Limits to classification performance by relating Kullback-Leibler Divergence to Cohen's Kappa

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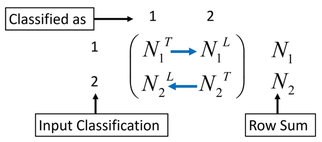
BACKGROUND

Performance of Machine Learning (ML) classification algorithms is evaluated using training data and cross-validation.

Q. How do you know if one has reached the best possible performance ?
A. The Kullback-Leibler Divergence through the Chernoff-Stein Lemma gives the rate at which performance improves due to the underlying pdf of the two classes.

METHOD

Write the confusion matrix as



True and Leaked entries for two classes with values, N_1 and N_2 $N=N_1+N_2$.

$$N_1^T = N_1 - N_1^L \qquad N_1^L = \frac{N_1 N_2}{N}\exp(-K_{12})$$

$$N_2^L = \frac{N_1 N_2}{N}\exp(-K_{21}) \qquad N_2^T = N_2 - N_2^L$$

Cohen's Kappa, κ can be calculated from this matrix. It measures the efficiency of the classifier, correcting for random chance. From kappa the parameter, K , is calculated, $K = -\log_2(1-\kappa)$. It can be shown that this is approximately the Resistor Average Distance, R(P,Q), which is the parallel combination of the Kullback-Leibler Divergences, D(P|Q) and D(Q|P). The kNN estimate of these divergences and this distance can be calculated from the training data.

Written up in paper of same title
https://arxiv.org/abs/2403.01571

METHOD + COMPARISON WITH DATA

Assume ML will try to get best performance for both classes. CDR is the kNN based estimator for R(P,Q).

Then, Cohens' Kappa, $\kappa \simeq 1 - 2^{-CDR(bits)}$

Data	S/B	Total	Continuous/ Discrete	Machine Learning (WEKA Software, [5])
Breast Cancer [1]	212/357	569	30/0	Simple Logistic Regression
Bankruptcy [2]	107/143	250	0/6	J48 Decision Tree
Particle [3]	3736/1264	5000	8/0	Random Forest
Heart Disease (CHD) [4]	302/160	462	8/1	Logistic Regression

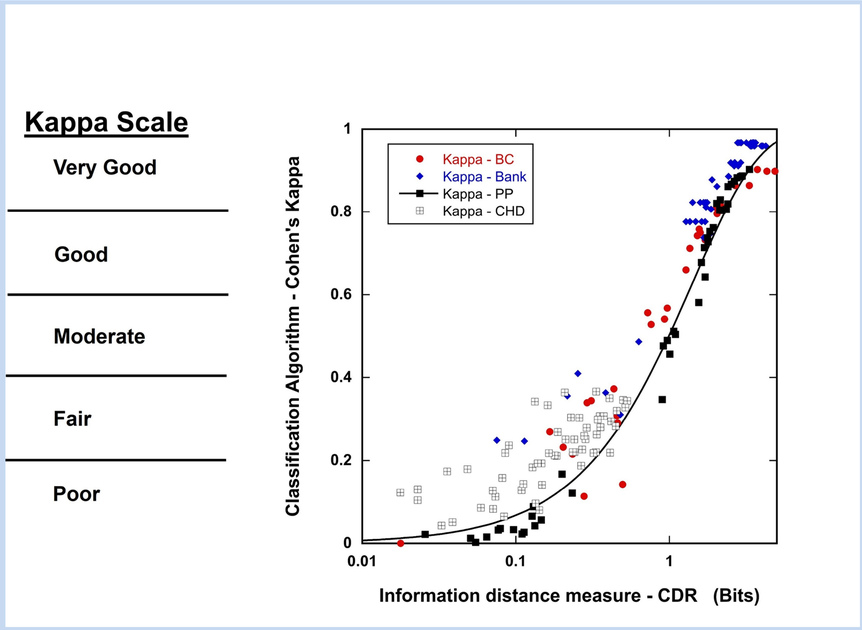


Figure 1. This figure combines the result of the classification algorithm performance using Cohen's Kappa versus the independently calculated Class Distance Resistance (CDR). CDR is an estimate of the Resistor Average Distance, which is an information distance measure. The curve gives the relation, $\kappa = 1 - 2^{-CDR}$. The points lie on this curve which indicates that the classification algorithm is performing as well as can be expected. The Kappa scale on the left-hand side is from D. G. Altman.

CONCLUSIONS

- First time that the performance of a Machine Learning Algorithm checked against predicted best case confusion matrix, estimated using the actual underlying probability density function of the two classes from training data.
- Method applies to discrete, continuous or mixed data.
- Any algorithm, no matter how clever, can better this performance limit. For example, the coronary heart disease (CHD) data is only able to deliver " Fair" performance. This type of data is useful for risk analysis but not prediction.
- Apply to multi-class data by taking the classes in pairs.
- This formulation leads naturally to methods to understand imbalanced class machine learning classification.

References and Acknowledgements

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