Introduction to Machine Learning NPFL 054

http://ufal.mff.cuni.cz/course/npf1054

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Outline

- Brief recap of the last lesson
- Entropy and conditional entropy
 - definition, calculation, and meaning
 - application for feature selection

Decision Trees

- building Decision Trees and using them as prediction function

WSD task — distribution of target class values

```
> examples <- read.table("wsd.development.csv", header=T)
> plot(examples$SENSE)
>
```



How much information do you gain when you observe a random event? According to the **Information Theory**, **amount of information** contained in an event is given by

$$I = \log_2 \frac{1}{p} = -\log_2 p$$

where p is probability of the event occurred.

Thus, the lower probability, the more information you get when you observe an event (e.g. a feature value). If an event is certain (p = 100 %), then the amount of information is zero.

```
### probability distribution of SENSE
> round(table(examples$SENSE)/nrow(examples), 3)
    cord division formation
                               phone
                                    product
                                                 text
                                        0.522
   0.095
            0.091
                      0.084
                               0.108
                                                 0.100
### amount of information contained in SENSE values
> round(-log2(table(examples$SENSE)/nrow(examples)), 3)
    cord division formation
                               phone product
                                                 text
                               3.213
                                        0.939
                                                 3.324
   3.391
            3.452
                      3.574
```

What is the average amount of information that you get when you observe values of the attribute SENSE?

Entropy

The average amount of information that you get when you observe random values is

$$\sum_{value} \Pr(value) \cdot \log_2 \frac{1}{\Pr(value)} = -\sum_{value} \Pr(value) \cdot \log_2 \Pr(value)$$

This is what information theory calls entropy.

• Entropy of a random variable X is denoted by H(X)

– or,
$$\mathsf{H}(p_1,p_2,\ldots,p_n)$$
 where $\sum_{i=1}^n p_i = 1$

- Entropy is a measure of the uncertainty in a random variable
 - or, measure of the uncertainty in a probability distribution
- The unit of entropy is bit; entropy says how many bits *on average* you necessarily need to encode a value of the given random variable

Properties of entropy

Normality

$$\mathsf{H}(\frac{1}{2},\frac{1}{2})=1$$

Continuity

H(p, 1-p) is a continuous function

Non negativity and maximality

$$0 \leq \mathsf{H}(p_1, p_2, \ldots, p_n) \leq \mathsf{H}(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n})$$

Symmetry

 $H(p_1, p_2, \ldots, p_n)$ is a symmetric function of its arguments

Recursivity

$$H(p_1, p_2, p_3, \dots, p_n) = H(p_1 + p_2, p_3, \dots, p_n) + (p_1 + p_2)H(\frac{p_1}{p_1 + p_2}, \frac{p_2}{p_1 + p_2})$$

Entropy of SENSE

Entropy of SENSE is 2.107129 bits.

```
### probability distribution of SENSE
> p.sense <- table(examples$SENSE)/nrow(examples)
>
### entropy of SENSE
> H.sense <- - sum( p.sense * log2(p.sense) )
> H.sense
[1] 2.107129
```

The maximum entropy value would be $\log_2(6) = 2.584963$ if and only if the distribution of the 6 senses was uniform.

```
> p.uniform <- rep(1/6, 6)
> p.uniform
[1] 0.16666667 0.16666667 0.16666667 0.16666667 0.16666667
>
#### entropy of uniformly distributed 6 senses
> - sum( p.uniform * log2(p.uniform) )
[1] 2.584963
```







Distribution of feature values - A4

```
> levels(examples$A4)
[1] "0" "1"
>
```



Entropy of A16 is 2.78 bits.

```
> p.A16 <- table(examples$A16)/nrow(examples)
> H.A16 <- - sum( p.A16 * log2(p.A16) )
> H.A16
[1] 2.777606
```

Entropy of A17 is 3.09 bits.

