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WALD TESTS WHEN RESTRICTIONS ARE LOCALLY SINGULAR

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This paper provides an exhaustive characterization of the asymptotic null distribution of Wald-type statistics for testing restrictions given by polynomial functions—which may involve singularities—when the limiting distribution of the parameter estimator is absolutely continuous (e.g., Gaussian). In addition to the well-known finite-sample noninvariance, there is also an asymptotic noninvariance (nonpivotality): with standard critical values, the test may either under-reject or over-reject, and even diverge under the null hypothesis. The asymptotic distribution of the test statistic can vary under the null hypothesis and depends on the true unknown parameter value. All these situations are possible in testing restrictions which arise in the statistical and econometric literatures, for example, for examining the specification of ARMA models, causality at different horizons, indirect effects, zero determinant hypotheses on matrices of coefficients, and other situations where singularities cannot be excluded. We provide the limit distribution and general bounds for the single restriction case. For multiple restrictions, we give a necessary and sufficient condition for the existence of a limit distribution, and its form if it exists.

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LARGE-DIMENSIONAL INDEPENDENT COMPONENT ANALYSIS: STATISTICAL OPTIMALITY AND COMPUTATIONAL TRACTABILITY

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In this paper, we investigate the optimal statistical performance and the impact of computational constraints for independent component analysis (ICA). Our goal is twofold. On the one hand, we characterize the precise role of dimensionality on sample complexity and statistical accuracy, and how computational consideration may affect them. In particular, we show that the optimal sample complexity is linear in dimensionality, and interestingly, the commonly used sample kurtosis-based approaches are necessarily suboptimal. However, the optimal sample complexity becomes quadratic, up to a logarithmic factor, in the dimension if we restrict ourselves to estimates that can be computed with low-degree polynomial algorithms. On the other hand, we develop computationally tractable estimates that attain both the optimal sample complexity and minimax optimal rates of convergence. We study the asymptotic properties of the proposed estimates and establish their asymptotic normality that can be readily used for statistical inferences. Our method is fairly easy to implement and numerical experiments are presented to further demonstrate its practical merits.

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FORWARD SELECTION AND POST-SELECTION INFERENCE IN FACTORIAL DESIGNS

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Ever since the seminal work of R. A. Fisher and F. Yates, factorial designs have been an important experimental tool to simultaneously estimate the effects of multiple treatment factors. In factorial designs, the number of treatment combinations grows exponentially with the number of treatment factors, which motivates the forward selection strategy based on the sparsity, hierarchy and heredity principles for factorial effects. Although this strategy is intuitive and has been widely used in practice, its rigorous statistical theory has not been formally established. To fill this gap, we establish design-based theory for forward factor selection in factorial designs based on the potential outcome framework. We not only prove a consistency property for the factor selection procedure but also discuss statistical inference after factor selection. In particular, with selection consistency, we quantify the advantages of forward selection based on asymptotic efficiency gain in estimating factorial effects. With inconsistent selection in higher-order interactions, we propose two strategies and investigate their impact on subsequent inference. Our formulation differs from the existing literature on variable selection and post-selection inference because our theory is based solely on the physical randomization of the factorial design and does not rely on a correctly specified outcome model.

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OBSERVABLE ADJUSTMENTS IN SINGLE-INDEX MODELS FOR REGULARIZED M-ESTIMATORS WITH BOUNDED P/N

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We consider observations $(\boldsymbol{X}, \boldsymbol{y})$ from single index models with unknown link function, Gaussian covariates and a regularized M-estimator $\hat{\boldsymbol{\beta}}$ constructed from convex loss function and regularizer. In the regime where sample size n and dimension p are both increasing such that p/n has a finite limit, the behavior of the empirical distribution of $\hat{\boldsymbol{\beta}}$ and the predicted values $\boldsymbol{X}\hat{\boldsymbol{\beta}}$ has been previously characterized in a number of models: The empirical distributions are known to converge to proximal operators of the loss and penalty in a related Gaussian sequence model, which captures the interplay between ratio $\frac{p}{n}$, loss, regularization and the data generating process. This connection between $(\hat{\boldsymbol{\beta}}, \boldsymbol{X}\hat{\boldsymbol{\beta}})$ and the corresponding proximal operators involves mean-field parameters defined as solutions to a nonlinear system of equations. This system typically involve unobservable quantities such as the prior distribution on the index or the link function, so the mean-field parameters need to be estimated. Although estimators for the mean-field parameters have been proposed in specific cases, a general framework that applies simultaneously to a broad class of loss and penalty has so far been missing.

