Dependency Discovery via Multiscale Graph Correlation

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Overview

1. Motivation

2. Methodology

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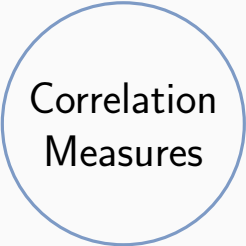$$(x_i, y_i) \overset{i.i.d.}{\sim} F_{XY}, \quad i = 1, \ldots, n$$

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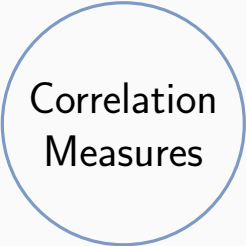$$H_A : F_{XY} \neq F_X F_Y.$$

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

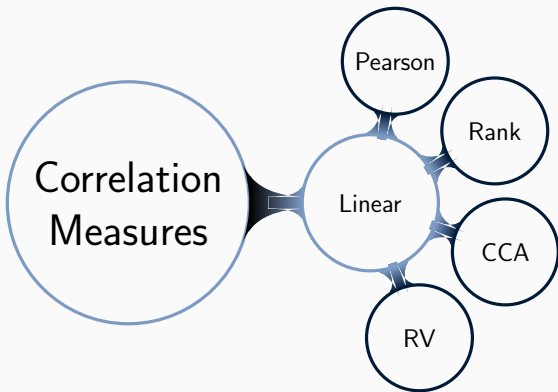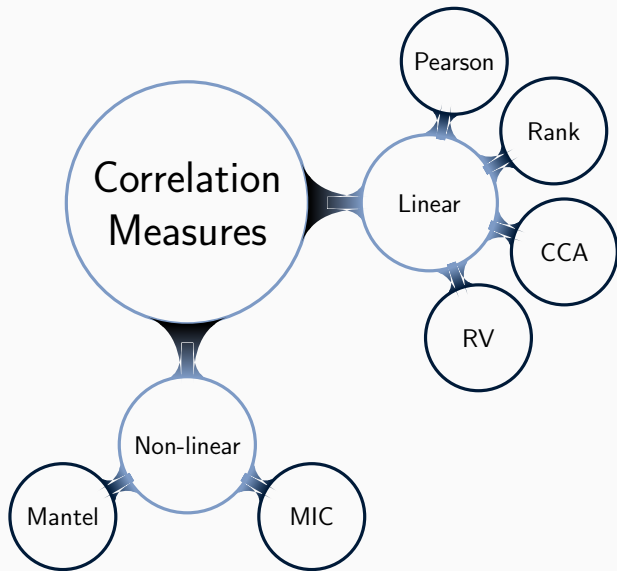# Benchmarks

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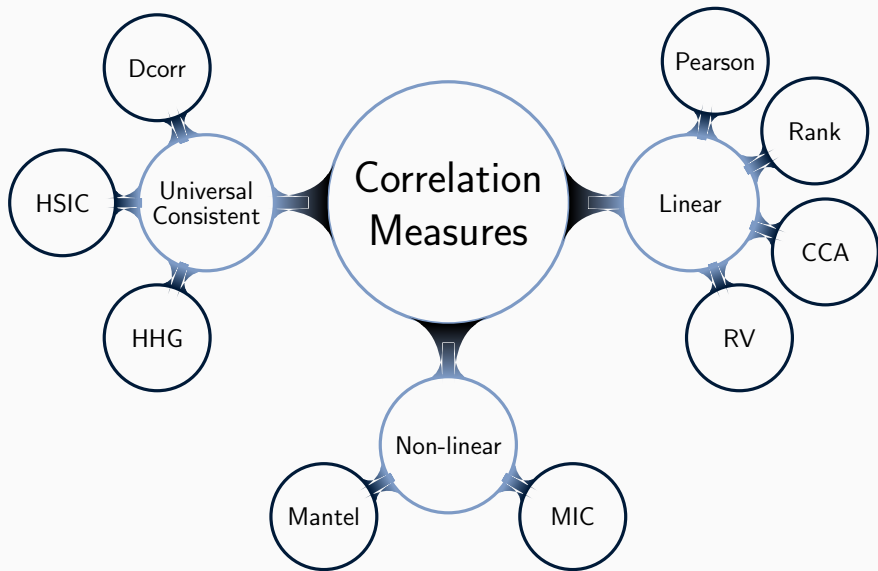
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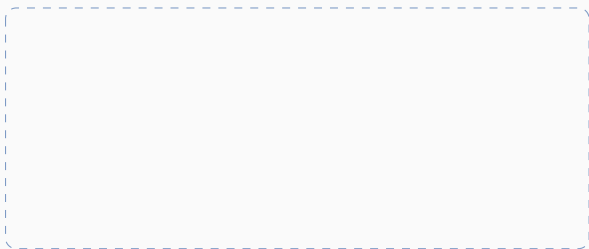
To that end, we propose the **multiscale graph correlation** in [*Shen et al.(2018)*].

