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

The performance of machine learning classification algorithms are evaluated by estimating metrics, often from the confusion matrix, using training data and cross-validation. However, these do not prove that the best possible performance has been achieved. Fundamental limits to error rates can be estimated using information distance measures. To this end, the confusion matrix has been formulated to comply with the Chernoff-Stein Lemma. This links the error rates to the Kullback-Leibler divergences between the probability density functions describing the two classes. This leads to a key result that relates Cohen's Kappa to the Resistor Average Distance which is the parallel resistor combination of the two Kullback-Leibler divergences. The Resistor Average Distance has units of bits and is estimated from the same training data used by the classification algorithm, using kNN estimates of the Kullback-Leibler divergences. The classification algorithm gives the confusion matrix and Kappa. Theory and methods are discussed in detail and then applied to Monte Carlo data and real datasets. Four very different real datasets - Breast Cancer, Coronary Heart Disease, Bankruptcy, and Particle Identification - are analysed, with both continuous and discrete values, and their classification performance compared to the expected theoretical limit. In all cases this analysis shows that the algorithms could not have performed any better due to the underlying probability density functions for the two classes. Important lessons are learnt on how to predict the performance of algorithms for imbalanced data. Preprint available at [arXiv:2403.01571](https://arxiv.org/abs/2403.01571).

Primary Field of Research

Particle Physics

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