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GRAPHICAL MODELS FOR NONSTATIONARY TIME SERIES

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We propose NonStGM, a general nonparametric graphical modeling framework, for studying dynamic associations among the components of a nonstationary multivariate time series. It builds on the framework of Gaussian graphical models (GGM) and stationary time series graphical models (StGM) and complements existing works on parametric graphical models based on change point vector autoregressions (VAR). Analogous to StGM, the proposed framework captures conditional noncorrelations (both intertemporal and contemporaneous) in the form of an undirected graph. In addition, to describe the more nuanced nonstationary relationships among the components of the time series, we introduce the new notion of conditional nonstationarity/stationarity and incorporate it within the graph. This can be used to search for small subnetworks that serve as the “source” of nonstationarity in a large system.

We explicitly connect conditional noncorrelation and stationarity between and within components of the multivariate time series to zero and Toeplitz embeddings of an infinite-dimensional inverse covariance operator. In the Fourier domain, conditional stationarity and noncorrelation relationships in the inverse covariance operator are encoded with a specific sparsity structure of its integral kernel operator. We show that these sparsity patterns can be recovered from finite-length time series by nodewise regression of discrete Fourier transforms (DFT) across different Fourier frequencies. We demonstrate the feasibility of learning NonStGM structure from data using simulation studies.

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BOOTSTRAPPING PERSISTENT BETTI NUMBERS AND OTHER STABILIZING STATISTICS

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We investigate multivariate bootstrap procedures for general stabilizing statistics, with specific application to topological data analysis. The work relates to other general results in the area of stabilizing statistics, including central limit theorems for geometric and topological functionals of Poisson and binomial processes in the critical regime, where limit theorems prove difficult to use in practice, motivating the use of a bootstrap approach. A smoothed bootstrap procedure is shown to give consistent estimation in these settings. Specific statistics considered include the persistent Betti numbers of Čech and Vietoris–Rips complexes over point sets in \mathbb{R}^d , along with Euler characteristics, and the total edge length of the k -nearest neighbor graph. Special emphasis is given to weakening the necessary conditions needed to establish bootstrap consistency. In particular, the assumption of a continuous underlying density is not required. Numerical studies illustrate the performance of the proposed method.

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ON LOWER BOUNDS FOR THE BIAS-VARIANCE TRADE-OFF

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It is a common phenomenon that for high-dimensional and nonparametric statistical models, rate-optimal estimators balance squared bias and variance. Although this balancing is widely observed, little is known whether methods exist that could avoid the trade-off between bias and variance. We propose a general strategy to obtain lower bounds on the variance of any estimator with bias smaller than a prespecified bound. This shows to which extent the bias-variance trade-off is unavoidable and allows to quantify the loss of performance for methods that do not obey it. The approach is based on a number of abstract lower bounds for the variance involving the change of expectation with respect to different probability measures as well as information measures such as the Kullback–Leibler or χ^2 -divergence. Some of these inequalities rely on a new concept of information matrices. In a second part of the article, the abstract lower bounds are applied to several statistical models including the Gaussian white noise model, a boundary estimation problem, the Gaussian sequence model and the high-dimensional linear regression model. For these specific statistical applications, different types of bias-variance trade-offs occur that vary considerably in their strength. For the trade-off between integrated squared bias and integrated variance in the Gaussian white noise model, we propose to combine the general strategy for lower bounds with a reduction technique. This allows us to reduce the original problem to a lower bound on the bias-variance trade-off for estimators with additional symmetry properties in a simpler statistical model. In the Gaussian sequence model, different phase transitions of the bias-variance trade-off occur. Although there is a non-trivial interplay between bias and variance, the rate of the squared bias and the variance do not have to be balanced in order to achieve the minimax estimation rate.

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A CROSS-VALIDATION FRAMEWORK FOR SIGNAL DENOISING WITH APPLICATIONS TO TREND FILTERING, DYADIC CART AND BEYOND

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This paper formulates a general cross-validation framework for signal denoising. The general framework is then applied to nonparametric regression methods such as trend filtering and dyadic CART. The resulting cross-validated versions are then shown to attain nearly the same rates of convergence as are known for the optimally tuned analogues. There did not exist any previous theoretical analyses of cross-validated versions of trend filtering or dyadic CART. To illustrate the generality of the framework, we also propose and study cross-validated versions of two fundamental estimators; lasso for high-dimensional linear regression and singular value thresholding for matrix estimation. Our general framework is inspired by the ideas in Chatterjee and Jafarov (2015) and is potentially applicable to a wide range of estimation methods which use tuning parameters.

