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LARGE COVARIANCE ESTIMATION THROUGH ELLIPTICAL FACTOR MODELS

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We propose a general Principal Orthogonal complEment Thresholding (POET) framework for large-scale covariance matrix estimation based on the approximate factor model. A set of high-level sufficient conditions for the procedure to achieve optimal rates of convergence under different matrix norms is established to better understand how POET works. Such a framework allows us to recover existing results for sub-Gaussian data in a more transparent way that only depends on the concentration properties of the sample covariance matrix. As a new theoretical contribution, for the first time, such a framework allows us to exploit conditional sparsity covariance structure for the heavy-tailed data. In particular, for the elliptical distribution, we propose a robust estimator based on the marginal and spatial Kendall's tau to satisfy these conditions. In addition, we study conditional graphical model under the same framework. The technical tools developed in this paper are of general interest to high-dimensional principal component analysis. Thorough numerical results are also provided to back up the developed theory.

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CURRENT STATUS LINEAR REGRESSION

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We construct $\sqrt{n}$-consistent and asymptotically normal estimates for the finite dimensional regression parameter in the current status linear regression model, which do not require any smoothing device and are based on maximum likelihood estimates (MLEs) of the infinite dimensional parameter. We also construct estimates, again only based on these MLEs, which are arbitrarily close to efficient estimates, if the generalized Fisher information is finite. This type of efficiency is also derived under minimal conditions for estimates based on smooth nonmonotone plug-in estimates of the distribution function. Algorithms for computing the estimates and for selecting the bandwidth of the smooth estimates with a bootstrap method are provided. The connection with results in the econometric literature is also pointed out.

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JUMP FILTERING AND EFFICIENT DRIFT ESTIMATION FOR LÉVY-DRIVEN SDES

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The problem of drift estimation for the solution X of a stochastic differential equation with Lévy-type jumps is considered under discrete high-frequency observations with a growing observation window. An efficient and asymptotically normal estimator for the drift parameter is constructed under minimal conditions on the jump behavior and the sampling scheme. In the case of a bounded jump measure density, these conditions reduce to $n\Delta_n^{3-\varepsilon} \to 0$, where n is the number of observations and Δ_n is the maximal sampling step. This result relaxes the condition $n\Delta_n^2 \to 0$ usually required for joint estimation of drift and diffusion coefficient for SDEs with jumps. The main challenge in this estimation problem stems from the appearance of the unobserved continuous part X^c in the likelihood function. In order to construct the drift estimator, we recover this continuous part from discrete observations. More precisely, we estimate, in a nonparametric way, stochastic integrals with respect to X^c. Convergence results of independent interest are proved for these nonparametric estimators.

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CONSISTENCY AND CONVERGENCE RATE OF PHYLOGENETIC INFERENCE VIA REGULARIZATION[2]

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It is common in phylogenetics to have some, perhaps partial, information about the overall evolutionary tree of a group of organisms and wish to find an evolutionary tree of a specific gene for those organisms. There may not be enough information in the gene sequences alone to accurately reconstruct the correct "gene tree." Although the gene tree may deviate from the "species tree" due to a variety of genetic processes, in the absence of evidence to the contrary it is parsimonious to assume that they agree. A common statistical approach in these situations is to develop a likelihood penalty to incorporate such additional information. Recent studies using simulation and empirical data suggest that a likelihood penalty quantifying concordance with a species tree can significantly improve the accuracy of gene tree reconstruction compared to using sequence data alone. However, the consistency of such an approach has not yet been established, nor have convergence rates been bounded. Because phylogenetics is a nonstandard inference problem, the standard theory does not apply. In this paper, we propose a penalized maximum likelihood estimator for gene tree reconstruction, where the penalty is the square of the Billera–Holmes–Vogtmann geodesic distance from the gene tree to the species tree. We prove that this method is consistent, and derive its convergence rate for estimating the discrete gene tree structure and continuous edge lengths (representing the amount of evolution that has occurred on that branch) simultaneously. We find that the regularized estimator is "adaptive fast converging," meaning that it can reconstruct all edges of length greater than any given threshold from gene sequences of polynomial length. Our method does not require the species tree to be known exactly; in fact, our asymptotic theory holds for any such guide tree.

