

Dependency Discovery via Multiscale Graph Correlation

Cencheng Shen

University of Delaware

*Collaborators: Joshua T. Vogelstein, Carey E. Priebe, Shangsi Wang, Youjin Lee,
Mauro Maggioni, Qing Wang, Alex Badea.*

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

Motivation

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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

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

$$H_0 : F_{XY} = F_X F_Y,$$

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Without loss of generality, we shall assume F_{XY} has finite second moments.

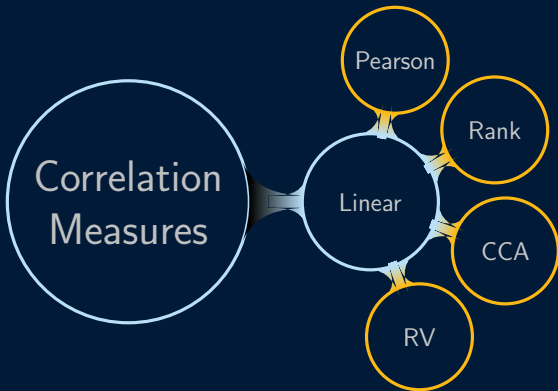


Correlation
Measures

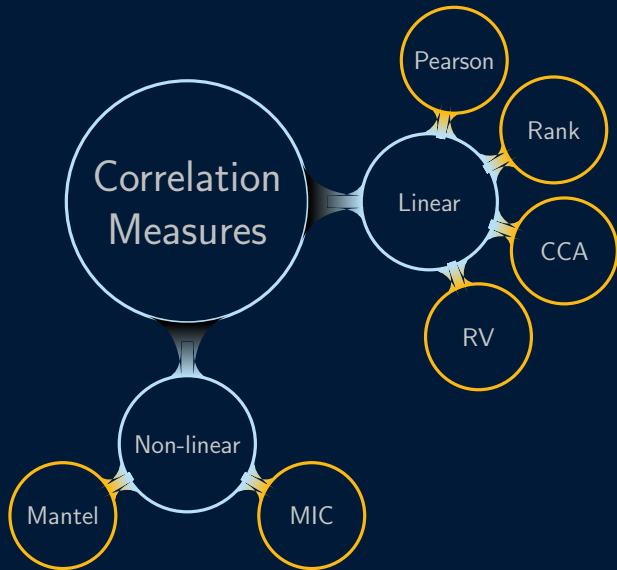


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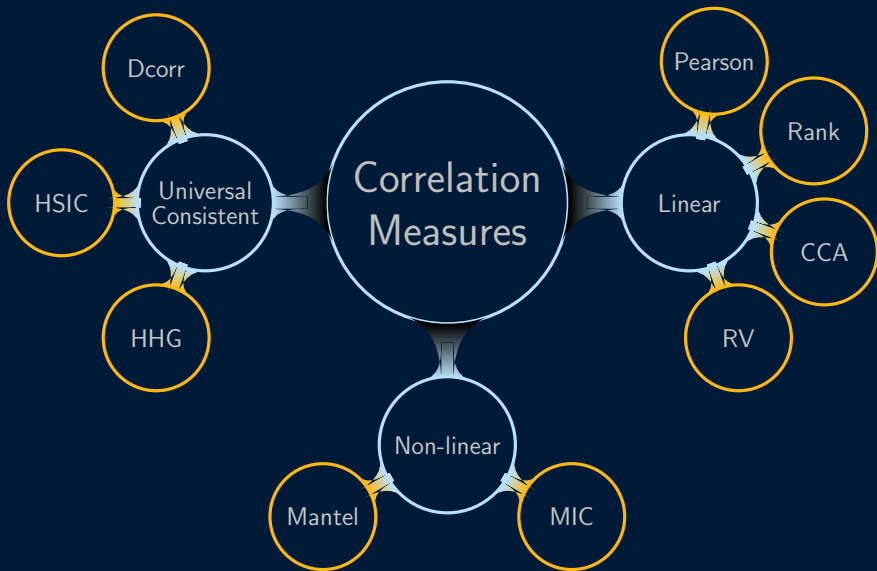
Benchmarks