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OFF-POLICY EVALUATION IN PARTIALLY OBSERVED MARKOV DECISION PROCESSES UNDER SEQUENTIAL IGNORABILITY

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We consider off-policy evaluation of dynamic treatment rules under sequential ignorability, given an assumption that the underlying system can be modeled as a partially observed Markov decision process (POMDP). We propose an estimator, partial history importance weighting, and show that it can consistently estimate the stationary mean rewards of a target policy, given long enough draws from the behavior policy. We provide an upper bound on its error that decays polynomially in the number of observations (i.e., the number of trajectories times their length) with an exponent that depends on the overlap of the target and behavior policies as well as the mixing time of the underlying system. Furthermore, we show that this rate of convergence is minimax, given only our assumptions on mixing and overlap. Our results establish that off-policy evaluation in POMDPs is strictly harder than off-policy evaluation in (fully observed) Markov decision processes but strictly easier than model-free off-policy evaluation.

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OPTIMAL CHANGE-POINT DETECTION AND LOCALIZATION

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Given a times series \mathbf{Y} in \mathbb{R}^n , with a piecewise constant mean and independent components, the twin problems of change-point detection and change-point localization, respectively amount to detecting the existence of times where the mean varies and estimating the positions of those change-points. In this work, we tightly characterize optimal rates for both problems and uncover the phase transition phenomenon from a global testing problem to a local estimation problem. Introducing a suitable definition of the energy of a change-point, we first establish in the single change-point setting that the optimal detection threshold is $\sqrt{2 \log \log(n)}$. When the energy is just above the detection threshold, then the problem of localizing the change-point becomes purely parametric: it only depends on the difference in means and not on the position of the change-point anymore. Interestingly, for most change-point positions, including all those away from the endpoints of the time series, it is possible to detect and localize them at a much smaller energy level. In the multiple change-point setting, we establish the energy detection threshold and show similarly that the optimal localization error of a specific change-point becomes purely parametric. Along the way, tight minimax rates for Hausdorff and l_1 estimation losses of the vector of all change-points positions are also established. Two procedures achieving these optimal rates are introduced. The first one is a least-squares estimator with a new multiscale penalty that favours well spread change-points. The second one is a two-step multiscale post-processing procedure whose computational complexity can be as low as $O(n \log(n))$. Notably, these two procedures accommodate with the presence of possibly many low-energy and therefore undetectable change-points and are still able to detect and localize high-energy change-points even with the presence of those nuisance parameters.

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NOISY LINEAR INVERSE PROBLEMS UNDER CONVEX CONSTRAINTS: EXACT RISK ASYMPTOTICS IN HIGH DIMENSIONS

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In the standard Gaussian linear measurement model $Y = X\mu_0 + \xi \in \mathbb{R}^m$ with a fixed noise level $\sigma > 0$, we consider the problem of estimating the unknown signal μ_0 under a convex constraint $\mu_0 \in K$, where K is a closed convex set in \mathbb{R}^n . We show that the risk of the natural convex constrained least squares estimator (LSE) $\hat{\mu}(\sigma)$ can be characterized exactly in high-dimensional limits, by that of the convex constrained LSE $\hat{\mu}_K^{\text{seq}}$ in the corresponding Gaussian sequence model at a different noise level. Formally, we show that

$$\|\hat{\mu}(\sigma) - \mu_0\|^2 / (nr_n^2) \rightarrow 1 \quad \text{in probability,}$$

where $r_n^2 > 0$ solves the fixed-point equation

$$\mathbb{E}\|\hat{\mu}_K^{\text{seq}}(\sqrt{(r_n^2 + \sigma^2)/(m/n)}) - \mu_0\|^2 = nr_n^2.$$

This characterization holds (uniformly) for risks r_n^2 in the maximal regime that ranges from constant order all the way down to essentially the parametric rate, as long as certain necessary nondegeneracy condition is satisfied for $\hat{\mu}(\sigma)$.