Methodology

Flowchart of MGC

$$d(\cdot, \cdot) : \mathbb{R}^{p+q} \times \mathbb{R}^{p+q} \to \mathbb{R}$$

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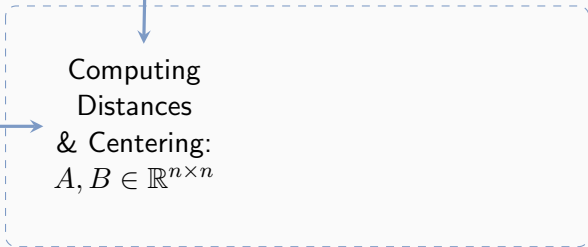
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$$Dcov^{k,l} = \sum_{i,j=1}^{n} A_{ij}^k B_{ji}^l - \sum_{i,j=1}^{n} A_{ij}^k \sum_{i,j=1}^{n} B_{ij}^l$$

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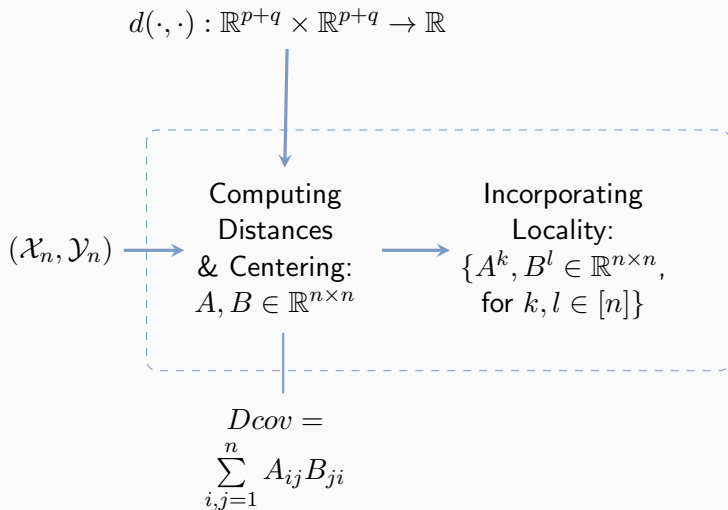
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Input: $\mathcal{X}_n = [x_1, \ldots, x_n]$ as the data matrix with each column representing one sample observation, and similarly $\mathcal{Y}_n$. A distance or kernel function $d(\cdot, \cdot) : \mathbb{R}^{p+q} \times \mathbb{R}^{p+q} \to \mathbb{R}$, by default the Euclidean distance.

