Local Distance Correlation

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Abstract

Understanding and discovering dependence between multiple properties or measurements of our world is a fundamental task not just in science, but also policy, commerce, and other domains. In the past hundred years, people have developed many different measures of dependence that can be applied in a wide variety of settings. An ideal dependence measure would have the following properties. (1) Strong theoretical support, guaranteeing rejecting independence no matter what the dependence structure is. (2) Strong empirical support on a wide variety of low- and high-dimensional simulation settings. (3) Provides insight into the local scale in which dependency is strongest. (4) Detects dependence when it exists, and fails to detect dependence when it does not exist, on real data. No existing test satisfies all of these properties. We develop a novel dependence statistic and test called "Local Graph Dependence". Briefly, we combine the ideas of distance correlation testing with nearest-neighbor testing, to obtain a nearest neighbor distance correlation test. LGD has all four of the above properties, as demonstrated by extensive theory, simulations, and real data examples. We can therefore use this test in a variety of settings in which previous tests failed to detect signal or provide insight.

Keywords: distance correlation, k-nearest-neighbor, independence test, permutation test

Contents

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1 Introduction

With the increasing type, size, and dimension of modern data sets, detecting dependency among multiple data sets is one of the most important and fundamental tasks in the big data age. The Pearson correlation coefficient **?**, Spearman's ρ **?**, Kendall's τ **?**, RV coefficient **?**, Procrustes coefficient **?**, information theoretic measures **?**, the energy distance **?**, and the Mantel test (see in Josse and Holmes (2013); Robert and Escoufier (1976); Mantel (1967)) have been the traditional tools for this task, but each has its limitations when dealing with the increasingly complex modern data sets, e.g., the Pearson correlation coefficient, RV coefficient and the Mantel test are mostly useful for finding linear relationship and may be zero for nonlinear dependent data sets, while mutual information performs poorly for high-dimensional data.

Many recent methods have been proposed to identify the existence of potential relationships between data sets, including Baringhaus and Franz (2004); Taskinen et al. (2005); Gretton et al. (2005); Szekely et al. (2007); Gretton and Gyorfi (2010); Reshef et al. (2011); Heller et al. (2013); Reimherr and Nicolae (2013); Szekely and Rizzo (2013a), etc. In particular, the distance correlation method from Szekely et al. (2007) has gained much popularity in the statistical community, due to its theoretical soundness and good numerical performance in testing independence. A similar method from the machine learning point of view is the kernel-based independence test, which is developed in Gretton et al. (2005); Gretton and Gyorfi (2010); Gretton et al. (2012), and connected to the distance-based method in Sejdinovic et al. (2013).

Despite of current progress in the area, it remains a difficult problem to test dependency on real data; and even the best method in theory may suffer from one or more real challenges underlying the data, such as small sample size, high dimensionality, non-linearity, noise, etc. For example, although distance correlation is consistent against all alternatives for testing independence on Euclidean data, the sample distance correlation (dcorr) under-performs in many high-dimensional or non-linear dependencies for finite-sample testing. The modified distance correlation (mcorr) from Szekely and Rizzo (2013a) adjusts the high-dimensional bias, but is still sub-optimal for non-linear dependencies. In comparison, the HHG statistic developed in Heller et al. (2013) performs much better for testing on non-linear data of small sample size, but it may lose some testing power for linear and high-dimensional dependency.

In a complementary literature, nearest-neighbor graphs have been used as a key computational primitive in many statistical approaches, ranging from classification and regression **?** to data com-

pression to recommender systems **?**. More recently, nearest-neighbor has been an invaluable tool in unfolding nonlinear geometry in many recent development of nonlinear embedding algorithms, including Isomap in Tenenbaum et al. (2000); de Silva and Tenenbaum (2003), LLE in Saul and Roweis (2000); Roweis and Saul (2003), and Laplacien eigenmaps in Belkin and Niyogi (2003), among many others. Furthermore, we have successfully applied joint neighborhood to unfold the non-linearity in multiple data sets in Shen et al. (2015), which shows that a good choice of joint neighborhood can better match the nonlinear data sets.

Most relevant to our work, a number of approaches to two-sample and dependence testing have utilizing nearest-beighbor graphs **????**. These approaches have the advantage of naturally operating on any kind of data, including categorical and structured data, as well as strong theoretical guarantees. Perhaps more importantly, they focus only on local distances, rather than global distances, enabling them to be robust to nonlinear and high-dimensional dependence structures. However, none of the previous nearest-neighbor based methods provided an automatic method for choosing the neighborhood size, therefore leaving a crucial tuning parameter unspecified, and impairing its finite sample performance. Moroever, they largely focused on two-sample testing, rather than dependence testing.

In this paper we propose graph correlation (GC), in order to better address those challenges from modern data analysis. By marrying ideas from the distance correlation literature to those from the nearest neighbor literature, and adding some of our own special sauce, we obtain a test better than those in either camp. More specifically, the local test statistic naturally inherits the advantages of the distance correlation, such as being consistent, but also inherits properties of graph dependence structures, such as robustness in high-dimensional dependency.

LDC significantly improves the finite-sample testing power over dcorr, for testing on data sets of non-linearity, noise, and/or small sample size. Those advantages make our new test statistic the best method thus far, for detecting dependency on real data and complex dependencies. Indeed in our comprehensive simulation setting, local distance correlation is able to achieve a superior performance comparing to the global distance correlation and HHG; and in the real data experiment, the local test statistic also returns the lowest p-value for testing dependency between human brain and human characteristics, XXX and fails to detect dependence when they are not there in a set of brain imaging experiments. XXX Thus, we expect LDC to find value in a wide range of applications. To facilitate, we make all of our code open source and incorporate LDC into FlashR.

2 Results

2.1 Intuition

2.2 Theoretical Properties

In this subsection we present the theoretical advantage of local distance correlation. Note that all proofs and additional propositions are provided in the appendix; and we always assume finite second moments of the joint distribution f_{XY}.

First, local distance correlation is consistent since it includes the global distance correlation.

Theorem 1. *Local distance correlation is consistent for testing independence against all alternatives, i.e., the testing power* $\beta \to 1$ *as* $n \to \infty$.

Note that the consistency holds for both the local original distance correlation and the local modified distance correlation.

Although global distance correlation is already consistent against all alternatives, it may not always yield a good finite-sample testing power for a particular dependency type; while our local distance correlation is able to improve the testing power by choosing the best neighborhood for a given joint distribution.

The advantage of using k-nearest-neighbor in local distance correlation, lies in its capability to exclude the product of small distances in one data set and large distances in the other data set: after double centering, the centered small distance is usually negative and the centered large distance is usually positive, and including such product reduces the magnitude of local distance covariance under the alternative. While excluding such product by k-nearest-neighbor can increase the magnitude of local distance covariance under the alternative, albeit at the cost of increasing its magnitude under the null as well.

