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A COMMON-CAUSE PRINCIPLE FOR ELIMINATING SELECTION BIAS IN CAUSAL ESTIMANDS THROUGH COVARIATE ADJUSTMENT

BY MAYA B. MATHUR^{1,a} , TYLER J. VANDERWEELE^{2,b} AND ILYA SHPITSER^{3,c}

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Average treatment effects (ATEs) may be subject to selection bias when they are estimated among only a nonrepresentative subset of the target population. Selection bias can sometimes be eliminated by conditioning on a “sufficient adjustment set” of covariates, even for some forms of missingness not at random (MNAR). Without requiring full specification of the causal structure, we consider sufficient adjustment sets to allow nonparametric identification of conditional ATEs in the target population. Covariates in the sufficient set may be collected among only the selected sample. We establish that if a sufficient set exists, then the set consisting of common causes of the outcome and selection, excluding the exposure and its descendants, also suffices. We establish simple graphical criteria for when a sufficient set will not exist, which could help indicate whether this is plausible for a given study. Simulations considering selection due to missing data indicated that sufficiently-adjusted complete-case analysis (CCA) can considerably outperform multiple imputation under MNAR and, if the sample size is not large, sometimes even under missingness at random. Analogous to the common-cause principle for confounding, these sufficiency results clarify when and how selection bias can be eliminated through covariate adjustment.

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NEAR-OPTIMAL INFERENCE IN ADAPTIVE LINEAR REGRESSION

BY KOULIK KHAMARU^{1,a}, YASH DESHPANDE^{2,b}, TOR LATTIMORE^{3,c},
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When data is collected in an adaptive manner, even simple methods like ordinary least squares can exhibit nonnormal asymptotic behavior. As an undesirable consequence, hypothesis tests and confidence intervals based on asymptotic normality can lead to erroneous results. We propose a family of online debiasing estimators to correct these distributional anomalies in least squares estimation. Our proposed methods take advantage of the covariance structure present in the dataset and provide sharper estimates in directions for which more information has accrued. We establish an asymptotic normality property for our proposed online debiasing estimators under mild conditions on the data collection process and provide asymptotically exact confidence intervals. We additionally prove a minimax lower bound for the adaptive linear regression problem, thereby providing a baseline by which to compare estimators. There are various conditions under which our proposed estimators achieve the minimax lower bound. We demonstrate the usefulness of our theory via applications to multi-armed bandit, autoregressive time series estimation, and active learning with exploration.

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ASYMPTOTICALLY-EXACT SELECTIVE INFERENCE FOR QUANTILE REGRESSION

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In modern data analysis, it is common to select a model before performing statistical inference. Selective inference tools make adjustments for the model selection process in order to ensure reliable inference post selection. In this paper, we introduce an asymptotic pivot to infer about the effects of selected variables on conditional quantile functions. Utilizing estimators from smoothed quantile regression, our proposed pivot is easy to compute and yields asymptotically-exact selective inference without making strict distributional assumptions about the response variable.

At the core of our pivot is the use of external randomization variables, which allows us to utilize all available samples for both selection and inference, without partitioning the data into independent subsets or discarding samples at any step. From simulation studies, we find that: (i) the asymptotic confidence intervals based on our pivot achieve the desired coverage rates, even in cases where sample splitting fails due to insufficient sample size for inference; (ii) our intervals are consistently shorter than those produced by sample splitting across various models and signal settings. We report similar findings when we apply our approach to study risk factors for low birth weights in a publicly accessible dataset of US birth records from 2022.

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COUNTERFACTUAL INFERENCE IN SEQUENTIAL EXPERIMENTS

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We consider after-study statistical inference for sequentially designed experiments wherein multiple units are assigned treatments for multiple time points using treatment policies that adapt over time. Our goal is to provide inference guarantees for the counterfactual mean at the smallest possible scale—mean outcome under different treatments *for each unit and each time*—with minimal assumptions on the adaptive treatment policy. Without any structural assumptions on the counterfactual means, this challenging task is infeasible due to more unknowns than observed data points. To make progress, we introduce a latent factor model over the counterfactual means that serves as a nonparametric generalization of the nonlinear mixed effects model and the bilinear latent factor model considered in prior works. For estimation, we use a nonparametric method, namely a variant of nearest neighbors, and establish a nonasymptotic high probability error bound for the counterfactual mean for each unit and each time. Under regularity conditions, this bound leads to asymptotically valid confidence intervals for the counterfactual mean as the number of units and time points grows to ∞ together at suitable rates. We illustrate our theory via several simulations and a case study involving data from a mobile health clinical trial HeartSteps.

