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HIGH-DIMENSIONAL INFERENCE FOR DYNAMIC TREATMENT EFFECTS

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Estimating dynamic treatment effects is a crucial endeavor in causal inference, particularly when confronted with high-dimensional confounders. Doubly robust (DR) approaches have emerged as promising tools for estimating treatment effects due to their flexibility. However, we showcase that the traditional DR approaches that only focus on the DR representation of the expected outcomes may fall short of delivering optimal results. In this paper, we propose a novel DR representation for intermediate conditional outcome models that leads to superior robustness guarantees. The proposed method achieves consistency even with high-dimensional confounders, as long as at least one nuisance function is appropriately parametrized for each exposure time and treatment path. Our results represent a significant step forward as they provide faster convergence rates and new robustness guarantees. The key to achieving these results lies in utilizing DR representations for intermediate conditional outcome models, which offer superior inferential performance while requiring weaker assumptions. Lastly, we examine finite sample behavior through simulations and a real data application.

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THE CURSE OF OVERPARAMETRIZATION IN ADVERSARIAL TRAINING: PRECISE ANALYSIS OF ROBUST GENERALIZATION FOR RANDOM FEATURES REGRESSION

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Successful deep learning models often involve training neural network architectures that contain more parameters than the number of training samples. Such overparametrized models have recently been extensively studied, and the virtues of overparametrization have been established from both the statistical perspective, via the double-descent phenomenon, and the computational perspective via the structural properties of the optimization landscape. Despite this success, it is also well known that these models are highly vulnerable to small adversarial perturbations in their inputs. Even when adversarially trained, their performance on perturbed inputs (robust generalization) is considerably worse than their best attainable performance on benign inputs (standard generalization). It is thus imperative to understand how overparametrization fundamentally affects robustness.

In this paper, we will provide a precise characterization of the role of overparametrization on robustness by focusing on random features regression models (two-layer neural networks with random first layer weights). We consider a regime where the sample size, the input dimension and the number of parameters grow proportionally, and derive an asymptotically exact formula for the robust generalization error when the model is adversarially trained. Our developed theory reveals the nontrivial effect of overparametrization on robustness and indicates that high overparametrization can hurt robust generalization.

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CONVERGENCE RATES OF OBLIQUE REGRESSION TREES FOR FLEXIBLE FUNCTION LIBRARIES

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We develop a theoretical framework for the analysis of oblique decision trees, where the splits at each decision node occur at linear combinations of the covariates (as opposed to conventional tree constructions that force axis-aligned splits involving only a single covariate). While this methodology has garnered significant attention from the computer science and optimization communities since the mid-80s, the advantages they offer over their axis-aligned counterparts remain only empirically justified, and explanations for their success are largely based on heuristics. Filling this long-standing gap between theory and practice, we show that oblique regression trees (constructed by recursively minimizing squared error) satisfy a type of oracle inequality and can adapt to a rich library of regression models consisting of linear combinations of ridge functions and their limit points. This provides a quantitative baseline to compare and contrast decision trees with other less interpretable methods, such as projection pursuit regression and neural networks, which target similar model forms. Contrary to popular belief, one needs not always trade-off interpretability with accuracy. Specifically, we show that, under suitable conditions, oblique decision trees achieve similar predictive accuracy as neural networks for the same library of regression models. To address the combinatorial complexity of finding the optimal splitting hyperplane at each decision node, our proposed theoretical framework can accommodate many existing computational tools in the literature. Our results rely on (arguably surprising) connections between recursive adaptive partitioning and sequential greedy approximation algorithms for convex optimization problems (e.g., orthogonal greedy algorithms), which may be of independent theoretical interest. Using our theory and methods, we also study oblique random forests.