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Distance Computation: Let $\tilde{A}$ be the $n \times n$ Euclidean distance matrices of $\mathcal{X}_n$:

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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 $\{R_{ij}^A\}$ as the "rank" of x_i relative to x_j, that is, $R_{ij}^A = k$ if x_i is the kth 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_{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

$$A_{ij}^k = A_{ij} \boldsymbol{I}(R_{ij}^A \leq k),$$
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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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for $k, l = 1, \ldots, n$. If $dVar^k(\mathcal{X}_n) \cdot dVar^l(\mathcal{X}_n) \leq 0$, we set $dCorr^{kl}(\mathcal{X}_n, \mathcal{Y}_n) = 0$ instead.

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

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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But directly taking the maximum local correlation

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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 $n \to \infty$), compute the set

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

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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

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

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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 $\mathcal{O}(n^2 log(n))$
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On a standard PC with Matlab, testing $n = 1000$ takes about 1 minutes.
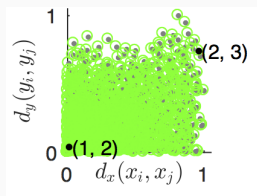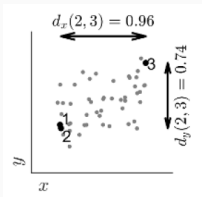
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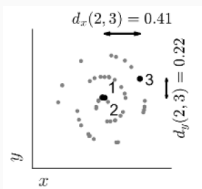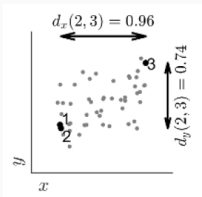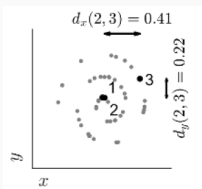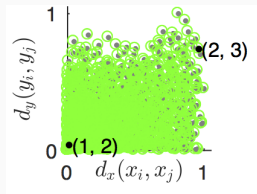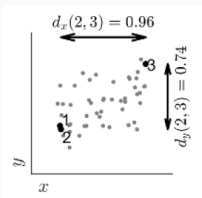
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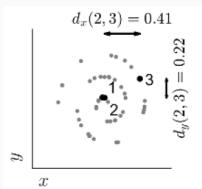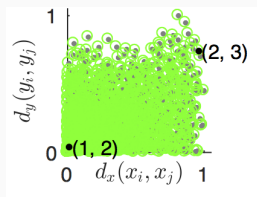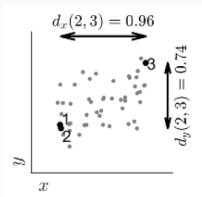# Examples

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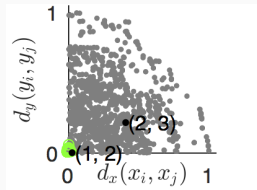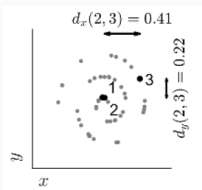$MGC(\mathcal{X}_n, \mathcal{Y}_n) = 0.15$
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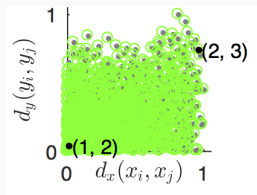

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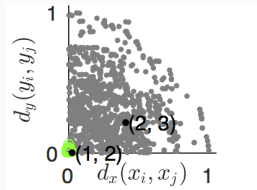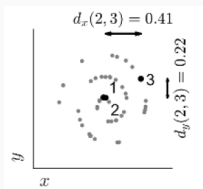
$Dcorr(\mathcal{X}_n, \mathcal{Y}_n) = 0.01$
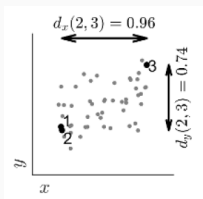$MGC(\mathcal{X}_n, \mathcal{Y}_n) = 0.13$
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MGC is applicable to similarity / kernel matrix

Theorem 1 (Transforming kernel to distance)

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

$$d(i, j) = 1 - k(i, j) / \max_{i, j = 1, \ldots, n} \{k(i, j)\}.$$

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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.

