

Dependence Discovery via Multiscale Generalized Correlation

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August, 2016

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- Multiscale Generalized Correlation
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Section 1

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- Indeed, prior to embarking on a predictive machine-learning investigation, one might first check whether any dependence is detectable; if not, high-quality predictions will be unlikely.
- Modern data sets may be high-dimensional, nonlinear, noisy, of small sample size; and different features may come from disparate spaces.
- A particular application is to investigate the association between brain activities and various phenotypes, such as brain vs disease, or brain vs personality. Despite recent inventions of many consistent test statistics, existing methods fall short for our real data.

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- To that end, we propose multiscale generalized correlation in [*Shen et al.(2016)*][1] for testing independence, which combines distance correlation and nearest-neighbor into the same framework.
- MGC is theoretically consistent and efficient to compute, achieves excellent testing powers in a comprehensive set of simulations, sheds light into the underlying dependency structures, and works well for our real data.

Section 2

Results

Generalized Correlation Coefficient

Start with n pairs of observations $(\mathbf{x}_i, \mathbf{y}_i)$ for $i = 1, \dots, n$, where \mathbf{x} 's and \mathbf{y} 's both might be vectors of arbitrary dimensions, shapes, networks, etc.

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Then $A = \{a_{ij}\}$ and $B = \{b_{ij}\}$ are the $n \times n$ interpoint comparison matrices for $X = \{\mathbf{x}_i\}$ and $Y = \{\mathbf{y}_i\}$, respectively. Assuming $\{a_{ij}\}$ and $\{b_{ij}\}$ have zero mean, a generalized correlation coefficient can then be written:

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$$c = \frac{1}{z} \sum_{i,j=1}^n a_{ij} b_{ij}, \quad (1)$$

where z is proportional to standard deviations of A and B , that is
 $z = n^2 \sigma_a \sigma_b$.

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- Using the doubly-centered distance entries for a_{ij} and b_{ij} yields the distance correlation [*Szekely et al.(2007)*][3], which is a consistent test for most dependencies.
- An unbiased version of dcorr can be achieved by slightly tweaking a_{ij}/b_{ij} of dcorr, which yields the modified distance correlation [*Szekely and Rizzo (2013)*] [4].

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$$\tilde{a}_{ij}^k = \begin{cases} a_{ij}, & \text{if } R(a_{ij}) \leq k, \\ 0, & \text{otherwise;} \end{cases} \quad \tilde{b}_{ij}^l = \begin{cases} b_{ij}, & \text{if } R(b_{ji}) \leq l, \\ 0, & \text{otherwise.} \end{cases} \quad (2)$$

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Then let $a_{ij}^k = \tilde{a}_{ij}^k - \bar{a}^k$, where \bar{a}^k is the local mean, and b_{ij}^k similarly.

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There are a maximum of $(n^2 - n)/2$ different local correlations, one for each possible combination of k and l . And our definition always yields symmetric local correlations, i.e. $c^{kl}(X, Y) = c^{lk}(Y, X)$, no matter A and B are symmetric or not.

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- Although each local correlation requires $O(n^2)$ to compute, our formulation allows all local correlations to be simultaneously calculated in $O(n^2)$ as well! (Note: sorting the distance matrix column-wise takes another $O(n^2 \log(n))$).
- 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

The formal testing scenario is as follows: assume that $\mathbf{x}_i, i = 1, \dots, n$ are identically independently distributed (i.i.d.) as $\mathbf{x} \sim f_{\mathbf{x}}$; similarly each \mathbf{y}_i are i.i.d. as $\mathbf{y} \sim f_{\mathbf{y}}$.

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$$H_0 : f_{\mathbf{xy}} = f_{\mathbf{x}}f_{\mathbf{y}},$$

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To test on a pair of sample data, we can use the p-value of a permutation test, and reject the null when the p-value is sufficiently small.

