# Measuring Association/Predictive power on Topological Spaces Using Kernels and Graphs 

Nabarun Deb

Department of Statistics
Columbia University

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Joint work with Promit Ghosal (MIT), Zhen Huang (Columbia U) and Bodhisattva Sen (Columbia U)

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$$
\begin{aligned}
& \text { https://arxiv.org/pdf/2010.01768.pdf } \\
& \text { https://arxiv.org/pdf/2012.14804.pdf }
\end{aligned}
$$

## Formal Introduction: Pearson's Correlation and beyond?

- $(X, Y) \sim \mu$ on $\mathcal{X} \times \mathcal{Y}$ (topological spaces) with marginals $\mu_{X}, \mu_{Y}$
- Informal goal: Construct a measure that can capture the strength of association between $X$ and $Y$
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What are truly nonparametric analogs of the Pearson's correlation?

## Think of nonparametric regression

- This asymmetry is fundamental in even simple regression problems, consider the noiseless version:

$$
Y=f(X)
$$

- If $f(\cdot)$ is a many-to-one function, predicting $X$ from $Y$ is not possible whereas predicting $Y$ from $X$ is immediate irrespective of $f(\cdot)$.
- Pearson's correlation being symmetric cannot distinguish between the two problems - same is the case for most measures of dependence.
- Design a directional measure that
(1) is "small" for "predicting" $X$ from $Y$.
(2) but large for "predicting" $Y$ from $X$.


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- Want a measure that equals 0 iff $X \Perp Y$, equals 1 iff $Y$ is "some function" of $X$.
- For the past century, most measures of association/dependence only focus on testing for independence, i.e., they equal 0 iff $Y \Perp X$; 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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## Recent advances

- In Dette et al., 2013, Chatterjee, 2019. When $\mathcal{X}=\mathcal{Y}=\mathbb{R}$, authors propose measures that equal 0 iff $Y \Perp X$ 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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## Structure

(1) A family of measures of association

- A measure on $\mathcal{X}=\mathbb{R}^{d_{1}}, \mathcal{Y}=\mathbb{R}^{d_{2}}$
- Interpretability and monotonicity
- Extending to a class of kernel measures
(2) Estimating the kernel measure
- Proposing the estimator
- Computational complexity
- Consistency
- Rate of estimation
- A central limit theorem when $X \Perp Y$


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## A measure on $\mathcal{X}=\mathbb{R}^{d_{1}}, \mathcal{Y}=\mathbb{R}^{d_{2}}$

## Basic strategy

- Most measures of dependence quantify a "discrepancy" between $\mu$ and $\mu_{X} \otimes \mu_{Y}$.


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- We construct a discrepancy between $\mu_{Y \mid X}$ (regular conditional distribution) and $\mu_{Y}$.
- When $Y \Perp X, \mu_{Y \mid X}=\mu_{Y}$. When $Y$ is a measurable function of $X$, $\mu_{Y \mid X}$ is a degenerate measure.
- Define

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T \equiv T(\mu):=1-\frac{\mathbb{E}\left\|Y^{\prime}-\tilde{Y}^{\prime}\right\|_{2}}{\mathbb{E}\left\|Y_{1}-Y_{2}\right\|_{2}} .
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- Generate $Y_{1}, Y_{2} \stackrel{\text { i.i.d. }}{\sim} \mu_{Y}$.
- $\left(X^{\prime}, Y^{\prime}, \tilde{Y}^{\prime}\right)$ is generated as: draw $X^{\prime} \sim \mu_{X}$ and then $Y^{\prime}\left|X^{\prime} \sim \mu_{Y \mid X^{\prime}}, \tilde{Y}^{\prime}\right| X^{\prime} \sim \mu_{Y \mid X^{\prime}}$ such that $Y^{\prime}$ and $\tilde{Y}^{\prime}$ are conditionally independent given $X^{\prime}$.


