

Measuring Association on Topological Spaces Using Kernels and Geometric Graphs

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Motivation: Pearson's correlation coefficient

- Given $(X, Y) \sim$ bivariate normal, Pearson's **correlation** ρ measures the **strength of association** between X and Y
- $\rho = 0$ iff X and Y are **independent**
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Question: What are **nonparametric analogs** of **Pearson's correlation**?

- **Want:** A **measure of association** that:
 - (a) equals **0** iff $X \perp\!\!\!\perp Y$,
 - (b) equals **1** iff Y is a (measurable) **function** of X , and
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- **Testing for independence:** For the past century, most measures of association/dependence only focus on **testing $X \perp\!\!\!\perp Y$** , i.e., they equal 0 iff $Y \perp\!\!\!\perp X$; e.g., **distance correlation** (Székely et al., 2007), Hilbert-Schmidt independence criterion (Gretton et al., 2008), graph-based measures (Friedman and Rafsky, 1983), etc.

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- Dette et al., 2013, Chatterjee, 2019: When $\mathcal{X} = \mathcal{Y} = \mathbb{R}$, authors propose measures that equal **0** iff $Y \perp\!\!\!\perp X$ and **1** iff Y is a **measurable function of X** ; extended to the case $\mathcal{X} = \mathbb{R}^{d_1}$ and $\mathcal{Y} = \mathbb{R}$ in Azadkia and Chatterjee, 2019.

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- Bottleneck: They rely on the canonical **ordering** of $\mathcal{Y} = \mathbb{R}$

We consider the case when \mathcal{X} and \mathcal{Y} are **general topological spaces** (e.g., metric spaces)

- 1 Family of Measures of Association
 - A measure of dependence on Euclidean spaces
 - Extending to a class of kernel measures
- 2 Estimating the Kernel Measure of Association (KMAc)
 - The estimator
 - Consistency and rate of convergence
 - Central limit theorem
 - Computational complexity
- 3 Other Applications of Kernels and Geometric Graphs
 - A measure of conditional dependence
 - A measure of dissimilarity between M -distributions

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A measure on $\mathcal{X} = \mathbb{R}^{d_1}$, $\mathcal{Y} = \mathbb{R}^{d_2}$

$(X, Y) \sim \mu$ on $\mathcal{X} \times \mathcal{Y}$ with marginals μ_X & μ_Y

Basic strategy

- Most measures quantify a “discrepancy” between μ and $\mu_X \otimes \mu_Y$
- We construct a discrepancy between $\mu_{Y|X}$ (regular conditional distribution of Y given X) and μ_Y

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Basic strategy

- Most measures quantify a “discrepancy” between μ and $\mu_X \otimes \mu_Y$
- We construct a discrepancy between $\mu_{Y|X}$ (regular conditional distribution of Y given X) and μ_Y
- When $Y \perp\!\!\!\perp X$, $\mu_{Y|X} = \mu_Y$. When Y is a measurable function of X , $\mu_{Y|X}$ is a **degenerate** measure

- Define

$$T \equiv T(\mu) := 1 - \frac{\mathbb{E} \|Y' - \tilde{Y}'\|_2}{\mathbb{E} \|Y_1 - Y_2\|_2}$$

- Generate $Y_1, Y_2 \stackrel{i.i.d.}{\sim} \mu_Y$
- (X', Y', \tilde{Y}') is generated as: $X' \sim \mu_X$ and then Y', \tilde{Y}' i.i.d. $\mu_{Y|X'}$ (i.e., Y' and \tilde{Y}' are conditionally independent given X')

- Recall $X' \sim \mu_X$, and $Y', \tilde{Y}' | X' \stackrel{iid}{\sim} \mu_{Y|X'}$, and

$$T = 1 - \frac{\mathbb{E} \| Y' - \tilde{Y}' \|_2}{\mathbb{E} \| Y_1 - Y_2 \|_2}.$$