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

Methodology

Flowchart of MGC

$(\mathcal{X}_n, \mathcal{Y}_n)$



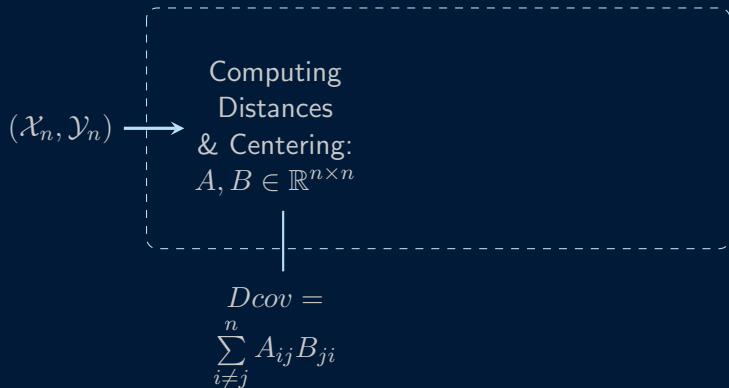
```
graph LR; A["(X_n, Y_n)"] --> B["Dashed Box"]; B --> C["Solid Box"];
```

Flowchart of MGC

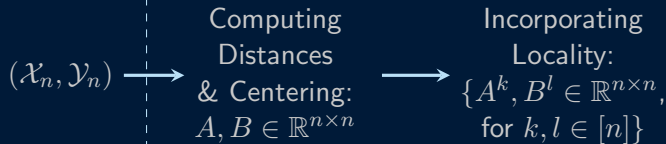
$(\mathcal{X}_n, \mathcal{Y}_n)$ → Computing
Distances
& Centering:
 $A, B \in \mathbb{R}^{n \times n}$

The flowchart illustrates the initial step of the MGC process. It starts with the input data $(\mathcal{X}_n, \mathcal{Y}_n)$, which is processed through a dashed box containing the text 'Computing Distances & Centering: $A, B \in \mathbb{R}^{n \times n}$ '. An arrow points from the input to this box. To the right of this box is a large, empty yellow rounded rectangle, which likely represents the subsequent steps in the flowchart.

Flowchart of MGC

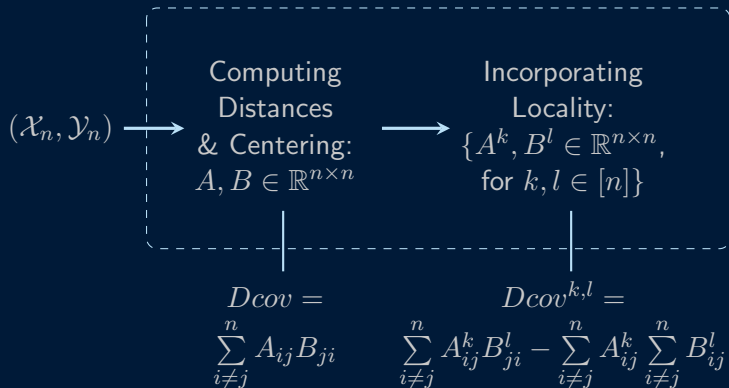


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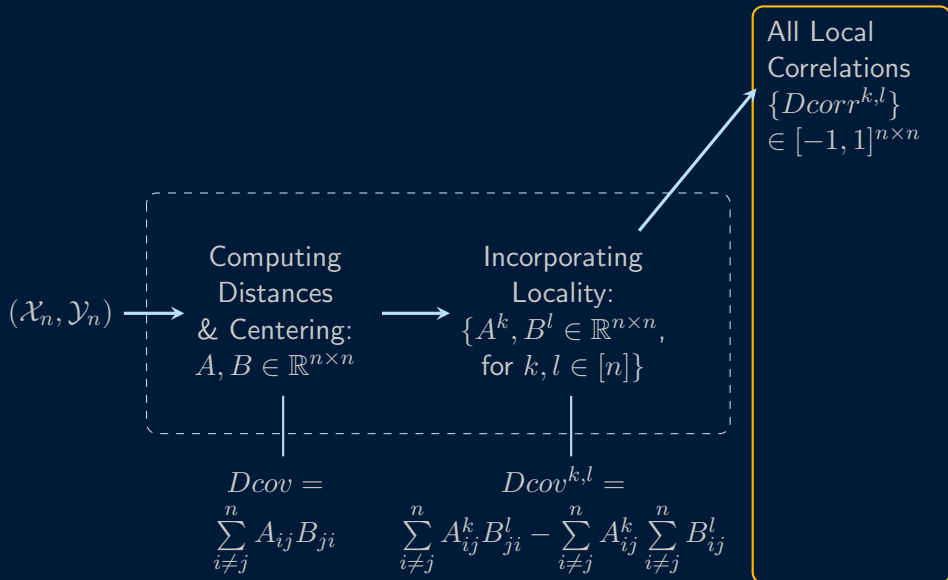


