Naïve Bayes. Evaluating Machine Learning Methods.

COMP5318 Machine Learning and Data Mining

semester 1, 2021, week 4

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Reference: 1) Witten ch.4.2, Tan ch.5.3

2) Witten ch.5: 128-131, Tan: ch.4.5, Müller & Guido: ch.5

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Outline

- Bayes theorem
- Naïve Bayes algorithm
- Evaluating ML models
  - Evaluation procedures
    - Holdout method
    - Cross validation
    - Leave-one-out cross validation
    - Cross-validation for parameter tuning
  - Performance measures
    - Accuracy, recall, precision and F1 score; confusion matrix

Probabilistic methods: Naïve Bayes

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Probabilistic classifiers

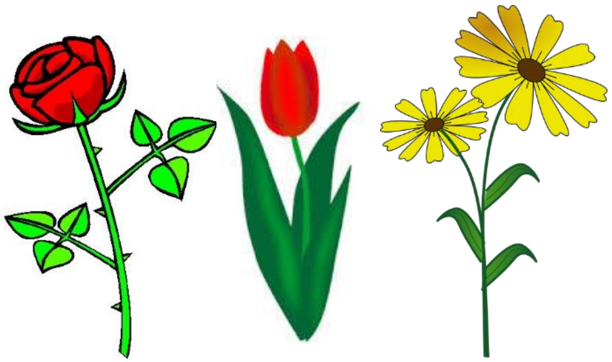
- Probabilistic classification methods compute the class membership probability, i.e. the probability that a given example belongs to a particular class
- Naive Bayes is a prominent example of this group
- It is based on the Bayes Theorem

Bayes Theorem

- Given a hypothesis H and evidence E for this hypothesis, then the probability of H given E is:

$$P(H \mid E) = \frac{P(E \mid H)P(H)}{P(E)}$$

- Example:
  - Given are examples of flowers, described by 2 features:
    - color = {red, yellow}
    - stem = {long, short}
  - Suppose that:
    - E is red and long
    - H is the hypothesis that E is a rose



P(H|E)=? P(H)=? P(E|H)=? P(E)=?

Probabilities for our example

- E is red and long
- H is the hypothesis that E is a rose

P(H|E)=? P(H)=? P(E|H)=? P(E)=?

- P(H|E) is the probability of the hypothesis (i.e. that E is a rose), given that we have seen that E is red and long
  - Called posteriori probability – probability of an event *after* seeing the evidence
  - Also called conditional probability – probability of H given E
- P(H) is the probability that any given example is a rose, regardless of how it looks
  - Called prior probability of H – probability of an event *before* seeing evidence
  - It is independent of E

Similarly:

- P(E|H) is the probability that E is red and long, given that we know that E is a rose
  - Called posteriori/conditional probability of E given H
- P(E) is the probability that any given example (flower) is red and long, regardless of the hypothesis
  - Called prior probability of E; it is independent of H

Naïve Bayes algorithm

- Uses the Bayes Theorem to solve classification tasks
- Two assumptions:
  1) Independence – (the values of the) attributes are conditionally independent of each other, given the class (i.e. for each class value)
  2) Equally importance – all attributes are equally important
- Unrealistic assumptions – almost never correct
  - => that's why the algorithm is called Naive Bayes
- However, these assumptions lead to a simple and easy to implement algorithm, which works surprisingly well in practice

Applying Naïve Bayes

- Consider the weather data:
- Use Naïve Bayes to predict the class (yes or no) of the new example:

outlook	temp.	humidity	windy	play
sunny	cool	high	true	?

