



národní
úložiště
šedé
literatury

Measures for Classification Results Evaluation

Řezanková, Hana
2015

Dostupný z <http://www.nusl.cz/ntk/nusl-200675>

Dílo je chráněno podle autorského zákona č. 121/2000 Sb.

Tento dokument byl stažen z Národního úložiště šedé literatury (NUŠL).

Datum stažení: 17.04.2024

Další dokumenty můžete najít prostřednictvím vyhledávacího rozhraní nusl.cz .



Institute of Computer Science
The Czech Academy of Sciences

Measures for Classification Results Evaluation

Hana Řezanková, Dušan Húsek

Technical report No. 1220

Jun 25 2015



Institute of Computer Science
The Czech Academy of Sciences

Measures for Classification Results Evaluation¹

Hana Řezanková, Dušan Húsek

Technical report No. 1220

Jun 25 2015

Abstract:

The paper focuses on measures which can be applied to evaluation of classification results. Objects with known assignment to certain groups are used for evaluation. Using a classification method the user obtains the assignment of objects to groups. Many coefficients have been proposed for evaluation of the success rate of classification. Most of them is determined for classification to two groups. Possibilities for classification to more groups are limited. The aim of this paper is to summarize different measures, discuss their origin and relationships. For classification to three or more groups we propose two novel measures which are more suitable. The first of them takes a variability of diagonal frequencies of the confusion matrix into account. The second one is based on the sum of squared differences between the maximum correctly assigned objects and real correctly assigned objects in each group.

Keywords:

Similarity measures, measures of agreement, success rate of classification

¹This research has been partly funded by long-term strategic development financing of the Institute of Computer Science (RVO:67985807).

1 Introduction

If a new method for object classification is developed or a model of object classification is estimated, evaluation of classification results is very useful and necessary. Many coefficients have been proposed for evaluation of the success rate of classification. Most of them is determined for classification to two groups. Possibilities for classification to more groups are limited. The aim of this paper is to summarize different measures, discuss their origin and relationships. For classification to three and more groups two novel measures, which better evaluate obtained results, are proposed. The first of them takes a variability of diagonal frequencies of the confusion matrix into account. The second one is based on the sum of squared differences between the maximum correctly assigned objects and real correctly assigned objects for each group. Measures evaluating classification are based on the confusion matrix including the frequencies n_{ij} . Each value n_{ij} expresses the number of objects observed in the i -th groups and classified in the j -th group.

2 Classification to two groups

In case of classification to two groups, more approaches are available to the users in comparison with classification to more than two groups. The confusion matrix includes four frequencies n_{ij} , see Table 2.1, where n is the total number of objects, $n_{1+} = n_{11} + n_{12}$, $n_{2+} = n_{21} + n_{22}$, $n_{+1} = n_{11} + n_{21}$, and $n_{+2} = n_{12} + n_{22}$ are the marginal frequencies.

		Classified (Predicted)		
		Group (Class) 1	Group (Class) 2	
Observed (Actual)	Group (Class) 1	n_{11}	n_{12}	n_{1+}
	Group (Class) 2	n_{21}	n_{22}	n_{2+}
		n_{+1}	n_{+2}	n

Table 2.1: Scheme of confusion matrix for two groups.

Let us suppose that group 1 expresses a positive situation (a patient is cured, a client repaid the installments, a document contains relevant information) and group 2 expresses a negative situation. In the process of classification evaluation, the number of objects from group 1 which are classified correctly is usually denoted TP (true positive), i.e. $n_{11} = TP$. The number of objects from group 1 which are not classified correctly is usually denoted FN (false negative), i.e. $n_{12} = FN$. Similarly, the number of objects from group 2 which are classified correctly is usually denoted TN (true negative), i.e. $n_{22} = TN$, and the number of objects from group 2 which are not classified correctly is usually denoted FP (false positive), i.e. $n_{21} = FP$.

The basic characteristics of classification to two groups are *sensitivity* (*true positive rate* or *recall*) and *specificity* (*true negative rate*). The former is defined as n_{11}/n_{1+} , the latter is expressed as n_{22}/n_{2+} . Further, the *precision* (*positive predictive value*) is defined as n_{11}/n_{+1} and the *false positive rate* is expressed as $(1 - \text{specificity})$, i.e. n_{21}/n_{+1} . The list of characteristics based on the frequencies in the confusion matrix and usually used for classification evaluation is shown in Table 2.2. Some terms comes from the area of information retrieval.

The confusion matrix is a contingency table in which different kinds of frequencies can be displayed, e.g. relative frequencies within the total table ($p_{ij} = n_{ij}/n$) with the marginal relative frequencies, $p_{1+} = p_{11} + p_{12}$, $p_{2+} = p_{21} + p_{22}$, $p_{+1} = p_{11} + p_{21}$, and $p_{+2} = p_{12} + p_{22}$ (see Table 2.3), the row relative frequencies (see Table 2.4) or column relative frequencies (see Table 2.5) which provide different views on the relationships between observed and suggested assignment of objects to groups.

The rates, predictive values, accuracy and *F1 score* have values from the interval $[0; 1]$. The true rates (*TPR* and *TNR*), predictive values (*PPV* and *NPV*), accuracy and *F1 score* should be close 1, false rates should be close 0.

