CLASSIFICATION

- Classification: Motivation and Applications
- Train-Validation Split and Cross-Validation
- Evaluation Metrics and Class Imbalance
- Overfitting
- kNN Classifier
- Naive Bayes Classifier
- Decision Tree
- Entroy, Conidtional Entropy, Information Gain

Imdad ullah Khan

Classification is a supervised task

Input: A collection of objects feature vectors with class labels

Output: A model for the class attribute as a function of other attributes



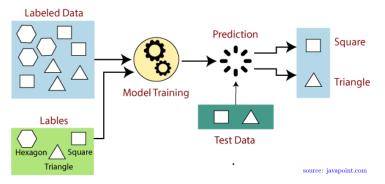
- Training Set: Instances whose class labels are used for learning
- Test Set: Instances with same attributes as training set but missing/hidden class labels
- **Goal:** Model should accurately assign class labels to unlabeled instances

Classification

Input: A collection of objects feature vectors with class labels

Output: A model for the class attribute as a function of other attributes





Classification

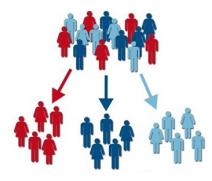
		orical	orical	UOUS
	cate	agorical cate	gorical cont	inuous class
Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Refund	Marital Status	Taxable Income	Cheat		
No	Single	75K	?		
Yes	Married	50K	?		
No	Married	150K	?	λ.	
Yes	Divorced	90K	?		
No	Single	40K	?	7	
No	Married	80K	?		Test

© Tan,Steinbach, Kumar Introduction to Data	a Mining 4/18/2004 «#»
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Targeted Advertisement

- Enhance marketing by identifying customers who are likely to buy a product
- Use customer purchase history, demographics etc. for similar (old) products
- buy/no buy as class labels

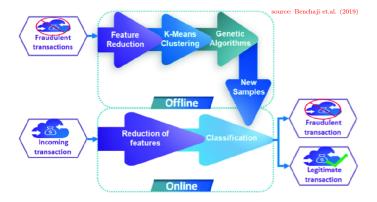




Classification: Applications

Credit Card Fraudulent Transaction Detection

- User transactions history and card holders characteristics
- fair/fraud as class labels



Predict Customer Attrition/Churn

- User customers transactions and feedback history
- churn/no-churn as class labels



Text Classification

Text is converted into feature vectors before classification



Document Classification

Sentiment Analysis

Emotion Mining



Sky Survey Cataloging

- Classify astronomical objects as stars or galaxies
- Use telescoping survey images (from Palomar Observatory)
- \blacksquare 3000 images with 23040 \times 23040 pixels per image
- Extract features values 40 features per object
- star/galaxy as class labels

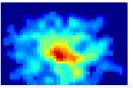
Classification: Applications

Courtesy: http://aps.umn.edu

Attributes:

- Image features,
- Characteristics of light waves received, etc.

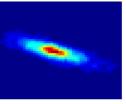




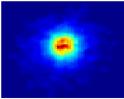
Class:

• Stages of Formation

Intermediate



Early



Data Size:

- 72 million stars, 20 million galaxies
- Object Catalog: 9 GB

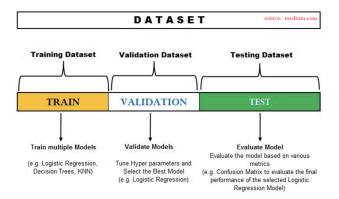
Classification Evaluation Metrics

Train-Validation Split and Cross-Validation

- The model (classifier) is learned by finding patterns in training set
- Performance on training set does not (necessarily) indicate generalization power of the model
- A validation set (a subset of training set) is used to learn parameters and tune architecture of classifier and estimate error
- For generalization of the model, validation set must be representative of the input instances
- Since test set is never used during training, it provides an unbiased estimate of generalization error

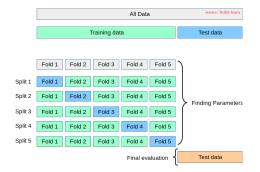
Classification: Training-Validation split

- Generally obtained by randomly splitting the dataset
- e.g. 70 30, 80 20 random Train-Validation split
- Use average performance of multiple random (splits)



