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COMPUTATION OF MAXIMUM LIKELIHOOD ESTIMATES IN CYCLIC STRUCTURAL EQUATION MODELS

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Software for computation of maximum likelihood estimates in linear structural equation models typically employs general techniques from nonlinear optimization, such as quasi-Newton methods. In practice, careful tuning of initial values is often required to avoid convergence issues. As an alternative approach, we propose a block-coordinate descent method that cycles through the considered variables, updating only the parameters related to a given variable in each step. We show that the resulting block update problems can be solved in closed form even when the structural equation model comprises feedback cycles. Furthermore, we give a characterization of the models for which the block-coordinate descent algorithm is well defined, meaning that for generic data and starting values all block optimization problems admit a unique solution. For the characterization, we represent each model by its mixed graph (also known as path diagram), which leads to criteria that can be checked in time that is polynomial in the number of considered variables.

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FRÉCHET REGRESSION FOR RANDOM OBJECTS WITH EUCLIDEAN PREDICTORS

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Increasingly, statisticians are faced with the task of analyzing complex data that are non-Euclidean and specifically do not lie in a vector space. To address the need for statistical methods for such data, we introduce the concept of Fréchet regression. This is a general approach to regression when responses are complex random objects in a metric space and predictors are in $\mathcal{R}^p$, achieved by extending the classical concept of a Fréchet mean to the notion of a conditional Fréchet mean. We develop generalized versions of both global least squares regression and local weighted least squares smoothing. The target quantities are appropriately defined population versions of global and local regression for response objects in a metric space. We derive asymptotic rates of convergence for the corresponding fitted regressions using observed data to the population targets under suitable regularity conditions by applying empirical process methods. For the special case of random objects that reside in a Hilbert space, such as regression models with vector predictors and functional data as responses, we obtain a limit distribution. The proposed methods have broad applicability. Illustrative examples include responses that consist of probability distributions and correlation matrices, and we demonstrate both global and local Fréchet regression for demographic and brain imaging data. Local Fréchet regression is also illustrated via a simulation with response data which lie on the sphere.

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DIVIDE AND CONQUER IN NONSTANDARD PROBLEMS AND THE SUPER-EFFICIENCY PHENOMENON

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We study how the divide and conquer principle works in non-standard problems where rates of convergence are typically slower than $\sqrt{n}$ and limit distributions are non-Gaussian, and provide a detailed treatment for a variety of important and well-studied problems involving nonparametric estimation of a monotone function. We find that for a fixed model, the pooled estimator, obtained by averaging nonstandard estimates across mutually exclusive subsamples, outperforms the nonstandard monotonicity-constrained (global) estimator based on the entire sample in the sense of pointwise estimation of the function. We also show that, under appropriate conditions, if the number of subsamples is allowed to increase at appropriate rates, the pooled estimator is asymptotically normally distributed with a variance that is empirically estimable from the subsample-level estimates. Further, in the context of monotone regression, we show that this gain in efficiency under a fixed model comes at a price—the pooled estimator's performance, in a *uniform sense* (maximal risk) over a class of models worsens as the number of subsamples increases, leading to a version of the super-efficiency phenomenon. In the process, we develop analytical results for the order of the bias in isotonic regression, which are of independent interest.

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RANK VERIFICATION FOR EXPONENTIAL FAMILIES

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Many statistical experiments involve comparing multiple population groups. For example, a public opinion poll may ask which of several political candidates commands the most support; a social scientific survey may report the most common of several responses to a question; or, a clinical trial may compare binary patient outcomes under several treatment conditions to determine the most effective treatment. Having observed the "winner" (largest observed response) in a noisy experiment, it is natural to ask whether that candidate, survey response or treatment is actually the "best" (stochastically largest response). This article concerns the problem of *rank verification*—post hoc significance tests of whether the orderings discovered in the data reflect the population ranks. For exponential family models, we show under mild conditions that an unadjusted two-tailed pairwise test comparing the first two-order statistics (i.e., comparing the "winner" to the "runner-up") is a valid test of whether the winner is truly the best. We extend our analysis to provide equally simple procedures to obtain lower confidence bounds on the gap between the winning population and the others, and to verify ranks beyond the first.

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SUB-GAUSSIAN ESTIMATORS OF THE MEAN OF A RANDOM VECTOR

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We study the problem of estimating the mean of a random vector X given a sample of N independent, identically distributed points. We introduce a new estimator that achieves a purely sub-Gaussian performance under the only condition that the second moment of X exists. The estimator is based on a novel concept of a multivariate median.