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

- Bayes theorem: $P(H|E) = \frac{P(E|H)P(H)}{P(E)}$
- What are H and E?
  - the evidence E is the new example
  - the hypothesis H is play=yes (and there is another H: play=no)
- How to use the Bayes theorem?
  - Calculate P(H|E) for each H (class), i.e. P(yes|E) and P(no|E)
  - Compare them and assign E to the class with the highest probability
  - For P(H|E) we need to calculate P(E), P(H) and P(E|H) – how to do this?
    - From the given training data

Applying Naïve Bayes (2)

- Step 1: Calculate P(H|E) for each H (class), i.e. P(yes|E) and P(no|E)

$$P(yes \mid E) = \frac{P(E \mid yes) P(yes)}{P(E)}$$

$$P(no \mid E) = \frac{P(E \mid no) P(no)}{P(E)}$$

where E:

outlook	temp.	humidity	windy	play
sunny	cool	high	true	?

outlook=sunny, temperature=cool, humidity=high, windy=true

- How to calculate P(E|yes) and P(E|no) ?
  - Split the evidence E into 4 smaller pieces of evidence (per-attribute evidences):

    E1 = outlook=sunny, E2 = temperature=cool

    E3 = humidity=high, E4 = windy=true
  - Use the Naïve Bayes's independence assumption:
  - E1, E2, E3 and E4 are independent given the class. Then, their combined probability is obtained by multiplication of per-attribute probabilities:

$$P(E \mid yes) = P(E_1 \mid yes)\, P(E_2 \mid yes)\, P(E_3 \mid yes)\, P(E_4 \mid yes)$$

$$P(E \mid no) = P(E_1 \mid no)\, P(E_2 \mid no)\, P(E_3 \mid no)\, P(E_4 \mid no)$$

Applying Naïve Bayes (3)

- Hence, we obtain:

$$P(yes \mid E) = \frac{P(E_1 \mid yes)\,P(E_2 \mid yes)\,P(E_3 \mid yes)\,P(E_4 \mid yes)\,P(yes)}{P(E)}$$

$$P(no \mid E) = \frac{P(E_1 \mid no)\,P(E_2 \mid no)\,P(E_3 \mid no)\,P(E_4 \mid no)\,P(no)}{P(E)}$$

- Top parts: the probabilities will be calculated from the training data
- Bottom parts: P(E) in both cases - the same for class yes and no. Since we take the decision by comparing P(yes|E) and P(yes|no), there is no need to calculate P(E), we will just compare the top parts.

Calculating probabilities from training data

E1 = outlook=sunny, E2 = temperature=cool

E3 = humidity=high, E4 = windy=true

$$P(yes \mid E) = \frac{P(E_1 \mid yes)\,P(E_2 \mid yes)\,P(E_3 \mid yes)\,P(E_4 \mid yes)\,P(yes)}{P(E)}$$

P(E1|yes)=P(outlook=sunny|yes)=?

P(E2|yes)=P(temp=cool|yes)=?

P(E3|yes)=P(humidity=high|yes)=?

P(E4|yes)=P(windy=true|yes)=?

P(yes)=?

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

Calculating probabilities from training data

E1 = outlook=sunny, E2 = temperature=cool

E3 = humidity=high, E4 = windy=true

$$P(yes \mid E) = \frac{P(E_1 \mid yes)\,P(E_2 \mid yes)\,P(E_3 \mid yes)\,P(E_4 \mid yes)\,P(yes)}{P(E)}$$

P(E1|yes)=P(outlook=sunny|yes)=?/9=2/9

P(E2|yes)=P(temp=cool|yes)=?

P(E3|yes)=P(humidity=high|yes)=?

P(E4|yes)=P(windy=true|yes)=?

P(yes)=?

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

proportions of days when outlook=sunny for days with play=yes
i.e. the probability of outlook=sunny, given that play=yes

Calculating probabilities from training data (2)

Similarly we calculate the other conditional probabilities:

$$P(yes \mid E) = \frac{P(E_1 \mid yes)\,P(E_2 \mid yes)\,P(E_3 \mid yes)\,P(E_4 \mid yes)\,P(yes)}{P(E)}$$

P(E1|yes)=P(outlook=sunny|yes)=?/9=2/9

P(E2|yes)=P(temp=cool|yes)=3/9

P(E3|yes)=P(humidity=high|yes)=3/9

P(E4|yes)=P(windy=true|yes)=3/9

P(yes)=?

