

Dependency Discovery via Multiscale Generalized Correlation

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Acknowledgment: NSF DMS, DARPA SIMPLEX.

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- Are they related?
- How are they related?

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

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

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

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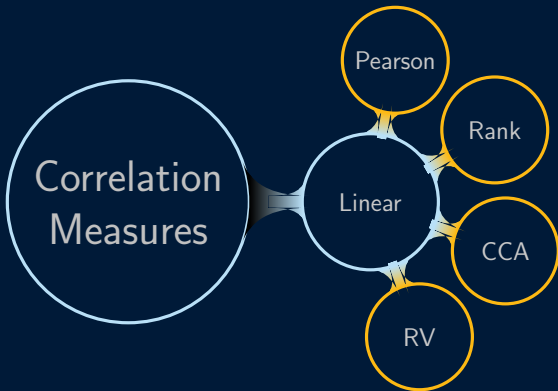
Without loss of generality, we shall assume F_{XY} has finite second moments.

Benchmarks

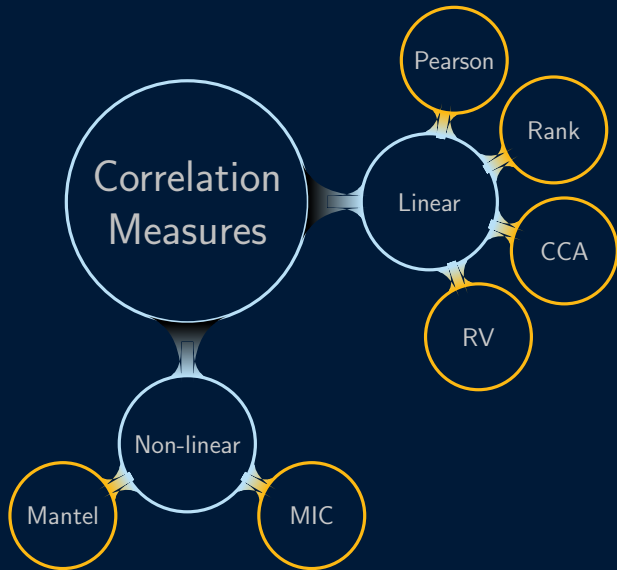


Correlation
Measures

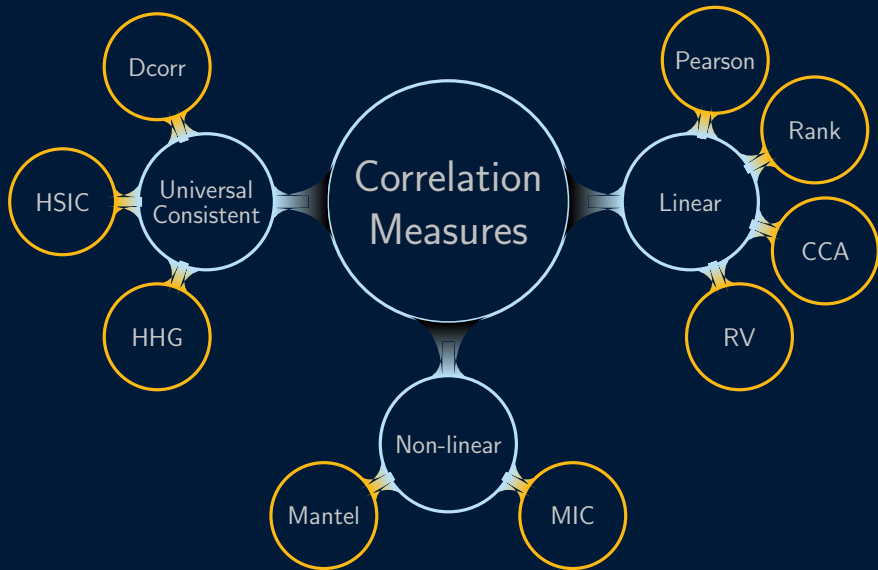
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To that end, we propose the **multiscale generalized correlation** in [*Shen et al.(2017a)*][1].