The *accuracy* is known as the *simple matching coefficient* (*SMC*) in the area of similarity measures for binary variables, applied e.g. in hierarchical cluster analysis. (The authors of this coefficient are

Name 1	Name 2 etc.	Equation
true positive rate (<i>TPR</i>)	sensitivity, recall	n_{11}/n_{1+}
true negative rate (<i>TNR</i>)	specificity (<i>SPC</i>)	n_{22}/n_{2+}
positive predictive value (<i>PPV</i>)	precision	n_{11}/n_{+1}
negative predictive value (<i>NPV</i>)		n_{22}/n_{+2}
false positive rate (<i>FPR</i>)	fall-out	n_{21}/n_{2+}
false negative rate (<i>FNR</i>)	miss rate	n_{12}/n_{1+}
false discovery rate (<i>FDR</i>)		n_{21}/n_{+1}
false omission rate (<i>FOR</i>)		n_{12}/n_{+2}
accuracy (<i>ACC</i>)		$(n_{11} + n_{22})/n$
prevalence		n_{+1}/n
F1 score		$2n_{11}/(n_{1+} + n_{+1})$
Matthews correlation coef. (<i>MCC</i>)		$\frac{n_{11}n_{22} - n_{12}n_{21}}{\sqrt{n_{1+}n_{2+}n_{+1}n_{+2}}}$

Table 2.2: Definitions of classification characteristics.

		Classified		
		Group 1	Group 2	
Observed	Group 1	p_{11}	p_{12}	p_{1+}
	Group 2	p_{21}	p_{22}	p_{2+}
		p_{+1}	p_{+2}	1

Table 2.3: Scheme of confusion matrix for two groups with total relative frequencies.

		Classified		
		Group 1	Group 2	
Observed	Group 1	$TPR = n_{11}/n_{1+}$	$FNR = n_{12}/n_{1+}$	1
	Group 2	$FPR = n_{21}/n_{2+}$	$TNR = n_{22}/n_{2+}$	1

Table 2.4: Scheme of confusion matrix for two groups with row relative frequencies.

		Classified		
		Group 1	Group 2	
Observed	Group 1	$PPV = n_{11}/n_{+1}$	$FOR = n_{12}/n_{+2}$	
	Group 2	$FDR = n_{21}/n_{+1}$	$NPV = n_{22}/n_{+2}$	
		1	1	

Table 2.5: Scheme of confusion matrix for two groups with column relative frequencies.

Sokal and Michener, who significantly affected research in the area of classification, see e.g. [16] or [22].) It is the weighted arithmetic average of sensitivity and specificity:

$$SMC = \frac{\frac{n_{11}}{n_{1+}}n_{1+} + \frac{n_{22}}{n_{2+}}n_{2+}}{n_{1+} + n_{2+}} = \frac{n_{11} + n_{22}}{n}. \quad (2.1)$$

The *F1 score* is a harmonic mean of sensitivity and precision. It is well known similarity measure for two asymmetric dichotomous variables, called *Dice* [6] or *Czekanowski* [5] or *Sorensen* [24]. Usually, it is expressed in the form

$$DICE = \frac{2n_{11}}{2n_{11} + n_{12} + n_{21}}. \quad (2.2)$$

The weighted harmonic mean of sensitivity and precision is the *F-measure*:

$$F_\alpha = \frac{(1 + \alpha) \cdot \frac{n_{11}}{n_{1+}} \cdot \frac{n_{11}}{n_{+1}}}{\alpha \cdot \frac{n_{11}}{n_{1+}} + \frac{n_{11}}{n_{+1}}} = \frac{(1 + \alpha) \cdot n_{11}}{(1 + \alpha) \cdot n_{11} + \alpha n_{12} + n_{21}}, \quad (2.3)$$

where α may be varied between 0 and 1. It is the significance level, see [1]. The arithmetic average of sensitivity and precision gives the *Kulczynski similarity measure 2*, i.e.

$$K2 = \frac{\frac{n_{11}}{n_{1+}} + \frac{n_{11}}{n_{+1}}}{2}. \quad (2.4)$$

The geometric mean of sensitivity and precision gives the *Ochiai similarity measure* [17] in the form

$$OCHIAI = \sqrt{\frac{n_{11}}{n_{1+}} \frac{n_{11}}{n_{+1}}}. \quad (2.5)$$

It is the special equation for the cosine similarity measure determined for quantitative variables.

The average of *TPR*, *TNR*, *PPV* and *NPV* is called *Sokal and Sneath similarity measure 4*, i.e.

$$SS4 = \frac{\frac{n_{11}}{n_{1+}} + \frac{n_{11}}{n_{+1}} + \frac{n_{22}}{n_{2+}} + \frac{n_{22}}{n_{+2}}}{4}. \quad (2.6)$$

The average of the values from the interval [0; 1] is the value from the same interval.

The ratio of the true positive rate and the false positive rate is called as the *positive likelihood ratio (LR+)*:

$$LR+ = \frac{\frac{n_{11}}{n_{1+}}}{\frac{n_{21}}{n_{2+}}}. \quad (2.7)$$

The ratio of the false negative rate and the true negative rate is called as the *negative likelihood ratio (LR)*:

$$LR- = \frac{\frac{n_{12}}{n_{1+}}}{\frac{n_{22}}{n_{2+}}}. \quad (2.8)$$

The ratio of the positive likelihood ratio and the negative likelihood ratio is called as the *diagnostic odds ratio (OR)*:

$$OR = \frac{\frac{\frac{n_{11}}{n_{1+}} \cdot \frac{n_{21}}{n_{2+}}}{\frac{n_{12}}{n_{1+}} \cdot \frac{n_{22}}{n_{2+}}}}{\frac{n_{11}n_{22}}{n_{1+}n_{21}}} = \frac{TPR \cdot TNR}{FNR \cdot FPR} = \frac{PPV \cdot NPV}{FOR \cdot FDR}. \quad (2.9)$$

Some suitable measures of association known from the contingency table analysis can be used for evaluation of classification. Further, some similarity measures for binary variables used in hierarchical cluster analysis can be also applied.