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

proportions of days when outlook=sunny for days with play=yes
i.e. the probability of outlook=sunny, given that play=yes

Calculating probabilities from training data (3)

Similarly we calculate the other conditional probabilities:

$$P(yes \mid E) = \frac{P(E_1 \mid yes)\,P(E_2 \mid yes)\,P(E_3 \mid yes)\,P(E_4 \mid yes)\,P(yes)}{P(E)}$$

P(E1|yes)=P(outlook=sunny|yes)=?/9=2/9

P(E2|yes)=P(temp=cool|yes)=3/9

P(E3|yes)=P(humidity=high|yes)=3/9

P(E4|yes)=P(windy=true|yes)=3/9

P(yes)=?

- the prior probability of play=yes - the probability of play=yes without E, i.e. without knowing anything about the particular day
- calculated from the "play" column = 9/14

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

Final probabilities

- For play=yes:

$$P(yes \mid E) = \frac{\frac{2}{9}\frac{3}{9}\frac{3}{9}\frac{3}{9}\frac{9}{14}}{P(E)} = \frac{0.0053}{P(E)}$$

- Similarly we can calculate the probability for play=no:

$$P(no \mid E) = \frac{\frac{3}{5}\frac{1}{5}\frac{4}{5}\frac{3}{5}\frac{5}{14}}{P(E)} = \frac{0.0206}{P(E)}$$

- Since P(no|E) > P(yes|E), Naïve Bayes predicts play=no for the new day

Task

- Ex.1 from the theoretical tutorial exercises (t4.pdf)
- Given is the following dataset where loan default is the class. Predict the class of the following new example using Naïve Bayes:

  home owner = no, marital status = married, annual income=very high

	home owner	marital status	income	loan default
1	yes	single	very high	yes
2	no	married	high	yes
3	no	single	medium	no
4	yes	married	very high	no
5	yes	divorced	high	yes
6	no	married	low	no
7	yes	divorced	very high	no
8	no	single	high	yes
9	no	married	medium	no
10	no	single	low	yes

$$P(H|E) = \frac{P(E|H)P(H)}{P(E)}$$

Solution

- New example:
  E= home owner = no, marital status = married, annual income = very high

- Split into 3 pieces of evidence, 1 per each attribute:
  E1 is home owner = no
  E2 is marital status = married
  E3 is annual income = very high

- Calculate P(yes|E) and P(no|E) and compare them:

$$P(yes|E) = \frac{P(E_1|yes)P(E_2|yes)P(E_3|yes)P(yes)}{P(E)}$$

$$P(no|E) = \frac{P(E_1|no)P(E_2|no)P(E_3|no)P(no)}{P(E)}$$

	home owner	marital status	income	loan default
1	yes	single	very high	yes
2	no	married	high	yes
3	no	single	medium	no
4	yes	married	very high	no
5	yes	divorced	high	yes
6	no	married	low	no
7	yes	divorced	very high	no
8	no	single	high	yes
9	no	married	medium	no
10	no	single	low	yes

Solution (2)

E1 is home owner = no, E2 is marital status = married, E3 is annual income=very high

P(yes)=5/10

P(no)=5/10

P(E1|yes)=P(home owner=no|yes)=3/5
P(E2|yes)=P(marital status=married|yes)=1/5
P(E3|yes)=P(annual income=very high|yes)=1/5

