Random Forests

The Bootstrap Sample and Bagging

Simple ideas to improve any model via ensemble

Bootstrap Samples

- Random samples of your data *with replacement* that are the same size as original data.
- Some observations will not be sampled. These are called *out-of-bag observations*

<u>Example:</u> Suppose you have 10 observations, labeled 1-10

Bootstrap Sample Number	Training Observations	Out-of-Bag Observations
1	{1,3,2,8,3,6,4,2,8,7}	{5,9,10}
2	{9,1,10,9,7,6,5,9,2,6}	{3,4,8}
3	{8,10,5,3,8,9,2,3,7,6}	{1,4}

(Efron 1983) (Efron and Tibshirani 1986)

Bootstrap Samples

- Can be proven that a bootstrap sample will contain approximately 63% of the observations.
- The sample size is the same as the original data as some observations are repeated.
- Some observations left out of the sample (~37% out-of-bag)

- Uses:
  - Alternative to traditional validation/cross-validation
  - **Create Ensemble Models using different training sets (Bagging)**

Bagging

(Bootstrap Aggregating)

- Let k be the number of bootstrap samples
- For each bootstrap sample, create a classifier using that sample as training data
  - Results in k different models
- Ensemble those classifiers
  - A test instance is assigned to the class that received the highest number of votes.

Bagging Example

input variable

target

x	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
y	1	1	1	-1	-1	-1	-1	1	1	1

- 10 observations in original dataset
- Suppose we build a decision tree with only 1 split.
- The best accuracy we can get is 70%
  - Split at x=0.35
  - Split at x=0.75
- A tree with one split called a **decision stump**

Bagging Example

Let’s see how bagging might improve this model:

1. Take 10 Bootstrap samples from this dataset.
2. Build a decision stump for each sample.
3. Aggregate these rules into a voting ensemble.
4. Test the performance of the voting ensemble on the whole dataset.

Bagging Example
Classifier 1

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Best decision stump splits at x=0.35

First bootstrap sample:

Some observations chosen multiple times.

Some not chosen.

Bagging Example
Classifiers 1-5

Bagging Round 1:

x	0.1	0.2	0.2	0.3	0.4	0.4	0.5	0.6	0.9	0.9
y	1	1	1	1	-1	-1	-1	-1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Bagging Round 2:

x	0.1	0.2	0.3	0.4	0.5	0.8	0.9	1	1	1
y	1	1	1	-1	-1	1	1	1	1	1

x <= 0.65 ==> y = 1
x > 0.65 ==> y = 1

Bagging Round 3:

x	0.1	0.2	0.3	0.4	0.4	0.5	0.7	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Bagging Round 4:

x	0.1	0.1	0.2	0.4	0.4	0.5	0.5	0.7	0.8	0.9
y	1	1	1	-1	-1	-1	-1	-1	1	1

x <= 0.3 ==> y = 1
x > 0.3 ==> y = -1

Bagging Round 5:

x	0.1	0.1	0.2	0.5	0.6	0.6	0.6	1	1	1
y	1	1	1	-1	-1	-1	-1	1	1	1

x <= 0.35 ==> y = 1
x > 0.35 ==> y = -1

Bagging Example

Classifiers 6-10

Bagging Round 6:

x	0.2	0.4	0.5	0.6	0.7	0.7	0.7	0.8	0.9	1
y	1	-1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 7:

x	0.1	0.4	0.4	0.6	0.7	0.8	0.9	0.9	0.9	1
y	1	-1	-1	-1	-1	1	1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 8:

x	0.1	0.2	0.5	0.5	0.5	0.7	0.7	0.8	0.9	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 9:

x	0.1	0.3	0.4	0.4	0.6	0.7	0.7	0.8	1	1
y	1	1	-1	-1	-1	-1	-1	1	1	1

x <= 0.75 ==> y = -1
x > 0.75 ==> y = 1

Bagging Round 10:

x	0.1	0.1	0.1	0.1	0.3	0.3	0.8	0.8	0.9	0.9
y	1	1	1	1	1	1	1	1	1	1

x <= 0.05 ==> y = -1
x > 0.05 ==> y = 1

Bagging Example

Predictions from each Classifier

Round	x=0.1	x=0.2	x=0.3	x=0.4	x=0.5	x=0.6	x=0.7	x=0.8	x=0.9	x=1.0
1	1	1	1	-1	-1	-1	-1	-1	-1	-1
2	1	1	1	1	1	1	1	1	1	1
3	1	1	1	-1	-1	-1	-1	-1	-1	-1
4	1	1	1	-1	-1	-1	-1	-1	-1	-1
5	1	1	1	-1	-1	-1	-1	-1	-1	-1
6	-1	-1	-1	-1	-1	-1	-1	1	1	1
7	-1	-1	-1	-1	-1	-1	-1	1	1	1
8	-1	-1	-1	-1	-1	-1	-1	1	1	1
9	-1	-1	-1	-1	-1	-1	-1	1	1	1
10	1	1	1	1	1	1	1	1	1	1
Sum	2	2	2	-6	-6	-6	-6	2	2	2
Sign	1	1	1	-1	-1	-1	-1	1	1	1
True Class	1	1	1	-1	-1	-1	-1	1	1	1