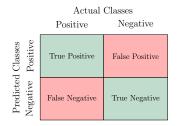
Classification: Cross-Validation

- The dataset is randomly split into k folds
- In each of k the ith fold is used for validation and the rest for training
- Every instance is used once for validation and k-1 times for training
- 5-fold, 10-fold cross-validation



Classification: Evaluation Metrics

Binary Classifiers (for classifying into two classes) are evaluated by tabulating the classification results in a Confusion Matrix

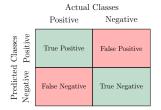


Some summary statistics of the confusion matrix are

 $ACCURACY = \frac{TP + TN}{TP + TN + FP + FN} \qquad ERROR = \frac{FP + FN}{TP + TN + FP + FN}$

ACCURACY and ERROR are usually reported as percentages

Classification: Evaluation Metrics



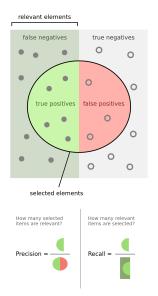


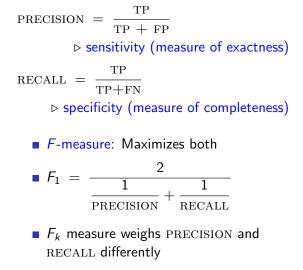
■ With big imbalance in classes, ACCURACY and ERROR are misleading

- In a tumors dataset 99% samples are negative
- (Blindly) predicting all as negatives gives 99% accuracy
- But cancer is not detected

Have to use cost matrix/loss function (essentially weighted accuracy)

Classification: Evaluation Metrics





Weighted harmonic mean

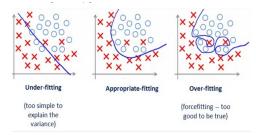
Classification: OVERFITTING

Overfitting: The phenomenon when model performs very well on training data but does not generalize to testing data

The model learns the data and not the underlying function

▷ Essentially learning by-rote

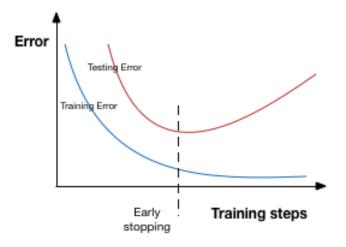
Model has too much freedom (many parameters with wider ranges)



 Validation, Cross-validation, early stopping, regularization, model comparison, Bayesian priors help avoiding overfitting

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Classification



- A classifier utilizes training data to understand how input variables are related to the class variable
- A model is built, which can be used to predict labels for unseen data
- Kinds of Classifiers
 - Lazy Classifiers
 - Eager Classifiers

Lazy Classifiers

- Store the training data and wait for testing data
- For an unseen test data record (data point), assign class label based on the most related points in the training data
- Less training time, more prediction time
- Examples: k-Nearest Neighbor (kNN) Classifier

Eager Classifiers

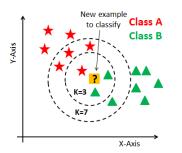
- Construct a classification model based on training data
- For a test data point, use the model to assign class label
- More training time but less prediction time
- Examples: Naive Bayes, Decision Tree

Nearest Neighbors Classification and Regression

k-Nearest Neighbor (kNN) Classifier

k-NN is a simple method used for classification \triangleright also for regression

The class label of a test instance x is predicted to be the most common class among the k nearest neighbors of x in the train set



- Assign the test instance (?) class A (★) or class B (▲)
- k = 3 nearest neighbors (ℓ_2 distance) 1 \bigstar and 2 \blacktriangle \implies assigned label = \blacktriangle

• k = 7 nearest neighbors (ℓ_2 distance) 4 \bigstar and 3 \blacktriangle \Longrightarrow assigned label = \bigstar The class label of a test instance x is predicted to be the most common class among the k nearest neighbors of x in the train set

