Dependency Discovery via Multiscale Graph Correlation

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Acknowledgment: NSF DMS, DARPA SIMPLEX.

R package available in CRAN and `https://github.com/neurodata/MGC/`
Matlab code available in `https://github.com/neurodata/mgc-matlab`

Overview

1. Motivation

2. Methodology

3. Theoretical Properties

4. Simulations and Experiments

5. Summary

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X	Y
brain connectivity	creativity / personality
brain shape	health
gene / protein	cancer
social networks	attributes
anything	anything else

Formal Definition of Independence Testing

$$(x_i, y_i) \stackrel{i.i.d.}{\sim} F_{XY}, \quad i = 1, \ldots, n$$

$$H_0 : F_{XY} = F_X F_Y,$$
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Without loss of generality, we shall assume F_{XY} has finite second moments.

Benchmarks

Correlation
Measures

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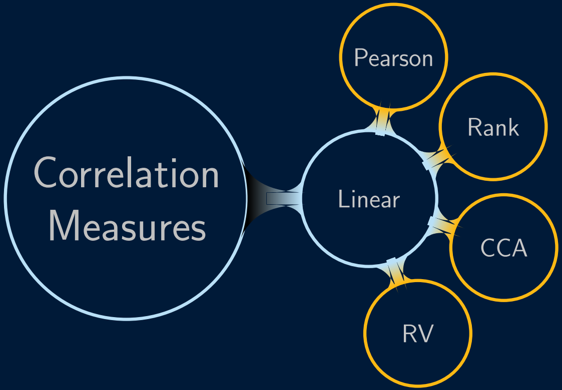

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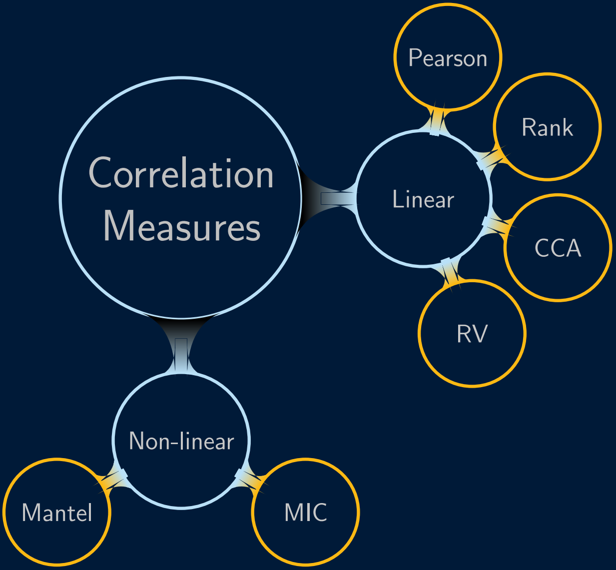
Correlation Measures
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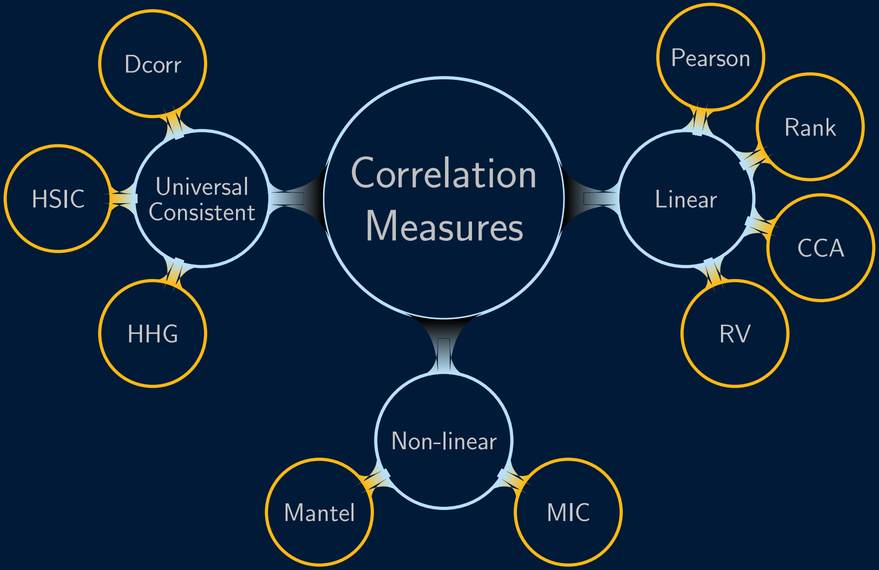
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To that end, we propose the **multiscale graph correlation** in [*Shen et al.(2018)*].

