JSC 270 - Lecture 5
Classifiers

https://jsc270.github.io/

Announcements

- Guest lecture by Benjamin Haibe-Kains on reproducibility today 2-3pm
- Perusall assignment is online, due on Saturday night
- Presentation for Assignment 2 is due on Feb 11th (instructions are on Quercus)
- Assignment 3 will be up online on Feb 12th
- Survey to give us feedback about how we are doing https://forms.gle/wYGYuSaCgNDbQgBv8

What classifiers have you heard of?

What classifiers have you heard of?

- Logistic Regression
- KNN
- Decision Tree
- Random Forest
- Naive Bayes
- SVM
- Neural Nets
- XGB (gradient boosting)
- Generalized additive models
- Ensemble classifiers

Data

N - number of records (samples, entries)

M - number of features (predictors)

D is N x M

N = ?

M = ?

Hero Name	Mask	Cape	Tech	Pointy Ears	Height (cm)	Good/ evil
Ant-Man	False	False	True	False	183	Good
Elastagirl	True	False	False	False	172	Good
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Dormammu	False	False	False	False	185	Evil
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Data

N - number of records (samples, entries)

M - number of features (predictors)

D is N x M

N = 8

M = 5

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Decision Trees Example.

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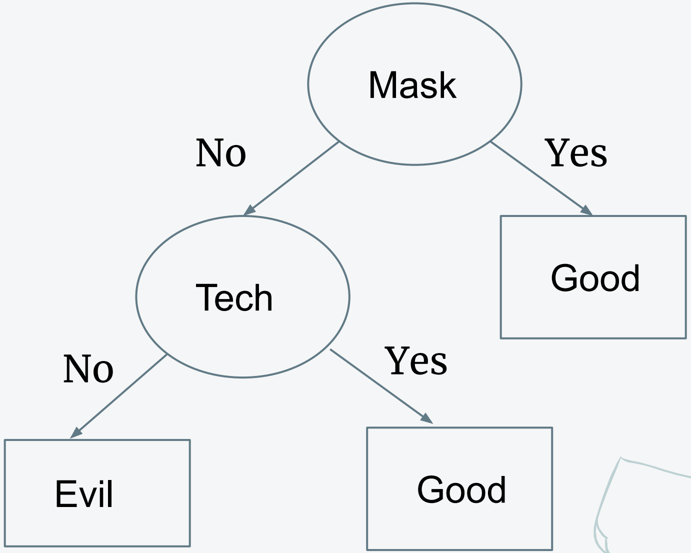

Decision Trees Example. Definitions

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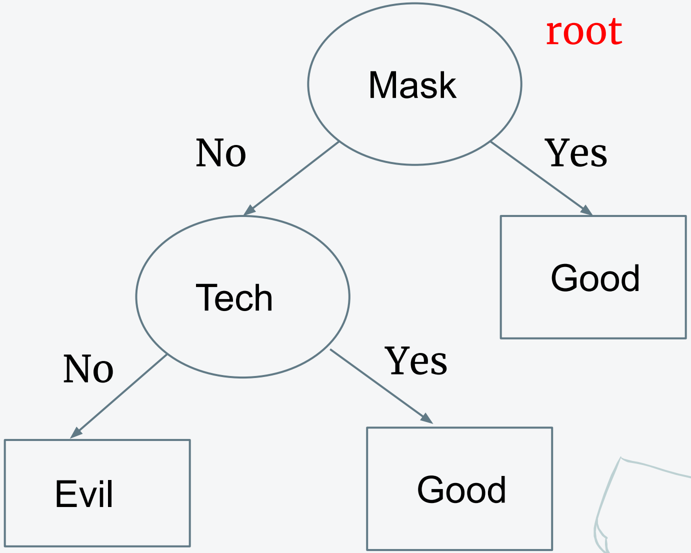

Depth = 2 (length of the longest path)

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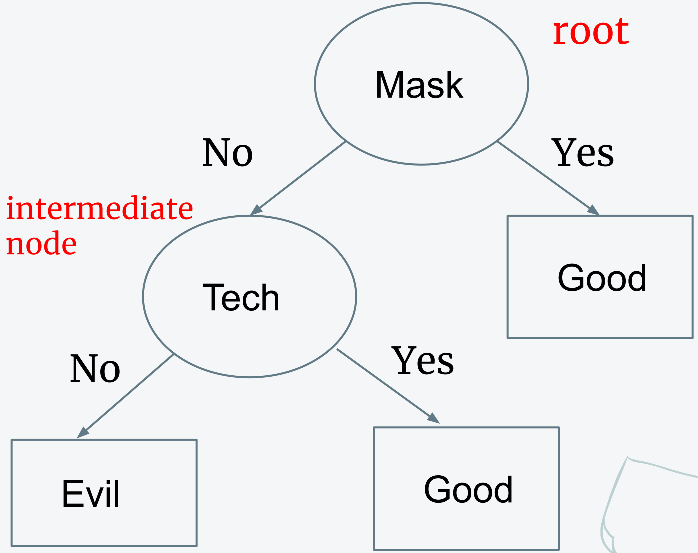

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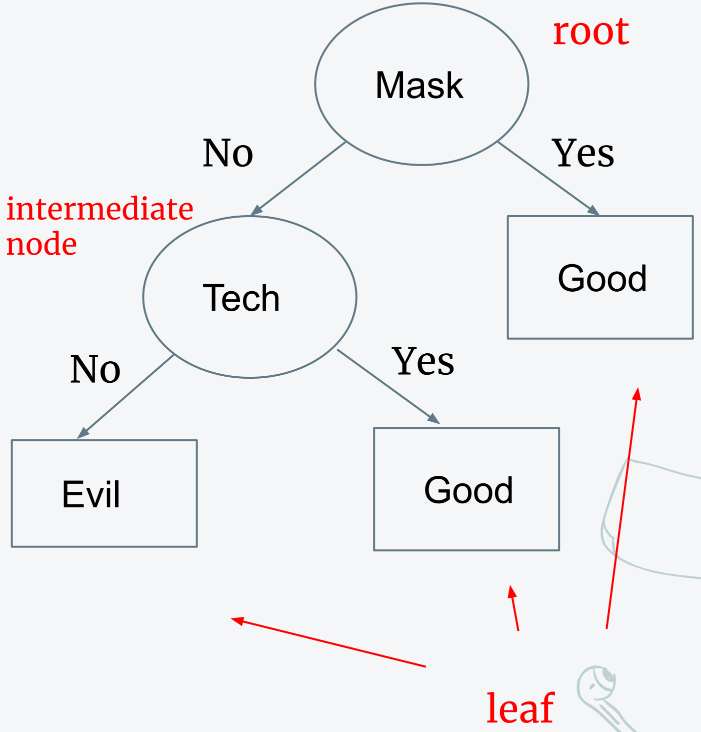