- Assumes that the proximity measure captures class membership
- Definition of proximity measure (defining 'nearest') is critical
- The parameter k is important and sensitive to local structure of data

k-Nearest Neighbor (kNN) Regression

- In k-NN regression, for a test instance x the value of target variable y is the 'average' of values of y of k-nearest neighbors of x in train set
- The 'average' can be the weighted mean (weighted by similarity), in this case generally take k so all points are included in neighborhood

$$y(x) = \frac{\sum_{x' \in D} sim(x, x') y(x')}{\sum_{x' \in D} sim(x, x')}$$

• y(x) is the value of target variable y in instance x

Naive Bayes Classifier

Naive Bayes Classifier

- Classify $\mathbf{x} = (x_1, \dots, x_n)$ into one of K classes C_1, \dots, C_K
- Naive Bayes is a conditional probability model
 - For instance **x** it computes probabilities $Pr[class = C_j | \mathbf{x}]$ for each class C_j
- Assumes that
 - 1 All attributes are equally important
 - 2 Attributes are statistically independent given the class label
 - knowing value of one attribute says nothing about value of another
- Independence assumption is almost never correct (thus the word Naive)
 but works well in practice
- Model is the probabilities calculated from training data for each attribute with respect to class label

Naive Bayes Classifier

Classify $\mathbf{x} = (x_1, \ldots, x_n)$ into one of K classes C_1, \ldots, C_K

We want to compute this. The **Posterior probability** of class C_i given the object **x**

The **Likelihood**: Probability of predictor(s) given a class C_j . Computed from frequencies of predictor(s) in class C_j in train set **Prior:** Probability of class C_j , without considering **x**. Estimated from frequency of labels C_j in train set

 $P(C_j \mid \mathbf{x}) = \frac{P(\mathbf{x} \mid C_j) \times P(C_j)}{P(\mathbf{x})}$

Evidence: Probability of observing \mathbf{x} , This is independent on classes C and \mathbf{x} is given. Effectively constant.

Apply the independence assumption

 $P(\mathbf{x} \mid C_j) = P(x_1 \mid C_j) \times P(x_2 \mid C_j) \times \dots \times P(x_n \mid C_j)$

Substitute in numerator and ignore the denominator

 $P(C_j \mid \mathbf{x}) = P(x_1 \mid C_j) \times P(x_2 \mid C_j) \times \dots \times P(x_n \mid C_j) \times [P(C_j)]$

Train on records of weather conditions and whether or not game was played. Given weather condition (test instance) predict whether game will be played

Outlook	Temp.	Humidity	Windy	Play
sunny	hot	high	false	no
sunny	hot	high	true	no
overcast	hot	high	false	yes
rainy	mild	high	false	yes
rainy	cool	normal	false	yes
rainy	cool	normal	true	no
overcast	cool	normal	true	yes
sunny	mild	high	false	no
sunny	cool	normal	false	yes
rainy	mild	normal	false	yes
sunny	mild	normal	true	yes
overcast	mild	high	true	yes
overcast	hot	normal	false	yes
rainy	mild	high	true	no

N. Milkic & U. Krcadinac @ Uni. of Belgrade

$$\begin{split} P(play = \mathbf{yes} \mid \mathbf{x}) &= P(outl = * \mid \mathbf{yes}) \times P(temp = * \mid \mathbf{yes}) \times P(humid = * \mid \mathbf{yes}) \times P(wind = * \mid \mathbf{yes}) \times [P(\mathbf{yes})] \\ P(play = \mathbf{no} \mid \mathbf{x}) &= P(outl = * \mid \mathbf{no}) \times P(temp = * \mid \mathbf{no}) \times P(humid = * \mid \mathbf{no}) \times P(wind = * \mid \mathbf{no}) \times [P(\mathbf{no})] \end{split}$$

Outlook	Temp.	Humidity	V	Windy		lay	
sunny	hot	high	1	false		10	
sunny	hot	high t		true	r	10	
overcast	hot	high	1	false	у	es	
rainy	mild	high	1	false	у	es	
rainy	cool	normal	normal f				
rainy	cool	normal		t		Play	_
overcast	cool	normal		Outlook		yes	no
sunny	mild	high				-	
sunny	cool	normal		sunn	y 🛛	2	3
rainy	mild	normal		over	ract	4	0
sunny	mild	normal		overcast		4	<u> </u>
overcast	mild	high		rainv		3	2
overcast	hot	normal	1	TOTA		0	
rainy	mild	high		ΤΟΤΑ	L	9	5

	Play		
Outlook	yes	no	
sunny	2	3	
overcast	4	0	
rainy	3	2	
TOTAL	9	5	
			•

For each attribute...