P(E1|no)= P(home owner=no|no)=3/5
P(E2|no)=P(marital status=married|no)=3/5
P(E3|no)=P(annual income=very high|no)=2/5

$$P(yes|E) = \frac{\frac{3}{5}\cdot\frac{1}{5}\cdot\frac{1}{5}\cdot\frac{5}{10}}{P(E)} = \frac{\frac{3}{250}}{P(E)} = \frac{0.012}{P(E)}$$

$$P(no|E) = \frac{\frac{3}{5}\cdot\frac{3}{5}\cdot\frac{2}{5}\cdot\frac{5}{10}}{P(E)} = \frac{\frac{9}{125}}{P(E)} = \frac{0.072}{P(E)}$$

P(no|E)>P(yes|E) => Naïve Bayes predicts
loan default = no for the new example

	home owner	marital status	income	loan default
1	yes	single	very high	yes
2	no	married	high	yes
3	no	single	medium	no
4	yes	married	very high	no
5	yes	divorced	high	yes
6	no	married	low	no
7	yes	divorced	very high	no
8	no	single	high	yes
9	no	married	medium	no
10	no	single	low	yes

The "zero-frequency" problem

- What if an attribute value does not occur with every class value?
- E.g. suppose that the training data was different:

  outlook=sunny had always occurred together with play=no, i.e.

  outlook=sunny had never occurred together with play=yes
- Then: P(outlook=sunny|yes)=0

$$P(yes \mid E) = \frac{\underbrace{P(E_1 \mid yes)}_{=0} P(E_2 \mid yes) P(E_3 \mid yes) P(E_4 \mid yes) P(yes)}{P(E)}$$

  => P(yes|E)=0, regardless of the other probability values
- This means that the prediction for new examples with outlook=sunny will always be play=no, completely ignoring the values of the other attributes
- Remedy: add 1 to the numerator and *m* to the denominator (*m* - number of attribute values = 3 for outlook)
- This is called Laplace correction or smoothing
  - it ensures that the probabilities will never be 0
- There is a generalization of the Laplace correction called *m*-estimate

Missing values

- Naïve Bayes can easily deal with missing values

- During classification: missing value in the new example
  - do not include this attribute, e.g.:
- outlook=?, temperature=cool, humidity=high, windy=true
- Then:

$$P(yes \mid E) = \frac{\frac{3}{9}\frac{3}{9}\frac{3}{9}\frac{9}{14}}{P(E)} = \frac{0.0238}{P(E)} \qquad P(no \mid E) = \frac{\frac{1}{5}\frac{4}{5}\frac{3}{5}\frac{5}{14}}{P(E)} = \frac{0.0343}{P(E)}$$

outlook is not included

- During training:
  - do not include the missing values in the counts
  - calculate the probabilities based on the actual number of training examples without missing values for each attribute

Naïve Bayes for Numeric Attributes

How to apply Naïve Bayes to numeric attributes?

- Now assume that temperature and humidity are numeric attributes (outlook and windy are still nominal)
- We would like to classify the following new example:

outlook	temperature	humidity	windy	play
sunny	66	90	true	?

- How to calculate the probabilities for the numeric attributes?

  P(temperature=66|yes)=?, P(humidity=90|yes)=?

  P(temperature=66|no)=?, P(humidity=90|no) ?

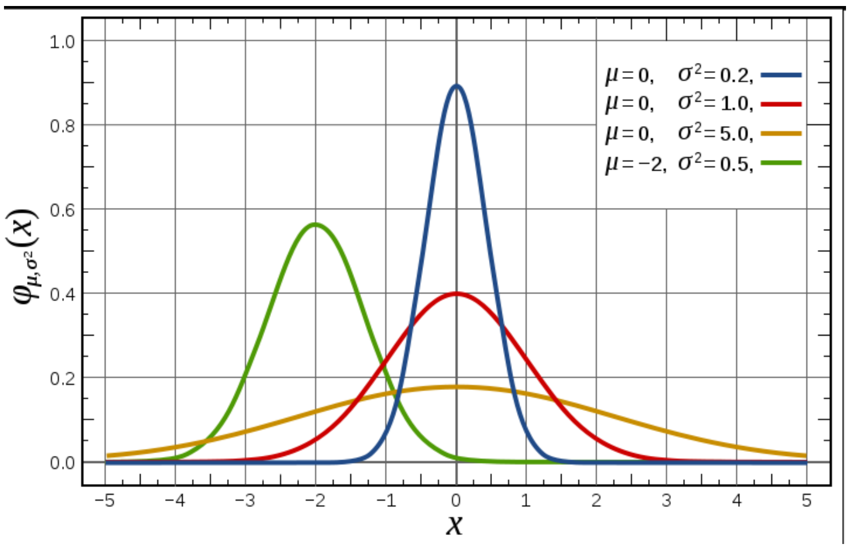
- Answer: assume that the numeric attributes follow a *normal* (or *Gaussian*) *distribution* and use *probability density function*