The Matthews correlation coefficient [14], see Table 2.2, is the classical *Pearson correlation coefficient* [18] expressed for two binary variables by frequencies from the contingency tables. In a case of two binary variables, the equation for the Pearson correlation coefficient is the same as the formulas for the Spearman and Kendall rank correlation coefficients (Kendall's tau-b). That means there is only one correlation coefficient for measurement of association of two dichotomous variable which can be used for classification evaluation. This coefficient has values from the interval [-1; 1]. Three examples of frequencies which give values 1, 0 and -1 are shown in Tables 2.6–2.8. The absolute values of the correlation coefficient are the same as the values of the *phi coefficient* of association based on the Pearson chi-squared statistic.

The correlation coefficient is a measure of linear dependence. There are two other coefficients proposed for linear dependence measurement of two ordinal variables which can be applied to binary variables – symmetric Somers's d and Goodman and Kruskal's gamma. *Somers's d* is a harmonic mean of two asymmetric coefficients. For the 2×2 contingency table it is defined as

		Classified		
		Group 1	Group 2	
Observed	Group 1	90	0	90
	Group 2	0	90	90
		90	90	180

Table 2.6: Example of frequencies which give the value 1 of the correlation coefficient.

		Classified		
		Group 1	Group 2	
Observed	Group 1	45	45	90
	Group 2	45	45	90
		90	90	180

Table 2.7: Example of frequencies which give the value 0 of the correlation coefficient.

		Classified		
		Group 1	Group 2	
Observed	Group 1	0	90	90
	Group 2	90	0	90
		90	90	180

Table 2.8: Example of frequencies which give the value -1 of the correlation coefficient.

$$d = \frac{2(n_{11}n_{22} - n_{12}n_{21})}{n_{1+}n_{2+} + n_{+1}n_{+2}}. \quad (2.10)$$

Its values are very close to values of the correlation coefficient, because generally Kendall's tau-b can be expressed as a geometric mean of two asymmetric Somers's coefficients. For classification we can consider a directional measure, it means if classification (C) with frequencies placed in columns of the confusion matrix is dependent on observed assignment of objects to groups placed in rows (R) or not. In this case

$$d_{C|R} = \frac{n_{11}n_{22} - n_{12}n_{21}}{n_{11}n_{22} + n_{12}n_{21} + n_{11}n_{21} + n_{12}n_{22}}. \quad (2.11)$$

If the confusion matrix is symmetric, then the values of all three Somers's coefficients are the same.

Goodman and Kruskal's gamma is called as *Yule's Q* [26] for the 2×2 contingency table. It is defined by the equation

$$Q = \frac{n_{11}n_{22} - n_{12}n_{21}}{n_{11}n_{22} + n_{12}n_{21}}. \quad (2.12)$$

This coefficient has also values from the interval $[-1; 1]$. Values 1, 0 and -1 correspond with situations in which correlation coefficient has the same values, see Tables 2.6–2.8. Yule's Q is used as a similarity measure in multivariate statistical methods. It is a function of the odds ratio:

$$Q = \frac{OR - 1}{OR + 1}. \quad (2.13)$$

Another coefficient with similar properties is *Yule's coefficient of colligation*. It can be expressed by the formula

$$Y = \frac{\sqrt{n_{11}n_{22}} - \sqrt{n_{12}n_{21}}}{\sqrt{n_{11}n_{22}} + \sqrt{n_{12}n_{21}}}. \quad (2.14)$$

Yule's coefficients assess the association between items as the predictability of one given the other. It is a function of the odds ratio:

$$Y = \frac{\sqrt{OR} - 1}{\sqrt{OR} + 1}. \quad (2.15)$$

The example in Table 2.6 is an ideal situation and the best classification. Beside of the measures mentioned above there are some different measure with this property, e.g. measures of agreement. One of them is *Kohen's kappa* which can be used for any square contingency table (two variables have the same number of categories which correspond with their senses). For the 2×2 table it is calculated according to the formula

$$\kappa = \frac{(n_{11} + n_{22}) - \left(\frac{n_{1+n_1}}{n} + \frac{n_{2+n_2}}{n}\right)}{n - \left(\frac{n_{1+n_1}}{n} + \frac{n_{2+n_2}}{n}\right)}. \quad (2.16)$$

This coefficient has values from the interval $[-1; 1]$. The value 0 means that the frequencies in the table are the same as the frequencies expected under the hypothesis of independence. The value -1 can be achieved only for the symmetric confusion matrix.

If all non-zero values are in the diagonal (see Table 2.6) then $n_{11} + n_{22} = n$ and $\kappa = 1$. If frequencies in the contingency table correspond to independence (see Table 2.7), then $\kappa = 0$. If the value in the diagonal are zero (see Table 2.8), then $n_{12} = n_{1+} = n_{+2}$ and $n_{21} = n_{2+} = n_{+1}$, i.e.

$$\kappa = \frac{-\left(\frac{n_{1+n_1}}{n} + \frac{n_{2+n_2}}{n}\right)}{n - \left(\frac{n_{1+n_1}}{n} + \frac{n_{2+n_2}}{n}\right)} = \frac{-\left(\frac{n_{1+n_1}}{n} + \frac{n_{2+n_2}}{n}\right)}{\left(\frac{n_{1+n_2}}{n} + \frac{n_{2+n_1}}{n}\right)} = -\frac{2n_{12}n_{21}}{n_{12}n_{12} + n_{21}n_{21}}. \quad (2.17)$$

If $n_{12} = n_{21}$ then $\kappa = -1$.