> p.A17 <- table(examples\$A17)/nrow(examples)
> H.A17 <- - sum(p.A17 * log2(p.A17))
> H.A17
[1] 3.093003

Entropy of A4 is 0.27 bits.

```
> p.A4 <- table(examples$A4)/nrow(examples)
> H.A4 <- - sum( p.A4 * log2(p.A4) )
> H.A4
[1] 0.270267
```

How much does target class entropy decrease if we have the knowledge of a feature?

The answer is conditional entropy:

$$H(C \mid A) = -\sum_{y \in C, x \in A} Pr(y, x) \cdot \log_2 Pr(y \mid x)$$

Conditional entropy and mutual information



WARNING

There are NO SETS in this picture! Entropy is a quantity, only a number!

Mutual information measures the amount of information that can be obtained about one random variable by observing another.

Mutual information is a symmetrical quantity.

$$H(C) - H(C | A) = I(C; A) = H(A) - H(A | C)$$

Another name for mutual information is information gain.

Conditional entropy – feature A4



Conditional entropy – feature A19



Conditional entropy – feature A17



Structure of a user-defined function

```
myfunction <- function(arg1, arg2, ... ){
    ... statements ...
    return(object)
}</pre>
```

Objects in a function are local to the function.

Example – a function to calculate entropy

```
> entropy <- function(x){
+   p <- table(x) / NROW(x)
+   return( -sum(p * log2(p)) )
+ }
>
# invoking the function
> entropy(examples$SENSE)
[1] 2.107129
```

Summary

- **Information theory provides a measure** for comparing how the knowledge of features *statistically* contribute to the knowledge about target class.
- The lower conditional entropy H(C | A), the better chance that A is a useful feature.
- However, since features typically interact, conditional entropy H(C | A) should NOT be the only criterion when you do feature selection. You need experiments to see if a feature with high information gain really helps.

Note

Also, decision tree learning algorithm makes use of entropy when it computes purity of training subsets.

 Write your own function for computing conditional entropy in R. New function entropy.cond(x,y) will take two factors of the same length and will compute H(x | y).

Example use: entropy.cond(examples\$SENSE, examples\$A4)

You should understand and be able to explain and practically use

- entropy
 - motivation
 - definition
 - main properties
 - calculation in R
- conditional entropy
 - definition and meaning
 - relation to mutual information
 - calculation in R
 - information gain application in feature selection

Decision Tree is a learning method suitable for both classification and regression tasks



Example classification task: WSD see the NPFL054 web page \rightarrow Materials \rightarrow wsd-attributes.pdf A decision tree T = (V, E) is a rooted tree where V is composed of internal decision nodes and terminal leaf nodes.



Decision tree learning corresponds to building a decision tree $T_D = (V, E)$ based on a training data set $D = \{ \langle \mathbf{x}, y \rangle : \mathbf{x} \in X, y \in Y \}$. When building a tree, each node is associated with a set $t, t \subseteq D$. The root node is associated with t = D.

Each leaf node is designated by an output value.



Building a decision tree from training data

A very basic idea: Assume binary decisions

• Step 1 Create a root node.



• **Step 2** Select decision *d* and add child nodes to an existing node.



Example

Associate the root node with the training set t. Example

- 1. Assume decision if $A_4 = TRUE$.
- 2. Split the training set t according to this decision into two subsets
 - "yellow" and "blue".

	SENSE	 A4	
	FORMATION	TRUE	
	FORMATION	FALSE	
t	PHONE	TRUE	
	CORD	TRUE	
		FALSE	

Building a decision tree from training data

 Add two child nodes, "yellow" and "blue", to the root. Associate each of them with the corresponding subset t_L, t_R, resp.



	SENSE	 A4	
tL	FORMATION	TRUE	
	CORD	TRUE	
	PHONE	TRUE	

	SENSE	 A4	
t _R	FORMATION	FALSE	

- Step 4 Repeat recursively steps (2) and (3) for both child nodes and their associated training subsets.
- **Step 5** Stop recursion for a node if a stopping criterion is fulfilled. Create a leaf node with an output value.

