Performance Evaluation

Pedro Larrañaga, Concha Bielza

Computational Intelligence Group
Artificial Intelligence Department
Universidad Politécnica de Madrid

Machine Learning

Master in Data Science + Master HMDA

Outline

Outline

1. The supervised classification learning problem
2. Performance measures
3. Performance estimation

The supervised classification learning problem

Three components

1. An instance space $\Omega_{\mathbf{X}}$
   - Random vectors $\mathbf{x} = (x_1, ..., x_n) \in \mathbb{R}^n$ are drawn independently according to some fixed but unknown probability distribution, $p(\mathbf{x})$
   - The i-th component of $\mathbf{x}$, x_i, has been drawn from the subspace Ω_{X_i} and contains the value of the i-th predictor variable, X_i, for one specific instance
   - $\Omega_{\mathbf{X}} = \Omega_{X_1} \times \cdots \times \Omega_{X_n}$
2. A label space, Ω_C, containing for each vector $\mathbf{x} = (x_1, ..., x_n)$ the value, c, of its label. The labels are obtained from a random variable, C
   - The conditional distribution of labels for a given vector of the instance space, $p(c|\mathbf{x})$, and
   - The joint distribution, $p(\mathbf{x}, c)$, of cases (instances + labels) are also unknown
3. A learning algorithm that implements a set of functions over the instance space, whose outputs are in the label space. The application of the learning algorithm to a data set of labelled instances, $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$, will provide a supervised classification model

The supervised classification learning problem

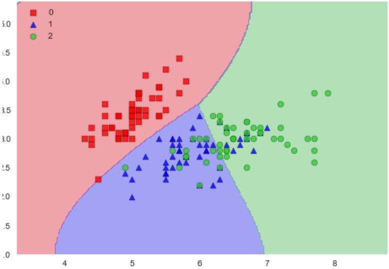
The data set $\mathcal{D}$ as a table

	X_1	$\ldots$	X_n	C
$(\boldsymbol{x}^{(1)}, c^{(1)})$	$x_1^{(1)}$	$\ldots$	$x_n^{(1)}$	$c^{(1)}$
$(\boldsymbol{x}^{(2)}, c^{(2)})$	$x_1^{(2)}$	$\ldots$	$x_n^{(2)}$	$c^{(2)}$
$\ldots$		$\ldots$		$\ldots$
$(\boldsymbol{x}^{(N)}, c^{(N)})$	$x_1^{(N)}$	$\ldots$	$x_n^{(N)}$	$c^{(N)}$
$\boldsymbol{x}^{(N+1)}$	$x_1^{(N+1)}$	$\ldots$	$x_n^{(N+1)}$	???

The supervised classification learning problem

Decision regions and decision boundaries

- The supervised classification model partitions the instance space into decision regions, one per class label. $\mathbf{x}$ is in the decision region associated with c if $\phi(\mathbf{x}) = c$.
- These regions are separated by decision boundaries, surfaces in the instance space corresponding to pairs of class labels reaching the same ϕ value
- The more flexible the decision boundaries, the better performance the classifier will have



Loss and risk functions

Loss and risk functions

- The loss function, $L(c, \phi(\mathbf{x}))$, is a quantitative measure of the loss when the label c of the vector $\mathbf{x}$ is different from the label assigned by the classifier, $\phi(\mathbf{x})$

$$\begin{array}{ccc} \Omega_C \times \Omega_C & \xrightarrow{L} & \mathbb{R}^+ \\ (c, \phi(\mathbf{x})) & \rightarrow & L(c, \phi(\mathbf{x})) \end{array}$$