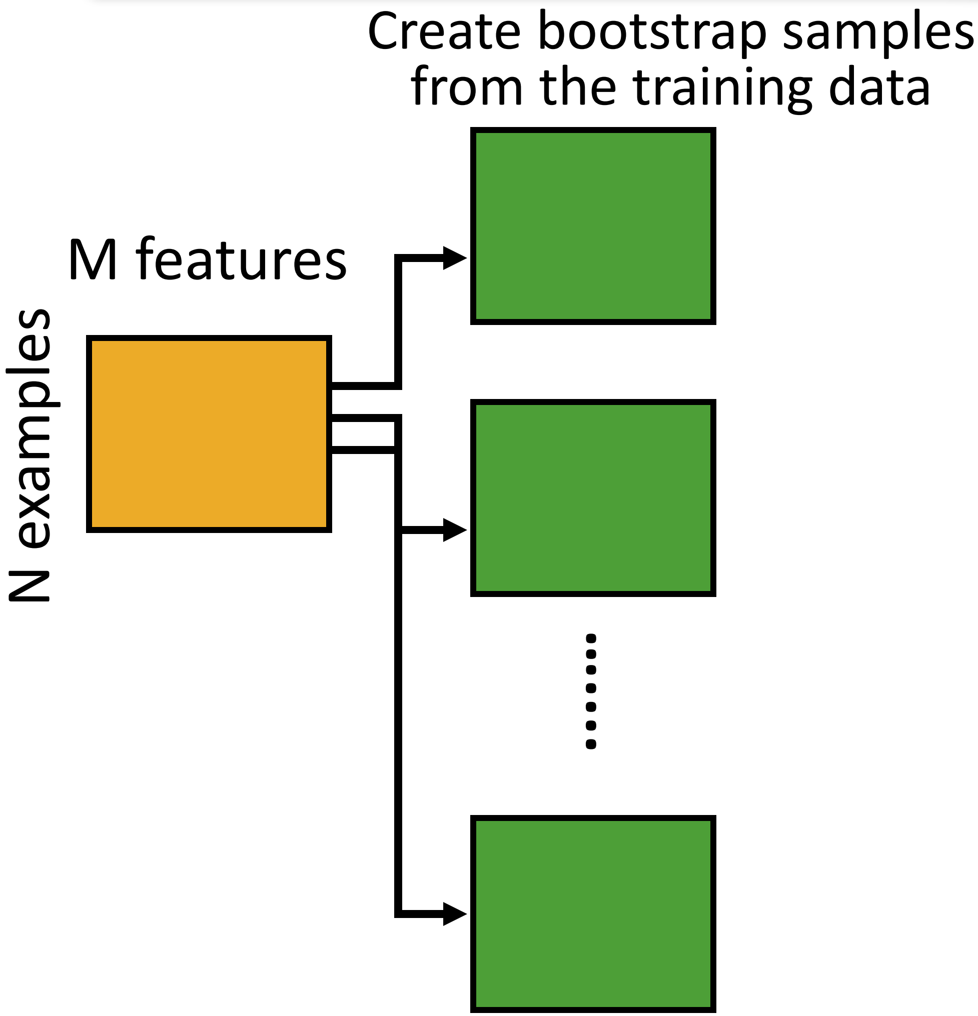
Ensemble Classifier has 100% Accuracy

Bagging

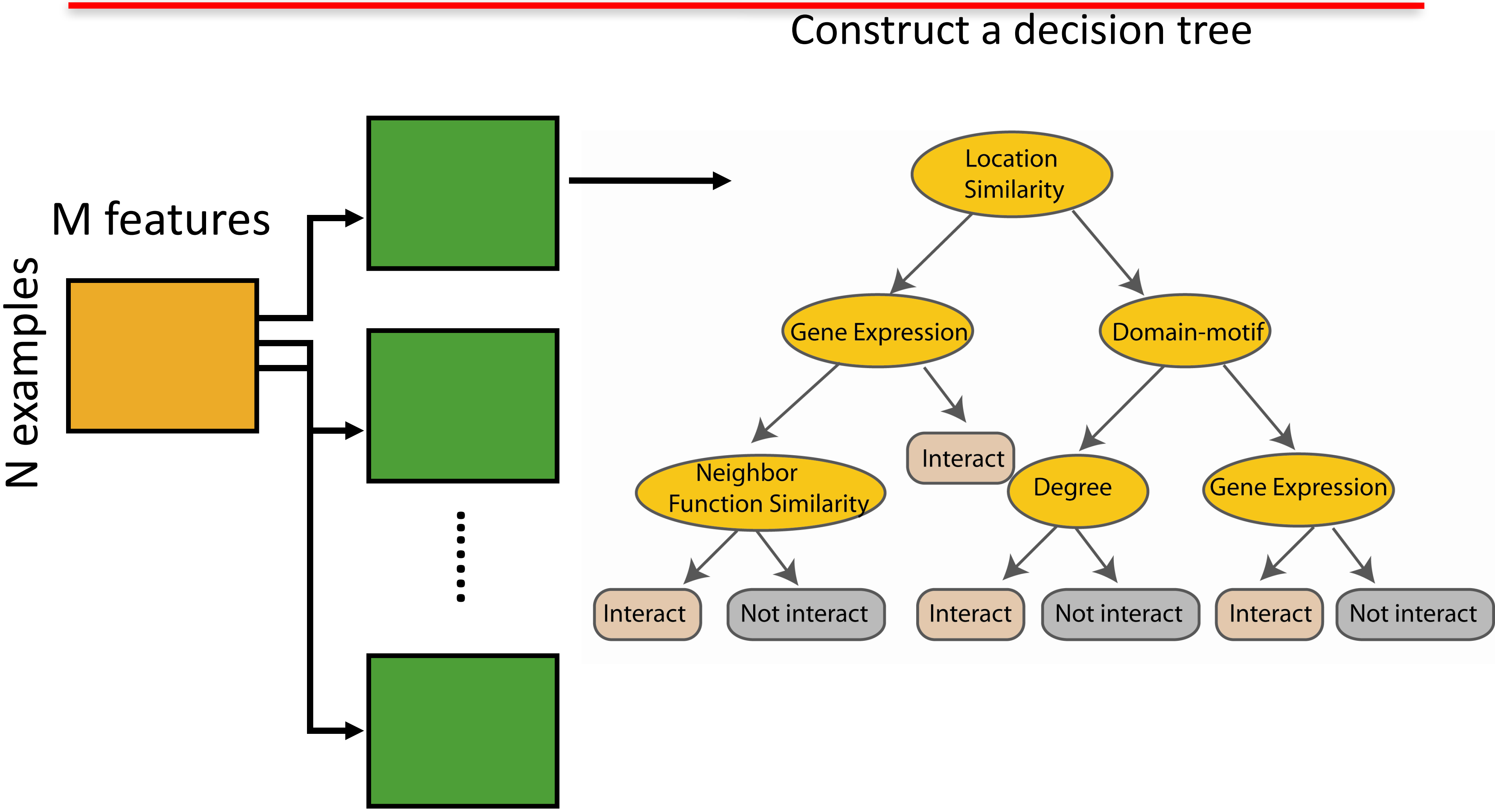
- Bagging or *bootstrap aggregation* a technique for reducing the variance of an estimated prediction function.

- For classification, a *committee* of trees each cast a vote for the predicted class.