Methodology

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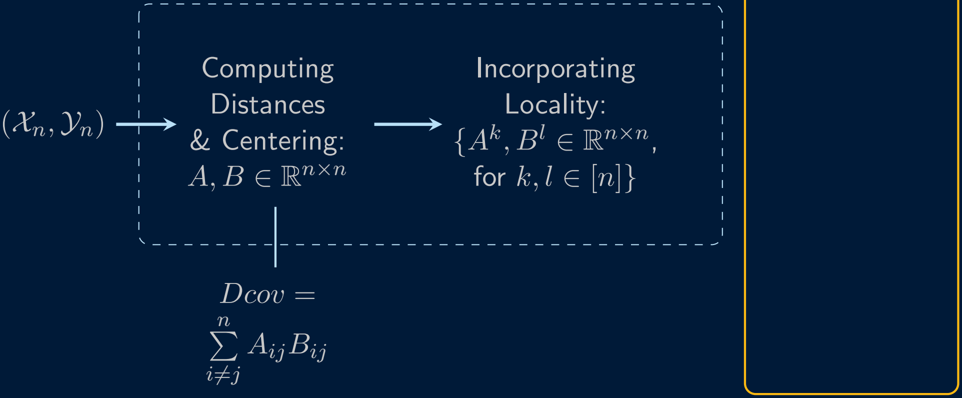

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$$Dcov^{k,l} = \sum_{i\neq j}^{n} A^k_{ij} B^l_{ij} - \sum_{i\neq j}^{n} A^k_{ij} \sum_{i\neq j}^{n} B^l_{ij}$$

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P-value by Permutation Test

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Centering: Then we center $\tilde{A}$ and $\tilde{B}$ by columns, with the diagonals excluded:

$$A_{ij} = \begin{cases} \tilde{A}_{ij} - \frac{1}{n-1}\sum_{s=1}^{n} \tilde{A}_{sj}, & \text{if } i \neq j, \\ 0, & \text{if } i = j; \end{cases} \tag{1}$$

similarly for B.

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Ranking: Define $\{R^A_{ij}\}$ as the "rank" of x_i relative to x_j, that is, $R^A_{ij} = k$ if x_i is the k^{th} closest point (or "neighbor") to x_j, as determined by ranking the set $\{\tilde{A}_{1j}, \tilde{A}_{2j}, \ldots, \tilde{A}_{nj}\}$ by ascending order. Similarly define R^B_{ij} for the y's.

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For any $(k, l) \in [n]^2$, define the rank truncated matrices A^k, B^l, and the joint distance matrix C^{kl} as

$$A^k_{ij} = A_{ij}\boldsymbol{I}(R^A_{ij} \leq k),$$
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When ties occur, minimal rank is recommended, e.g., if Y only takes two value, R^B_{ij} takes value in $\{1, 2\}$ only. We assume no ties for each of presentation.

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$$\begin{aligned}
dCov^{k,l}(\mathcal{X}_n, \mathcal{Y}_n) &= \hat{E}(A^k \circ B^{l'}) - \hat{E}(A^k)\hat{E}(B^l), \\
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There are a maximum of n^2 different local correlations. At $k = l = n$, $dCorr^{kl}(\mathcal{X}_n, \mathcal{Y}_n)$ equals the "global" distance correlation $dCorr(\mathcal{X}_n, \mathcal{Y}_n)$ by *Szekely et al.(2007)*.

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Instead, we take a smoothed maximum, by finding a connected region in the local correlation map with significant local correlatons – if such a region exists, use the maximum within the region.

Smoothed Maximum

Pick a threshold $\tau \geq 0$ (we choose by an approximate null distribution of $Dcorr$, which is symmetric beta and converges to 0 as $n \rightarrow \infty$), compute the set

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Permutation Test

To get a p-value by MGC for any given data, we utilize the permutation test: randomly permute index the second data set for r times, compute the permuted MGC statistic for each, and compute the percentage that the original MGC is no larger than the permuted MGC statistic, and take it as the p-value.

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This is a standard nonparametric testing procedure employed by Mantel, Dcorr, HHG, HSIC, where the null distribution of the dependency measure cannot be exactly derived.

Computation Complexity

Distance computation takes $\mathcal{O}(n^2 \max(p, q))$, centering takes $\mathcal{O}(n^2)$, ranking takes $\mathcal{O}(n^2 log(n))$, **all local correlations can be iteratively computed in** $\mathcal{O}(n^2)$, and the smoothing step takes $\mathcal{O}(n^2)$.