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When the metric is of strong negative type or the kernel is characteristic, $c^*(X, Y) = 0$ if and only if independence. For arbitrary metric or kernel, the if direction is still true but not the only if direction.

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

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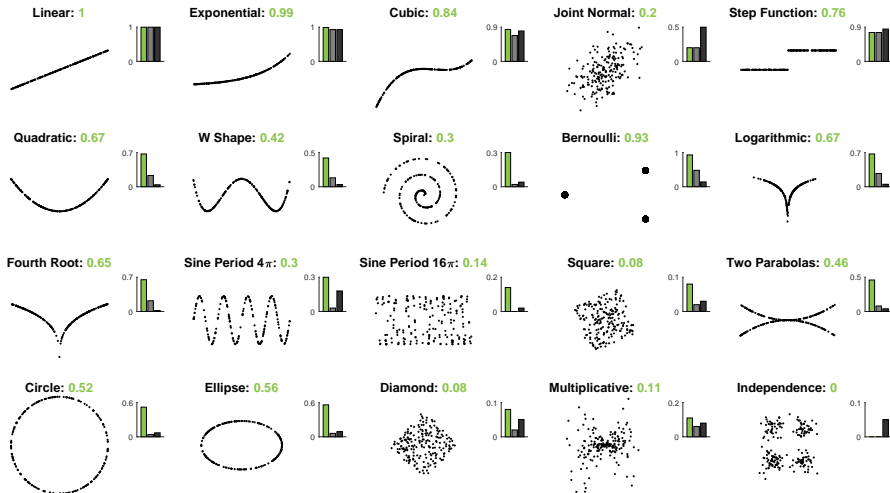
Conversely, the optimal scale being local, i.e., $c^*(X, Y) > Dcorr(X, Y)$, implies a non-linear relationship.

Simulations and Experiments

Visualizations of 20 Simulation Settings

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

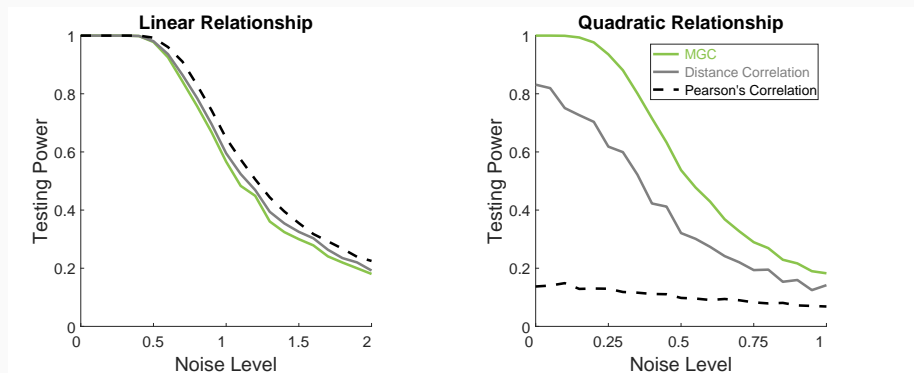# Testing Power: Linear vs Nonlinear

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

Required Sample Size

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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

Extracting Signal Brain Region from fMRI images

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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 altas, which has 70 regions. They are transformed to graph structure using the NeuroDatas MRI Graphs pipeline [1].

We compute the dependency measure between each brain region and sex. Rank the brain region via magnitude of the measure, and include all significant ($p - val < 0.05$) brain regions. Then run leave-one-out cross validation with K-Nearest Neighbor classifier to verify the results. Repeat it for the site property.

