Dependence Discovery from Multimodal Data via Multiscale Graph Correlation

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Overview

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   - Global Correlation Coefficient
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Section 1

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- In particular, we are investigating the association between brain activities and various phenotypes, such as brain Connectome vs certain disease, or brain vs personality, where the brain data is usually obtained via fMRI scans for a number of brain regions at consecutive time steps.
- Before we try all kinds of regression / classification methods, the first task is to determine whether there exists strong dependency for given pair of data.

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- To that end, we propose multiscale graph correlation in Shen et al. [2016] for testing independence, which combines distance correlation and nearest-neighbor into the same testing framework.

Section 2

Results

General Correlation Coefficient

A general correlation coefficient $\mathcal{G}$ can be expressed as follows:

$$\mathcal{G} = \frac{\sum_{i,j=1}^{n}(a_{ij} - \bar{a})(b_{ij} - \bar{b})}{\sqrt{\sum_{i,j=1}^{n}(a_{ij} - \bar{a})^2 \sum_{i,j=1}^{n}(b_{ij} - \bar{b})^2}}, \tag{1}$$

where $\bar{a}$ and $\bar{b}$ denote the sample means of a_{ij} and b_{ij}.

Examples

- Suppose $X = [x_1, \cdots, x_n] \in \mathbb{R}^{d_x \times n}$ and $Y = [y_1, \cdots, y_n] \in \mathbb{R}^{d_y \times n}$ are the corresponding data sets.

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- The distance correlation (dcorr) proposed in Szekely et al. [2007] uses the doubly-centered distance entries for a_{ij} and b_{ij}.
- The modified distance correlation (mcorr) proposed in Szekely and Rizzo [2013] slightly modifies a_{ij}/b_{ij} of dcorr to make the resulting $\mathcal{G}$ unbiased.

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- Then for any general correlation coefficient $\mathcal{G}$ in the form of Equation 1, we define its *local* variants by

$$\mathcal{G}_{kl} = \frac{\sum_{i,j=1}^{n}(a_{ij}^{k} - \bar{a}^{k})(b_{ij}^{l} - \bar{b}^{l})}{\sqrt{\sum_{i,j=1}^{n}(a_{ij}^{k} - \bar{a}^{k})^2 \sum_{i,j=1}^{n}(b_{ij}^{l} - \bar{b}^{l})^2}}, \tag{2}$$

for $k = 1, \ldots, \max(rank(a_{ij}))$, $l = 1, \ldots, \max(rank(b_{ij}))$, where

$$a_{ij}^{k} = \begin{cases} a_{ij}, & \text{if } 0 < rank(a_{ij}) \leq k, \\ 0, & \text{otherwise;} \end{cases} \qquad b_{ij}^{l} = \begin{cases} b_{ij}, & \text{if } 0 < rank(b_{ij}) \\ 0, & \text{otherwise;} \end{cases} \tag{3}$$

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- Although each local correlation requires $O(n^2)$ to compute, we provide a fast algorithm to compute all local correlations simultaneously in $O(n^2)$, assuming the rank information is given (note: sorting the distance matrix column-wise takes $O(n^2 \log(n))$).

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- This allows the optimal scale to be efficiently determined for MGC, unlike many other applications by nearest-neighbor (say knn classification, manifold learning, etc.).

The Testing Framework

- Given two data sets $X = [x_1, \cdots, x_n] \in \mathcal{R}^{d_X \times n}$ and $Y = [y_1, \cdots, y_n] \in \mathcal{R}^{d_Y \times n}$.

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- The null and the alternative hypothesis for testing independence are

$$H_0 : f_{xy} = f_x f_y,$$
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  where f_{xy} denotes the joint distribution of $(\boldsymbol{x}, \boldsymbol{y})$.
- For a given pair of data with unknown model, we can use the permutation test, and reject the null when the p-value is sufficiently small.