  The zero-one loss function is $L(c, \phi(\mathbf{x})) = 1$ when $c \neq \phi(\mathbf{x})$ and 0 otherwise
- The expected risk of the classifier ϕ, $R(\phi) = \int L(c, \phi(\mathbf{x}))\mathrm{d}p(\mathbf{x}, c)$ computes the expectation of the loss (risk) function over the unknown distribution, $p(\mathbf{x}, \mathbf{c})$
  For the zero-one loss function, the expected risk associated with a classifier ϕ is calculated as $R_{0-1}(\phi) = p(C \neq \phi(\mathbf{X}))$ with cases drawn according to $p(\mathbf{x}, c)$
- The expected risk should be estimated using the information in $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$, by the empirical risk function, $R_{\mathcal{D}}(\phi)$, according to

$$R_{\mathcal{D}}(\phi) = \frac{1}{N} \sum_{i=1}^{N} L(c^i, \phi(\mathbf{x}^i))$$

Loss and risk functions

	X_1	...	X_n	C	$\phi(\mathbf{x})$
$(\mathbf{x}^1, c^1)$	7.2	...	10.4	P	I
$(\mathbf{x}^2, c^2)$	7.1	...	11.7	P	P
$(\mathbf{x}^3, c^3)$	6.4	...	13.2	P	P
$(\mathbf{x}^4, c^4)$	6.7	...	10.1	P	P
$(\mathbf{x}^5, c^5)$	8.9	...	8.4	I	P
$(\mathbf{x}^6, c^6)$	9.2	...	7.9	I	I
$(\mathbf{x}^7, c^7)$	10.7	...	5.9	I	I
$(\mathbf{x}^8, c^8)$	8.1	...	8.8	I	I
$(\mathbf{x}^9, c^9)$	9.9	...	7.2	I	I
$(\mathbf{x}^{10}, c^{10})$	11.5	...	6.9	I	I

- The output of the classifier is incorrect for Cases 1 and 5
- If each class is equally important, the loss associated with both types of mistakes is the same, and we have $L(c^i, \phi(\mathbf{x}^i)) = 1$ for $i \in \{1, 5\}$ and $L(c^j, \phi(\mathbf{x}^j)) = 0$ for $j \in \{2, 3, 4, 6, 7, 8, 9, 10\}$
- The empirical risk for this zero-one loss function would then be $R_{\mathcal{D}}(\phi) = 1/10 \times 2 = 0.20$. This empirical risk represents an estimation of the probability of the classifier being wrong

Outline

Binary classification

Two possible values for the class variable, C, represented, for example, as positive, $+$, and negative, $-$. $|\Omega_C| = 2 = |\Omega_{\phi(\mathbf{x})}| = 2$

Confusion matrix

$$\begin{array}{cc} & \phi(\mathbf{x}) \\ & \begin{array}{cc} + & - \end{array} \\ C \begin{array}{c} + \\ - \end{array} & \begin{pmatrix} \mathtt{TP} & \mathtt{FN} \\ \mathtt{FP} & \mathtt{TN} \end{pmatrix} \end{array}$$

- TP: true positives
- FP: false positives
- FN: false negatives
- TN: true negatives

Binary classification

Performance measures

Name	Formula
Accuracy	$\frac{\text{TP}+\text{TN}}{\text{TP}+\text{FN}+\text{FP}+\text{TN}}$
Sensitivity or Recall	$\frac{\text{TP}}{\text{TP}+\text{FN}}$
Specificity	$\frac{\text{TN}}{\text{FP}+\text{TN}}$
Positive predictive value or Precision	$\frac{\text{TP}}{\text{TP}+\text{FP}}$
Negative predictive value	$\frac{\text{TN}}{\text{TN}+\text{FN}}$
F_1-measure	$\frac{2\text{Prec}(\phi)\text{Rec}(\phi)}{\text{Prec}(\phi)+\text{Rec}(\phi)}$
Cohen's kappa statistic	$\frac{(\frac{\text{TP}}{N}+\frac{\text{TN}}{N})-[(\frac{\text{FN}+\text{TP}}{N})(\frac{\text{FP}+\text{TP}}{N})+(\frac{\text{FP}+\text{TN}}{N})(\frac{\text{FN}+\text{TN}}{N})]}{1-[(\frac{\text{FN}+\text{TP}}{N})(\frac{\text{FP}+\text{TP}}{N})+(\frac{\text{FP}+\text{TN}}{N})(\frac{\text{FN}+\text{TN}}{N})]}$