## Some intuition

- Suppose $d_{2}=1$.
- Consider a slight modification:

$$
T^{*} \equiv T^{*}(\mu):=1-\frac{\mathbb{E}\left|Y^{\prime}-\tilde{Y}^{\prime}\right|^{2}}{\mathbb{E}\left|Y_{1}-Y_{2}\right|^{2}}
$$

- Plug-in $\mathbb{E}\left|Y^{\prime}-\tilde{Y}^{\prime}\right|^{2}=\mathbb{E}\left|Y^{\prime}\right|^{2}+\mathbb{E}\left|\tilde{Y}^{\prime}\right|^{2}-2 \mathbb{E} Y^{\prime} \tilde{Y}^{\prime}$.
- Do the same for the denominator.
- Simplify $T^{*}(\mu)$ to get:

$$
T^{*}(\mu)=\frac{\operatorname{Var}(\mathbb{E}[Y \mid X])}{\operatorname{Var}(Y)} \in[0,1] .
$$

- $T$ can be interpreted as the proportion of the variance of $Y$ explained by $X$.


## Back to $T(\mu)$ - More intuition

- Recall $X^{\prime} \sim \mu_{X}$ and $Y^{\prime}\left|X^{\prime} \sim \mu_{Y \mid X^{\prime}}, \tilde{Y}^{\prime}\right| X^{\prime} \sim \mu_{Y \mid X^{\prime}}$ such that $Y^{\prime}$ and $\tilde{Y}^{\prime}$ are conditionally independent given $X^{\prime}$.

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T=1-\frac{\mathbb{E}\left\|Y^{\prime}-\tilde{Y}^{\prime}\right\|_{2}}{\mathbb{E}\left\|Y_{1}-Y_{2}\right\|_{2}} .
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$Y^{\prime} \sim \mu_{Y}, \tilde{Y}^{\prime} \sim \mu_{Y}$ but $Y^{\prime}$ and $\tilde{Y}^{\prime}$ are not independent.

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- Suppose $Y \Perp X$, then

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and so $T=0$.

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

$$
Y^{\prime}=\tilde{Y}^{\prime}=h\left(X^{\prime}\right), \quad\left\|Y^{\prime}-\tilde{Y}^{\prime}\right\|_{2}=0
$$

and so $T=1$.

## A formal result

## Theorem

Suppose $\mathbb{E}\left\|Y_{1}\right\|_{2}<\infty$. Then

- $T \in[0,1]$.
- $T=0$ iff $Y \Perp X$.
- $T=1$ iff $Y$ is a noiseless measurable function of $X$.


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- $T=0$ iff $Y \Perp X$.
- $T=1$ iff $Y$ is a noiseless measurable function of $X$.
- The choice $\|\cdot\|_{2}$ is important. For instance,

$$
1-\frac{\mathbb{E}\left\|Y^{\prime}-\tilde{Y}^{\prime}\right\|_{2}^{2}}{\mathbb{E}\left\|Y_{1}-Y_{2}\right\|_{2}^{2}}
$$

can be 0 even when $Y \not \Perp X$.

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What happens in the interval $(0,1)$ ?

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## $T$ for bivariate normal

Suppose $\mu$ is the bivariate normal distribution with means $\mu_{X}, \mu_{Y}$, variances $\sigma_{X}^{2}, \sigma_{Y}^{2}$ and correlation $\rho$. Then

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T(\mu)=1-\sqrt{1-\rho^{2}} .
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Other examples: Let

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Y=\lambda g(X)+\epsilon
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where $\lambda \geq 0, \epsilon, X$ are independent, $\epsilon^{\prime} \stackrel{\text { i.i.d. }}{\sim} \epsilon$ such that $\epsilon-\epsilon^{\prime}$ is unimodal. Then $T(\mu)$ is montonic in $\lambda$.

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In nonparametric regression models with additive noise, $T$ turns out to be a monotonic function of the noise variance.