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CLUSTERING RISK IN NONPARAMETRIC HIDDEN MARKOV AND I.I.D. MODELS

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We conduct an in-depth analysis of the Bayes risk of clustering in the context of hidden Markov and i.i.d. models. In both settings, we identify the situations where this risk is comparable to the Bayes risk of classification and those where its minimizer, the Bayes clusterer, can be derived from the Bayes classifier. While we demonstrate that clustering based on the Bayes classifier does not always match the optimal Bayes clusterer, we show that this difference is primarily theoretical and that the Bayes classifier remains nearly optimal for clustering. A key quantity emerges, capturing the fundamental difficulty of both classification and clustering tasks. Furthermore, by leveraging the identifiability of HMMs, we establish bounds on the clustering excess risk of a plug-in Bayes classifier in the general nonparametric setting, offering theoretical justification for its widespread use in practice. Simulations further illustrate our findings.

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CAUSAL EFFECT ESTIMATION UNDER NETWORK INTERFERENCE WITH MEAN-FIELD METHODS

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We study causal effect estimation from observational data under interference. The interference pattern is captured by an observed network. We adopt the chain graph framework of (*J. Amer. Statist. Assoc.* **116** (2021) 833–844), which allows (i) interaction among the outcomes of distinct study units connected along the graph and (ii) long range interference, whereby the outcome of an unit may depend on the treatments assigned to distant units connected along the interference network. For “mean-field” interaction networks, we develop a new scalable iterative algorithm to estimate the causal effects. For Gaussian weighted networks, we introduce a novel causal effect estimation algorithm based on Approximate Message Passing (AMP). Our algorithms are provably consistent under a “high temperature” condition on the underlying model. We estimate the (unknown) parameters of the model from data using maximum pseudo-likelihood and establish $\sqrt{n}$ -consistency of this estimator in all parameter regimes. Finally, we prove that the downstream estimators obtained by plugging in estimated parameters into the aforementioned algorithms are consistent at high temperature. Our methods can accommodate dense interactions among the study units—a setting beyond reach using existing techniques. Our algorithms originate from the study of variational inference approaches in high-dimensional statistics; overall, we demonstrate the usefulness of these ideas in the context of causal effect estimation under interference.

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THE EMPIRICAL COPULA PROCESS IN HIGH DIMENSIONS: STUTE’S REPRESENTATION AND APPLICATIONS

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The empirical copula process, a fundamental tool for copula inference, is studied in the high dimensional regime where the dimension is allowed to grow to infinity exponentially in the sample size. Under natural, weak smoothness assumptions on the underlying copula, it is shown that Stute’s representation is valid in the following sense: all low-dimensional margins of fixed dimension of the empirical copula process can be approximated by a functional of the low-dimensional margins of the standard empirical process, with the almost sure error term being uniform in the margins. The result has numerous potential applications, and is exemplarily applied to the problem of testing pairwise stochastic independence in high dimensions, leading to various extensions of recent results in the literature: for certain test statistics based on pairwise association measures, type-I error control is obtained for models beyond mutual independence. Moreover, bootstrap-based critical values are shown to yield strong control of the familywise error rate for a large class of data generating processes.

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SEMI-SUPERVISED U-STATISTICS

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Semi-supervised datasets are ubiquitous across diverse domains where obtaining fully labeled data is costly or time-consuming. The prevalence of such datasets has consistently driven the demand for new tools and methods that exploit the potential of unlabeled data. Responding to this demand, we introduce semi-supervised U-statistics enhanced by the abundance of unlabeled data, and investigate their statistical properties. We show that the proposed approach is asymptotically Normal and exhibits notable efficiency gains over classical U-statistics by effectively integrating various powerful prediction tools into the framework. To understand the fundamental difficulty of the problem, we derive minimax lower bounds in semi-supervised settings and showcase that our procedure is semi-parametrically efficient under regularity conditions. Moreover, tailored to bivariate kernels, we propose a refined approach that outperforms the classical U-statistic across all degeneracy regimes, and demonstrate its optimality properties. Simulation studies are conducted to corroborate our findings and to further demonstrate our framework.