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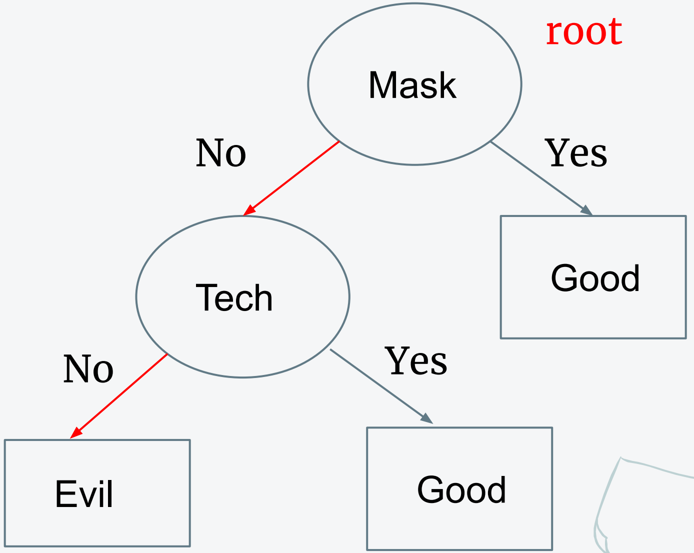

Depth – length of the longest path

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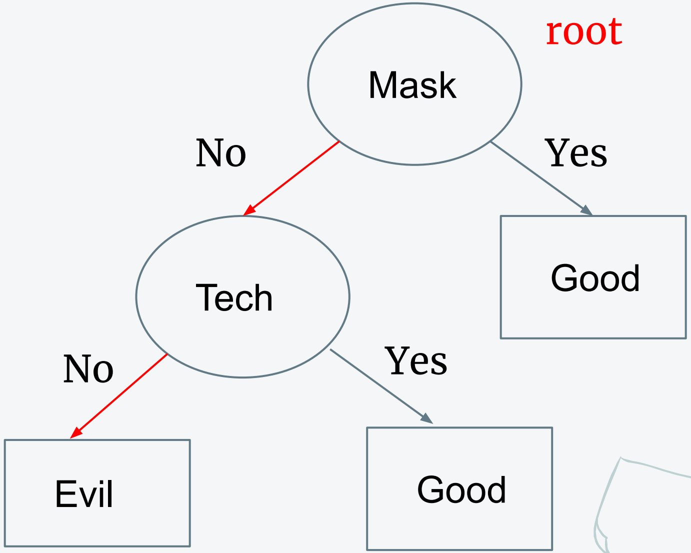

Depth – length of the longest path
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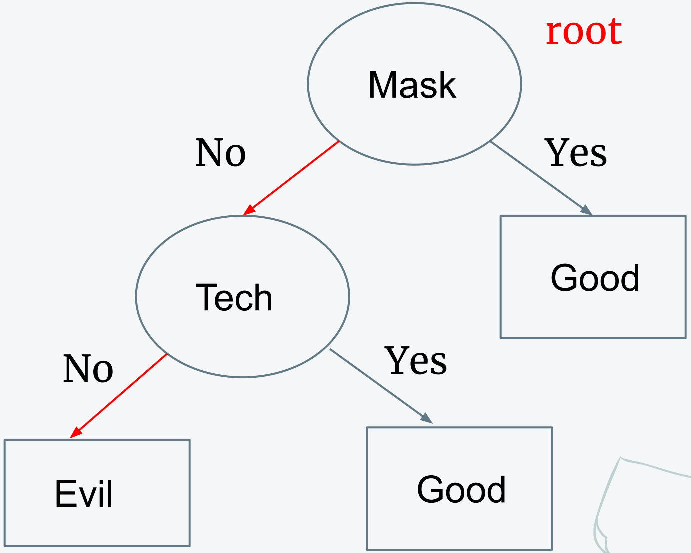

Each path is a classification rule!
No mask, no tech -> evil

Decision Trees Example. A possible tree.

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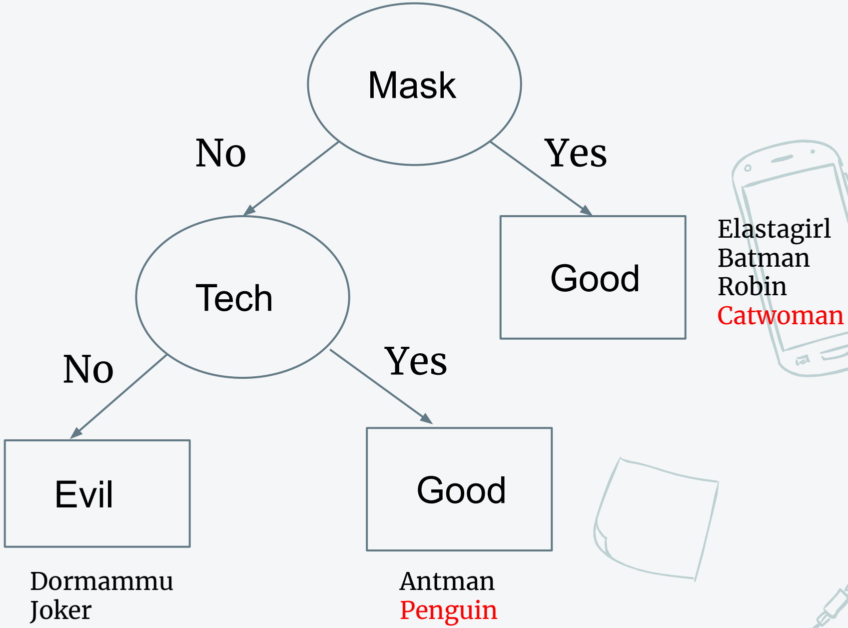