## Preliminaries: reproducing kernel Hilbert spaces (RKHS)

- RKHS on $\mathcal{Y}$ : linear, complete, inner product space of functions from $\mathcal{Y} \rightarrow \mathbb{R}$; non-negative definite kernel; "reproducing property".
- Consider a non-negative definite kernel function on $\mathcal{Y}$ $K: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ satisfying

$$
\sum_{i, j=1}^{m} \alpha_{i} \alpha_{j} K\left(y_{i}, y_{j}\right) \geq 0
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for all $\alpha_{i} \in \mathbb{R}, y_{i} \in \mathcal{Y}$ and $m \geq 1$.

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- Note $K(y, \cdot): \mathcal{Y} \rightarrow \mathbb{R}$.
- Identify $y \mapsto K(y, \cdot)$ (feature map).
- (Reproducing property) For all $f \in \mathcal{H}, y \in \mathcal{Y},\langle f, K(y, \cdot)\rangle_{\mathcal{H}}=f(y)$.


## RKHS (continued) - useful identities

As a consequence of the reproducing property:

- $\left\langle K\left(y_{1}, \cdot\right), K\left(y_{2}, \cdot\right)\right\rangle_{\mathcal{H}}=K\left(y_{1}, y_{2}\right)$.


## RKHS (continued) - useful identities

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- Using the above,

$$
\begin{aligned}
& \left\|K\left(y_{1}, \cdot\right)-K\left(y_{2}, \cdot\right)\right\|_{\mathcal{H}}^{2} \\
= & \left\langle K\left(y_{1}, \cdot\right), K\left(y_{1}, \cdot\right)\right\rangle_{\mathcal{H}}+\left\langle K\left(y_{2}, \cdot\right), K\left(y_{2}, \cdot\right)\right\rangle_{\mathcal{H}}-2\left\langle K\left(y_{1}, \cdot\right), K\left(y_{2}, \cdot\right)\right\rangle_{\mathcal{H}} \\
= & K\left(y_{1}, y_{1}\right)+K\left(y_{2}, y_{2}\right)-2 K\left(y_{1}, y_{2}\right) .
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## 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

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T=1-\frac{\mathbb{E}\left\|Y^{\prime}-\tilde{Y}^{\prime}\right\|_{2}}{\mathbb{E}\left\|Y_{1}-Y_{2}\right\|_{2}}
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& =1-\frac{\mathbb{E} K\left(Y^{\prime}, Y^{\prime}\right)+\mathbb{E} K\left(\tilde{Y}^{\prime}, \tilde{Y}^{\prime}\right)-2 \mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)}{\mathbb{E} K\left(Y_{1}, Y_{1}\right)+\mathbb{E} K\left(Y_{2}, Y_{2}\right)-2 \mathbb{E} K\left(Y_{1}, Y_{2}\right)}
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& =\frac{\mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)-\mathbb{E} K\left(Y_{1}, Y_{2}\right)}{\mathbb{E} K\left(Y_{1}, Y_{1}\right)-\mathbb{E} K\left(Y_{1}, Y_{2}\right)} .
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## KMAc (continued)

## Theorem (informal)

Suppose $K(\cdot, \cdot)$ is characteristic and $\mathbb{E} K\left(Y_{1}, Y_{1}\right)<\infty$, then:

- $\eta_{K} \in[0,1]$.
- $\eta_{k}=0$ iff $Y \Perp X$.
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- $\eta_{k}=0$ iff $Y \Perp X$.
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- A kernel is characteristic if

$$
\mathbb{E}_{P}[K(Y, \cdot)]=\mathbb{E}_{Q}[K(Y, \cdot)] \Longrightarrow P=Q
$$

for probability measures $P$ and $Q$.