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EARLY STOPPING FOR L^2-BOOSTING IN HIGH-DIMENSIONAL LINEAR MODELS

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Increasingly high-dimensional data sets require that estimation methods do not only satisfy statistical guarantees but also remain computationally feasible. In this context, we consider L^2-boosting via orthogonal matching pursuit in a high-dimensional linear model and analyze a data-driven early stopping time τ of the algorithm, which is sequential in the sense that its computation is based on the first τ iterations only. This approach is much less costly than established model selection criteria, that require the computation of the full boosting path, which may even be computationally infeasible in truly high-dimensional applications. We prove that sequential early stopping preserves statistical optimality in this setting in terms of a fully general oracle inequality for the empirical risk and recently established optimal convergence rates for the population risk. Finally, an extensive simulation study shows that at a significantly reduced computational cost, the performance of early stopping methods is on par with other state of the art algorithms such as the cross-validated Lasso or model selection via a high-dimensional Akaike criterion based on the full boosting path.

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CONSISTENT INFERENCE FOR DIFFUSIONS FROM LOW FREQUENCY MEASUREMENTS

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Let (X_t) be a reflected diffusion process in a bounded convex domain in $\mathbb{R}^d$, solving the stochastic differential equation

$$dX_t = \nabla f(X_t)\,dt + \sqrt{2f(X_t)}\,dW_t, \quad t \geq 0,$$

with W_t a d-dimensional Brownian motion. The data $X_0, X_D, \dots, X_{ND}$ consist of discrete measurements and the time interval D between consecutive observations is fixed so that one cannot 'zoom' into the observed path of the process. The goal is to infer the diffusivity f and the associated transition operator $P_{t,f}$. We prove injectivity theorems and stability inequalities for the maps $f \mapsto P_{t,f} \mapsto P_{D,f}$, $t < D$. Using these estimates, we establish the statistical consistency of a class of Bayesian algorithms based on Gaussian process priors for the infinite-dimensional parameter f, and show optimality of some of the convergence rates obtained. We discuss an underlying relationship between the degree of ill-posedness of this inverse problem and the 'hot spots' conjecture from spectral geometry.

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A GENERAL FRAMEWORK TO QUANTIFY DEVIATIONS FROM STRUCTURAL ASSUMPTIONS IN THE ANALYSIS OF NONSTATIONARY FUNCTION-VALUED PROCESSES

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We present a general theory to quantify the uncertainty from imposing structural assumptions on the second-order structure of nonstationary Hilbert space-valued processes, which can be measured via functionals of time-dependent spectral density operators. The second-order dynamics are well known to be elements of the space of trace class operators, the latter is a Banach space of type 1 and of cotype 2, which makes the development of statistical inference tools more challenging. A part of our contribution is to obtain a weak invariance principle as well as concentration inequalities for (functionals of) the sequential time-varying spectral density operator. In addition, we introduce deviation measures in the nonstationary context, and derive corresponding estimators that are asymptotically pivotal. We then apply this framework and propose statistical methodology to investigate the validity of structural assumptions for nonstationary functional data, such as low-rank assumptions in the context of time-varying dynamic fPCA and principle separable component analysis, deviations from stationarity with respect to the square root distance, and deviations from zero functional canonical coherency.

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THE EDGE OF DISCOVERY: CONTROLLING THE LOCAL FALSE DISCOVERY RATE AT THE MARGIN

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Despite the popularity of the false discovery rate (FDR) as an error control metric for large-scale multiple testing, its close Bayesian counterpart the local false discovery rate (lfdr), defined as the posterior probability that a particular null hypothesis is false, is a more directly relevant standard for justifying and interpreting individual rejections. However, the lfdr is difficult to work with in small samples, as the prior distribution is typically unknown. We propose a simple multiple testing procedure and prove that it controls the expectation of the maximum lfdr across all rejections; equivalently, it controls the probability that the rejection with the largest p-value is a false discovery. Our method operates without knowledge of the prior, assuming only that the p-value density is uniform under the null and decreasing under the alternative. We also show that our method asymptotically implements the oracle Bayes procedure for a weighted classification risk, optimally trading off between false positives and false negatives. We derive the limiting distribution of the attained maximum lfdr over the rejections, and the limiting empirical Bayes regret relative to the oracle procedure.

