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EMPIRICAL PARTIALLY BAYES MULTIPLE TESTING AND COMPOUND χ^2 DECISIONS

BY NIKOLAOS IGNATIADIS^{1,a}  AND BODHISATTVA SEN^{2,b} 

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A common task in high-throughput biology is to screen for associations across thousands of units of interest, for example, genes or proteins. Often, the data for each unit are modeled as Gaussian measurements with unknown mean and variance and are summarized as per-unit sample averages and sample variances. The downstream goal is multiple testing for the means. In this domain, it is routine to “moderate” (i.e., to shrink) the sample variances through parametric empirical Bayes methods before computing p -values for the means. Such an approach is asymmetric in that a prior is posited and estimated for the nuisance parameters (variances) but not the primary parameters (means). Our work initiates the formal study of this paradigm, which we term “empirical partially Bayes multiple testing.” In this framework, if the prior for the variances were known, one could proceed by computing p -values conditional on the sample variances—a strategy called partially Bayes inference by Sir David Cox. We show that these conditional p -values satisfy an Eddington/Tweedie-type formula and are approximated at nearly-parametric rates when the prior is estimated by nonparametric maximum likelihood. The estimated p -values can be used with the Benjamini–Hochberg procedure to guarantee asymptotic control of the false discovery rate. Even in the compound setting, wherein the variances are fixed, the approach retains asymptotic type-I error guarantees.

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CONCENTRATION OF DISCREPANCY-BASED APPROXIMATE BAYESIAN COMPUTATION VIA RADEMACHER COMPLEXITY

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There has been an increasing interest on summary-free solutions for approximate Bayesian computation (ABC) that replace distances among summaries with discrepancies between the empirical distributions of the observed data and the synthetic samples generated under the proposed parameter values. The success of these strategies has motivated theoretical studies on the limiting properties of the induced posteriors. However, there is still the lack of a theoretical framework for summary-free ABC that (i) is unified, instead of discrepancy-specific, (ii) does not necessarily require to constrain the analysis to data generating processes and statistical models meeting specific regularity conditions, but rather facilitates the derivation of limiting properties that hold uniformly, and (iii) relies on verifiable assumptions that provide more explicit concentration bounds clarifying which factors govern the limiting behavior of the ABC posterior. We address this gap via a novel theoretical framework that introduces the concept of Rademacher complexity in the analysis of the limiting properties for discrepancy-based ABC posteriors, including in non-i.i.d. and misspecified settings. This yields a unified theory that relies on constructive arguments and provides more informative asymptotic results and uniform concentration bounds, even in those settings not covered by current studies. These key advancements are obtained by relating the asymptotic properties of summary-free ABC posteriors to the behavior of the Rademacher complexity associated with the chosen discrepancy within the family of integral probability semimetrics (IPS). The IPS class extends summary-based distances, and also includes the widely implemented Wasserstein distance and maximum mean discrepancy (MMD), among others. As clarified in specialized theoretical analyses of popular IPS discrepancies and via illustrative simulations, this new perspective improves the understanding of summary-free ABC.

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ON THE SAMPLE COMPLEXITY OF ENTROPIC OPTIMAL TRANSPORT

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We study the sample complexity of entropic optimal transport in high dimensions using computationally efficient plug-in estimators. We significantly advance the state of the art by establishing dimension-free, parametric rates for estimating various quantities of interest, including the entropic regression function, which is a natural analog to the optimal transport map. As an application, we propose a practical model for transfer learning based on entropic optimal transport and establish parametric rates of convergence for nonparametric regression and classification.

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DEFLATED HETEROPCA: OVERCOMING THE CURSE OF ILL-CONDITIONING IN HETEROSKEDASTIC PCA

