Statistical Science
2018, Vol. 33, No. 4, 469–472
https://doi.org/10.1214/18-STS673

Editorial: Special Issue on "Nonparametric Inference Under Shape Constraints"

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1. INTRODUCTION

Shape-constrained inference usually refers to nonparametric function estimation and uncertainty quantification under qualitative shape restrictions such as monotonicity, convexity, log-concavity and so on. One of the earliest contributions to the field was by Grenander (1956). Motivated by the theory of mortality measurement, he studied the nonparametric maximum likelihood estimator of a decreasing density function on the nonnegative half-line. A great attraction of this estimator is that, unlike other nonparametric density estimators such as histograms or kernel density estimators, there are no tuning parameters (e.g., bandwidths) to choose.

Over subsequent years, this idea has been extended and developed in many different directions. On the applied side, there has been a gradual realisation that nonparametric shape constraints are very natural to impose in many situations. For instance, monotonicity of a regression function arises in many contexts such as genetics (Luss, Rosset and Shahar, 2012), medicine (Schell and Singh, 1997) and dose-response modelling (Lin et al., 2012). Shape-constrained procedures are also commonly used in economics (Matzkin, 1991, Varian, 1984) and survival analysis, for instance in the interval-censoring problem and hazard function estimation; see the recent book by Groeneboom and Jongbloed (2014). Many other applications, and further developments, including the computational aspects of these shape-constrained estimators, are nicely summarised in the books by Barlow et al. (1972), Robertson, Wright and Dykstra (1988) and Groeneboom and Wellner (1992).

On the theoretical side, it has been known since the work of Prakasa Rao (1969) that the Grenander estimator exhibits nonstandard asymptotic behaviour (more precisely, it converges at rate $n^{-1/3}$, where n is the sample size, at points at which the true decreasing density is differentiable with negative derivative). Moreover, Groeneboom (1985) obtained the limiting distribution of the L_1-distance between the Grenander estimator and true density. The study of the likelihood ratio test for monotone functions was initiated by Banerjee and Wellner (2001), while the adaptive behaviour of monotonicity-constrained estimators was highlighted by Birgé (1989) and Zhang (2002), using finite-sample risk bounds.

However, since the turn of the millennium (and the last decade in particular) the area of shape constraints has witnessed substantially increased activity. On the one hand, researchers started studying systematically the behaviour of univariate shape-constrained procedures beyond monotonicity, for instance in convexity-constrained models (Groeneboom, Jongbloed and Wellner, 2001) and log-concave density estimation (Dümbgen and Rufibach, 2009, Balabdaoui, Rufibach and Wellner, 2009). On the other hand, there has been a realisation that shape-constrained methods have much to offer in multi-dimensional problems (e.g., Cule, Samworth and Stewart, 2010, Seijo and Sen, 2011, Koenker and Mizera, 2010, Han et al., 2018, Seregin and Wellner, 2010). The scope of the field has been broadened by the emergence of new applications, including convex set estimation (Brunel, 2013, Guntuboyina, 2012, Gardner, Kiderlen and Milanfar, 2006, Gardner, 2006), shape-constrained dimension reduction (Chen and Samworth, 2016, Xu, Chen and Lafferty, 2016, Groeneboom and Hendrickx, 2018) and ranking and pairwise comparisons (Shah et al., 2017). New theoretical tools have been developed that have allowed us to make progress in understanding how shape-constrained procedures behave (Dümbgen, Samworth and Schuhmacher, 2011, Kim and Samworth, 2016, Cai and Low, 2015, Guntuboyina and Sen, 2013). Last but not least, increased computing power together with algorithmic advances mean that certain estimators have become computationally feasible (Koenker and Mizera, 2014, Mazumder et al.,

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2018). Four recent workshops, at the Lorentz Center in Leiden (October, 2015), the International Centre for Mathematical Sciences in Edinburgh (May, 2016), the Mathematisches Forschungsinstitut Oberwolfach in Germany (July, 2016) and the Banff International Research Station in Canada (January, 2018) also attest to the vitality of the area.

This unprecedented growth has signalled the need for a special issue on shape-constrained statistical methods and, as Guest Editors, we hope that it will serve as a gateway to this exciting field of research. We have eight articles, as well as one conversation piece, written by experts in their respective sub-fields that showcase the main shape-constrained models of interest, a variety of applications of such models, and the major recent theoretical, methodological and computational advances in some of these problems. We briefly describe the main highlights of each of the papers appearing in this special issue.