$$Dcov = \sum_{i \neq j}^n A_{ij} B_{ji}$$

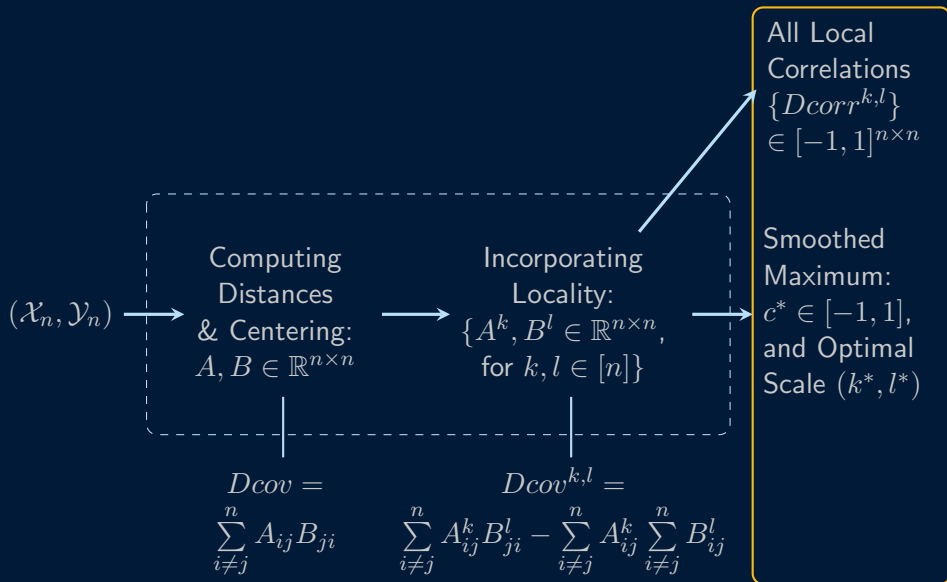
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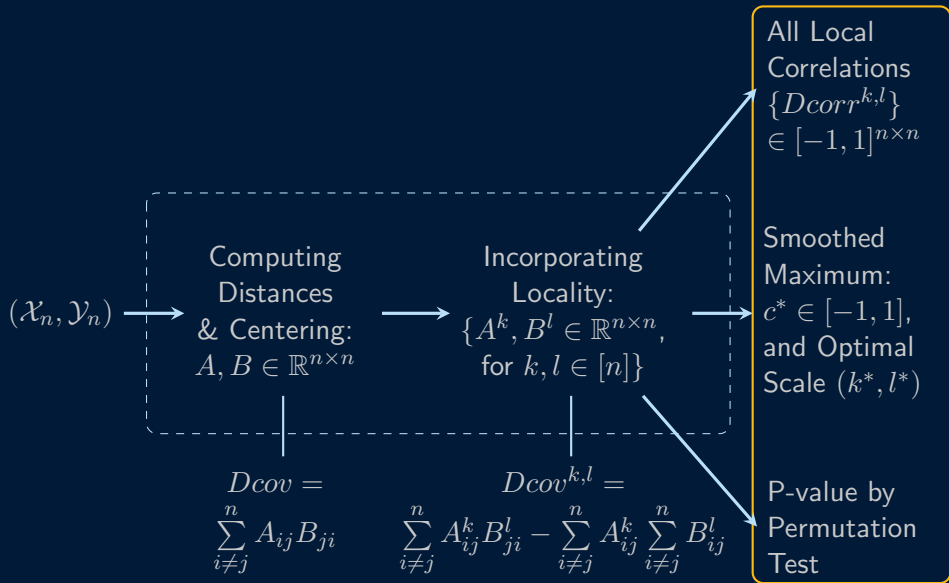
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Computing Distance and Centering

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

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

similarly for B .