The special measure of agreement proposed for the 2×2 table is *Hamann's coefficient (HC)* [8] defined by the equation

$$HC = \frac{(n_{11} + n_{22}) - (n_{12} + n_{21})}{n}. \quad (2.18)$$

This coefficient has values from the interval $[-1; 1]$. It is applied as a similarity measure in multivariate methods. The examples of frequencies which give the values 1, 0 and -1 are in Tables 2.6–2.8.

Beside of the simple matching coefficient with a range from 0 to 1, some other similarity measures with this range can be applied. We can mention *Sokal and Sneath similarity measure 5* calculated as

$$SS5 = \frac{n_{11}n_{22}}{\sqrt{n_{1+}n_{2+}n_{+1}n_{+2}}}. \quad (2.19)$$

Some similarity measures favor the correct classification. The example are the *Sokal and Sneath similarity measure 1*

$$SS1 = \frac{2(n_{11} + n_{22})}{2(n_{11} + n_{22}) + n_{12} + n_{21}}. \quad (2.20)$$

and the *Rogers and Tanimoto similarity measure* [19]

$$RT = \frac{n_{11} + n_{22}}{n_{11} + n_{22} + 2(n_{12} + n_{21})}. \quad (2.21)$$

These coefficients have also values from the interval $[0; 1]$. It is a special case of the Tversky index [25] which has a form

$$TV = \frac{n_{11} + n_{22}}{n_{11} + n_{22} + \alpha \cdot n_{12} + \beta \cdot n_{21}}. \quad (2.22)$$

If $\alpha = \beta = 2$, then we get the Rogers and Tanimoto coefficient. If $\alpha = \beta = 0.5$, we get the Sokal and Sneath similarity measure 1. There are also similarity measures which have not values either from the interval $[0; 1]$ nor $[-1; 1]$. These measures have a minimum value of 0 and have no upper limit. We will not evaluate them in this study.

Moreover, there are several coefficients which represent only the proportion of correct classification to the first group as the F1 score (or the Dice similarity measure) or the K2 or Ochiai similarity measures express. They have values from the interval $[0; 1]$. There are Russel and Rao (RR , also *support*), Jaccard ($JACC$), and Sokal and Sneath ($SS2$) similarity measures. The *Russel and Rao similarity measure* [20] is defined as

$$RR = \frac{n_{11}}{n}, \quad (2.23)$$

the *Jaccard coefficient* [9],[10], [11]:

$$JACC = \frac{n_{11}}{n_{11} + n_{12} + n_{21}} = \frac{n_{11}}{n - n_{22}}, \quad (2.24)$$

and the *Sokal and Sneath similarity measure 2* as

$$SS2 = \frac{n_{11}}{n_{11} + 2(n_{12} + n_{21})}. \quad (2.25)$$

Some publications summarize and compare similarity coefficients, e.g. [23], [3], [12], [21], [15], [2], [4].

In Table 2.9, there are examples of frequencies and corresponding values of coefficients. Different frequencies for all marginal frequencies equal 90 are considered (as in Tables 2.6–2.8). It means that the confusion matrix is symmetric. For the reason that given marginal frequencies and the frequencies in one cell determine frequencies in three other cells, only the value of n_{11} is included in the table. The coefficients are ordered according their values (from higher to lower values in the group of a certain coefficient type). We can see that for the symmetric confusion matrix some coefficients give the same results. Graphical representation of coefficient values is shown in Figures 2.1 and 2.2. Some other examples are shown in Figures 2.3 and 2.4.

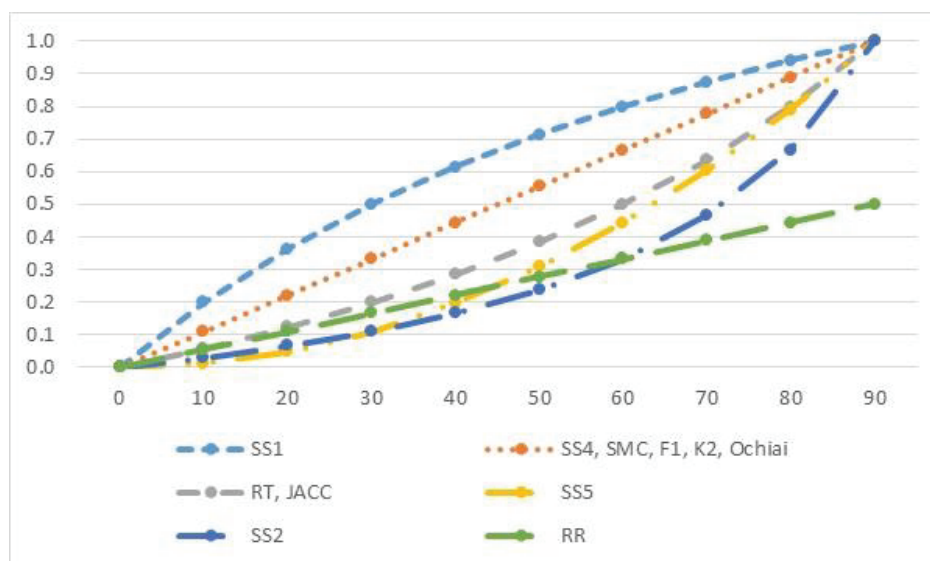


Figure 2.1: Dependence of coefficient values on selected frequencies in the first cell of the confusion matrix with marginal frequencies 90, 90, 90 90 (coefficients with range from 0).