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A FLEXIBLE DEFENSE AGAINST THE WINNER’S CURSE

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Across science and policy, decision-makers often need to draw conclusions about the best candidate among competing alternatives. For instance, researchers may seek to infer the effectiveness of the most successful treatment or determine which demographic group benefits most from a specific treatment. Similarly, in machine learning, practitioners are often interested in the population performance of the model that performs best empirically. However, cherry-picking the best candidate leads to the winner’s curse: the observed performance for the winner is biased upwards, rendering conclusions based on standard measures of uncertainty invalid. We introduce the *zoom correction*, a novel approach for valid inference on the winner. Our method is flexible: it can be employed in both parametric and nonparametric settings, can handle arbitrary dependencies between candidates, and automatically adapts to the level of selection bias. The method easily extends to important related problems, such as inference on the top k winners, inference on the value and identity of the population winner, and inference on “near-winners.”

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CLUSTERING BY HILL-CLIMBING: CONSISTENCY RESULTS

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We consider several hill-climbing approaches to clustering as formulated by Fukunaga and Hostetler (*IEEE Trans. Inf. Theory* **IT-21** (1975) 32–40) in the 1970s. We study both continuous-space and discrete-space (i.e., medoid) variants and establish their consistency.

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KURTOSIS-BASED PROJECTION PURSUIT FOR MATRIX-VALUED DATA

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We develop projection pursuit for data that admit a natural representation in matrix form. For projection indices, we propose extensions of the classical kurtosis and Mardia's multivariate kurtosis. The first index estimates projections for both sides of the matrices simultaneously, while the second index finds the two projections separately. Both indices are shown to recover the optimally separating projection for two-group Gaussian mixtures in the absence of any label information. We further establish the strong consistency of the corresponding sample estimators, as well as the asymptotic normality and high-dimensional consistency for the first estimator. Simulations and real data examples on hand-written postal codes and video data are used to demonstrate the method.

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A GEOMETRICAL ANALYSIS OF KERNEL RIDGE REGRESSION AND ITS APPLICATIONS

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We obtain upper bounds for the estimation error of Kernel Ridge Regression (KRR) for all nonnegative regularization parameters, offering a geometric perspective on various phenomena in KRR. As applications: 1. We address the Multiple Descents problem, unifying the proofs of (In *Proceedings of Thirty Third Conference on Learning Theory* (2020) 2683–2711 PMLR) and (*Ann. Statist.* **49** (2021) 1029–1054) for polynomial kernels in nonasymptotic regime and we establish Multiple Descents for the generalization error of KRR for polynomial kernel under sub-Gaussian design in asymptotic regimes. 2. In the nonasymptotic regime, we have established a one-sided isomorphic version of the Gaussian Equivalence Conjecture for sub-Gaussian design vectors. 3. We offer a novel perspective on the linearization of kernel matrices of nonlinear kernels, extending it to the power regime for polynomial kernels. 4. Our theory extends the results in (*J. Mach. Learn. Res.* **24** (2023) Paper No. [123]) under weak moment assumption.

Our proof is based on three mathematical tools developed in this paper that can be of independent interest: 1. Dvoretzky–Milman theorem for ellipsoids under (very) weak moment assumptions. 2. Restricted isomorphic property in reproducing kernel Hilbert spaces with embedding index conditions. 3. A concentration inequality for finite-degree polynomial kernel functions.

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A TWO-WAY HETEROGENEITY MODEL FOR DYNAMIC NETWORKS

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Analysis of networks that evolve dynamically requires the joint modelling of individual snapshots and time dynamics. This paper proposes a new flexible two-way heterogeneity model towards this goal. The new model equips each node of the network with two heterogeneity parameters, one to characterize the propensity to form ties with other nodes statically and the other to differentiate the tendency to retain existing ties over time. With n observed networks each having p nodes, we develop a new asymptotic theory for the maximum likelihood estimation of $2p$ parameters when $np \rightarrow \infty$. We overcome the global nonconvexity of the negative log-likelihood function by the virtue of its local convexity, and propose a novel method of moment estimator as the initial value for a simple algorithm that leads to the consistent local maximum likelihood estimator (MLE). To establish the upper bounds for the estimation error of the MLE, we derive a new uniform deviation bound, which is of independent interest. The theory of the model and its usefulness are further supported by extensive simulation and the analysis of some real network data sets.