Overview

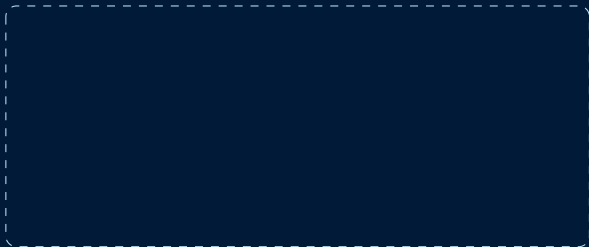
1. Illustration
2. Experiments
3. Theory
4. Summary

Illustration

Introducing MGC

Introducing MGC

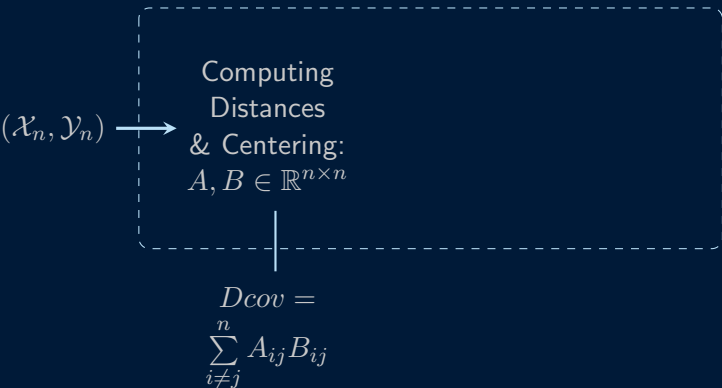
$(\mathcal{X}_n, \mathcal{Y}_n)$



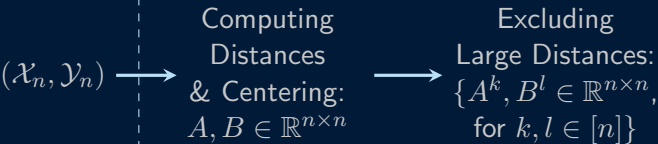
Introducing MGC

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

Introducing MGC

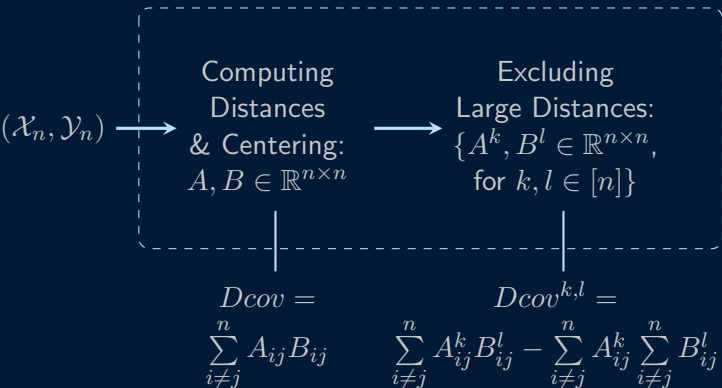


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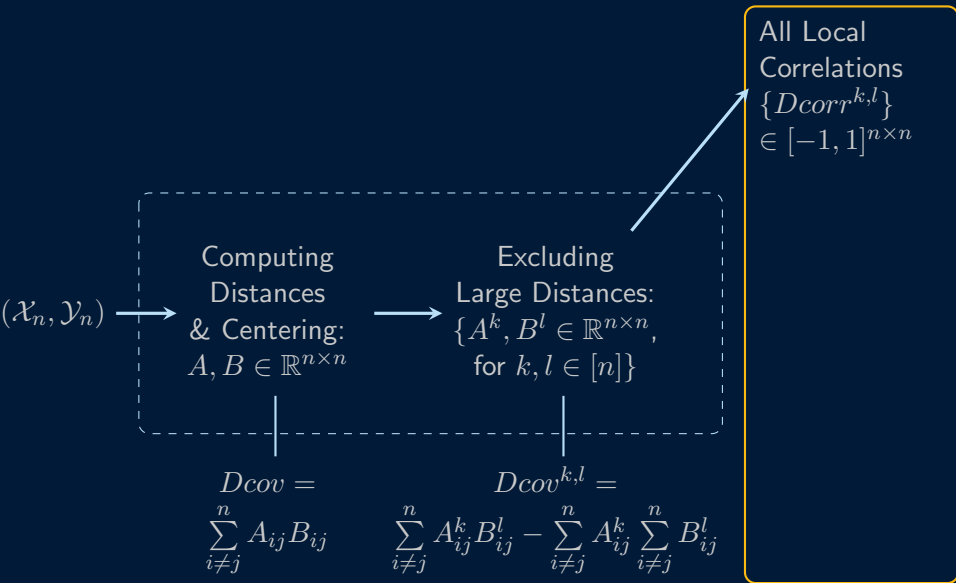