3 Classification to three and more groups

If we consider more than two groups, then the number of possibilities for evaluation of classification is considerably less. We can evaluate classification to individual groups separately (assignment to

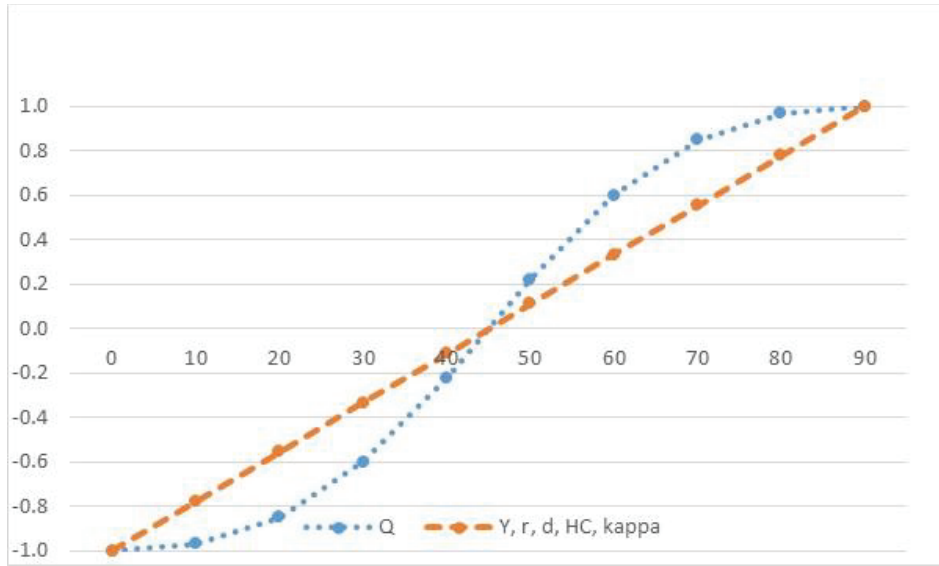


Figure 2.2: Dependence of coefficient values on selected frequencies in the first cell of the confusion matrix with marginal frequencies 90, 90, 90 90 (coefficients with range $[-1; 1]$).

	Frequencies – examples								
	1	2	3	4	5	6	7	8	9
n_{11}	0	10	20	30	45	60	70	80	90
	Values of coefficients								
Measures for symmetric binary variables with range $[0; 1]$									
$SS1$	0	0.20	0.36	0.50	0.67	0.80	0.88	0.94	1
$SS4$	0	0.11	0.22	0.33	0.50	0.67	0.78	0.89	1
$ACC (SMC)$	0	0.11	0.22	0.33	0.50	0.67	0.78	0.89	1
RT	0	0.06	0.13	0.20	0.33	0.50	0.64	0.80	1
$SS5$	0	0.01	0.05	0.11	0.25	0.44	0.60	0.79	1
Measures for asymmetric binary variables									
$F1\ score\ (Dice)$	0	0.11	0.22	0.33	0.50	0.67	0.78	0.89	1
$F-0.7$	0	0.11	0.22	0.33	0.50	0.67	0.78	0.89	1
$K2$	0	0.11	0.22	0.33	0.50	0.67	0.78	0.89	1
$Ochiai$	0	0.11	0.22	0.33	0.50	0.67	0.78	0.89	1
$JACC$	0	0.06	0.13	0.20	0.33	0.50	0.64	0.80	1
$SS2$	0	0.03	0.07	0.11	0.20	0.33	0.47	0.67	1
RR	0	0.06	0.11	0.17	0.25	0.33	0.39	0.44	0.5
Measure with range $[-1; 1]$									
Q	-1	-0.97	-0.85	-0.60	0	0.60	0.85	0.97	1
Y	-1	-0.78	-0.56	-0.33	0	0.33	0.56	0.78	1
$MCC (r)$	-1	-0.78	-0.56	-0.33	0	0.33	0.56	0.78	1
$Som. d$	-1	-0.78	-0.56	-0.33	0	0.33	0.56	0.78	1
HC	-1	-0.78	-0.56	-0.33	0	0.33	0.56	0.78	1
$kappa$	-1	-0.78	-0.56	-0.33	0	0.33	0.56	0.78	1

Table 2.9: Examples of frequencies and corresponding values of coefficients.

a certain groups and to all other groups) and use the approaches mentioned above. However, for evaluation of assignment to all groups simultaneously only the simple matching coefficient and the

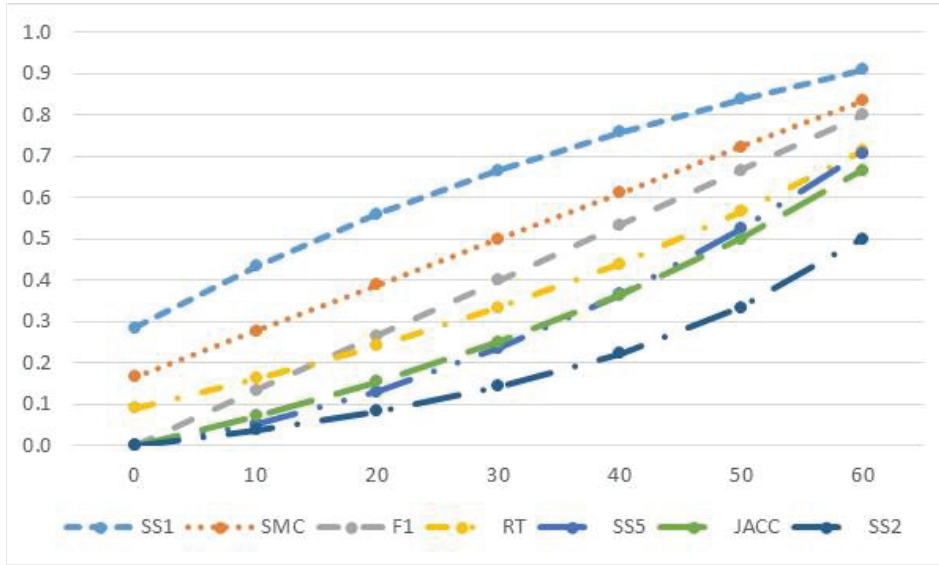


Figure 2.3: Dependence of coefficient values on selected frequencies in the first cell of the confusion matrix with marginal frequencies 90, 90, 60, 120 (coefficients with range [0; 1])