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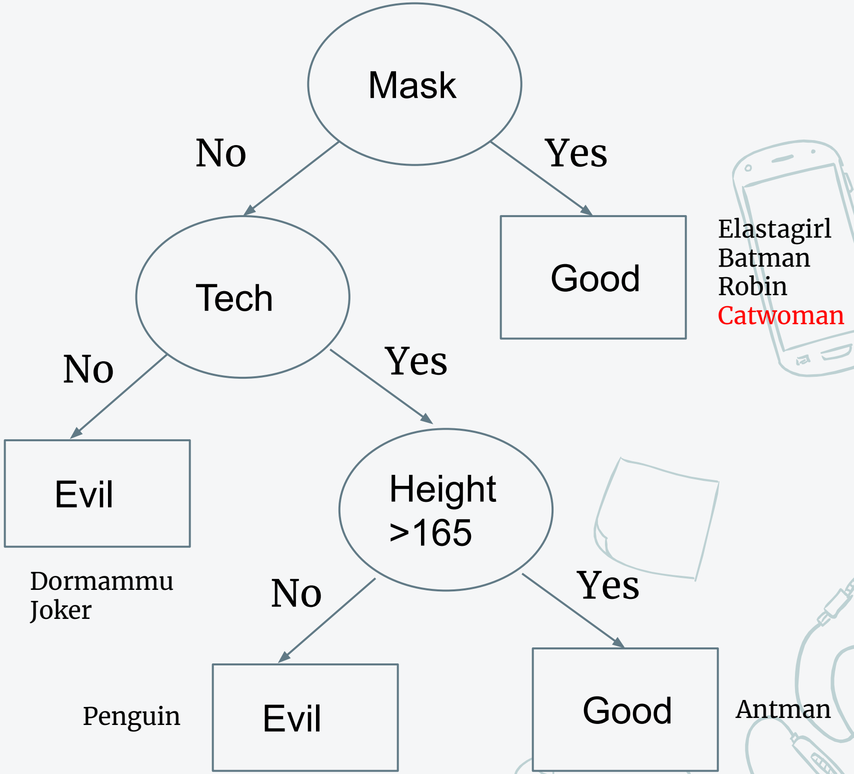

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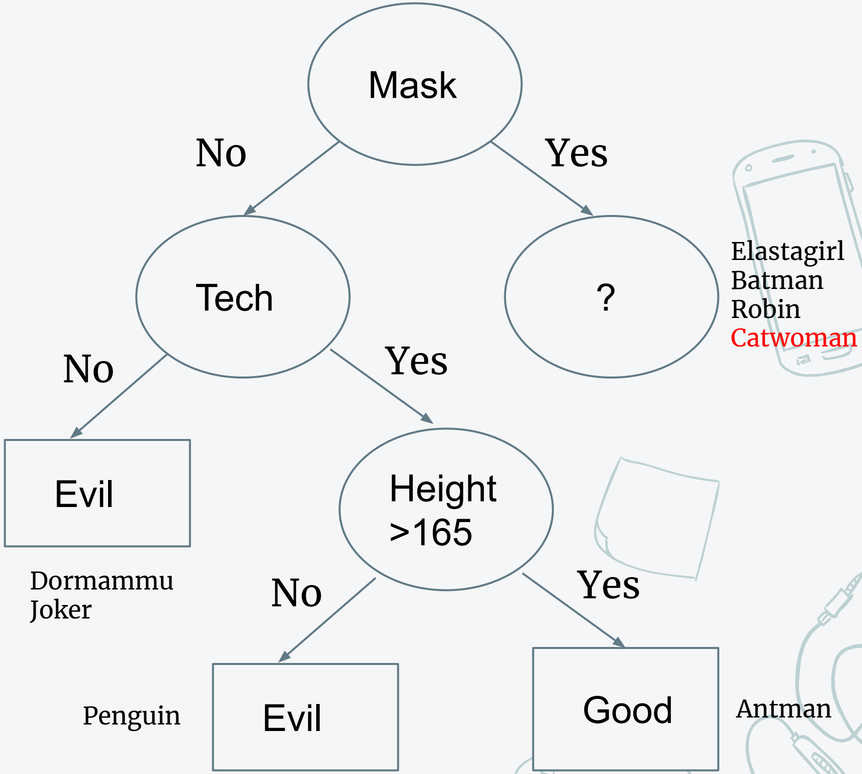

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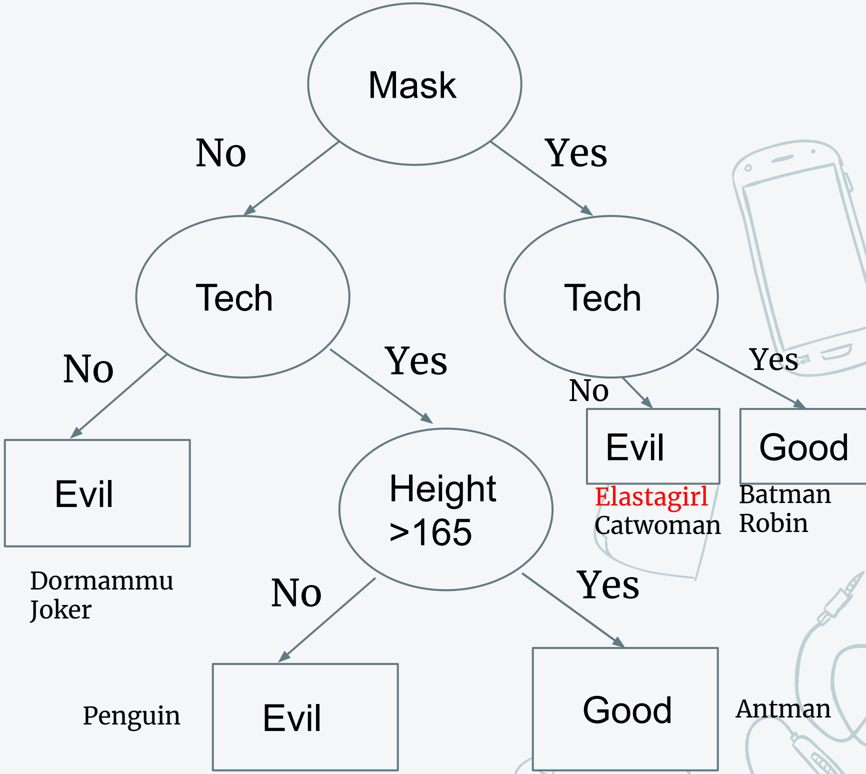