This paper develops a different theory to describe the empirical distribution of $\hat{\boldsymbol{\beta}}$ and $\boldsymbol{X}\hat{\boldsymbol{\beta}}$: Approximations of $(\hat{\boldsymbol{\beta}}, \boldsymbol{X}\hat{\boldsymbol{\beta}})$ in terms of proximal operators are provided that only involve observable adjustments in place of the mean-field parameters. These proposed observable adjustments are data-driven, for example, do not require prior knowledge of the index or the link function. These new adjustments yield confidence intervals for individual components of the index, as well as estimators of the correlation of $\hat{\boldsymbol{\beta}}$ with the index, enabling parameter tuning to maximize the correlation. The interplay between loss, regularization and the model is captured in a data-driven manner, without relying on the nonlinear systems studied in previous works. The results are proved to hold both strongly convex regularizers and unregularized M-estimation.

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A STATISTICAL FRAMEWORK FOR ANALYZING SHAPE IN A TIME SERIES OF RANDOM GEOMETRIC OBJECTS

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We introduce a new framework to analyze shape descriptors that capture the geometric features of an ensemble of point clouds. At the core of our approach is the point of view that the data arises as sampled recordings from a metric space-valued stochastic process, possibly of nonstationary nature, thereby integrating geometric data analysis into the realm of functional time series analysis. Our framework allows for natural incorporation of spatial-temporal dynamics, heterogeneous sampling, and the study of convergence rates. Further, we derive complete invariants for classes of metric space-valued stochastic processes in the spirit of Gromov, and relate these invariants to so-called ball volume processes. Under mild dependence conditions, a weak invariance principle in $D([0,1] \times [0,\mathscr{R}])$ is established for sequential empirical versions of the latter, assuming the probabilistic structure possibly changes over time. Finally, we use this result to introduce novel test statistics for topological change, which are distribution-free in the limit under the hypothesis of stationarity. We explore these test statistics on time series of single-cell mRNA expression data, using shape descriptors coming from topological data analysis.

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APPROXIMATION ERROR FROM DISCRETIZATIONS AND ITS APPLICATIONS

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Converting a continuous variable into a discrete one is a commonly used technique for solving various problems in both statistics and machine learning. It is well known that discretizations result in biases. However, this issue has not been studied systematically. In this paper, a general framework is proposed to understand and compare the approximation errors of different slicing strategies. Poincaré-type inequalities are first established for univariate discretizations and then generalized to the multivariate and other settings. It is shown that the bias is controlled by two factors: the distance between two specific distributions that are generated with and without discretizations respectively, and the smoothness of the functions involved. Several important applications are considered to illustrate the usefulness of the results. Our results help to understand the approximation error of some matrix used in the literature of dimension reduction. Furthermore, as an illustration of the usefulness of discretizations, we propose an algorithm for regression problems, by combining random forest with partial discretizations of responses. Simulation results confirm the advantages of this algorithm over the classical random forest.

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EMBEDDING DISTRIBUTIONAL DATA

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We adapt concepts, methodology, and theory originally developed in the areas of multidimensional scaling and dimensionality reduction for Euclidean data to be applicable to distributional data. We focus on classical scaling and Isomap—prototypical methods that have played important roles in these areas—and showcase their use in the context of distributional data analysis. In the process, we highlight the crucial role that the ambient metric plays.

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A NEW CENTRAL LIMIT THEOREM FOR THE AUGMENTED IPW ESTIMATOR: VARIANCE INFLATION, CROSS-FIT COVARIANCE AND BEYOND

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Estimation of the average treatment effect (ATE) is a central problem in causal inference. In recent times, inference for the ATE in the presence of high-dimensional covariates has been extensively studied. Among diverse approaches that have been proposed, augmented inverse propensity weighting (AIPW) with cross-fitting has emerged a popular choice in practice. In this work, we study this cross-fit AIPW estimator under well-specified outcome regression and propensity score models in a high-dimensional regime where the number of features and samples are both large and comparable. Under assumptions on the covariate distribution, we establish a new central limit theorem for the suitably scaled cross-fit AIPW that applies without *any* sparsity assumptions on the underlying high-dimensional parameters. Our CLT uncovers two crucial phenomena among others: (i) the AIPW exhibits a substantial variance inflation that can be precisely quantified in terms of the signal-to-noise ratio and other problem parameters, (ii) the asymptotic covariance between the precross-fit estimators is nonnegligible even on the $\sqrt{n}$ scale. These findings are strikingly different from their classical counterparts. On the technical front, our work utilizes a novel interplay between three distinct tools—approximate message passing theory, the theory of deterministic equivalents and the leave-one-out approach. We believe our proof techniques should be useful for analyzing other two-stage estimators in this high-dimensional regime. We complement our theoretical results with simulations that demonstrate both the finite sample efficacy of our CLT and its robustness to our assumptions. Finally, we provide some theoretical evidence for the universality of our CLT to the law of the covariates, and explore the effects of certain forms of model misspecification.