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ℓ^2 INFERENCE FOR CHANGE POINTS IN HIGH-DIMENSIONAL TIME SERIES VIA A TWO-WAY MOSUM

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We propose an inference method for detecting multiple change points in high-dimensional time series, targeting dense or spatially clustered signals. Our method aggregates moving sum (MOSUM) statistics cross-sectionally by an ℓ^2-norm and maximizes them over time. We further introduce a novel Two-Way MOSUM, which utilizes spatial-temporal moving regions to search for breaks, with the added advantage of enhancing testing power when breaks occur in only a few groups. The limiting distribution of an ℓ^2-aggregated statistic is established for testing break existence by extending a high-dimensional Gaussian approximation theorem to spatial-temporal nonstationary processes. Simulation studies exhibit promising performance of our test in detecting nonsparse weak signals. Two applications on equity returns and COVID-19 cases in the United States show the real-world relevance of our algorithms. The R package "L2hdchange" is available on CRAN.

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TESTING FOR PRACTICALLY SIGNIFICANT DEPENDENCIES IN HIGH DIMENSIONS VIA BOOTSTRAPPING MAXIMA OF U-STATISTICS

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This paper takes a different look on the problem of testing the mutual independence of the components of a high-dimensional vector. Instead of testing if all pairwise associations (e.g., all pairwise Kendall's τ) between the components vanish, we are interested in the (null) hypothesis that all pairwise associations do not exceed a certain threshold in absolute value. The consideration of these hypotheses is motivated by the observation that in the high-dimensional regime, it is rare, and perhaps impossible, to have a null hypothesis that can be exactly modeled by assuming that all pairwise associations are precisely equal to zero.

The formulation of the null hypothesis as a composite hypothesis makes the problem of constructing tests nonstandard and in this paper we provide a solution for a broad class of dependence measures, which can be estimated by U-statistics. In particular, we develop an asymptotic and a bootstrap level α-test for the new hypotheses in the high-dimensional regime. We also prove that the new tests are minimax-optimal and investigate their finite sample properties by means of a small simulation study and a data example.

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TRANSFER LEARNING FOR FUNCTIONAL MEAN ESTIMATION: PHASE TRANSITION AND ADAPTIVE ALGORITHMS

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This paper studies transfer learning for estimating the mean of random functions based on discretely sampled data, where in addition to observations from the target distribution, auxiliary samples from similar but distinct source distributions are available. The paper considers both common and independent designs and establishes the minimax rates of convergence for both designs. The results reveal an interesting phase transition phenomenon under the two designs and demonstrate the benefits of utilizing the source samples in the low sampling frequency regime.

For practical applications, this paper proposes novel data-driven adaptive algorithms that attain the optimal rates of convergence within a logarithmic factor simultaneously over a large collection of parameter spaces. The theoretical findings are complemented by a simulation study that further supports the effectiveness of the proposed algorithms.

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FINDING THE OPTIMAL DYNAMIC TREATMENT REGIMES USING SMOOTH FISHER CONSISTENT SURROGATE LOSS