- The F_1 measure (van Rijsbergen, 1979) is the harmonic mean of the precision and recall measures
- Cohen's kappa statistic (Cohen, 1960) corrects the accuracy measure considering the result of a mere chance match between the classifier, $\phi(\mathbf{x})$, and the label generation process, C
- All measure values fall within the interval $[0, 1]$, where values close to 1 are preferred

Binary classification

Performance measures. An example

$$\begin{array}{cc} & \phi(\mathbf{x}) \\ & \begin{array}{cc} + & - \end{array} \\ C \begin{array}{c} + \\ - \end{array} & \begin{pmatrix} 120 & 8 \\ 60 & 139 \end{pmatrix} \end{array}$$

The values for the seven performance measures are:

1. $\text{Acc}(\phi) = 0.79$
2. $\text{Sensitivity}(\phi) = \text{Rec}(\phi) = 0.94$
3. $\text{Specificity}(\phi) = 0.74$
4. $\text{PPV}(\phi) = \text{Prec}(\phi) = 0.67$
5. $\text{NPV}(\phi) = 0.95$
6. $F_1(\phi) = 0.78$
7. $\kappa(\phi) = 0.59$

Binary classification

Cost matrix

$$
\begin{array}{ccc}
 & \multicolumn{2}{c}{\phi(\mathbf{x})} \\
 & + & - \\
C \begin{array}{c} + \\ - \end{array} & \multicolumn{2}{c}{\begin{pmatrix} 0 & \mathrm{L}(+,-) \\ \mathrm{L}(-,+) & 0 \end{pmatrix}}
\end{array}.
$$

- Total cost error: $\mathrm{TCE}(\phi) = \mathtt{FN} \cdot L(+,-) + \mathtt{FP} \cdot L(-,+)$
- Total cost error in terms of the empirical risk as $\mathrm{TCE}(\phi) = N \cdot R_{\mathcal{D}}(\phi)$
- The total cost error verifies $0 \leq \mathrm{TCE}(\phi) \leq N \cdot \max\{L(+,-), L(-,+)\}$
- If the domain expert is not able to provide this information, costs are assumed to be symmetric: $L(+,-) = L(-,+)$

Binary classification

- The Brier score (Brier, 1950) measures the accuracy of probabilistic classifications over cases
- Measure of the calibration of a set of probabilistic predictions or as a quadratic cost function

Brier score

$$\text{Brier}(\phi) = \frac{1}{N}\sum_{i=1}^{N} d^2\left(p_\phi(\mathbf{c}|\mathbf{x}^i), \mathbf{c}^i\right)$$

- N denotes the number of cases in $\mathcal{D}$
- $p_\phi(\mathbf{c}|\mathbf{x}^i)$ is the vector $(p_\phi(+|\mathbf{x}^i), p_\phi(-|\mathbf{x}^i))$ containing the output of the probabilistic classifier
- $\mathbf{c}^i = (1,0)$ or $\mathbf{c}^i = (0,1)$ when the label of the i-th instance is $+$ or $-$, respectively
- The difference between the predicted probability assigned to the possible outcomes for each instance and its actual label is measured with the squared Euclidean distance, $d^2\left(p_\phi(\mathbf{c}|\mathbf{x}^i), \mathbf{c}^i\right)$
- The Brier score for a binary classification problem verifies $0 \leq \text{Brier}(\phi) \leq 2$

