

Chapter ML:II (continued)

II. Machine Learning Basics

- ❑ Regression
- ❑ Concept Learning: Search in Hypothesis Space
- ❑ Concept Learning: Search in Version Space
- ❑ Evaluating Effectiveness

Evaluating Effectiveness

True Misclassification Rate

Definition 8 (True Misclassification Rate)

Let X be a feature space with a finite number of elements. Moreover, let C be a set of classes, let $y : X \rightarrow C$ be a classifier, and let c be the target concept to be learned. Then the true misclassification rate, denoted as $Err^*(y)$, is defined as follows:

$$Err^*(y) = \frac{|\{\mathbf{x} \in X : y(\mathbf{x}) \neq c(\mathbf{x})\}|}{|X|}$$

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Problem:

- Usually the *total function* c is unknown.

Solution:

- **Estimation** of $Err^*(y)$ with $Err(y, D_{ts})$, i.e., evaluating y on a subset $D_{ts} \subseteq D$ of carefully chosen examples D . Recall that for the feature vectors in D the target concept c is known.

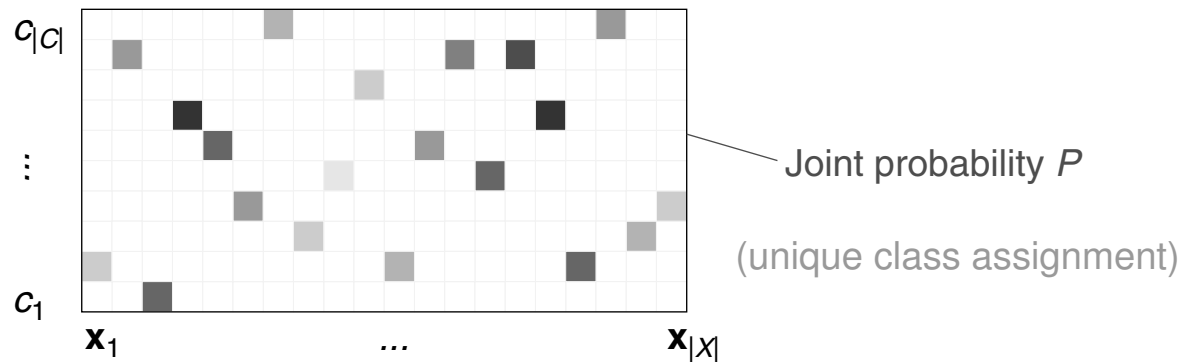
Remarks:

- ❑ Instead of the term “true misclassification rate” we may also use the term “true misclassification error” or simply “true error”.
- ❑ The English word “rate” can be used to denote both the mathematical concept of a *flow quantity* (a change of a quantity per time unit) as well as the mathematical concept of a *portion*, a *percentage*, or a *ratio*, which has a stationary (= time-independent) semantics. Note that the latter semantics is meant here when talking about the misclassification rate.
- ❑ Unfortunately, the German word „Rate“ is often (mis)used to denote the mathematical concept of a portion, a percentage, or a ratio. Taking a precise mathematical standpoint, the correct German words are „Anteil“ or „Quote“. I.e., a semantically correct translation of misclassification rate is „Missklassifikationsanteil“, and not „Missklassifikationsrate“.

