Dependency Discovery via Multiscale Graph Correlation

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Acknowledgment: NSF DMS, DARPA SIMPLEX.

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

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

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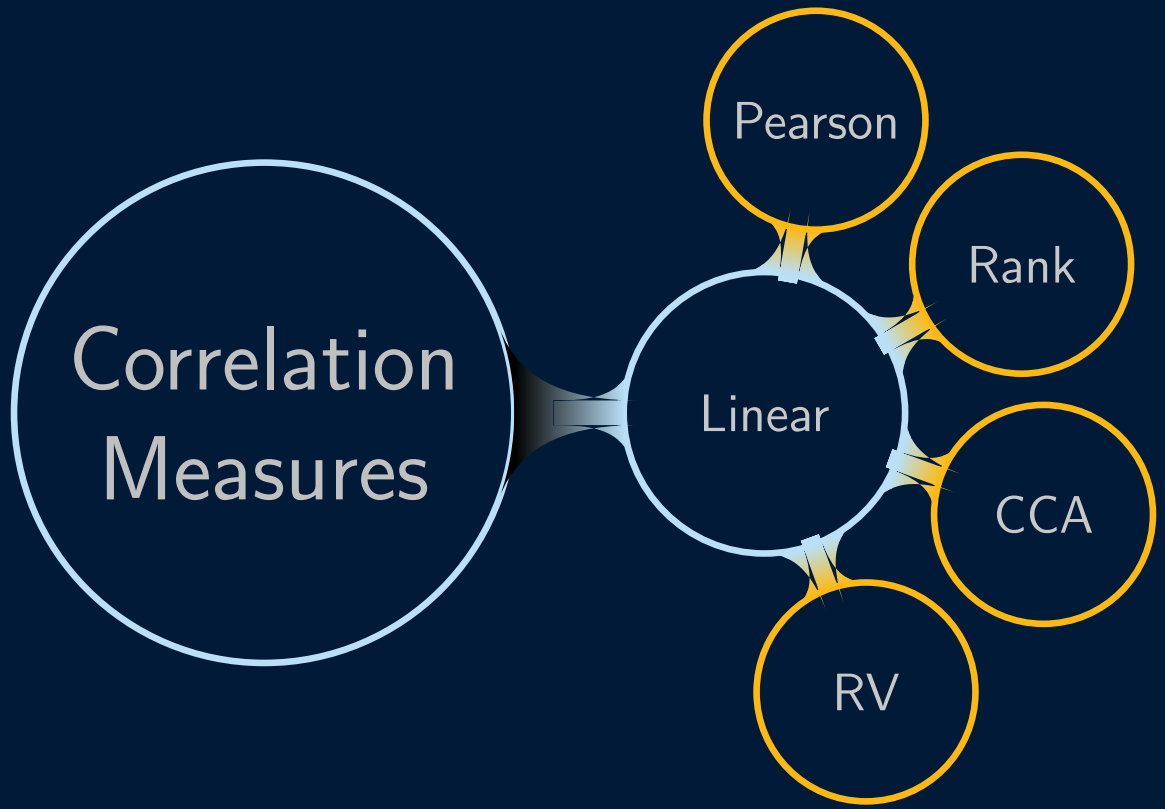