Binary classification

Brier score

	X_1	...	X_n	C	$p_\phi(\mathbf{c}\|\mathbf{x})$
$(\mathbf{x}^1, c^1)$	7.2	...	10.4	P	(0.20, 0.80)
$(\mathbf{x}^2, c^2)$	7.1	...	11.7	P	(0.65, 0.35)
$(\mathbf{x}^3, c^3)$	6.4	...	13.2	P	(0.70, 0.30)
$(\mathbf{x}^4, c^4)$	6.7	...	10.1	P	(0.87, 0.13)
$(\mathbf{x}^5, c^5)$	8.9	...	8.4	I	(0.55, 0.45)
$(\mathbf{x}^6, c^6)$	9.2	...	7.9	I	(0.25, 0.75)
$(\mathbf{x}^7, c^7)$	10.7	...	5.9	I	(0.12, 0.88)
$(\mathbf{x}^8, c^8)$	8.1	...	8.8	I	(0.07, 0.93)
$(\mathbf{x}^9, c^9)$	9.9	...	7.2	I	(0.37, 0.63)
$(\mathbf{x}^{10}, c^{10})$	11.5	...	6.9	I	(0.18, 0.82)

$$\mathrm{Brier}(\phi) = \frac{1}{10}\left[(0.20-1)^2 + (0.80-0)^2 + \cdots + (0.18-0)^2 + (0.82-1)^2\right] = 0.2971$$

Multi-class classification

Confusion matrix

$$
\begin{array}{cc}
 & \phi(\mathbf{x}) \\
 & \begin{array}{ccccc} c_1 & \cdots & c_j & \cdots & c_R \end{array} \\
C \begin{array}{c} c_1 \\ \cdots \\ c_j \\ \cdots \\ c_R \end{array} & \begin{pmatrix} N_{11} & \cdots & N_{1j} & \cdots & N_{1R} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ N_{j1} & \cdots & N_{jj} & \cdots & N_{jR} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ N_{R1} & \cdots & N_{Rj} & \cdots & N_{RR} \end{pmatrix}
\end{array}
$$

Measures from the confusion matrix

Name	Notation	Formula
Accuracy	$\mathrm{Acc}(\phi)$	$\frac{\sum_{i=1}^{R} N_{ii}}{N}$
PPV or Prec for class c_j	$\mathrm{PPV}_j(\phi) = \mathrm{Prec}_j(\phi)$	$\frac{N_{jj}}{\sum_{i=1}^{R} N_{ij}}$
Total cost error	$\mathrm{TCE}(\phi)$	$\sum_{i=1}^{R} \sum_{j>i}^{R} N_{ij} \cdot L(c_i, c_j)$
Brier score	$\mathrm{Brier}(\phi)$	$\frac{1}{N} \sum_{i=1}^{N} d^2 \left(p_\phi(\mathbf{c}\vert\mathbf{x}^i), \mathbf{c}^i \right)$

$N = \sum_{i=1}^{R} \sum_{i=1}^{R} N_{ij}$

Binary classification

- A receiver operating characteristic (ROC), or simply ROC curve (Lusted, 1960), is a graphical plot that illustrates the performance of a binary classifier system as its discrimination threshold is varied
- The discrimination threshold is a cutoff value for the posterior probability $p_\phi(c|\mathbf{x})$ for which the predicted label is $+$
- A given discrimination threshold returns a point of the plot
- The ROC curve is created by plotting (on the Y-axis) the true positive rate ($\texttt{TPR}= \frac{\texttt{TP}}{\texttt{TP}+\texttt{FN}}$), versus (on the X-axis) the false positive rate ($\texttt{FPR} = \frac{\texttt{FP}}{\texttt{FP}+\texttt{TN}}$), at various threshold settings. $\texttt{TP}+\texttt{FN} = N_+$ number of real positive. $\texttt{FP}+\texttt{TN} = N_-$ number of real negative
- The ROC curve is the polygonal curve plotted by connecting all pairs of consecutive points
- The ROC space is a unit square because $0 \leq \texttt{FPR} \leq 1$ and $0 \leq \texttt{TPR} \leq 1$

$$
\begin{array}{cc}
 & \phi(\mathbf{x}) \\
 & \begin{array}{cc} + & - \end{array} \\
C \begin{array}{c} + \\ - \end{array} & \begin{pmatrix} \texttt{TP} & \texttt{FN} \\ \texttt{FP} & \texttt{TN} \end{pmatrix}
\end{array}
$$