Evaluating Effectiveness

True Misclassification Rate: Probabilistic Foundation

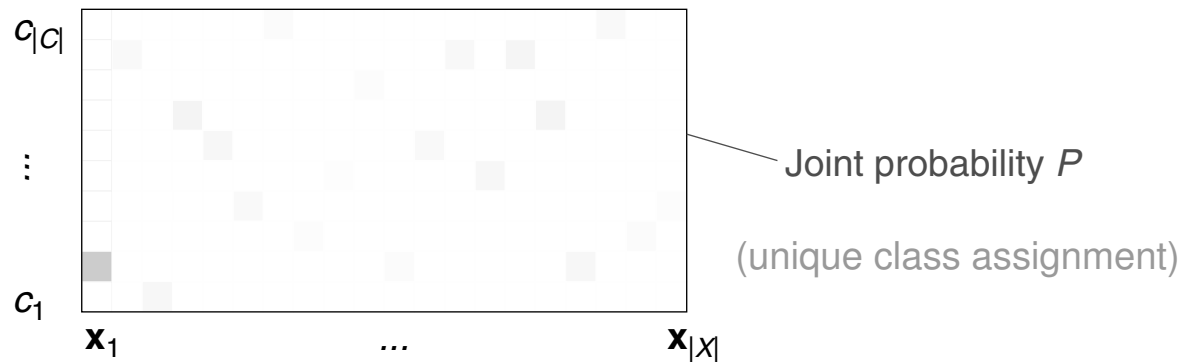
Let X be a feature space, C a set of classes, and P a probability measure on $X \times C$. Then $P(\mathbf{x}, c)$ (precisely: $P(\mathcal{H} = \mathbf{x}, \mathcal{C} = c)$) denotes the probability (1) to observe the vector $\mathbf{x} \in X$ and (2) that \mathbf{x} belongs to class $c \in C$. Illustration:



Evaluating Effectiveness

True Misclassification Rate: Probabilistic Foundation (continued)

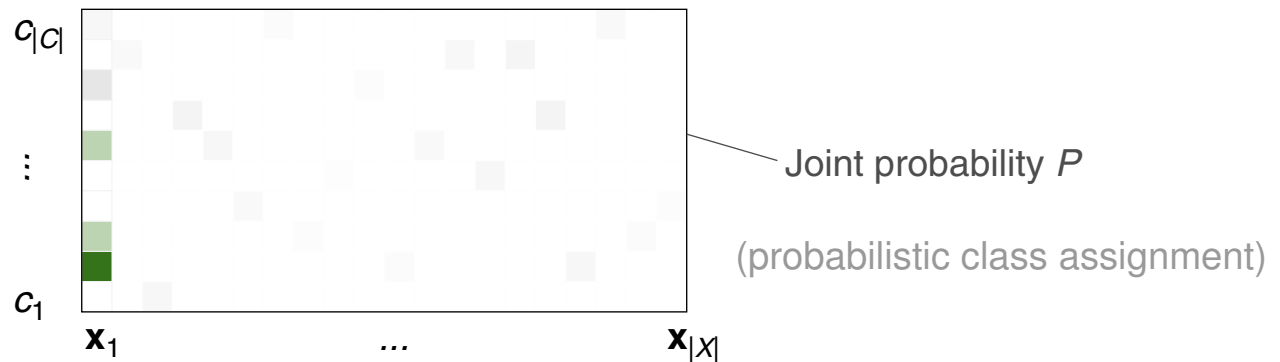
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Evaluating Effectiveness

True Misclassification Rate: Probabilistic Foundation (continued)

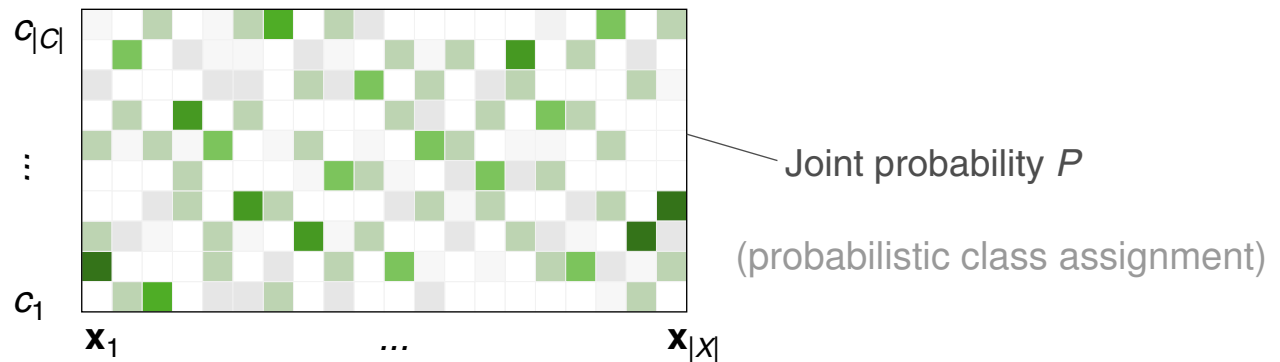
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Evaluating Effectiveness