Probability density function for normal distribution

- Probability density function for a *normal* distribution with mean μ and standard deviation σ:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

  - The probability density function is not exactly the probability but it is closely related



Reminder about μ and σ :

$$\mu = \frac{\sum_{i=1}^{n} x_i}{n} \qquad \sigma = \sqrt{\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{n-1}}$$

Calculating probabilities

- For each numeric attribute:
  - Split the values per class
  - Calculate μ and σ (for each attribute-class combination)

outlook			temperature			humidity			windy			play	
	yes	*no*		*yes*	*no*		*yes*	*no*		*yes*	*no*	*yes*	*no*
sunny	2	3		83	85		86	85	false	6	2	9	5
overcast	4	0		70	80		96	90	true	3	3		
rainy	3	2		68	65		80	70					
				64	72		65	95					
				69	71		70	91					
				75			80						
				75			70						
				72			90						
				81			75						
sunny	2/9	3/5	*mean*	73	74.6	*mean*	79.1	86.2	false	6/9	2/5	9/14	5/14
overcast	4/9	0/5	*std dev*	6.2	7.9	*std dev*	10.2	9.7	true	3/9	3/5		
rainy	3/9	2/5											

numeric

Probability density function for normal distribution

$$f(temperature=66\,|\,yes)=\frac{1}{6.2\sqrt{2\pi}}e^{-\frac{(66-73)^2}{2*6.2^2}}=0.034$$

μ for temp. for play=yes

σ for temp. for play=yes

- Similarly: $f(humidity=90\,|\,yes)=0.0221$

$$P(yes|E)=\frac{\frac{2}{9}\,0.034\;0.0221\,\frac{3}{9}\,\frac{9}{14}}{P(E)}=\frac{0.000036}{P(E)}$$

$$P(no|E)=\frac{\frac{3}{5}\,0.0279\;0.038\,\frac{3}{5}\,\frac{5}{14}}{P(E)}=\frac{0.000137}{P(E)}$$

- P(no|E) >P(yes|E) => Naïve Bayes predicts play=no

Task

- Ex.2 from the theoretical tutorial exercises (t4.pdf)
- The same as before but now income is numeric attribute
- Predict the class of the following new example using Naïve Bayes:

home owner = no, marital status = married, annual income=120

	home owner	marital status	income (in K)	loan default
1	yes	single	125	yes
2	no	married	100	yes
3	no	single	70	no
4	yes	married	120	no
5	yes	divorced	95	yes
6	no	married	60	no
7	yes	divorced	220	no
8	no	single	85	yes
9	no	married	75	no
10	no	single	90	yes

Solution

1) Calculate the mean and standard deviation values for income:

$$\mu = \frac{\sum_{i=1}^{n} X_i}{n} \qquad \sigma^2 = \frac{\sum_{i=1}^{n} (X_i - \mu)^2}{n-1}$$

We need to do this separately for class=yes and class=no:

class yes income		**class no income**
125		70
100		120
95		60
85		220
90		75
μ_income_yes=99		μ_income_no=109
σ_income_yes=15.57		σ_income_no=66.18

Solution (2)