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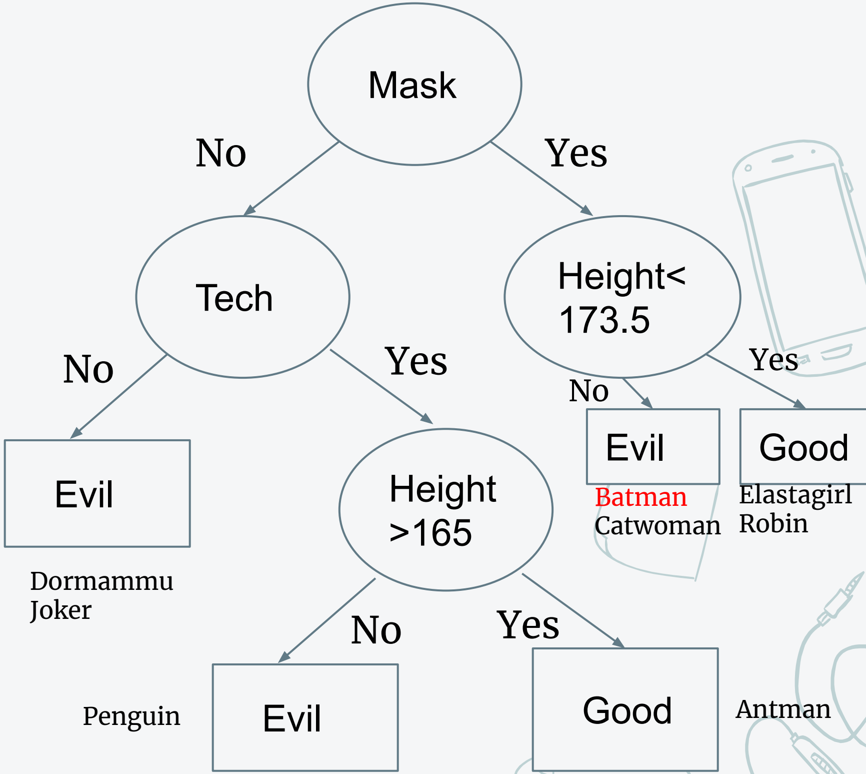


How do you find a good tree?

Important concept: Impurity Function

Impurity? As it sounds – error in class assignment

Most common impurity functions:

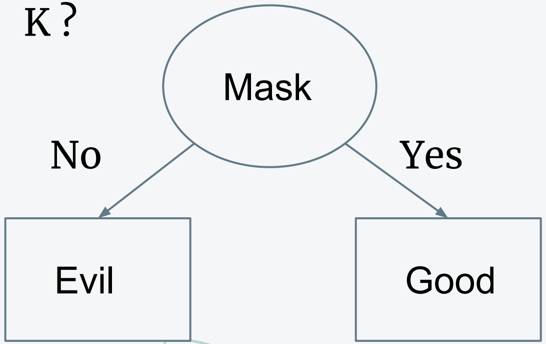
- Gini
- Entropy
- Gain Ratio

Some annotation

S - data to split into K classes: $\{(\mathbf{x}_1,y_1), (\mathbf{x}_2,y_2),\dots,(\mathbf{x}_n,y_n)\}$

$p_k = |S_k|/|S|$, where $S_k = \{(\mathbf{x}_j,y_j) \in S \text{ for all } j: y_j = k\}$

K ?



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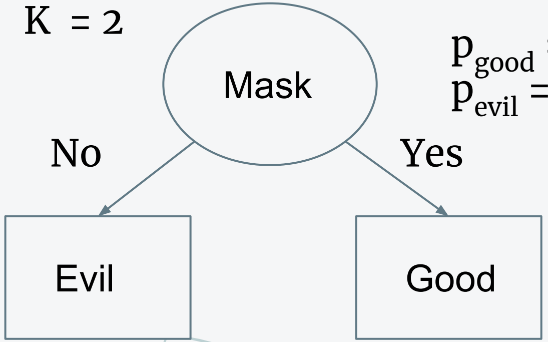
$K = 2$

$p_{good} =$
$p_{evil} =$



$p_{good} =$
$p_{evil} =$

$p_{good} =$
$p_{evil} =$

Some annotation

S - data to split into K classes: $\{(x_1,y_1), (x_2,y_2),\ldots,(x_n,y_n)\}$

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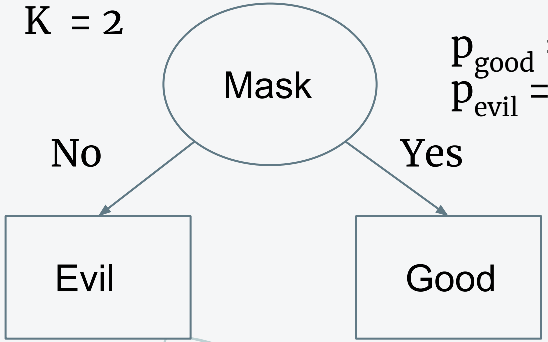

$p_{good} = 0.5$
$p_{evil} = 0.5$

$p_{good} =$
$p_{evil} =$

Some annotation

S - data to split into K classes: $\{(x_1,y_1), (x_2,y_2),...,(x_n,y_n)\}$

$p_k = |S_k|/|S|$, where $S_k = \{(x_j,y_j) \in S \text{ for all } j: y_j = k\}$

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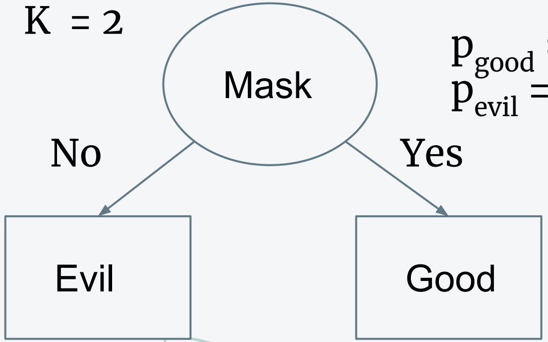


