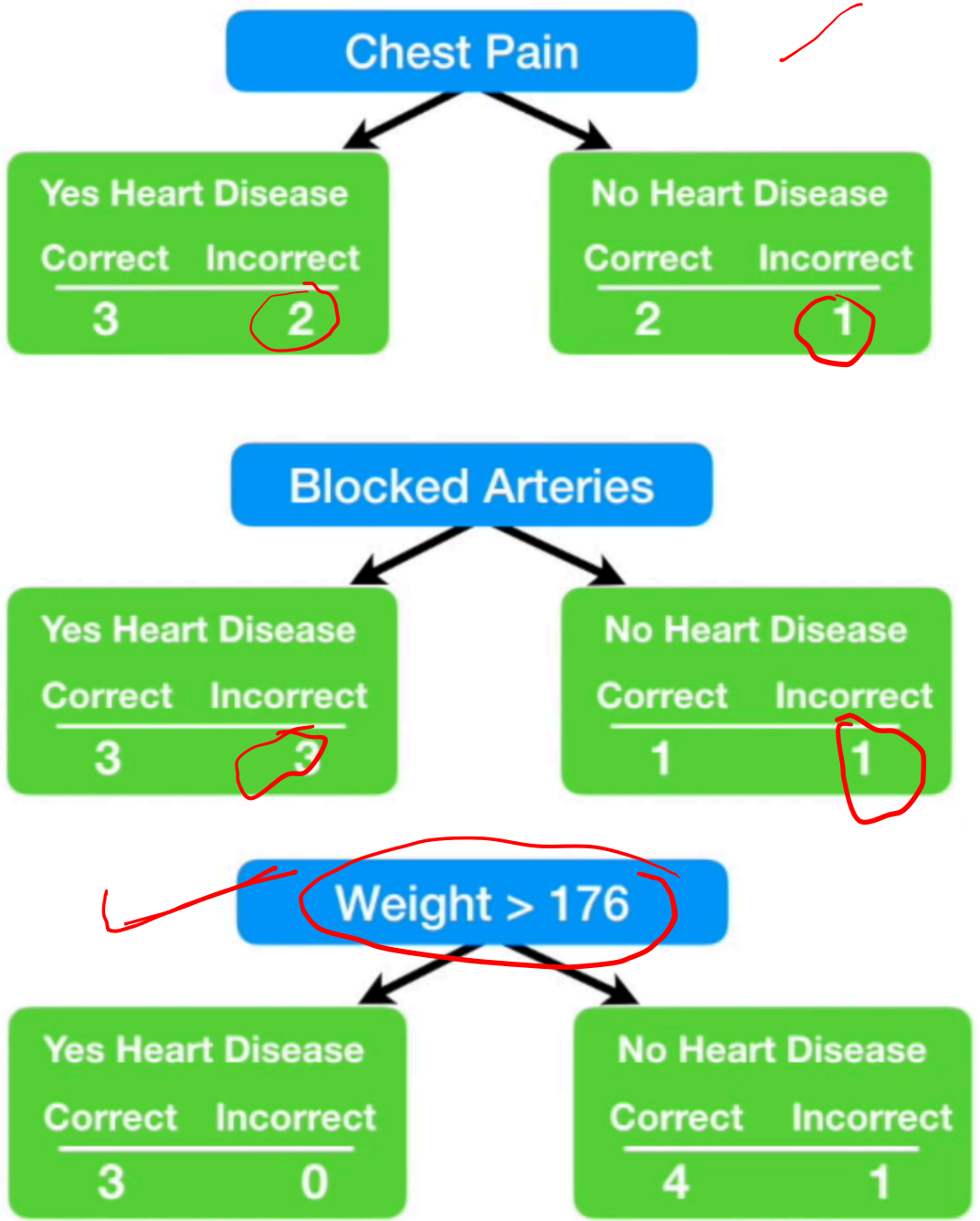

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Thus, in this case, the **Total Error** is **1/8**.

