

EFFICIENT INFERENCE FOR SPATIAL AND SPATIO-TEMPORAL STATISTICAL MODELS USING BASIS-FUNCTION AND DEEP-LEARNING METHODS

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Inference in spatial and spatio-temporal models can be challenging for a variety of reasons. For example, non-Gaussianity often leads to analytically intractable integrals; we may be in a ‘big’ data setting, whereby the number of observations renders traditional methods too computationally expensive; we may wish to make inferences over spatial supports that are different to those of our measurements; or, we may wish to use a statistical model whose likelihood function is either unavailable or computationally intractable. In this thesis, I develop several techniques that help to alleviate these challenges.

First, I develop a unifying framework and accompanying software for modelling spatial and spatio-temporal data with both point- and area-support that are big, irregularly spaced, and non-Gaussian. This framework facilitates the modelling of large data sets through the use of spatial/spatio-temporal basis functions; it caters for arbitrary observation supports by discretising the domain into basic areal units; and it caters for non-Gaussian data by employing a spatial/spatio-temporal generalised linear mixed model. This contribution is described in [1].

Second, I contribute to the emerging field of neural Bayes estimation. Neural Bayes estimators are neural networks that map data to point estimates of parameters; they are approximate Bayes estimators, likelihood-free, and amortised, in the sense that, once trained with simulated data, inference from observed data is extremely fast. In this thesis, I formalise the connection between neural Bayes estimators and classical point estimation, and I propose a principled way to construct neural Bayes estimators for replicated data from general statistical models via the use of permutation-invariant

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neural networks. The resulting estimators may be applied to data sets with an arbitrary number of replicates, and they can be used for highly parametrised spatial dependence models. This contribution is described in [2].

Finally, I tackle the important problem of neural Bayes estimation from data collected over arbitrary spatial locations, by employing graph neural networks: the resulting estimators can be used with data collected over any set of spatial locations, thereby amortising the cost of training for a given spatial model. I also propose a novel approach to performing rigorous uncertainty quantification in an amortised manner, by training a neural Bayes estimator to jointly approximate a set of low and high marginal posterior quantiles. This contribution is described in [3].

To facilitate their adoption by the broader statistical community, all of the methodological contributions are incorporated in user-friendly, comprehensively documented, open-source software packages in the Julia and R programming languages.

References

- [1] M. Sainsbury-Dale, A. Zammit-Mangion and N. Cressie, ‘Modelling big, heterogeneous, non-Gaussian spatial and spatio-temporal data using FRK’, *J. Stat. Softw.* **108**(10) (2024), 1–39.
- [2] M. Sainsbury-Dale, A. Zammit-Mangion and R. Huser, ‘Likelihood-free parameter estimation with neural Bayes estimators’, *Amer. Statist.* **78** (2024), 1–14.
- [3] M. Sainsbury-Dale, A. Zammit-Mangion, J. Richards and R. Huser, ‘Neural Bayes estimators for irregular spatial data using graph neural networks’, Preprint, 2023, [arXiv:2310.02600](https://arxiv.org/abs/2310.02600).

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