$p_{good} = 0.5$
$p_{evil} = 0.5$

$p_{good} =$
$p_{evil} =$

$p_{good} = 0.75$
$p_{evil} = 0.25$

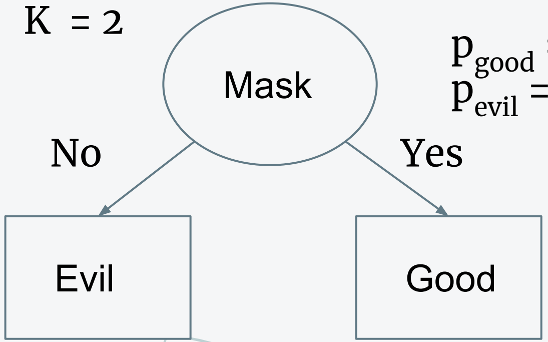
Some annotation

S - data to split into K classes: $\{(x_1,y_1), (x_2,y_2),\ldots,(x_n,y_n)\}$

$p_k = |S_k|/|S|$, where $S_k = \{(x_j,y_j) \in S \text{ for all } j: y_j = k\}$

$K = 2$

$p_{good} = 0.5$
$p_{evil} = 0.5$



$p_{good} = 0.25$
$p_{evil} = 0.75$

$p_{good} = 0.75$
$p_{evil} = 0.25$

What's the worst possible split?

What's the worst possible split?