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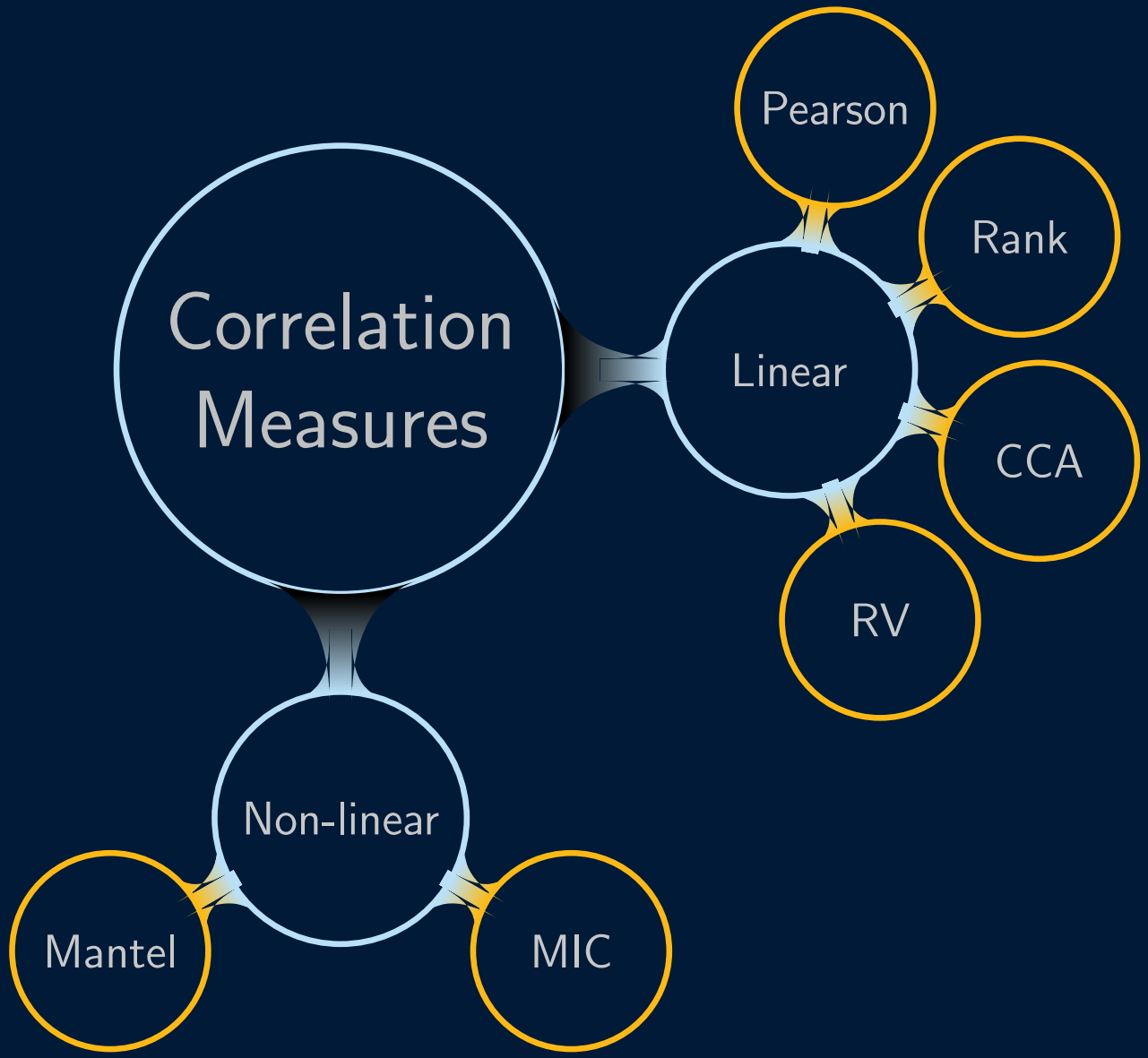
Correlation Measures
Linear
Pearson
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CCA
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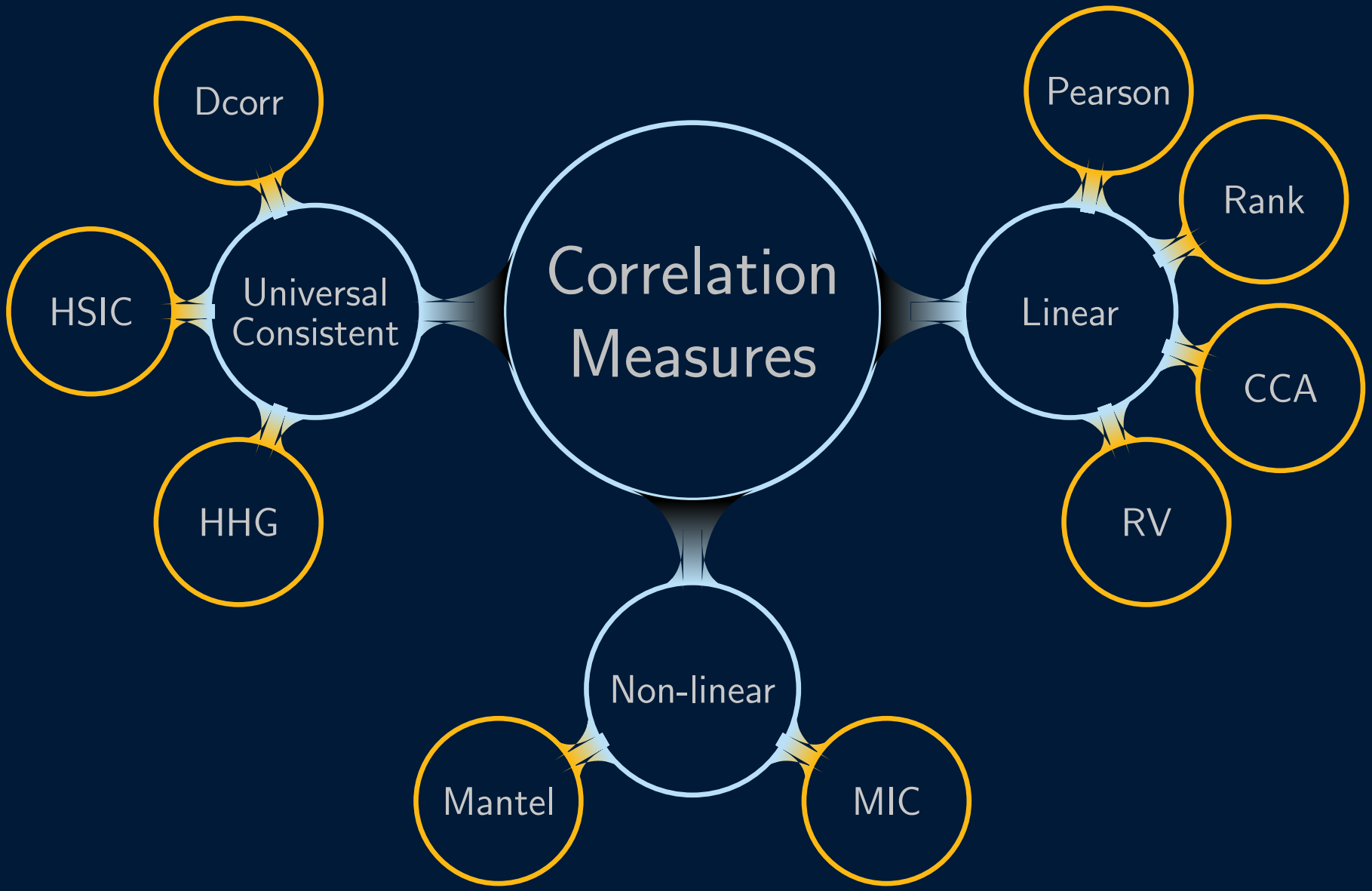
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To that end, we propose the **multiscale graph correlation** in [*Shen et al.(2017a)*][1].

Overview

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

Illustration

Introducing MGC

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

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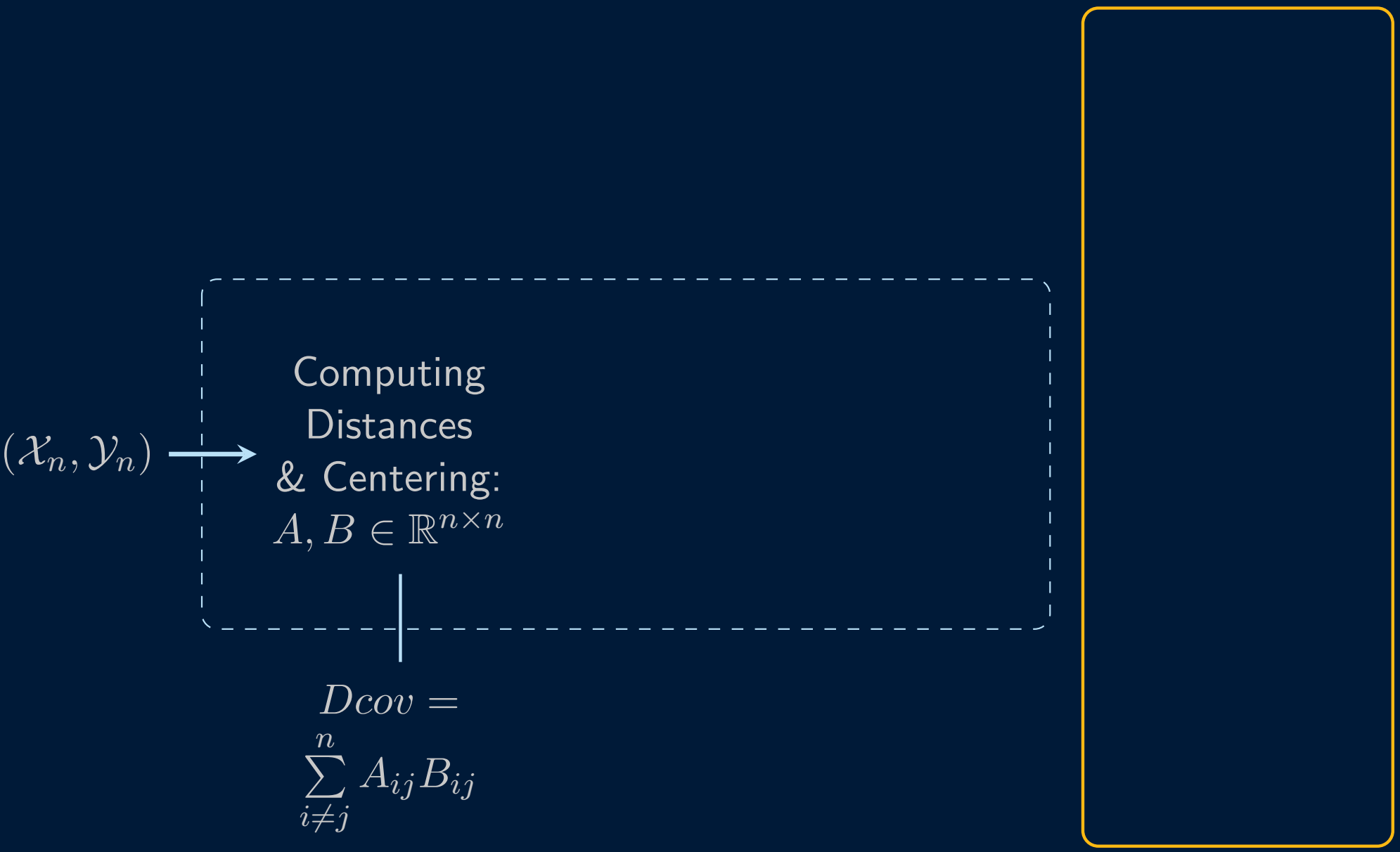