Once the decision tree predictor is built, an unseen instance is predicted by starting at the root node and moving down the tree branch corresponding to the feature values asked in decisions.



Assign the correct sense of *line* in the sentence "Draw a line between the points P and Q."

True prediction: DIVISION

First, get twenty feature values from the sentence

	A_1	A_2	A ₃	A	$_4 \mid A_5$	A_6	A ₇	A ₈	A ₉	A ₁₀	A ₁₁
ſ	0	0	0	0	0	0	0	0	1	0	0
_	A_{12}	A ₁₃	A	14	A_{15}	A	-16	A ₁₇	A_{18}	A_{19}	A_{20}
	а	drav	v X		betwee	n D	т	IN	DT	line	dobj

Second, get the classification of the instance using the decision tree



Assign the correct sense of *line* in the sentence "Draw a line that passes through the points P and Q." **True prediction**: DIVISION

First, get twenty feature values from the sentence

	A_1	A_2	A ₃	A ₄	A ₅	A ₆	A_7	A ₈	A ₉	A ₁₀	A ₁₁
	0	0	0	0	0	0	0	0	0	0	0
	A ₁₂	A ₁	3	A ₁₄	A ₁₅	A ₁₆	A ₁₇	,	A ₁₈	A_{19}	A_{20}
;	a	dra	aw	X	that	DT	WD)T	VB	line	dobi
Decision tree predictor for the WSD-line task

Second, get the classification of the instance using the decision tree



Classification trees

• Y is a categorical output feature



Figure: Tree for predicting the sense of *line* based on binary features.

Regression trees

• Y is a numerical output feature



Figure: Tree for predicting the salary of a baseball player based on the number of years that he has played in the major leagues (Year) and the number of hits that he made in the previous year (Hits). See the ISLR Hitters data set.

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Historical excursion



- ID3 \sim Iterative Dichotomiser
- AID \sim Automatic Interaction Detection
- CART \sim Classification and Regression Trees

Probably most well-known is the "C 5.0" algorithm (Quinlan), which has become the industry standard.

Packages in R: rpart

- **1** Tree growing
- 2 Tree pruning

Basic idea: First, grow a large tree that fits the training data. Second, prune this tree to avoid overfitting.

Building a decision tree from training data

Tree growing
 Tree pruning

The growing process is based on subdividing the feature space recursively into non-overlapping regions.



Building a decision tree from training data



Each terminal node in the decision tree is associated with one of the regions in the feature space. Then

Classification trees

• **output value**: the most common class in the data associated with the terminal node

Regression trees

• **output value**: the mean output value of the training instances associated with the terminal node

Notation

- $Attr = \{A_1, A_2, ..., A_m\},$
- $Y = \{y_1, y_2, \dots, y_k\}$
- Values(A_i) is a set of all possible values for feature A_i.
- $D_{i,v} = \{ \langle \mathbf{x}, y \rangle \in D | x_i = v \}.$

 	Ai	
 	V	

Building a classification tree from training data

We work with decisions on the value of only a single feature

• For each categorical feature A_j having values $Values(A_j) = \{b_1, b_2, ..., b_L\}$

is
$$x_j = b_i$$
? as $i = 1, ..., L$

• For each categorical feature A_j

is
$$x_j \in a \text{ subset} \in 2^{Values(A_j)}$$
?

• For each numerical feature A_j

is
$$x_j \leq k$$
?, $k \in (-\infty, +\infty)$

- Focus on a distribution of target class values in associated subsets of training examples.
- Then select the decision that splits training data into subsets as pure as possible.

We say a data set is **pure** (or **homogenous**) if it contains only a single class. If a data set contains several classes, then the data set is **impure** (or **heterogenous**).