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SPARSE ANOMALY DETECTION ACROSS REFERENTIALS: A RANK-BASED HIGHER CRITICISM APPROACH

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Detecting anomalies in large sets of observations is crucial in various applications, such as epidemiological studies, gene expression studies, and systems monitoring. We consider settings where the units of interest result in multiple independent observations from potentially distinct referentials. Scan statistics and related methods are commonly used in such settings, but rely on stringent modeling assumptions for proper calibration. We instead propose a rank-based variant of the higher criticism statistic that only requires independent observations originating from ordered spaces. We show under what conditions the resulting methodology is able to detect the presence of anomalies. These conditions are stated in a general, nonparametric manner, and depend solely on the probabilities of anomalous observations exceeding nominal observations. The analysis requires a refined understanding of the distribution of the ranks under the presence of anomalies, and in particular of the rank-induced dependencies. The methodology is robust against heavy-tailed distributions through the use of ranks. Within the exponential family and a family of convolutional models, we analytically quantify the asymptotic performance of our methodology and the performance of the oracle, and show the difference is small for many common models. Simulations confirm these results. We show the applicability of the methodology through an analysis of quality control data of a pharmaceutical manufacturing process.

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STUDENTIZED TESTS OF INDEPENDENCE: RANDOM-LIFTER APPROACH

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The exploration of associations between random objects with complex geometric structures has catalyzed the development of various novel statistical tests encompassing distance-based and kernel-based statistics. These methods have various strengths and limitations. One problem is that their test statistics tend to converge to asymptotic null distributions involving second-order Wiener chaos, which are hard to compute and need approximation or permutation techniques that use much computing power to build rejection regions. In this work, we take an entirely different and novel strategy by using the so-called "random-lifter." This method is engineered to yield test statistics with the standard normal limit under null distributions without the need for sample splitting. In other words, we set our sights on having simple limiting distributions and finding the proper statistics through reverse engineering. We use the Central Limit Theorems (CLTs) for degenerate U-statistics derived from our novel association measures to do this. As a result, the asymptotic distributions of our proposed tests are straightforward to compute. Our test statistics also have the minimax property. We further substantiate that our method maintains competitive power against existing methods with minimal adjustments to constant factors. Both numerical simulations and real-data analysis corroborate the efficacy of the random-lifter method.

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RESIDUAL PERMUTATION TEST FOR REGRESSION COEFFICIENT TESTING

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We consider the problem of testing whether a single coefficient is equal to zero in linear models when the dimension of covariates p can be up to a constant fraction of sample size n. In this regime, an important topic is to propose tests with *finite-sample valid* size control without requiring the noise to follow strong distributional assumptions. In this paper, we propose a new method, called the *residual permutation test* (RPT), which is constructed by projecting the regression residuals onto the space orthogonal to the union of the column spaces of the original and permuted design matrices. RPT can be proved to achieve finite-sample size validity under fixed design with just exchangeable noises, whenever $p < n/2$. Moreover, RPT is shown to be asymptotically powerful for heavy-tailed noises with bounded $(1+t)$th order moment when the true coefficient is at least of order $n^{-t/(1+t)}$ for $t \in [0, 1]$. We further proved that this signal size requirement is essentially rate-optimal in the minimax sense. Numerical studies confirm that RPT performs well in a wide range of simulation settings with normal and heavy-tailed noise distributions.

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ARK: ROBUST KNOCKOFFS INFERENCE WITH COUPLING

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We investigate the robustness of the model-X knockoffs framework with respect to the misspecified or estimated feature distribution. We achieve such a goal by theoretically studying the feature selection performance of a practically implemented knockoffs algorithm, which we name as the approximate knockoffs (ARK) procedure, under the measures of the false discovery rate (FDR) and k-familywise error rate (k-FWER). The approximate knockoffs procedure differs from the model-X knockoffs procedure only in that the former uses the misspecified or estimated feature distribution. A key technique in our theoretical analyses is to couple the approximate knockoffs procedure with the model-X knockoffs procedure so that random variables in these two procedures can be close in realizations. We prove that if such coupled model-X knockoffs procedure exists, the approximate knockoffs procedure can achieve the asymptotic FDR or k-FWER control at the target level. We showcase three specific constructions of such coupled model-X knockoff variables, verifying their existence and justifying the robustness of the model-X knockoffs framework. Additionally, we formally connect our concept of knockoff variable coupling to a type of Wasserstein distance.