$$p_1 = p_2 = \ldots = p_K$$

Gini Impurity

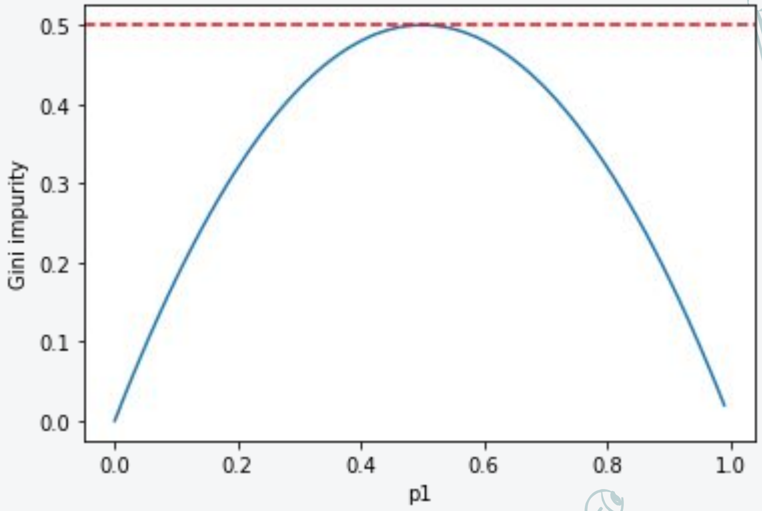
$$G(S) = \sum_{k=1}^{K} p_k(1 - p_k)$$

For K = 2: p_1, p_2, where $p_1+p_2=1$

Then $G(S) = p_1(1-p_1) + p_2(1-p_2)$

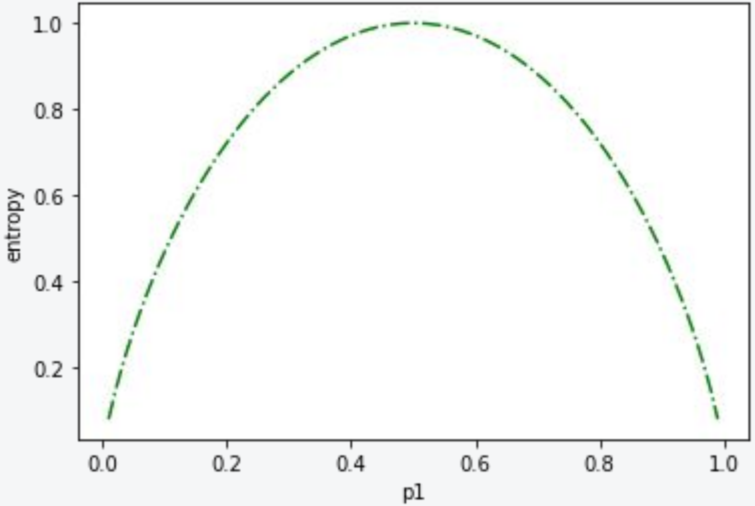
$= p_1p_2 + p_2p_1 = 2p_1p_2$

$= 2p_1(1-p_1)$

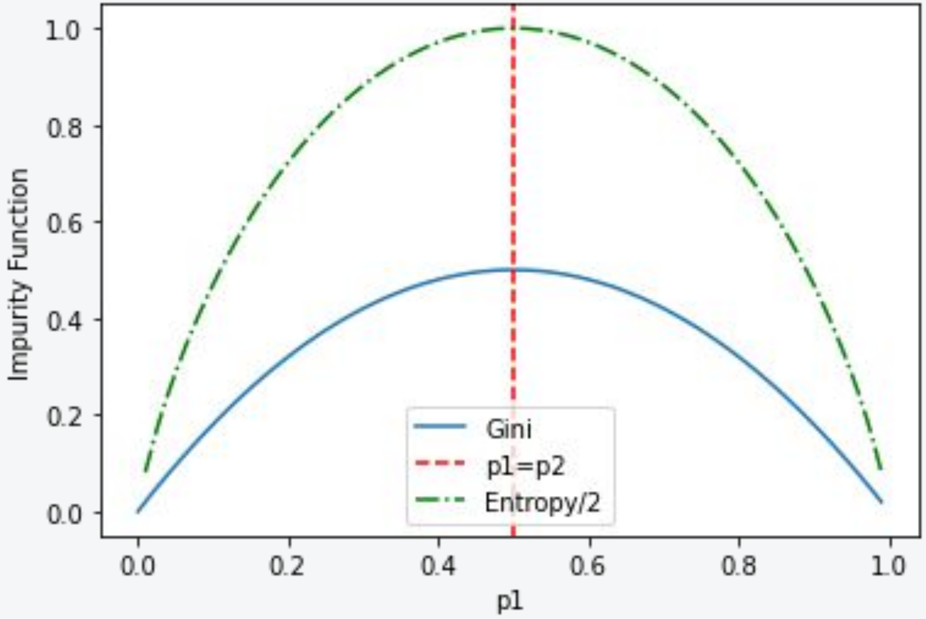


Entropy

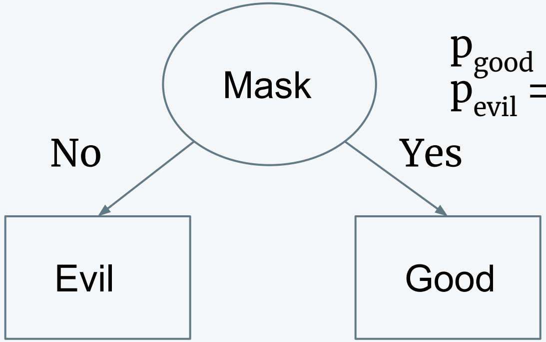
$$H(S) = -\sum_{k=1}^{K} p_k log(p_k)$$



Comparison of G(S) and H(S)



Computing Impurity



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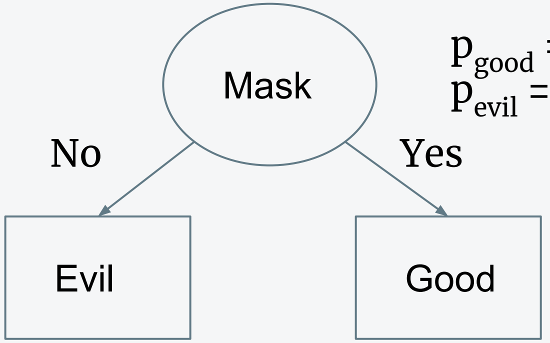
Gini: $G(Mask) =$
Entropy: $H(Mask) =$

Computing Impurity



$p_{good} = 0.5$
$p_{evil} = 0.5$

Gini: $G(Mask) = 0.5$
Entropy: $H(Mask) = 1$

How to construct a tree using an Impurity function?

NP-hard to find the best tree

Greedy approach:

1.
2.
3.

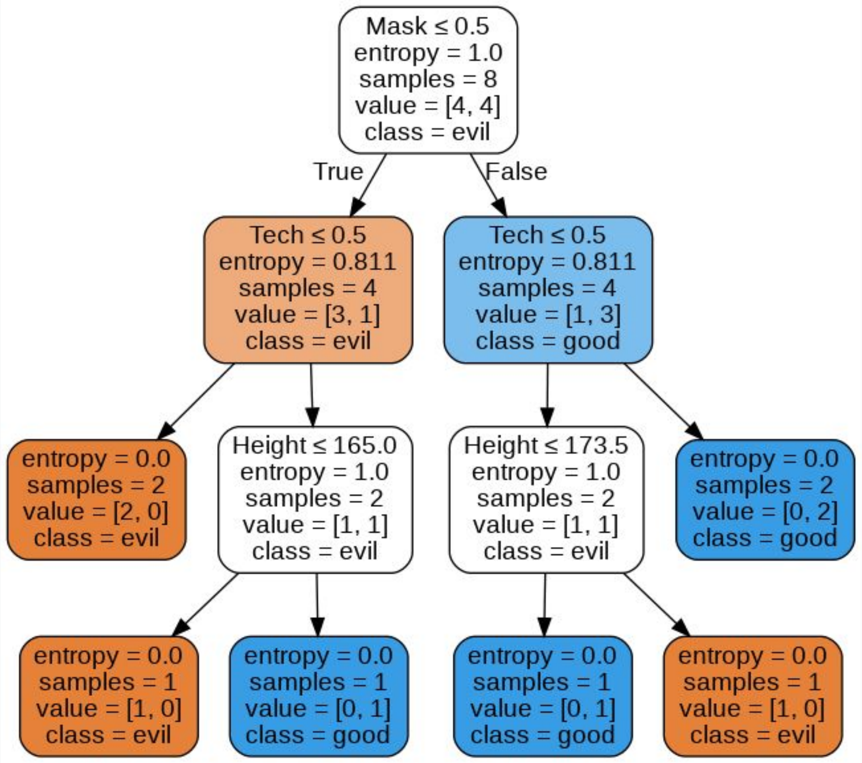
How to construct a tree using an Impurity function?

NP-hard to find the best tree

Greedy approach:

1. Check all potential splits for all features
2. Get the one with the lowest impurity
3. Split and repeat

A tree from our superhero example

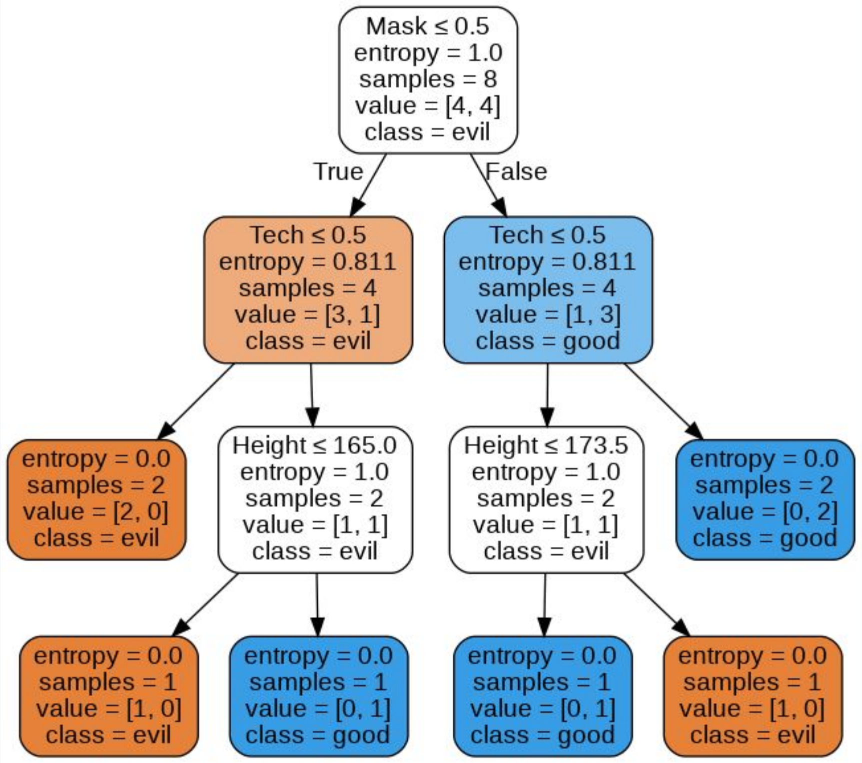


Impurity = entropy
Depth = ?

