Dependency Discovery via Multiscale Generalized Correlation

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

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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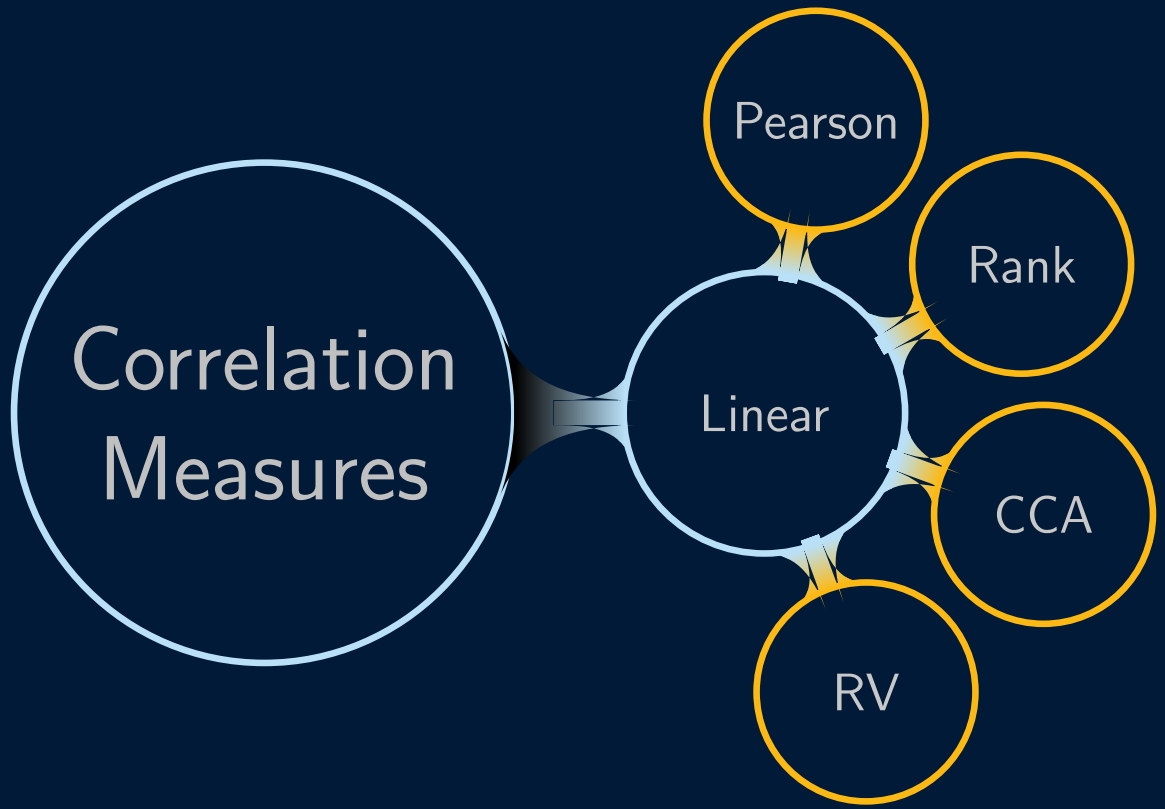