$Y' \sim \mu_Y, \tilde{Y}' \sim \mu_Y$ but Y' and \tilde{Y}' are **not** necessarily **independent**

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- Suppose $Y = h(X)$ for some measurable $h(\cdot)$, then

$$Y' = \tilde{Y}' = h(X') \Leftrightarrow \|Y' - \tilde{Y}'\|_2 = 0 \text{ a.s.} \Leftrightarrow T = 1$$

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- Showing that $T = 0 \Rightarrow Y \perp\!\!\!\perp X$ is more **complicated!**

Theorem [Deb, Ghosal and S. (2020+)]

Suppose $\mathbb{E}\|Y_1\|_2 < \infty$. Then

- $T \in [0, 1]$
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Interpretability and Monotonicity: What happens when $T \in (0, 1)$?

- Suppose μ is the **bivariate normal** distribution with means μ_X, μ_Y , variances σ_X^2, σ_Y^2 and **correlation** ρ . Then

$$T(\mu) = 1 - \sqrt{1 - \rho^2}.$$

The above function is **strictly convex and increasing** in $|\rho|$.

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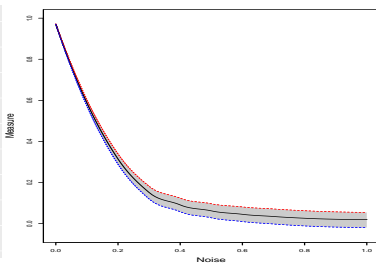
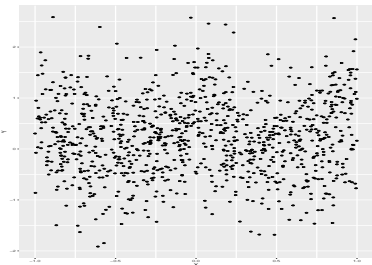
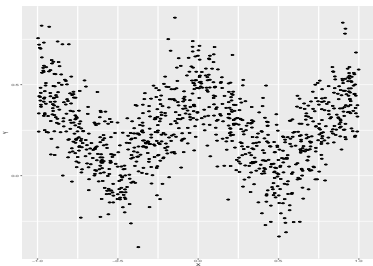
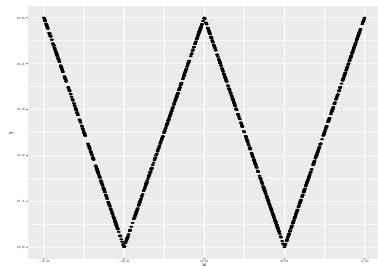
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- In many nonparametric regression models, T turns out to be a **monotonic** function of the degree of **dependence** between Y and X

T captures the **strength** of the **relationship** between Y and X

$(X^{(1)}, X^{(2)}, Y^{(1)}, Y^{(2)}) \sim \mu$ on \mathbb{R}^4 ; $(X^{(1)}, Y^{(1)}), (X^{(2)}, Y^{(2)})$ are i.i.d.

W-shape: $Y^{(1)} = |X^{(1)} + 0.5|\mathbf{1}_{X^{(1)} \leq 0} + |X^{(1)} - 0.5|\mathbf{1}_{X^{(1)} > 0} + 0.75\lambda\epsilon$,
where $\epsilon \sim \mathcal{N}(0, 1)$ with varying λ ; $X \sim \text{Uniform}[-1, 1]$



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Reproducing kernel Hilbert spaces (RKHS)

- \mathcal{H} : Hilbert space² of functions from \mathcal{Y} to \mathbb{R}
- **Kernel function**: A symmetric nonnegative definite function on \mathcal{Y} , i.e., $K : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ satisfying

$$\sum_{i,j=1}^m \alpha_i \alpha_j K(y_i, y_j) \geq 0$$

for all $\alpha_i \in \mathbb{R}$, $y_i \in \mathcal{Y}$ and $m \geq 1$

²A Hilbert space is a complete inner product space

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- For all $y \in \mathcal{Y}$, $K(y, \cdot) \in \mathcal{H}$, (note $K(y, \cdot) : \mathcal{Y} \rightarrow \mathbb{R}$, $\forall y \in \mathcal{Y}$)
- Identify $y \mapsto K(y, \cdot)$ (feature map)
- **Gaussian kernel**: $k(u, v) := \exp(-\|u - v\|_2^2)$