2) Calculate P(income=120|yes) and P(income=120|no) using the probability density function for normal distribution:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$f(income = 120|yes) = \frac{1}{15.57\sqrt{2\pi}} e^{-\frac{(120-99)^2}{2*15.57^2}} = 0.01032$$

$$f(income = 120|no) = \frac{1}{66.18\sqrt{2\pi}} e^{-\frac{(120-109)^2}{2*66.18^2}} = 0.00595$$

class yes income		**class no income**
125		70
100		120
95		60
85		220
90		75
μ_income_yes=99		μ_income_no=109
σ_income_yes=15.57		σ_income_no=66.18

Solution (3)

3) Calculating the probabilities P(yes|E) and P(no|E) using the Bayes Theorem

- We already have the probabilities for the nominal attributes from the previous exercise:

$$P(yes|E) = \frac{\frac{3}{5}\frac{1}{5}0.01032\frac{5}{10}}{P(E)} = \frac{0.000619}{P(E)}$$

$$P(no|E) = \frac{\frac{3}{5}\frac{3}{5}0.00595\frac{5}{10}}{P(E)} = \frac{0.001071}{P(E)}$$

- P(no|E)>P(yes|E) => Naïve Bayes predicts **loan default = no** for the new example

Naïve Bayes - discussion

- Probabilities are calculated easily due to the independence assumption
- Fast - requires 1 scan of the training data to calculate all statistics for both nominal and continuous attributes
- In many cases outperforms more sophisticated learning methods
- Robust to isolated noise points – such points have only negligible impact on the conditional probabilities
- Correlated attributes reduce the power of Naïve Bayes - violation of the independence assumption
  - Solution: apply feature selection beforehand to identify and discard correlated (redundant) attributes
- Normal distribution assumption for numeric attributes - many features are not normally distributed – solutions:
- Discretize the data first, i.e. numerical -> nominal attributes
- Use other probability density functions, e.g. Poisson, binomial, gamma

Evaluating Machine Learning Algorithms

Evaluating performance

- How to evaluate the generalization performance of ML models?
  - i.e. the performance on new, unseen data

- Evaluation procedures?
- Performance measures?

Evaluation Procedures

- Holdout method
- Cross validation
- Leave-one-out cross validation
- Cross-validation for parameter tuning

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Holdout method

- Split the data randomly into 2 sets: training set and test set
  - typically 2/3 and 1/3
- Build the model using the training data
- Evaluate the model on the test data
  - calculate accuracy or other performance measures

Accuracy

- Accuracy = proportion of correctly classified examples
  - predicted class = actual class
- We can calculate it on training and test set
  - accuracy on training set - overly optimistic, not a good indicator of generalization performance
  - accuracy on test set – used to evaluate generalization performance

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

training data

outlook	temp.	humidity	windy	play
sunny	hot	normal	false	no
overcast	mild	normal	false	yes
rainy	hot	normal	false	no
rainy	cool	high	true	no
sunny	mild	high	true	no

test data

Classifier:

if humidity=high then play=yes

elseif humidity=normal then play=no

Accuracy on test set =?

Validation set

- Sometimes we need to use a third set: validation set
  - The data is split into: training, validation and test set
- For example, some classification methods (decision trees, neural networks) operate in two stages:
  - Stage 1: Build the classifier
  - Stage 2: Tune its hyperparameters (see next slide)
- The test data can not be used for hyperparameter tuning
- Proper evaluation procedure - 3 datasets:
  - 1) Training set - to build the classifier
  - 2) Validation set - to tune its hyperparameters
  - 3) Test set - to evaluate accuracy

Parameters and hyperparameters

- Hyperparameter – parameter that can be tuned to optimize the performance of a ML algorithm
- Different from basic parameter that is part of a model, such as a coefficient in a linear regression model

- Examples of hyperparameters
  - in k-nearest neighbor algorithm: k
  - in neural networks: number of hidden layers and nodes in them; number of training epochs, etc.

