



COSTNET FINAL MEETING 2020

On the Mathematical Foundation of Approximate Bayesian Computation A Robust Set for Estimating Mechanistic Network Models

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24–25 September 2020

Abstract

We research relations between optimal transport theory, OTT, and the innovative methodology of approximate Bayesian computation, ABC, possibly connected to relevant metrics defined on probability measures.

Those of ABC are computational methods based on Bayesian statistics and applicable to a given generative model to estimate its a posteriori distribution in case the likelihood function is intractable. The idea is therefore to simulate sets of synthetic data from the model with respect to assigned parameters and, rather than comparing prospects of these data with the corresponding observed values as typically ABC requires, to employ just a distance between a chosen distribution associated to the synthetic data and another of the observed values.

Such methods have become increasingly popular especially thanks to the various fields of applicability which go from finance to biological science, and yet an ABC methodology relying on OTT as the one we're trying to develop was born specifically with the hope of esteem mechanistic network models, i.e. models for data network growth or evolution over time, thus particularly suitable for processing dynamic data domains; but which indeed, by definition, don't have a manageable likelihood, main reason why those models are opposed to probabilistic ones which instead can always count on powerful inferential tools.

Our focus lies in theoretical and methodological aspects, although there would exist a remarkable part of algorithmic implementation, and more precisely issues regarding mathematical foundation and asymptotic properties are carefully analyzed, inspired by an in-depth study of what is then our main bibliographic reference, that is [1], carrying out what follows: a rigorous formulation of the set-up for the ABC rejection algorithm, also to regain a transparent and general result of convergence as the ABC threshold goes to zero whereas the number n of samples from the prior stays fixed; general technical proposals about distances leaning on OTT; weak assumptions which lead to lower bounds for small values of threshold and as n goes to infinity, ultimately showing a reasonable possibility of lack of concentration which is contrary to what is proposed in [1] itself.

References. ABC: [12]. Network or mechanistic models: [2], [3], [4], [5]. Wasserstein distance in ABC: [7], [9]. More of ABC: [6], [8], [10], [13], [14]. The mathematics: [11], [15].

Keywords. Approximate Bayesian computation. Asymptotic properties. Bayesian statistics. Borel measurable. Concentration properties. Generative models. Likelihood-free inference. Measure theory. Mechanistic network models. Monge-Kantorovich problem. Networks. Optimal coupling. Optimal transport theory. Probability metric. Radon's metric. Radon probability measure. Transportation of measure. Wasserstein distance.

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