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COMBINATORIAL INFERENCE FOR GRAPHICAL MODELS

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We propose a new family of combinatorial inference problems for graphical models. Unlike classical statistical inference where the main interest is point estimation or parameter testing, combinatorial inference aims at testing the global structure of the underlying graph. Examples include testing the graph connectivity, the presence of a cycle of certain size, or the maximum degree of the graph. To begin with, we study the information-theoretic limits of a large family of combinatorial inference problems. We propose new concepts including structural packing and buffer entropies to characterize how the complexity of combinatorial graph structures impacts the corresponding minimax lower bounds. On the other hand, we propose a family of novel and practical structural testing algorithms to match the lower bounds. We provide numerical results on both synthetic graphical models and brain networks to illustrate the usefulness of these proposed methods.

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ESTIMATION AND PREDICTION USING GENERALIZED WENDLAND COVARIANCE FUNCTIONS UNDER FIXED DOMAIN ASYMPTOTICS

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We study estimation and prediction of Gaussian random fields with covariance models belonging to the generalized Wendland (GW) class, under fixed domain asymptotics. As for the Matérn case, this class allows for a continuous parameterization of smoothness of the underlying Gaussian random field, being additionally compactly supported. The paper is divided into three parts: first, we characterize the equivalence of two Gaussian measures with GW covariance function, and we provide sufficient conditions for the equivalence of two Gaussian measures with Matérn and GW covariance functions. In the second part, we establish strong consistency and asymptotic distribution of the maximum likelihood estimator of the microergodic parameter associated to GW covariance model, under fixed domain asymptotics. The third part elucidates the consequences of our results in terms of (misspecified) best linear unbiased predictor, under fixed domain asymptotics. Our findings are illustrated through a simulation study: the former compares the finite sample behavior of the maximum likelihood estimation of the microergodic parameter with the given asymptotic distribution. The latter compares the finite-sample behavior of the prediction and its associated mean square error when using two equivalent Gaussian measures with Matérn and GW covariance models, using covariance tapering as benchmark.

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CHEBYSHEV POLYNOMIALS, MOMENT MATCHING, AND OPTIMAL ESTIMATION OF THE UNSEEN

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We consider the problem of estimating the support size of a discrete distribution whose minimum nonzero mass is at least $\frac{1}{k}$. Under the independent sampling model, we show that the sample complexity, that is, the minimal sample size to achieve an additive error of εk with probability at least 0.1 is within universal constant factors of $\frac{k}{\log k}\log^2\frac{1}{\varepsilon}$, which improves the state-of-the-art result of $\frac{k}{\varepsilon^2\log k}$ in [In *Advances in Neural Information Processing Systems* (2013) 2157–2165]. Similar characterization of the minimax risk is also obtained. Our procedure is a linear estimator based on the Chebyshev polynomial and its approximation-theoretic properties, which can be evaluated in $O(n+\log^2 k)$ time and attains the sample complexity within constant factors. The superiority of the proposed estimator in terms of accuracy, computational efficiency and scalability is demonstrated in a variety of synthetic and real datasets.

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PARTIAL LEAST SQUARES PREDICTION IN HIGH-DIMENSIONAL REGRESSION

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We study the asymptotic behavior of predictions from partial least squares (PLS) regression as the sample size and number of predictors diverge in various alignments. We show that there is a range of regression scenarios where PLS predictions have the usual root-n convergence rate, even when the sample size is substantially smaller than the number of predictors, and an even wider range where the rate is slower but may still produce practically useful results. We show also that PLS predictions achieve their best asymptotic behavior in abundant regressions where many predictors contribute information about the response. Their asymptotic behavior tends to be undesirable in sparse regressions where few predictors contribute information about the response.

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SIGNAL ALIASING IN GAUSSIAN RANDOM FIELDS FOR EXPERIMENTS WITH QUALITATIVE FACTORS

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Signal aliasing is an inevitable consequence of using fractional factorial designs. Unlike linear models with fixed factorial effects, for Gaussian random field models advocated in some Bayesian design and computer experiment literature, the issue of signal aliasing has not received comparable attention. In the present article, this issue is tackled for experiments with qualitative factors. The signals in a Gaussian random field can be characterized by the random effects identified from the covariance function. The aliasing severity of the signals is determined by two key elements: (i) the aliasing pattern, which depends only on the chosen design, and (ii) the effect priority, which is related to the variances of the random effects and depends on the model parameters. We first apply this framework to study the signal-aliasing problem for regular fractional factorial designs. For general factorial designs including nonregular ones, we propose an aliasing severity index to quantify the severity of signal aliasing. We also observe that the aliasing severity index is highly correlated with the prediction variance.

