Multivariate conformal prediction distributions

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Confidence distributions can be seen as a frequentist alternative to Bayesian posteriors for summarizing the knowledge available for an unknown quantity based on the observed data and a model, but without the need for a Bayesian prior. Two equally important parts of a confidence distribution are (i) A distribution estimator, ii) A matching family of confidence-credibility regions. This is illustrated by examples for two-dimensional parameters, but also for one-dimensional parameters. The main tools for construction are given by a) Data generating algorithms, b) Pivots, and c) p-value functions. Presently, confidence distributions are in practice not anywhere near the success of Bayesian posteriors due to a lack of general available software and a lack of a fully developed theory. This can and will be changed as part of the focus in machine learning is directed towards uncertainty quantification in its predictions. It will be explained that a prediction distribution generalizes the concept of a confidence distribution by being defined by two equally important parts: (i) A distribution estimator, ii) A matching family of prediction-credibility regions. The methods can also be used to construct multivariate conformal prediction distributions of use in an on-line setting in which multivariate labels are predicted successively, each one being revealed before the next is predicted. The corresponding sequence of families of conformal prediction regions are characterized by successive predictions being right a fraction of the time given by the corresponding credibility level even though they are based on an accumulating data set rather than on independent data sets. Optimality is discussed in terms of frequentist properties of the distribution estimator and of the family of credibility regions separately. Uniformly most powerful unbiased distributions and regions are obtained for exponential families and group families in concrete cases. More generally, Bayes optimal regions are obtained using Bayes informed frequentist methods.



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