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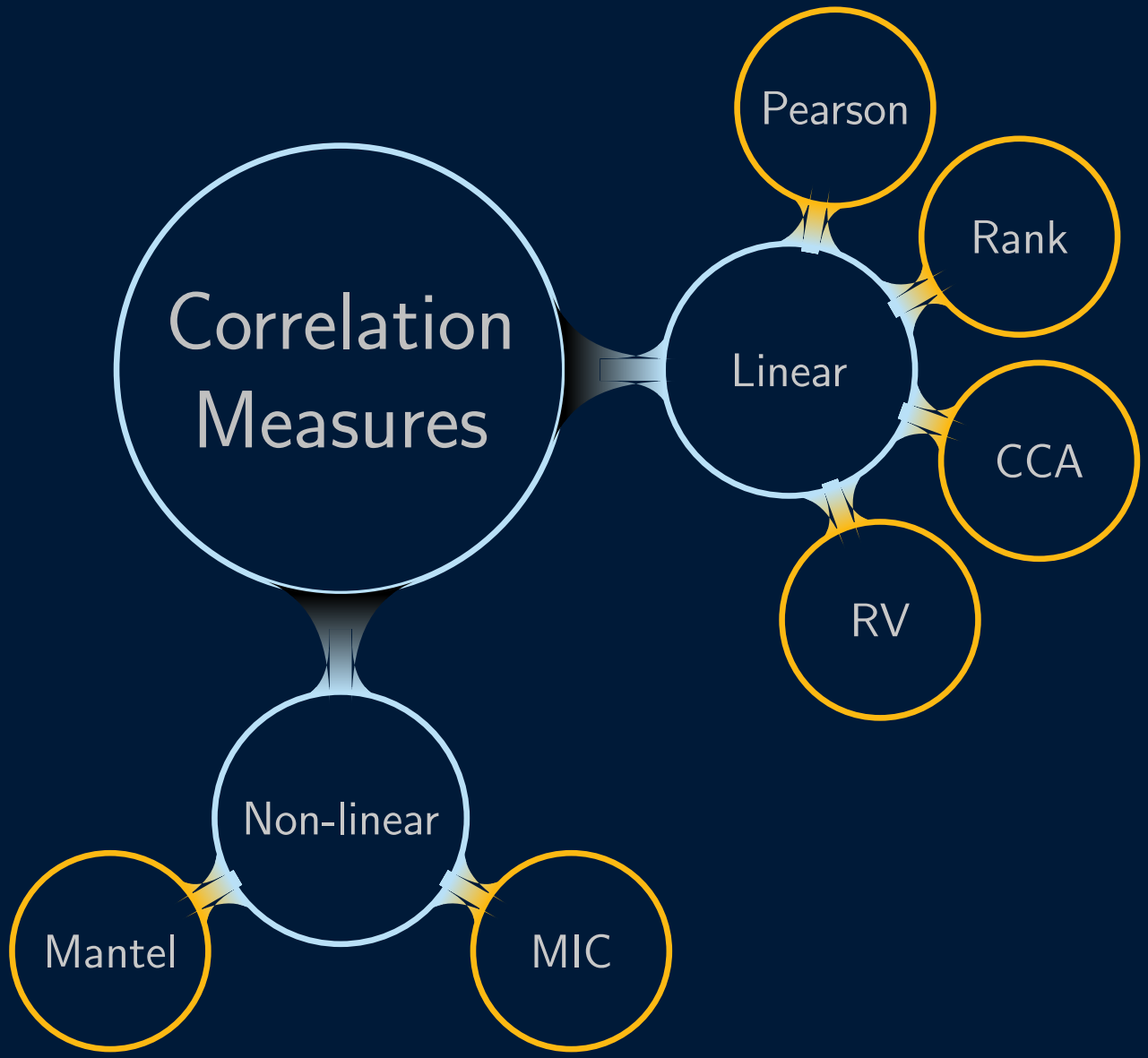
Correlation Measures
Linear
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CCA
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Non-linear
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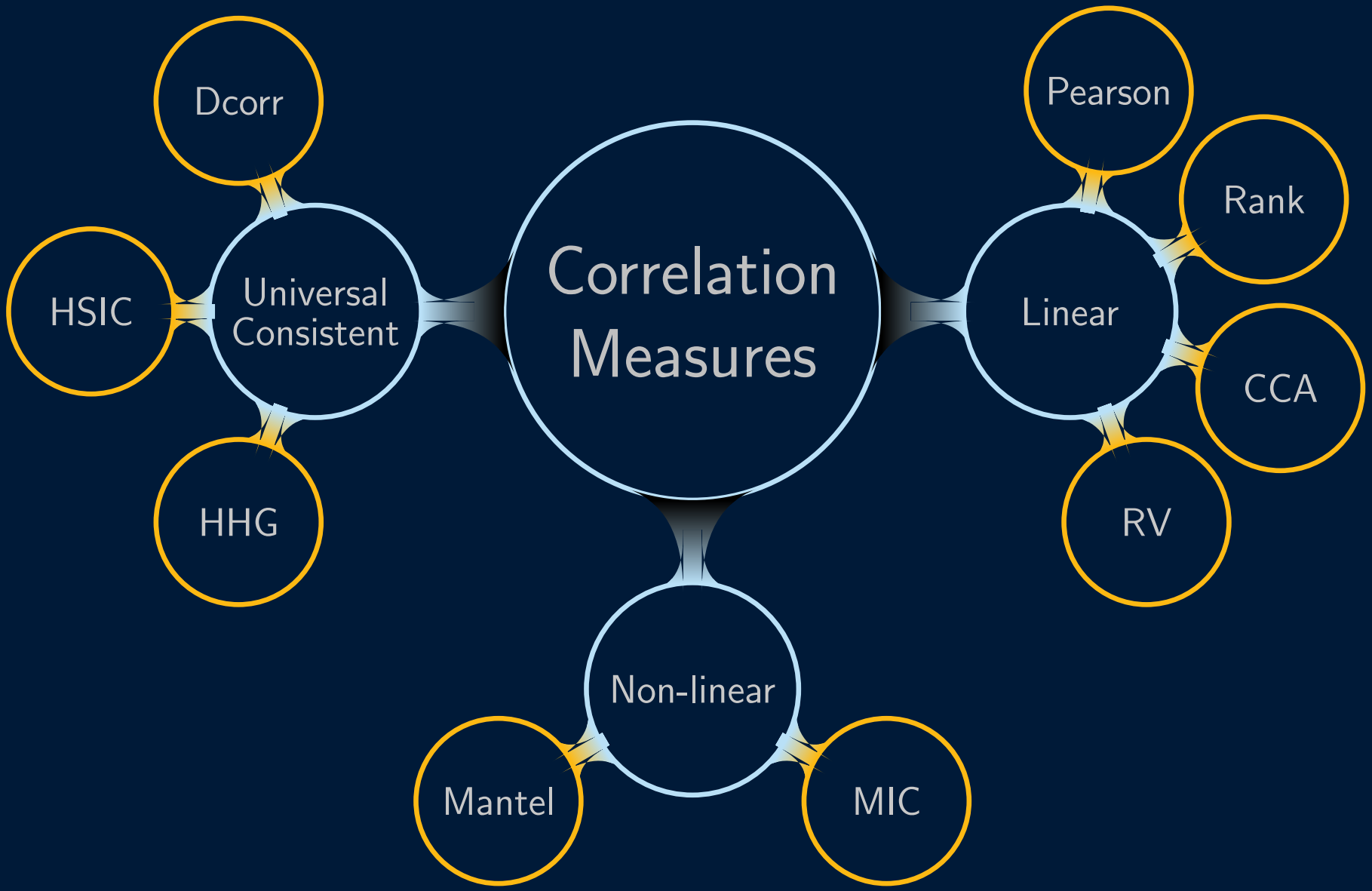
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To that end, we propose the **multiscale generalized correlation** in [*Shen et al.(2017a)*][1].

Overview

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

Illustration

Introducing MGC

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

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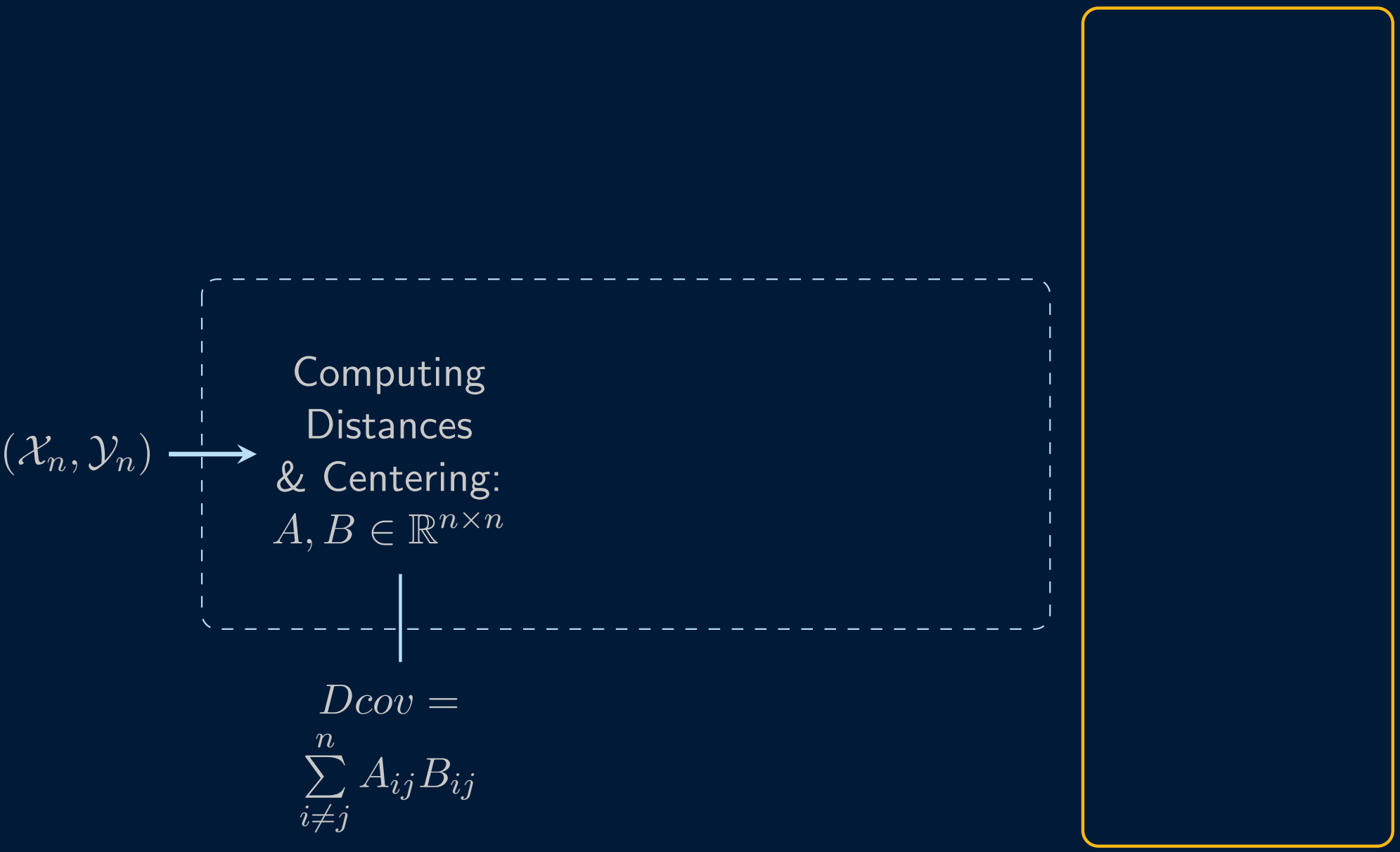

