

# STATISTICAL SCIENCE

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# Probabilistic Integration: A Role in Statistical Computation?

François-Xavier Briol, Chris J. Oates, Mark Girolami, Michael A. Osborne and Dino Sejdinovic

*Abstract.* A research frontier has emerged in scientific computation, wherein discretisation error is regarded as a source of epistemic uncertainty that can be modelled. This raises several statistical challenges, including the design of statistical methods that enable the coherent propagation of probabilities through a (possibly deterministic) computational work-flow, in order to assess the impact of discretisation error on the computer output. This paper examines the case for probabilistic numerical methods in routine statistical computation. Our focus is on numerical integration, where a *probabilistic integrator* is equipped with a full distribution over its output that reflects the fact that the integrand has been discretised. Our main technical contribution is to establish, for the first time, rates of posterior contraction for one such method. Several substantial applications are provided for illustration and critical evaluation, including examples from statistical modelling, computer graphics and a computer model for an oil reservoir.

*Key words and phrases:* Computational statistics, nonparametric statistics, probabilistic numerics, uncertainty quantification.

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# Comment on “Probabilistic Integration: A Role in Statistical Computation?”

Fred J. Hickernell and R. Jagadeeswaran

*Abstract.* Probabilistic integration provides a criterion for stopping a simulation when a specified error tolerance is satisfied with high confidence. We comment on some of the modeling assumptions and implementation issues involved in designing an automatic Bayesian cubature.

*Key words and phrases:* Bayesian, fast algorithms, quasi-Monte Carlo.

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# Comment: Unreasonable Effectiveness of Monte Carlo

Art B. Owen

*Abstract.* There is a role for statistical computation in numerical integration. However, the competition from incumbent methods looks to be stiffer for this problem than for some of the newer problems being handled by probabilistic numerics. One of the challenges is the unreasonable effectiveness of the central limit theorem. Another is the unreasonable effectiveness of pseudorandom number generators. A third is the common  $O(n^3)$  cost of methods based on Gaussian processes. Despite these advantages, the classical methods are weak in places where probabilistic methods could bring an improvement.

*Key words and phrases:* Probabilistic numerics, quasi-Monte Carlo.

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# Comment on “Probabilistic Integration: A Role in Statistical Computation?”

Michael L. Stein and Ying Hung

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# Rejoinder: Probabilistic Integration: A Role in Statistical Computation?

François-Xavier Briol, Chris J. Oates, Mark Girolami, Michael A. Osborne and Dino Sejdinovic

*Abstract.* This article is the rejoinder for the paper “Probabilistic Integration: A Role in Statistical Computation?” (*Statist. Sci.* **34** (2019) 1–22). We would first like to thank the reviewers and many of our colleagues who helped shape this paper, the Editor for selecting our paper for discussion, and of course all of the discussants for their thoughtful, insightful and constructive comments. In this rejoinder, we respond to some of the points raised by the discussants and comment further on the fundamental questions underlying the paper: (i) Should Bayesian ideas be used in numerical analysis? and (ii) If so, what role should such approaches have in statistical computation?

*Key words and phrases:* Computational statistics, nonparametric statistics, probabilistic numerics, uncertainty quantification.

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# Automated versus Do-It-Yourself Methods for Causal Inference: Lessons Learned from a Data Analysis Competition