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LOW COORDINATE DEGREE ALGORITHMS I: UNIVERSALITY OF COMPUTATIONAL THRESHOLDS FOR HYPOTHESIS TESTING

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We study when *low coordinate degree functions (LCDF)*—linear combinations of functions depending on small subsets of entries of a vector—can hypothesis test between high-dimensional probability measures. These functions are a generalization, proposed in Hopkins' 2018 thesis but seldom studied since, of *low degree polynomials (LDP)*, a class widely used in recent literature as a proxy for all efficient algorithms for tasks in statistics and optimization. Instead of the orthogonal polynomial decompositions used in LDP calculations, our analysis of LCDF is based on the *Efron–Stein* or *ANOVA decomposition*, making it much more broadly applicable. By way of illustration, we prove *channel universality* for the success of LCDF in testing for the presence of sufficiently "dilute" random signals through noisy channels: the efficacy of LCDF depends on the channel only through the scalar *Fisher information* for a class of channels including nearly arbitrary additive i.i.d. noise and nearly arbitrary exponential families. As applications, we extend lower bounds against LDP for spiked matrix and tensor models under additive Gaussian noise to lower bounds against LCDF under general noisy channels. We also give a simple and unified treatment of the effect of *censoring* models by erasing observations at random and of *quantizing* models by taking the sign of the observations. These results are the first computational lower bounds against any large class of algorithms for all of these models when the channel is not one of a few special cases, and thereby give the first substantial evidence for the universality of several statistical-to-computational gaps.

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DEEP APPROXIMATE POLICY ITERATION

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In this paper, we consider deep approximate policy iteration (DAPI) with the Bellman residual minimization in reinforcement learning. In each iteration of DAPI, we apply convolutional neural networks (CNNs) with ReLU activation, called ReLU CNNs, to estimate the fixed point of the Bellman equation by minimizing an unbiased minimax loss. To bound the estimation error in each iteration, we control the statistical and approximation errors using the tools of the empirical process theory with dependent data and deep approximation theory, respectively. We establish a novel statistical error bound for ReLU CNNs on dependent data that is $\mathcal{C}$-mixing, and an approximation error bound for ReLU CNNs on Hölder class. Combining with error propagation, we obtain a nonasymptotic error bound between the optimal action-value function Q^* and the estimated Q function induced by the greedy policy in DAPI. This bound depends on the sample size and ambient dimension of the data, as well as the size, weight bound, and depth of the CNNs, providing prior guidance on how to set these hyperparameters to achieve the desired convergence rate when training DAPI in practice. Moreover, this bound circumvents the curse of dimensionality if the distribution of state-action pairs is supported on a set with a low intrinsic dimension.

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THE GENERALIZATION ERROR OF MAX-MARGIN LINEAR CLASSIFIERS: BENIGN OVERFITTING AND HIGH DIMENSIONAL ASYMPTOTICS IN THE OVERPARAMETRIZED REGIME

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Modern machine learning classifiers often exhibit vanishing classification error on the training set. They achieve this by learning nonlinear representations of the inputs that map the data into linearly separable classes.

Motivated by these phenomena, we revisit high-dimensional maximum margin classification for linearly separable data. We consider a stylized setting in which data $(y_i, \boldsymbol{x}_i)$, $i \le n$ are i.i.d. with $\boldsymbol{x}_i \sim \mathsf{N}(\mathbf{0}, \boldsymbol{\Sigma})$ a p-dimensional Gaussian feature vector, and $y_i \in \{+1, -1\}$ a label whose distribution depends on a linear combination of the covariates $\langle \boldsymbol{\theta}_*, \boldsymbol{x}_i \rangle$. Recent universality results can be used to show that the results derived in the Gaussian setting also apply when $\boldsymbol{x}_i = \boldsymbol{\phi}(z_i)$ for standard Gaussian z_i and $\boldsymbol{\phi}$ a nonlinear featurization map.

