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Score test for a separable covariance structure with the first component as compound symmetric correlation matrix

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A B S T R A C T

Likelihood ratio tests (LRTs) for separability of a covariance structure for doubly multivariate data are widely studied in the literature. There are three types of LRT: biased tests based on an asymptotic chi-square null distribution; unbiased/unmodified tests based on an empirical null distribution; and unbiased/modified tests with a test statistic modified to follow a theoretical chi-square null distribution. The Rao's score test (RST) statistic, an alternative for both biased and unbiased/unmodified versions of the corresponding LRT test statistics, is derived for a common case. In this paper the separability of a covariance structure with the first component as a compound symmetric correlation matrix under the assumption of multivariate normality is tested. For this purpose Monte Carlo simulation studies, which compare the biased LRT to biased RST, and unbiased/unmodified LRT to unbiased/unmodified RST, are conducted. It is shown that the RSTs outperform their corresponding LRTs in the sense of empirical Type I error as well as empirical null distribution. Moreover, since the RST does not require estimation of a general variance–covariance matrix (the alternative hypothesis), RST can be performed for small sample sizes, where the variance–covariance matrix could not be estimated for the corresponding LRT, making the LRT infeasible. Three examples are presented to illustrate and compare statistical inference based on LRT and RST.

1. Introduction

This article is concerned with a very important hypothesis testing problem of a 2-separable covariance structure (defined in Section 2) as found in two-level or doubly multivariate data. Modern experimental techniques allow to collect and store *multi-level* multivariate data (Leiva and Roy [14]) in almost all fields such as agriculture, biology, biomedical, medical, environmental and engineering research, where the observations are collected on more than one response variable (q) at different locations (p) repeatedly over time (t) and at different depths (d), etc. These multi-level multivariate observations may have variances that differ across locations, time and depths, and developing efficient techniques for accounting these variations is of great importance for any statistical analysis.

In many practical problems, where the repeated measures occur, the covariance matrix of these repeated measures is found to have some structure. For measurements of the same type made in the same way it is usual to assume variance

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homogeneity too. Crowder and Hand [4, p. 60] say "While it is robust not to assume knowledge of the covariance structure, this can result in rather weak inference in the sense that too many degrees of freedom are used up in estimating the covariance parameters, leaving too few for the parameters of interest". The unstructured (UN) covariance matrix does not require stationarity, but is overparameterized since correlation should decay as the space or time points become more widely separated and estimating parameters which are close to zero only adds extra variability due to estimation of excessive parameters, and as a consequence losing the degrees of freedom. Thus, for example, we assume stationarity as a consequence of the assumption of equicorrelated covariance structure – compound symmetry (CS) – which may be appropriate where the repeated measurements are all made at about the same time, as in the often used 'split-plots' set-up. The CS structure is also plausible where the measurements are made at unequally spaced times over a longer period. The advantages of using CS structure over repeated measures include flexibility in using the structured covariance matrices for the repeated measures and savings in degrees of freedom for testing of hypothesis. In other cases, there might be some strict temporal sequence where the covariance matrix has autoregressive of order one (AR(1)) structure, as often seen in medical data.

For doubly multivariate data, separable structure can additionally be used to model data without losing many degrees of freedom and still avoid an over-constrained model. Consider an example of a medical data set where the detection of a cancerous region from surrounding tissues (skeletonization) of patients suffering from breast cancer is the focus. Pinto Pereira et al. [19] divided each breast image into 48 regions and then estimated the percent density (PD) for each one of its regions. However, they only used one marker, the PD, in their analysis. A better result with a high reliability may be achieved if joint analysis of the PD and a measure of microcalcifications, which are often the only detectable sign of breast cancer, can be done together. These two measurements ($q = 2$), the PD and a measure of microcalcifications, are not only correlated among themselves, but also exploit the strong regional covariance over the 48 regions ($p = 48$). In this example equicorrelated covariance structure could be one of the plausible structures over 48 regions. Besides CS, a few other plausible correlation structures over repeated measures among many are AR(1), circular or Toeplitz. Non-stationary unstructured (UN) and antedependent variance–covariance matrices are other possibilities. All structures on the repeated measures are tentative; so before any statistical analysis of doubly multivariate data one needs to perform tests for the most suitable separable structures with the first component (structure on repeated measurements) as one of the above plausible structures, i.e., (CS $\otimes$ UN), or (AR(1) $\otimes$ UN) or (UN $\otimes$ UN), etc.

1.1. Existing tests

The most common hypotheses testing procedures for large samples are the likelihood ratio (Wilks [40]), the Wald (Wald [38]), and the Rao's score (Rao [20]) tests. These were all developed using one-level multivariate models. These tests have earned the status of default methods, with a neat and unified asymptotic theory. They are widely used in almost all areas from agriculture to engineering research among many others even for the smallest possible sample size (n). The likelihood ratio test criterion Λ (Anderson [1]) or a function of it, $\mathcal{L} = -2 \ln \Lambda$ (Wald [38]), is the most commonly used test statistic. The quantity $\mathcal{L}$ is asymptotically distributed as a χ^2 under the null hypothesis and normality assumption and is used as the test statistic with large sample size. When the data are not large enough, χ^2 distribution is generally an inadequate approximation thus resulting in erroneous conclusions. When the sample size is small or moderate, Korin [12] studied the accuracy of the approximation and expressed the null distribution of $\mathcal{L}$ in the form of an asymptotic series of central χ^2 distribution and then derived the distribution of $\mathcal{L}$ using this series.

All the above mentioned tests have been established for traditional multivariate data (say with q response variables); in other words, just for 'one-level multivariate data' in a large sample setting. Hypothesis testing of a 2-separable covariance structure with both unstructured components has been widely studied by many authors, e.g. Roy and Khattree [25], Lu and Zimmerman [15], Roy [24], Srivastava et al. [34], Werner et al. [39]. Roy and Khattree [26,27] have also studied this 2-separable covariance structure by assuming a CS or AR(1) correlation structures on the first component just to avoid the identifiability problem. Roy and Khattree [28] have shown that the choice of appropriate covariance structure is crucial for two-level multivariate data in the context of classification, and it almost always affects the misclassification error rate, in a major way. Thus, it is vital to test the appropriate covariance structure on the multi-level multivariate observations before any statistical analysis. Roy and Leiva [30] further studied the 2-separable covariance structure by assuming both the components as structured (CS or AR(1)) which is useful for spatio-temporal repeated measurements. For example, for modeling the covariance of multivariate environmental monitoring data obtained repeatedly over time and space, or for modeling covariance structure of glucose measurement at 15 different regions ($p = 15$) in both the hemispheres ($q = 2$) of the brain (Worsley et al. [41]). All these authors used likelihood ratio test (LRT) statistic for testing various permutations of patterns of 2-separable covariance structures. Among these authors Lu and Zimmerman [15] and Roy and Leiva [30] have used unbiased/unmodified LRT, and simulations are used to build its sampling distribution and find quantiles. Others worked on biased LRT, based on the theoretical chi-square null distribution; in this case the rejection rate of null hypothesis is not equal to the nominal Type I error when the null hypothesis is true. It is worthwhile to mention here that using biased LRT, *MIXED* procedure of SAS Software can test the hypotheses for 2-separable covariance structure with the first component as CS or AR(1) correlation or UN covariance structures. Therefore, it can be seen that hypotheses tests for separable structures are a well developed area, and biased and unbiased/unmodified LRTs are available.

Several authors also proposed unbiased/modified LRT statistic in which the test statistic is modified in order to match the theoretical chi-square distribution to test the separability of variance–covariance structure. Simpson [17] derived a modified