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There are a number of ways to speed up the method for big data: faster implementation when $p = q = 1$, null distribution approximation by subsampling and spectral embedding.

Examples

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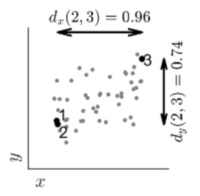

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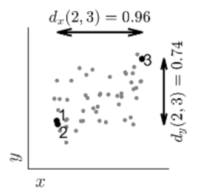

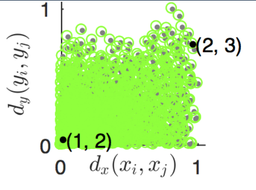

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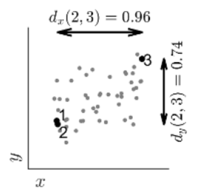

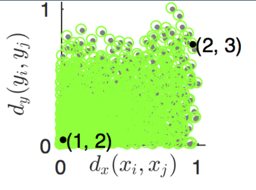

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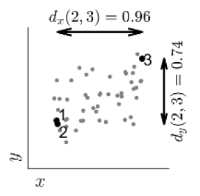

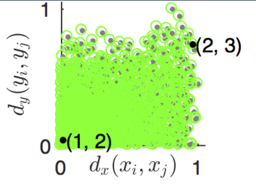

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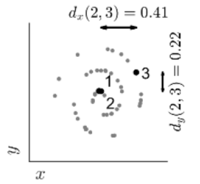

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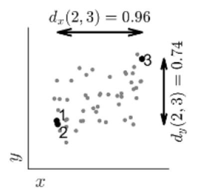

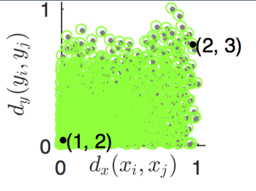

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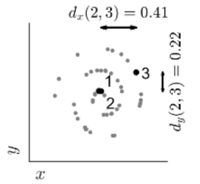
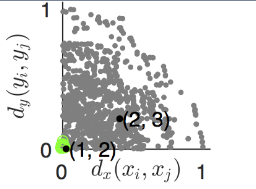
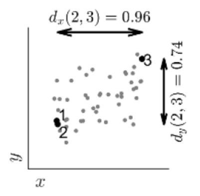
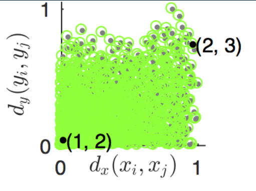




Examples





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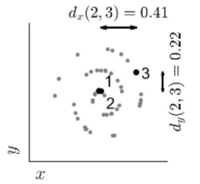

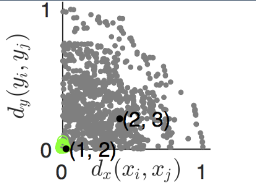

$Dcorr(\mathcal{X}_n, \mathcal{Y}_n) = 0.01$
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Theoretical Properties

Basic Properties of Sample MGC

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5. 1-Linear: $c(\mathcal{X}_n, \mathcal{Y}_n) = 1$ *if and only if* F_X *is non-degenerate and* (X, uY) *are dependent via an isometry for some non-zero constant* u.

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Defining Population MGC

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Normalizing and taking a smoothed maximum yield population MGC.

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Can be similarly adapted to the local correlation.

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The last three properties also hold for any local correlation by $(\rho_k, \rho_l) = (\frac{k-1}{n-1}, \frac{l-1}{n-1})$.

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If the relationship is linear (or with independent noise), the global scale is always optimal and $MGC(X, Y) = Dcorr(X, Y)$.

Conversely, the optimal scale being local, i.e., $MGC(X, Y) > Dcorr(X, Y)$, implies a non-linear relationship.

MGC is applicable to similarity / kernel matrix

Theorem 6 (Transforming kernel to distance)

Given any characteristic kernel function $k(\cdot,\cdot)$, define an induced semi-metric as

$$d(\cdot,\cdot) = 1 - k(\cdot,\cdot)/\max\{k(\cdot,\cdot)\}.$$

Then $d(\cdot,\cdot)$ is of strong negative type, and the resulting MGC is universally consistent.

Namely, given a sample kernel matrices $K_{n\times n}$, one can compute the induced distance matrix by

$$D = J - K/\max_{i,j\in[1,\ldots,n]^2}\{K(i,j)\},$$

and apply MGC to the induced distance matrices.