- However, in ML we often just say *parameter tuning*, not *hyperparameter tuning*

Stratification

- Since the split into training and test set is random, without stratification some classes might be missing from the training or test sets, or be under-represented
  - e.g. if all examples with a certain class are missing in the training set (they went to the test set), the classifier cannot learn to predict this class
- Solution: stratification
- Can be used together with the holdout method -> an improved holdout method
- Ensures that each class is represented with approximately equal proportions in both data sets (training and testing)
  - e.g. if the class proportion in the whole dataset is 60% class1 and 40% class2, this ratio is maintained in the training and test split

Repeated holdout method

- The holdout method can be made more reliable by repeating the random split into training and test set several times and calculating average accuracy
  - e.g. repeating 10 times: in each of the 10 runs, a certain proportion (e.g. 2/3) is randomly selected for training (possibly with stratification) and the reminder is used for testing
  - the 10 accuracies are averaged to produce an overall average accuracy
- This is called repeated holdout method

- We can do better than this, e.g., by preventing the overlapping between the test sets

Cross-validation

- Avoids the overlapping test sets
- 10-fold cross-validation – typically used

Step 1: Split data into 10 sets set1,.., set10 of approximately equal size

Step 2: A classifier is built 10 times. Each time the testing is on 1 set (blue) and the training is on the remaining 9 sets together (white)

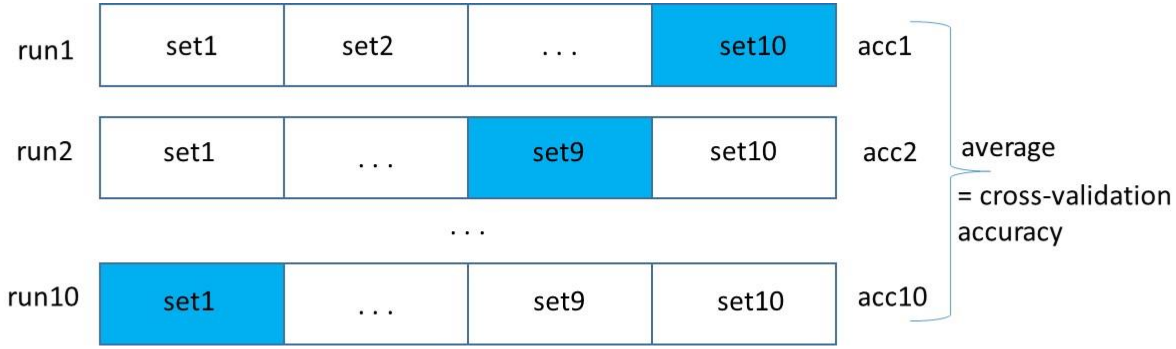
Run1: train on set1+…set9, test on set10 and calculate accuracy (acc1)

Run2: train on set1+…set8+set10, test on set9 and calculate accuracy (acc2)

….

Run10: train on set2+…set10, test on set1 and calculate accuracy (acc10)

Step 3: Calculate the cross validation accuracy = average (acc1, acc2,…acc10)



Cross-validation with stratification

- Stratified 10-fold cross-validation – this is a standard method for evaluation used in ML
  - each subset is stratified
- Why 10?
  - Extensive experiments have shown that this is the best choice to get an accurate estimate
  - There is also some theoretical evidence for this
- Even better: repeated stratified 10-fold cross-validation
  - e.g. 10-fold cross-validation is repeated 10 times and results are averaged – reduces the variance in splitting the data

Leave-one-out cross-validation

- A special form of n-fold cross-validation
  - Set the number of folds to the number of training examples
  - => for n training examples, build classifier n times

- Advantages:
  - Makes the best use of data - the greatest possible amount of data is used for training
  - Deterministic procedure – no random sampling is involved - the same result will be obtained every time
- Disadvantage
  - High computational cost, especially for large datasets