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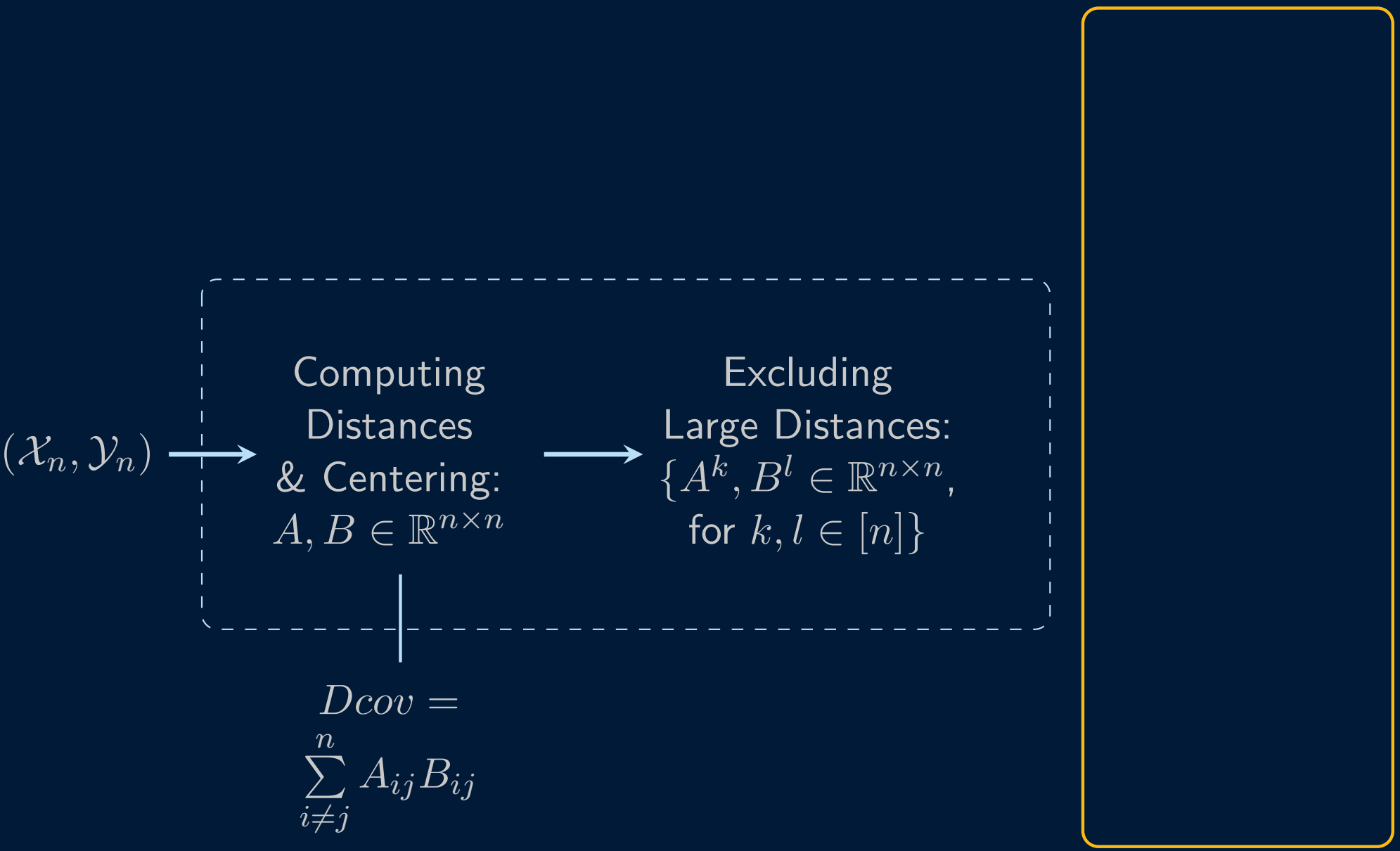