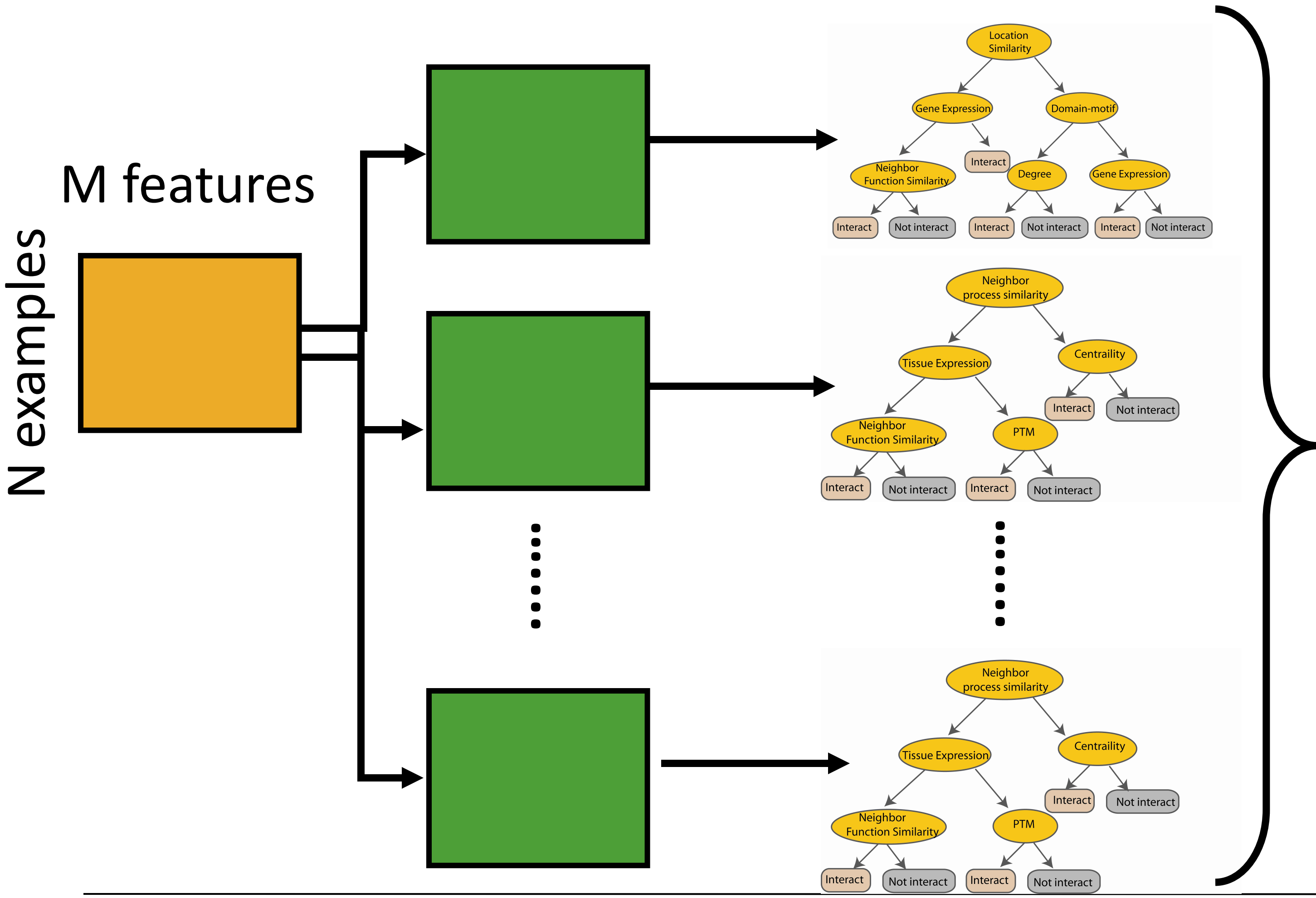
Bagging


Create bootstrap samples
from the training data
M features
N examples

Bagging


M features
N examples
Construct a decision tree
Location Similarity
Gene Expression
Domain-motif
Neighbor Function Similarity
Interact
Degree
Gene Expression
Interact
Not interact
Interact
Not interact
Interact
Not interact

Bagging



Take the majority vote

Bagging Summary

- Improves generalization error on models with high variance
- Bagging helps reduce errors associated with random fluctuations in training data (high variance)
- If base classifier is stable (not suffering from high variance), bagging can actually make it worse

- Bagging does not focus on any particular observations in the training data (unlike boosting)

Random Forests

Tin Kam Ho (1995, 1998)

Leo Breiman (2001)

Random Forests

- Random Forests are ensembles of decision trees similar to the one we just saw

- Ensembles of decision trees work best when their predictions are not correlated – they each find different patterns in the data

- <u>Problem</u>: Bagging tends to create correlated trees
- <u>Two Solutions</u>: (a) Randomly subset features considered for each split. (b) Use unpruned decision trees in the ensemble.

Random Forests

- A collection of unpruned decision or regression trees.
- Each tree is build on a bootstrap sample of the data ***and*** a subset of features are considered at each split.
  - The number of features considered for each split is a parameter called $mtry$.
  - Brieman (2001) suggests $mtry = \sqrt{p}$ where p is the number of features
  - I'd suggest setting $mtry$ equal to 5-10 values evenly spaced between 2 and p and choosing the parameter by validation
  - Overall, the model is relatively insensitive to values for $mtry$.
- The results from the trees are ensembled into one voting classifier.

Random Forests

Based on slides by Oznur Tastan et.al

Basic idea of Random Forests

Grow a forest of many trees.

Each tree is a little different (slightly different data, different choices of predictors).

Combine the trees to get predictions for new data.

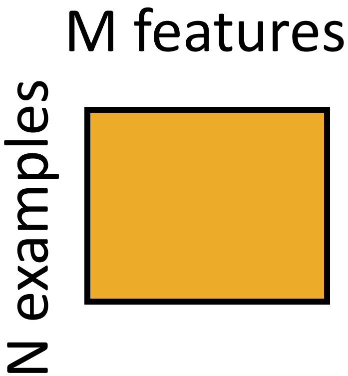
Idea: most of the trees are good for most of the data and make mistakes in different places.