For linear dependency, local distance correlation does not benefit from the above trade-off; but for nonlinear dependency, $dCorr_{kl}$ for $(k,l) \neq (n,n)$ may enjoy a better finite-sample testing power. We characterize the behaviors in the following two theorems.

Theorem 2. *Suppose* $Y = cX$ *for a non-zero scalar* c*, then for any* n *we always have*

$$\beta(dCorr_n) \geq \beta(dCorr_{kl}) \tag{1}$$

for all $k, l = 2, \ldots, n$*, where* β *is the permutation test power at a given type* 1 *error* α.

Thus local distance correlation is no better than global distance correlation under linear dependency.

Theorem 3. *There exists f_{XY}, n and α such that*

$$\beta(dCorr_n) > \beta(dCorr_{kl}) \tag{2}$$

for some $(k,l) \neq (n,n)$, where β is the permutation test power at the type 1 error α.

Thus local distance correlation can be better than global distance correlation under certain nonlinear dependency.

Note that Theorem 2 and the example used in the proof of Theorem 3 correspond to the linear and quadratic relationship in the simulation. Indeed in Figure **??** we observe the global distance correlation has the best empirical testing power for linear dependency, while local distance correlation yields a better power for the quadratic relationship.

3 Numerical Experiments

In this section we show the numerical advantage of local distance correlation via simulations and real data experiments. We carry out the independence test and report the empirical testing power for simulations, and report the empirical p-value of permutation test for the real data. The benchmarks are the global distance correlation, HHG, and the Mantel test.

Overall, we observe that local modified distance correlation combines the best aspects of global distance correlation and HHG: it performs similarly to the global distance correlation for dependencies that are close to linear, yields similar or better power than HHG in most nonlinear dependencies, and is robust against high-dimensionality throughout all simulations. For real data testing, its superior performance is reflected in the relatively small p-value.

3.1 Simulations

Here we consider 20 different distributions f_{XY} based on the simulations in Szekely et al. (2007); Simon and Tibshirani (2012); Gorfine et al. (2012); Heller et al. (2013). They consist of various polynomial relationships such as linear and quadratic, a variety of complex nonlinear relationship such as circle, trigonometry, and multiplicative noise; we also include two useful benchmark scenarios, the uncorrelated binomial and an independent relationship.

In Figure 6 we offer a visualization of each dependency, by plotting $\mathcal{X}$ against $\mathcal{Y}$ generated by each pair of (X, Y) at dimension 1 and $n = 1000$ with no noise. Clearly type 1, 3, 8, 9, 18 are either linear dependency or very close to linear, while type 2, 4, 5-7, 10-16, 19-20 are nonlinear dependencies. Note that the uncorrelated binomial without noise concentrates on just three points $(0, 0)$, $(1, -1)$ and $(1, 1)$, and the independent clouds does not have any dependency. More details about the simulation set-up and each distribution can be found in the appendix or the simulation code.

We consider two different scenarios for those 20 distributions: a dimension 1 scenario with increasing sample size, and an increasing dimension scenario with fixed sample size. For the first scenario, we always set $m_X = m_Y = 1$ and plot the power with respect to increasing sample size, so as to observe how fast the testing power of each method converges to 1 for various dependencies; for the second scenario, we fix $n = 100$ and plot the power with respect to increasing m_X, so as to determine how robust each method is for increasing dimension of each dependency.

For either scenario, $\mathcal{X}$ and $\mathcal{Y}$ are generated accordingly, then appropriate level of white noise may be added to $\mathcal{Y}$ depending on the distribution (otherwise certain dependency like perfect linear is too easy), and the sample test statistic can be calculated on the sample data. As described in Section E, we carry out the independence test to estimate the testing power for $r = 10000$ Monte-Carlo replicates at $\alpha = 0.05$. The empirical powers are shown in Figure **??** for both the dimension 1 and increasing dimension scenarios in two separate panels.

For the dimension 1 scenario, one may observe that for dependencies that are close to linear, global and local distance correlation always yield similar testing powers, which are better than HHG and Mantel; for the remaining nonlinear dependencies, HHG is usually much better than global distance correlation and Mantel, while local distance correlation performs similarly or even better than HHG in most cases due to its significant improvement over the respective global version. Note that for all distributions other than the independent clouds, the empirical powers eventually increase to 1 as the sample size increases, implying that all methods are consistent (the only exception is the Mantel test, whose powers stay low in many nonlinear dependencies); and for the independent relationship, all testing powers should be exactly the type 1 error level, which approximately holds for the empirical testing powers.

For the increasing dimension scenario, local modified distance correlation significantly surpasses all other methods: for dependencies that are close to linear, the powers of both global and local modified distance correlation deteriorate much slower than others; and for the remaining nonlinear

dependencies, local modified distance correlation is much better than all other methods including the global modified distance correlation or the local original distance correlation, due to its capability to better handle non-linearity and high-dimensionality at the same time. Note that a quarter of the distributions (e.g. sine period, square, diamond) cannot be detected by any method at dimension higher than 1, since all testing powers quickly degrade to around α.

To intuitively summarize the simulation performance of each method in all settings, we apply the performance profiles introduced by Dolan and More (2002) to the testing powers, which is an evaluation tool to compare different algorithms throughout all given settings. Suppose there are S methods and T different settings, and we denote the respective powers as β_s^t for $s = 1, \ldots, S$ and $t = 1, \ldots, T$. Then the relative performance for each method is defined as follows:

$$performance_s(x) = \frac{1}{T} \sum_{t=1}^{T} I((\beta_*^t - \beta_s^t) \leq x)$$

where $x \in [0, 1]$ and $\beta_*^t = \max_s \beta_s^t$ denotes the best testing power in the tth setting. Namely x stands for the difference with respect to the best power, and the performance profile of each method equals the proportion of simulations that the method is worse than the best method by no more than x. For example, at $x = 0.1$, local modified distance correlation has a relative performance of 0.75 if and only if there are 15 out of 20 simulations that local modified distance correlation is worse than the best method by no more than 0.1 in testing power; the relative performance at $x = 0$ stands for the proportion of simulations that the method has the best power; and the performance profile curve always increases to 1 at $x = 1$. The best method should have a similar or higher curve than others; and we also show the area under curve for each profile profile in the legend, which is a numerical way of viewing the advantage of each method.

In Figure **??** we show the performance profiles at fixed dimension and sample size that are determined by a power threshold, for both the dimension 1 and increasing dimension scenarios: for the dimension 1 scenario, the dimension is always fixed at 1, so the sample size is determined by the first sample size that any method has a power of 0.8 (otherwise pick the largest sample size); and for the increasing dimension scenario, the sample size is already fixed at 100, so we determine the dimension choice by the first dimension that any method has a power that is lower than 0.5 (otherwise pick the smallest dimension). The threshold choices are arbitrary, and additional plots of varying power thresholds are provided in the appendix.