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PARETO QUANTILES OF UNLABELED TREE OBJECTS

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In this paper, we consider a set of unlabeled tree objects with topological and geometric properties. For each data object, two curve representations are developed to characterize its topological and geometric aspects. We further define the notions of topological and geometric medians as well as quantiles based on both representations. In addition, we take a novel approach to define the Pareto medians and quantiles through a multi-objective optimization problem. In particular, we study two different objective functions which measure the topological variation and geometric variation, respectively. Analytical solutions are provided for topological and geometric medians and quantiles, and in general, for Pareto medians and quantiles, the genetic algorithm is implemented. The proposed methods are applied to analyze a data set of pyramidal neurons.

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EFFICIENT AND ADAPTIVE LINEAR REGRESSION IN SEMI-SUPERVISED SETTINGS[1]

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We consider the linear regression problem under semi-supervised settings wherein the available data typically consists of: (i) a small or moderate sized "labeled" data, and (ii) a *much larger* sized "unlabeled" data. Such data arises naturally from settings where the outcome, unlike the covariates, is expensive to obtain, a frequent scenario in modern studies involving large databases like electronic medical records (EMR). Supervised estimators like the ordinary least squares (OLS) estimator utilize only the labeled data. It is often of interest to investigate if and when the unlabeled data can be exploited to improve estimation of the regression parameter in the adopted linear model.

In this paper, we propose a class of "Efficient and Adaptive Semi-Supervised Estimators" (EASE) to improve estimation efficiency. The EASE are two-step estimators adaptive to model mis-specification, leading to improved (optimal in some cases) efficiency under model mis-specification, and equal (optimal) efficiency under a linear model. This adaptive property, often unaddressed in the existing literature, is crucial for advocating "safe" use of the unlabeled data. The construction of EASE primarily involves a flexible "semi-nonparametric" imputation, including a smoothing step that works well even when the number of covariates is not small; and a follow up "refitting" step along with a cross-validation (CV) strategy both of which have useful practical as well as theoretical implications towards addressing two important issues: under-smoothing and over-fitting. We establish asymptotic results including consistency, asymptotic normality and the adaptive properties of EASE. We also provide influence function expansions and a "double" CV strategy for inference. The results are further validated through extensive simulations, followed by application to an EMR study on auto-immunity.

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CONVEXIFIED MODULARITY MAXIMIZATION FOR DEGREE-CORRECTED STOCHASTIC BLOCK MODELS

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The stochastic block model (SBM), a popular framework for studying community detection in networks, is limited by the assumption that all nodes in the same community are statistically equivalent and have equal expected degrees. The degree-corrected stochastic block model (DCSBM) is a natural extension of SBM that allows for degree heterogeneity within communities. To find the communities under DCSBM, this paper proposes a *convexified modularity maximization* approach, which is based on a convex programming relaxation of the classical (generalized) modularity maximization formulation, followed by a novel doubly-weighted ℓ_1-norm k-medoids procedure. We establish nonasymptotic theoretical guarantees for approximate and perfect clustering, both of which build on a new *degree-corrected density gap condition*. Our approximate clustering results are insensitive to the minimum degree, and hold even in sparse regime with bounded average degrees. In the special case of SBM, our theoretical guarantees match the best-known results of computationally feasible algorithms. Numerically, we provide an efficient implementation of our algorithm, which is applied to both synthetic and real-world networks. Experiment results show that our method enjoys competitive performance compared to the state of the art in the literature.

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NEAR-OPTIMALITY OF LINEAR RECOVERY IN GAUSSIAN OBSERVATION SCHEME UNDER $\|\cdot\|_2^2$-LOSS

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We consider the problem of recovering linear image Bx of a signal x known to belong to a given convex compact set $\mathcal{X}$ from indirect observation $\omega = Ax + \sigma\xi$ of x corrupted by Gaussian noise ξ. It is shown that under some assumptions on $\mathcal{X}$ (satisfied, e.g., when $\mathcal{X}$ is the intersection of K concentric ellipsoids/elliptic cylinders), an easy-to-compute linear estimate is near-optimal in terms of its worst case, over $x \in \mathcal{X}$, expected $\|\cdot\|_2^2$-loss. The main novelty here is that the result imposes no restrictions on A and B. To the best of our knowledge, preceding results on optimality of linear estimates dealt either with one-dimensional Bx (estimation of linear forms) or with the "diagonal case" where A, B are diagonal and $\mathcal{X}$ is given by a "separable" constraint like $\mathcal{X} = \{x : \sum_i a_i^2 x_i^2 \le 1\}$ or $\mathcal{X} = \{x : \max_i |a_i x_i| \le 1\}$.