Any problems?

DecisionTreeClassifier from the scikitlearn tree package

A tree from our superhero example



Entropy impurity
Depth = 3

Any problems?
Overfitting!!

DecisionTreeClassifier from the scikitlearn tree package

WHAT'S OVERFITTING?

Definition:

Is it high bias or high variance scenario?

What's overfitting?

Definition: fitting the data too well (usually capturing the noise) with the consequence that it doesn't generalize to new examples

Is it high bias or high variance scenario?

Low bias high variance

Decision Trees Summary

Advantages?

Disadvantages?

Decision Trees Summary

Advantages?

- ❑ Simple
- ❑ Easy to analyze
- ❑ Features can have very different scales

Disadvantages?

- ❑ Poor accuracy
- ❑ Deep tree – high variance
- ❑ Shallow tree – high bias
- ❑ NP hard to find best tree

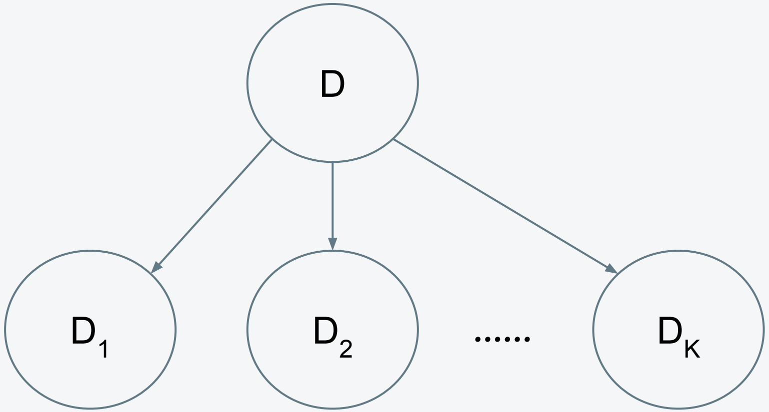
Bagging

An effective way to reduce the variance of a classifier

Helps with high variance classifiers (overfitting)

Bagging

N - number of records (samples, entries)
M - number of features (predictors)
D is N x M



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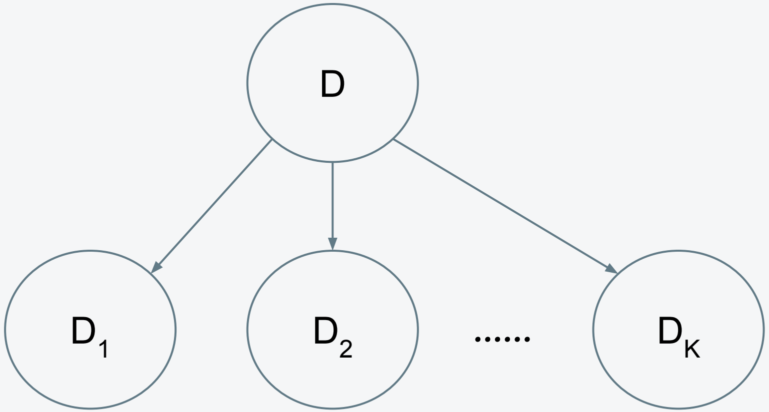
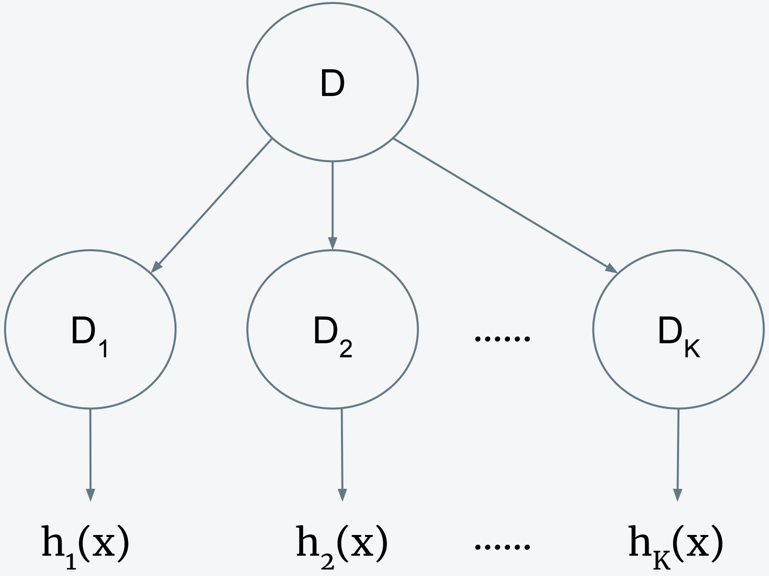


$D_1 \ldots D_K$ are NxM

(sampled independently with replacement)