Vincent Dorie, Jennifer Hill, Uri Shalit, Marc Scott and Dan Cervone

*Abstract.* Statisticians have made great progress in creating methods that reduce our reliance on parametric assumptions. However, this explosion in research has resulted in a breadth of inferential strategies that both create opportunities for more reliable inference as well as complicate the choices that an applied researcher has to make and defend. Relatedly, researchers advocating for new methods typically compare their method to at best 2 or 3 other causal inference strategies and test using simulations that may or may not be designed to equally tease out flaws in all the competing methods. The causal inference data analysis challenge, “Is Your SATT Where It’s At?”, launched as part of the 2016 Atlantic Causal Inference Conference, sought to make progress with respect to both of these issues. The researchers creating the data testing grounds were distinct from the researchers submitting methods whose efficacy would be evaluated. Results from 30 competitors across the two versions of the competition (black-box algorithms and do-it-yourself analyses) are presented along with post-hoc analyses that reveal information about the characteristics of causal inference strategies and settings that affect performance. The most consistent conclusion was that methods that flexibly model the response surface perform better overall than methods that fail to do so. Finally new methods are proposed that combine features of several of the top-performing submitted methods.

*Key words and phrases:* Causal inference, competition, machine learning, automated algorithms, evaluation.

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# Comment: Spherical Cows in a Vacuum: Data Analysis Competitions for Causal Inference

Miguel A. Hernán

*Abstract.* A recent data analysis competition compared the performance of several methods for causal inference from observational data. However, sound causal inference requires not only adequate data analysis techniques but also subject-matter expertise about the causal structure of the problem under study. Therefore, until a methodology is developed to combine data analysis and subject-matter knowledge, causal inference competitions may only provide advice to practitioners under ideal conditions.

*Key words and phrases:* Causal inference, data analysis competitions.

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# Comment: Will Competition-Winning Methods for Causal Inference Also Succeed in Practice?

Qingyuan Zhao, Luke J. Keele and Dylan S. Small

*Abstract.* First, we would like to congratulate the authors for successfully hosting the causal inference data competition (referred to as Competition henceforth) and contributing a unique and thought-provoking article to the literature. The authors have provided a comprehensive and timely platform to evaluate the ever-growing number of methods used for covariate adjustment in observational studies. In our comment, we don't generally question the results of the competition, but we do wish to emphasize several other key elements about the role statistics plays in causal inference and observational studies.

*Key words and phrases:* Observational studies, machine learning, study design.

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# Comment: Strengthening Empirical Evaluation of Causal Inference Methods

David Jensen

*Abstract.* This is a contribution to the discussion of the paper by Dorie et al. (*Statist. Sci.* **34** (2019) 43–68), which reports the lessons learned from 2016 Atlantic Causal Inference Conference Competition. My comments strongly support the authors’ focus on empirical evaluation, using examples and experience from machine learning research, particularly focusing on the problem of algorithmic complexity. I argue that even broader and deeper empirical evaluation should be undertaken by the researchers who study causal inference. Finally, I highlight a few key conclusions that suggest where future research should focus.

*Key words and phrases:* Causal inference, empirical evaluation, machine learning, algorithmic complexity, constructed observational studies, alignment.

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# Comment on “Automated Versus Do-It-Yourself Methods for Causal Inference: Lessons Learned from a Data Analysis Competition”

Susan Gruber and Mark J. van der Laan

*Abstract.* Dorie and co-authors (DHSSC) are to be congratulated for initiating the ACIC Data Challenge. Their project engaged the community and accelerated research by providing a level playing field for comparing the performance of a priori specified algorithms. DHSSC identified themes concerning characteristics of the DGP, properties of the estimators, and inference. We discuss these themes in the context of targeted learning.

*Key words and phrases:* Targeted learning, causal inference, TMLE.

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# Comment: Causal Inference Competitions: Where Should We Aim?

Ehud Karavani, Tal El-Hay, Yishai Shimoni and Chen Yanover

*Abstract.* Data competitions proved to be highly beneficial to the field of machine learning, and thus expected to provide similar advantages in the field of causal inference. As participants in the 2016 and 2017 Atlantic Causal Inference Conference (ACIC) data competitions and co-organizers of the 2018 competition, we discuss the strengths of simulation-based competitions and suggest potential extensions to address their limitations. These suggested augmentations aim at making the data generating processes more realistic and gradually increase in complexity, allowing thorough investigations of algorithms' performance. We further outline a community-wide competition framework to evaluate an end-to-end causal inference pipeline, beginning with a causal question and a database, and ending with causal estimates.