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AN MCMC APPROACH TO EMPIRICAL BAYES INFERENCE AND BAYESIAN SENSITIVITY ANALYSIS VIA EMPIRICAL PROCESSES

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Consider a Bayesian situation in which we observe $Y \sim p_\theta$, where $\theta \in \Theta$, and we have a family $\{\nu_h, h \in \mathcal{H}\}$ of potential prior distributions on Θ. Let g be a real-valued function of θ, and let $I_g(h)$ be the posterior expectation of $g(\theta)$ when the prior is ν_h. We are interested in two problems: (i) selecting a particular value of h, and (ii) estimating the family of posterior expectations $\{I_g(h), h \in \mathcal{H}\}$. Let $m_y(h)$ be the marginal likelihood of the hyperparameter h: $m_y(h) = \int p_\theta(y)\nu_h(d\theta)$. The empirical Bayes estimate of h is, by definition, the value of h that maximizes $m_y(h)$. It turns out that it is typically possible to use Markov chain Monte Carlo to form point estimates for $m_y(h)$ and $I_g(h)$ for each individual h in a continuum, and also confidence intervals for $m_y(h)$ and $I_g(h)$ that are valid pointwise. However, we are interested in forming estimates, with confidence statements, of the entire families of integrals $\{m_y(h), h \in \mathcal{H}\}$ and $\{I_g(h), h \in \mathcal{H}\}$: we need estimates of the first family in order to carry out empirical Bayes inference, and we need estimates of the second family in order to do Bayesian sensitivity analysis. We establish strong consistency and functional central limit theorems for estimates of these families by using tools from empirical process theory. We give two applications, one to latent Dirichlet allocation, which is used in topic modeling, and the other is to a model for Bayesian variable selection in linear regression.

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CURVATURE AND INFERENCE FOR MAXIMUM LIKELIHOOD ESTIMATES[1]

BY BRADLEY EFRON

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Maximum likelihood estimates are sufficient statistics in exponential families, but not in general. The theory of statistical curvature was introduced to measure the effects of MLE insufficiency in one-parameter families. Here, we analyze curvature in the more realistic venue of multiparameter families—more exactly, *curved exponential families*, a broad class of smoothly defined nonexponential family models. We show that within the set of observations giving the same value for the MLE, there is a "region of stability" outside of which the MLE is no longer even a local maximum. Accuracy of the MLE is affected by the location of the observation vector within the region of stability. Our motivating example involves "g-modeling," an empirical Bayes estimation procedure.

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EMPIRICAL BAYES ESTIMATES FOR A TWO-WAY CROSS-CLASSIFIED MODEL

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We develop an empirical Bayes procedure for estimating the cell means in an unbalanced, two-way additive model with fixed effects. We employ a hierarchical model, which reflects exchangeability of the effects within treatment and within block but not necessarily between them, as suggested before by Lindley and Smith [*J. R. Stat. Soc., B* **34** (1972) 1–41]. The hyperparameters of this hierarchical model, instead of considered fixed, are to be substituted with data-dependent values in such a way that the point risk of the empirical Bayes estimator is small. Our method chooses the hyperparameters by minimizing an unbiased risk estimate and is shown to be asymptotically optimal for the estimation problem defined above, under suitable conditions. The usual empirical Best Linear Unbiased Predictor (BLUP) is shown to be substantially different from the proposed method in the unbalanced case and, therefore, performs suboptimally. Our estimator is implemented through a computationally tractable algorithm that is scalable to work under large designs. The case of missing cell observations is treated as well.