Simulations and Experiments

Visualizations of 20 Simulation Settings

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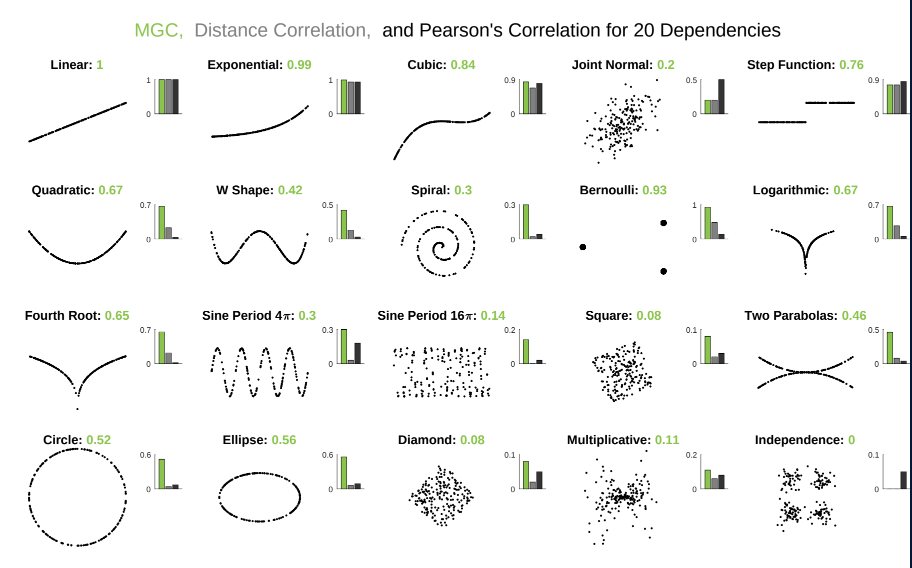

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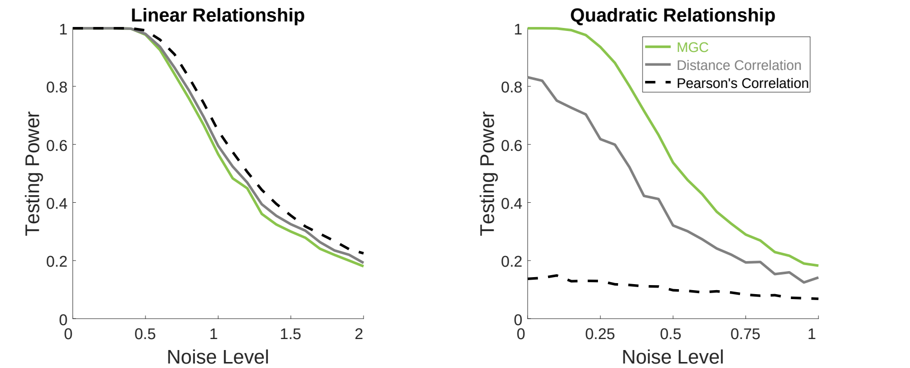

$$n = 30, p = q = 1,$$
$$X \sim Uniform(-1, 1),$$
$$\epsilon \sim Normal(0, noise),$$
$Y = X + \epsilon$ and $Y = X^2 + \epsilon.$

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We consider univariate (1D) and multivariate (10D) cases.

Median Size Table

Testing Methods	1D Lin	1D Non-Lin	10D Lin	10D Non-Lin
MGC	**50**	**90**	60	**165**
Dcorr	**50**	250	60	515
Pearson / RV / CCA	**50**	>1000	**50**	>1000
HHG	70	**90**	100	315
HSIC	70	95	100	400
MIC	120	180	n/a	n/a

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Adjusted for multiple testing, MGC uniquely revealed one particular protein, neurogranin, which is exclusively expressed in brain tissue among normal tissues and has not been linked with any other cancer type.

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   - Any dissimilarity / similarity / kernel matrix.

Advantages of MGC

1. Performant under any joint distribution of finite second moments:
   - Equals 0 asymptotically if and only if independence.
   - Amplify the dependency signal while mostly avoiding the sample bias.
   - Superior finite-sample performance over all benchmarks, against linear / nonlinear / noisy / high-dimensional relationships.
2. It works for:
   - Low- and high-dimensional data.
   - Euclidean and structured data (e.g., images, networks, shapes).
   - Any dissimilarity / similarity / kernel matrix.
3. Intuitive to understand and efficient to implement in $\mathcal{O}(n^2 logn)$.

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