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CROSS: EFFICIENT LOW-RANK TENSOR COMPLETION

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The completion of tensors, or high-order arrays, attracts significant attention in recent research. Current literature on tensor completion primarily focuses on recovery from a set of uniformly randomly measured entries, and the required number of measurements to achieve recovery is not guaranteed to be optimal. In addition, the implementation of some previous methods are NP-hard. In this article, we propose a framework for low-rank tensor completion via a novel tensor measurement scheme that we name Cross. The proposed procedure is efficient and easy to implement. In particular, we show that a third-order tensor of Tucker rank-(r_1, r_2, r_3) in p_1-by-p_2-by-p_3 dimensional space can be recovered from as few as $r_1r_2r_3 + r_1(p_1 - r_1) + r_2(p_2 - r_2) + r_3(p_3 - r_3)$ noiseless measurements, which matches the sample complexity lower bound. In the case of noisy measurements, we also develop a theoretical upper bound and the matching minimax lower bound for recovery error over certain classes of low-rank tensors for the proposed procedure. The results can be further extended to fourth or higher-order tensors. Simulation studies show that the method performs well under a variety of settings. Finally, the procedure is illustrated through a real dataset in neuroimaging.

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COVARIATE BALANCING PROPENSITY SCORE BY TAILORED LOSS FUNCTIONS[1]

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In observational studies, propensity scores are commonly estimated by maximum likelihood but may fail to balance high-dimensional pretreatment covariates even after specification search. We introduce a general framework that unifies and generalizes several recent proposals to improve covariate balance when designing an observational study. Instead of the likelihood function, we propose to optimize special loss functions—covariate balancing scoring rules (CBSR)—to estimate the propensity score. A CBSR is uniquely determined by the link function in the GLM and the estimand (a weighted average treatment effect). We show CBSR does not lose asymptotic efficiency in estimating the weighted average treatment effect compared to the Bernoulli likelihood, but CBSR is much more robust in finite samples. Borrowing tools developed in statistical learning, we propose practical strategies to balance covariate functions in rich function classes. This is useful to estimate the maximum bias of the inverse probability weighting (IPW) estimators and construct honest confidence intervals in finite samples. Lastly, we provide several numerical examples to demonstrate the tradeoff of bias and variance in the IPW-type estimators and the tradeoff in balancing different function classes of the covariates.

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THE GEOMETRY OF HYPOTHESIS TESTING OVER CONVEX CONES: GENERALIZED LIKELIHOOD RATIO TESTS AND MINIMAX RADII

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We consider a compound testing problem within the Gaussian sequence model in which the null and alternative are specified by a pair of closed, convex cones. Such cone testing problem arises in various applications, including detection of treatment effects, trend detection in econometrics, signal detection in radar processing and shape-constrained inference in nonparametric statistics. We provide a sharp characterization of the GLRT testing radius up to a universal multiplicative constant in terms of the geometric structure of the underlying convex cones. When applied to concrete examples, this result reveals some interesting phenomena that do not arise in the analogous problems of estimation under convex constraints. In particular, in contrast to estimation error, the testing error no longer depends purely on the problem complexity via a volume-based measure (such as metric entropy or Gaussian complexity); other geometric properties of the cones also play an important role. In order to address the issue of optimality, we prove information-theoretic lower bounds for the minimax testing radius again in terms of geometric quantities. Our general theorems are illustrated by examples including the cases of monotone and orthant cones, and involve some results of independent interest.

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NONPARAMETRIC IMPLIED LÉVY DENSITIES[1]

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This paper develops a nonparametric estimator for the Lévy density of an asset price, following an Itô semimartingale, implied by short-maturity options. The asymptotic setup is one in which the time to maturity of the available options decreases, the mesh of the available strike grid shrinks and the strike range expands. The estimation is based on aggregating the observed option data into nonparametric estimates of the conditional characteristic function of the return distribution, the derivatives of which allow to infer the Fourier transform of a known transform of the Lévy density in a way which is robust to the level of the unknown diffusive volatility of the asset price. The Lévy density estimate is then constructed via Fourier inversion. We derive an asymptotic bound for the integrated squared error of the estimator in the general case as well as its probability limit in the special Lévy case. We further show rate optimality of our Lévy density estimator in a minimax sense. An empirical application to market index options reveals relative stability of the left tail decay during high and low volatility periods.