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ESTIMATING VARIANCE OF RANDOM EFFECTS TO SOLVE MULTIPLE PROBLEMS SIMULTANEOUSLY

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The two-level normal hierarchical model (NHM) has played a critical role in statistical theory for the last several decades. In this paper, we propose random effects variance estimator that simultaneously (i) improves on the estimation of the related shrinkage factors, (ii) protects empirical best linear unbiased predictors (EBLUP) [same as empirical Bayes (EB)] of the random effects from the common overshrinkage problem, (iii) avoids complex bias correction in generating strictly positive second-order unbiased mean square error (MSE) (same as integrated Bayes risk) estimator either by the Taylor series or single parametric bootstrap method. The idea of achieving multiple desirable properties in an EBLUP or EB method through a suitably devised random effects variance estimator is the first of its kind and holds promise in providing good inferences for random effects under the EBLUP or EB framework. The proposed methodology is also evaluated using a Monte Carlo simulation study and real data analysis.

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OPTIMAL SHRINKAGE OF EIGENVALUES IN THE SPIKED COVARIANCE MODEL[1]

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To the memory of Charles M. Stein, 1920–2016

We show that in a common high-dimensional covariance model, the choice of loss function has a profound effect on optimal estimation.

In an asymptotic framework based on the spiked covariance model and use of orthogonally invariant estimators, we show that optimal estimation of the population covariance matrix boils down to design of an optimal shrinker η that acts elementwise on the sample eigenvalues. Indeed, to each loss function there corresponds a unique admissible eigenvalue shrinker η^* dominating all other shrinkers. The shape of the optimal shrinker is determined by the choice of loss function and, crucially, by inconsistency of both eigenvalues *and* eigenvectors of the sample covariance matrix.

Details of these phenomena and closed form formulas for the optimal eigenvalue shrinkers are worked out for a menagerie of 26 loss functions for covariance estimation found in the literature, including the Stein, Entropy, Divergence, Fréchet, Bhattacharya/Matusita, Frobenius Norm, Operator Norm, Nuclear Norm and Condition Number losses.

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A BAYESIAN APPROACH TO THE SELECTION OF TWO-LEVEL MULTI-STRATUM FACTORIAL DESIGNS

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In a multi-stratum factorial experiment, there are multiple error terms (strata) with different variances that arise from complicated structures of the experimental units. For unstructured experimental units, minimum aberration is a popular criterion for choosing regular fractional factorial designs. One difficulty in extending this criterion to multi-stratum factorial designs is that the formulation of a word length pattern based on which minimum aberration is defined requires an order of desirability among the relevant words, but a natural order is often lacking. Furthermore, a criterion based only on word length patterns does not account for the different stratum variances. Mitchell, Morris and Ylvisaker [*Statist. Sinica* **5** (1995) 559–573] proposed a framework for Bayesian factorial designs. A Gaussian process is used as the prior for the treatment effects, from which a prior distribution of the factorial effects is induced. This approach is applied to study optimal and efficient multi-stratum factorial designs. Good surrogates for the Bayesian criteria that can be related to word length and generalized word length patterns for regular and nonregular designs, respectively, are derived. A tool is developed for eliminating inferior designs and reducing the designs that need to be considered without requiring any knowledge of stratum variances. Numerical examples are used to illustrate the theory in several settings.

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ACCURACY ASSESSMENT FOR HIGH-DIMENSIONAL LINEAR REGRESSION[1]

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This paper considers point and interval estimation of the ℓ_q loss of an estimator in high-dimensional linear regression with random design. We establish the minimax rate for estimating the ℓ_q loss and the minimax expected length of confidence intervals for the ℓ_q loss of rate-optimal estimators of the regression vector, including commonly used estimators such as Lasso, scaled Lasso, square-root Lasso and Dantzig Selector. Adaptivity of confidence intervals for the ℓ_q loss is also studied. Both the setting of the known identity design covariance matrix and known noise level and the setting of unknown design covariance matrix and unknown noise level are studied. The results reveal interesting and significant differences between estimating the ℓ_2 loss and ℓ_q loss with $1 \le q < 2$ as well as between the two settings.