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This paper is concerned with estimating the column subspace of a low-rank matrix $\mathbf{X}^* \in \mathbb{R}^{n_1 \times n_2}$ from contaminated data. How to obtain optimal statistical accuracy while accommodating the widest range of signal-to-noise ratios (SNRs) becomes particularly challenging in the presence of heteroskedastic noise and unbalanced dimensionality (i.e., $n_2 \gg n_1$). While the state-of-the-art algorithm HeteroPCA emerges as a powerful solution for solving this problem, it suffers from “the curse of ill-conditioning,” namely, its performance degrades as the condition number of $\mathbf{X}^*$ grows. In order to overcome this critical issue without compromising the range of allowable SNRs, we propose a novel algorithm, called Deflated – HeteroPCA, that achieves near-optimal and condition-number-free theoretical guarantees in terms of both ℓ_2 and $\ell_{2,\infty}$ statistical accuracy. The proposed algorithm divides the spectrum of $\mathbf{X}^*$ into well-conditioned and mutually well-separated subblocks, and applies HeteroPCA to conquer each subblock successively. Further, an application of our algorithm and theory to two canonical examples—the factor model and tensor PCA—leads to remarkable improvement for each application.

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NONLINEAR GLOBAL FRÉCHET REGRESSION FOR RANDOM OBJECTS VIA WEAK CONDITIONAL EXPECTATION

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Random objects are complex non-Euclidean data taking values in general metric spaces, possibly devoid of any underlying vector space structure. Such data are becoming increasingly abundant with the rapid advancement in technology. Examples include probability distributions, positive semidefinite matrices and data on Riemannian manifolds. However, except for regression for object-valued response with Euclidean predictors and distribution-on-distribution regression, there has been limited development of a general framework for object-valued response with object-valued predictors in the literature. To fill this gap, we introduce the notion of a weak conditional Fréchet mean based on Carleman operators and then propose a global nonlinear Fréchet regression model through the reproducing kernel Hilbert space (RKHS) embedding. Furthermore, we establish the relationships between the conditional Fréchet mean and the weak conditional Fréchet mean for both Euclidean and object-valued data. We also show that the state-of-the-art global Fréchet regression developed by Petersen and Müller (*Ann. Statist.* **47** (2019) 691–719) emerges as a special case of our method by choosing a linear kernel. We require that the metric space for the predictor admits a reproducing kernel, while the intrinsic geometry of the metric space for the response is utilized to study the asymptotic properties of the proposed estimates. Numerical studies, including extensive simulations and a real application, are conducted to investigate the finite-sample performance.

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SIMPLEX QUANTILE REGRESSION WITHOUT CROSSING

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Noncrossing quantile regression with an emphasis on model misspecification is investigated. While many sophisticated methods for noncrossing quantile have been developed under the assumption of correct model specification, model misspecification and extrapolation are two issues rarely considered in the literature. In this paper, a monotonicity representation for quantile regression models is obtained under simplex embedding, which leads to the simplex quantile regression (SQR) method. SQR model advocates the use of the Barycentric coordinate system and is immune to quantile crossing. An innovative concept, the maximum effective region, which defines the allowable region for extrapolation without quantile crossing is introduced. Under model misspecification, the existence of pseudo true quantile regression parameters, the asymptotic property of SQR estimator and asymptotic optimality of cross-validation for model selection and model averaging are established. The advantages of our new approach are also illustrated by numerical results. The proposed method is applied to U.S. financial market data. Our SQR-based strategy of asset pricing analysis allows for head-to-head transparent comparisons of five periods between October 1987 (Black Monday crash period) and February 2020 (COVID-19 pandemic).

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BAYESIAN NONPARAMETRIC INFERENCE IN MCKEAN-VLASOV MODELS

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We consider nonparametric statistical inference on a periodic interaction potential W from noisy discrete space-time measurements of solutions $\rho = \rho_W$ of the nonlinear McKean–Vlasov equation, describing the probability density of the mean field limit of an interacting particle system. We show how Gaussian process priors assigned to W give rise to posterior mean estimators that exhibit fast convergence rates for the implied estimated densities $\bar{\rho}$ towards ρ_W . We further show that if the initial condition ϕ is not too smooth and satisfies a standard deconvolvability condition, then one can consistently infer Sobolev-regular potentials W at convergence rates $N^{-\theta}$ for appropriate $\theta > 0$, where N is the number of measurements. The exponent θ can be taken to approach $1/2$ as the regularity of W increases corresponding to ‘near-parametric’ models.

