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Statistical inference for functions of the covariance matrix in the stationary Gaussian time-orthogonal principal components model

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Abstract We consider inference for functions of the marginal covariance matrix under a class of stationary vector time series models, referred to as time-orthogonal principal components models. The main application which motivated this work involves the estimation of configurational entropy from molecular dynamics simulations in computational chemistry, where current methods of entropy estimation involve calculations based on the sample covariance matrix. The theoretical results we obtain provide a basis for approximate inference procedures, including confidence interval calculations for scalar quantities of interest; these results are applied to the molecular dynamics application, and some further applications are discussed briefly.

Keywords Autoregressive · Central limit theorem · Configurational entropy · Principal components · Procrustes · Sample covariance · Shape · Size-and-shape