⊕: 5, ⊖: 5		⊕: 9, ⊖: 1		
heterogenous		almost homogenous		
high degree of impurity	- I	ow degree of impurity		

- **1.** Define a candidate set *S* of splits at each node using possible decisions. $s \in S$ splits *t* into *L* subsets t_1, t_2, \ldots, t_L .
- Define the node proportions p(y_j|t), j = 1,..., k, to be the proportion of instances (x, y_j) in t.
- **3.** Define an impurity measure i(t), i.e. splitting criterion, as a nonnegative function Φ of the $p(y_1|t), p(y_2|t), \ldots, p(y_k|t)$,

$$i(t) = \Phi(p(y_1|t), p(y_2|t), \dots, p(y_k|t)),$$
 (1)

such that

- $\Phi(\frac{1}{k}, \frac{1}{k}, ..., \frac{1}{k}) = max$, i.e. the node impurity is largest when all examples are equally mixed together in it.
- $\Phi(1, 0, ..., 0) = 0, \Phi(0, 1, ..., 0) = 0, ..., \Phi(0, 0, ..., 1) = 0$, i.e. the node impurity is smallest when the node contains instances of only one class

Building a classification tree from training data

Which decision is the best?

- 4. Define the goodness of split s to be the decrease in impurity $\Delta i(s,t) = i(t) \sum_{l=1}^{L} p_l * i(t_l)$, where p_l is the proportion of instances in t that go to t_l .
- **5.** Find split s^* with the largest decrease in impurity: $\Delta i(s^*, t) = \max_{s \in S} \Delta i(s, t).$
- **6.** Use splitting criterion i(t) to compute $\Delta i(s, t)$ and get s^* .



Splitting criteria – examples that are really used

- Misclassification Error $-i(t)_{ME}$
- Information Gain $i(t)_{IG}$
- Gini Index i(t)_{GI}

Which decision is the best? Splitting criteria

$$i(t)_{ME} = 1 - \max_{j=1,...,k} p(y_j|t)$$
 (2)

	\oplus : 0, \ominus : 6	⊕: 1, ⊖: 5	⊕: 2, ⊖: 4	⊕: 3, ⊖: 3
ME	$1 - \frac{6}{6} = 0$	$1 - \frac{5}{6} = 0.17$	$1 - \frac{4}{6} = 0.33$	$1 - \frac{3}{6} = 0.5$

Which decision is the best? Splitting criteria

$$i(t)_{IG} = -\sum_{j=1}^{k} p(y_j|t) * \log p(y_j|t).$$
(3)

Recall the notion of entropy H(t), $i(t)_{IG} = H(t)$.

$$Gain(s,t) = \Delta i(s,t)_{IG} \tag{4}$$

Which decision is the best? Splitting criteria

$$i(t)_{GI} = 1 - \sum_{j=1}^{k} p^2(y_j|t) = \sum_{j=1}^{k} p(y_j|t)(1 - p(y_j|t)).$$
 (5)

Building a classification tree from training data

Which decision is the best? Splitting criteria

	⊕: 0	\oplus : 1	⊕: 2	⊕: 3
	⊖: 6	⊖: 5	⊕: 4	⊕: 3
Gini	0	0.278	0.444	0.5
Entropy	0	0.65	0.92	1.0
ME	0	0.17	0.333	0.5

For two classes (k = 2), if p is the proportion of the class "1", the measures are:

• Misclassification error: 1 - max(p, 1 - p)

• Entropy:
$$-p * \log p - (1-p) * \log(1-p)$$

• Gini: 2p * (1 - p)

Building a classification tree from training data

Which decision is the best? Splitting criteria



Each terminal node in the decision tree is associated with one of the regions in the feature space. Then

Classification trees

- Output value: the most common class in the data associated with the terminal node
- A criterion for making splits, e.g.
 - Misclassification error
 - Information gain
 - Gini index

Regression trees

• Output value: the mean output value of the training instances associated with the terminal node

Notation

- $Attr = \{A_1, A_2, ..., A_m\}$
- $Y = \mathcal{R}$
- Values(A_i) is a set of all possible values for feature A_i

Again, we work with decisions on the value of only a single feature

Which decision is the best?