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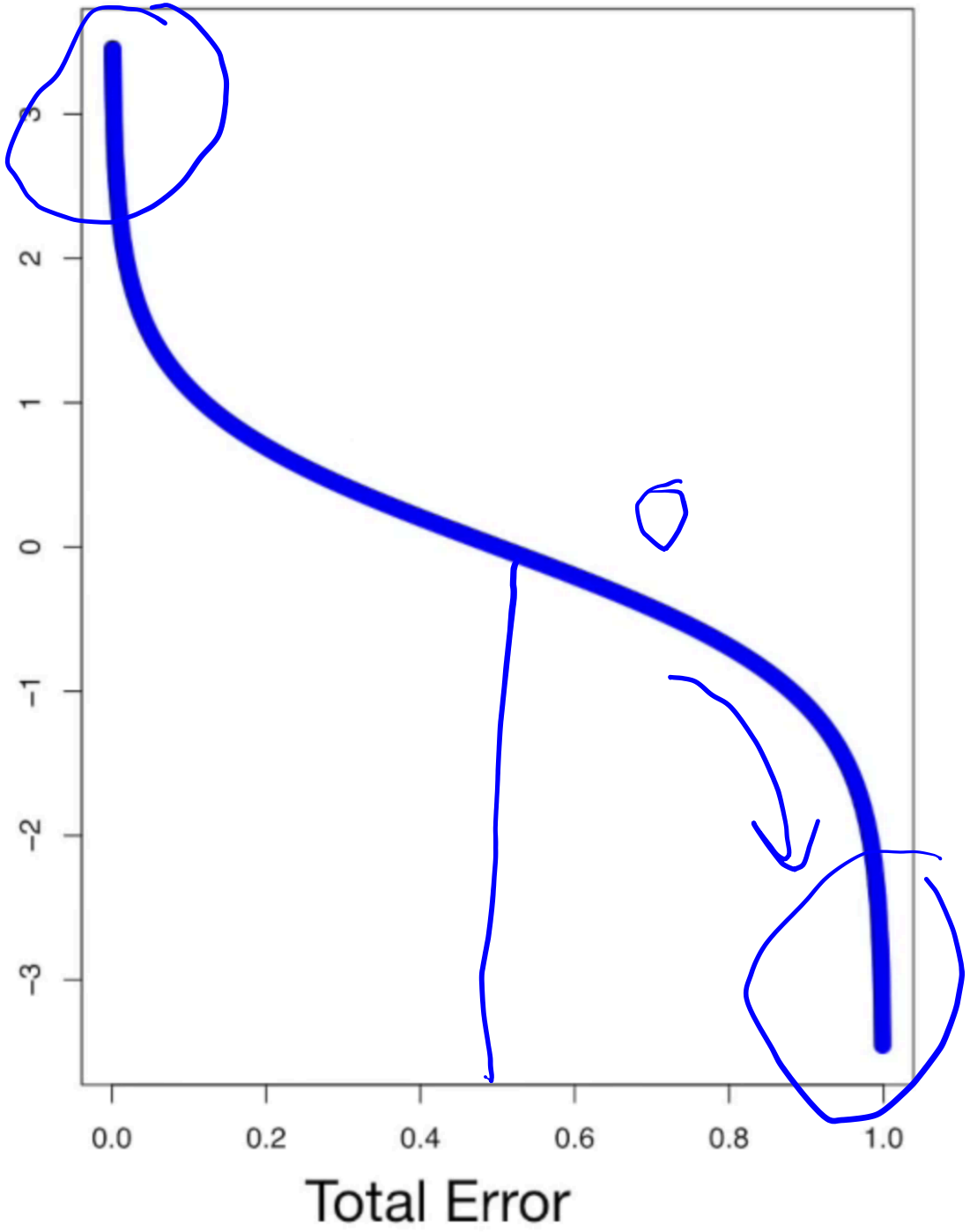
Thus, in this case, the **Total Error** is **1/8**.

$$\text{Amount of Say} = \frac{1}{2}\log_2\left(\frac{1 - \text{Total Error}}{\text{Total Error}}\right)$$



$$\text{Amount of Say} = \frac{1}{2}\log\left(\frac{1 - \text{Total Error}}{\text{Total Error}}\right)$$

$$\text{Amount of Say} = \frac{1}{2}\log(7) = 0.97$$

$\alpha_m = 0$

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$$\text{New Sample Weight} = \text{sample weight} \times e^{\text{amount of say}}$$

$$= \frac{1}{8} e^{0.97} = \frac{1}{8} \times 2.64 = 0.33$$

$$\text{New Sample Weight} = \text{sample weight} \times e^{-\text{amount of say}}$$

$$= \frac{1}{8} e^{-0.97} = \frac{1}{8} \times 0.38 = 0.05$$

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight	New Weight	Norm. Weight
Yes	Yes	205	Yes	1/8	0.05	0.07
No	Yes	180	Yes	1/8	0.05	0.07
Yes	No	210	Yes	1/8	0.05	0.07
Yes	Yes	167	Yes	1/8	0.33	0.49
No	Yes	156	No	1/8	0.05	0.07
No	Yes	125	No	1/8	0.05	0.07
Yes	No	168	No	1/8	0.05	0.07
Yes	Yes	172	No	1/8	0.05	0.07

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Yes	Yes	172	No	0.07

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Yes	Yes	167	Yes
Yes	Yes	167	Yes
Yes	Yes	172	No
Yes	Yes	205	Yes
Yes	Yes	167	Yes

Ultimately, the patient is classified as **Has Heart Disease** because this is the larger sum.

Has Heart Disease

Total = 2.7

Total = 1.23

Does Not Have Heart Disease

Amount of Say

0.97

0.32

0.78

0.63

Amount of Say

0.41

0.82