The precise risk characterization reveals a fundamental difference between noiseless (or low noise limit) and noisy linear inverse problems in terms of the sample complexity for signal recovery. A concrete example is given by the isotonic regression problem: While exact recovery of a general monotone signal requires $m \gg n^{1/3}$ samples in the noiseless setting, consistent signal recovery in the noisy setting requires as few as $m \gg \log n$ samples. Such a discrepancy occurs when the low and high noise risk behavior of $\hat{\mu}_K^{\text{seq}}$ differ significantly. In statistical languages, this occurs when $\hat{\mu}_K^{\text{seq}}$ estimates 0 at a faster “adaptation rate” than the slower “worst-case rate” for general signals. Several other examples, including nonnegative least squares and generalized Lasso (in constrained forms), are also worked out to demonstrate the concrete applicability of the theory in problems of different types.

The proof relies on a collection of new analytic and probabilistic results concerning estimation error, log likelihood ratio test statistics and degree-of-freedom associated with $\hat{\mu}_K^{\text{seq}}$, regarded as stochastic processes indexed by the noise level. These results are of independent interest in and of themselves.

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PROJECTED STATE-ACTION BALANCING WEIGHTS FOR OFFLINE REINFORCEMENT LEARNING

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Off-policy evaluation is considered a fundamental and challenging problem in reinforcement learning (RL). This paper focuses on value estimation of a target policy based on pre-collected data generated from a possibly different policy, under the framework of infinite-horizon Markov decision processes. Motivated by the recently developed marginal importance sampling method in RL and the covariate balancing idea in causal inference, we propose a novel estimator with approximately projected state-action balancing weights for the policy value estimation. We obtain the convergence rate of these weights, and show that the proposed value estimator is asymptotically normal under technical conditions. In terms of asymptotics, our results scale with both the number of trajectories and the number of decision points at each trajectory. As such, consistency can still be achieved with a limited number of subjects when the number of decision points diverges. In addition, we develop a necessary and sufficient condition for establishing the well-posedness of the operator that relates to the nonparametric Q -function estimation in the off-policy setting, which characterizes the difficulty of Q -function estimation and may be of independent interest. Numerical experiments demonstrate the promising performance of our proposed estimator.

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POST-SELECTION INFERENCE VIA ALGORITHMIC STABILITY

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When the target of statistical inference is chosen in a data-driven manner, the guarantees provided by classical theories vanish. We propose a solution to the problem of inference after selection by building on the framework of *algorithmic stability*, in particular its branch with origins in the field of differential privacy. Stability is achieved via *randomization* of selection and it serves as a quantitative measure that is sufficient to obtain nontrivial post-selection corrections for classical confidence intervals. Importantly, the underpinnings of algorithmic stability translate directly into computational efficiency—our method computes simple corrections for selective inference without recourse to Markov chain Monte Carlo sampling.

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BRIDGING FACTOR AND SPARSE MODELS

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Factor and sparse models are widely used to impose a low-dimensional structure in high-dimensions. However, they are seemingly mutually exclusive. We propose a lifting method that combines the merits of these two models in a supervised learning methodology that allows for efficiently exploring all the information in high-dimensional datasets. The method is based on a flexible model for high-dimensional panel data with observable and/or latent common factors and idiosyncratic components. The model is called the factor-augmented regression model. It includes principal components and sparse regression as specific models, significantly weakens the cross-sectional dependence, and facilitates model selection and interpretability. The method consists of several steps and a novel test for (partial) covariance structure in high dimensions to infer the remaining cross-section dependence at each step. We develop the theory for the model and demonstrate the validity of the multiplier bootstrap for testing a high-dimensional (partial) covariance structure. A simulation study and applications support the theory.

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MATCHING RECOVERY THRESHOLD FOR CORRELATED RANDOM GRAPHS

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For two correlated graphs which are independently sub-sampled from a common Erdős–Rényi graph $G(n, p)$, we wish to recover their *latent* vertex matching from the observation of these two graphs *without labels*. When $p = n^{-\alpha+o(1)}$ for $\alpha \in (0, 1]$, we establish a sharp information-theoretic threshold for whether it is possible to correctly match a positive fraction of vertices. Our result sharpens a constant factor in a recent work by Wu, Xu and Yu.