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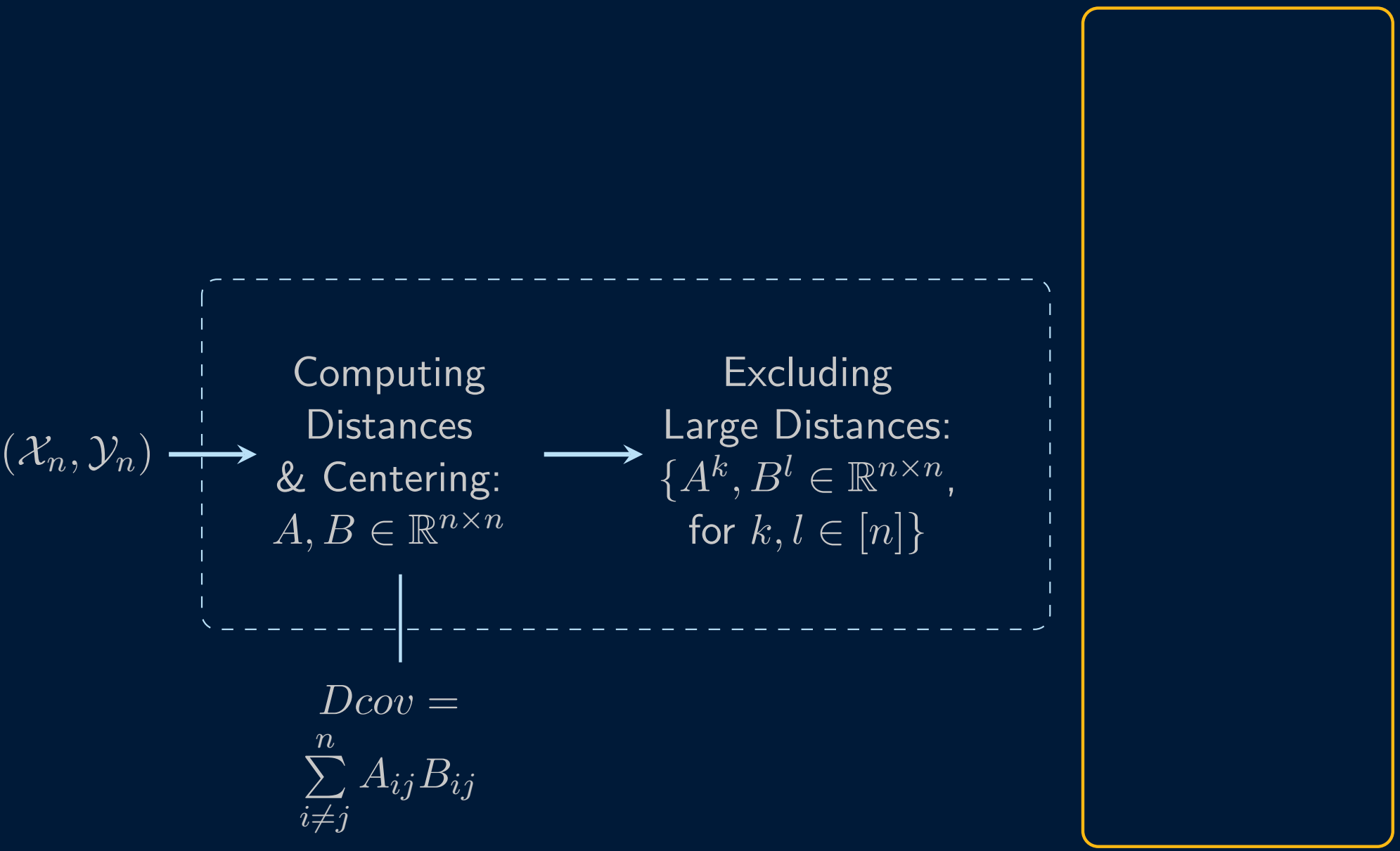