Outlook	Temp.	Humidity	Windy	Play
sunny	hot	high	false	no
sunny	hot	high	true	no
overcast	hot	high	false	yes
rainy	mild	high	false	yes
rainy	cool	normal	false	yes
rainy	cool	normal	true	no
overcast	cool	normal	true	yes
sunny	mild	high	false	no
sunny	cool	normal	false	yes
rainy	mild	normal	false	yes
sunny	mild	normal	true	yes
overcast	mild	high	true	yes
overcast	hot	normal	false	yes
rainy	mild	high	true	no

	Play			Play			Play			Play			Play
Outlook	yes	no	Temp.	yes	no	Humid.	yes	no	Windy	yes	no		
sunny	2	3	hot	2	2	high	3	4	false	6	2	yes	9
overcast	4	0	mild	4	2	normal	6	1	true	3	3	no	5
rainy	3	2	cool	3	1								
TOTAL	9	5	TOTAL	9	5	TOTAL	9	5	TOTAL	9	5	TOTAL	14

	Play			Play	Play		Play		Play				Play
Outlook	yes	no	Temp.	yes	no	Humid.	yes	no	Windy	yes	no		
sunny	2	3	hot	2	2	high	3	4	false	6	2	yes	9
overcast	4	0	mild	4	2	normal	6	1	true	3	3	no	5
rainy	3	2	cool	3	1								
TOTAL	9	5	TOTAL	9	5	TOTAL	9	5	TOTAL	9	5	TOTAL	14

Covert values to ratios

	Play			Play			Play			Play			Play
Outlook	yes	no	Temp.	yes	no	Humid.	yes	no	Windy	yes	no		
sunny	0.22	0.60	hot	0.22	0.40	high	0.33	0.80	false	0.67	0.40	yes	0.64
overcast	0.44	0.00	mild	0.44	0.40	normal	0.67	0.20	true	0.33	0.60	no	0.36
rainy	0.3	0.40	ool	0.33	0.20								
	_												

2 occurences of Play = no, where Outlook = rainy

5 occurrences of Play = no

Given weather condition $\mathbf{x} = (sunny, cool, high, true)$ will game be played?

$$\begin{split} P(play = \mathbf{yes} \mid \mathbf{x}) &= P(sunny \mid \mathbf{yes}) \times P(cool \mid \mathbf{yes}) \times P(high \mid \mathbf{yes}) \times P(true \mid \mathbf{yes}) \times [P(\mathbf{yes})] \\ &= 0.22 \times 0.33 \times 0.33 \times 0.33 \times [0.64] = \mathbf{0.0053} \end{split}$$

 $\begin{aligned} P(play = \mathbf{no} \,|\, \mathbf{x}) &= P(sunny | \mathbf{no}) \times P(cool | \mathbf{no}) \times P(high | \mathbf{no}) \times P(true | \mathbf{no}) \times [P(\mathbf{no})] \\ &= 0.60 \times 0.20 \times 0.80 \times 0.80 \times [0.36] = \mathbf{0.0206} \end{aligned}$

	Play		Play		Play		Play			Play			
Outlook	yes	no	Temp.	yes	no	Humid.	yes	no	Windy	yes	no		
sunny	0.22	0.60	hot	0.22	0.40	high	0.33	0.80	false	0.67	0.40	yes	0.64
overcast	0.44	0.00	mild	0.44	0.40	normal	0.67	0.20	true	0.33	0.60	no	0.36
rainy	0.33	0.40	cool	0.33	0.20								

Some issues for Naive Bayes classifier: you are encouraged to read about

Zero frequency problem: probability = 0 for an attribute in a class

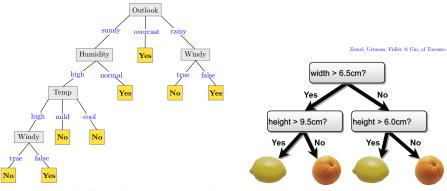
- For example: P[Outlook = sunny|yes] = 0
- One zero would make whole product zero
- Solution: Laplace smoothing (add-one smoothing)
- Missing value of an attribute for a test instance
 - usually attribute is omitted from probability calculation
- What if values of attributes are continuous?
 - Discretization solves the problem in many cases
 - Can also assume a probability distribution for each continuous attribute and learn distribution parameters from training set

Decision Tree Classifier

Decision Tree

- Fundamentally, an if-then rule set for classifying objects
- Builds model in the form of a tree structure