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ENSEMBLE PROJECTION PURSUIT FOR GENERAL NONPARAMETRIC REGRESSION

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Projection pursuit regression (PPR) and artificial neural networks (ANNs), both introduced around the same time, share a similar approach to approximating complex structures in data. However, PPR has received far less attention than ANNs and other popular statistical learning methods such as random forests (RF) and support vector machines (SVM). In this paper, we revisit the estimation of PPR and propose an *optimal* greedy algorithm and an ensemble approach via feature bagging, hereafter referred to as ePPR, to improve its effectiveness. Compared to RF, ePPR has two main advantages. First, its theoretical consistency can be proved for more general regression functions, as long as they are L^2 integrable, and higher consistency rates can be achieved. Second, ePPR does not split the samples, so each term of the PPR is estimated using the entire data, making minimisation more efficient and ensuring the smoothness of the estimator. Extensive comparisons on real data sets show that ePPR is more efficient in regression and classification than RF and other competitors.

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RATE-OPTIMAL ESTIMATION OF MIXED SEMIMARTINGALES

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Consider the sum $Y = B + B(H)$ of a Brownian motion B and an independent fractional Brownian motion $B(H)$ with Hurst parameter $H \in (0, 1)$. Even though $B(H)$ is not a semimartingale, it was shown by Cheridito (Bernoulli 7 (2001) 913–934) that Y is a semimartingale if $H > 3/4$. Moreover, Y is locally equivalent to B in this case, so H cannot be consistently estimated from local observations of Y . This paper pivots on another unexpected feature in this model: if B and $B(H)$ become correlated, then Y will never be a semimartingale, and H can be identified, regardless of its value. This and other results will follow from a detailed statistical analysis of a more general class of processes called *mixed semimartingales*, which are semiparametric extensions of Y with stochastic volatility in both the martingale and the fractional component. In particular, we derive consistent estimators and feasible central limit theorems for all parameters and processes that can be identified from high-frequency observations. We further show that our estimators achieve optimal rates in a minimax sense.

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SOME THEORY ABOUT EFFICIENT DIMENSION REDUCTION REGARDING THE INTERACTION BETWEEN TWO RESPONSES

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Efficient dimension reduction regarding the interaction between two response variables, which facilitates statistical analysis in multiple important application scenarios, was initially discussed by Luo (*J. R. Stat. Soc. Ser. B. Stat. Methodol.* **84** (2022) 269–294). The efficient dimension reduction subspaces were introduced, and, under mild conditions on the predictor, they were equated with the family of dual inverse regression subspaces. Besides the general framework, however, limited theory has been proposed to uncover the mystery of these spaces. In this paper, we propose a thorough characterization of the family of dual inverse regression subspaces, including their uniform lower and upper bounds, their explicit forms, their consistent and exhaustive estimation, some interesting special cases, and certain subfamilies that have desired sparsity. In addition, we extend some of these results to provide more insights into the efficient dimension reduction subspaces under the general settings, including their uniform lower and upper bounds, and the sufficient and necessary conditions for the uniqueness of the space that are assessable in practice. These results largely complete the theoretical foundation for the new type of dimension reduction, and, as such, enhance its applicability in statistical problems such as missing data analysis and causal inference. The latter is illustrated by simulation studies and a real data example at the end.

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GENERAL SPATIO-TEMPORAL FACTOR MODELS FOR HIGH-DIMENSIONAL RANDOM FIELDS ON A LATTICE

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Motivated by the need for analysing large spatio-temporal panel data, we introduce a novel nonparametric methodology for n -dimensional random fields observed across S spatial locations and T time periods. We call it general spatio-temporal factor model (GSTFM). First, we provide the probabilistic and mathematical underpinning needed for the representation of a random field as the sum of two components: the common component (driven by a small number q of latent factors) and the idiosyncratic component (mildly cross-correlated). We show that the two components are identified as $n \rightarrow \infty$. Second, we propose an estimator of the common component and derive its statistical guarantees (consistency and rate of convergence) as $\min(n, S, T) \rightarrow \infty$. Third, we propose an information criterion to determine the number of factors. Estimation makes use of Fourier analysis in the frequency domain and thus it fully exploits the information on the spatio-temporal covariance structure of the whole panel. Synthetic data examples illustrate the applicability of GSTFM and its advantages over the extant generalized dynamic factor model that ignores the spatial correlations.

