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Conformal and probabilistic prediction with applications: editorial

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This special issue of *Machine Learning* is devoted to conformal prediction, an emerging technique in machine learning that focuses on designing prediction algorithms that are provably valid, in various senses. There have been annual meetings on this subject over the past seven years. The basis for this special issue is formed by selected papers presented in the last year's meeting, the *Sixth Symposium on Conformal and Probabilistic Prediction with Applications* (COPA 2017) that took place on June 14–16, 2017, in Stockholm (with tutorials on 13 June). The authors' of the best papers presented at COPA 2017, as judged by the Programme Committee, have been invited to submit revised and expanded versions of their papers to this special issue, and in addition, there was an open call for papers on conformal prediction and related topics. Naturally, the whole set of the submitted papers went through several rounds of peer review before they were accepted for publication.

One of the advantages of conformal prediction is its flexibility; e.g., almost any known classification or regression algorithm can be turned into a conformal predictor. The simplest mode of using conformal prediction and its sister method of Venn prediction is to use it on top of traditional machine-learning techniques as a "wrapper" method that complements their predictions with valid measures of confidence. The underlying algorithms that have been used successfully with conformal prediction include neural networks, support vector machines, nearest neighbours methods, random forests, boosting, as well as older statistical techniques such as ridge regression and discriminant analysis. Newer ways of applying conformal and Venn prediction is to produce different kinds of predictions, such as predictive probability

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distributions, rather than merely complementing predictions produced by the underlying algorithms with further information.

Conformal and Venn prediction have been successfully applied to many challenging real world problems in medicine, engineering, and other application areas. These methods have been extended to such settings as semi-supervised learning, anomaly detection, feature selection, outlier detection, change detection in streams, and active learning. Recent developments in collecting large volumes of data have also required their adjustment to handle "big data". An ongoing EU Horizon 2020 project on drug design has adopted conformal predictors as one of the main tools for selecting useful chemical compounds. Industrial companies have started applying conformal prediction, with a recent example being its use by AstraZeneca to accelerate the process of development of new drugs.

Overall, seven papers were accepted for this special issue after being reviewed by three (occasionally two) independent referees. The issue is divided into two parts. The first part presents an invited paper by Vladimir Vapnik and Rauf Izmailov, *Rethinking Statistical Learning Theory: Learning Using Statistical Invariants*.

The second part is devoted to conformal prediction and related methods of probabilistic prediction. The theoretical papers in this part are *Online aggregation of unbounded losses using shifting experts with confidence* by Vladimir V'yugin and Vladimir Trunov, *Nonparametric predictive distributions based on conformal prediction* by Vladimir Vovk, and *Majority vote ensembles of conformal predictors* by Giovanni Cherubin. There are also several experimental papers: *Combination of inductive Mondrian conformal predictors* by Paolo Toccaceli and Alexander Gammerman, *Automatic face recognition with well-calibrated confidence measures* by Harris Papadopoulos, Charalambos Eliades, Ladislav Lenc, and Pavel Kral, and *Efficient Venn predictors using random forests* by Ulf Johansson, Tuwe Löfström, Henrik Linusson, and Henrik Boström.

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