Groeneboom and Jongbloed (2018) begin with an article on "*Some developments in the theory of shape constrained inference*". This paper introduces some of the common applications where monotonicity is a natural constraint, discusses the characterisation and computation of the nonparametric maximum likelihood (least squares) estimator in these regression and density estimation problems and describes some of the key results. Potential procedures for quantifying uncertainty, for example, bootstrap methods, are also considered. In recognition of the fundamental contributions, Piet Groeneboom has made to shape constraints and other areas, an interview with him, carried out by Geurt Jongbloed, will appear in a forthcoming issue of *Statistical Science*.

A central nonparametric shape constraint arising in density estimation is log-concavity, where the logarithm of the underlying probability density is concave. Many standard probability densities (e.g., normal/uniform and beta/gamma for certain parameter regions) are log-concave. In the article "*Recent progress in log-concave density estimation*", Samworth (2018) describes some of the attractive theoretical properties of this class of densities and discusses the computation, consistency, and rates of convergence of the nonparametric maximum likelihood estimator. The paper also points to many statistical applications where these ideas have been successfully employed.

Log-concave densities are unimodal with exponentially decaying tails. Recently, there has also been focus on weaker forms of concavity constraints that allow heavier tail behaviour and sharper modal peaks, and that may offer additional modelling flexibility. Koenker and Mizera (2018) explore this area in the paper "*Shape constrained density estimation via penalized Rényi divergence*". Their work discusses estimation strategies based on the Rényi α-divergence criterion. The authors show the existence, uniqueness and continuity properties of the obtained estimator and propose tractable convex optimisation schemes to compute the estimator effectively.

The field of shape constraints is starting to have significant impact in a variety of disciplines, and the survey paper "*Shape constraints in economics and operations research*" (Johnson and Jiang, 2018) highlights the utility of shape-constrained estimation in two application areas. In the first part of the paper, applications to consumer preferences, demand functions and production economics are described, with an emphasis on the relevant shape constraints and estimation strategies. The second part deals with sequential decision making where the authors describe the natural shape restrictions that arise when enforcing structure in (i) value function estimation, (ii) approximate dynamic programming and (iii) optimal policy determination.

The paper "*Limit theory in monotone function estimation*" (Durot and Lopuhaä, 2018) returns to the theme of estimating monotone functions, but has a greater focus on limiting distributions of estimators and their derivations, both in the pointwise case and for global L_p loss functions. They also consider the problem of smoothing isotonic estimators. Guntuboyina and Sen (2018) take a complementary perspective in "*Nonparametric shape-restricted regression*", where they outline the oracle inequality approach to studying the performance of estimators. Attractive features of these results include the facts that it may be possible to consider simultaneously the cases of correct and incorrect model specification, and the potential for the results to reveal the remarkable adaptive behaviour that shape-constrained estimation procedures often enjoy. The extent of this phenomenon is still yet to be fully understood, particularly in multivariate cases, but the authors give several examples where nonparametric shape-constrained estimators can attain near-parametric risk bounds in special cases.

Meyer (2018) introduces "*A framework for estimation and inference in generalized additive models with shape and order restrictions*". Additive structures are often appealing as methods for reducing the space of regression functions to be considered. The author proposes to model the components for continuous covariates with splines, and those for ordinal covariates with partial orderings. In particular, it is shown that regression functions can be constrained to respect common shape restrictions by maximising the likelihood over appropriate convex cones.

While most of the papers mentioned above consider the estimation of functions, Brunel (2018) considers a dual problem in his paper "*Methods for estimation of convex sets*". Important examples include the estimation of the support or level sets of a density, as well as depth functions. As is often the case with shape-constrained problems, the understanding of geometric properties turns out to be key, and the interesting statistical and computational trade-off in the estimation of convex sets is described.

This volume concludes with a conversation with one of the doyens of shape-constrained inference, namely Jon Wellner (Banerjee and Samworth, 2018). Jon provides a fascinating insight into his life and career, and we are sure that readers will enjoy the challenge of trying to identify him from a wonderful teenage group photo of his scooter gang.

We hope that these papers will stimulate readers to explore this fascinating area of nonparametric shape-constrained estimation in more detail.

ACKNOWLEDGMENTS

R. J. Samworth is supported by EPSRC Grants EP/P031447/1 and EP/N031938/1. B. Sen is supported by NSF Grants DMS-17-12822 and AST-16-14743.

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