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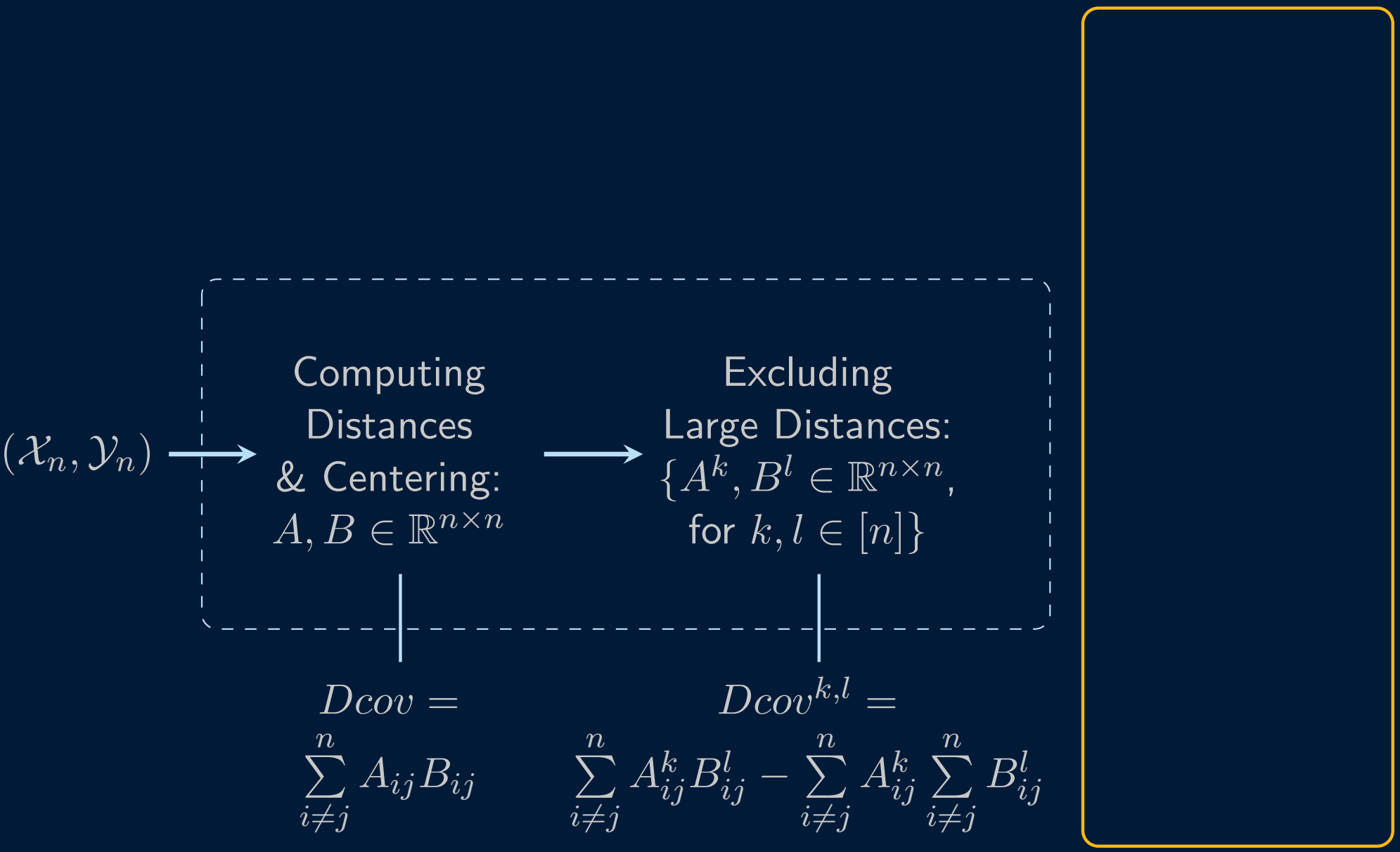

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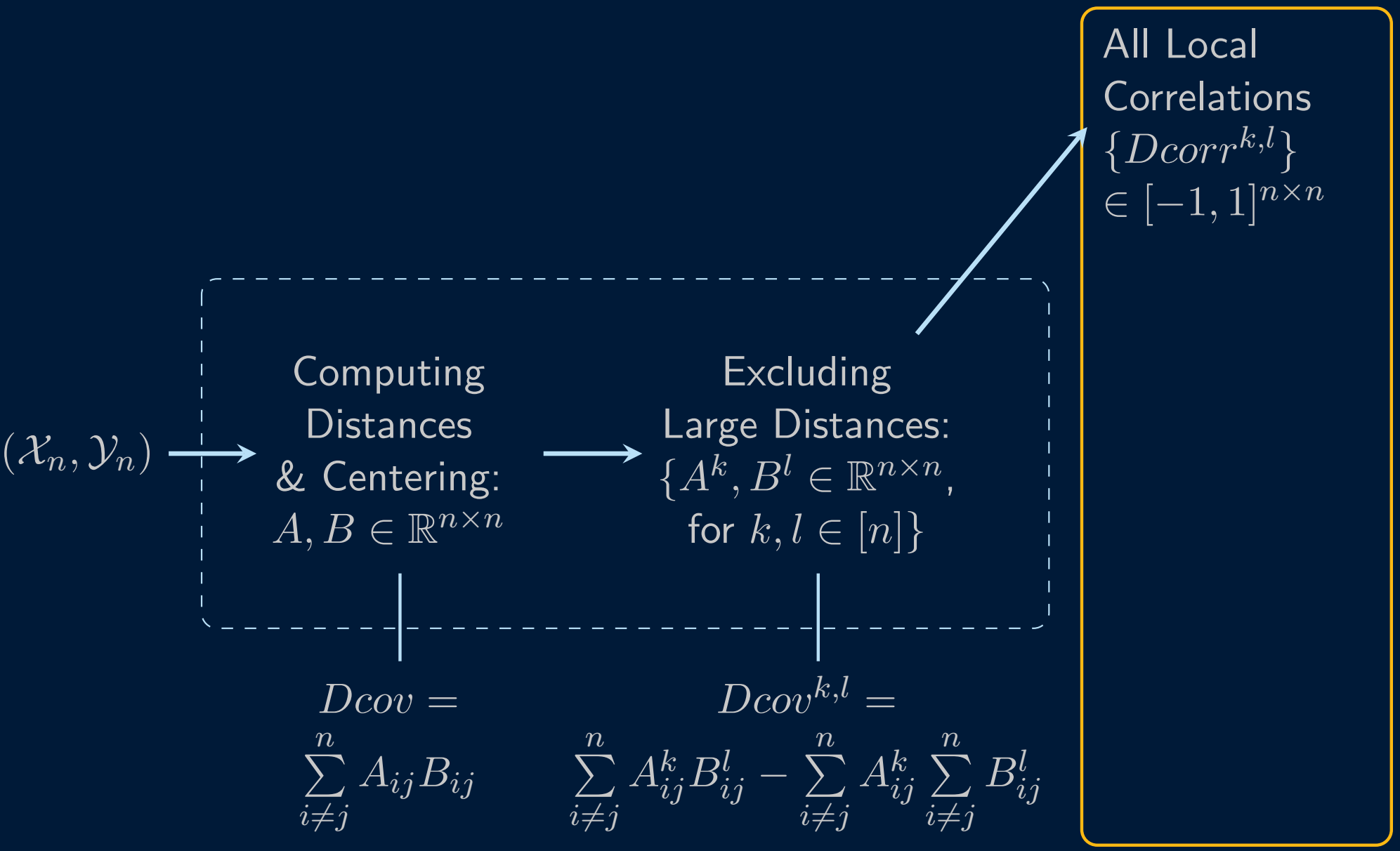