$$D_{cov} = \sum_{i \neq j}^n A_{ij} B_{ij}$$

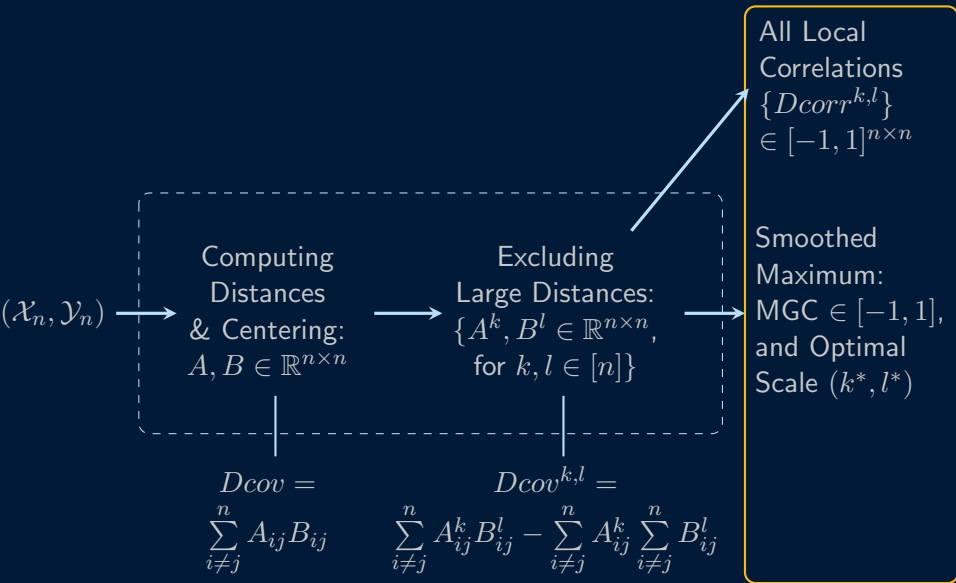
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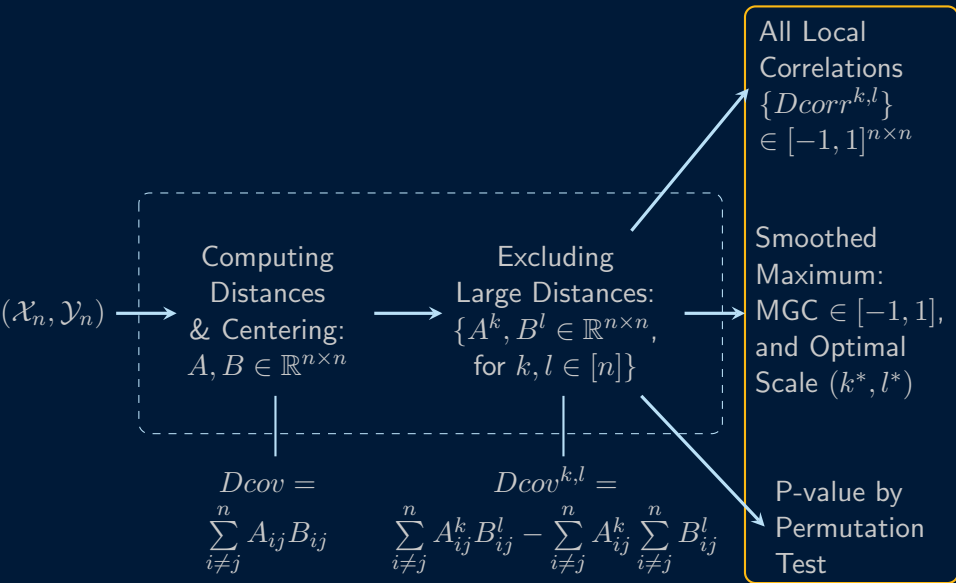
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Direct Maximum

Direct Maximum

Directly taking the maximum local correlation

$$\max_{(k,l) \in [n]^2} \{Dcorr^{k,l}(\mathcal{X}_n, \mathcal{Y}_n)\}$$

will yield a biased statistic under independence, i.e., the maximum is always larger than 0 in expectation even under independent relationship!