Splitting criterion – usually used

• Squared Error $-i(t)_{SE}$

$$i(t)_{SE} = rac{1}{|t|} \sum_{\mathbf{x}_i \in t} (y_i - y^t)^2,$$

where $y^t = \frac{1}{|t|} \sum_{\mathbf{x}_i \in t} y_i$.

Each terminal node in the decision tree is associated with one of the regions in the feature space. Then

Classification trees

- Output value: the most common class in the data associated with the terminal node
- A criterion for making splits, e.g.
 - Misclassification error
 - Information gain
 - Gini index

Regression trees

- Output value: the mean output value of the training instances associated with the terminal node
- A criterion for making splits, e.g. Squared error

The recursive binary splitting is stopped when a stopping criterion is fulfilled. Then a leaf node is created with an output value.

Stopping criteria, e.g.

- the leaf node is associated with less than five training instances
- the maximum tree depth has been reached
- the best splitting criteria is not greater than a certain threshold

As a splitting criterion, ID3 algorithm uses information gain.

Main idea

- Calculate the entropy of every attribute using the data set S
- Split the set S into subsets using the attribute for which entropy is minimum (or, equivalently, information gain is maximum)
- Make a decision tree node containing that attribute
- Recurse on subsets using remaining attributes

ID3 algorithm is nicely described on the Wikiedia:

— https://en.wikipedia.org/wiki/ID3_algorithm

$\text{ID3} \longrightarrow \text{C4.5}$

ID3 is originally designed with two restrictions:

- classification task
- 2 categorical features used to train a decision tree \rightarrow Let's extend ID3 for the continuous-valued features

C4.5 algorithm: Incorporating continuous-valued features

For a continuous-valued feature A, define a boolean-valued feature A_c so that if $A(\mathbf{x}) \leq c$ then $A_c(\mathbf{x}) = 1$ else $A_c(\mathbf{x}) = 0$.

C4.5 algorithm: Handling training examples with missing feature values

Consider the situation in which Gain(t, A) is to be calculated at node associated with a training data set t in the decision tree. Suppose that $\langle \mathbf{x}, y \rangle$ is one of the training examples in t and that the value $A(\mathbf{x})$ is unknown.

Possible solutions

- Assign the value that is most common among training instances associated with the node.
- Alternatively, assign the most common value among instances associated with the node *t* having the classification *y*.

- 1 Tree growing $\sqrt{}$
- 2 Tree pruning

Basic idea: First, grow a large tree that fits the training data. Second, prune this tree to avoid overfitting.

Models built with different cp values



Overfitting can be avoided by

- applying a stopping criterion that prevents some sets of training instances from being subdivided,
- removing some of the structure of the decision tree after it has been produced.

Preferred strategy

Grow a large tree T_0 , stop the splitting process when only some minimum node size (say 5) is reached. Then prune T_0 using some pruning criteria.

Decision trees — implementation in R

There are two widely used packages in R

- rpart
- tree

The algorithms used are very similar.

References

- An Introduction to Recursive Partitioning Using the RPART Routines by Terry M. Therneau, Elizabeth J. Atkinson, and Mayo Foundation (available online)
- An Introduction to Statistical Learning with Application in R Chapters 8.1, 8.3.1, and 8.3.2 by Gareth James, Daniela Witten, Trevor Hastie and Rob Tibshirani (available online)
- R packages documentation rpart, tree (available online)

data splitting

- deeper nodes can learn only from small data portions

sensitivity to training data set (unstable algorithm)

- learning algorithm is called unstable if small changes in the training set cause large differences in generated models

- Breiman Leo, Friedman Jerome H., Olshen Richard A., Stone Charles J. *Classification and Regression Trees.* Chapman & Hall/CRC, 1984.
- Hunt, E. B. Concept Learning: An Information Processing Problem, Wiley. 1962.
- Morgan, J. N., Sonquist, J. A. Problems in the analysis of survey data, and a proposal. Journal of the American Statistical Association 58, pp. 415–434. 1963.
- Quinlan, J. R. Discovering rules from large collections of examples: A case study, in D. Michie, ed., Expert Systems in the Micro Electronic Age. Edinburgh University Press. 1979.
- Quinlan, J. R. C4.5: Programs for Machine Learning, Morgan Kaufmann, San Mateo, California. 1993.