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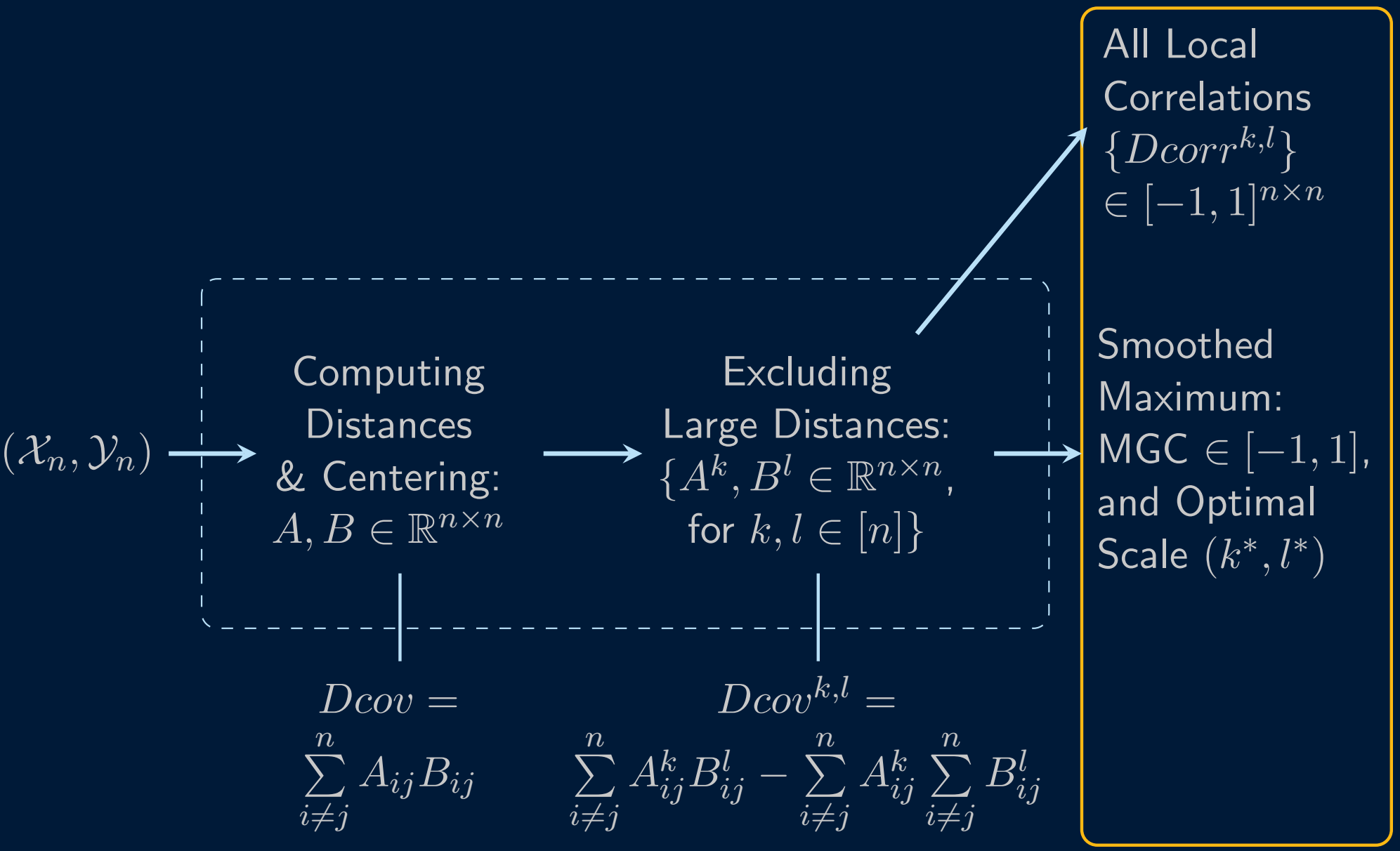

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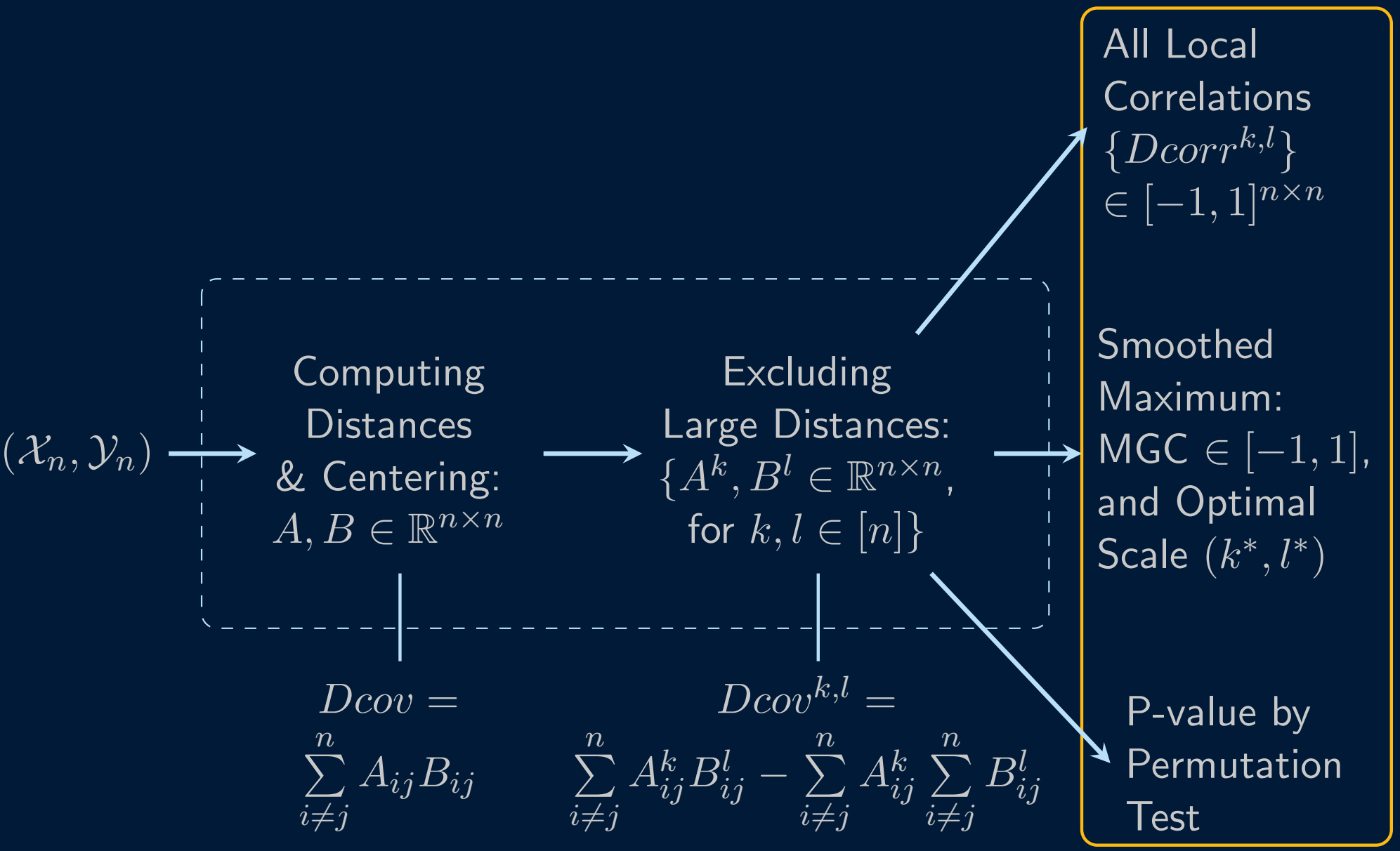