Decision Tree



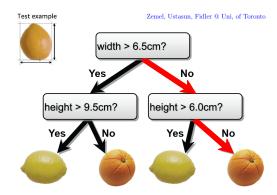
Decision tree for binary classification of instance with nominal attributes



- Each internal node tests an attribute x_i
- Branches correspond to possible (subsets of) values of x_i
- Each leaf node assigns a class label y

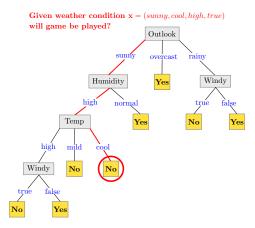
Classification using Decision Trees

- To classify a test instance x traverse the tree from root to leaf
- Take branches at internal nodes according to results of their tests
- Predict the class label at the leaf node reached



Classification using Decision Trees

- To classify a test instance **x** traverse the tree from root to leaf
- Take branches at internal nodes according to results of their tests
- Predict the class label at the leaf node reached



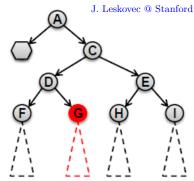
Building the optimal decision tree is $\operatorname{NP-HARD}$ problem

|D|=10 $X_1 < v_1$ |D|=45 $Z_2 < v_2$ |D|=45 $X_2 < v_2$ |D|=45 $Z_2 < v_2$ |D|=45 $Z_2 < v_3$ |D|=25 |D|=15 $Z_2 < v_3$ |D|=30 |D|=26 |D|=15 $Z_2 < v_3$ |D|=30 |D|=15 $Z_3 < v_3$ |D|=20 |D|=15 |D|=15

Training dataset D*, |D*|=100 examples

- Recursively build the tree top-down, using greedy heuristics
- Start with an empty decision tree
- Split the current dataset by the best attribute until stopping condition

Suppose at some node G in the tree built so far

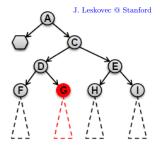


Shall we continue building the tree?

- If **Yes**, *G* is internal, which attribute to split on (test)?
- If **No**, *G* is leaf, what is the prediction rule?

Stop when the leaf (subtree at G)

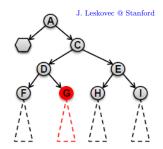
- is pure (purity?) or
- When the size of sub-dataset at G is small e.g. $|D_G| \le 5$



. . .

If we stop at G, then prediction at G can be

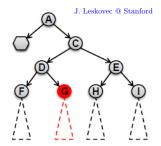
- mode of class labels in sub-dataset D_G
- For a numeric target variable prediction could be an average of target variable values in D_G
- When target variable is numeric it is called Regression Tree



Attribute Selection

Top attributes are selected based on metrics e.g.

- Entropy
- Information Gain
- Gini Index



Common algorithms for Decision Tree are ID3, C4.5, ...

Entropy

In information theory, entropy quantify the average level of information content or uncertainty in a random variable



- Entropy values range between 0 and 1 bit ▷ unit of entropy
- Max surprise is for fair coin (p = 1/2) ▷ no reason to expect an outcome over another
- Min entropy value is 0 bit for p = 0 or p = 1

These slides about information theory concepts are adapted from Grosse, Farahmand, & Carrasquilla, Uni. of Toronto

Entropy

A random variable X taking value x_1, \ldots, x_n has entropy

$$H(X) = -\sum_{i=1}^{n} p(x_i) \log p(x_i)$$

For fair coin,
$$p = 1/2$$
, $H(\cdot) = -1/2 \log 1/2 - 1/2 \log 1/2 = 1$

- For 1-sided coin, p = 1/0, $H(\cdot) = -1 \log 1 0 \log 0 = 0$
- For coin-1 in example, $H(\cdot) = -\frac{16}{20} \log \frac{16}{20} \frac{4}{20} \log \frac{4}{20} = 0.721928$
- For coin-2 in example, $H(\cdot) = -\frac{9}{20} \log \frac{9}{20} \frac{11}{20} \log \frac{11}{20} = 0.99277$

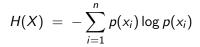


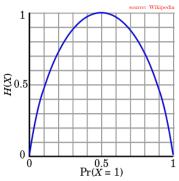
In which case would we be more surprised if the next outcome is a 1?