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Large health care data repositories such as electronic health records (EHR) open new opportunities to derive individualized treatment strategies for complicated diseases such as sepsis. In this paper, we consider the problem of estimating sequential treatment rules tailored to a patient's individual characteristics, often referred to as dynamic treatment regimes (DTRs). Our main objective is to find the optimal DTR that maximizes a discontinuous value function through direct maximization of Fisher consistent surrogate loss functions. In this regard, we demonstrate that a large class of concave surrogates fails to be Fisher consistent—a behavior that differs from the classical binary classification problems. We further characterize a nonconcave family of Fisher consistent smooth surrogate functions, which is amenable to gradient-descent type optimization algorithms. Compared to the existing direct search approach under the support vector machine framework (*J. Amer. Statist. Assoc.* **110** (2015) 583–598), our proposed DTR estimation via surrogate loss optimization (DTRESLO) method is more computationally scalable to large sample sizes and allows for broader functional classes for treatment policies. We establish theoretical properties for our proposed DTR estimator and obtain a sharp upper bound on the regret corresponding to our DTRESLO method. The finite sample performance of our proposed estimator is evaluated through extensive simulations. We also illustrate the working principles and benefits of our method for estimating an optimal DTR for treating sepsis using EHR data from sepsis patients admitted to intensive care units.

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EDGE DIFFERENTIALLY PRIVATE ESTIMATION IN THE β-MODEL VIA JITTERING AND METHOD OF MOMENTS

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A standing challenge in data privacy is the trade-off between the level of privacy and the efficiency of statistical inference. Here, we conduct an in-depth study of this trade-off for parameter estimation in the β-model (*Ann. Appl. Probab.* **21** (2011) 1400–1435) for edge differentially private network data released via jittering (*J. R. Stat. Soc. Ser. C. Appl. Stat.* **66** (2017) 481–500). Unlike most previous approaches based on maximum likelihood estimation for this network model, we proceed via the method of moments. This choice facilitates our exploration of a substantially broader range of privacy levels—corresponding to stricter privacy—than has been to date. Over this new range, we discover our proposed estimator for the parameters exhibits an interesting phase transition, with both its convergence rate and asymptotic variance following one of three different regimes of behavior depending on the level of privacy. Because identification of the operable regime is difficult, if not impossible in practice, we devise a novel adaptive bootstrap procedure to construct uniform inference across different phases. In fact, leveraging this bootstrap we are able to provide for simultaneous inference of all parameters in the β-model (i.e., equal to the number of nodes), which, to our best knowledge, is the first result of its kind. Numerical experiments confirm the competitive and reliable finite sample performance of the proposed inference methods, next to a comparable maximum likelihood method, as well as significant advantages in terms of computational speed and memory.

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INFERENCE FOR HETEROSKEDASTIC PCA WITH MISSING DATA

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This paper studies how to construct confidence regions for principal component analysis (PCA) in high dimension, a problem that has been vastly underexplored. While computing measures of uncertainty for nonlinear/nonconvex estimators is in general difficult in high dimension, the challenge is further compounded by the prevalent presence of missing data and heteroskedastic noise. We propose a novel approach to performing valid inference on the principal subspace, on the basis of an estimator called HeteroPCA (*Ann. Statist.* **50** (2022b) 53–80). We develop nonasymptotic distributional guarantees for HeteroPCA, and demonstrate how these can be invoked to compute both confidence regions for the principal subspace and entrywise confidence intervals for the spiked covariance matrix. Our inference procedures are fully data-driven and adaptive to heteroskedastic random noise, without requiring prior knowledge about the noise levels.

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METRIC STATISTICS: EXPLORATION AND INFERENCE FOR RANDOM OBJECTS WITH DISTANCE PROFILES

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This article provides an overview on the statistical modeling of complex data as increasingly encountered in modern data analysis. It is argued that such data can often be described as elements of a metric space that satisfies certain structural conditions and features a probability measure. We refer to the random elements of such spaces as random objects and to the emerging field that deals with their statistical analysis as metric statistics. Metric statistics provides methodology, theory and visualization tools for the statistical description, quantification of variation, centrality and quantiles, regression and inference for populations of random objects, inferring these quantities from available data and samples. In addition to a brief review of current concepts, we focus on distance profiles as a major tool for object data in conjunction with the pairwise Wasserstein transports of the underlying one-dimensional distance distributions. These pairwise transports lead to the definition of intuitive and interpretable notions of transport ranks and transport quantiles as well as two-sample inference. An associated profile metric complements the original metric of the object space and may reveal important features of the object data in data analysis. We demonstrate these tools for the analysis of complex data through various examples and visualizations.