## Examples

Characteristic kernels - Gretton et al., 2012, Sejdinovic et al., 2013, Lyons 2013, 2014. Some examples include:

- (Distance) $K\left(y_{1}, y_{2}\right):=\left\|y_{1}\right\|_{2}+\left\|y_{2}\right\|_{2}-\left\|y_{1}-y_{2}\right\|_{2}$. In this case,

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- Bounded kernels: (Gaussian) $K\left(y_{1}, y_{2}\right):=\exp \left(-\left\|y_{1}-y_{2}\right\|_{2}^{2}\right)$ and (Laplacian) $K\left(y_{1}, y_{2}\right):=\exp \left(-\left\|y_{1}-y_{2}\right\|_{1}\right)$.
- 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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- A measure on $\mathcal{X}=\mathbb{R}^{d_{1}}, \mathcal{Y}=\mathbb{R}^{d_{2}}$
- Interpretability and monotonicity
- Extending to a class of kernel measures
(2) Estimating the kernel measure
- Proposing the estimator
- Computational complexity
- Consistency
- Rate of estimation
- A central limit theorem when $X \Perp Y$


## Estimation strategy

- Suppose $\left(X_{1}, Y_{1}\right), \ldots,\left(X_{n}, Y_{n}\right) \sim \mu$.
- $\mathcal{X}$ is endowed with metric $\rho_{\mathcal{X}}(\cdot, \cdot)$.
- Recall

$$
\eta_{K}=\frac{\mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)-\mathbb{E} K\left(Y_{1}, Y_{2}\right)}{\mathbb{E} K\left(Y_{1}, Y_{1}\right)-\mathbb{E} K\left(Y_{1}, Y_{2}\right)} .
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$$

- From standard U-Statistic theory,

$$
\mathbb{E} K\left(Y_{1}, Y_{1}\right) \approx \frac{1}{n} \sum_{i=1}^{n} K\left(Y_{i}, Y_{i}\right)
$$

and

$$
\frac{1}{n} \sum_{i=1}^{n} K\left(Y_{i}, Y_{i+1}\right) \approx \mathbb{E} K\left(Y_{1}, Y_{2}\right) \approx \frac{1}{n(n-1)} \sum_{i \neq j} K\left(Y_{i}, Y_{j}\right)
$$

- Hardest term to estimate is $\mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)$.


## Estimation (continued)

- Suppose $X$ is supported on a finite set. A natural estimator

$$
\mathbb{E}\left[\mathbb{E}\left[K\left(Y^{\prime}, \tilde{Y}^{\prime}\right) \mid X^{\prime}\right]\right] \approx \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\left|\left\{j: X_{j}=X_{i}\right\}\right|} \sum_{j: X_{j}=X_{i}} K\left(Y_{i}, Y_{j}\right)
$$

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$$

- If $X$ is continuous, replace $X_{j}=X_{i}$ with $\rho_{\mathcal{X}}\left(X_{i}, X_{j}\right)$ being "small".
- Construct a graph $G_{n}$ on $\left\{X_{1}, \ldots, X_{n}\right\}$ which joins points that are "close" to each other.
- For example, consider a $k$-nearest neighbor graph ( $k$-NNG) - join every point to its first $k$ nearest neighbors.


## Estimation (continued)

- Replace

$$
\frac{1}{n} \sum_{i=1}^{n} \frac{1}{\left|\left\{j: X_{j}=X_{i}\right\}\right|} \sum_{j: X_{j}=X_{i}} K\left(Y_{i}, Y_{j}\right)
$$

with

$$
\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i, j) \in E\left(G_{n}\right)} K\left(Y_{i}, Y_{j}\right)
$$

where $E\left(G_{n}\right)$ - edge/neighbor set of $G_{n}$ and $d_{i}$ - degree of $X_{i}$.

## Estimation (continued)

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$$
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$$

where $E\left(G_{n}\right)$ - edge/neighbor set of $G_{n}$ and $d_{i}$ - degree of $X_{i}$.