We can clearly see from Figure **??** that local distance correlation is indeed the most reliable method in finite-sample testing, in accordance with the individual power plots in Figure **??**: for

the dimension 1 scenario the performance profiles of local original distance correlation and local modified distance correlation are similar to each other and much better than others; and for the increasing dimension scenario local modified distance correlation is significantly better than all other methods. Note that HHG is slightly better than global distance correlation in the performance profiles, because there are more nonlinear distributions than linear in the 20 dependencies, and HHG has a larger advantage for nonlinear dependency than its disadvantage in linear dependency when compared to global distance correlation; and the Mantel test has the lowest performance profile in both scenarios.

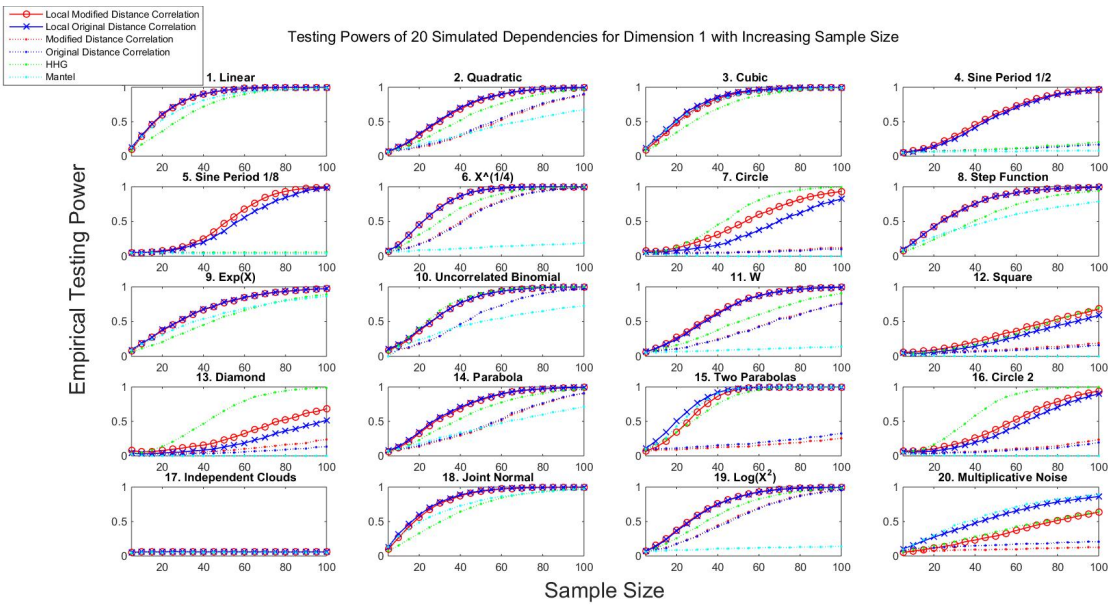

Figure 1: Power of different methods on 20 different one-dimensional simulation settings—estimated on the basis of XXX k repititions XXX—including those used in Heller et al. (2013) and Reshef et al. (2011). Each panel shows empirical testing power on the absicca, and sample size on the ordinate. Our method empirically achieves as high or higher power than the previous state of the art approaches for nearly all sample sizes on nearly all problems.

3.2 Real Data

Here we apply the local distance correlation to test independence between brain features and personal characteristics from two different experiments, for which the data sets are relatively small in sample size due to the expensive data collection process.

The first experiment is to detect the relationship between the brain connectome and personality

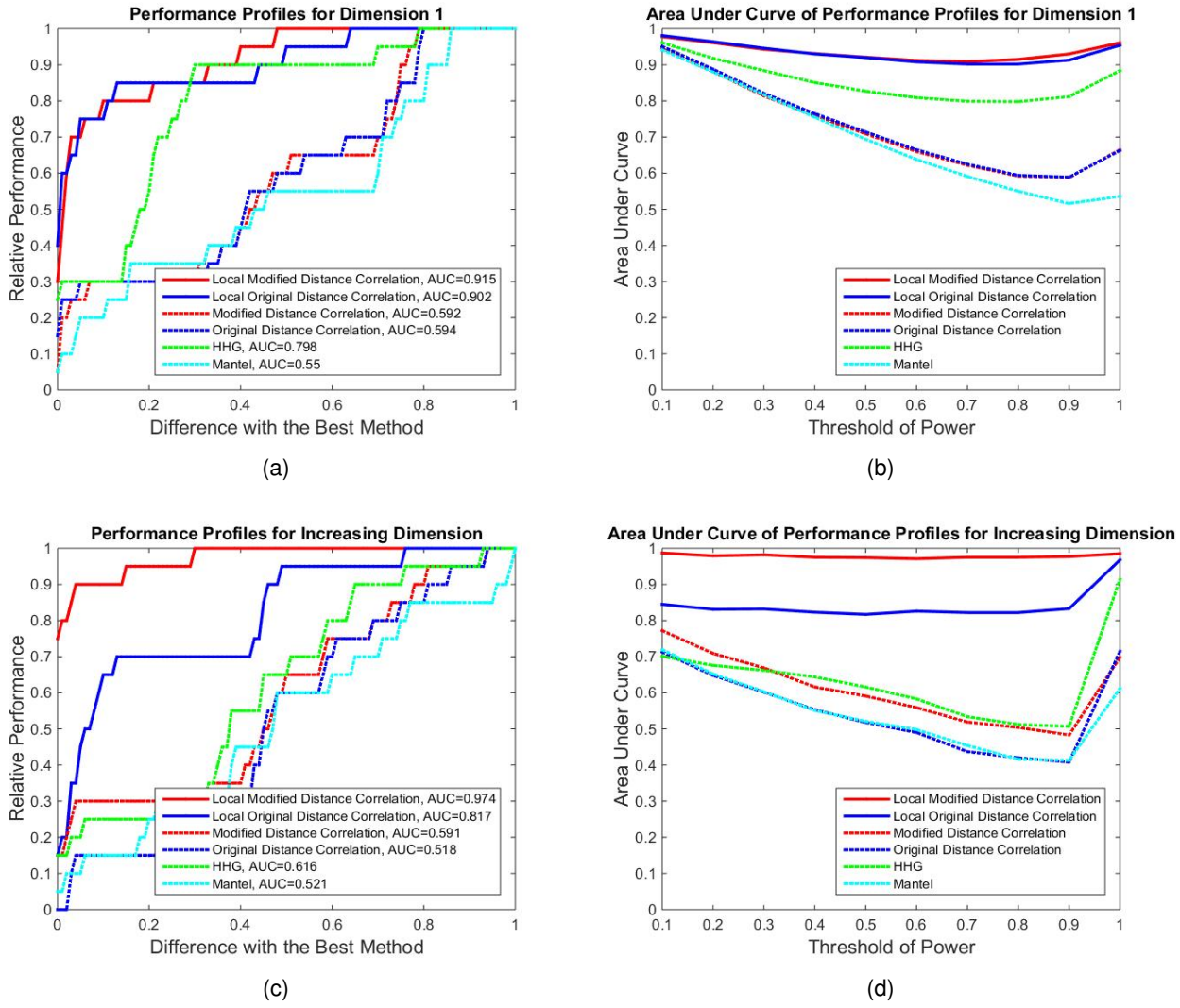

Figure 2: Quantitative comparisons of the power of the various algorithms across all simulations into a single number. (a) Performance profile plots comparing the different algorithms on all 1-dimensional problems at XXX a fixed sample size XXX. The legend provides the Area-Under-the-Curve (AUC) for each method; larger is better. (b) AUC for each method sweeping over all different power thresholds. (c) Same as (a) but for the high-dimensional simulations. (d) Same as (b) but for the high-dimensional simulations. It is clear that our method outperforms the previous state of the art, regardless of function, sample size, and dimensionality.