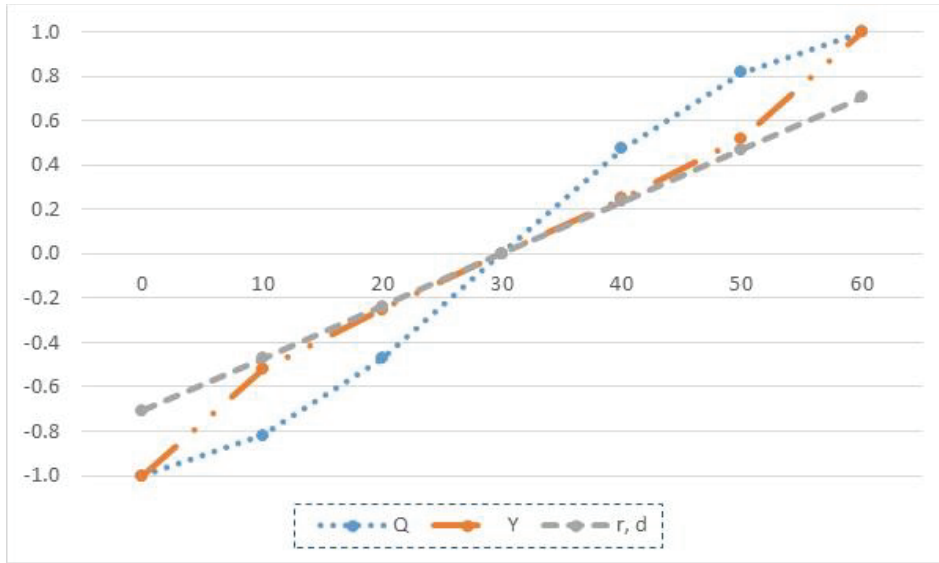


Figure 2.4: Dependence of coefficient values on selected frequencies in the first cell of the confusion matrix with marginal frequencies 90, 90, 60, 120 (coefficients with range [-1; 1]).

kappa coefficient are usually applied. The *simple matching coefficient* is defined as

$$SMC = \frac{\sum_{i=1}^K n_{ii}}{n}, \quad (3.1)$$

where K is the number of groups. This coefficient has values from the interval [0; 1]. The *SMC* measure is a weighted arithmetic average of individual sensitivities for each group:

$$SMC = \sum_{i=1}^K \frac{n_{ii}}{n_{i+}} \cdot \frac{n_{i+}}{n} = \sum_{i=1}^K \frac{n_{ii}}{n} = \frac{\sum_{i=1}^K n_{ii}}{n}. \quad (3.2)$$

This coefficient does not distinguish variability of diagonal frequencies.

For K groups the *kappa coefficient* is expressed as

$$\kappa = \frac{\sum_{i=1}^K n_{ii} - \sum_{i=1}^K \frac{n_{i+}n_{+i}}{n}}{n - \sum_{i=1}^K \frac{n_{i+}n_{+i}}{n}}. \quad (3.3)$$

It has values from the interval $[-1; 1]$. If the frequencies in the confusion matrix are the same as the frequencies expected under the hypothesis of independence, then the value of kappa is 0. However, if the value is 0, then random frequencies are only one from several possibilities. For this reason, the kappa coefficient is the suitable measure of agreement, but it is not a suitable measure for evaluation of classification results.

The modified *Hamann's coefficient* for K groups can be applied for evaluation of classification results in the form

$$HC = \frac{\sum_{i=1}^K n_{ii} - \sum_{i=1}^K \sum_{j=1; j \neq i}^K n_{ij}}{n}. \quad (3.4)$$

This coefficient has values from the interval $[-1; 1]$. The value 0 means that the number of correct assigned objects and the number of incorrect assigned objects are the same. However, we obtain similar information as using the SMC measure, only in the different interval. The comparison of three mentioned coefficients applied for the symmetric confusion matrix for 90 objects is shown in Figure 3.1.

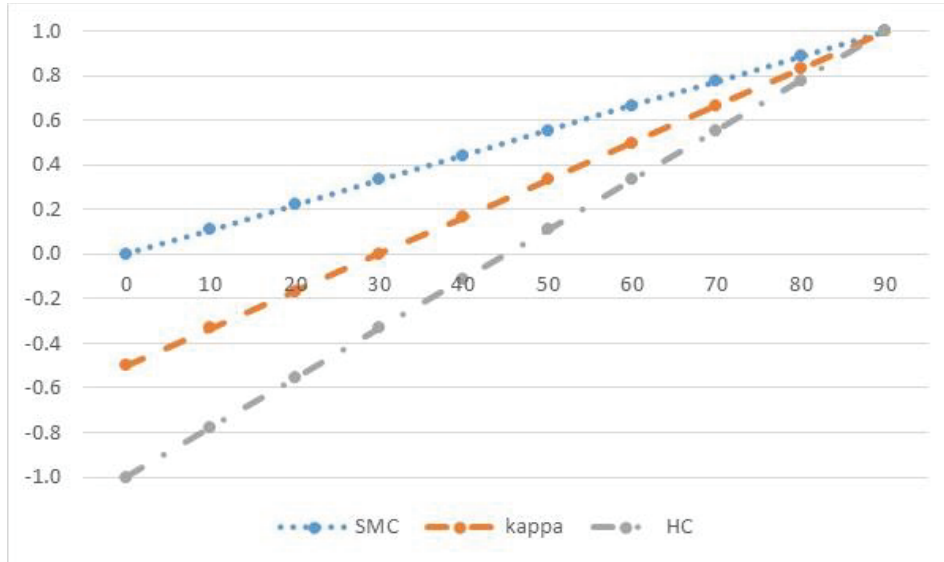


Figure 3.1: Dependence of coefficient values on selected diagonal frequencies.