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OPTIMAL HETEROSKEDASTICITY TESTING IN NONPARAMETRIC REGRESSION

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Heteroskedasticity testing in nonparametric regression is a classic statistical problem with important practical applications, yet fundamental limits are unknown. Adopting a minimax perspective, this article considers the testing problem in the context of an α -Hölder mean and a β -Hölder variance function. For $\alpha > 0$ and $\beta \in (0, 1/2)$, the sharp minimax separation rate $n^{-4\alpha} + n^{-4\beta/(4\beta+1)} + n^{-2\beta}$ is established. To achieve the minimax separation rate, a kernel-based statistic using first-order squared differences is developed. Notably, the statistic estimates a proxy rather than a natural quadratic functional (the squared distance between the variance function and its best L^2 approximation by a constant) suggested in previous work.

The setting where no smoothness is assumed on the variance function is also studied; the variance profile across the design points can be arbitrary. Despite the lack of structure, consistent testing turns out to still be possible by using the Gaussian character of the noise, and the minimax rate is shown to be $n^{-4\alpha} + n^{-1/2}$. Exploiting noise information happens to be a fundamental necessity, as consistent testing is impossible if nothing more than zero mean and unit variance is known about the noise distribution. Furthermore, in the setting where the variance function is β -Hölder but heteroskedasticity is measured only with respect to the design points, the minimax separation rate is shown to be $n^{-4\alpha} + n^{-((1/2) \vee (4\beta/(4\beta+1)))}$ when the noise is Gaussian and $n^{-4\alpha} + n^{-4\beta/(4\beta+1)} + n^{-2\beta}$ when the noise distribution is unknown.

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A STATISTICAL FRAMEWORK OF WATERMARKS FOR LARGE LANGUAGE MODELS: PIVOT, DETECTION EFFICIENCY AND OPTIMAL RULES

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Since ChatGPT was introduced in November 2022, embedding (nearly) unnoticeable statistical signals into text generated by large language models (LLMs), also known as watermarking, has been used as a principled approach to provable detection of LLM-generated text from its human-written counterpart. In this paper, we introduce a general and flexible framework for reasoning about the statistical efficiency of watermarks and designing powerful detection rules. Inspired by the hypothesis testing formulation of watermark detection, our framework starts by selecting a pivotal statistic of the text and a secret key—provided by the LLM to the verifier—to control the false positive rate (the error of mistakenly detecting human-written text as LLM-generated). Next, this framework allows one to evaluate the power of watermark detection rules by obtaining a closed-form expression of the asymptotic false negative rate (the error of incorrectly classifying LLM-generated text as human-written). Our framework further reduces the problem of determining the optimal detection rule to solving a minimax optimization program. We apply this framework to two representative watermarks—one of which has been internally implemented at OpenAI—and obtain several findings that can be instrumental in guiding the practice of implementing watermarks. In particular, we derive optimal detection rules for these watermarks under our framework. These theoretically derived detection rules are demonstrated to be competitive and sometimes enjoy a higher power than existing detection approaches through numerical experiments.

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EMPIRICAL LIKELIHOOD BASED TESTING FOR MULTIVARIATE REGULAR VARIATION

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Multivariate regular variation is a common assumption in the statistics literature and needs to be verified in real-data applications. We develop a novel hypothesis test for multivariate regular variation, employing localized empirical likelihood. We establish the weak convergence of the test statistic to a nonstandard, distribution-free limit and hence can provide universal critical values for the test. We show the very good finite-sample behavior of the procedure through simulations and apply the test to several real-data examples.

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COMPUTATIONALLY EFFICIENT AND STATISTICALLY OPTIMAL ROBUST HIGH-DIMENSIONAL LINEAR REGRESSION