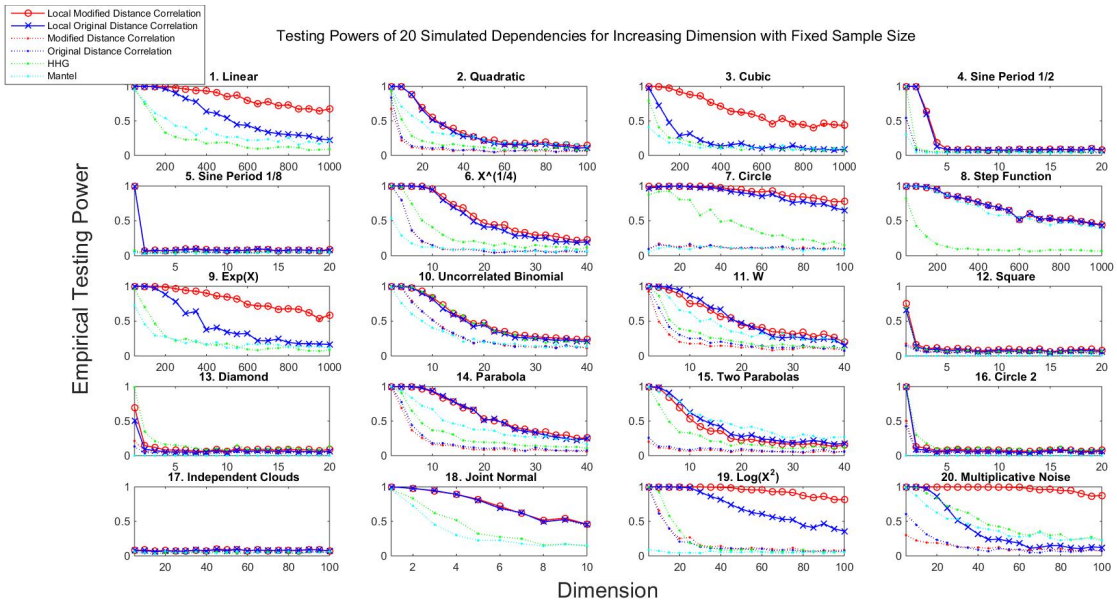

Figure 3: Power of different methods on 20 different simulation settings, for dimensionality ranging from 1 to 1000. Details as in Figure 1. Again, our method empirically achieves as high or higher power than the previous state of the art approaches for nearly all sample sizes on nearly all problems and dimensions.

from Adelstein et al. (2011). The sample size is $n = 42$, and each person has a 5 dimensional personality data based on questionnaires and the five-factor personality model. Then the brain activity of each person is measured by fMRI for 197 brain regions and 194 time steps. Thus the brain connectome feature is high-dimensional while the personality data is low-dimensional. There seems to exist certain correlation between the brain activity and personality as experimentally shown in Adelstein et al. (2011), but whether the dependency can be detected from the raw data is the question here.

To apply distance correlation and HHG, first we need to find two distance measures for the different data sources: for the personality data, the distance matrix A is formed by the Euclidean distance directly; for the connectome data, we run a spectrum analysis for each region, bandpass and normalize it, then calculate the Kullback-Leibler divergence among regions and use the normalized Hellinger distance as the distance matrix B. Once the distance matrices A and B are obtained, we apply the permutation test in Section E for $r = 10000$ random permutations, and show the log scaled p-value in the first plot of Figure 5: The x-axis is the neighborhood choice of k from 2 to n, and the y-axis for local distance correlation stands for the empirical p-value of

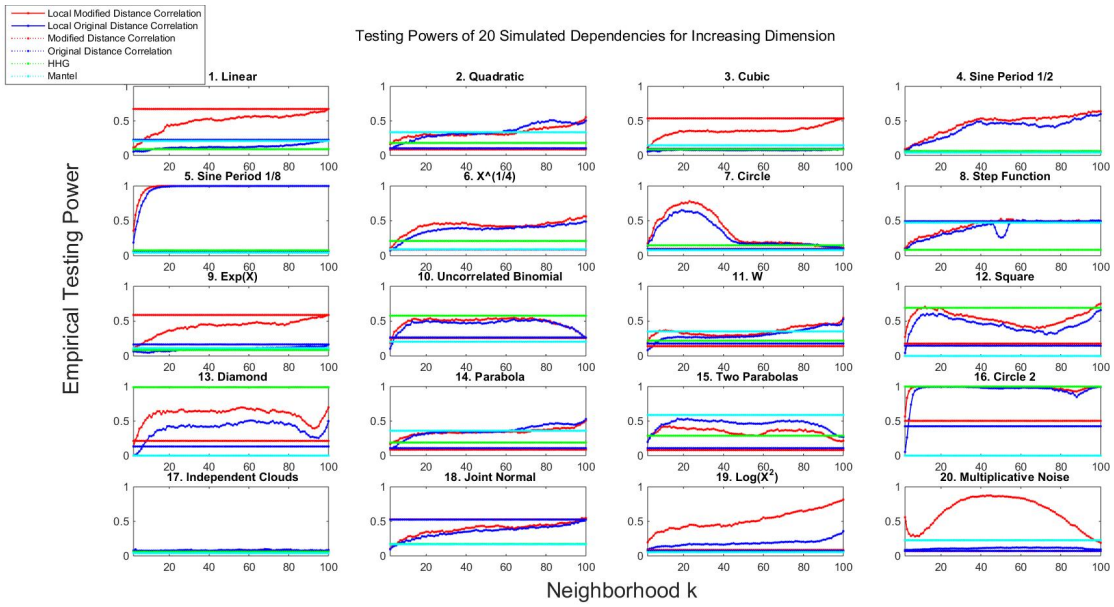

Figure 4: Understanding how dependence varies with the local scale of the dependence. For each of the 20 panels, the abscissa shows power and the ordinate is the number of neighbors for XXX X XXX (we actually sweep over all pairs of locality for X and Y, so this plot only shows a line in that plane). Each different simulation yields a different curve, highlighting the importance of understanding local scale in terms of understanding the data.

$\min_l\{\text{p-value}(dCorr_{kl})\}$ at each k in log scale, and all other global benchmarks are always dashed straight lines.