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OPTIMAL SEQUENCING DEPTH FOR SINGLE-CELL RNA-SEQUENCING IN WASSERSTEIN SPACE

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How many samples should one collect for an empirical distribution to be as close as possible to the true population? This question is not trivial in the context of single-cell RNA-sequencing. With limited sequencing depth, profiling more cells comes at the cost of fewer reads per cell. Therefore, one must strike a balance between the number of cells sampled and the accuracy of each measured gene expression profile. In this paper, we analyze an empirical distribution of cells and obtain upper and lower bounds on the Wasserstein distance to the true population. Our analysis holds for general, nonparametric distributions of cells, and is validated by simulation experiments on a real single-cell dataset.

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HIGH-DIMENSIONAL HILBERT–SCHMIDT LINEAR REGRESSION WITH HILBERT MANIFOLD VARIABLES

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In this paper, we propose a novel high-dimensional linear regression technique for variables taking values in Hilbert manifolds. Our approach offers a flexible framework where the response and covariates originate from distinct spaces and are interconnected by Hilbert–Schmidt operators. Our methodology is designed for situations where the number of the covariates grows exponentially fast as the sample size increases and some of the covariates together with the response take values in infinite dimensional spaces. It is formulated under a general penalization scheme that includes various nonconvex penalty functions. Leveraging modern statistical theory for data residing on Hilbert manifolds, we establish the oracle property and derive error bounds for the proposed estimators. We also provide an efficient computational algorithm to solve the associated constrained optimization problem. The practical performance of the proposed method is demonstrated via numerical simulation and real data applications.

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ONLINE ESTIMATION WITH ROLLING VALIDATION: ADAPTIVE NONPARAMETRIC ESTIMATION WITH STREAMING DATA

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Online nonparametric estimators are gaining popularity due to their efficient computation and competitive generalization abilities. An important example includes variants of stochastic gradient descent. These algorithms often take one sample point at a time and incrementally update the parameter estimate of interest. In this work, we consider model selection/hyperparameter tuning for such online algorithms. We propose a weighted rolling validation procedure, an online variant of leave-one-out cross-validation, that costs minimal extra computation for many typical stochastic gradient descent estimators and maintains their online nature. Similar to batch cross-validation, it can boost base estimators to achieve better heuristic performance and adaptive convergence rate. Our analysis is straightforward, relying mainly on some general statistical stability assumptions. The simulation study underscores the significance of diverging weights in practice and demonstrates its favorable sensitivity even when there is only a slim difference between candidate estimators.

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FUNDAMENTAL LIMITS OF COMMUNITY DETECTION FROM MULTI-VIEW DATA: MULTI-LAYER, DYNAMIC AND PARTIALLY LABELED BLOCK MODELS

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Multi-view data arises frequently in modern network analysis for example, relations of multiple types among individuals in social network analysis, longitudinal measurements of interactions among observational units, annotated networks with noisy partial labeling of vertices etc. We study community detection in these disparate settings via a unified theoretical framework, and investigate the fundamental thresholds for community recovery. We characterize the mutual information between the data and the latent parameters, provided the degrees are sufficiently large. Based on this general result, (i) we derive a sharp threshold for community detection in an inhomogeneous multi-layer block model (*Ann. Statist.* **50** (2022) 2664–2693), (ii) characterize a sharp threshold for weak recovery in a dynamic stochastic block model (*J. R. Stat. Soc. Ser. B. Stat. Methodol.* **79** (2017) 1119–1141), and (iii) identify the limiting mutual information in an unbalanced partially labeled block model. Finally, we introduce iterative algorithms based on Approximate Message Passing for community detection in these problems.

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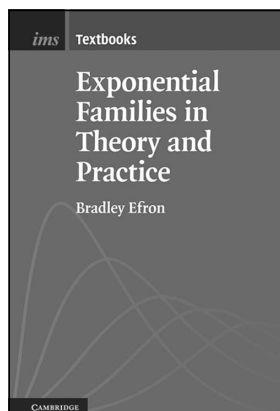
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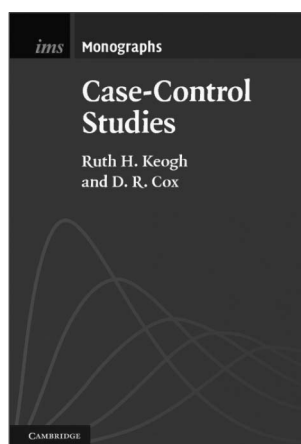
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