*Key words and phrases:* Causal inference, competition, data challenge, machine learning, automated algorithms, evaluation.

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et al. (2017). Many analysts, one dataset: Making transparent how variations in analytical choices affect results. PsyArXiv.

# Comment: Contributions of Model Features to BART Causal Inference Performance Using ACIC 2016 Competition Data

Nicole Bohme Carnegie

*Abstract.* With a thorough exposition of the methods and results of the 2016 Atlantic Causal Inference Competition, Dorie et al. have set a new standard for reproducibility and comparability of evaluations of causal inference methods. In particular, the open-source **R** package `aciccomp2016`, which permits reproduction of all datasets used in the competition, will be an invaluable resource for evaluation of future methodological developments.

Building upon results from Dorie et al., we examine whether a set of potential modifications to Bayesian Additive Regression Trees (BART)—multiple chains in model fitting, using the propensity score as a covariate, targeted maximum likelihood estimation (TMLE), and computing symmetric confidence intervals—have a stronger impact on bias, RMSE, and confidence interval coverage in combination than they do alone. We find that bias in the estimate of SATT is minimal, regardless of the BART formulation. For purposes of CI coverage, however, all proposed modifications are beneficial—alone and in combination—but use of TMLE is least beneficial for coverage and results in considerably wider confidence intervals.

*Key words and phrases:* Bayesian additive regression trees, TMLE, propensity score.

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# Rejoinder: Response to Discussions and a Look Ahead

Vincent Dorie, Jennifer Hill, Uri Shalit, Marc Scott and Dan Cervone

*Abstract.* Response to discussion of Dorie (2017), in which the authors of that piece express their gratitude to the discussants, rebut some specific criticisms, and argue that the limitations of the 2016 Atlantic Causal Inference Competition represent an exciting opportunity for future competitions in a similar mold.

*Key words and phrases:* Causal inference, competition, machine learning, automated algorithms, evaluation.

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# Gaussian Integrals and Rice Series in Crossing Distributions—to Compute the Distribution of Maxima and Other Features of Gaussian Processes

Georg Lindgren

*Abstract.* We describe and compare how methods based on the classical Rice’s formula for the expected number, and higher moments, of level crossings by a Gaussian process stand up to contemporary numerical methods to accurately deal with crossing related characteristics of the sample paths.

We illustrate the relative merits in accuracy and computing time of the Rice moment methods and the exact numerical method, developed since the late 1990s, on three groups of distribution problems, the maximum over a finite interval and the waiting time to first crossing, the length of excursions over a level, and the joint period/amplitude of oscillations.

We also treat the notoriously difficult problem of dependence between successive zero crossing distances. The exact solution has been known since at least 2000, but it has remained largely unnoticed outside the ocean science community.

Extensive simulation studies illustrate the accuracy of the numerical methods. As a historical introduction an attempt is made to illustrate the relation between Rice’s original formulation and arguments and the exact numerical methods.

*Key words and phrases:* Computational statistics, distribution of maximum, Durbin’s formula, excursion length distribution, first passage, independent interval assumption, level crossings, multivariate normal probabilities, period/amplitude distribution, Rice’s formula, RIND program, statistical computation, stochastic process, successive crossing distance distribution, truncated normal moments, Wafo toolbox.

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# Generalized Multiple Importance Sampling

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*Abstract.* Importance sampling (IS) methods are broadly used to approximate posterior distributions or their moments. In the standard IS approach, samples are drawn from a single proposal distribution and weighted adequately. However, since the performance in IS depends on the mismatch between the targeted and the proposal distributions, several proposal densities are often employed for the generation of samples. Under this multiple importance sampling (MIS) scenario, extensive literature has addressed the selection and adaptation of the proposal distributions, interpreting the sampling and weighting steps in different ways. In this paper, we establish a novel general framework with sampling and weighting procedures when more than one proposal is available. The new framework encompasses most relevant MIS schemes in the literature, and novel valid schemes appear naturally. All the MIS schemes are compared and ranked in terms of the variance of the associated estimators. Finally, we provide illustrative examples revealing that, even with a good choice of the proposal densities, a careful interpretation of the sampling and weighting procedures can make a significant difference in the performance of the method.