- Define

$$
\begin{aligned}
& \hat{\eta}_{n}:=\frac{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i, j) \in E\left(G_{n}\right)} K\left(Y_{i}, Y_{j}\right)-\frac{1}{n(n-1)} \sum_{i \neq j} K\left(Y_{i}, Y_{j}\right)}{\frac{1}{n} \sum_{i=1}^{n} K\left(Y_{i}, Y_{i}\right)-\frac{1}{n(n-1)} \sum_{i \neq j} K\left(Y_{i}, Y_{j}\right)} . \\
& \hat{\eta}_{n}^{\text {lin }}:=\frac{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i, j) \in E\left(G_{n}\right)} K\left(Y_{i}, Y_{j}\right)-\frac{1}{n} \sum_{i=1}^{N} K\left(Y_{i}, Y_{i+1}\right)}{\frac{1}{n} \sum_{i=1}^{n} K\left(Y_{i}, Y_{i}\right)-\frac{1}{n} \sum_{i=1}^{N} K\left(Y_{i}, Y_{i+1}\right)} .
\end{aligned}
$$

## Computational complexity

- Suppose $G_{n}$ is the $k$-NNG; computed in $\mathcal{O}(k n \log n)$ time.
- Recall

$$
\hat{\eta}_{n}^{\operatorname{lin}}=\frac{\underbrace{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i, j) \in E\left(G_{n}\right)} K\left(Y_{i}, Y_{j}\right)}_{\mathcal{O}(k n \log n)}-\frac{1}{n} \sum_{i=1}^{N} K\left(Y_{i}, Y_{i+1}\right)}{\underbrace{\frac{1}{n} \sum_{i=1}^{n} K\left(Y_{i}, Y_{i}\right)-\frac{1}{n} \sum_{i=1}^{N} K\left(Y_{i}, Y_{i+1}\right)}_{\mathcal{O}(n)}} .
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$$

- $\hat{\eta}_{n}^{\text {lin }}$ is computable in near linear time as opposed to $\hat{\eta}_{n}$ which may be quadratic. In practice, for certain kernels, one may compute $\hat{\eta}_{n}$ approximately, in near linear time.


## Estimation (continued)

## Theorem (informal)

Suppose $G_{n}$ satisfies the "close"-ness condition in the sense that:

$$
\frac{\sum_{(i, j) \in E\left(G_{n}\right)} \rho_{\mathcal{X}}\left(X_{i}, X_{j}\right)}{\left|E\left(G_{n}\right)\right|} \xrightarrow{\mathbb{P}} 0
$$

and $\mathbb{E} K\left(Y_{1}, Y_{1}\right)^{2+\epsilon}<\infty$, then

$$
\hat{\eta}_{n} \xrightarrow{\mathbb{P}} \eta_{K}, \quad \hat{\eta}_{n}^{\text {lin }} \xrightarrow{\mathbb{P}} \eta_{K} .
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- Under additional moments, convergence happens almost surely in $\mu$ (not required if bounded kernels are used).
- No smoothness assumption needed on $\mathbb{E} K[(\cdot, Y) \mid X]$.


## Examples of graphs (Euclidean)

- Minimum spanning trees, $k$-nearest neighbor graphs - join every point to its first $k$ nearest neighbors.
- For $k-N N G, \hat{\eta}_{n}$ is consistent provided $k=o(n / \log n)$.


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- Minimum spanning trees, $k$-nearest neighbor graphs - join every point to its first $k$ nearest neighbors.
- For $k-N N G, \hat{\eta}_{n}$ is consistent provided $k=o(n / \log n)$.
- Recall

$$
\hat{\eta}_{n}-\eta_{K}=\underbrace{\left(\hat{\eta}_{n}-\mathbb{E} \hat{\eta}_{n}\right)}_{\text {Variance term }}+\underbrace{\left(\mathbb{E} \hat{\eta}_{n}-\eta_{K}\right)}_{\text {Bias term }}
$$

. The bias $\uparrow$ with $k$. However the variances stabilizes because

$$
\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i, j) \in E\left(G_{n}\right)} K\left(Y_{i}, Y_{j}\right)
$$

- For consistent estimation, a 1-NNG can be chosen (no tuning required).