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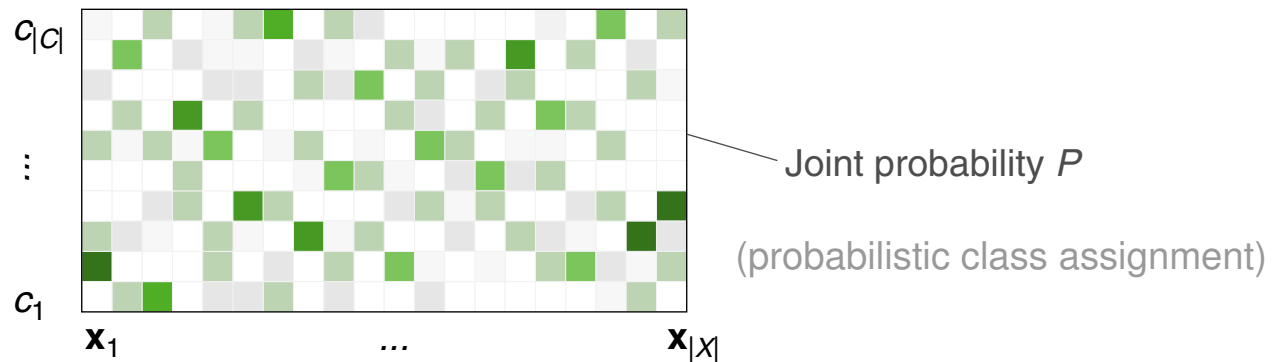
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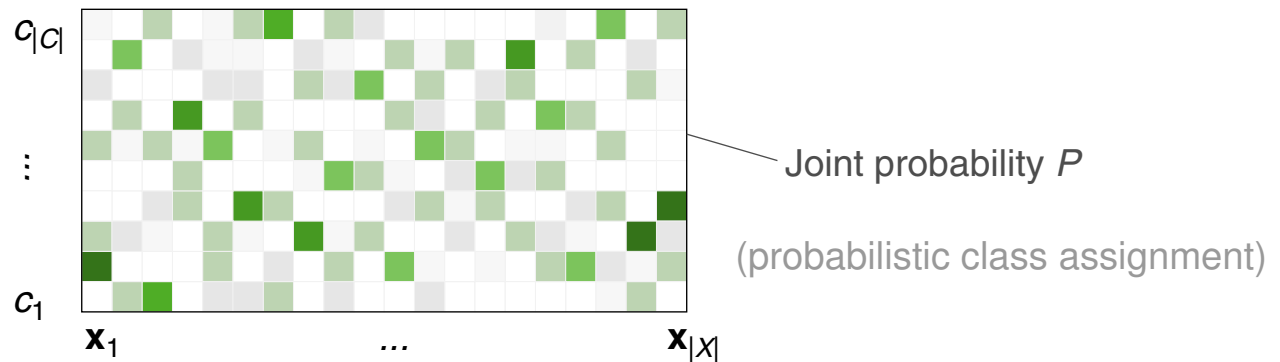


$$\underline{Err^*}(y) = \sum_{\mathbf{x} \in X} \sum_{c \in C} P(\mathbf{x}, c) \cdot I(y(\mathbf{x}), c), \quad \text{with } I(y(\mathbf{x}), c) = \begin{cases} 0 & \text{if } y(\mathbf{x}) = c \\ 1 & \text{otherwise} \end{cases}$$

Evaluating Effectiveness

True Misclassification Rate: Probabilistic Foundation (continued)

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$$\underline{Err^*(y)} = \sum_{\mathbf{x} \in X} \sum_{c \in C} P(\mathbf{x}, c) \cdot I(y(\mathbf{x}), c), \quad \text{with } I(y(\mathbf{x}), c) = \begin{cases} 0 & \text{if } y(\mathbf{x}) = c \\ 1 & \text{otherwise} \end{cases}$$

$D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\} \subseteq X \times C$ is a set of examples whose elements are drawn independently and according to the same P .