*Key words and phrases:* Monte Carlo methods, multiple importance sampling, Bayesian inference.

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# A Conversation with Piet Groeneboom

Geurt Jongbloed

*Abstract.* Petrus (Piet) Groeneboom was born in Scheveningen in 1941 and grew up in Voorburg. Both villages are located near The Hague in The Netherlands; Scheveningen actually being part of The Hague. He attended the gymnasium of the Huygens lyceum. In 1959, he entered the University of Amsterdam, where he studied psychology. After his “candidate” exam (comparable to BSc) in 1963, he worked at the psychological laboratory of the University of Amsterdam until 1966. In 1965, he took up mathematics as a part-time study. After having obtained his master’s degree in 1971, he had a position at the psychological laboratory again until 1973, when he was appointed to the Mathematical Center in Amsterdam. There, he wrote between 1975 and 1979 his Ph.D. thesis with Kobus Oosterhoff as advisor, graduating in 1979. After a period of two years as visiting professor at the University of Washington (UW) in Seattle, Piet moved back to the Mathematical Center until he was appointed full professor of statistics at the University of Amsterdam in 1984. Four years later, he moved to Delft University of Technology where he became professor of statistics and stayed until his retirement in 2006. Between 2000 and 2006 he also held a part-time professorship at the Vrije Universiteit in Amsterdam. From 1999 till 2013 he was Affiliate Professor at the statistics department of UW, Seattle. Apart from being visiting professor at the UW in Seattle, he was also visiting professor at Stanford University, Université Paris 6 and ETH Zürich.

Piet is well known for his work on shape constrained statistical inference. He worked on asymptotic theory for these problems, created algorithms to compute nonparametric estimates in such models and applied these models to real data. He also worked on interacting particle systems, extreme value analysis and efficiency theory for testing procedures. Piet (co-)authored four books and 64 papers and served as promotor of 13 students. He is the recipient of the 1985 Rollo Davidson prize, a fellow of the IMS and elected member of the ISI. In 2015, he delivered the Wald lecture at the Joint Statistical Meeting in Montreal.

Piet and his wife Marijke live in Naarden. He has two sons, Thomas and Tim, and (since June 12, 2018) one grandson, Tarik. This conversation was held at Piet’s house in Naarden, on February 28 and April 24, 2018.

*Key words and phrases:* University of Amsterdam, Mathematical Center (CWI), Delft University of Technology, violin playing.

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# A Conversation with Dick Dudley

Vladimir Koltchinskii, Richard Nickl and Philippe Rigollet

*Abstract.* Richard Mansfield Dudley (Dick Dudley) was born in 1938. He received the A.B. from Harvard in 1952 and the Ph.D. from Princeton in 1962 (under the supervision of Gilbert Hunt and Edward Nelson). Following an appointment at UC Berkeley as an assistant professor, he joined the Department of Mathematics at MIT in 1967. Dick Dudley has made fundamental contributions to the theory of Gaussian processes and Probability in Banach Spaces. Among his major achievements is the development of a general framework for empirical processes theory, in particular, for uniform central limit theorems. These results have had and continue having tremendous impact in contemporary statistics and in mathematical foundations of machine learning. A more extensive biographical sketch is contained in the preface to the *Selected works of R. M. Dudley* (editors: E. Giné, V. Koltchinskii and R. Norvaiša) published in 2010.

This conversation took place (mostly, via email) in the fall of 2017.

*Key words and phrases:* Biography, probability, statistics.

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