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High-dimensional linear regression under heavy-tailed noise or outlier corruption is challenging, both computationally and statistically. Convex approaches have been proven statistically optimal but suffer from high computational costs, especially since the robust loss functions are usually nonsmooth. More recently, computationally fast nonconvex approaches via subgradient descent are proposed, which, unfortunately, fail to deliver a statistically consistent estimator even under sub-Gaussian noise. In this paper, we introduce a projected subgradient descent algorithm for both the sparse linear regression and low-rank linear regression problems. The algorithm is not only computationally efficient with linear convergence but also statistically optimal, be the noise Gaussian or heavy-tailed with a finite $1 + \varepsilon$ moment. The convergence theory is established for a general framework and its specific applications to absolute loss, Huber loss and quantile loss are investigated. Compared with existing nonconvex methods, ours reveals a surprising phenomenon of *two-phase convergence*. In phase one, the algorithm behaves as in typical nonsmooth optimization that requires gradually decaying stepsizes. However, phase one only delivers a statistically suboptimal estimator, which is already observed in the existing literature. Interestingly, during phase two, the algorithm converges linearly *as if* minimizing a smooth and strongly convex objective function, and thus a constant stepsize suffices. Underlying the phase-two convergence is the *smoothing effect* of random noise to the nonsmooth robust losses in an area *close but not too close* to the truth. Numerical simulations confirm our theoretical discovery and showcase the superiority of our algorithm over prior methods.

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MULTIVARIATE DYNAMIC MEDIATION ANALYSIS UNDER A REINFORCEMENT LEARNING FRAMEWORK

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Mediation analysis is an important analytic tool commonly used in a broad range of scientific applications. In this article, we study the problem of mediation analysis when there are multivariate and conditionally dependent mediators, and when the variables are observed over multiple time points. The problem is challenging, because the effect of a mediator involves not only the path from the treatment to this mediator itself at the current time point, but also all possible paths pointed to this mediator from its upstream mediators, as well as the carryover effects from all previous time points. We propose a novel multivariate dynamic mediation analysis approach. Drawing inspiration from the Markov decision process model that is frequently employed in reinforcement learning, we introduce a Markov mediation process paired with a system of time-varying linear structural equation models to formulate the problem. We then formally define the individual mediation effect, built upon the idea of simultaneous interventions and intervention calculus. We next derive the closed-form expression, propose an iterative estimation procedure under the Markov mediation process model and develop a bootstrap method to infer the individual mediation effect. We study both the asymptotic property and the empirical performance of the proposed methodology, and further illustrate its usefulness with a mobile health application.

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UNIFIED ALGORITHMS FOR RL WITH DECISION-ESTIMATION COEFFICIENTS: PAC, REWARD-FREE, PREFERENCE-BASED LEARNING AND BEYOND

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Modern Reinforcement Learning (RL) is more than just learning the optimal policy; alternative learning goals such as exploring the environment, estimating the underlying model and learning from preference feedback are all of practical importance. While provably sample-efficient algorithms for each specific goal have been proposed, these algorithms often depend strongly on the particular learning goal, and thus admit different structures correspondingly. It is an urging open question whether these learning goals can rather be tackled by a single unified algorithm.

We make progress on this question by developing a unified algorithm framework for a large class of learning goals, building on the Decision-Estimation Coefficient (DEC) framework. Our framework handles many learning goals such as no-regret RL, PAC RL, reward-free learning, model estimation and preference-based learning, all by simply instantiating the same generic complexity measure called “Generalized DEC,” and a corresponding generic algorithm. The generalized DEC also yields a sample complexity lower bound for each specific learning goal. As applications, we propose “decouplable representation” as a natural sufficient condition for bounding generalized DEC, and use it to obtain many new sample-efficient results (and recover existing results) for a wide range of learning goals and problem classes as direct corollaries. Finally, as a connection, we reanalyze two existing optimistic model-based algorithms based on posterior sampling and maximum likelihood estimation, showing that they enjoy sample complexity bounds under similar structural conditions as the DEC.

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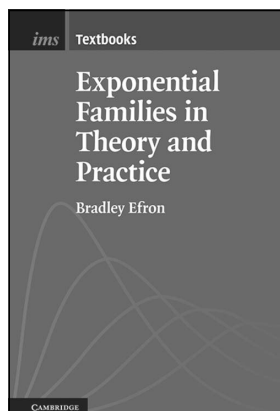
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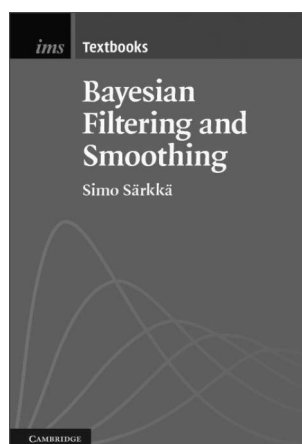
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