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Moore-Aronszajn Theorem

Suppose $K(\cdot, \cdot) : \mathcal{Y} \rightarrow \mathbb{R}$ is a nonnegative definite kernel. Then there exists a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ comprising $\{f : \mathcal{Y} \rightarrow \mathbb{R}\}$ such that:

- $K(y, \cdot) \in \mathcal{H}, \quad \forall y \in \mathcal{Y};$
- (**Reproducing property**) For all $f \in \mathcal{H}, y \in \mathcal{Y},$

$$\langle f, K(y, \cdot) \rangle_{\mathcal{H}} = f(y).$$

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- $\langle K(y_1, \cdot), K(y_2, \cdot) \rangle_{\mathcal{H}} = K(y_1, y_2)$
- Using the above,

$$\begin{aligned} & \|K(y_1, \cdot) - K(y_2, \cdot)\|_{\mathcal{H}}^2 \\ &= \langle K(y_1, \cdot), K(y_1, \cdot) \rangle_{\mathcal{H}} + \langle K(y_2, \cdot), K(y_2, \cdot) \rangle_{\mathcal{H}} - 2\langle K(y_1, \cdot), K(y_2, \cdot) \rangle_{\mathcal{H}} \\ &= K(y_1, y_1) + K(y_2, y_2) - 2K(y_1, y_2) \end{aligned}$$

Kernel Measure of Association (KMAc)

- **Recall:** $K(y, \cdot) : \mathcal{Y} \rightarrow \mathbb{R}$ for all $y \in \mathcal{Y}$, y identified with $K(y, \cdot)$, and

$$T = 1 - \frac{\mathbb{E} \|Y' - \tilde{Y}'\|_2}{\mathbb{E} \|Y_1 - Y_2\|_2}.$$

- **Idea:** Replace $Y_1 - Y_2$ with $K(Y_1, \cdot) - K(Y_2, \cdot)$

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- Define our **kernel measure of association** (KMAc) as

$$\eta_K := 1 - \frac{\mathbb{E} \|K(Y', \cdot) - K(\tilde{Y}', \cdot)\|_{\mathcal{H}}^2}{\mathbb{E} \|K(Y_1, \cdot) - K(Y_2, \cdot)\|_{\mathcal{H}}^2}$$

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Theorem [Deb, Ghosal and S. (2020+)]

Suppose $K(\cdot, \cdot)$ is **characteristic** and $\mathbb{E}K(Y_1, Y_1) < \infty$. Then:

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- A kernel is **characteristic** if

$$\mathbb{E}_P[K(Y, \cdot)] = \mathbb{E}_Q[K(Y, \cdot)] \implies P = Q$$

for probability measures P and Q .

Examples of Characteristic Kernels

Some examples of characteristic kernels [Gretton et al., 2012, Sejdinovic et al., 2013, Lyons 2013, 2014] include:

- (Distance) $K(y_1, y_2) := \|y_1\|_2 + \|y_2\|_2 - \|y_1 - y_2\|_2$. In this case,

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- Bounded kernels: (Gaussian) $K(y_1, y_2) := \exp(-\|y_1 - y_2\|_2^2)$ and (Laplacian) $K(y_1, y_2) := \exp(-\|y_1 - y_2\|_1)$
- For **non-Euclidean domains** such as video filtering, robotics, text documents, human action recognition, **characteristic kernels** constructed in Fukumizu et al., 2009, Danafar et al., 2010, Christmann and Steinwart, 2010, ...