Random forest classifier

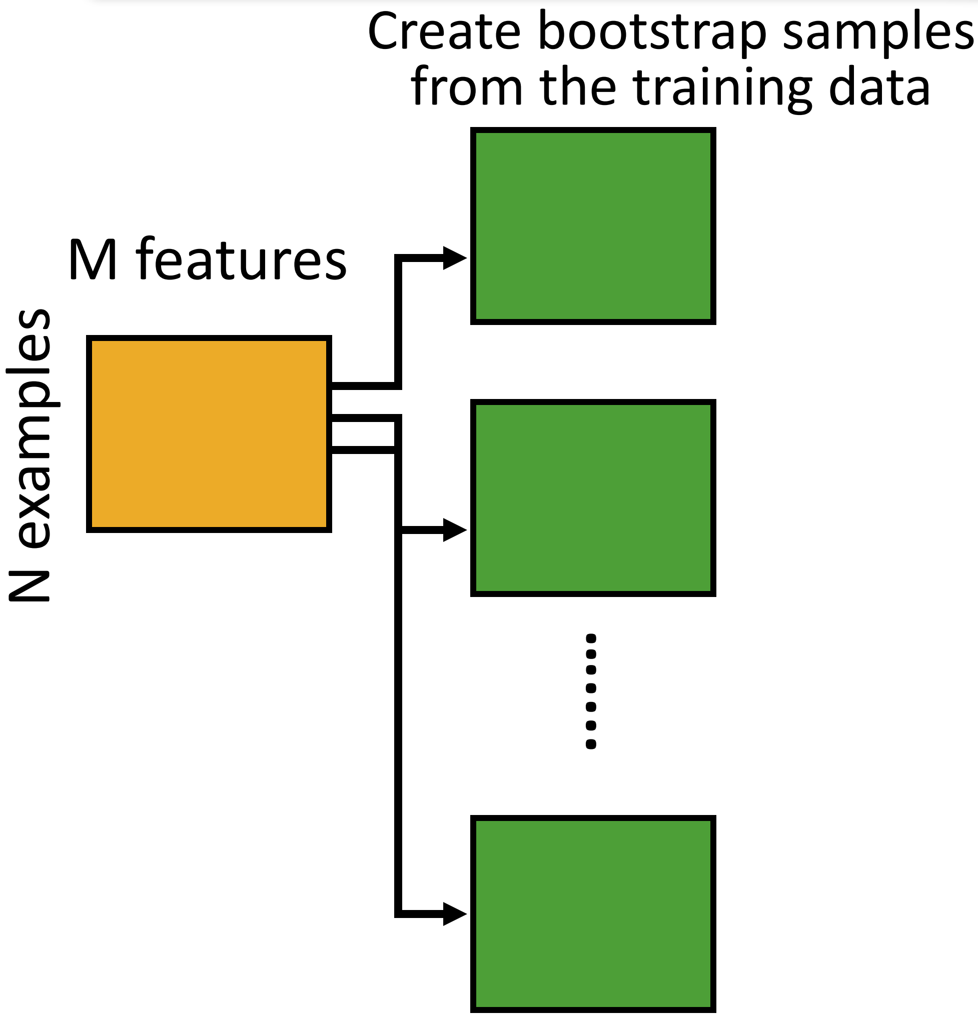
Random forest classifier, an extension to bagging which uses *de-correlated* trees.

