hyppo: A Multivariate Hypothesis Testing Python Package

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Abstract. We introduce \texttt{hyppo}, a unified library for performing multivariate hypothesis testing, including independence, two-sample, and $k$-sample testing. While many multivariate independence tests have \texttt{R} packages available, the interfaces are inconsistent and most are not available in \texttt{Python}. \texttt{hyppo} includes many state of the art multivariate testing procedures. The package is easy-to-use and is flexible enough to enable future extensions. The documentation and all releases are available at https://hyppo.neurodata.io.

Key words. Python, multivariate, independence, $k$-sample, hypothesis

1 Introduction

Examining and identifying relationships between sets of high-dimensional variables is critical to advance understanding and planning of future numerical and physical experiments. Hypothesis testing enables formally testing models to identify such discrepancies.

Many correlation measures have been proposed to solve the problem of independence testing, such as Pearson’s correlation [1], but many are unsuited to detect nonlinear and high-dimensional dependence structures within data. Recently, several statistics have been proposed that operate well on high-dimensional (potentially non-Euclidean) data, such as distance correlation [2–5] and Hilbert-Schmidt independence criterion [6–8], which are actually exactly equivalent in Sejdinovic et al. [9], Shen and Vogelstein [10]. Heller, Heller and Gofrine proposed another nonparametric independence test with particularly high power in certain nonlinear relationships [11]. Multiscale Graph Correlation is a test that has demonstrated higher statistical power on many multivariate, nonlinear, and structured data when compared to other independence tests [12–14], which combines and extends the nearest neighbors and energy statistics to detect underlying relationships. For each of these tests, $p$-values can be calculated using a random permutation test [15–17]. These tests can be modified and extended to such applications as time-series testing [18].

To approach the problem of two-sample testing, Student’s t-test [19] is traditionally used, while a few nonparametric alternatives have been proposed that operate well on multivariate, nonlinear data such as Energy [20], and maximal mean discrepancy [21], and Heller Heller and Gorfine’s test [11]. The two-sample testing problem can be generalized to the $k$-sample testing problem and here analysis of variance (ANOVA) [22] or its multivariate analogue multivariate ANOVA (MANOVA) [23] can be used, but these statistics either fail to, or operate poorly upon, non-Gaussian data [24, 25]. There are a few nonparametric alternatives to ANOVA and MANOVA, such as multivariate $k$-sample Heller Heller Gorfine [26], and distance components (DISCO) [27]. Recently, Panda et al. [28] has shown that nonparametric distance and kernel $k$-sample tests can be formulated by reducing the $k$-sample testing problem to the independence testing problem.

This manuscript introduces \texttt{hyppo}, a hypothesis package that provides various tests with high finite-sample statistical power on multivariate and nonlinear relationships. \texttt{hyppo} is a well-tested, multi-platform, \texttt{Python} 3 compatible library that allows users to conduct hypothesis tests on their data, and is also extensible enough to allow developers to easily add in their own tests. \texttt{hyppo} also provides benchmarks for each of these tests by comparing statistical power over many statistical models. The contribution of this manuscript is therefore to provide: (1) an overview of the library and examples of how to use some of the tests in the package, and (2) comparisons of the test statistics and wall times with similar \texttt{R} packages.

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2 Library Overview

Inspired by the desire to allow for convenient use of these independence tests, hyppo has been developed as a hypothesis testing package. The package structure is modeled on the scikit-learn and energy R packages' API. Links to source code, documentation, and tutorials can be found here: https://hyppo.neurodata.io.

Included Tests

We have included a host of notable and novel hypothesis tests that we determined to be useful for the end user. Shen and Vogelstein [10] has shown that distance and kernel methods are equivalent and thus, we have one implementation that is able to perform both with a proper bijective transformation. We have implemented $k$-sample tests as specified in Panda et al. [28] and every algorithm in the following list can be used as a two-sample or $k$-sample test this way. The included algorithms are:

- Multivariate generalizations of Pearson's product moment correlation: RV [29, 30] and Canonical correlation analysis (CCA) [31].
- Heller-Heller-Gorfine (HHG) [11]: Multivariate distance-based test.
- Distance correlation (Dcorr): Both biased [4] and unbiased [32] and a fast $O(n \log n)$ variant that runs on Euclidean one-dimensional data [33].
- Hilbert-Schmidt independence criterion (Hsic): Both biased and unbiased [34] kernel-based statistics. A chi-square fast statistic is also implemented [35].
- Multiscale graph correlation (Mgc) [14]: An independence tests that combines $k$-nearest neighbors and energy statistics. Recently, Mgc has been accepted into scipy.stats and this implementation wraps the scipy implementation.
- Friedman Rafsky [36]: A tree-based two sample test.
- dHsic [37]: A d-variate independence test based on Hsic
- Multivariate analysis of variance (MANOVA) [24, 38] and Hotelling $T^2$ (HOTELLING) [39].
- Maximum mean discrepancy ($\text{MMD}$) [21]: A kernel two-sample test.
- ENERGY [20]: A distance two-sample test.
- Distance components (DISCO) [27]: A distance-based $k$-sample test.
- Smooth CF Test [40]: A test using analytic analogues of characteristic functions.
- Mean Embedding Test [40]: A test based on the analytical mean embeddings between two distributions.
- KSample HHG [41]: A $k$-sample test for HHG.
- Fast Conditional Independence Test [42]: A fast, nonparametric conditional independence test.
- Kernel Conditional Independence Test [43]: An efficient, kernel conditional independence test.
- Finite Set Stein Discrepancy [44]: A linear time kernel goodness of fit test.
- Discriminability test [45]: A highly accurate and powerful discriminability test.
- Partial Dcorr [46]: A method to perform conditional independence testing using distance correlation.
- Conditional Dcorr [47]: Conditional independence testing using Dcorr with strong theoretical properties.
- LjungBox [48]: Tests if groups of autocorrelations of time series are different from 0.

A number of algorithms have been implemented that lack an open source implementation elsewhere. These include:

- Kernel mean embedding random forest (KMERF) [49]: A kernel test that leverages random forest kernel induced similarity matrix to generate a test statistic.
- Fast Implementations of Dcorr (FAST DCORR) [50]: An approximation to Dcorr when calculating the p-value.
- Universally consistent $k$-sample tests via independence testing [28]: Transforms the $k$-sample testing problem into the independence testing problem and then uses non-parametric independence tests from hyppo.
- Time-series Mgc and Dcorr: Applying Mgc and Dcorr to time-series data.
- Maximal Margin Correlation (MAXMARGIN) [50]: A highly accurate formulation of independence...
Figure 1a shows the computational efficiency of hyppo’s implementations against existing implementations in commonly used R packages—specifically energy [51], kernlab [52], and HHG [53]. When comparing performance, wall times are averages of p-value computations (1000 replications when permutation tests are used) 3 trials calculated on a univariate noisy linear simulation with number of samples increasing from 50 to 10,000. All computations were performed on an Ubuntu 18.04.3 LTS system with access to 96 cores. When sample sizes are above a few hundred, all algorithms achieve approximately quadratic times, with different slopes. HHG was the slowest as expected, though had comparable speeds to the other algorithms at low sample sizes. MGC and Dcorr are next, and still only requires tens of minutes to run when sample sizes are around 10,000. At low sample sizes, the energy package’s Dcorr is faster than kernlab’s implementation of MMD (Dcorr is equivalent to MMD for all finite sample sizes [10]) even at a sample size of 10,000. hyppo’s Fast Dcorr, which uses a fast statistic [33] and p-value approximation [35] is the fastest, even though both energy and kernlab both use highly optimized C++ versions.

Implementation Validation Next, we verify that hyppo’s test statistics are equivalent to existing R implementations of the tests. Specifically, hyppo’s implementations were compared to: Dcorr from the energy package [51], MMD from the kernlab package [52], and HHG from the HHG package [53]. The evaluation uses a spiral simulation with 1000 samples and 2 dimensions for each test and compares test statistics over 20 repetitions. Figure 1b shows the difference between the hyppo implementation
of the independence test and the respective R package implementation of the independence test. Test statistics are nearly equivalent for each implementation.

4 Conclusion hyppo is an extensive and extensible open-source Python package for multivariate hypothesis testing. As hyppo continues to grow and add functionality, it will enhance tools scientists use when determining relationships within their investigations.

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