The power of a test is defined as the probability that it correctly rejects the null when the null is indeed false, and has power equal to the type 1 error level when the null is true. And a test is universally consistent if its power converges to 1 as $n \rightarrow \infty$ whenever $f_{\mathbf{xy}} \neq f_{\mathbf{x}}f_{\mathbf{y}}$.

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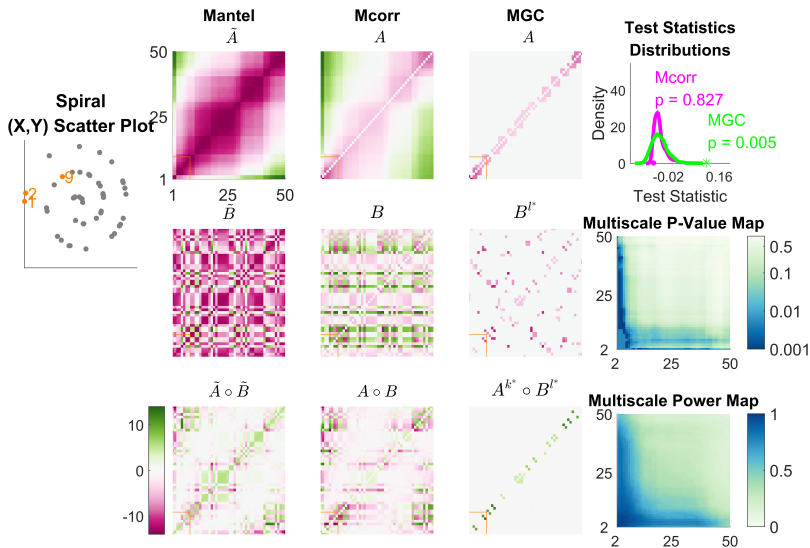
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Theorem 3

There exists f_{xy} and n such that MGC is better than its global counterpart in testing power.

Illustration of Utilizing locality



Advantage of Utilizing Locality

	Mantel	Mcorr	MGC
$\delta_x(1,2)$	-2.42	-5.21	-5.07
$\delta_y(1,2)$	-1.58	-0.91	-0.12
$\delta_x \times \delta_y$	3.82	4.74	0.61
<hr/>			
$\delta_x(2,9)$	0.70	0.61	0.14
$\delta_y(2,9)$	-0.91	-0.28	0.12
$\delta_x \times \delta_y$	-0.63	-0.17	0.02
<hr/>			
$\sum \delta_x \times \delta_y$	-162.14	-93.04	116.41
$\sum \delta_x \times \delta_y / \sum \delta_x^2 \sum \delta_y^2$	-0.02	-0.02	0.16

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- Our MGC implementation is based on modified distance correlation.

Visualizations of Simulation Settings

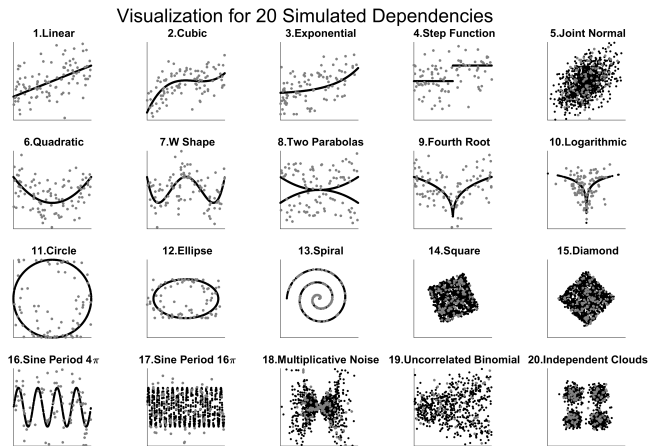


Figure: Visualization of the 20 dependencies for one-dimensional simulations.