Binary classification

- Point $(0,0)$, with both $\texttt{FPR}$ and $\texttt{TPR}$ equal to zero, denotes the model that classifies all instances as negative
- Point $(1,1)$, with both $\texttt{FPR}$ and $\texttt{TPR}$ equal to one, represents the classifier labeling all instances as positive
- The diagonal of the ROC space, that is, the line connecting points $(0,0)$ and $(1,1)$, verifies $\texttt{FPR} = \texttt{TPR}$ at all points. The classifiers represented with points along this diagonal are regarded as random classifiers. The random classifier at point (a,a) means that, for a positive labelled case, $C = +$, the probability that the classifier, ϕ, classifies it as positive, $\phi = +$, equals a. In mathematical notation, $p(\phi = +|C = +) = a$. For a negative labelled case, $p(\phi = +|C = -) = a$.
- The classifiers represented by points above (or below) the diagonal perform better (or worse) than random
- $(\texttt{FPR}_1, \texttt{TPR}_1)$ represents a better classifier than $(\texttt{FPR}_2, \texttt{TPR}_2)$ if $(\texttt{FPR}_1, \texttt{TPR}_1)$ is on the left and higher up than $(\texttt{FPR}_2, \texttt{TPR}_2)$, because these positions signify that $\texttt{FPR}_1 < \texttt{FPR}_2$ and $\texttt{TPR}_1 > \texttt{TPR}_2$
- For point $(1,0)$, $\texttt{FPR} = 1$ and $\texttt{TPR} = 0$. It denotes a classifier that gets all its predictions wrong
- Point $(0,1)$ represents the best classifier, which gets all the positive cases right and none the negative ones wrong

Binary classification

Notation used by Algorithm 1 for building a ROC curve

ROC analysis in binary classification

- $\mathcal{D}$: the set of cases
- $\phi(\mathbf{x}^i)$: the continuous output of the classifier for instance $\mathbf{x}^i$
- *min* and *max*: the smallest and largest values returned by $\phi(\mathbf{x})$, respectively,
- *incr*: the smallest difference between any two output values
- N_+ and N_-: the number of real positive and negative cases, respectively
- The range of the threshold values t is $min, min + incr, min + 2 \cdot incr, ..., max$
- `TP` and `FP` are initialized as 0 (lines 2 and 3)
- For each case whose classification output exceeds threshold t (line 5), the `TP` counter is incremented by one if the case is positive (lines 6-7); for negative cases (lines 8-9) the `FP` counter is incremented by one
- `TPR` and `FPR` are respectively computed (lines 12 and 13) and the associated (`FPR`, `TPR`) is added to the ROC curve (line 14)

Binary classification

ROC analysis in binary classification

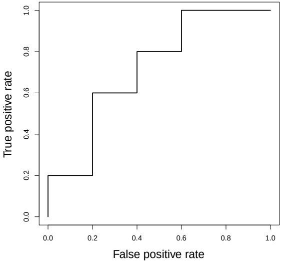
Algorithm 1: A simple algorithm for building a ROC curve (Fawcett, 2006)

Input : A classifier ϕ, and constants *min*, *max*, *incr*, N_+, N_-
Output: A ROC curve

```
for t = min to max by incr do
    TP = 0
    FP = 0
    for x^i ∈ D do
        if φ(x^i) ≥ t then
            if x^i is a positive case then
                TP = TP +1
            else
                FP = FP +1
        endif
    endfor
    TPR = TP/N_+
    FPR = FP/N_-
    Add point (FPR, TPR) to ROC curve
endfor
```

Binary classification

Instances	$\mathbf{x}^i$	1	2	3	4	5	6	7	8	9	10
Output	$p(+\|\mathbf{x}^i)$	0.97	0.91	0.84	0.80	0.68	0.67	0.66	0.61	0.49	0.46
True class	c^i	+	−	+	+	−	+	−	+	−	−