The p-value by local modified distance correlation is 0.0276 achieved at $k = 11, l = 5$; the p-value by local original distance correlation is 0.3833 achieved at $k = 11, l = 35$; original distance correlation has a p-value of 0.6745; modified distance correlation has a p-value of 0.3759; HHG has a p-value of 0.0576; and the Mantel test has a p-value of 0.9886. Therefore only local distance correlation has significant (less than 0.05) p-value, although HHG is quite close to significant as well. Note that the p-value of local modified distance correlation is validated by adjacent p-values, and one may also observe from the first plot of Figure 5 that $mdCorr_{kl}$ has low p-values for consecutive neighborhoods.

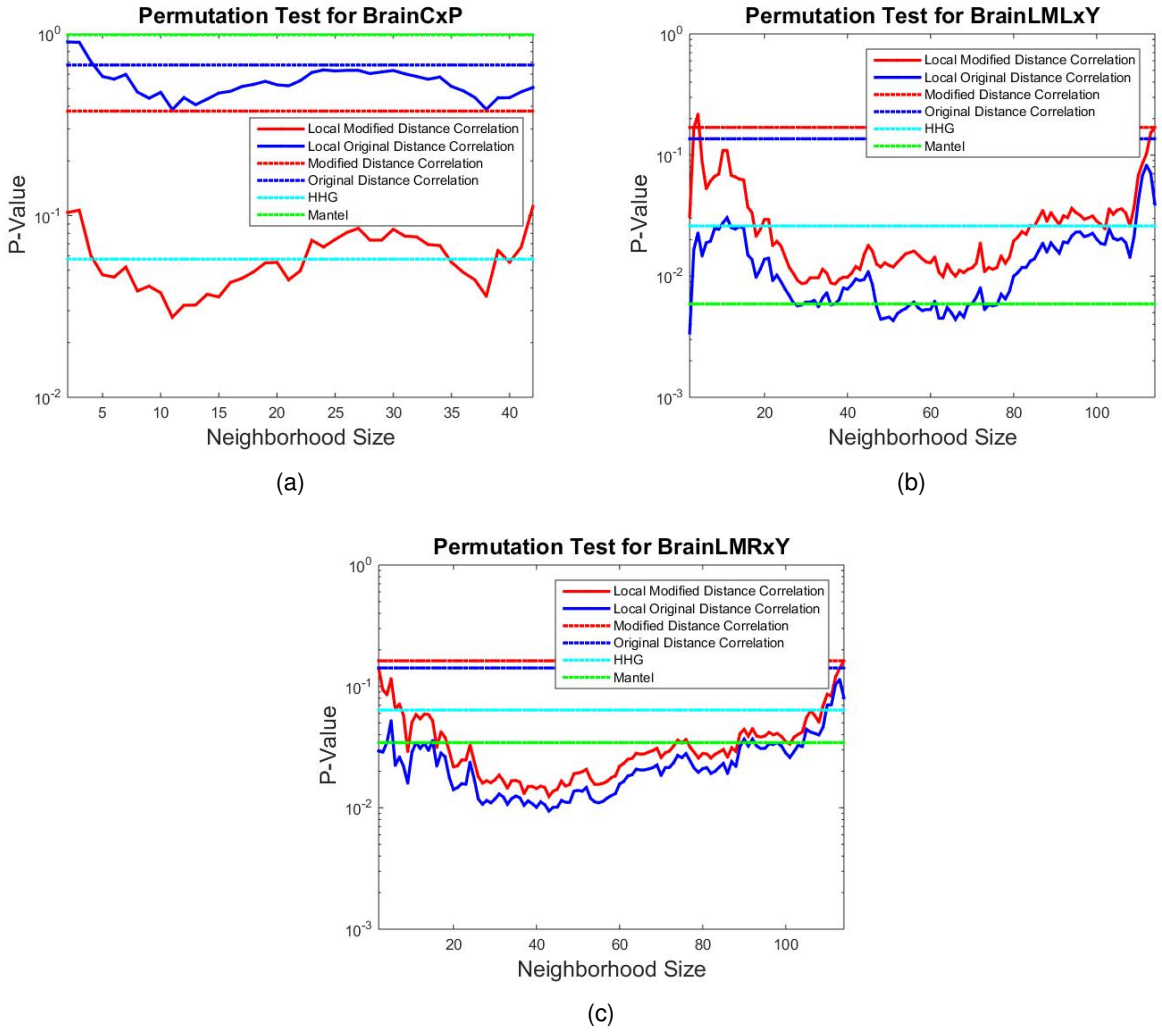

Figure 5: P-value of Real Data Testing

Next we carry out the same testing procedure on another experiment regarding brain hippocampus shape and major depressive disorder. There are $n = 114$ subjects, and the brain images of each person are obtained by very high resolution MRI scans on the hippocampus; and we also have available a categorical vector containing the disease information, including clinically depressed subject, high-risk subject, and non-affected subject.

The brain data is transformed into two dissimilarity matrices LML and LMR, representing the left and right hippocampus data based on landmark matching (see Park et al. (2008) for more details on data processing); and the label vector is transformed into a binary dissimilarity matrix D, where $D(i, j) = 0$ if and only if the ith subject has a different label from the jth subject.

There has been evidences that relate major depressive disorder to the hippocampus shape in Park et al. (2008) and Posener et al. (2003), and we would like to test the significance of such relationship in the data. In the second plot of Figure 5, we show the log scaled p-value of permutation test between LML and D, and in the last plot of Figure 5 we show the log scaled p-value for testing between LMR and D.

In both plots, local distance correlation yields lower p-values than its global version and HHG. For testing between LML and D, the actual p-value of local modified distance correlation is 0.0086 achieved at $k = 37, l = 23$, 0.0048 for local original distance correlation achieved at $k = 51, l = 9$, 0.1690 and 0.1362 for global modified and original distance correlation, 0.0260 for HHG, and 0.0059 for Mantel. Note that the lowest p-value of local original distance correlation is achieved at $k = 5, l = 2$ for 0.0034, but is not used...

For testing between LMR and D, the actual p-value of local modified distance correlation is 0.0124 achieved at $k = 43, l = 114$, 0.0094 for local original distance correlation achieved at $k = 43, l = 114$ too, 0.1624 and 0.1419 for global modified and original distance correlation, 0.0638 for HHG, and 0.0344 for Mantel. Again the p-values of local distance correlation are very significant.

Furthermore, the p-value is always 0 for any test statistic when testing independence between LML and LMR, implying strong linear dependency between the left and right brain.

4 Conclusion

In short, we propose the local distance correlation to test independence between data sets, which has been shown to be perform well for testing independence on data of small sample size, high-

dimensionality, linearity or non-linearity. It not only enjoys theoretical guarantee such as being consistent in testing independence, but also exhibits superior numerical performances in a comprehensive simulation setting and real data experiments, comparing to other popular methods.