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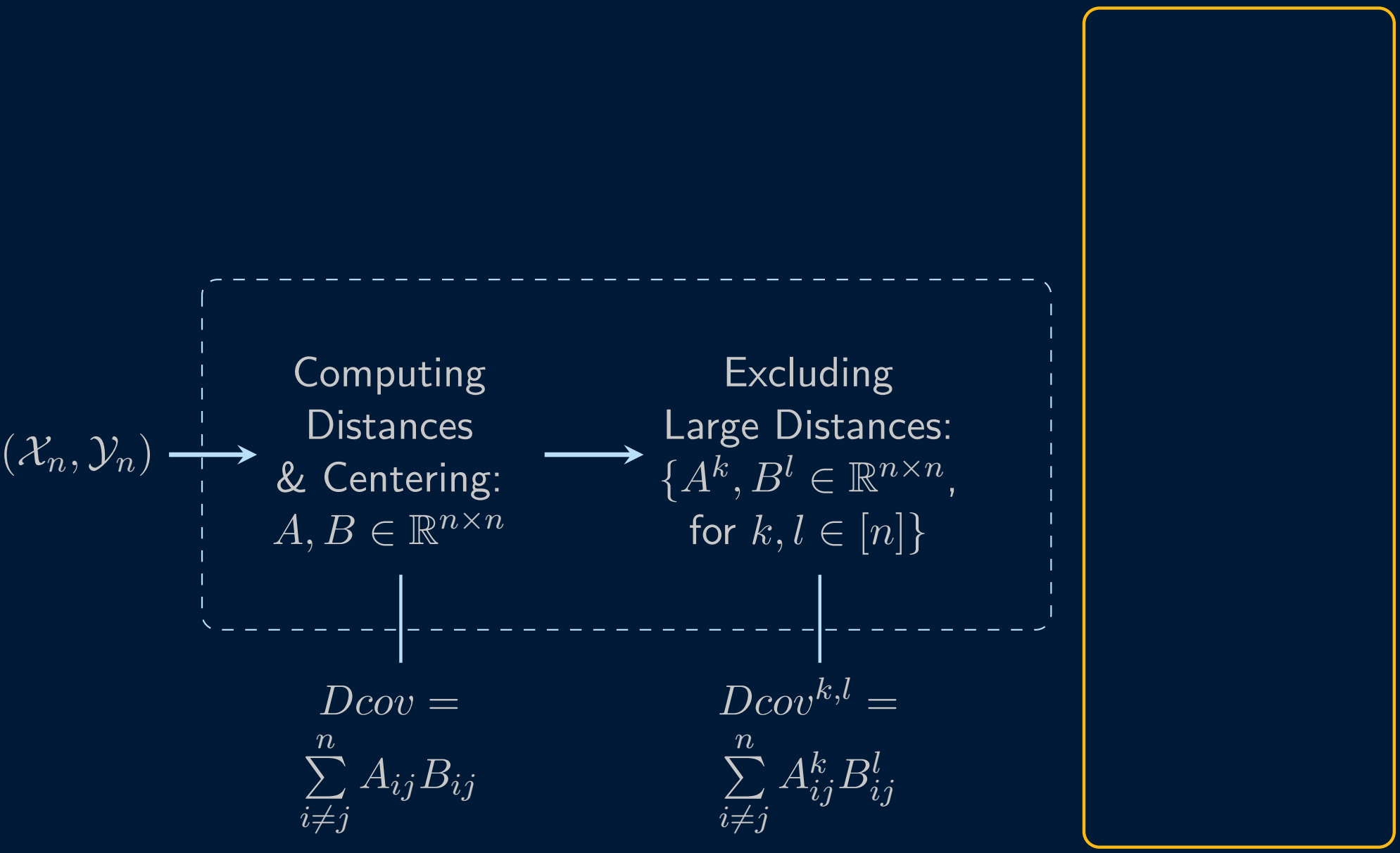

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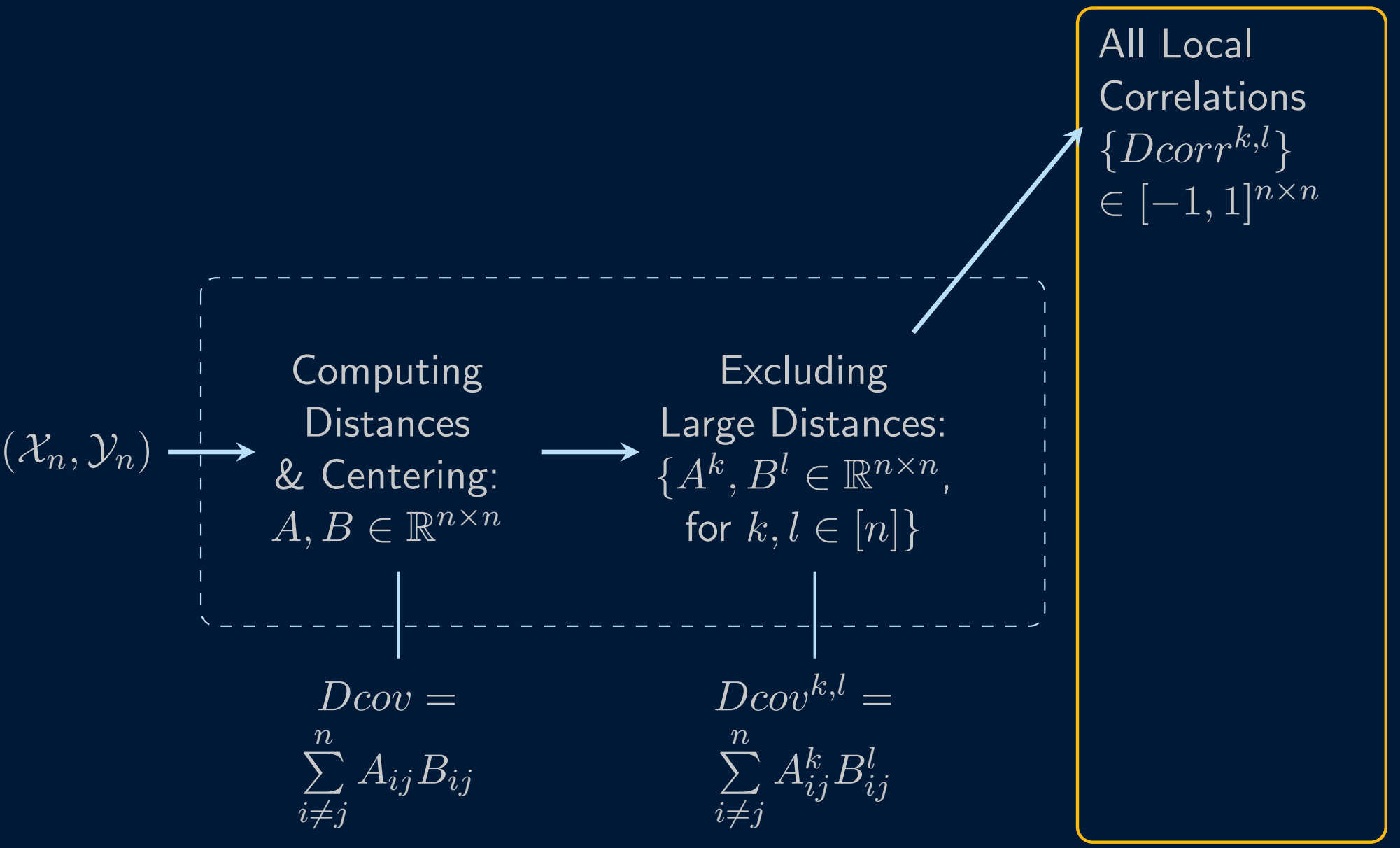