Smoothed Maximum

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Pick a threshold $\tau \geq 0$, 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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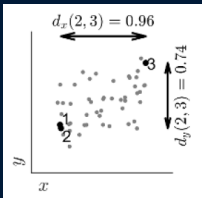
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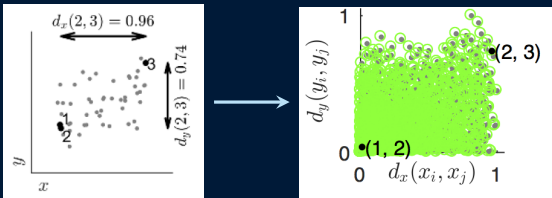
It is a critical step for both the finite-sample performance and certain theoretical properties of MGC.

Examples

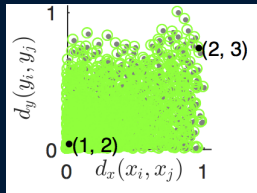
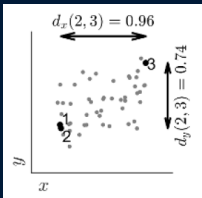
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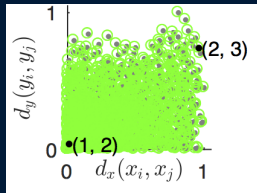
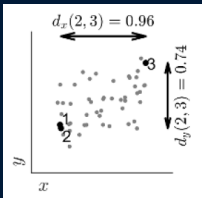
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$$Dcorr(\mathcal{X}_n, \mathcal{Y}_n) = 0.15$$
$$MGC(\mathcal{X}_n, \mathcal{Y}_n) = 0.15$$

p-vals: < 0.001

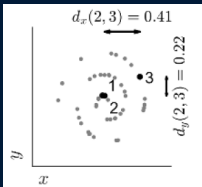
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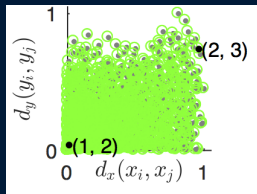
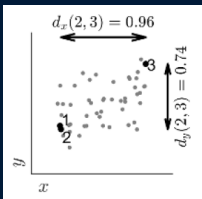
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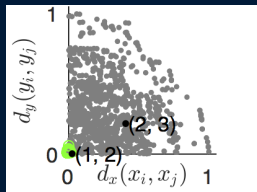
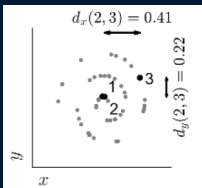
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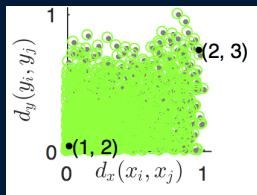
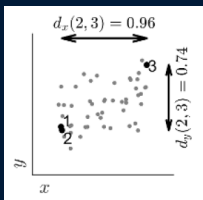
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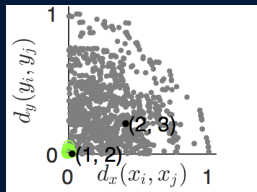
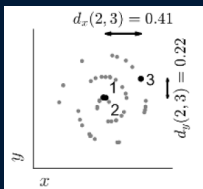
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$$Dcorr(\mathcal{X}_n, \mathcal{Y}_n) = 0.01$$