Acknowledgment

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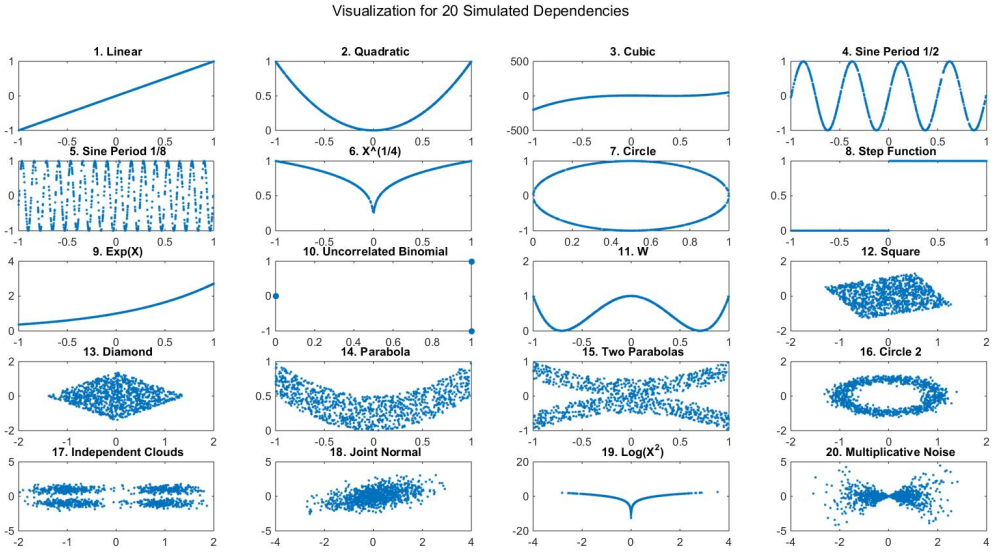
A Functions



(a)

Figure 6: Visualization of 20 different at dimension 1 and $n = 1000$ with no noise

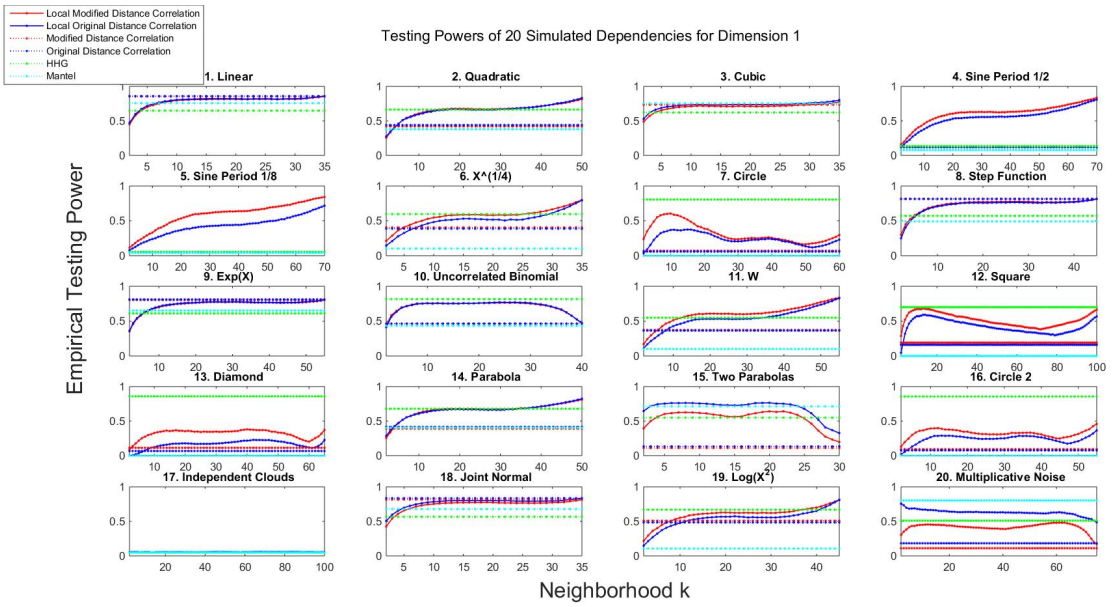


Figure 7: Testing Power for 20 Simulations of Increasing Neighborhood at Fixed Sample Size and Dimension

B Locality

C Distance Correlation

C.1 Global Distance Correlation

Suppose we are given two data sets $\mathcal{X} = [X_1, \cdots, X_n] \in \mathcal{R}^{m_X \times n}$ and $\mathcal{Y} = [Y_1, \cdots, Y_n] \in \mathcal{R}^{m_Y \times n}$, where n is the sample size, m_X and m_Y are the dimensions for each data set. Under the classical hypothesis testing framework, we assume that $X_i, i = 1, \ldots, n$ are identically independently distributed (i.i.d.) as X, similarly $Y_i \overset{i.i.d.}{\sim} Y$. Throughout the paper, we always assume that X and Y have finite second moments, which is a necessary assumption to guarantee the consistency of distance correlation.

For testing independence between X and Y, the null and the alternative hypothesis are

$$H_0 : X \text{ is independent of } Y, i.e., f_{XY} = f_X f_Y,$$
$$H_A : f_{XY} \neq f_X f_Y,$$

where f_{XY} denotes the joint distribution of $(X, Y) \in \mathcal{R}^{m_X + m_Y}$, and f_X and f_Y are the marginal distributions.

To test independence by distance correlation on sample data, we first calculate two Euclidean distance matrices $A, B \in \mathcal{R}^{n\times n}$ for $\mathcal{X}$ and $\mathcal{Y}$ respectively, i.e., $A_{ij} = \|X_i - X_j\|_2$. The sample distance covariance is defined as

$$dCov_n(\mathcal{X}, \mathcal{Y}) = \frac{1}{n^2}\sum_{i,j=1}^{n} A^H_{ij} B^H_{ij}, \tag{3}$$

where $A^H = HAH$, $B^H = HBH$ with $H = I_n - \frac{J_n}{n}$. Then the sample distance variance is defined as

$$dVar_n(\mathcal{X}) = \frac{1}{n^2}\sum_{i,j=1}^{n} A^H_{ij} A^H_{ij}$$

$$dVar_n(\mathcal{Y}) = \frac{1}{n^2}\sum_{i,j=1}^{n} B^H_{ij} B^H_{ij}.$$

The squared sample distance correlation is obtained by normalizing the distance covariance

$$dCorr_n(\mathcal{X}, \mathcal{Y}) = \frac{dCov_n(\mathcal{X}, \mathcal{Y})}{\sqrt{dVar_n(\mathcal{X}) \cdot dVar_n(\mathcal{Y})}}, \tag{4}$$

where all of $dCov_n, dVar_n, dCorr_n$ are always non-negative. Note that the $dCor_n/dCorr_n$ above is actually the square of distance covariance/correlation in Szekely et al. (2007); but for simplicity we drop the square in the name throughout this paper.