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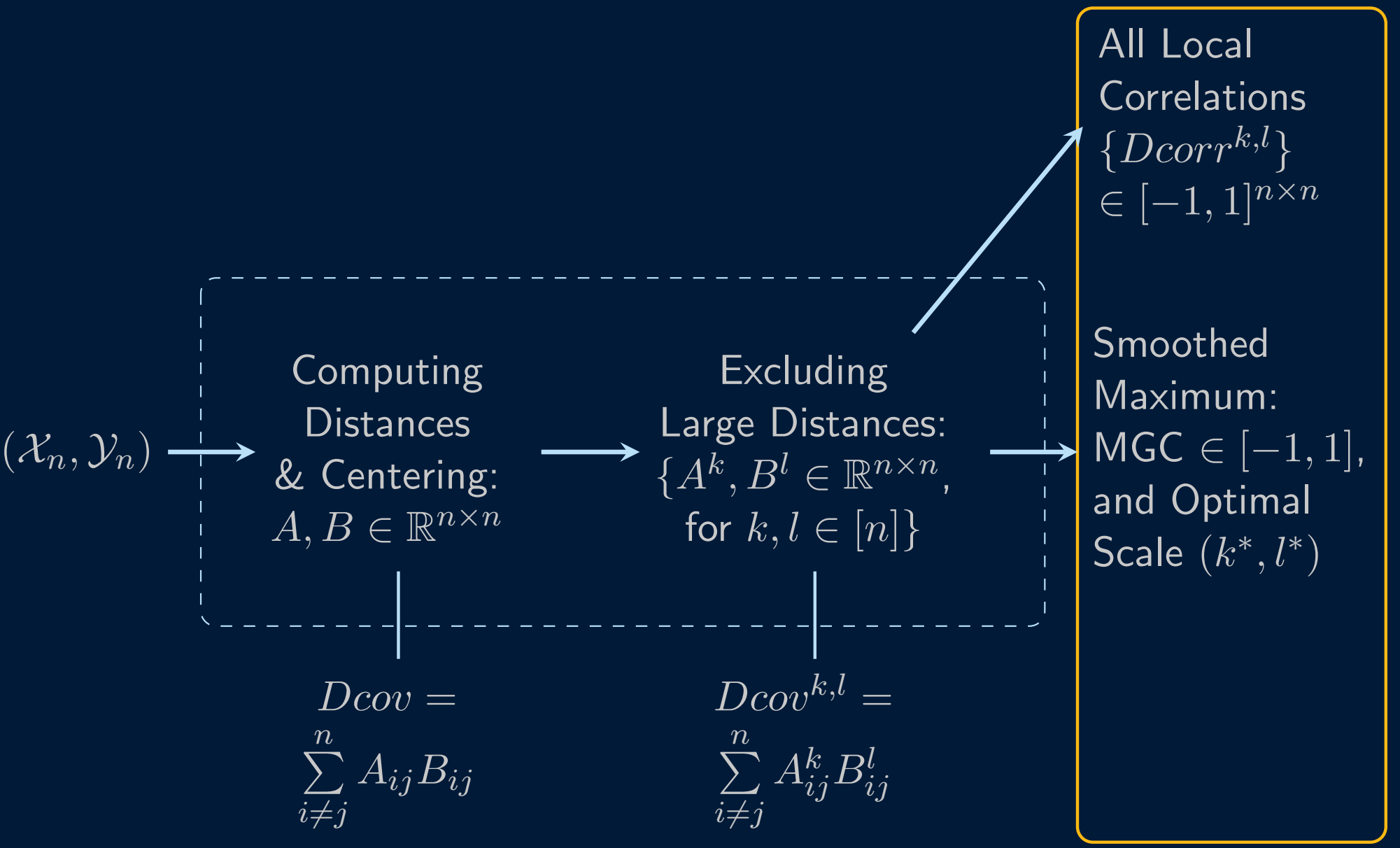

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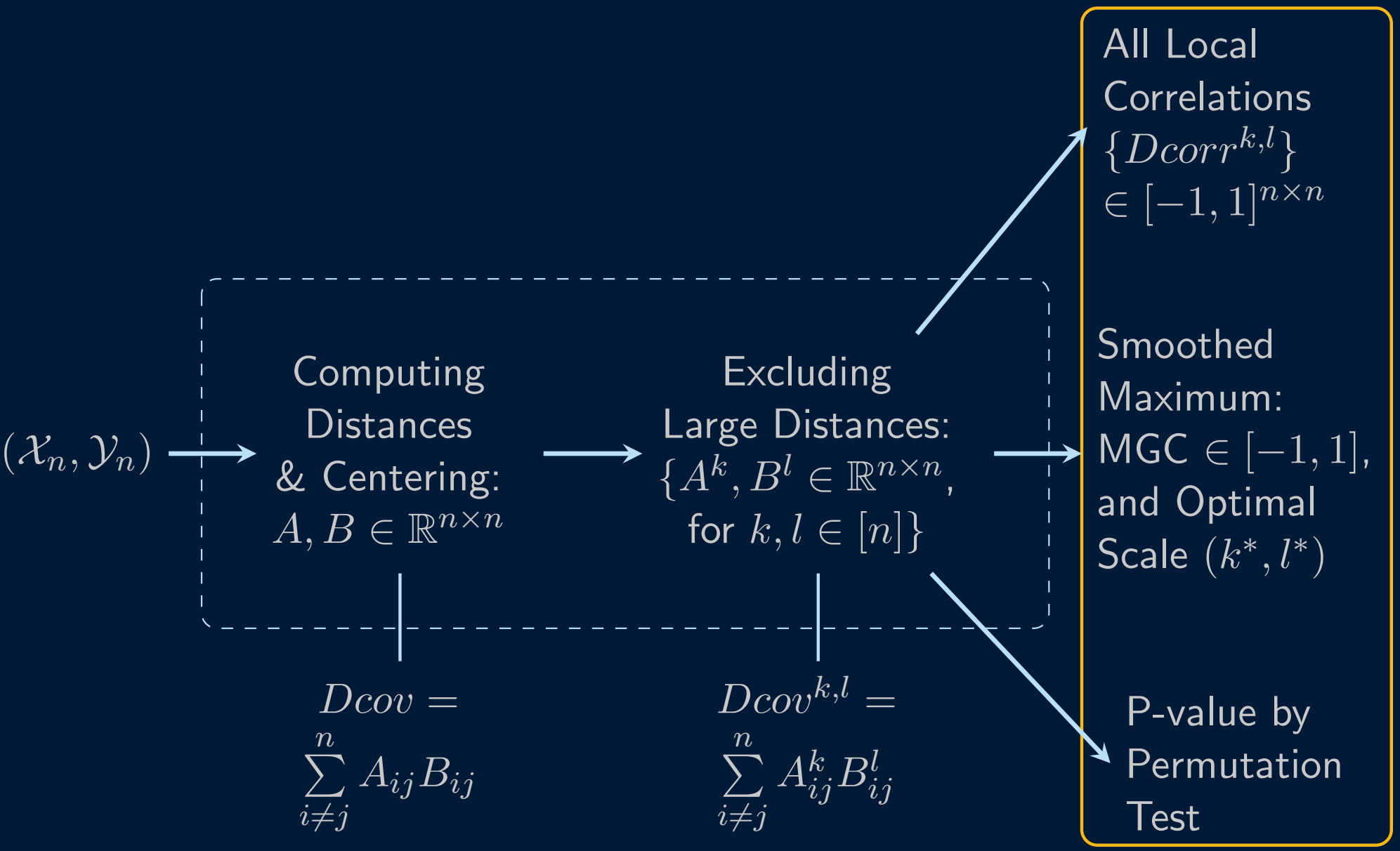

Direct Maximum

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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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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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It is a critical step for both the finite-sample performance and certain theoretical properties of MGC.