Direct Maximum

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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!

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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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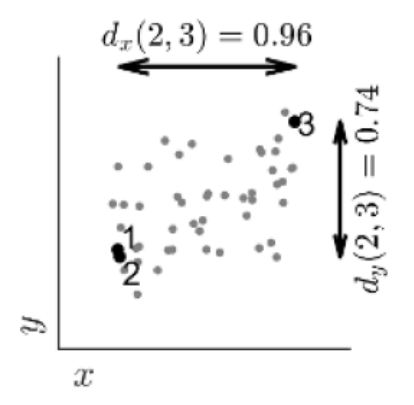

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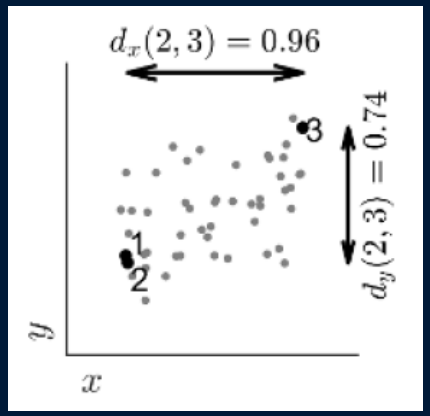

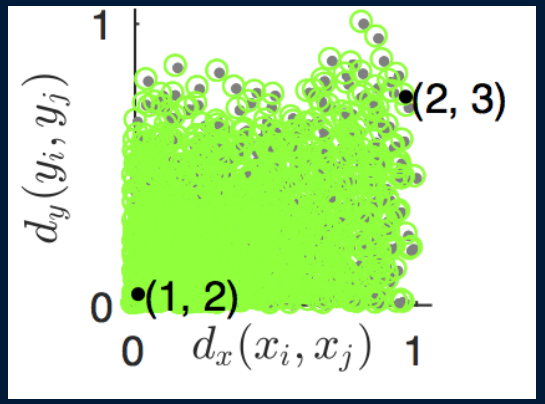

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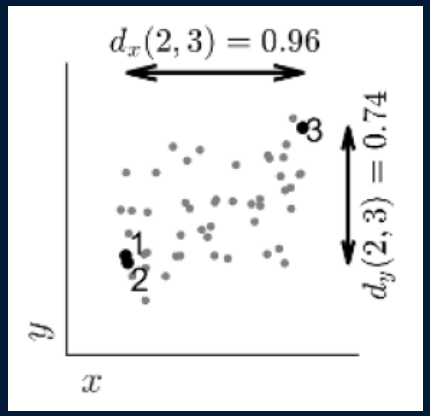

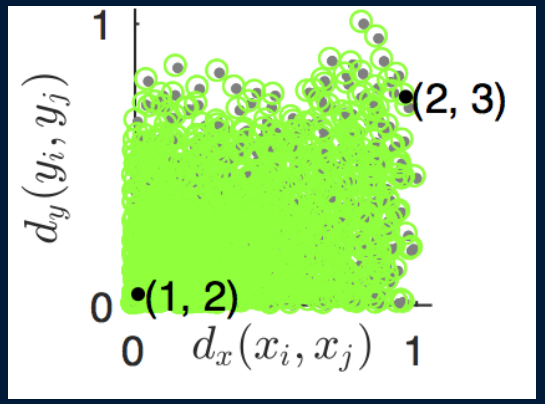

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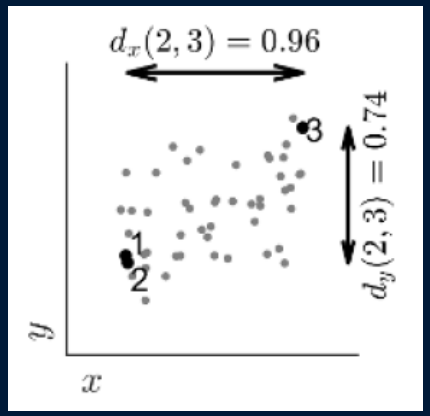

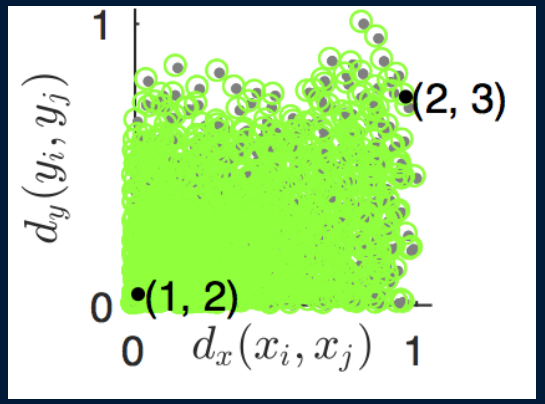

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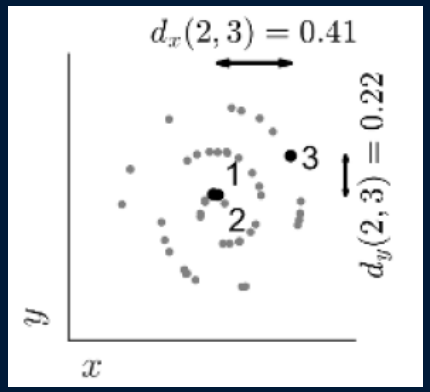

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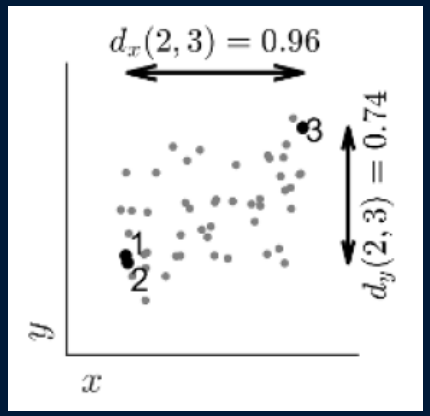