Cross-validation for parameter tuning

- We can also use cross-validation to search through different parameter combinations and select the best one
- Let's consider k-Nearest Neighbor and 2 of its parameters - k and distance measure type; we can search through the following combinations:
  - number of nearest neighbours k = 1, 3, 5, 11 and 13
  - distance measure - Manhattan and Euclidean
- => 5 x 2 combinations of parameter values
- We would like to find the best combination - the one that will generalise well on new examples

- We will use the following procedure, called grid-search with cross-validation for parameter tuning

Grid search with cross-validation for parameter tuning

Create the parameter grid (i.e. the parameter combinations)

Split the data into training set and test set

For each parameter combination:

    Train a k-NN classifier on the training data using 10-fold cross-validation

    Compute the cross-validation accuracy cv_acc

    If cv_acc > best_cv_acc

        best_cv_acc = cv_acc

        best_parameters = current parameters

Rebuild the k-NN model using the whole training data and best_parameters

Evaluate it on the test data and report the results

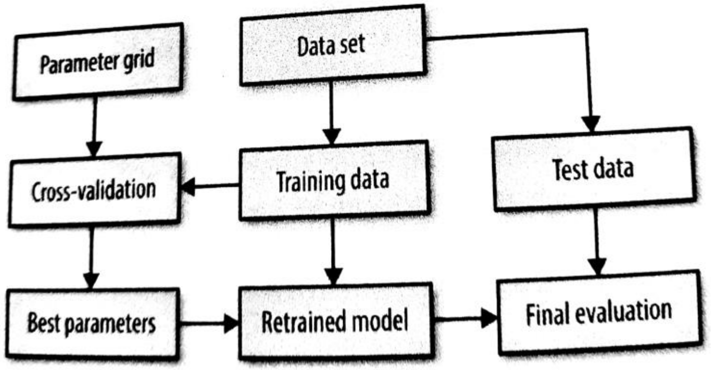


Image from Müller and Guido, Introduction to ML with Python

Grid search with cross-validation for parameter tuning (2)

- The data is split into training set and test set
- The cross-validation loop uses the training data
  - It is performed for every parameter combination
  - Its purpose is to select the best parameter combination - the one with the highest cross-validation accuracy
  - This involves, for every parameter combination, building 10 models on 90% of the training data (9 folds) and evaluating them on the remaining 10% (1 fold)
- Once this is done, a new model is trained using the selected best parameter combination on the whole training set and evaluated on the test set

- In sklearn, we can use GridSearchCV to do this – see the tutorial exercises using Python

More Performance Measures

- Confusion matrix
- Recall, precision and F1 score

Confusion matrix

- 2 class problem: yes and no
- 4 different outcomes - confusion matrix:

examples	# assigned to class yes	# assigned to class no
# from class yes	true positives (tp)	false negatives (fn)
# from class no	false positives (fp)	true negatives (tn)

- accuracy in terms of tp, fn, fp and tn? accuracy= (tp+tn)/(tp+fn+fp+tn)
- The confusion matrix is not a performance measure, it allows us to calculate performance measures

Confusion matrix for more than two classes

- E.g. iris data classification - confusion matrix:

```
  a  b  c   <-- classified as
 50  0  0 |  a = Iris-setosa
  0 44  6 |  b = Iris-versicolor
  0  3 47 |  c = Iris-virginica
```

- accuracy =?

- accuracy = (50+44+47)/(50+0+0+0+44+6+0+3+47) =141/150 =94%

Precision, recall and F1 score

- In addition to accuracy, other performance measures are precision (P), recall (R) and their combination - F1 score classification

$$P = \frac{tp}{tp + fp} \qquad R = \frac{tp}{tp + fn} \qquad F1 = \frac{2PR}{P + R}$$

examples	# assigned to class yes	# assigned to class no
# from class yes	true positives (tp)	false negatives (fn)
# from class no	false positives (fp)	true negatives (tn)