

Marginally calibrated deep distributional regression

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Abstract

Deep neural network (DNN) regression models are widely used in applications requiring state-of-the-art predictive accuracy. However, until recently there has been little work on accurate uncertainty quantification for predictions from such models. We add to this literature by outlining an approach to constructing predictive distributions that are ‘marginally calibrated’. This is where the long run average of the predictive distributions of the response variable matches the observed empirical margin. Our approach considers a DNN regression with a conditionally Gaussian prior for the final layer weights, from which an implicit copula process on the feature space is extracted. This copula process is combined with a non-parametrically estimated marginal distribution for the response. The end result is a scalable distributional DNN regression method with marginally calibrated predictions, and our work complements existing methods for probability calibration. The approach is first illustrated using two applications of dense layer feed-forward neural networks. However, our main motivating applications are in likelihood-free inference, where distributional deep regression is used to estimate marginal posterior distributions. In two complex ecological time series examples we employ the implicit copulas of convolutional networks, and show that marginal calibration results in improved uncertainty quantification. Our approach also avoids the need for manual specification of summary statistics, a requirement that is burdensome for users and typical of competing likelihood-free inference methods. This is joint work with Nadja Klein and Michael Smith.

References

- [1] N. Klein, D. J. Nott, M.S. Smith. Marginally-calibrated deep distributional regression, *J. Comput. Graph. Stat.*, [arXiv:2006.14126](https://arxiv.org/abs/2006.14126), doi [10.1080/10618600.2020.1807996](https://doi.org/10.1080/10618600.2020.1807996).