For the reason that the coefficients mentioned above do not express a success rate of classification in a suitable way, we propose a new coefficient including variability of frequencies. Sensitivities are

relative frequencies. However, the sum of them usually is not 1. If these relative frequencies are recalculated for the sum equal 1, then we can express variability of corrected classification.

We suggest to apply nominal variance (i.e. mutability) proposed by [7], reviewed in [13], as a variability measure. So each sensitivity is divided by the sum of sensitivities and then the normalized nominal variance of these proportions are calculated. The *SMC* coefficient is multiplied by the obtained value, i.e.

$$RH = \frac{1}{n} \sum_{i=1}^K n_{ii} \cdot \left(\frac{K}{K-1} \sum_{i=1}^K \frac{n_{ii}}{n_{i+}} \left(1 - \frac{\frac{n_{ii}}{n_{i+}}}{\sum_{i=1}^K \frac{n_{ii}}{n_{i+}}} \right) \right). \quad (3.5)$$

If all proportions are the same, then the normalized nominal variance is 1 and $RH = SMC$. If only one class is classified correctly, then variance is 0 and $RH = 0$.

If there are the same numbers of objects in all groups, then variability of diagonal frequencies instead variability of sensitivities can be calculated. Then the RH coefficient can be expressed as

$$RH = \frac{1}{n} \sum_{i=1}^K n_{ii} \cdot \left(\frac{K}{K-1} \sum_{i=1}^K \frac{n_{ii}}{\sum_{i=1}^K n_{ii}} \left(1 - \frac{n_{ii}}{\sum_{i=1}^K n_{ii}} \right) \right). \quad (3.6)$$

We can illustrate taking variability into account with the following example. Let us suppose that there are 3 groups and 9 objects. In each group there are 3 objects correctly. The values of the *SMC* and RH coefficients are in Table 3.1.

Another way to take into account different sensitivities in individual groups is to compute the sum of squared differences between the maximum correctly assigned objects and real correctly assigned objects for each group:

$$Dif2 = \sum_{i=1}^K (n_{i+} - n_{ii})^2. \quad (3.7)$$

For obtaining values from the interval from 0 to 1, the *Dif2Norm* measure can be expressed in the form

$$Dif2Norm = \frac{\sum_{i=1}^K n_{i+}^2 - Dif2}{\sum_{i=1}^K n_{i+}^2}. \quad (3.8)$$

The values of *Dif2* and *Dif2Norm* for the example mentioned above are in Table 3.1. In this table the rows are ordered according to values of the RH and *Dif2Norm* measures. We can see that both measures give the same order for the given marginal frequencies. Both measures give for two cases of frequencies the same values but the pairs of frequencies are different.

According to our opinion the RH and *Dif2Norm* measures are more suitable for evaluation of classification results than usually used measures because the successful classification to all groups is preferred over the total number of correctly classified objects.

4 Conclusion

Many different measures have been proposed for evaluation of classification results. For classification to two groups, the possibilities are varied. If the numbers of objects observed in two groups are the same and the numbers of objects predicted to two groups are also the same, then the obtained values of some coefficients are the same. In this paper we point out which coefficients have the same dependence on the frequencies in the confusion matrix.

Diagonal frequencies	<i>SMC</i>	<i>Normalized mutability</i>	<i>RH</i>	<i>Dif2</i>	<i>Dif2Norm</i>
0,0,0,	0	0	0	27	0
1,0,0	0.111	0	0	23	0.148
2,0,0	0.222	0	0	19	0.296
3,0,0,	0.333	0	0	18	0.333
1,1,0	0.222	0.750	0.167	17	0.370
2,1,0	0.333	0.667	0.222	14	0.481
3,1,0	0.444	0.563	0.250	13	0.519
1,1,1	0.333	1.000	0.333	12	0.556
2,2,0	0.444	0.750	0.333	11	0.593
3,2,0	0.556	0.720	0.400	10	0.630
2,1,1	0.444	0.938	0.417	9	0.667
3,3,0	0.667	0.750	0.500	9	0.667
2,2,1	0.556	0.960	0.533	6	0.778
3,2,1	0.667	0.917	0.611	5	0.815
2,2,2	0.667	1.000	0.667	3	0.889
3,2,2	0.778	0.980	0.762	2	0.926
3,3,2	0.889	0.984	0.875	1	0.963
3,3,3	1	1.000	1	0	1

Table 3.1: Examples of diagonal frequencies and values of *SMC*, *RH* and *Dif2Norm* measures.

For evaluation of assignment to three or more groups simultaneously, only the simple matching coefficient and the kappa coefficient are usually applied. If the value of the kappa coefficient is zero, it can mean that the frequencies in the confusion matrix are the same as the frequencies expected under the hypothesis of independence, however it is only one from many possibilities. The simple matching coefficient, which is a weighted arithmetic average of individual sensitivities for each group, does not distinguish variability of diagonal frequencies.

For this reason we proposed two novel coefficients, the *HR* and *Dif2Norm* coefficients. The former takes a variability of diagonal frequencies into account. The normalized nominal variance is used as a variability measure in this case. The *HR* coefficient is a product of the simple matching coefficient and the normalized nominal variance. The *Dif2Norm* coefficient is based on the sum of squared differences between the maximum correctly assigned objects and real correctly assigned objects for each group. The obtained value is normalized to the interval [0;1]. We believe that the proposed coefficients evaluate the results of classification suitably.