## Rate of estimation ( $k$-NNG)

## Theorem (informal)

Suppose $K(\cdot, \cdot)$ is bounded, $\mathbb{E}[K(Y, \cdot) \mid X=x]$ is Lipschitz with respect to $\rho_{\mathcal{X}}(\cdot, \cdot)$ and the support of $\mu_{X}$ has intrinsic dimension $d_{0}$. Then

$$
\hat{\eta}_{n}^{\text {lin }}-\eta_{K}= \begin{cases}\mathcal{O}_{\mathbb{P}}((\sqrt{k / n})(\log n)) & \text { if } d_{0} \leq 2, \\ \mathcal{O}_{\mathbb{P}}\left((k / n)^{1 / d_{0}}(\log n)\right) & \text { if } d_{0}>2 .\end{cases}
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- The rate of estimation adapts to the intrinsic dimension of $\mu_{X}$ (extension of Azadkia and Chatterjee, 2019).
- Recall

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\hat{\eta}_{n}-\eta_{K}=\underbrace{\left(\hat{\eta}_{n}-\mathbb{E} \hat{\eta}_{n}\right)}_{\text {Variance term } n^{-1 / 2}}+\underbrace{\left(\mathbb{E} \hat{\eta}_{n}-\eta_{K}\right)}_{\text {Bias term } \uparrow_{k}} .
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$$

- When $Y \Perp X$, bias is always 0 and variance improves with $k$ useful in independence testing.


## Limiting null (general graph)

## Theorem (informal)

Suppose $\mu=\mu_{X} \otimes \mu_{Y}$, then there exists sequences of random variables $V_{n}=\mathcal{O}_{\mathbb{P}}(1)$ and $V_{n}^{\text {lin }}$ such that

$$
\frac{\sqrt{n} \hat{\eta}_{n}^{\text {lin }}}{V_{n}^{\operatorname{lin}}} \xrightarrow{d} \mathcal{N}(0,1), \quad \frac{\sqrt{n} \hat{\eta}_{n}}{V_{n}} \xrightarrow{d} \mathcal{N}(0,1) .
$$

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$$

- (Proof) Uses U-statistics projection theory and Stein's method on dependency graphs.
- (General) a uniform CLT holds for a suitable class of graphs $\mathcal{G}_{n}$, i.e.,

$$
\sup _{G_{n} \in \mathcal{G}_{n}} \sup _{x \in \mathbb{R}}\left|\mathbb{P}\left(\sqrt{n} \hat{\eta}_{n}^{\operatorname{lin}} / V_{n} \leq x\right)-\Phi(x)\right| \xrightarrow{n \rightarrow \infty} 0 .
$$

- Theorem holds for data driven choices $\hat{G}_{n}$ provided $\mathbb{P}\left(\hat{G}_{n} \in \mathcal{G}_{n}\right) \xrightarrow{n \rightarrow \infty} 1$.


## Independence testing

- Consider the testing problem:

$$
\mathrm{H}_{0}: \mu=\mu_{X} \otimes \mu_{Y} \quad \text { vs } \quad \mathrm{H}_{1}: \mu \neq \mu_{X} \otimes \mu_{Y}
$$

- 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 test:

$$
\text { Reject if } \sqrt{n} \hat{\eta}_{n}^{\text {lin }} / V_{n} \geq z_{\alpha} \text {. }
$$

- Consistent and maintains level, i.e.,

$$
\lim _{n \rightarrow \infty} \mathbb{P}_{\mathrm{H}_{0}}\left(\text { Reject } \mathrm{H}_{0}\right)=\alpha, \quad \lim _{n \rightarrow \infty} \mathbb{P}_{\mathrm{H}_{1}}\left(\text { Reject } \mathrm{H}_{0}\right)=1
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$$

- Near linear complexity.


## Summary

- Class of kernel measures of association (KMAc) when $\mathcal{Y}$ admits a non-negative 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 adapts to the intrinsic dimension of the support $\mu_{X}$.
- Established a pivotal Gaussian limit uniformly over a class of graphs.
- A linear time estimator + a near linear time test of statistical independence.