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Ranking: Define $\{R_{ij}^A\}$ as the “rank” of x_i relative to x_j , that is, $R_{ij}^A = k$ if x_i is the k^{th} closest point (or “neighbor”) to x_j , as determined by ranking the set $\{\tilde{A}_{1j}, \tilde{A}_{2j}, \dots, \tilde{A}_{nj}\}$ by ascending order. Similarly define R_{ij}^B 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

$$A_{ij}^k = A_{ij} \mathbf{I}(R_{ij}^A \leq k),$$

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When ties occur, minimal rank is recommended, e.g., if Y only takes two value, R_{ij}^B takes value in $\{1, 2\}$ only. We assume no ties for each of presentation.

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A Family of Local Correlations: Let \circ denote the entry-wise product, $\hat{E}(\cdot) = \frac{1}{n(n-1)} \sum_{i \neq j}^n (\cdot)$ denote the diagonal-excluded sample mean of a square matrix, then the sample local covariance, variance, and correlation are defined as:

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for $k, l = 1, \dots, n$. If $dVar^k(\mathcal{X}_n) \cdot dVar^l(\mathcal{Y}_n) \leq 0$, we set $dCorr^{kl}(\mathcal{X}_n, \mathcal{Y}_n) = 0$ instead.

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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 correlations – 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 D_{corr} , which is symmetric beta and converges to 0 as $n \rightarrow \infty$), compute the set

$$\{(k, l) \text{ such that } D_{corr}^{k,l}(\mathcal{X}_n, \mathcal{Y}_n) > \max\{\tau, D_{corr}(\mathcal{X}_n, \mathcal{Y}_n)\}\},$$

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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 of the second data set for r times, compute the permuted MGC statistic $c^*(\mathcal{X}_n, \mathcal{Y}_n^\pi)$ for each permutation π , and estimate

$$\text{Prob}(c^*(\mathcal{X}_n, \mathcal{Y}_n) > c^*(\mathcal{X}_n, \mathcal{Y}_n^\pi))$$

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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 $\mathcal{O}(n^2)$**
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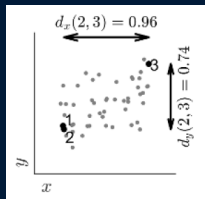
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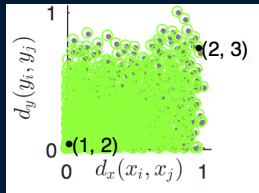
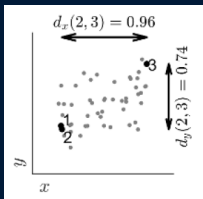
There are a number of ways to speed up the method for big data: faster implementation when $p = q = 1$, null distribution approximation by subsampling and spectral embedding.

Examples

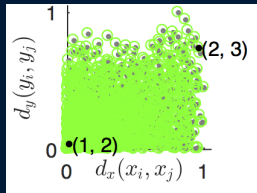
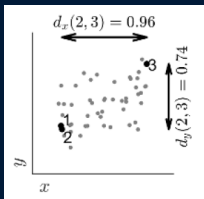
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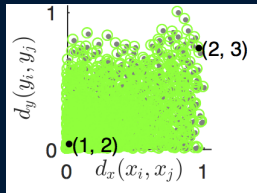
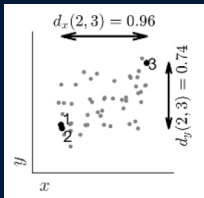
Examples



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$$MGC(\mathcal{X}_n, \mathcal{Y}_n) = 0.15$$

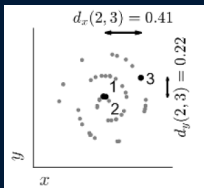
p-vals: < 0.001

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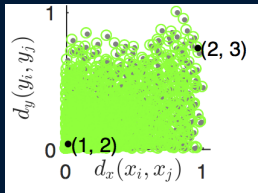
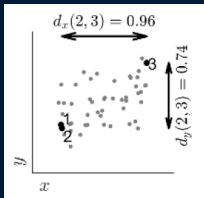