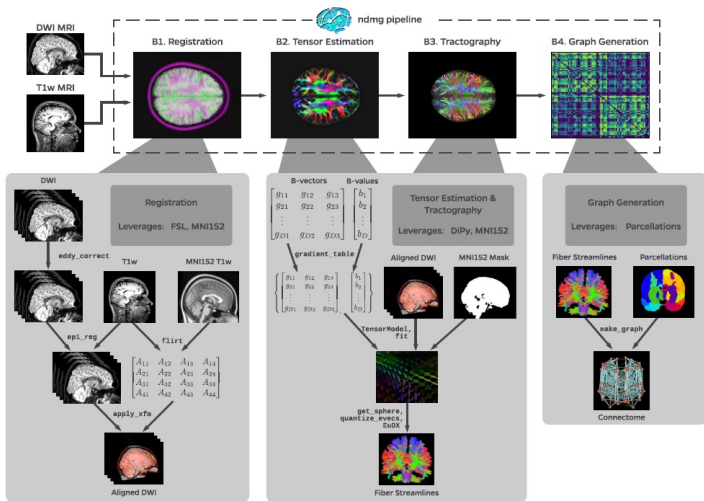[1] https://github.com/neurodata/ndmg

Figure 7: **ndmg detailed pipeline**. The NDMG pipeline consists of 4 main steps: Registration (**B1**), Tensor Estimation (**B2**), Tractography (**B3**), and Graph Generation (**B4**). Each of these sections leverages pubicly available tools and data to robustly produce the desired derivative of each step. Alongside derivative production, NDMG produces QA figures at each stage, as can be seen in **B1-4**, that enable qualitative evaluation of the pipeline's performance.

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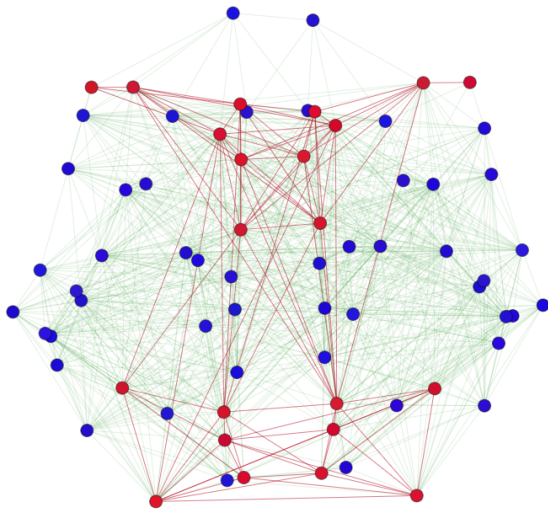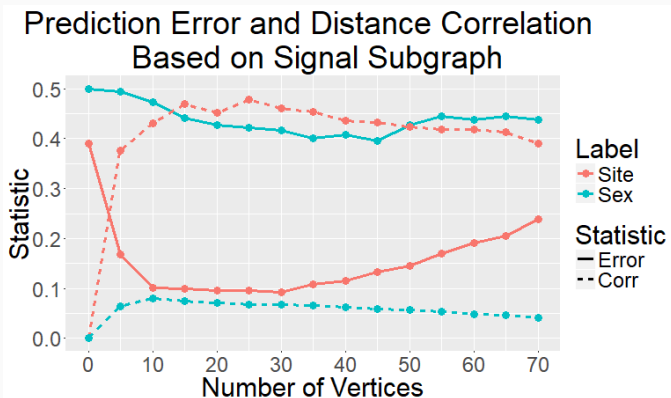
Figure: A total of 22 regions are recognized for site difference, which maximizes the MGC statistic and almost minimizes the leave-one-out cross validation error. It is no longer the case for sex, for which neither the MGC nor the error are too significant for any size of subgraph.

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- Using a proper distance or kernel ensures the universal consistency.
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- The optimal scale gives information on linear vs nonlinear dependency.
- It can be used in a variety of applications to replace the Pearson's correlation.

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

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Thus when n is small (say less than a few thousands), MGC is the better choice; whereas distance correlation can better handle extremely large data.

Open Source Packages

Python package in https://github.com/neurodata/mgcpy/ and
forthcoming in scikit-learn

R package in https://github.com/neurodata/MGC/ and CRAN

Matlab code https://github.com/neurodata/mgc-matlab

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