- $\mathtt{FPR} = \frac{\mathtt{FP}}{N_-}$ and $\mathtt{TPR} = \frac{\mathtt{TP}}{N_+}$
- First threshold at 0.46. At it, the five positive instances are well classified, whereas the five negative instances are misclassified. We get $\mathtt{FPR} = \mathtt{TPR} = 1$
- All the thresholds output by increments of 0.01 (value of `incr`) up to 0.49 yield the same results
- At 0.49, the instance $\mathbf{x}^{10}$ is correctly classified as $-$, and we get $\mathtt{FPR} = 0.80$, and $\mathtt{TPR} = 1$
- The next significant threshold is 0.61, where we get the third point, $(0.60, 1)$
- The other points are output in a similar fashion

Binary classification

The area under the ROC curve (AUC)

- The AUC is the most popular summary statistic for the ROC curve: $\text{AUC}(\phi) \in [0, 1]$
- A perfect classifier, ($\texttt{FPR} = 0$, $\texttt{TPR} = 1$): $\text{AUC}(\phi_{\text{perfect}}) = 1$
- A random classifier: $\text{AUC}(\phi_{\text{random}}) = 0.5$
- The AUC can be computed as: $\text{AUC}(\phi) = 1 - \frac{\sum_{i=1}^{N_+}(i - \text{rank}_i)}{N_+ \cdot N_-}$
    - rank_i is the rank (according to the posterior probability of $C = +$) of the i-th case in the subset of positive labels given by classifier ϕ
    - N_+ and N_- denote the number of real positive and negative cases in $\mathcal{D}$, respectively
- AUC can be interpreted as a measurement indicator of whether a classifier is able to rank a randomly chosen positive instance higher than a negative one

$$\text{AUC}(\phi) = 1 - \frac{(1-1)+(3-2)+(4-3)+(6-4)+(8-5)}{5 \cdot 5} = 0.72$$

The AUC directly from the Figure:

$$\text{AUC}(\phi) = 0.20 \cdot 0.20 + 0.20 \cdot 0.60 + 0.20 \cdot 0.80 + 0.40 \cdot 1 = 0.72$$

Multi-class classification

ROC analysis in multi-class problems

- For multi-class problems the AUC can be generalized as the volume under the ROC surface (Ferri et al., 2003)
- Alternatively, as an average AUC of all possible two-class ROC curves that can be generated from the multi-class problem (Hand and Till, 2001)

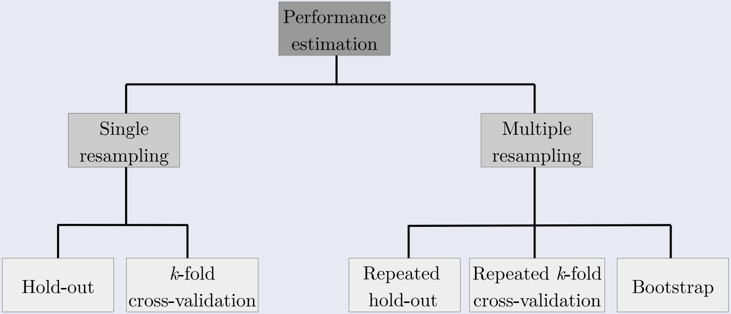
$$\mathrm{AUC}_{\text{multi-class}}(\phi) = \frac{2}{R(R-1)} \sum_{\substack{c_i, c_j \in \Omega_C \\ c_i \neq c_j}} \mathrm{AUC}_{c_i, c_j}(\phi)$$

  - $\mathrm{AUC}_{\text{multi-class}}(\phi)$ is the total AUC of the multi-class ROC for classifier ϕ
  - $\mathrm{AUC}_{c_i, c_j}(\phi)$ is the AUC of the two-class ROC curve of ϕ for classes c_i and c_j