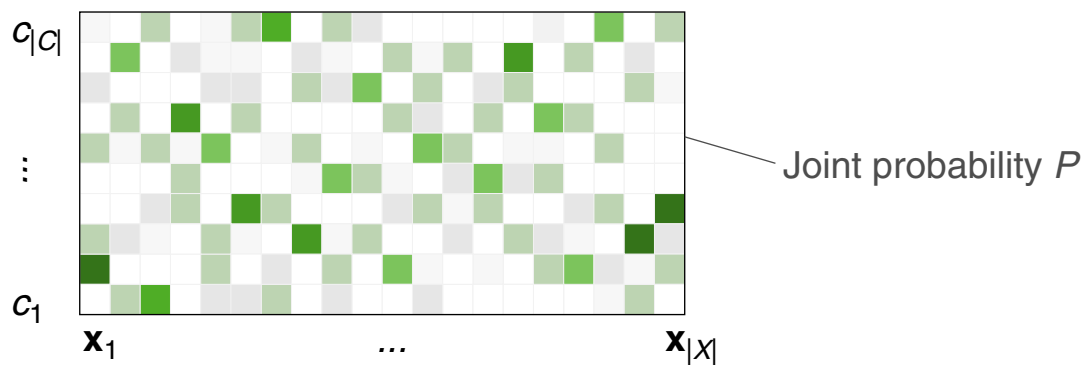
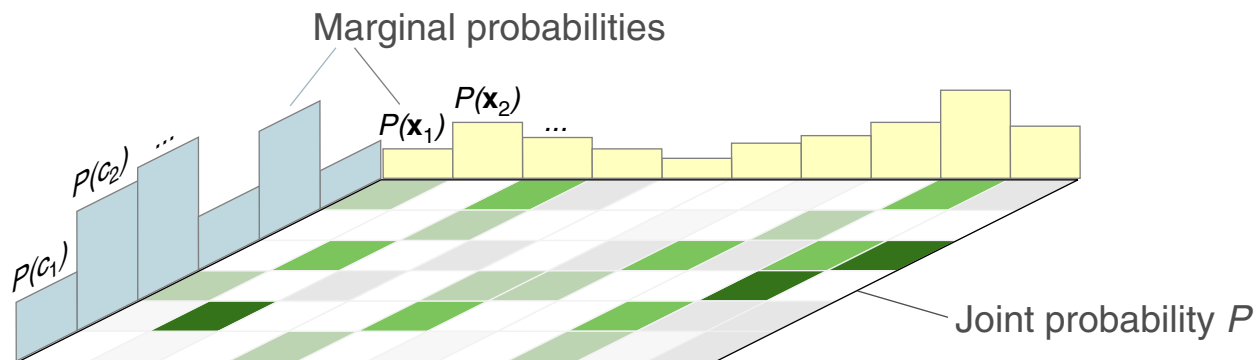
Remarks:

- ❑ \mathcal{H} and \mathcal{C} are random variables with domains X and C respectively. In particular, X may not be restricted to contain a finite number of elements.
- ❑ \mathbf{x} is modeled as random variable, \mathcal{H} , to account for the fact that each observation process is governed by a probability distribution, rendering certain observations more likely than others. Note that in the definition of the True Misclassification Rate the set X is implicitly treated as uniformly distributed: each element in X contributes to the same amount to Err^* .
- ❑ The function $c(\mathbf{x})$ is modeled as random variable, \mathcal{C} , since in the real world the classification of a feature vector \mathbf{x} may not be deterministic but the result of a random (measuring) process. Keyword: label noise.
- ❑ Let A and B denote two events, e.g., $A = “\mathcal{H} = \mathbf{x}”$ and $B = “\mathcal{C} = c”$. Then the following expressions are syntactic variants, i.e., they are semantically equivalent: $P(A, B)$, $P(A \text{ and } B)$, $P(A \wedge B)$.
- ❑ Also the sampling process is a stochastic process: The elements in D and D_{ts} are considered as random variables that are both independent of each other and identically distributed. This property of a set of random variables is abbreviated with “i.i.d.”
If the elements in D or D_{ts} are not chosen according to P , then $Err(y, D_{ts})$ cannot be used as an estimation of $Err^*(y)$. Keyword: sample selection bias