Examples

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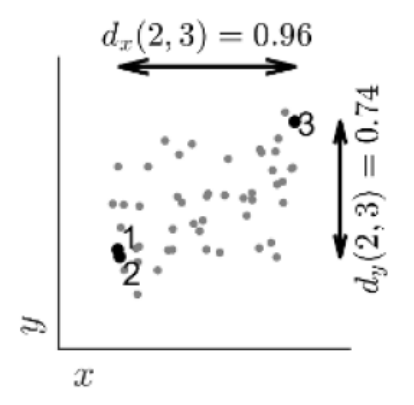

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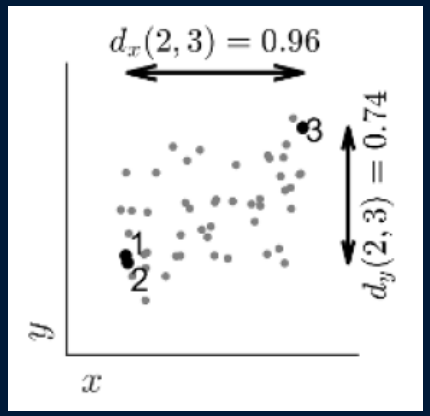

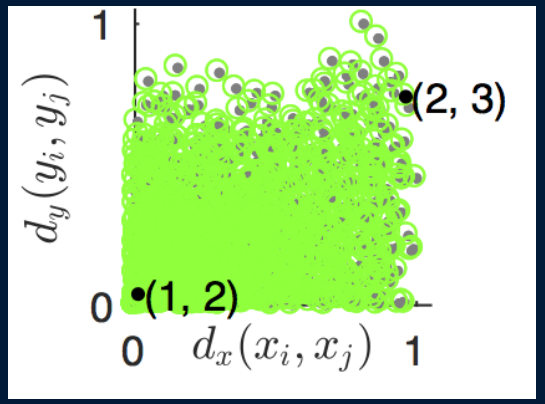

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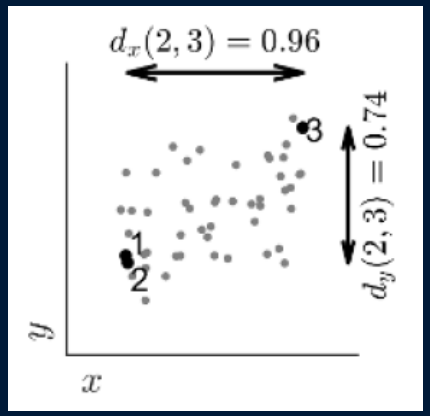

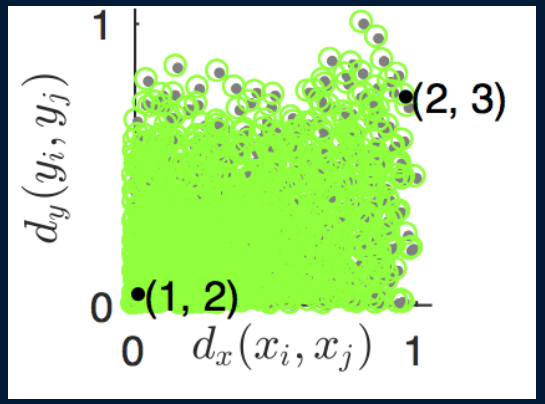

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p-vals: < 0.001

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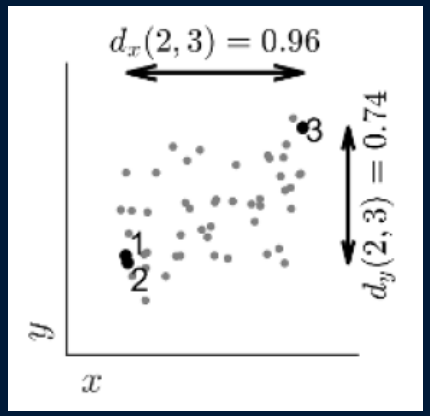

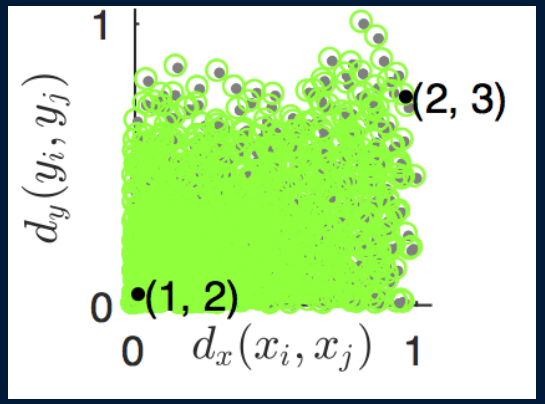

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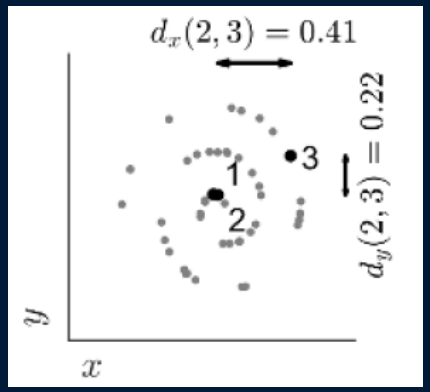

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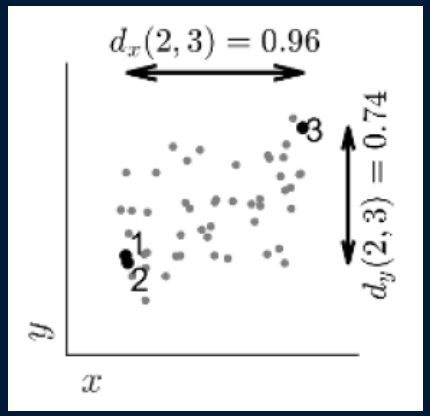