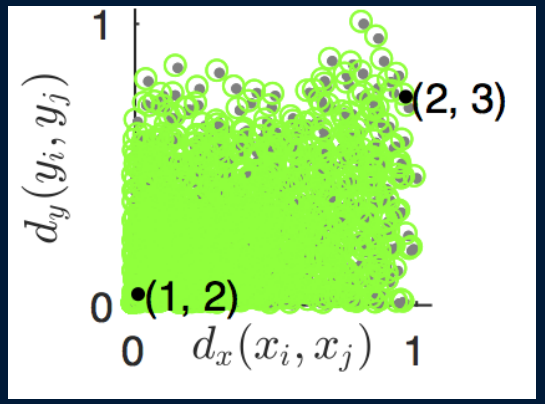

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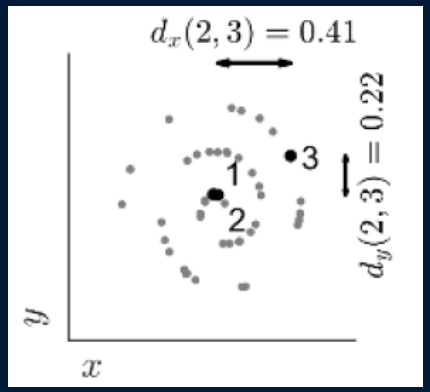

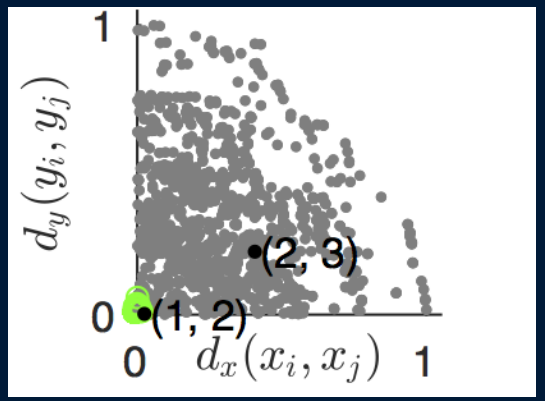

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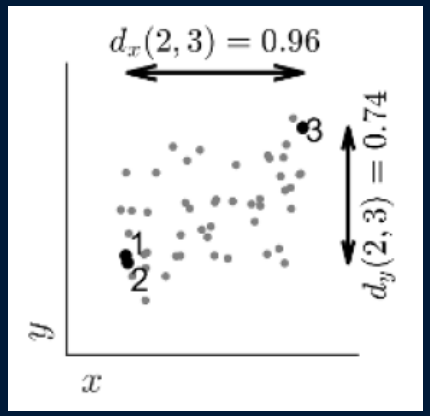

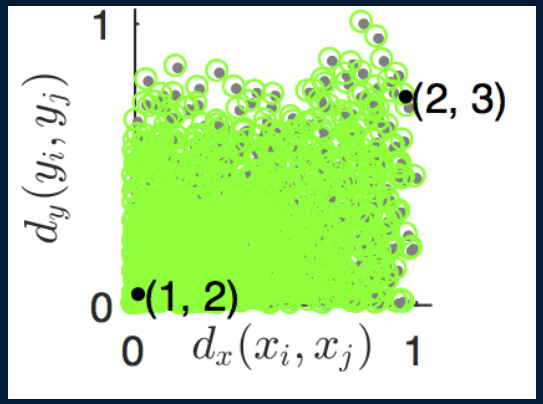

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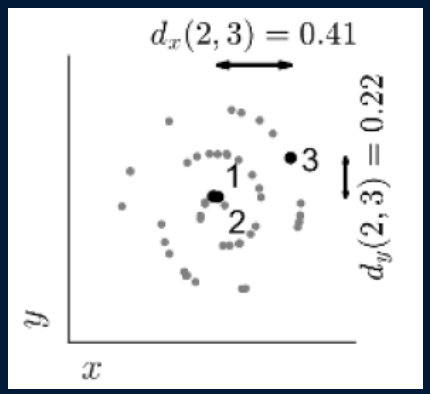

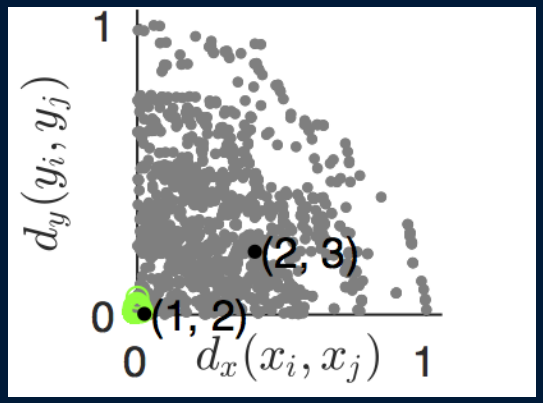

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Theory

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6. *Consistency: At any type 1 error level* α*, testing power* $\beta(c(\mathcal{X}_n, \mathcal{Y}_n)) \overset{n\to\infty}{\to} 1$ *against any dependent* F_{XY}.

Defining Population MGC

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

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

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

$$d_X^{\rho_k} = (\|X - X'\| - \|X - X''\|)\boldsymbol{I}_{X,X'}^{\rho_k}$$
$$d_{Y'}^{\rho_l} = (\|Y' - Y\| - \|Y' - Y'''\|)\boldsymbol{I}_{Y',Y}^{\rho_l}$$

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Suppose $(X, Y), (X', Y'), (X'', Y''), (X''', Y''')$ are *iid* as F_{XY}. Let $\boldsymbol{I}(\cdot)$ be the indicator function, define two random variables

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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

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

Then $d(\cdot, \cdot)$ is negative definite, and

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

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

and apply MGC / Dcorr to the transformed dissimilarity matrices.