Evaluating Effectiveness

True Misclassification Rate: Probabilistic Foundation (continued)

Illustration of the marginal probabilities $P(c_i)$ and $P(\mathbf{x}_j)$:



Remarks:

- $P(\mathbf{x} \mid c_i)$ is the probability distribution of \mathcal{H} under class $\mathcal{C} = c_i$.
 $P(\mathbf{x} \mid c_i)$ is also called “class-conditional *probability [density]* function”.

In the illustration: the distribution of \mathbf{x} (consider a row) for a certain class c .
Summation (integration) over the $\mathbf{x} \in X$ yields the marginal probability $P(c_i)$.

- $P(c \mid \mathbf{x}_j)$ is the probability distribution of \mathcal{C} under feature vector $\mathcal{H} = \mathbf{x}_j$.
 $P(c \mid \mathbf{x}_j)$ is also called “conditional *class probability* function”.

In the illustration: the distribution of c (consider a column) for a certain feature vector \mathbf{x} .
Summation over the $c \in C$ yields the marginal probability $P(\mathbf{x}_j)$.

- $P(\mathbf{x}_j, c_i) = P(\mathbf{x}_j \mid c_i) \cdot P(c_i)$, where $P(c_i)$ is the a-priori probability for (observing) event c_i , and $P(\mathbf{x}_j \mid c_i)$ is the probability for (observing) event \mathbf{x}_j given event c_i .

Likewise, $P(\mathbf{x}_j, c_i) = P(c_i, \mathbf{x}_j) = P(c_i \mid \mathbf{x}_j) \cdot P(\mathbf{x}_j)$, where $P(\mathbf{x}_j)$ is the a-priori probability for (observing) event \mathbf{x}_j , and $P(c_i \mid \mathbf{x}_j)$ is the probability for (observing) event c_i given event \mathbf{x}_j .

- Let both events $\mathcal{H} = \mathbf{x}_j$ and $\mathcal{C} = c_i$ have occurred already, and, let \mathbf{x}_j be known and c_i be unknown. Then, $P(\mathbf{x}_j \mid c_i)$ is called *likelihood* (for event \mathbf{x}_j given event c_i).

Evaluating Effectiveness

Training Error [True Misclassification Rate]

- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \dots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.
- $D_{tr} = D$ is the training set.
- $y : X \rightarrow C$ is a classifier learned on the basis of D_{tr} .

Training error = misclassification rate with respect to D_{tr} :

$$Err(y, D_{tr}) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_{tr} : y(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D_{tr}|}$$

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Training Error [True Misclassification Rate]

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Problems:

- $Err(y, D_{tr})$ is based on examples that are also exploited to learn y .
- $Err(y, D_{tr})$ quantifies **memorization** but **not** the **generalization** capability of y .
- $Err(y, D_{tr})$ is an optimistic estimation, i.e., it is constantly lower compared to the error incurred when applying y in the wild.

Evaluating Effectiveness

2-Fold Cross-Validation (Holdout Estimation) [True Misclassification Rate]

- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \dots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.
- $D_{tr} \subset D$ is the training set.
- $y : X \rightarrow C$ is a classifier learned on the basis of D_{tr} .
- $D_{ts} \subset D$ with $D_{ts} \cap D_{tr} = \emptyset$ is a test set.

Holdout estimation = misclassification rate with respect to D_{ts} :

$$Err(y, D_{ts}) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_{ts} : y(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D_{ts}|}$$

Evaluating Effectiveness

2-Fold Cross-Validation (Holdout Estimation) [True Misclassification Rate]

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Holdout estimation = misclassification rate with respect to D_{ts} :

$$Err(y, D_{ts}) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_{ts} : y(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D_{ts}|}$$

Requirements:

- D_{tr} and D_{ts} must be **governed by the same distribution**.
- D_{tr} and D_{ts} should have similar sizes.