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Estimation Strategy

- Suppose $(X_1, Y_1), \dots, (X_n, Y_n) \stackrel{iid}{\sim} \mu$ on $\mathcal{X} \times \mathcal{Y}$
- \mathcal{X} is endowed with **metric** $\rho_{\mathcal{X}}(\cdot, \cdot)$
- Recall

$$\eta_{\kappa} = \frac{\mathbb{E}K(Y', \tilde{Y}') - \mathbb{E}K(Y_1, Y_2)}{\mathbb{E}K(Y_1, Y_1) - \mathbb{E}K(Y_1, Y_2)}$$

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- By standard U-statistics theory,

$$\mathbb{E}K(Y_1, Y_1) \approx \frac{1}{n} \sum_{i=1}^n K(Y_i, Y_i)$$

and

$$\mathbb{E}K(Y_1, Y_2) \approx \frac{1}{n(n-1)} \sum_{i \neq j} K(Y_i, Y_j)$$

- **Hardest** term to estimate is $\mathbb{E}K(Y', \tilde{Y}')$!

- Suppose \mathcal{X} is a **finite** set. Then, $\mathbb{E}K(Y', \tilde{Y}')$ can be handled as

$$\mathbb{E}K(Y', \tilde{Y}') = \mathbb{E}[\mathbb{E}[K(Y', \tilde{Y}')|X']] \approx \frac{1}{n} \sum_{i=1}^n \frac{1}{|\{j : X_j = X_i\}|} \sum_{j: X_j = X_i} K(Y_i, Y_j)$$

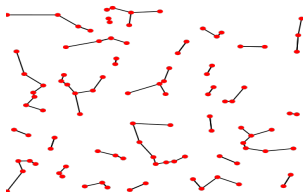
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- If X is continuous, replace $X_j = X_i$ with $\rho_{\mathcal{X}}(X_i, X_j)$ being “**small**”

Geometric graph

- A **graph** G_n on $\{X_1, \dots, X_n\}$ which joins points that are “**close**” to each other
- For example, consider a **k -nearest neighbor graph (k -NNG)**: Join every point on $\{X_1, \dots, X_n\}$ to its first k nearest neighbors



Estimate $\mathbb{E}K(Y', \tilde{Y}')$ by replacing

$$\frac{1}{n} \sum_{i=1}^n \frac{1}{|\{j : X_j = X_i\}|} \sum_{j: X_j = X_i} K(Y_i, Y_j)$$

with

$$\frac{1}{n} \sum_{i=1}^n \frac{1}{d_i} \sum_{j:(i,j) \in E(G_n)} K(Y_i, Y_j)$$

where $E(G_n)$ is edge set of G_n and d_i is the degree of X_i

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Geometric graph-based estimator

Now

$$\eta_K = \frac{\mathbb{E}K(Y', \tilde{Y}') - \mathbb{E}K(Y_1, Y_2)}{\mathbb{E}K(Y_1, Y_1) - \mathbb{E}K(Y_1, Y_2)}$$

can be estimated by

$$\hat{\eta}_n := \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{d_i} \sum_{j:(i,j) \in E(G_n)} K(Y_i, Y_j) - \frac{1}{n(n-1)} \sum_{i \neq j} K(Y_i, Y_j)}{\frac{1}{n} \sum_{i=1}^n K(Y_i, Y_i) - \frac{1}{n(n-1)} \sum_{i \neq j} K(Y_i, Y_j)}.$$

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Theorem (informal) [Deb, Ghosal and S. (2020+)]

Suppose G_n satisfies the “close”-ness condition in the sense that:

$$\frac{\sum_{(i,j) \in E(G_n)} \rho_{\mathcal{X}}(X_i, X_j)}{|E(G_n)|} \xrightarrow{\mathbb{P}} 0,$$

and $\mathbb{E}K(Y_1, Y_1)^{2+\epsilon} < \infty$ (and other mild technical conditions), then

$$\hat{\eta}_n \xrightarrow{\mathbb{P}} \eta_K.$$

- In particular, $\frac{1}{n} \sum_{i=1}^n \frac{1}{d_i} \sum_{j:(i,j) \in E(G_n)} K(Y_i, Y_j) \xrightarrow{\mathbb{P}} \mathbb{E}K(Y', \tilde{Y}')$