Experiments

Visualizations of 20 Simulation Settings

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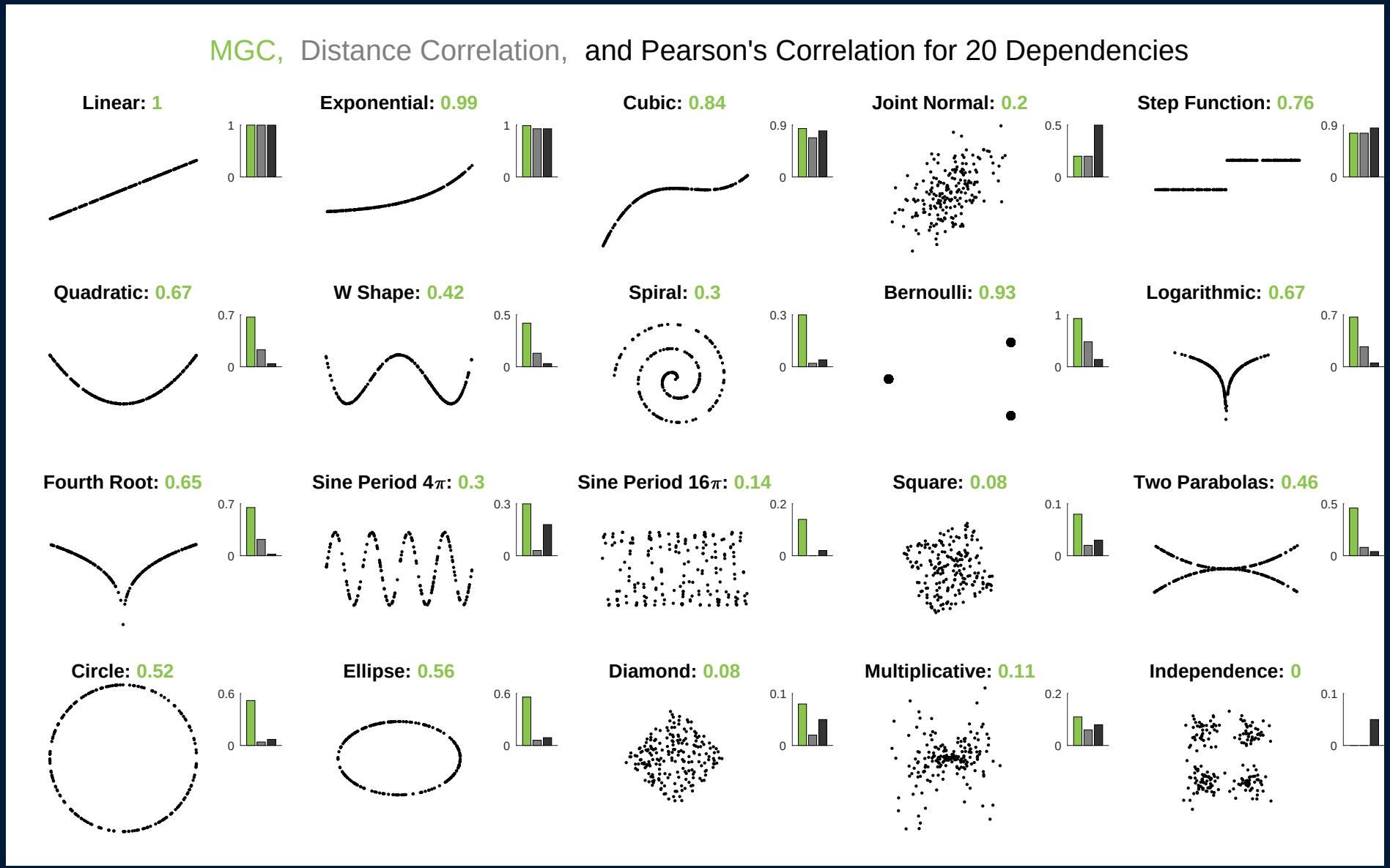

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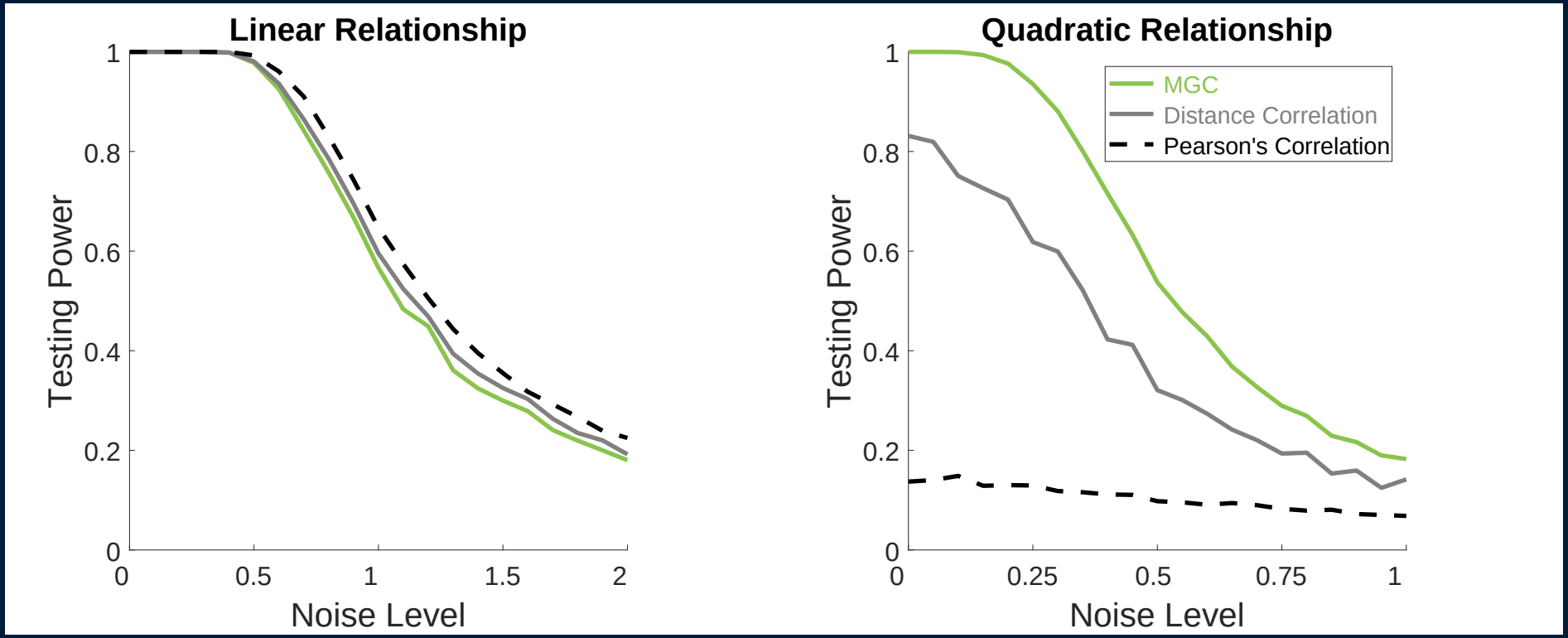

$$n = 30, p = q = 1,$$
$$X \sim Uniform(-1, 1),$$
$$\epsilon \sim Normal(0, noise),$$
$$Y = X + \epsilon \text{ and } Y = X^2 + \epsilon.$$

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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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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.

References

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