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MINIMAX RATES FOR HETEROGENEOUS CAUSAL EFFECT ESTIMATION

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Estimation of heterogeneous causal effects—that is, how effects of policies and treatments vary across subjects—is a fundamental task in causal inference. Many methods for estimating conditional average treatment effects (CATEs) have been proposed in recent years, but questions surrounding optimality have remained largely unanswered. In particular, a minimax theory of optimality has yet to be developed, with the minimax rate of convergence and construction of rate-optimal estimators remaining open problems. In this paper, we derive the minimax rate for CATE estimation, in a Hölder-smooth nonparametric model, and present a new local polynomial estimator, giving high-level conditions under which it is minimax optimal. Our minimax lower bound is derived via a localized version of the method of fuzzy hypotheses, combining lower bound constructions for nonparametric regression and functional estimation. Our proposed estimator can be viewed as a local polynomial R-Learner, based on a localized modification of higher-order influence function methods. The minimax rate we find exhibits several interesting features, including a nonstandard elbow phenomenon and an unusual interpolation between nonparametric regression and functional estimation rates. The latter quantifies how the CATE, as an estimand, can be viewed as a regression/functional hybrid.

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THE ONLINE CLOSURE PRINCIPLE

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The closure principle is fundamental in multiple testing and has been used to derive many efficient procedures with familywise error rate control. However, it is often unsuitable for modern research, which involves flexible multiple testing settings where not all hypotheses are known at the beginning of the evaluation. In this paper, we focus on online multiple testing where a possibly infinite sequence of hypotheses is tested over time. At each step, it must be decided on the current hypothesis without having any information about the hypotheses that have not been tested yet. Our main contribution is a general and stringent mathematical definition of online multiple testing and a new online closure principle, which ensures that the resulting closed procedure can be applied in the online setting. We prove that any familywise error rate controlling online procedure can be derived by this online closure principle and provide admissibility results. In addition, we demonstrate how shortcuts of these online closed procedures can be obtained under a suitable consonance property.

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PARAMETER ESTIMATION IN NONLINEAR MULTIVARIATE STOCHASTIC DIFFERENTIAL EQUATIONS BASED ON SPLITTING SCHEMES

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The likelihood functions for discretely observed nonlinear continuous time models based on stochastic differential equations are not available except for a few cases. Various parameter estimation techniques have been proposed, each with advantages, disadvantages and limitations depending on the application. Most applications still use the Euler–Maruyama discretization, despite many proofs of its bias. More sophisticated methods, such as Kessler's Gaussian approximation, Ozaki's local linearization, Aït–Sahalia's Hermite expansions or MCMC methods, might be complex to implement, do not scale well with increasing model dimension or can be numerically unstable. We propose two efficient and easy-to-implement likelihood-based estimators based on the Lie–Trotter (LT) and the Strang (S) splitting schemes. We prove that S has L^p convergence rate of order 1, a property already known for LT. We show that the estimators are consistent and asymptotically efficient under the less restrictive one-sided Lipschitz assumption. A numerical study on the 3-dimensional stochastic Lorenz system complements our theoretical findings. The simulation shows that the S estimator performs the best when measured on precision and computational speed compared to the state-of-the-art.

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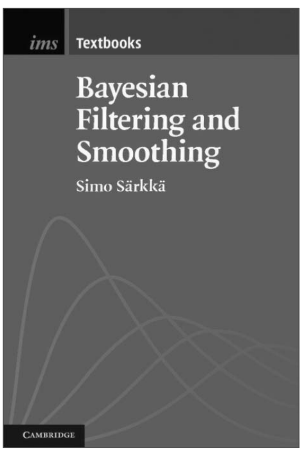

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Simo Särkkä

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