It is shown in Szekely et al. (2007) that as $n \to \infty$, $dCorr_n(\mathcal{X}, \mathcal{Y}) \to dCorr(X, Y) \geq 0$, where $dCorr(X, Y)$ is the population distance correlation of X and Y defined by their characteristic functions. The population distance correlation is 0 if and only if X and Y are independent, so that the sample distance correlation is a consistent test for independence, i.e., the testing power converges to 1 as n increases, at any fixed type 1 error level. Note that in this paper distance correlation always means the sample statistic rather than the population statistic, unless otherwise mentioned.

However, in case of high-dimensional data where the dimension m_X or m_Y increases with the sample size n, the original distance correlation $dCorr_n$ is no longer appropriate. For example, even for independent Gaussian distribution, $dCorr_n \to 1$ as $m_X, m_Y \to \infty$, such that it is no longer a consistent test in high dimension. This problem is solved by the modified distance correlation proposed in Szekely and Rizzo (2013a):

$$mdCov_n(\mathcal{X}, \mathcal{Y}) = \frac{1}{n(n-3)}\Big(\sum_{i,j=1}^{n} A^{H*}_{ij} B^{H*}_{ij} - \frac{n}{n-2}\sum_{i=1}^{n} A^{H*}_{ii} B^{H*}_{ii}\Big), \tag{5}$$

where A^{H*}_{ij} adjusts the entries of A^H by

$$A^{H*}_{ij} = \begin{cases} \frac{n}{n-1}(A^H_{ij} - \frac{A_{ij}}{n}), & \text{if } i \neq j \\ \frac{n}{n-1}(\frac{\sum_i A_{ij}}{n} - \frac{\sum_{i,j} A_{ij}}{n^2}), & \text{if } i = j \end{cases}$$

and similarly for B_{ij}^{H*}. Then $mdVar_n(\mathcal{X})$ can be defined by replacing all B_{ij}^{H*} in Equation 5 by A_{ij}^{H*}, similarly define $mdVar_n(\mathcal{Y})$.

If $mdVar_n(\mathcal{X}) \cdot mdVar_n(\mathcal{Y}) \leq 0$, the modified distance correlation is set to 0; otherwise it is defined as

$$mdCorr_n(\mathcal{X}, \mathcal{Y}) = \frac{mdCov_n(\mathcal{X}, \mathcal{Y})}{\sqrt{mdVar_n(\mathcal{X}) \cdot mdVar_n(\mathcal{Y})}}. \tag{6}$$

It is shown in Szekely and Rizzo (2013a) that $mdCorr_n(\mathcal{X}, \mathcal{Y}) \to dCorr(X, Y) \geq 0$, and is an unbiased estimator of the population distance correlation $dCorr(X, Y)$; furthermore, $mdCorr_n$ is approximately normal even if $m_X, m_Y \to \infty$. Thus it is a consistent test of independence for high-dimension data.

To summarize this subsection, both the distance correlation and modified distance correlation are great for testing independence of Euclidean data due to their theoretical consistency, with the modified test statistic being more robust against high-dimensionality. Indeed it is a flourishing concept by a series of papers Bakirov et al. (2006); Szekely et al. (2007); Szekely and Rizzo (2009); Bickel and Xu (2009); Kosorok (2009); Remillard (2009); Li et al. (2012); Szekely and Rizzo (2013a,b, 2014); and the test statistic is not limited to the Euclidean metric as shown in Lyons (2013).

However, the required sample size for achieving a good testing power very much depends on the type of dependency underlying the given data, e.g. for perfect linear relationship, sample distance correlation usually requires less than 10 points for a permutation test to declare significance; but for some nonlinear relationships like circle, sample distance correlation yields no significance even at $n = 100$. Because real data rarely exhibits perfect linear relationship, and in practice large amount of data may not always be available, a better finite-sample method is of tremendous value: it not only yields a better testing power for the same sample size, but may also requires much less sample data for the permutation test to declare significance, which in turn saves the running time and data collection process.

There exists another distance-based method that is consistent and works particularly well for non-linear dependencies, which is called the HHG statistics in Heller et al. (2013). It applies Pearson's chi-square test to ranks of distances within each column rather than directly summing up the products of distances, and is shown to be better than distance correlation and other methods for finite-sample testing of many common nonlinear relationships in Gorfine et al. (2012) and Heller et al. (2013). However, in our numerical simulations HHG seems to fall a bit short when testing against high-dimensional or close to linear dependency, but is otherwise a strong competitor of

the global distance correlation.

The other method we use as the benchmark in the numerical section is the Mantel test, which simply applies Pearson's correlation to the distance matrices, see in Mantel (1967). Despite its lack of theoretical guarantee (for example, unlike distance correlation and HHG, it is not consistent against all alternatives), it has been a very popular method so far and commonly used in biology and ecology. In our numerical simulations we will observe that the Mantel test is not consistent for many nonlinear dependencies, and is sub-optimal in almost all types of dependency we consider.

Since there has not been a method that perform well against all possible alternatives in finite-sample testing, it motivates us to propose a local distance correlation that is concurrently robust against small sample size, high-dimensionality, linearity or non-linearity in the following subsection.

D Local Distance Correlation

In this subsection we define the local distance correlation, which is based on k-nearest-neighbor and applicable to both the original distance correlation and the modified distance correlation. From now on, we distinguish the local test statistic as either the local original distance correlation or the local modified distance correlation when they have different behaviors in the context, otherwise we call both as local/global distance correlation since they often share the same properties.

Under the same setting and notation as the global distance correlation in Section C.1, we further sort the distance matrix A within column and denote the ranks as $r(A_{ij})$: for each $i = 1, \ldots, n$, we always set $r(A_{ii}) = 0$; then set $r(A_{ij}) = k$ if and only if A_{ij} is the kth smallest distance in $\{A_{ij}, i = 1, \ldots, n \,\&\, i \neq j\}$; for ties, we take the minimum rank among them (alternatively, one can break ties randomly). Similarly sort the distance matrix B within column and denote the ranks by $r(B_{ij})$.

Then for each $k, l = 1, \ldots, n$, we can calculate a "local" version of distance covariance as

$$dCov_{kl}(\mathcal{X}, \mathcal{Y}) = \frac{1}{n^2} \sum_{i,j=1}^{n} A_{ij}^H B_{ij}^H I(r(A_{ij}) < k) I(r(B_{ij}) < l), \tag{7}$$

and calculate a local version of distance variance as

$$dVar_k(\mathcal{X}) = \frac{1}{n^2}\sum_{i,j=1}^{n} A_{ij}^H A_{ij}^H I(r(A_{ij}) < k)$$
$$dVar_l(\mathcal{Y}) = \frac{1}{n^2}\sum_{i,j=1}^{n} B_{ij}^H B_{ij}^H I(r(B_{ij}) < l),$$

where $I(\cdot)$ is the indicator function. After normalizing, we have a family of distance correlation:

$$dCorr_{kl}(\mathcal{X},\mathcal{Y}) = \frac{dCov_{kl}(\mathcal{X},\mathcal{Y})}{\sqrt{dVar_k(\mathcal{X})\cdot dVar_l(\mathcal{Y})}}. \quad (8)$$

When $k = l$, we simplify the notations to $dCov_k$ and $dCorr_k$; and the family of local test statistics $\{dCorr_{kl}, k, l = 2,\ldots,n\}$ includes the original distance correlation $dCorr_n$ as well. Note that in the family we exclude $dCorr_{1l}$ and $dCorr_{k1}$, because it holds that $dCorr_{1l} = dCorr_{k1} = dCorr_{11}$, which does not consider any neighbor, merely counts the diagonal terms in the distance matrices, and not meaningful for testing independence.