Outline

Honest estimation methods

Honest estimation methods according to their sampling characteristics

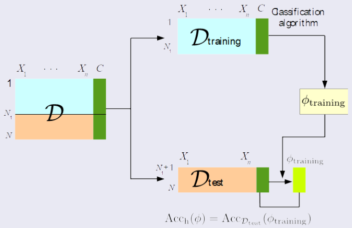


Single resampling-based estimation methods

$\mathcal{D} = \{(\mathbf{x}^1, c^1), \ldots, (\mathbf{x}^N, c^N)\}$ is partitioned into two disjoint data subsets:

- The training data set: $\mathcal{D}_{\text{training}} = \{(\mathbf{x}^1, c^1), \ldots, (\mathbf{x}^{N_1}, c^{N_1})\}$ with N_1 cases and
- The test data set: $\mathcal{D}_{\text{test}} = \mathcal{D} \setminus \mathcal{D}_{\text{training}} = \{(\mathbf{x}^{N_1+1}, c^{N_1+1}), \ldots, (\mathbf{x}^N, c^N)\}$ with $N - N_1$ cases

Hold-out estimation



A general empirical risk function is estimated as follows: $R_{\mathcal{D}_{\text{test}}}(\phi_{\text{training}}) = \frac{1}{N-N_1} \sum_{(\mathbf{x}^i, c^i) \in \mathcal{D}_{\text{test}}} L(c^i, \phi_{\text{training}}(\mathbf{x}^i))$

The hold-out estimation of classification accuracy:

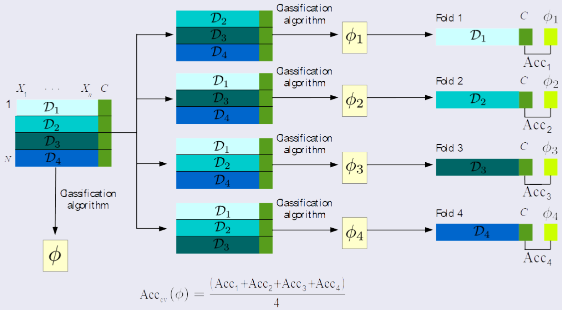
$$\text{Acc}_h(\phi) = \text{Acc}_{\mathcal{D}_{\text{test}}}(\phi_{\text{training}}) = \frac{1}{N - N_1} \sum_{(\mathbf{x}^i, c^i) \in \mathcal{D}_{\text{test}}} \mathbb{I}(c^i = \phi_{\text{training}}(\mathbf{x}^i))$$

where $\mathbb{I}(a)$ is the indicator function

Single resampling-based estimation methods

$\mathcal{D} = \{(\mathbf{x}^1, c^1), \ldots, (\mathbf{x}^N, c^N)\}$, is partitioned into k folds: $\mathcal{D}_1, \ldots, \mathcal{D}_k$, verifying $\mathcal{D} = \bigcup_{l=1}^{k} \mathcal{D}_l$ with $\mathcal{D}_w \bigcap \mathcal{D}_t = \varnothing$

k-fold cross-validation (Kurtz, 1948)



Accuracy of ϕ estimated as $\mathrm{Acc}_{\mathrm{cv}}(\phi) = \frac{1}{k}\sum_{l=1}^{k} \mathrm{Acc}_l$ with $\mathrm{Acc}_l = \frac{1}{|\mathcal{D}_l|} \sum_{(\mathbf{x}^i, c^i) \in \mathcal{D}_l} \mathbb{I}(c^i = \phi_l(\mathbf{x}^i))$

- The k-fold cross-validation estimator is very nearly unbiased, but its variance can be large (Stone, 1977)
- Leave-one-out cross-validation when $k = N$
- Stratified k-fold cross-validation for unbalanced data sets