New technical tools are developed to establish rate sharp lower bounds for the minimax estimation error and the expected length of minimax and adaptive confidence intervals for the ℓ_q loss. A significant difference between loss estimation and the traditional parameter estimation is that for loss estimation the constraint is on the performance of the estimator of the regression vector, but the lower bounds are on the difficulty of estimating its ℓ_q loss. The technical tools developed in this paper can also be of independent interest.

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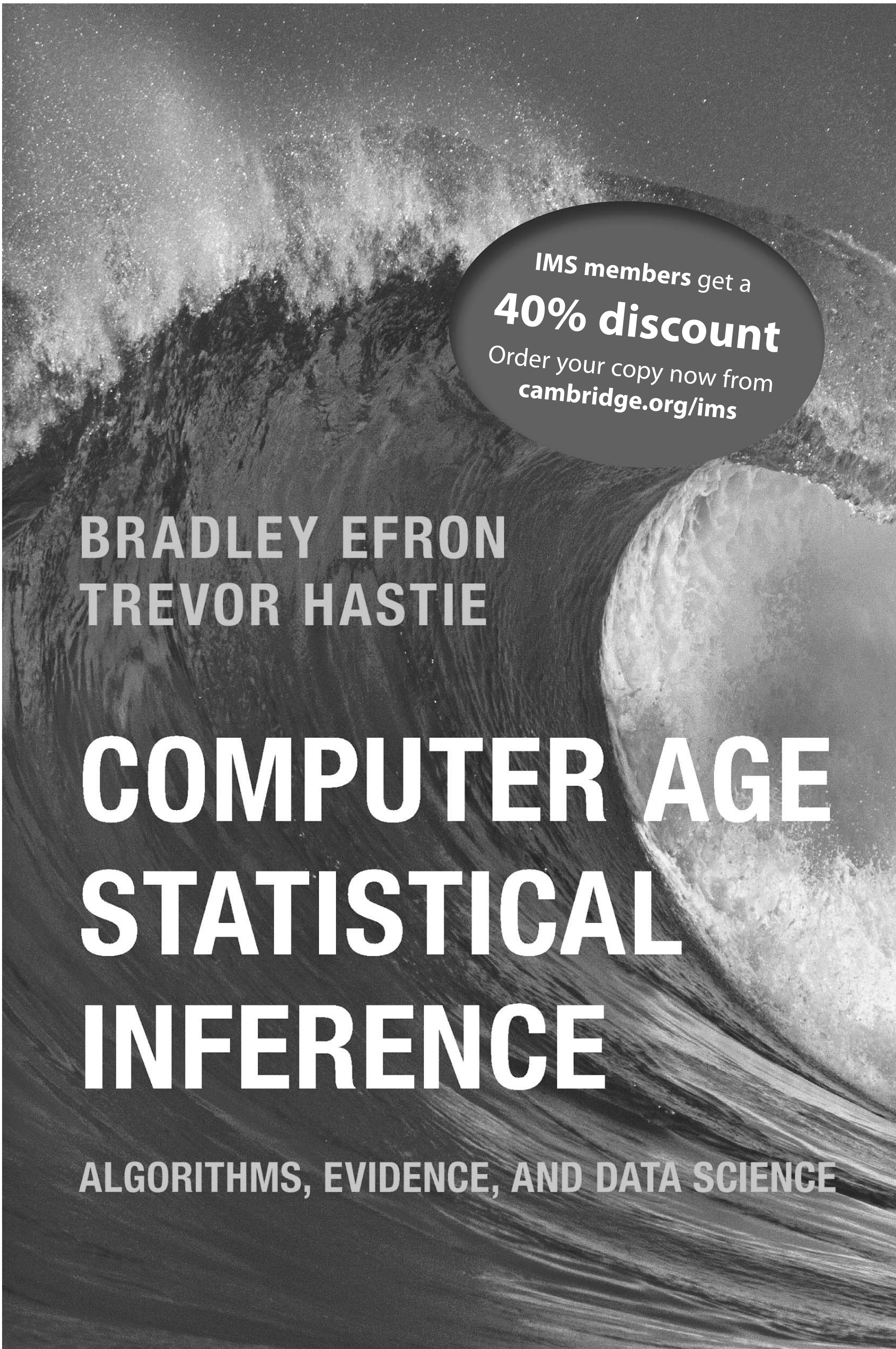
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