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- No **smoothness assumptions** needed on **conditional distribution of $Y|X$** — motivated directly from the approach used in [Chatterjee, 2019](#), [Azadkia and Chatterjee, 2019](#).
- For **k -NNGs**, $\hat{\eta}_n$ is consistent provided $k = o(n/\log n)$
- Thus, for consistent estimation, a **1-NNG** can be chosen

Rate of convergence (for k -NNG)

Theorem (informal) [Deb, Ghosal and S. (2020+)]

Suppose $K(\cdot, \cdot)$ is **bounded**, $\mathbb{E}[K(Y, \cdot)|X = \cdot]$ is **Lipschitz** with respect to $\rho_X(\cdot, \cdot)$ and the support of μ_X has **intrinsic dimension d_0** . Then

$$\hat{\eta}_n - \eta_K = \begin{cases} \mathcal{O}_{\mathbb{P}}\left(\sqrt{\frac{k}{n}} \log n\right) & \text{if } d_0 \leq 2, \\ \mathcal{O}_{\mathbb{P}}\left(\left(\frac{k}{n}\right)^{1/d_0} \log n\right) & \text{if } d_0 > 2. \end{cases}$$

- Estimation rate **automatically adapts** to **intrinsic dimension** of μ_X

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- Note:
$$\hat{\eta}_n - \eta_K = \underbrace{(\hat{\eta}_n - \mathbb{E}\hat{\eta}_n)}_{\text{Variance term} \sim n^{-1/2}} + \underbrace{(\mathbb{E}\hat{\eta}_n - \eta_K)}_{\text{Bias term} \uparrow k}$$

- **When $Y \perp\!\!\!\perp X$** : Bias is **always 0**, and variance **improves with k** — useful in independence testing.

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Limiting Distribution under Independence (general graph)

Theorem (informal) [Deb, Ghosal and S. (2020+)]

Suppose $\mu = \mu_X \otimes \mu_Y$, then there exists a sequence of random variables $V_n = \mathcal{O}_{\mathbb{P}}(1)$ such that

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- **Result:** A **uniform CLT** holds for a suitable class of graphs \mathcal{G}_n , i.e.,

$$\sup_{G_n \in \mathcal{G}_n} \sup_{x \in \mathbb{R}} \left| \mathbb{P} \left(\frac{\sqrt{n} \hat{\eta}_n}{V_n} \leq x \right) - \Phi(x) \right| \xrightarrow{n \rightarrow \infty} 0$$

- Theorem holds for **data driven** choices \hat{G}_n if $\mathbb{P}(\hat{G}_n \in \mathcal{G}_n) \xrightarrow{n \rightarrow \infty} 1$
- V_n can be computed from the data

Test of Independence

- Consider the **testing** problem:

$$H_0 : \mu = \mu_X \otimes \mu_Y \quad \text{vs} \quad H_1 : \mu \neq \mu_X \otimes \mu_Y.$$

- Recall:** $\eta_K = 0$ iff $\mu = \mu_X \otimes \mu_Y$, $\eta_K > 0$ otherwise, $\hat{\eta}_n \xrightarrow{\mathbb{P}} \eta_K$.
- A natural **level- α** test (for $\alpha \in (0, 1)$):

$$\text{Reject } H_0 \quad \text{if} \quad \frac{\sqrt{n} \hat{\eta}_n}{V_n} \geq z_\alpha$$

- Consistent** and maintains level, i.e.,

$$\lim_{n \rightarrow \infty} \mathbb{P}_{H_0}(\text{Reject } H_0) = \alpha, \quad \lim_{n \rightarrow \infty} \mathbb{P}_{H_1}(\text{Reject } H_0) = 1$$

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- What is the **computational complexity**?