• library **rpart** (but there are also other libraries **tree**, **party**, ...)

Model=rpart(formula, data=, method=, control=)

- ?rpart
- formula in the format TargetClass~Feature1+Feature2+...
- data specifies the input data frame
- method is "class" for decision trees
- control other optional parameters

Visualisation of the model with library rpart.plot



hypothesis parameters - parameters of the prediction function

• output of the learning algorithm, define the structure of the decision tree

learning parameters - parameters of the learning process

• "configuration" of the learning algorithm
- 2 phases of decision tree learning:
 - growing
 - pruning

Learning parameters are used to control these two phases:

- when to stop growing
- how much to prune the tree
- ... to avoid overfitting and improve performance

rpart.control

minsplit

• the minimum number of observations that must exist in a node in order for a split to be attempted

ср

• complexity parameter, influences the depth of the tree

... and others, see ?rpart.control

T: try to set different cp and minsplit values in the M1 model learning and observe the resulting tree

Any split that does not decrease the **relative training error** by a factor of cp is not attempted

 \Rightarrow That means, the learning algorithm measures for each split how it improves the tree relative error and if the improvement is too small, the split will not be performed.

Relative error is the error relative to the misclassification error (without any splitting relative error is 100%)

<pre>> M <- rpart(SENSE ~ A1+A2+A3+A4+A5+A6+A7+A8+A9+A10+A11, data=train,</pre>	
method="class", minsplit=5, cp=0.001) > M\$cptable CP nsplit rel error xerror xstd	
> M\$cptable CP nsplit rel error xerror xstd	
CP nsplit rel error xerror xstd	
1 0.093053735 0 1.0000000 1.0000000 0.01844043	
2 0.057667104 1 0.9069463 0.9069463 0.01830335	
3 0.048492792 2 0.8492792 0.8591088 0.01817412	
4 0.040629096	
5 0.009174312 4 0.7601573 0.7601573 0.01777550	
6 0.003931848	
7 0.001000000 10 0.7024902 0.7044561 0.01746957	

rel error relative error on training data

xerror relative error in x-fold cross-validation

xstd standard deviation of xerror on x validation folds

Models built with different cp value



plotcp(model) visualisation of the cross-validation error depending on cp va

prune(model, cp=) prune the model based on cp value

> M5\$cptable[which.min(M5\$cptable[,"xerror"]),"CP"]
[1] 0.001

plotcp

- visualisation of the cross-validation error depending on cp value
- the horizontal line shows the minimal xerror + its standard deviation





demo code cp-and-pruning.Forbes.R on course page

```
m = rpart(profits ~ category + sales + assets + marketvalue,
           data=F[data.train, 1:8], cp=0.001)
 m$cptable
           CP nsplit rel error xerror
                                              xstd
  0.543259557
1
                   0 1.0000000 1.0482897 0.03178559
2
  0.027162978
                   1 0.4567404 0.4607646 0.02673551
3
  0.007042254
                   3 0.4024145 0.4446680 0.02640028
  0.006036217
4
                   6 0.3762575 0.4507042 0.02652763
5
  0.005030181
                  8 0.3641851 0.4567404 0.02665301
6
  0.004024145
                 15 0.3279678 0.4768612 0.02705703
7
  0.003018109
                 19 0.3118712 0.4688129 0.02689795
  0.002012072
8
                 21 0.3058350 0.4869215 0.02725122
  0.001006036 23 0.3018109 0.5171026 0.02780383
9
10 0.001000000
                 25 0.2997988 0.5412475 0.02821490
```

How to choose the optimal cp value?



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Lecture 2, page 81/81