Theorems of MGC

Theorem 1

Multiscale graph correlation is consistent against all dependent alternatives of finite second moments, i.e., $\beta_\alpha(\mathcal{G}^*) \to 1$ *as* $n \to \infty$ *at any type 1 error level* α*, when distance correlation or modified distance correlation is used as the global correlation* $\mathcal{G}$*.*

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Theorem 2

*Suppose **x** is linearly dependent of **y**. Then for any n and α it always holds that*

$$\beta_\alpha(\mathcal{G}^*) = \beta_\alpha(\mathcal{G}). \tag{4}$$

Thus multiscale graph correlation is equivalent to the global correlation coefficient under linear dependency.

Theorems of MGC

Theorem 3

There exists f_{xy}, n and α such that

$$\beta_{\alpha}(\mathcal{G}^{*}) > \beta_{\alpha}(\mathcal{G}). \tag{5}$$

Thus multiscale graph correlation can be better than its global correlation coefficient under certain nonlinear dependency.

We use a quadratic relationship and finite n to prove theorem 3.

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- The benchmarks are distance correlation, modified distance correlation, the Mantel test, and the HHG method proposed in Heller et al. [2013].
- To better illustrate the effectiveness of distance-based local correlation, we consider three MGC implementations by dcorr / mcorr / Mantel respectively in the simulation.

Visualization of Sample Data for Each Joint Distribution

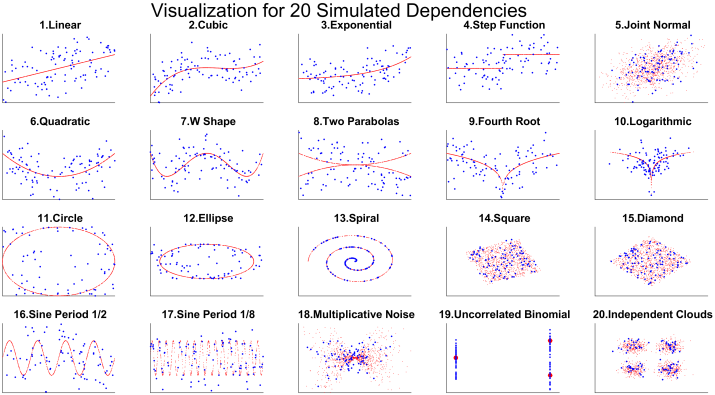

Figure: Visualization of the 20 dependencies for 1-dimensional simulations. The blue points are generated with noise (c=1) for $n = 100$ to show the actual sample data in testing, and the red points are generated with no noise for $n = 1000$ to highlight each underlying dependency.

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- For 1-dimensional simulations, each panel shows empirical testing power on the absicca, and sample size on the ordinate, with dimension fixed at 1; for high-dimensional simulations, the dimension choice is on the ordinate, with the sample size fixed at 100.