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LEARNING LOW-DIMENSIONAL NONLINEAR STRUCTURES FROM HIGH-DIMENSIONAL NOISY DATA: AN INTEGRAL OPERATOR APPROACH

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We propose a kernel-spectral embedding algorithm for learning low-dimensional nonlinear structures from noisy and high-dimensional observations, where the data sets are assumed to be sampled from a nonlinear manifold model and corrupted by high-dimensional noise. The algorithm employs an adaptive bandwidth selection procedure which does not rely on prior knowledge of the underlying manifold. The obtained low-dimensional embeddings can be further utilized for downstream purposes such as data visualization, clustering and prediction. Our method is theoretically justified and practically interpretable. Specifically, for a general class of kernel functions, we establish the convergence of the final embeddings to their noiseless counterparts when the dimension grows polynomially with the size, and characterize the effect of the signal-to-noise ratio on the rate of convergence and phase transition. We also prove the convergence of the embeddings to the eigenfunctions of an integral operator defined by the kernel map of some reproducing kernel Hilbert space capturing the underlying nonlinear structures. Our results hold even when the dimension of the manifold grows with the sample size. Numerical simulations and analysis of real data sets show the superior empirical performance of the proposed method, compared to many existing methods, on learning various nonlinear manifolds in diverse applications.

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SINGLE INDEX FRÉCHET REGRESSION

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Single index models provide an effective dimension reduction tool in regression, especially for high-dimensional data, by projecting a general multivariate predictor onto a direction vector. We propose a novel single-index model for regression models where metric space-valued random object responses are coupled with multivariate Euclidean predictors. The responses in this regression model include complex, non-Euclidean data, including covariance matrices, graph Laplacians of networks and univariate probability distribution functions, among other complex objects that lie in abstract metric spaces. While Fréchet regression has proved useful for modeling the conditional mean of such random objects given multivariate Euclidean vectors, it does not provide for regression parameters such as slopes or intercepts, since the metric space-valued responses are not amenable to linear operations. As a consequence, distributional results for Fréchet regression have been elusive. We show here that for the case of multivariate Euclidean predictors, the parameters that define a single index and projection vector can be used to substitute for the inherent absence of parameters in Fréchet regression. Specifically, we derive the asymptotic distribution of suitable estimates of these parameters, which then can be utilized to test linear hypotheses for the parameters, subject to an identifiability condition. Consistent estimation of the link function of the single index Fréchet regression model is obtained through local linear Fréchet regression. We demonstrate the finite sample performance of estimation and inference for the proposed single index Fréchet regression model through simulation studies, including the special cases where responses are probability distributions and graph adjacency matrices. The method is illustrated for resting-state functional Magnetic Resonance Imaging (fMRI) data from the ADNI study.

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UNIVERSALITY OF REGULARIZED REGRESSION ESTIMATORS IN HIGH DIMENSIONS

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The Convex Gaussian Min–Max Theorem (CGMT) has emerged as a prominent theoretical tool for analyzing the precise stochastic behavior of various statistical estimators in the so-called high-dimensional proportional regime, where the sample size and the signal dimension are of the same order. However, a well-recognized limitation of the existing CGMT machinery rests in its stringent requirement on the exact Gaussianity of the design matrix, therefore rendering the obtained precise high-dimensional asymptotics, largely a specific Gaussian theory in various important statistical models.

This paper provides a structural universality framework for a broad class of regularized regression estimators that is particularly compatible with the CGMT machinery. Here, universality means that if a “structure” is satisfied by the regression estimator $\hat{\mu}_G$ for a standard Gaussian design G , then it will also be satisfied by $\hat{\mu}_A$ for a general non-Gaussian design A with independent entries. In particular, we show that with a good enough ℓ_∞ bound for the regression estimator $\hat{\mu}_A$, any “structural property” that can be detected via the CGMT for $\hat{\mu}_G$ also holds for $\hat{\mu}_A$ under a general design A with independent entries.

As a proof of concept, we demonstrate our new universality framework in three key examples of regularized regression estimators: the Ridge, Lasso and regularized robust regression estimators, where new universality properties of risk asymptotics and/or distributions of regression estimators and other related quantities are proved. As a major statistical implication of the Lasso universality results, we validate inference procedures using the degrees-of-freedom adjusted debiased Lasso under general design and error distributions. We also provide a counterexample, showing that universality properties for regularized regression estimators do not extend to general isotropic designs.

The proof of our universality results relies on new comparison inequalities for the optimum of a broad class of cost functions and Gordon’s max–min (or min–max) costs, over arbitrary structure sets subject to ℓ_∞ constraints. These results may be of independent interest and broader applicability.