Multiple resampling-based estimation methods

Repeated hold-out

- $\mathcal{D} = \{(\mathbf{x}^1, c^1), ..., (\mathbf{x}^N, c^N)\}$, is randomly partitioned B times as training data sets, $\mathcal{D}^l_{\text{training}}$, and test data sets, $\mathcal{D}^l_{\text{test}}$. For each partition $l \in \{1, ..., B\}$: $\mathcal{D} = \mathcal{D}^l_{\text{training}} \bigcup \mathcal{D}^l_{\text{test}}$ and $\mathcal{D}^l_{\text{training}} \bigcap \mathcal{D}^l_{\text{test}} = \varnothing$
- The final model, ϕ, is learned from $\mathcal{D}$, and its accuracy is estimated as

$$\text{Acc}_{\text{rh}}(\phi) = \frac{1}{B} \sum_{l=1}^{B} \text{Acc}^l$$

where Acc^l denotes the estimation of the accuracy of model ϕ^l_{training} , learned from $\mathcal{D}^l_{\text{training}}$, and tested over $\mathcal{D}^l_{\text{test}}$

- Repeated hold-out extends the main idea of the hold-out scheme to a multiple resampling scenario. The partition in the hold-out scheme is repeated several times, each with a random assignment of training and test cases
- Advantage: stability of the estimates (variance is low), resulting from a large number of sampling repetitions
- Drawback: there is no control of how many times each case is used in the training data sets or in the test data sets

Multiple resampling-based estimation methods

Repeated k-fold cross-validation

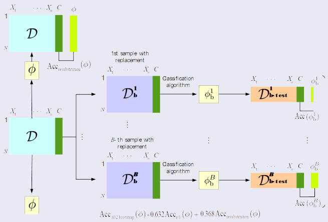
Repeated k-fold cross-validation reduces the variability of the estimator by multiple rounds of k-fold cross-validation performed using different partitions

- The 5×2 cross-validation (Dietterich, 1998) performs five repetitions of two-fold cross-validation
- The 10×10 cross-validation (Bouckaert, 2003) based on 10 repetitions of 10-fold cross-validation

Multiple resampling-based estimation methods

- Bootstrap sampling method consists of sampling with replacement N cases from $\mathcal{D} = \{(\mathbf{x}^1, c^1), \ldots, (\mathbf{x}^N, c^N)\}$
- Repeated B times: $\mathcal{D}_{\mathrm{b}}^l$, with $l \in \{1, \ldots, B\}$, all of size N
- The probability of a case not being chosen after N selections is $(1 - \frac{1}{N})^N \approx \frac{1}{e} \approx 0.368$
- The expected number of distinct cases in each of the B data sets $\mathcal{D}_{\mathrm{b}}^l$ used for training the classifier is $0.632N$
- $\mathcal{D}_{\mathrm{b-test}}^l = \mathcal{D} \setminus \mathcal{D}_{\mathrm{b}}^l$ and $\mathrm{Acc}(\phi_{\mathrm{b}}^l) = \frac{1}{|\mathcal{D}_{\mathrm{b-test}}^l|} \sum_{(\mathbf{x}^i, c^i) \in \mathcal{D}_{\mathrm{b-test}}^l} \mathbb{I}(c^i = \phi_{\mathrm{b}}^l(\mathbf{x}^i))$
- The **e0** bootstrap estimate, $\mathrm{Acc}_{\mathrm{e0}}(\phi) = \frac{1}{B} \sum_{l=1}^{B} \mathrm{Acc}(\phi_{\mathrm{b}}^l)$ can be pessimistic

0.632 bootstrap method (Efron, 1979)



$$\mathrm{Acc}_{.632\mathrm{bootstrap}}(\phi) = 0.632\mathrm{Acc}_{\mathrm{e0}}(\phi) + 0.368\mathrm{Acc}_{\mathrm{resubstitution}}(\phi)$$

where the resubstitution estimation is: $\mathrm{Acc}_{\mathrm{resubstitution}}(\phi) = \frac{1}{N} \sum_{(\mathbf{x}^i, c^i) \in \mathcal{D}} \mathbb{I}(c^i = \phi(\mathbf{x}^i))$

- Bootstrap estimation is asymptotically (large values of B) unbiased and its variance is small. These are interesting properties when working with small data sets.

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