Simulation Powers

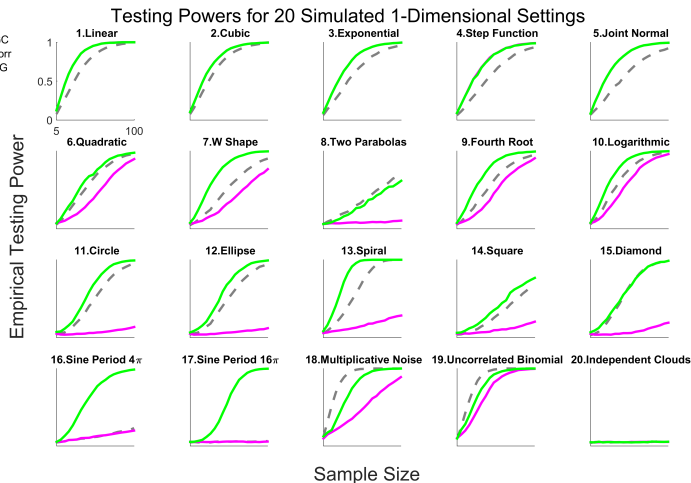


Figure: Powers of different methods for 20 different one-dimensional dependence structures.

Simulation Power Map

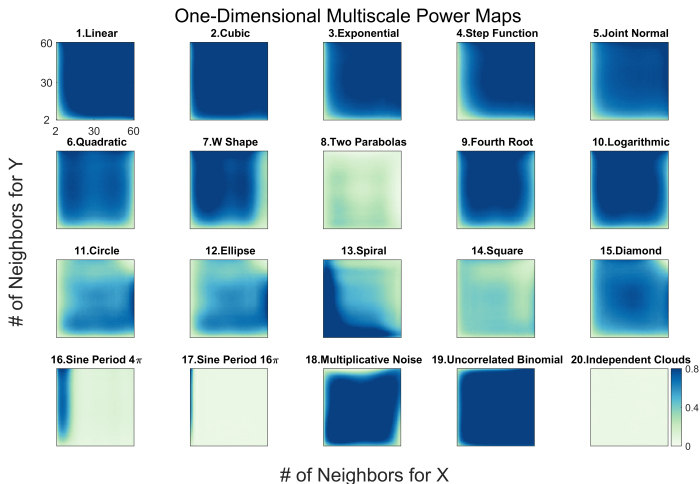


Figure: Multiscale Power Maps indicating the influence of neighborhood size on MGC testing power.

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The raw brain activity was processed using CPAC [*Craddock et al.(2015)*][7] resulting in 197 brain regions. We ran a spectral analysis on each region, bandpassed and normalized it, and then calculated the Kullback-Leibler divergence across regions and the normalized Hellinger distance between each subject.

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For the five-factor personality data, we use the Euclidean distance.

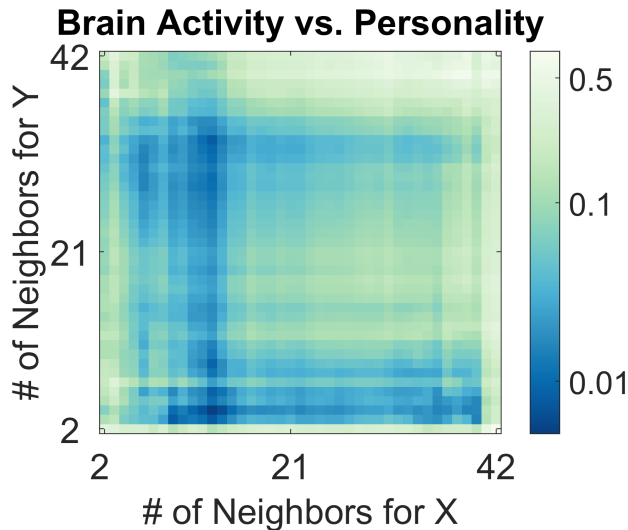


Figure: P-value map (log scale) for brain fMRI scan vs five-factor personality.

Section 3

Conclusion

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- 5) MGC not only yields a p-value in real data testing, but also provides useful information on the local scale where the dependency is the strongest, which implies the geometry of the underlying dependency.

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- When applying MGC to sample data without known model or training data, we provide a heuristic algorithm to accurately select the optimal scale by finding consecutive regions of significant p-values.

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