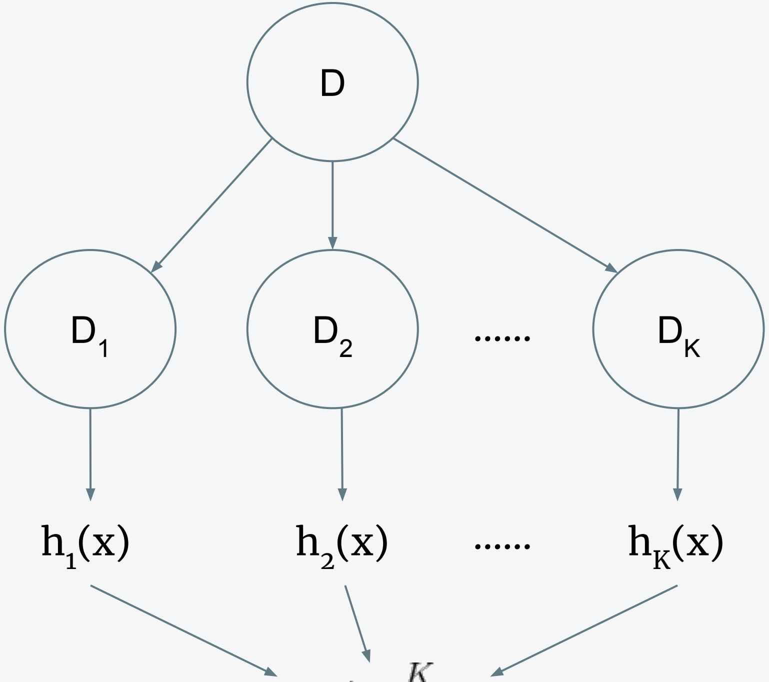
BAGGING



D_1... D_K are NxM

(sampled independently with replacement)

Bagging



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

$D_1 \ldots D_K$ are NxM

(sampled independently with replacement)

- average of classifiers

Bagging

Advantages?

Disadvantages?

BAGGING

Advantages?

- Reduce variance
- Calibrated probabilities
- Can estimate uncertainty of the prediction (by looking at how many classifiers predicted the label out of K)

Disadvantages?

-

Bagging

Advantages?

- Reduce variance
- Calibrated probabilities
- Can estimate uncertainty of the prediction (by looking at how many classifiers predicted the label out of K)

Disadvantages?

- Requires more space and compute (can do in parallel)

Random Forests

Best example of bagging

Algorithm?

Learn a decision tree on each of the "bags" $D_1 \ldots D_K$, except...

Random Forests

Best example of bagging

Algorithm?

Learn a decision tree on each of the "bags" $D_1 \ldots D_K$, except… at each tree split pick a subset of variables!!!

Random Forests

Learn a decision tree on each of the samples, except... at each tree-split pick a subset of variables at random (without replacement)!!!

How many new parameters?

Random Forests

Learn a decision tree on each of the samples, except... at each tree-split pick a subset of variables at random (without replacement)!!!

How many new parameters?

- How many trees to build
- Number of variables to subset

Random Forests

Learn a decision tree on each of the samples, except... at each tree-split pick a subset of variables at random (without replacement)!!!

How many new parameters?

- How many trees to build - as many as possible
- Number of variables to subset - $\lceil\sqrt{M}\rceil$

Random Forests

Advantages?

- Fast
- Robust
- Accurate
- Nonlinear
- No need to rescale features
- Few parameters
- Out of bag error
- Feature importance

Disadvantages?

- Treat each dimension independently (e.g. not as good for images)
- May need to prune (extra)

Out of bag (OOB) error

In principle, don't need to split data into train and test. Why?

Out of bag (OOB) error

In principle, don't need to split data into train and test. Why?

Since we get bags of samples, there are trees which were built with a subset of samples withheld

Testing those trees with unseen samples will give you a test (OOB) error!

Feature Importance

Get feature importance for free! How?

Feature Importance

Get feature importance for free! How?

Compute by how much impurity is reduced when splitting on the feature (on average)!

Summary

- There are many classifiers
- Today we learned about decision trees, bagging (not a classifier in itself but helps with overfitting!) and random forests
- Decision tree - simple and usually wrong
- Random forest - very powerful

Reading Material

Original paper on bagging by Leo Breiman, 1996:

https://link.springer.com/article/10.1007/BF00058655

Original paper on random forests by Leo Breiman, 2001 (quite theoretical):
https://link.springer.com/article/10.1023/A:1010933404324

Machine learning classifiers and fMRI (nice overview of classification itself):

https://www.sciencedirect.com/science/article/pii/S1053811908012263?casa_token=kFvmrR_QnxsAAAAA:H7tk36DYja_88DmfYyIbEEuVGXksXMkZX5LNv3tQoFrKippiZT3UdOfawidRksQoViYqKQlOqKTY

Elements of statistical learning by

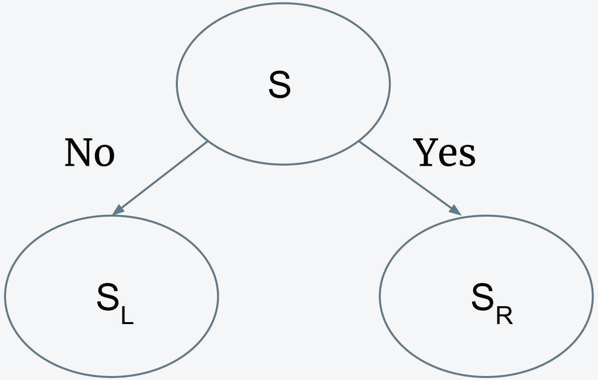
https://web.stanford.edu/~hastie/Papers/ESLII.pdf

Entropy of a tree

- $H(S)$

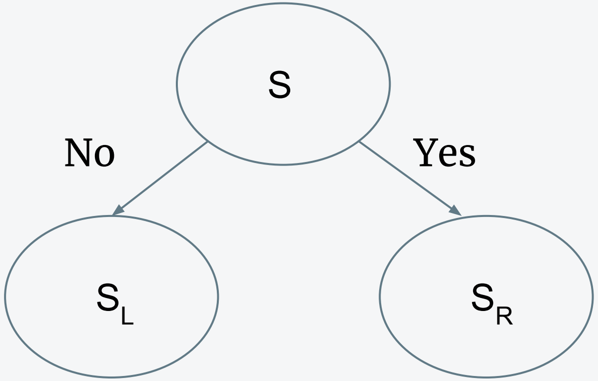
minimize

$H(S_L)$ -



- $H(S_R)$

Entropy of a tree



- $H(S_L)$
  $p_L = |S_L|/|S|$

- $H(S) = p_L H(S_L) + p_R H(S_R)$

minimize

- $H(S_R)$
  $p_R = |S_R|/|S|$