Acknowledgment

This research has been partly funded by long-term strategic development financing of the Institute of Computer Science (RVO:67985807).

Bibliography

- [1] BILLINGER, M. – DALY, I. – KAISER, V. – JIN, J. – ALLISON, B. Z. – MÜLLER-PUTZ, G.R. – BRUNNER, C.: Is it significant? Guidelines for reporting BCI performance. In: ALLISON, B. Z. et al. (Eds.): *Towards Practical Brain Computer Interfaces, Biological and Medical Physics, Biomedical Engineering*. Berlin Heidelberg: Springer-Verlag, 2012.
- [2] CHA, S.H.: Comprehensive survey on distance/similarity measures between probability density functions. In: *International Journal of Mathematical Models and Methods in Applied Sciences*, vol. 1, no. 4, 2007, p. 300–307.
- [3] CHEETHAM, A.H. – HAZEL, J.E.: Binary (presence-absence) similarity coefficients. In: *Journal of Paleontology*, vol. 43, no. 5, 1969, p. 1130–1136.
- [4] CHOI, S.S. – CHA, S.H. – TAPPERT, C.C.: A survey of binary similarity and distance measures. In: *Journal of Systemics, Cybernetics and Informatics*, vol. 8, no. 1, 2010, p. 43–48.
- [5] CZEKANOWSKI, J.: Coefficient of racial likeness und durchschnittliche Differenz. In: *Anthrop. Anz.*, vol. 9, 1932, p. 227–249.
- [6] DICE, L.R.: Measures of the amount of ecologic association between species. In: *Ecology*, vol. 26, no. 3, 1945, p. 297–302.
- [7] GINI, C.W.: Variability and mutability. Contribution to the study of statistical distributions and relations. *Studi Economico-Giuridici della R. Universita de Cagliari*, 1912.
- [8] HAMANN, U.: Merkmalbestand und Verwandtschaftsbeziehungen der Farinosae. Ein Beitrag zum System der Monokotyledonen. In: *Willdenowia*, vol. 2, 1961, p. 639–768.
- [9] JACCARD, P.: tude comparative de la distribution florale dans une portion des Alpes et des Jura. In: *Bulletin de la Socit Vaudoise des Sciences Naturelles*, vol. 37, 1901, p. 547–579.
- [10] JACCARD, P.: Nouvelles recherches sur la distribution florale. In: *Bulletin de la Socit Vaudoise des Sciences Naturelles*, vol. 44, 1908, p. 223–270.
- [11] JACCARD, P.: The distribution of the flora in the alpine zone. In: *New Phytologist*, vol. 11, 1912, p. 37–50.
- [12] KURCZYNSKI, T.W.: Generalized distance and discrete variable. In: *Biometrics*, vol. 26, 1970, p. 525–534.
- [13] LIGHT, R.J., MARGOLIN, B.H. *An Analysis of Variance for Categorical Data*. J. American Statistical Association, vol. 66, 1971, p. 534–544.
- [14] MATTHEWS, B.W. 1975. Comparison of the predicted and observed secondary structure of T4 phage lysozyme. In: *Biochimica et Biophysica Acta (BBA) – Protein Structure*, vol. 405, no. 2, 1975, p. 442–451.
- [15] MEYER, A.S. – GARCIA, A.A.F. – SOUZA, A.P. – SOUZA, C.L.: Comparison of similarity coefficients used for cluster analysis with dominant markers in maize (*Zea mays* L). In: *Genetics and Molecular Biology*, vol. 27, no. 1, 2004.

- [16] MICHENER, C.D. – SOKAL, R.R.: A quantitative approach to a problem in classification. In: *Evolution*, vol. 11, 1957, p. 130–162.
- [17] OCHIAI, A.: Zoogeographic studies on the soleoid fishes found in Japan and its neighbouring regions. In: *Bull Jnp Soc Sci Fish*, vol. 22, 1957, p. 526–530.
- [18] PEARSON, K.: On the coefficient of racial likeness. In: *Biometrika*, vol. 18, 1926, p. 105–117.
- [19] ROGERS, D.J. – TANIMOTO, T.T.: A computer program for classifying plants. In: *Science*, vol. 132, 1960, p. 1115–1118.
- [20] RUSSEL, P.F. – RAO, T.R.: On habitat and association of species of anophelinae larvae in south-eastern Madras. In: *Journal of the Malaria Institute of India*, vol. 3, no. 1, 1940, p. 153–178.
- [21] SNEATH, P.H. – SOKAL, R.R.: *Numerical Taxonomy*. San Francisco: W.H. Freeman and Company, 1973.
- [22] SOKAL R.R. – MICHENER C.D.: A statistical method for evaluating systematic relationships. In: *The University of Kansas Scientific Bulletin*, vol. 38, 1958, s. 1409–1438.
- [23] SOKAL, R.R. – SNEATH, P.H.: *Principles of Numerical Taxonomy*. San Francisco: W. H. Freeman and Company, 1963.
- [24] SORENSEN, T.: A method of establishing groups of equal amplitude in plant sociology based on similarity of species content and its application to analyses of the vegetation on Danish commons. In: *Kongelige Danske Videnskabernes Selskab*, vol. 5, no. 4, 1948, p. 134.
- [25] TVERSKY, A.: Features of similarity. *Psychological reviews*, vol. 84, no. 4, 1977, p. 327352.
- [26] YULE, G.U.: A mathematical theory of evolution, based on the conclusions of Dr. J.C. Willis, F.R.S. In: *Phil. Trans. Roy. Soc. Lond. Ser. B*, vol. 213, 1924, p. 2187.