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STATISTICAL INFERENCE ON A CHANGING EXTREME VALUE DEPENDENCE STRUCTURE

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We analyze the extreme value dependence of independent, not necessarily identically distributed multivariate regularly varying random vectors. More specifically, we propose estimators of the spectral measure locally at some time point and of the spectral measures integrated over time. The uniform asymptotic normality of these estimators is proved under suitable nonparametric smoothness and regularity assumptions. We then use the process convergence of the integrated spectral measure to devise consistent tests for the null hypothesis that the spectral measure does not change over time.

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RELAXING THE I.I.D. ASSUMPTION: ADAPTIVELY MINIMAX OPTIMAL REGRET VIA ROOT-ENTROPIC REGULARIZATION

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We consider prediction with expert advice when data are generated from distributions varying arbitrarily within an unknown constraint set. This *semi-adversarial* setting includes (at the extremes) the classical i.i.d. setting, when the unknown constraint set is restricted to be a singleton, and the unconstrained adversarial setting, when the constraint set is the set of all distributions. The Hedge algorithm—long known to be minimax (rate) optimal in the adversarial regime—was recently shown to be simultaneously minimax optimal for i.i.d. data. In this work, we propose to relax the i.i.d. assumption by seeking adaptivity at all levels of a natural ordering on constraint sets. We provide matching upper and lower bounds on the minimax regret at all levels, show that Hedge with deterministic learning rates is suboptimal outside of the extremes and prove that one can adaptively obtain minimax regret at all levels. We achieve this optimal adaptivity using the follow-the-regularized-leader (FTRL) framework, with a novel adaptive regularization scheme that implicitly scales as the square root of the entropy of the current predictive distribution, rather than the entropy of the initial predictive distribution. Finally, we provide novel technical tools to study the statistical performance of FTRL along the semi-adversarial spectrum.

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ORDER-OF-ADDITION ORTHOGONAL ARRAYS TO STUDY THE EFFECT OF TREATMENT ORDERING

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The effect of the order in which a set of m treatments is applied can be modeled by relative-position factors that indicate whether treatment i is carried out before or after treatment j , or by the absolute position for treatment i in the sequence. A design with the same normalized information matrix as the design with all $m!$ sequences is D- and G-optimal for the main-effects model involving the relative-position factors. We prove that such designs are also I-optimal for this model and D-optimal as well as G- and I-optimal for the first-order model in the absolute-position factors. We propose a methodology for a complete or partial enumeration of nonequivalent designs that are optimal for both models.

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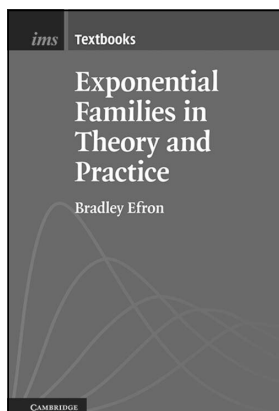
Key words and phrases. Average prediction variance, component-position model, D-optimality, equivalence class, I-optimality, pairwise order factors, projection.

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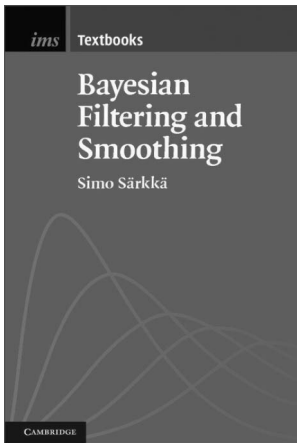
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Bayesian Filtering and Smoothing

Simo Särkkä

Filtering and smoothing methods are used to produce an accurate estimate of the state of a time-varying system based on multiple observational inputs (data). Interest in these methods has exploded in recent years, with numerous applications emerging in fields such as navigation, aerospace engineering, telecommunications and medicine. This compact, informal introduction for graduate students and advanced undergraduates presents the current state-of-the-art filtering and smoothing methods in a unified Bayesian framework. Readers learn what non-linear Kalman filters and particle filters are, how they are related, and their relative advantages and disadvantages. They also discover how state-of-the-art Bayesian parameter estimation methods can be combined with state-of-the-art filtering and smoothing algorithms. The book's practical and algorithmic approach assumes only modest mathematical prerequisites. Examples include MATLAB computations, and the numerous end-of-chapter exercises include computational assignments. MATLAB/GNU Octave source code is available for download at www.cambridge.org/sarkka, promoting hands-on work with the methods.

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