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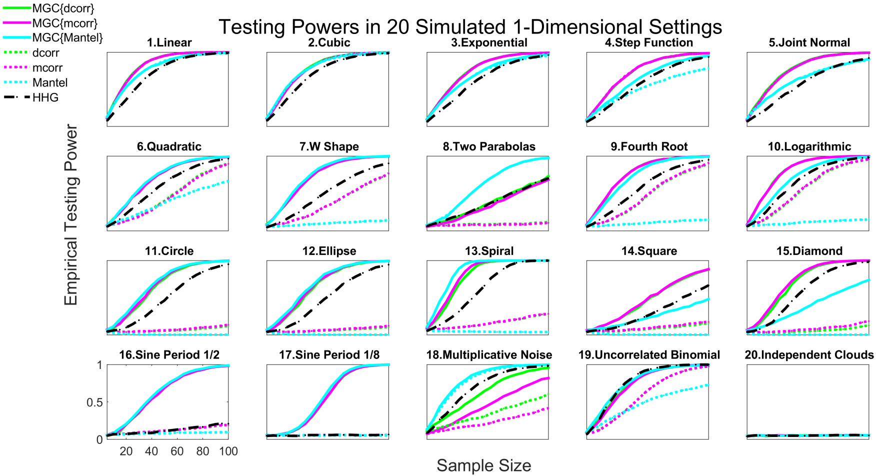
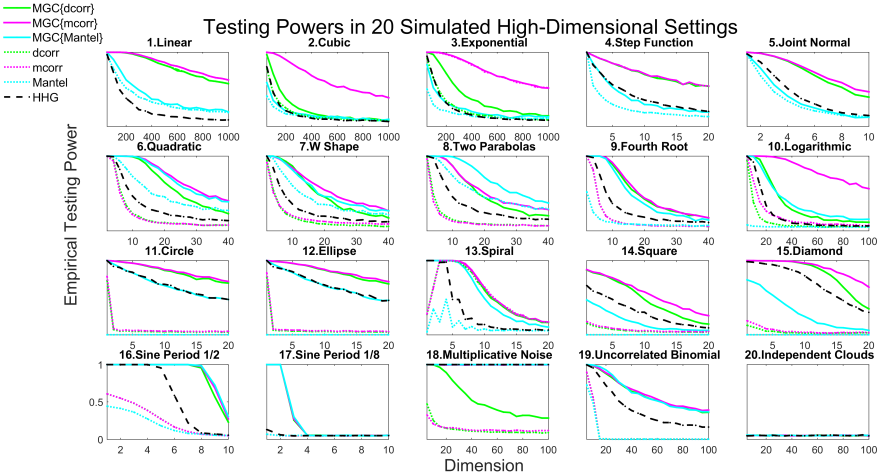
- We also show the MGC power heatmap with respect to neighborhood choices, where we can observe that: linear dependency always favors the largest scale (i.e., $\mathcal{G}^* = \mathcal{G}$), while nonlinear dependency always favors a smaller scale such that ($\mathcal{G}^* > \mathcal{G}$); and similar dependency structure usualy yield similar optimal scales.

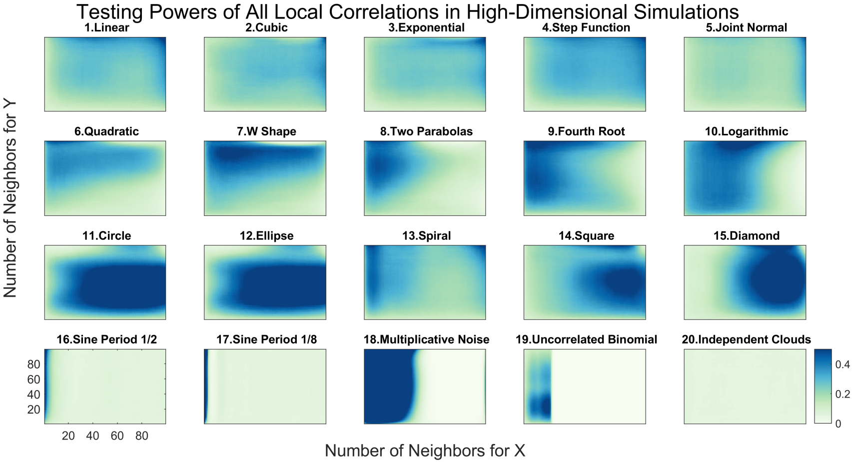
1-Dimensional Testing Powers



High-Dimensional Testing Powers



High-Dimensional Local Mcorr Power Heatmap



Section 3

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- 6) Does not inflate the false positive rate.
- 7) MGC is a better scalable method, for big data where distance-based testing method is often performed on sub-samples.

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- In case of one pair of given data of unknown model, how to choose the optimal scale heuristically;
- Real data experiments where MGC is used to detect local signals between brain data vs phenotypes.

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- Local correlation is potentially useful for nonlinear embedding, variable selection, etc.

Section 4

References

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