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Computational Complexity

- Suppose G_n is the k -NNG; computable in $\mathcal{O}(kn \log n)$ time
- Recall

$$\hat{\eta}_n = \frac{\underbrace{\frac{1}{n} \sum_{i=1}^n \frac{1}{d_i} \sum_{j:(i,j) \in E(G_n)} K(Y_i, Y_j)}_{\mathcal{O}(kn \log n)} - \frac{1}{n(n-1)} \sum_{i \neq j} K(Y_i, Y_j)}{\underbrace{\frac{1}{n} \sum_{i=1}^n K(Y_i, Y_i)}_{\mathcal{O}(n)} - \underbrace{\frac{1}{n(n-1)} \sum_{i \neq j} K(Y_i, Y_j)}_{(*)}}$$

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- $\sum_{i,j} K(Y_i, Y_j) = \|\sum_{i=1}^n K(Y_i, \cdot)\|_{\mathcal{H}}^2$
- $(*)$ can be computed in **linear time** if $\|\cdot\|_{\mathcal{H}}^2$ is exactly computable, e.g., $K(y_i, y_j) = \langle y_i, y_j \rangle$ Otherwise
- Yields a **near linear time test for independence**; cf. distance correlation (or HSIC) takes $\mathcal{O}(n^2 B)$ time if B permutations are used

Summary

- Class of kernel measures of association (KMAc) when \mathcal{Y} admits a nonnegative definite kernel
- Class of graph-based, consistent estimators (\mathcal{X} — metric space) for KMAc without smoothness on the conditional distribution
- When k -NNG is used, the rate of convergence automatically adapts to the intrinsic dimension of the support of $\mu_{\mathcal{X}}$
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- In the paper, when \mathcal{X} and \mathcal{Y} are Euclidean, we propose another class of measures and estimators that is distribution-free under H_0

Simulations (choice of k)

$(X^{(1)}, X^{(2)}, Y^{(1)}, Y^{(2)}) \sim \mu$ on \mathbb{R}^4 ; $(X^{(1)}, Y^{(1)}), (X^{(2)}, Y^{(2)})$ are i.i.d.

- **W-shape:**

$$Y^{(1)} = |X^{(1)} + 0.5| \mathbf{1}_{X^{(1)} \leq 0} + |X^{(1)} - 0.5| \mathbf{1}_{X^{(1)} > 0} + 0.75\lambda\epsilon,$$

where $\epsilon \sim \mathcal{N}(0, 1)$ with varying λ ; $X \sim \text{Uniform}[-1, 1]$

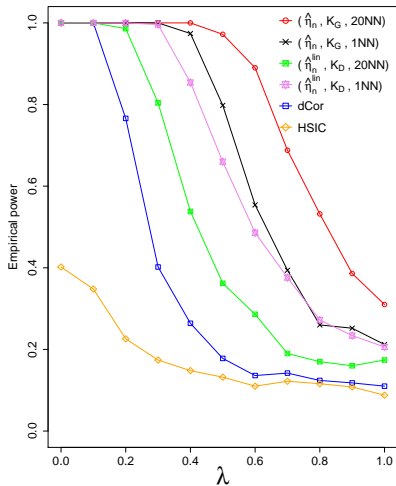
- **Sinusoidal:**

$$Y^{(1)} = \cos(8\pi X^{(1)}) + 3\lambda\epsilon,$$

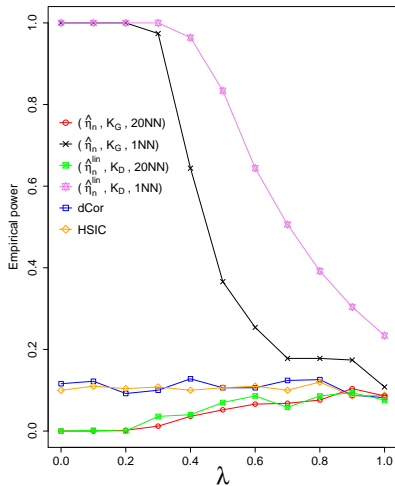
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Sample size $n = 300$