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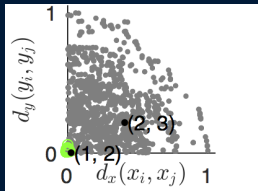
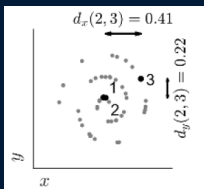


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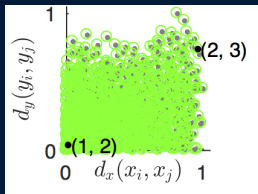
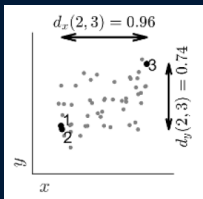


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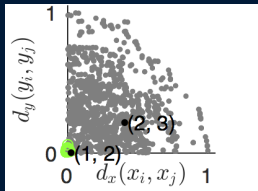
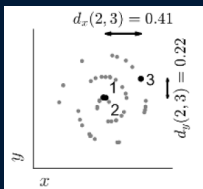


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p-vals: < 0.001



$$Dcorr(\mathcal{X}_n, \mathcal{Y}_n) = 0.01$$
$$MGC(\mathcal{X}_n, \mathcal{Y}_n) = 0.13$$

p-vals: 0.3 vs < 0.001

Theoretical Properties

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4. *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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Normalizing and taking a smoothed maximum yield population MGC.

Sample to Population

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Alternatively, the population version can be equivalently defined via characteristic functions of F_{XY} :

$$D_{cov}^{\rho_k=1, \rho_l=1}(X, Y) = \int_{t,s} |g_{XY}(t, s) - g_X(t)g_Y(s)|^2 dw(t, s)$$

with respect to a non-negative weight function $w(t, s)$ on $(t, s) \in \mathbb{R}^p \times \mathbb{R}^q$.

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$$w(t, s) = (d_p d_q |t|^{1+p} |s|^{1+q})^{-1},$$

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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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Theorem 5 (Optimal Scale of MGC Implies Geometry Structure)

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

Conversely, the optimal scale being local, i.e., $c^(X, Y) > Dcorr(X, Y)$, 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

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

and apply MGC to the induced distance matrices.

Simulations and Experiments

Visualizations of 20 Simulation Settings

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MGC, Distance Correlation, and Pearson's Correlation for 20 Dependencies