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ON MODEL SELECTION FROM A FINITE FAMILY OF POSSIBLY MISSPECIFIED TIME SERIES MODELS

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Consider finite parametric time series models. "I have n observations and k models, which model should I choose on the basis of the data alone" is a frequently asked question in many practical situations. This poses the key problem of selecting a model from a collection of candidate models, none of which is necessarily the true data generating process (DGP). Although existing literature on model selection is vast, there is a serious lacuna in that the above problem does not seem to have received much attention. In fact, existing model selection criteria have avoided addressing the above problem directly, either by assuming that the true DGP is included among the candidate models and aiming at choosing this DGP, or by assuming that the true DGP can be asymptotically approximated by an increasing sequence of candidate models and aiming at choosing the candidate having the best predictive capability in some asymptotic sense. In this article, we propose a misspecification-resistant information criterion (MRIC) to address the key problem directly. We first prove the asymptotic efficiency of MRIC whether the true DGP is among the candidates or not, within the fixed-dimensional framework. We then extend this result to the high-dimensional case in which the number of candidate variables is much larger than the sample size. In particular, we show that MRIC can be used in conjunction with a high-dimensional model selection method to select the (asymptotically) best predictive model across several high-dimensional misspecified time series models.

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ESTIMATING THE ALGORITHMIC VARIANCE OF RANDOMIZED ENSEMBLES VIA THE BOOTSTRAP[1]

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Although the methods of bagging and random forests are some of the most widely used prediction methods, relatively little is known about their algorithmic convergence. In particular, there are not many theoretical guarantees for deciding when an ensemble is "large enough"—so that its accuracy is close to that of an ideal infinite ensemble. Due to the fact that bagging and random forests are randomized algorithms, the choice of ensemble size is closely related to the notion of "algorithmic variance" (i.e., the variance of prediction error due only to the training algorithm). In the present work, we propose a bootstrap method to estimate this variance for bagging, random forests and related methods in the context of classification. To be specific, suppose the training dataset is fixed, and let the random variable ERR_t denote the prediction error of a randomized ensemble of size t. Working under a "first-order model" for randomized ensembles, we prove that the centered law of ERR_t can be consistently approximated via the proposed method as $t \to \infty$. Meanwhile, the computational cost of the method is quite modest, by virtue of an extrapolation technique. As a consequence, the method offers a practical guideline for deciding when the algorithmic fluctuations of ERR_t are negligible.

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EFFICIENT NONPARAMETRIC BAYESIAN INFERENCE FOR *X*-RAY TRANSFORMS

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We consider the statistical inverse problem of recovering a function $f : M \to \mathbb{R}$, where M is a smooth compact Riemannian manifold with boundary, from measurements of general X-ray transforms $I_a(f)$ of f, corrupted by additive Gaussian noise. For M equal to the unit disk with "flat" geometry and $a = 0$ this reduces to the standard Radon transform, but our general setting allows for anisotropic media M and can further model local "attenuation" effects—both highly relevant in practical imaging problems such as SPECT tomography. We study a nonparametric Bayesian inference method based on standard Gaussian process priors for f. The posterior reconstruction of f corresponds to a Tikhonov regulariser with a reproducing kernel Hilbert space norm penalty that does not require the calculation of the singular value decomposition of the forward operator I_a. We prove Bernstein–von Mises theorems for a large family of one-dimensional linear functionals of f, and they entail that posterior-based inferences such as credible sets are valid and optimal from a frequentist point of view. In particular we derive the asymptotic distribution of smooth linear functionals of the Tikhonov regulariser, which attains the semiparametric information lower bound. The proofs rely on an invertibility result for the "Fisher information" operator $I_a^* I_a$ between suitable function spaces, a result of independent interest that relies on techniques from microlocal analysis. We illustrate the performance of the proposed method via simulations in various settings.

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GENERALIZED RANDOM FORESTS

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We propose generalized random forests, a method for nonparametric statistical estimation based on random forests (Breiman [*Mach. Learn.* **45** (2001) 5–32]) that can be used to fit any quantity of interest identified as the solution to a set of local moment equations. Following the literature on local maximum likelihood estimation, our method considers a weighted set of nearby training examples; however, instead of using classical kernel weighting functions that are prone to a strong curse of dimensionality, we use an adaptive weighting function derived from a forest designed to express heterogeneity in the specified quantity of interest. We propose a flexible, computationally efficient algorithm for growing generalized random forests, develop a large sample theory for our method showing that our estimates are consistent and asymptotically Gaussian and provide an estimator for their asymptotic variance that enables valid confidence intervals. We use our approach to develop new methods for three statistical tasks: nonparametric quantile regression, conditional average partial effect estimation and heterogeneous treatment effect estimation via instrumental variables. A software implementation, `grf` for `R` and `C++`, is available from `CRAN`.