Remarks:

- ❑ A typical value for splitting D into training set D_{tr} and test set D_{ts} is 2:1.
- ❑ When splitting D into D_{tr} and D_{ts} one has to ensure that the underlying distribution is maintained. Keywords: stratification, sample selection bias

Evaluating Effectiveness

k -Fold Cross-Validation [Holdout Estimation]

- Form k test sets by splitting D into disjoint sets D_1, \dots, D_k of similar size.
- For $i = 1, \dots, k$ do:
 1. $y_i : X \rightarrow C$ is a classifier learned on the basis of $D \setminus D_i$
 2. $Err(y_i, D_i) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_i : y_i(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D_i|}$

Cross-validated misclassification rate:

$$Err_{cv}(y, D) = \frac{1}{k} \sum_{i=1}^k Err(y_i, D_i)$$

Evaluating Effectiveness

n -Fold Cross-Validation (Leave One Out)

Special case with $k = n$:

- Determine the cross-validated misclassification rate for $D \setminus D_i$ where $D_i = \{(\mathbf{x}_i, c(\mathbf{x}_i))\}$, $i \in \{1, \dots, n\}$.

Evaluating Effectiveness

n -Fold Cross-Validation (Leave One Out)

Special case with $k = n$:

- Determine the cross-validated misclassification rate for $D \setminus D_i$ where $D_i = \{(\mathbf{x}_i, c(\mathbf{x}_i))\}$, $i \in \{1, \dots, n\}$.

Problems:

- High computational effort if D is large.
- Singleton test sets ($|D_i| = 1$) are never stratified since they contain a single class only.

Remarks:

- ❑ For large k the set $D \setminus D_i$ is of similar size as D . Hence $Err(y_i, D_i)$ is close to $Err(y, D)$, where y is the classifier learned on the basis of the entire set D .
- ❑ n -fold cross-validation is a special case of exhaustive cross-validation methods, which learn and test on all possible ways to divide the original sample into a training and a validation set.
[\[Wikipedia\]](#)

Evaluating Effectiveness

Bootstrapping [Holdout Estimation]

Resampling the example set D :

- For $j = 1, \dots, l$ do:
 1. Form training set D_j by drawing m examples from D with replacement.
 2. $y_j : X \rightarrow C$ is a classifier learned on the basis of D_j
 3. $Err(y_j, D \setminus D_j) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D \setminus D_j : y_j(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D \setminus D_j|}$

Bootstrapped misclassification rate:

$$Err_{bt}(y, D) = \frac{1}{l} \sum_{j=1}^l Err(y_j, D \setminus D_j)$$

Remarks:

- ❑ Let $|D| = n$. The probability that an example is not considered is $(1 - 1/n)^m$. Hence, the probability that an example is considered at least once is $1 - (1 - 1/n)^m$.
- ❑ If m gets closer to n , then $1 - (1 - 1/n)^m \approx 1 - 1/e \approx 0.632$. I.e., each training set contains about 63.2% of the examples in D .
- ❑ The classifiers y_1, \dots, y_l can be used in a combined fashion, called *ensemble*, where the class is determined by means of a majority decision:

$$y(\mathbf{x}) = \operatorname{argmax}_{c \in C} |\{j \in \{1, \dots, l\} : y_j(\mathbf{x}) = c\}|$$

Evaluating Effectiveness

Misclassification Costs [Holdout Estimation]

Use of a cost measure for the misclassification of a feature vector \mathbf{x} in class c' instead of in class c :

$$\text{cost}(c' \mid c) \begin{cases} \geq 0 & \text{if } c' \neq c \\ = 0 & \text{otherwise} \end{cases}$$

Estimation of $Err_{cost}^*(y)$ based on a sample $D_{ts} \subseteq D$:

$$Err_{cost}(y, D_{ts}) = \frac{1}{|D_{ts}|} \cdot \sum_{(\mathbf{x}, c(\mathbf{x})) \in D_{ts}} \text{cost}(y(\mathbf{x}) \mid c(\mathbf{x}))$$

Remarks:

- ❑ The misclassification rate Err is a special case of Err_{cost} with $cost(c' | c) = 1$ for $c' \neq c$.