(K_G -Gaussian kernel, K_D -Distance kernel)



W-shaped



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Measure of Conditional Dependence³

- Suppose $(X, Y, Z) \sim \mu$ on some topological space $\mathcal{X} \times \mathcal{Y} \times \mathcal{Z}$
- **Goal:** Measure the **strength** of **conditional dependence** between **Y** and **X** given **Z**

³Joint work with Zhen Huang and Nabarun Deb

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- **Applications:** Model-free **variable selection**, modeling causal relations in graphical models, ...
- We propose and study a class of **nonparametric** yet **interpretable** measures and their **estimates**, a sub-class of which can be computed in **near linear time**

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- Recall **KMAc** (for measuring dependence between **Y** and **X**):

$$\eta_K = \frac{\mathbb{E}K(Y', \tilde{Y}') - \mathbb{E}K(Y_1, Y_2)}{\mathbb{E}K(Y_1, Y_1) - \mathbb{E}K(Y_1, Y_2)} = \frac{\mathbb{E}[\text{MMD}^2(\mu_{Y|X}, \mu_Y)]}{\mathbb{E}[\text{MMD}^2(\delta_Y, \mu_Y)]}$$

where $X' \sim \mu_X$, Y', \tilde{Y}' are drawn independently from $\mu_{Y|X'}$

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- Kernel partial correlation** (KPC) coefficient:

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where: (i) $(X', Z') \sim \mu_{XZ}$ and Y'_2, \tilde{Y}'_2 are i.i.d. $\mu_{Y|(X', Z')}$,
 (ii) $Z' \sim \mu_Z$ and Y', \tilde{Y}' are i.i.d. $\mu_{Y|Z'}$

Can again employ a **geometric graph-based** estimation strategy

- For example, we can estimate

$$\tau_K = \frac{\mathbb{E} \left[\mathbb{E}[k(Y'_2, \tilde{Y}'_2) | X, Z] \right] - \mathbb{E} \left[\mathbb{E}[k(Y', \tilde{Y}') | Z] \right]}{\mathbb{E}[k(Y_1, Y_1)] - \mathbb{E}[\mathbb{E}[k(Y', \tilde{Y}') | Z]]}$$

by a 1-NNG by

$$\hat{\tau}_n := \frac{\frac{1}{n} \sum_{i=1}^n k(Y_i, Y_{\tilde{N}(i)}) - \frac{1}{n} \sum_{i=1}^n k(Y_i, Y_{N(i)})}{\frac{1}{n} \sum_{i=1}^n k(Y_i, Y_i) - \frac{1}{n} \sum_{i=1}^n k(Y_i, Y_{N(i)})}$$

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- **Consistency:** $\hat{\tau}_n \xrightarrow{\mathbb{P}} \tau_K$
- Automatic **adaptation** to the **intrinsic dimensions** of μ_X and μ_{XZ}
- Can develop a fully automatic **stepwise variable selection algorithm** which is provably **consistent** (cf. **Azadkia and Chatterjee, 2019**)

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- M -distributions P_1, \dots, P_M on \mathcal{X} (e.g., metric space)
- **Data:** $\{X_{ij}\}_{j=1}^{n_i} \stackrel{iid}{\sim} P_i$ for $i = 1, \dots, M$
- **Question:** How **different** are the M distributions?