Classification

Entropy

A random variable X taking value x_1, \ldots, x_n has entropy





Entropy H(X) (expected surprisal) of a coin flip (in bits) plotted versus the bias of the coin Pr(X = 1) = P(heads)

Classification

Entropy of joint distribution

Entropy of the joint distribution of random variables X and Y

• Example: $X = \{\text{Raining}, \text{Not raining}\}, Y = \{\text{Cloudy}, \text{Not cloudy}\}$

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

$$H(X, Y) = -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(x, y)$$

= $-\frac{24}{100} \log_2 \frac{24}{100} - \frac{1}{100} \log_2 \frac{1}{100} - \frac{25}{100} \log_2 \frac{25}{100} - \frac{50}{100} \log_2 \frac{50}{100}$
 ≈ 1.56 bits

Conditional Entropy

• Example: $X = \{\text{Raining}, \text{Not raining}\}, Y = \{\text{Cloudy}, \text{Not cloudy}\}$

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

What is the entropy of cloudiness Y, given that it is raining?

$$H(Y|X = x) = -\sum_{y \in Y} p(y|x) \log_2 p(y|x)$$

= $-\frac{24}{25} \log_2 \frac{24}{25} - \frac{1}{25} \log_2 \frac{1}{25}$
 ≈ 0.24 bits

• We used: $p(y|x) = \frac{p(x,y)}{p(x)}$, and $p(x) = \sum_{y} p(x,y)$ (sum in a row) Grosse, Farahmand, & Carrasouilla, Uni, of Toronto

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	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

The expected conditional entropy:

$$H(Y|X) = \sum_{x \in X} p(x)H(Y|X = x)$$

= $-\sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(y|x)$

Conditional Entropy

• Example: $X = \{\text{Raining}, \text{Not raining}\}, Y = \{\text{Cloudy}, \text{Not cloudy}\}$

		Cloudy	Not Cloudy
Raining	3	24/100	1/100
Not Raini	ng	25/100	50/100

• What is the entropy of cloudiness, given the knowledge of whether or not it is raining?

$$H(Y|X) = \sum_{x \in X} p(x)H(Y|X = x)$$

= $\frac{1}{4}H(cloudy|is raining) + \frac{3}{4}H(cloudy|not raining)$
 $\approx 0.75 \text{ bits}$
Grosse, Farahmand, & Carrasquilla, Uni. of Toronto

- Some useful properties:
 - H is always non-negative
 - Chain rule: H(X, Y) = H(X|Y) + H(Y) = H(Y|X) + H(X)
 - ► If X and Y independent, then X doesn't tell us anything about Y: H(Y|X) = H(Y)
 - But Y tells us everything about Y: H(Y|Y) = 0
 - ► By knowing X, we can only decrease uncertainty about Y: $H(Y|X) \le H(Y)$

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

How much information about cloudiness do we get by discovering whether it is raining?

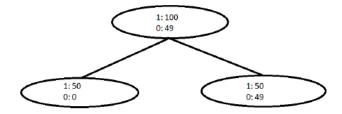
$$IG(Y|X) = H(Y) - H(Y|X)$$

$$\approx 0.25 \text{ bits}$$

- This is called the information gain in Y due to X, or the mutual information of Y and X
- If X is completely uninformative about Y: IG(Y|X) = 0
- If X is completely informative about Y: IG(Y|X) = H(Y)

Information Gain

- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!
- What is the information gain of this split?



- Root entropy: $H(Y) = -\frac{49}{149} \log_2(\frac{49}{149}) \frac{100}{149} \log_2(\frac{100}{149}) \approx 0.91$
- Leafs entropy: H(Y|left) = 0, $H(Y|right) \approx 1$.
- $IG(split) \approx 0.91 (\frac{1}{3} \cdot 0 + \frac{2}{3} \cdot 1) \approx 0.24 > 0$

Classification: Some other Concepts

Some other concepts related to classification you should be familiar with

- Decision boundary
- ROC-Curve
- Multi-Class classification form binary classifier
 - ONE-VS-ALL
 - One-vs-Rest
- Some classifiers you should read about, (at least wikipedia level is essential for reading papers and using them in your projects)
- Random Forest, Support Vector Machine, Neural Networks, Deep Learning