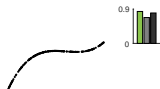
Linear: 1



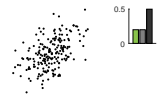
Exponential: 0.99



Cubic: 0.84



Joint Normal: 0.2



Step Function: 0.76



Quadratic: 0.67



W Shape: 0.42



Spiral: 0.3



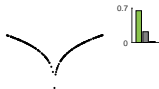
Bernoulli: 0.93



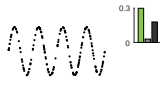
Logarithmic: 0.67



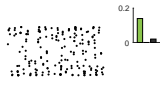
Fourth Root: 0.65



Sine Period 4π : 0.3



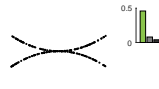
Sine Period 16π : 0.14



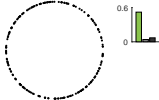
Square: 0.08



Two Parabolas: 0.46



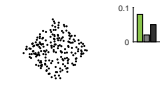
Circle: 0.52



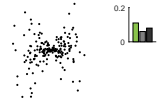
Ellipse: 0.56



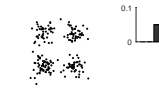
Diamond: 0.08



Multiplicative: 0.11



Independence: 0



Evaluation Criterion

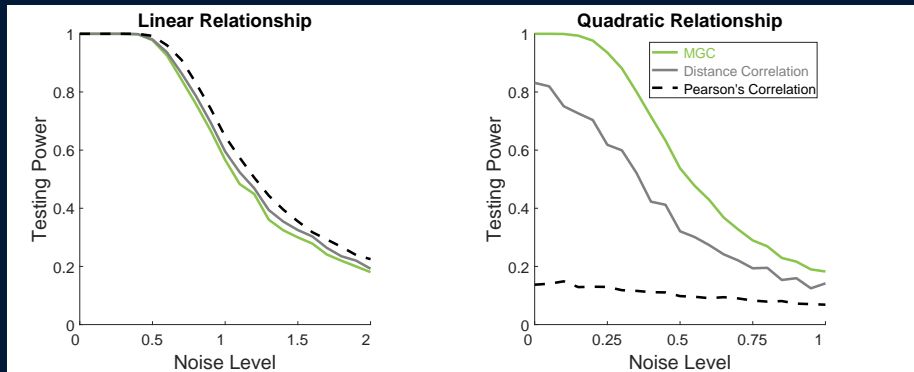
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Evaluation Criterion

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- Required sample size $N_{\alpha,\beta}(c)$ to achieve a power of β at type 1 error level α using a statistic c .

Testing Power: Linear vs Nonlinear

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$$\begin{aligned}n &= 30, p = q = 1, \\ X &\sim \text{Uniform}(-1, 1), \\ \epsilon &\sim \text{Normal}(0, \text{noise}), \\ Y &= X + \epsilon \text{ and } Y = X^2 + \epsilon.\end{aligned}$$

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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

Signal Subgraph via MGC

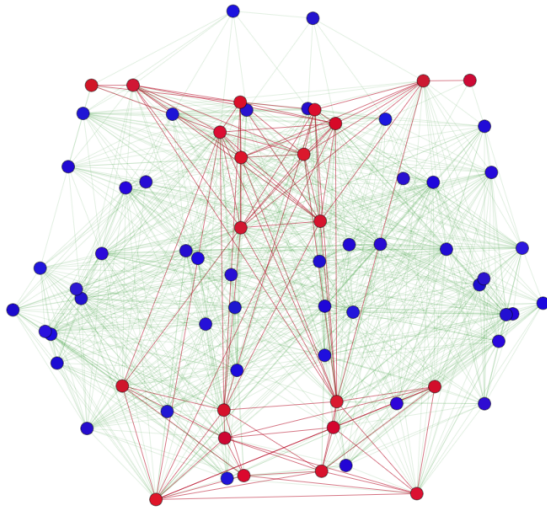
Signal Subgraph via MGC

We consider predicting the site and sex based on functional magnetic resonance image (fMRI) graphs. Two datasets used are SWU4 and HNU1, which have 467 and 300 samples respectively.

Each sample is an fMRI scan registered to the MNI152 template using the Desikan atlas, which has 70 regions.

We used an iterative screening method (similar to backward selection) via MGC from [Wang *et al.*(2018)] to extract signal subgraph (in this case brain regions) that are most dependent with sites and sex, and also run leave-one-out cross validation with K -Nearest Neighbor classifier to verify the results.

Desikan Atlas With Site Difference Highlighted



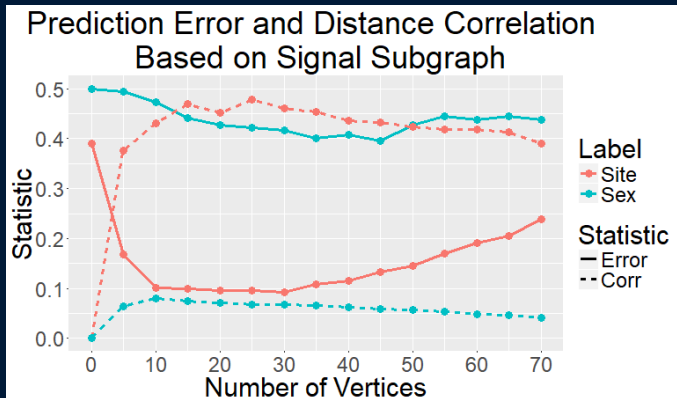


Figure: A total of 22 regions are recognized for site difference, which maximizes the MGC statistic and almost minimizes the leave-one-out cross validation error. It is no longer the case for sex, for which neither the MGC nor the error are too significant for any size of subgraph.

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They made MGC advantageous in theory and practice.

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3. Intuitive to understand and efficient to implement in $\mathcal{O}(n^2 \log n)$.

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