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- **Define:** $Y_{ij} = i$, for $i = 1, \dots, M$
- Consider $\{ \{(X_{ij}, Y_{ij})\}_{j=1}^{n_i} \}_{i=1}^M$; $X \sim \sum_{i=1}^M \pi_i P_{Y_i}$; $\pi_i \approx \frac{n_i}{\sum_{\ell=1}^M n_\ell}$

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- We want to find a class of measures $\gamma \equiv \gamma(P_1, \dots, P_M)$ such that:
 - (i) $\gamma \in [0, 1]$;
 - (ii) $\gamma = 0$ iff $P_1 = \dots = P_M$ (i.e., all the distributions are same);
 - (iii) $\gamma = 1$ iff P_1, \dots, P_M have **disjoint supports**
- **Define:** $Y_{ij} = i$, for $i = 1, \dots, M$
- Consider $\{\{(X_{ij}, Y_{ij})\}_{j=1}^{n_i}\}_{i=1}^M$; $X \sim \sum_{i=1}^M \pi_i P_{Y_i}$; $\pi_i \approx \frac{n_i}{\sum_{\ell=1}^M n_\ell}$
- **Result:** (a) $P_1 = \dots = P_M$ iff $X \perp\!\!\!\perp Y$;
(b) P_1, \dots, P_M have disjoint supports iff Y is a **deterministic function of X**

A measure of dissimilarity between M -distributions

- M -distributions P_1, \dots, P_M on \mathcal{X} (e.g., metric space)
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(b) P_1, \dots, P_M have disjoint supports iff Y is a **deterministic function of X**
- “Similar” **kernel** and **graph-based** strategy yields a desired measure

Summary

- Measure the **strength of association** between X and Y on \mathcal{X} and \mathcal{Y}
- **Class of kernel measures of association** (KMAc) when \mathcal{Y} admits a nonnegative definite kernel
- **Class of geometric graph-based**, consistent estimators (\mathcal{X} — metric space) for KMAc without smoothness on the conditional distribution
- When k -NNG is used, the rate of convergence automatically adapts to the **intrinsic dimension** of the support of μ_X
- Established a **pivotal Gaussian** limit uniformly over a class of graphs

Thank you very much!

Questions?

Near Linear time Estimator

- Note

$$\frac{1}{n(n-1)} \sum_{i \neq j} K(Y_i, Y_j) \approx \mathbb{E}K(Y_1, Y_2)$$

- Replace with

$$\frac{1}{n-1} \sum_{i=1}^{n-1} K(Y_i, Y_{i+1}) \approx \mathbb{E}K(Y_1, Y_2)$$

- Define

$$\hat{\eta}_n^{\text{lin}} := \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{d_i} \sum_{j:(i,j) \in E(G_n)} K(Y_i, Y_j) - \frac{1}{n-1} \sum_{i=1}^{n-1} K(Y_i, Y_{i+1})}{\frac{1}{n} \sum_{i=1}^n K(Y_i, Y_i) - \frac{1}{n-1} \sum_{i=1}^{n-1} K(Y_i, Y_{i+1})}$$

Properties of $\hat{\eta}_n^{\text{lin}}$

- When G_n is k -NNG with $k = \mathcal{O}(1)$, $\hat{\eta}_n^{\text{lin}}$ takes $\mathcal{O}(n \log n)$ time
- $\hat{\eta}_n^{\text{lin}} \xrightarrow{\mathbb{P}} \eta_K$ (the **same measure** of association)
- $\hat{\eta}_n^{\text{lin}}$ has the **same rate of convergence** as $\hat{\eta}_n$
- There exists a sequence of random variables $\tilde{V}_n = \mathcal{O}_{\mathbb{P}}(1)$ such that:

$$\frac{\sqrt{n} \hat{\eta}_n^{\text{lin}}}{\tilde{V}_n} \xrightarrow{d} \mathcal{N}(0, 1)$$

where \tilde{V}_n can be computed in **near linear time**

- Yields a **near linear time test for independence**; cf. distance correlation (or HSIC) takes $\mathcal{O}(n^2 B)$ time if B permutations are used

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- Yields a **near linear time test for independence**; cf. distance correlation (or HSIC) takes $\mathcal{O}(n^2 B)$ time if B permutations are used
- **Price to pay**: Has a **higher** asymptotic variance than $\hat{\eta}_n$