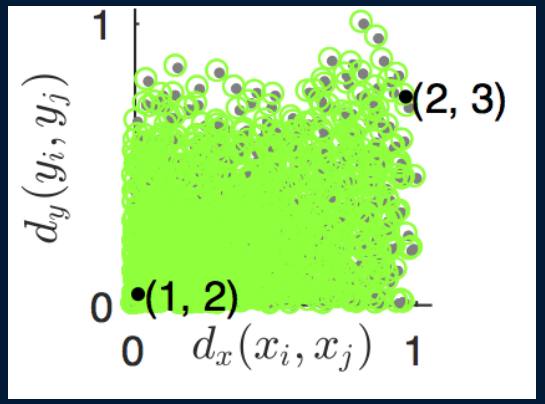

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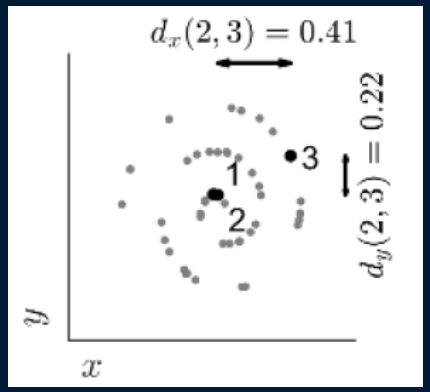

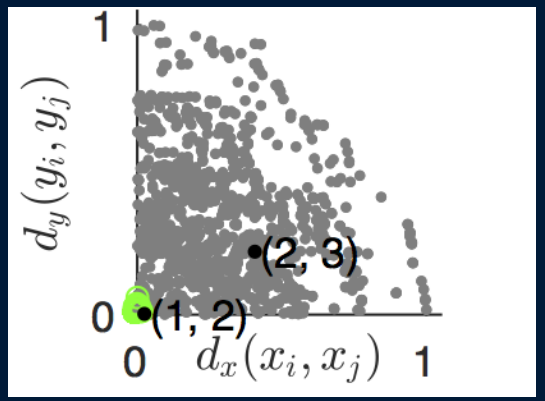

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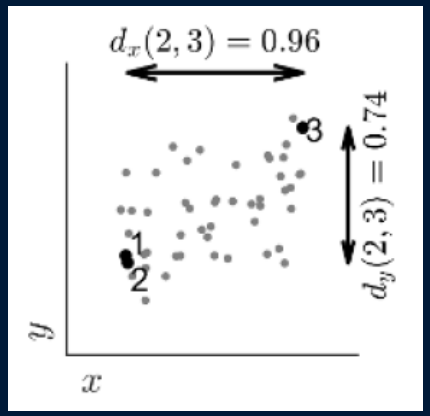

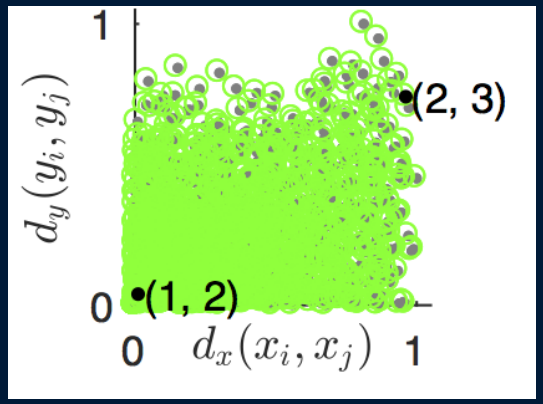

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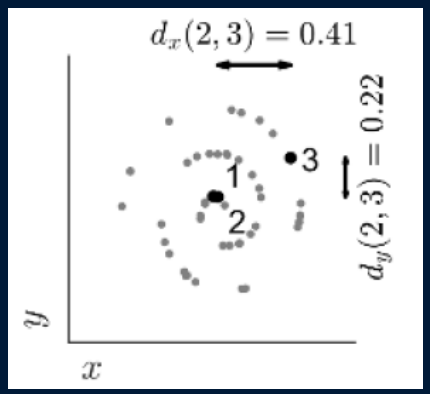

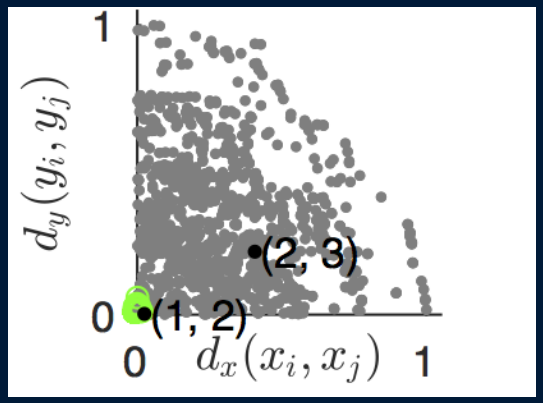

$Dcorr(\mathcal{X}_n, \mathcal{Y}_n) = 0.01$
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p-vals: 0.3 vs < 0.001