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

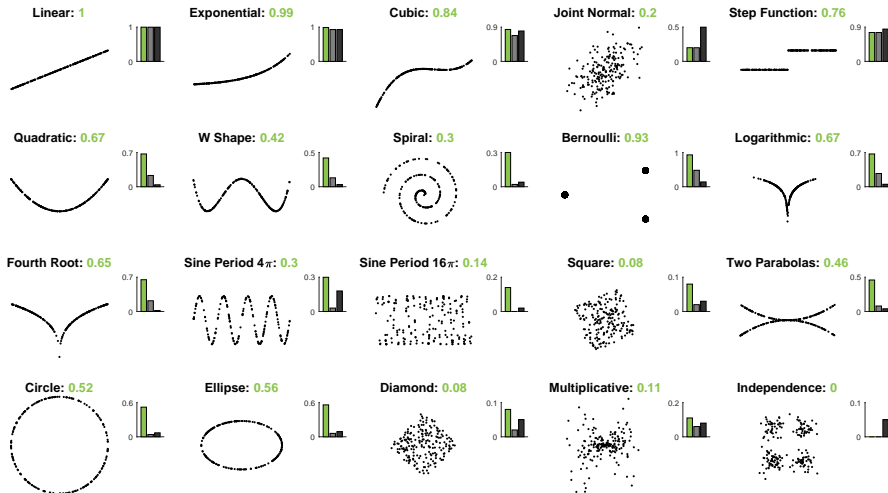
p-vals: 0.3 vs < 0.001

Experiments

Visualizations of 20 Simulation Settings

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



Evaluation Criterion

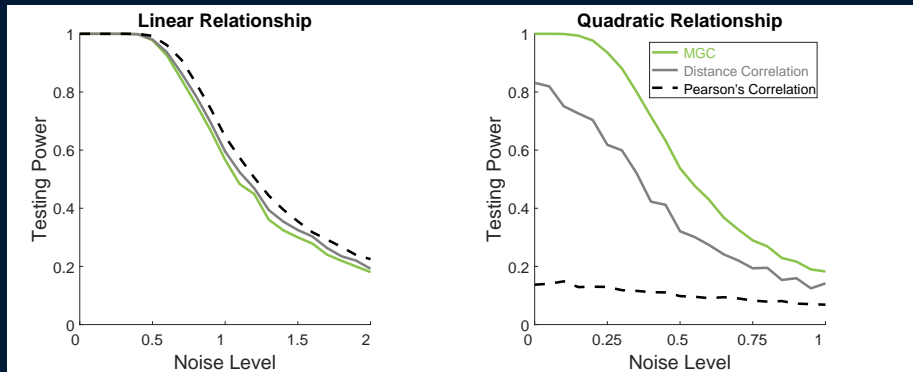
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- Required sample size $N_{\alpha,\beta}(c)$ to achieve a power of β at type 1 error level α using a statistic c .

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$$n = 30, p = q = 1,$$

$$X \sim \text{Uniform}(-1, 1),$$

$$\epsilon \sim \text{Normal}(0, \text{noise}),$$

$$Y = X + \epsilon \text{ and } Y = X^2 + \epsilon.$$

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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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Theory

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5. *0-Indep:* $c(\mathcal{X}_n, \mathcal{Y}_n) \xrightarrow{n \rightarrow \infty} 0$ if and only if independence.
6. *Consistency:* At any type 1 error level α , testing power $\beta(c(\mathcal{X}_n, \mathcal{Y}_n)) \xrightarrow{n \rightarrow \infty} 1$ against any dependent F_{XY} .

Defining Population MGC

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$$I_{X, X'}^{\rho_k} = I(\text{Prob}\{B(X, \|X' - X\|)\} \leq \rho_k)$$

$$I_{Y', Y}^{\rho_l} = I(\text{Prob}\{B(Y', \|Y - Y'\|)\} \leq \rho_l)$$

for $\rho_k, \rho_l \in [0, 1]$.

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Normalizing and taking a smoothed maximum yield population MGC.

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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)

For a positive definite kernel function $k(\cdot, \cdot)$, define an induced semi-metric as

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

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For any sample kernel matrices $K_{n \times n}$, one can transform it to a dissimilarity matrix by

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

and apply MGC / Dcorr to the transformed dissimilarity matrices.

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They made MGC advantageous in theory and practice.

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MGC shares the same intrinsic idea as in nonlinear embedding, random forest, multiple kernel learning, deep learning.

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