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A CLASSIFICATION CRITERION FOR DEFINITIVE SCREENING DESIGNS

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A conference design is a rectangular matrix with orthogonal columns, one zero in each column, at most one zero in each row and -1's and $+1$'s elsewhere. A definitive screening design can be constructed by folding over a conference design and adding a row vector of zeroes. We prove that, for a given even number of rows, there is just one isomorphism class for conference designs with two or three columns. Next, we derive all isomorphism classes for conference designs with four columns. Based on our results, we propose a classification criterion for definitive screening designs founded on projections into four factors. We illustrate the potential of the criterion by studying designs with 24 and 82 factors.

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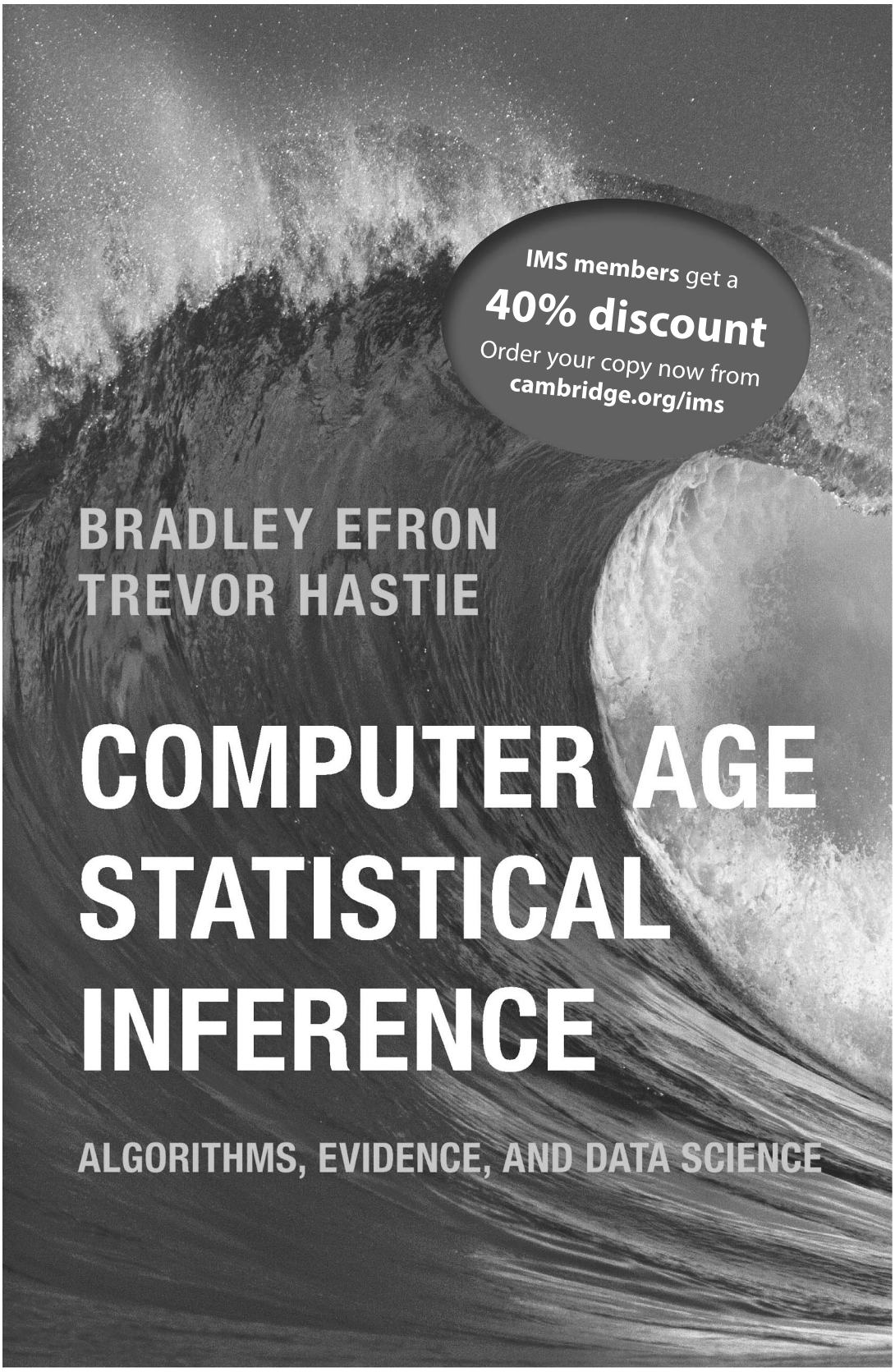
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