Experiments

Visualizations of 20 Simulation Settings

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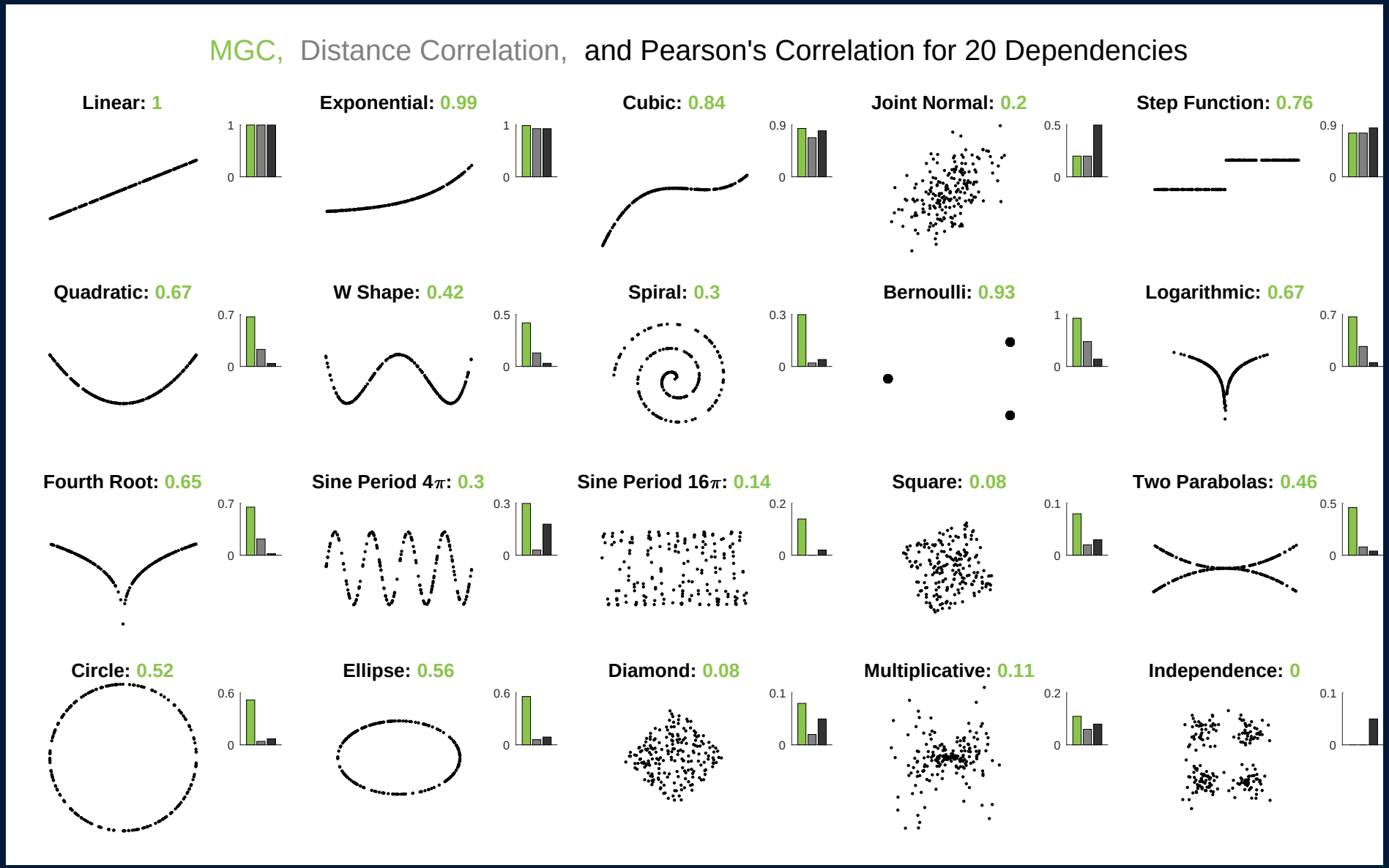

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- Required sample size $N_{\alpha,\beta}(c)$ to achieve a power of β at type 1 error level α using a statistic c.

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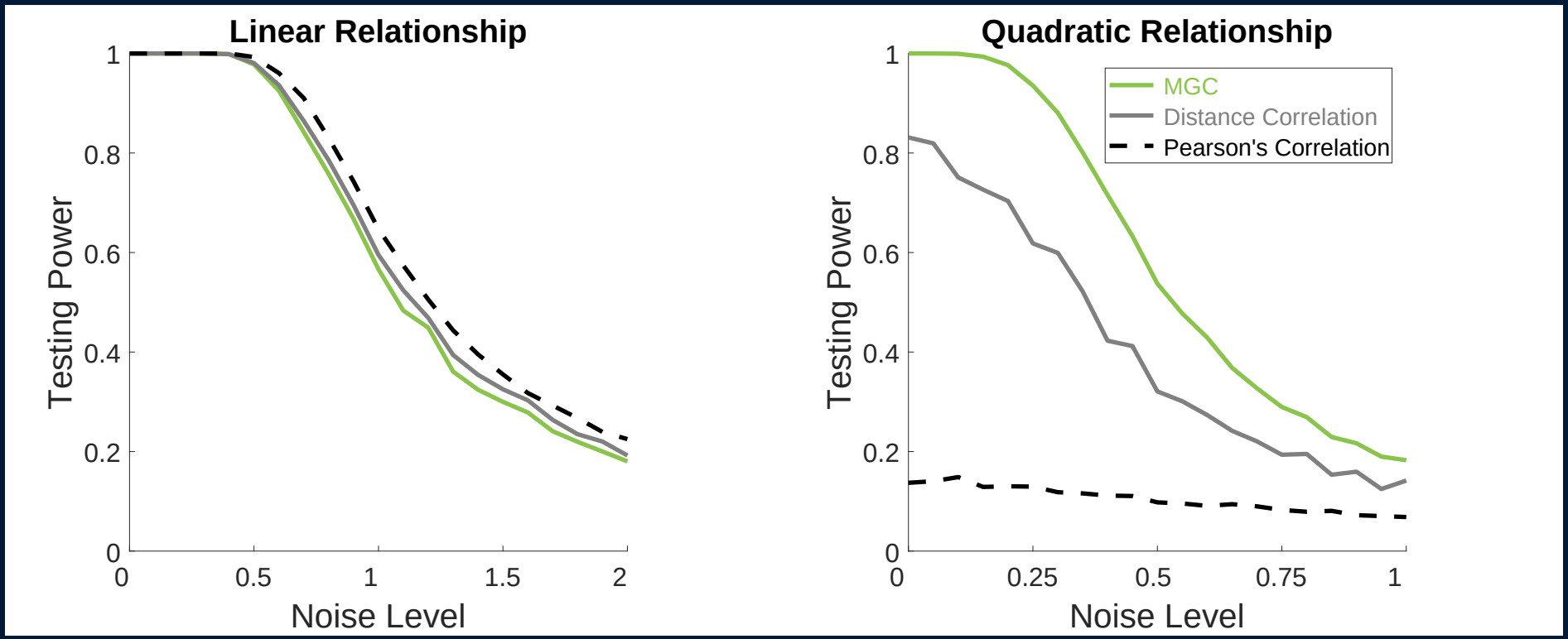

$$n = 30, p = q = 1,$$
$$X \sim Uniform(-1, 1),$$
$$\epsilon \sim Normal(0, noise),$$
$$Y = X + \epsilon \text{ and } Y = X^2 + \epsilon.$$

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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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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.

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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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- MGC is utilized for iterative signal subgraph extraction in [*Wang et al.(2018)*][4].

References

1. C. Shen, C. E. Priebe, M. Maggioni, Q. Wang, and J. T. Vogelstein, "Discovering relationships and their structures across disparate data modalities," *https://arxiv.org/abs/1609.05148*.

2. C. Shen, C. E. Priebe, and J. T. Vogelstein, "From distance correlation to the multiscale generalized correlation," *https://arxiv.org/abs/1710.09768*.

3. Y. Lee, C. Shen, and J. T. Vogelstein, "Network dependence testing via diffusion maps and distance-based correlations," *https://arxiv.org/abs/1703.10136*.

4. S. Wang, C. Shen, A. Badea, C. E. Priebe, and J. T. Vogelstein, "Signal subgraph estimation via vertex screening," *https://arxiv.org/abs/1801.07683*.