We consider the proportional asymptotics $n, p \to \infty$ with $p/n \to \psi$, and derive exact expressions for the limiting generalization error. We use this theory to derive two results of independent interest: (i) Sufficient conditions on $(\boldsymbol{\Sigma}, \boldsymbol{\theta}_*)$ for "benign overfitting" that are parallel to previously derived conditions in the case of linear regression; (ii) An asymptotically exact expression for the generalization error when max-margin classification is used in conjunction with feature vectors produced by random one-layer neural networks.

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PRECISE ERROR RATES FOR COMPUTATIONALLY EFFICIENT TESTING

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We revisit the fundamental question of simple-versus-simple hypothesis testing with an eye toward computational complexity, as the statistically optimal likelihood ratio test is often computationally intractable in high-dimensional settings. In the classical spiked Wigner model with a general i.i.d. spike prior, we show (conditional on a conjecture) that an existing test based on linear spectral statistics achieves the best possible trade-off curve between type-I and type-II error rates among all computationally efficient tests, even though there are exponential-time tests that do better. This result is conditional on an appropriate complexity-theoretic conjecture, namely a natural strengthening of the well-established low-degree conjecture. Our result shows that the spectrum is a sufficient statistic for computationally bounded tests (but not for all tests).

To our knowledge, our approach gives the first tool for reasoning about the precise asymptotic testing error achievable with efficient computation. The main ingredients required for our hardness result are a sharp bound on the norm of the low-degree likelihood ratio along with (counterintuitively) a positive result on achievability of testing. This strategy appears to be new even in the setting of unbounded computation, in which case it gives an alternate way to analyze the fundamental statistical limits of testing.

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ASYMPTOTIC EQUIVALENCE OF LOCALLY STATIONARY PROCESSES AND BIVARIATE GAUSSIAN WHITE NOISE

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We consider a general class of statistical experiments, in which an n-dimensional centered Gaussian random variable is observed and its covariance matrix is the parameter of interest. The covariance matrix is assumed to be well-approximable in a linear space of lower dimension K_n with eigenvalues uniformly bounded away from zero and infinity. We prove asymptotic equivalence of this experiment and a class of K_n-dimensional Gaussian models with informative expectation in Le Cam's sense when n tends to infinity and K_n is allowed to increase moderately in n at a polynomial rate. For this purpose we derive a new localization technique for non-i.i.d. data and a novel high-dimensional Central Limit Law in total variation distance. These results are key ingredients to show asymptotic equivalence between the experiments of locally stationary Gaussian time series and a bivariate Wiener process with the log spectral density as its drift. On this way a novel class of matrices is introduced which generalizes circulant Toeplitz matrices traditionally used for strictly stationary time series.

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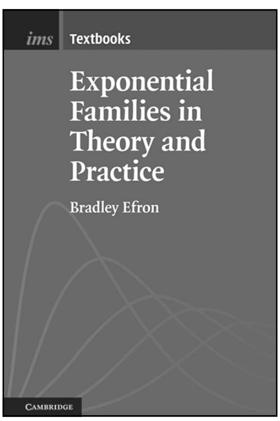

Exponential Families in Theory and Practice

Bradley Efron, Stanford University

During the past half-century, exponential families have attained a position at the center of parametric statistical inference. Theoretical advances have been matched, and more than matched, in the world of applications, where logistic regression by itself has become the go-to methodology in medical statistics, computer-based prediction algorithms, and the social sciences. This book is based on a one-semester graduate course for first year Ph.D. and advanced master's students. After presenting the basic structure of univariate and multivariate exponential families, their application to generalized linear models including logistic and Poisson regression is described in detail, emphasizing geometrical ideas, computational practice, and the analogy with ordinary linear regression. Connections are made with a variety of current statistical methodologies: missing data, survival analysis and proportional hazards, false discovery rates, bootstrapping, and empirical Bayes analysis. The book connects exponential family theory with its applications in a way that doesn't require advanced mathematical preparation.

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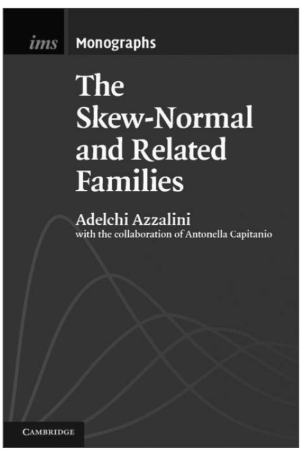

The Skew-Normal and Related Families

Adelchi Azzalini
in collaboration with Antonella Capitanio

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