Random Forest Classifier

Training Data

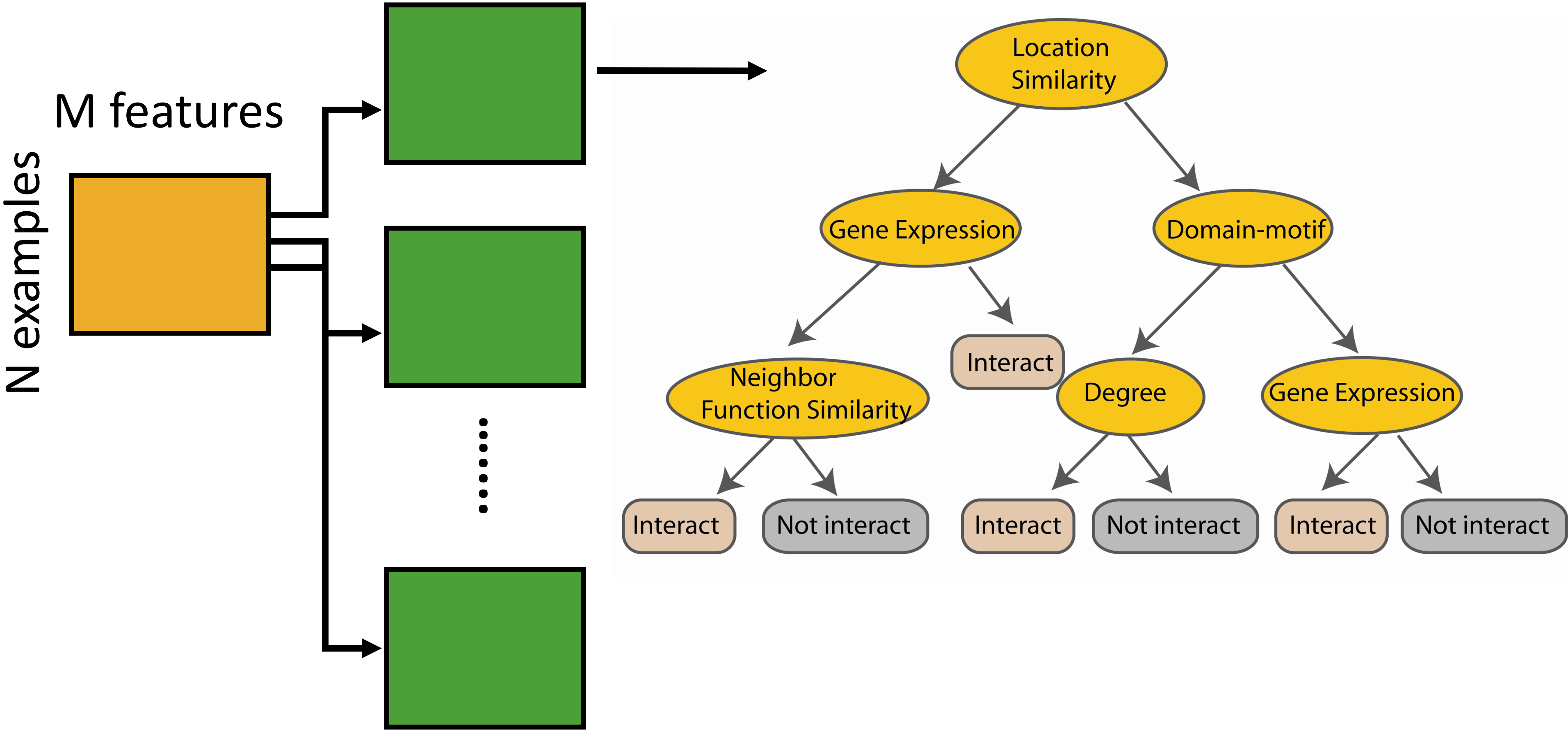


Random Forest Classifier



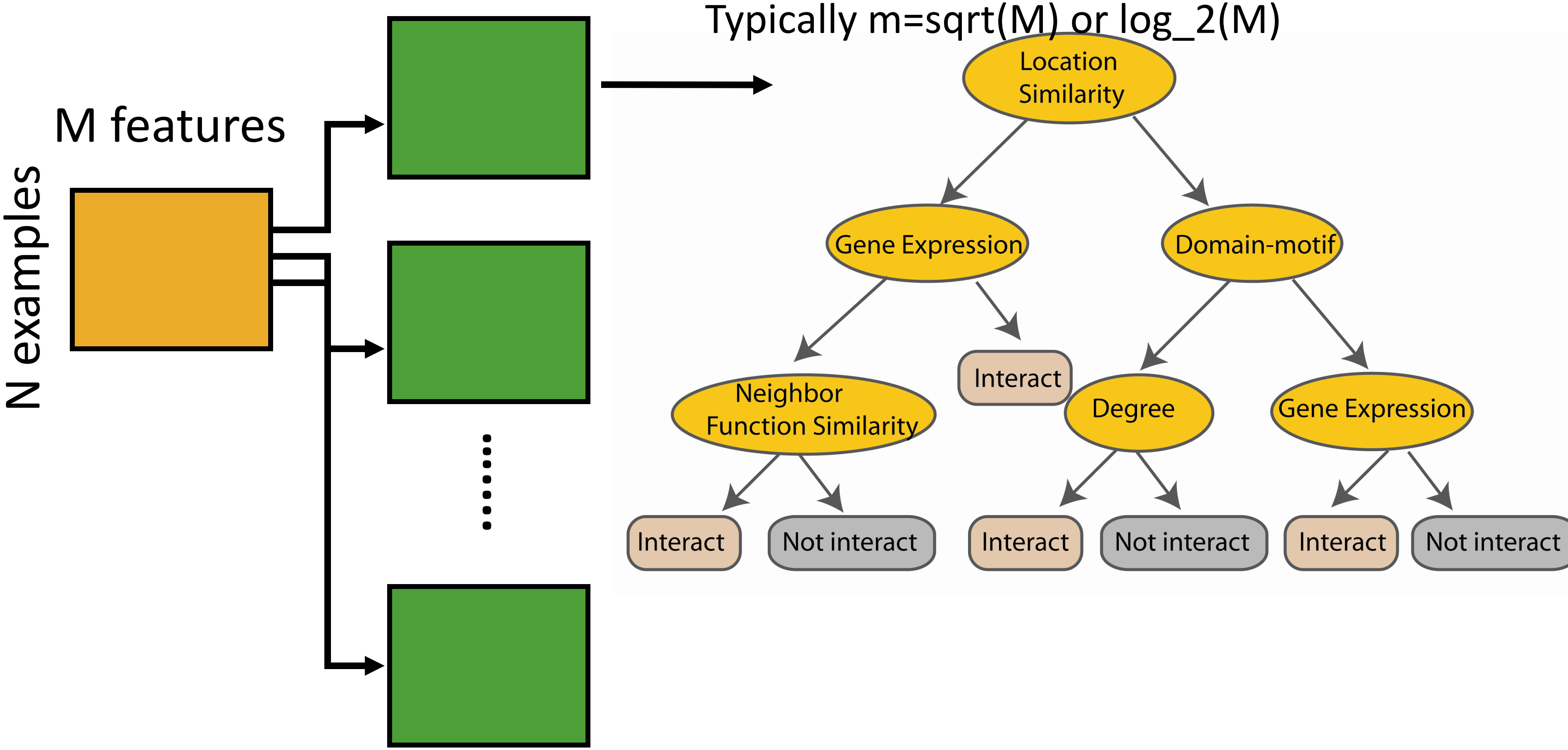
Random Forest Classifier

Construct a decision tree

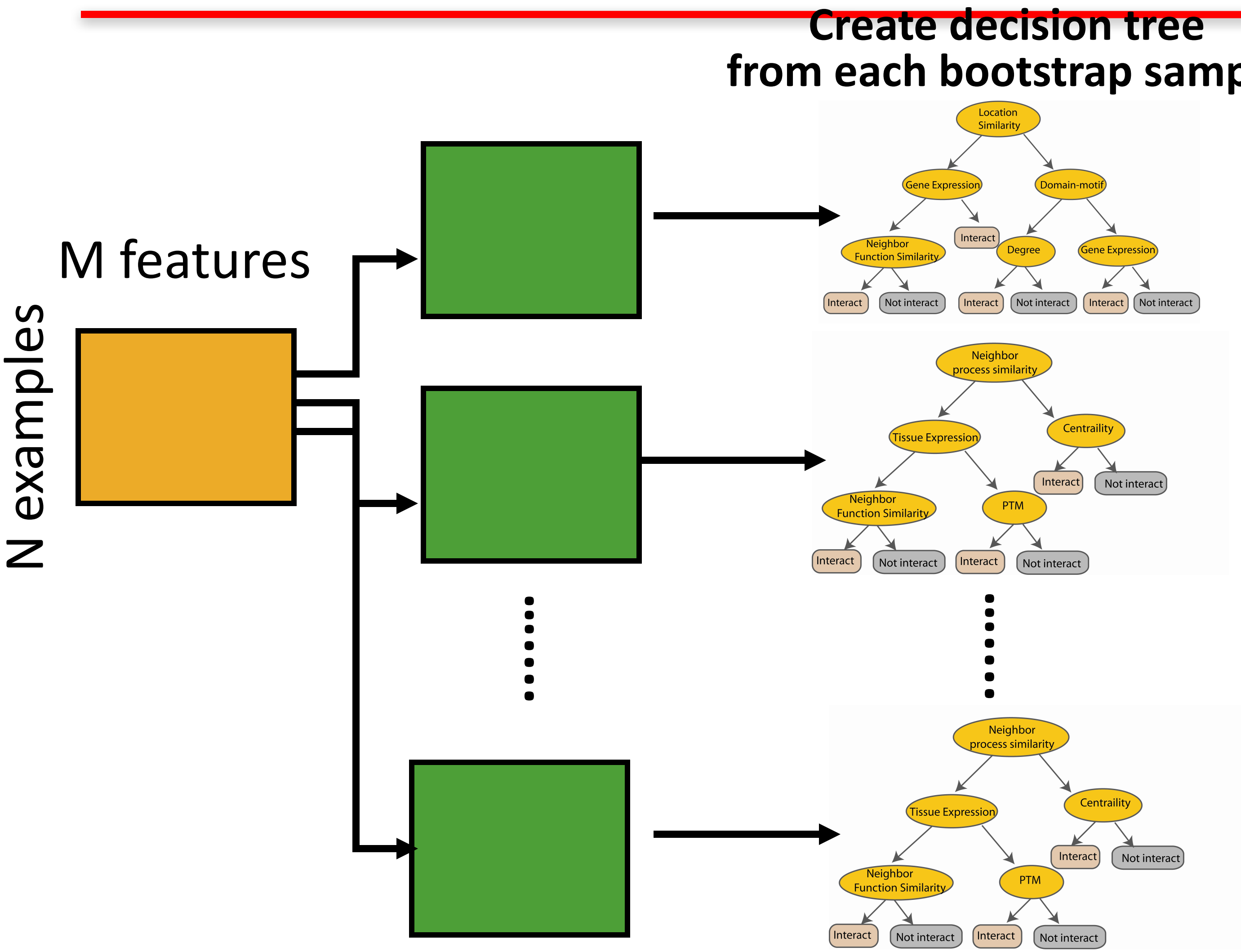


Random Forest Classifier

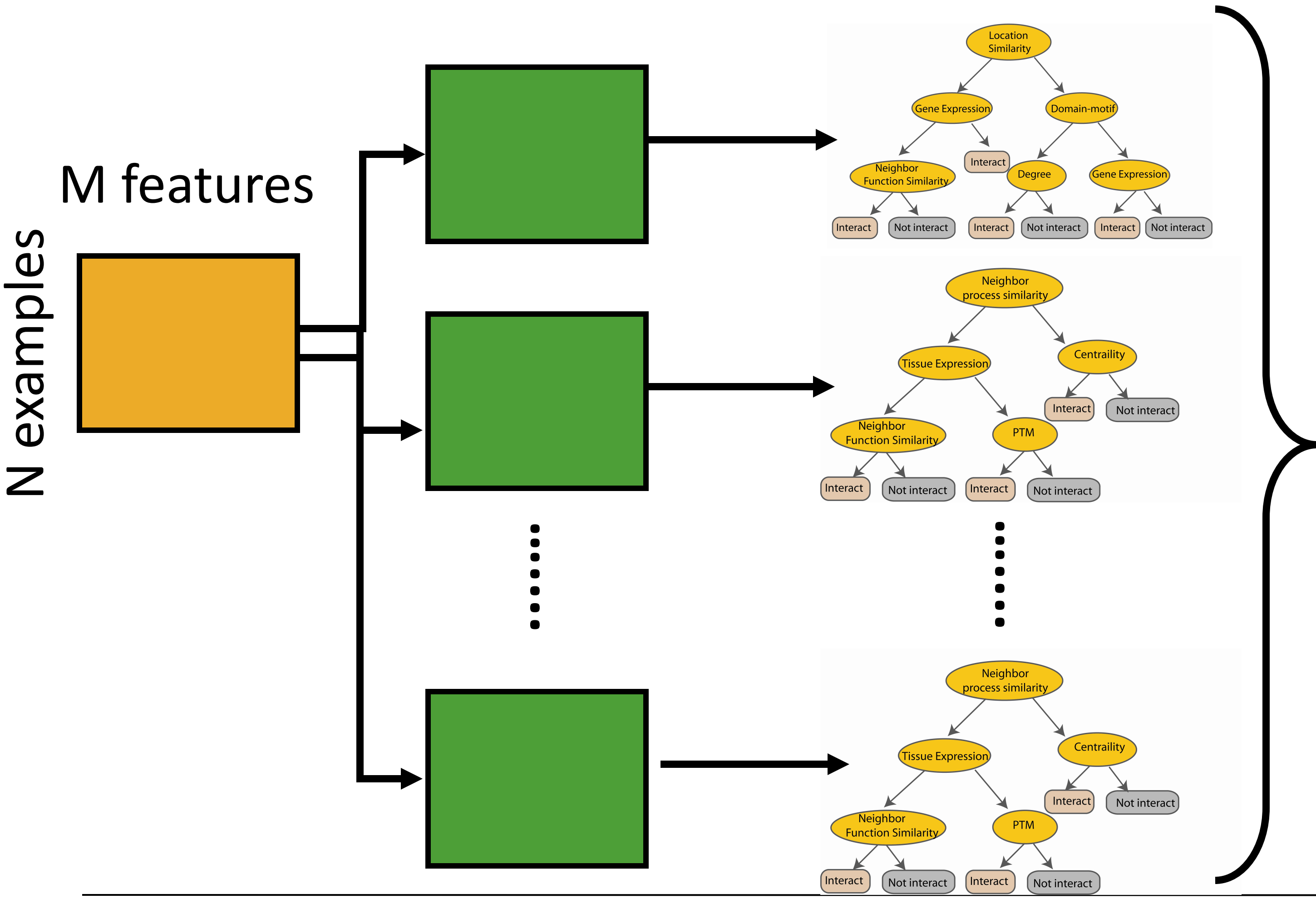
At each node in choosing the split feature
choose only among *m*<*M* features
Typically m=sqrt(M) or log_2(M)



Random Forest Classifier



Random Forest Classifier



Take he majority vote

Random Forests Summary

- Advantages
  - Computationally Fast – can handle thousands of input variables
  - Trees can be trained simultaneously
  - Exceptional Classifiers – one of most accurate available
  - Provide information on variable importance for the purposes of feature selection
  - Can effectively handle missing data
- Disadvantages
  - No interpretability in final model aside from variable importance
  - Prone to overfitting
  - Lots of tuning parameters like the number of trees, the depth of each tree, the percentage of variables passed to each tree