From now on, local distance correlation refers to the family of the test statistics $\{dCorr_{kl}, k, l = 2,\ldots,n\}$ rather than each individual $dCorr_{kl}$; and the testing power of local distance correlation refers to the best testing power achieved in the family. Since k, l are finite, the optimal testing power always exists; and it is clear that the optimal power and the corresponding best local test statistic are dependent on the joint distribution f_{XY} and may not be unique.

In the same manner, we can apply the above to modified distance covariance:

$$mdCov_{kl}(\mathcal{X},\mathcal{Y}) = \frac{1}{n(n-3)}\Big(\sum_{i,j=1}^{n} A_{ij}^{H*} B_{ij}^{H*} I(r(A_{ij}) < k) I(r(B_{ij}) < l) - \frac{n}{n-2}\sum_{i=1}^{n} A_{ii}^{H*} B_{ii}^{H*}\Big), \quad (9)$$

then $mdCorr_{kl}$ is obtained by normalizing each $mdCov_{kl}(\mathcal{X},\mathcal{Y})$ by the square root of $mdVar_k(\mathcal{X})\cdot mdVar_l(\mathcal{Y})$; 0 if the square root is either 0 or not a real number. It follows that local modified distance correlation refers to the family $\{mdCorr_{kl}, k, l = 2,\ldots,n\}$.

Because $\{mdCorr_{kl}\}$ has the same asymptotic properties as $\{dCorr_{kl}\}$ other than its robustness against high-dimensionality, we will mostly use $\{dCorr_{kl}\}$ for explanation purposes in Section C. Indeed in the numerical section, local modified distance correlation has almost the same numerical performance as the local original distance correlation at dimension 1, but much more superior at higher dimensions due to its bias adjustment.

Moreover, testing dependency by local distance correlation can be a more elegant solution than nonlinear embedding: choosing an optimal neighborhood size and an appropriate dimension in nonlinear algorithms can be computationally expensive by cross validation, but the family of local

test statistics can be easily computed for all possible neighborhoods. In fact, once the distance matrices A and B are sorted within column, computing $\{dCorr_{kl}\}$ has the same running time as computing any individual $dCorr_{kl}$; and the overall computation always takes $O(n^2 \log(n))$, which comes from sorting.

E Testing Procedure

XXX fix this section XXX

In this subsection we explain how to test independence by local distance correlation, which is necessary for understanding their theoretical properties in Section 2.2, and also used as the testing procedure in our numerical experiment.

E.1 Independence Test

When the true joint distribution f_{XY} is known, we carry out the following independence test for evaluation: We first derive the distribution of $dCorr_{kl}(\mathcal{X}, \mathcal{Y})$ under the null and the alternative.

E.2 Permutation Test

For given sample data, the permutation test and its p-value is a nature choice of evaluation, especially when the underlying random variables X and Y have unknown distributions. We first calculate $dCorr_{kl}(\mathcal{X}, \mathcal{Y})$, then permute the second data set and calculate $dCorr_{kl}(\mathcal{X}, \mathcal{Y}P)$ for all possible permutation matrices P; next we calculate the p-value for each $k, l = 2, \ldots, n$ by comparing $dCorr_{kl}(\mathcal{X}, \mathcal{Y})$ and $\{dCorr_{kl}(\mathcal{X}, \mathcal{Y}P), \forall P\}$; finally we pick the neighborhood that minimizes the p-value (or the mean p-values from bootstrap samples, see below), and use the corresponding p-value as the p-value of local distance correlation. In the numerical section, the permutation test is carried out for r randomly generated permutations rather than all permutations, and the resulting empirical p-value is an estimation of the true p-value. A small p-value (say less than 0.05) from the permutation test implies significant dependency between $\mathcal{X}$ and $\mathcal{Y}$.

E.2.1 Power Calculations

then calculate the testing power of $dCorr_{kl}$ at a fixed type 1 error level α. This can be done for all $k, l \in [2, \ldots, n]$, and the power β of local distance correlation equals the maximum power in the family, i.e., $\beta = \max_{k,l}\{\beta(dCorr_{kl}), k, l \in [2, \ldots, n]\}$. We call the neighborhood choice having power β as the optimal neighborhood, which exists but may not be unique. In the numerical experiment, we compute the empirical distribution of $dCorr_{kl}$ by generating $(X_i, Y_i), i = 1, \ldots, n$ under the null and the alternative respectively for r Monte-Carlo replicates, then calculate the empirical testing power of local distance correlation by $\hat{\beta} = \max_{k,l}\{\hat{\beta}(dCorr_{kl}), k, l \in [2, \ldots, n]\}$ at a fixed type 1 error level α.

E.2.2 Bias Adjustment

Since the independence test is an approximation of the permutation test by Lehmann and Romano (2008), the power of local distance correlation β in the independence test approximates its testing power in the permutation test, assuming the optimal neighborhood in the independent test is used in the permutation test. But if we pick the neighborhood in the permutation test by minimizing the p-value on the given data, it is likely to be different from the actual optimal neighborhood that maximizes the testing power. Although $dCorr_{kl}$ are strongly dependent for adjacent neighborhoods, such that the powers of $dCorr_{kl}$ are close to each other for adjacent neighborhoods; so the estimated neighborhood by minimizing the p-value may still have power that is close to optimal.

Alternatively, one may estimate the optimal neighborhood in the permutation test by a procedure similar to re-sampling/smoothed bootstrap: Suppose two distance matrices A and B are given, we generate a vector of random noise by $N(0, \frac{1}{n})$, form the corresponding distance matrix E, and calculate the p-values of $dCorr_{kl}$ between A and $B + E$ for all neighborhoods; after certain number of Monte-Carlo replicates, we estimate the optimal neighborhood by minimizing the sum of p-values from the bootstrap samples. Clearly as the sample size n and the number of MC replicates increases, the estimated neighborhood converges to the true optimal neighborhood, and we report the p-value at the estimated neighborhood for local distance correlation XXX is the previous sentence true? did somebody else prove it? if not, do we need to? i would think so XXX. if the estimated neighborhood is not unique, we use the mean p-value from all estimated neighborhoods. This is the procedure we use in the real data experiment for the permutation test on local test statistics.

In our numerical experiments, for simulations of known distributions we evaluate the test statistics by the empirical testing powers of the independence test, while for real data of unknown distributions we evaluate all methods by the empirical p-values of the permutation test.

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