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Column PhD thesis

Confidence in Bayesian Uncertainty Quantification?

Botond Szabó received the Willem R. van Zwet Award 2014 for his thesis *Adaptation and Confidence in Nonparametric Bayes*. The Willem R. van Zwet Award is the annual prize of the Netherlands Society of Statistics and Operations Research for an excellent PhD thesis in the area of statistics or operations research, in 2014 awarded to two people. In this article Botond Szabó introduces us to his research.

In recent years there has been a rapid increase in computational power and available information, leading to the rise of Bayesian methods in many practical applications. The popularity of the Bayesian approach comes from its natural framework for combining experts' beliefs with observed data. Bayesian methods have been successfully applied in many real world problems, including for instance recovering Air France Flight 447 which crashed into the Atlantic Ocean, improving the prevention of the spread of malaria or constructing self-driving cars, just to mention but a few. However, despite its wide applicability, we still don't have a good theoretical understanding of its behaviour. My thesis focuses on the theoretical investigation of Bayesian methods.

Bayesian modeling

In the Bayesian approach one can incorporate prior experience or intuition about the problem into the model in a straightforward manner. This is done through the *prior distribution*, which represents our initial opinion about certain unknown characteristics (i.e. parameters) of the model that are of interest to us. The next step is to incorporate the observed data into our prior belief resulting in an updated belief about the problem. This revised opinion is formulated via the *posterior distribution*, which is the conditional distribution of the unknown parameters given the data. In Bayesian statistics, the posterior distribution is used to make approximations and decisions about the unknown parameters of interest.

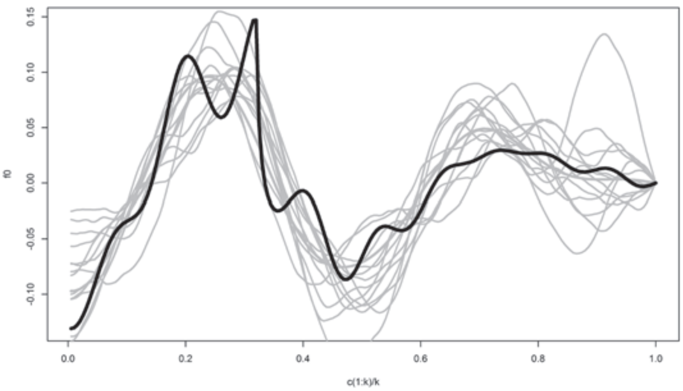

Figure 1 Simulation results for a polished tail function. The unknown functional parameter of interest is drawn in black, while the gray curves represent typical draws from the posterior distribution.

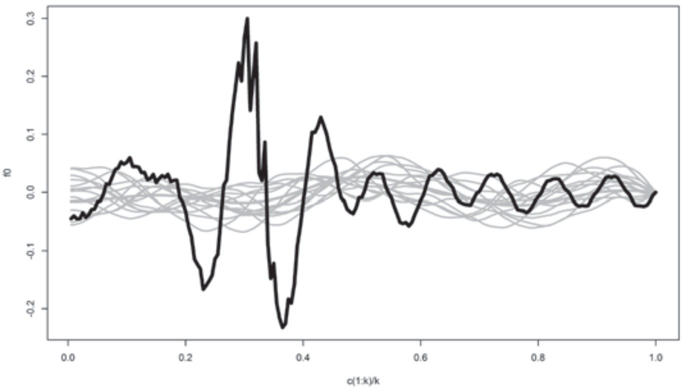

Figure 2 Simulation results for a nonpolished tail function. The unknown functional parameter of interest is drawn in black, while the gray curves represent typical draws from the posterior distribution.

However, the behaviour of the posterior distribution depends highly on the choice of the prior, especially in complex models. Naive use of Bayesian statistics can result in misleading or even false conclusions. An objective way of comparing Bayesian methods is via classical (also known as frequentist) statistics: one assumes that the data is generated according to a fixed 'true" parameter and investigates how well the posterior distribution recovers this.

Bayesian uncertainty quantification

Another particularly appealing aspect of Bayesian techniques is that they naturally include a quantification of their precision. Assessing the reliability of a statistical procedure is of central importance, since reporting only a single estimate without any information about how certain we are about it can be profoundly misleading. Therefore, the goal is to give a set of probable parameter values instead of a single one. Larger sets thus correspond to less certainty in the estimates, while smaller sets represent confidence in the procedure. Such confidence statements can then be immediately applied in statistical decision making.

The problem is that although Bayesian techniques come with built-in uncertainty statements and are therefore widely used in practice because of their convenience, it was shown that they can be far off, giving haphazard and false uncertainty quantification. The goal of my PhD project was to investigate the theoretical properties of Bayesian based uncertainty quantification in complex models.

Polished tail condition

In general one would like to quantify uncertainty in an optimal way. Too conservative confidence statements, i.e. large sets of possible parameter values, obviously provide only a limited amount of information. It has been shown in the literature that in general it is not possible to give reliable and optimal uncertainty quantification at the same time. Therefore certain additional modeling assumptions have to be introduced.

In our work we developed the so called *polished tail* condition under which the investigated Bayesian methods provide reliable and optimally precise uncertainty statements. In the polished tail condition we roughly assume that the 'information level' of the unknown functional parameter of interest that we can extract from the data is not dominated by the information level of the functional parameter hidden by the noise (i.e. a random object corrupting our observations). In other words we assume that just by looking at the data we can extrapolate certain aspects about the model which are hidden by the noise. We also gave topological, statistical, and Bayesian arguments to verify the optimality of this assumption. We illustrate our findings via a simulation study in Figure 1, respectively Figure 2, where we consider a functional parameter satisfying, respectively violating, the polished tail condition. We draw the unknown function in black and the gray curves represent typical samples from the posterior distribution resulting from a Gaussian process prior. One can observe that the gray curves cover the true function in Figure 1, while fail to cover it in Figure 2. These pictures intuitively indicate that under a polished tail assumption, Bayesian methods can measure the uncertainty of the statistical procedure correctly. Without it one can get misleading uncertainty statements.

Further questions, applications

The thesis considers the behaviour of the Bayesian approach in an idealized statistical model. This serves as a platform to investigate more realistic, real world problems with high practical relevance, including various network models and machine learning algorithms. It can then provide a guideline to practitioners how to calibrate their Bayesian procedures. Possible fields of applications include machine learning, genomics, finance, legal and medical practice, and epidemiology just to mention but a few.

Bibliography

Botond Szabó has defended his PhD thesis on the 19th of February 2014 at the Eindhoven University of Technology under the supervision of prof. dr. Aad van der Vaart and prof. dr. Harry van Zanten. The title of the dissertation is *Adaptation and Confidence in Nonparametric Bayes*. After defending his thesis he obtained a half a year long post-doc position at CREST in Paris and then an assistant professor position at Budapest University of Technology in Hungary. In the beginning of 2015 he returned to the Netherlands and was a post-doc in Amsterdam for a year. Currently he holds an assistant professor position at Leiden University. His research interests include Bayesian nonparametric statistics, asymptotic statistics, graph theory, and machine learning.