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- Established a pivotal Gaussian limit uniformly over a class of graphs.
- A linear time estimator + a near linear time test of statistical independence.
- A wide array of numerical experiments with real and simulated datasets - see https://arxiv.org/pdf/2012.14804.pdf.
Thou Enod


## Simulations (choice of $k$ )

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

- (W-shaped)

$$
\begin{aligned}
& Y^{(1)}=\left|X^{(1)}+0.5\right| 1\left(X^{(1)} \leq 0\right)+\left|X^{(1)}-0.5\right| 1\left(X^{(1)}>0\right)+0.75 \lambda \epsilon, \\
& \epsilon \sim \mathcal{N}(0,1) \text { with varying } \lambda .
\end{aligned}
$$

- (Sinusoidal)

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

$\epsilon \sim \mathcal{N}(0,1)$ with varying $\lambda$.

Sample size $n=300$.

## W-shaped ( $K_{G}$-Gaussian kernel, $K_{D}$-Distance kernel)



## Sinusoidal ( $K_{G}$-Gaussian kernel, $K_{D}$-Distance kernel)



## Conditional association

- Recall

$$
\frac{\underbrace{\mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)}_{{ }^{*} \mu_{Y \mid X}}-\underbrace{\mathbb{E} K\left(Y_{1}, Y_{2}\right)}_{* \mu_{\gamma}}}{\mathbb{E} K\left(Y_{1}, Y_{1}\right)-\mathbb{E} K\left(Y_{1}, Y_{2}\right)}
$$

where $X^{\prime} \sim \mu_{X}, Y^{\prime}, \tilde{Y}^{\prime}$ are drawn independently from $\mu_{Y \mid X^{\prime}}$.

- The surrogate in the numerator show we are comparing $\mu_{Y \mid X}$ with $\mu_{Y}$.


## Conditional association

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$$
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- The surrogate in the numerator show we are comparing $\mu_{Y \mid X}$ with $\mu_{Y}$.
- For conditional association, i.e., how closely is $Y$ associated with $Z$ given $X$, define:

$$
\tilde{\eta}_{K}:=\frac{\underbrace{\mathbb{E} K\left(Y_{2}^{\prime}, \tilde{Y}_{2}^{\prime}\right)}_{{ }^{\prime} \mu_{Y \mid X, Z}}-\underbrace{\mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)}_{{ }_{\mu_{Y \mid X}}}}{\mathbb{E} K\left(Y_{1}, Y_{1}\right)-\mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)}
$$

where $\left(X^{\prime}, Z^{\prime}\right) \sim \mu_{X Z}$ and $Y_{2}^{\prime}, \tilde{Y}_{2}^{\prime}$ are drawn independently from $\mu_{Y \mid\left(X^{\prime}, Z^{\prime}\right)}$.

## Estimating Conditional association

- Recall

$$
T_{1, n}:=\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i, j) \in E\left(G_{n}\right)} K\left(Y_{i}, Y_{j}\right) \approx \mathbb{E} K\left(Y^{\prime}, \tilde{Y}^{\prime}\right)
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where $E\left(G_{n}\right)$ - edge/neighbor set of $G_{n}$, the nearest neighbor graph on $\left(X_{1}, \ldots, X_{n}\right)$ and $d_{i}$ - degree of $X_{i}$.

- Use the estimator

$$
\hat{\tilde{\eta}}_{K}:=\frac{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{\tilde{d}_{i}} \sum_{j:(i, j) \in E\left(\tilde{G}_{n}\right)} K\left(Y_{i}, Y_{j}\right)-T_{1, n}}{\frac{1}{n} \sum_{i=1}^{n} K\left(Y_{i}, Y_{i}\right)-T_{1, n}},
$$

$\tilde{G}_{n}$ — edge/neighbor set of $G_{n}$, the nearest neighbor graph on $\left(X_{1}, Z_{1}\right), \ldots,\left(X_{n}, Z_{n}\right)$ and $\tilde{d}_{i}$ - degree of $\left(X_{i}, Z_{i}\right)$.

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- Then

$$
\hat{\tilde{\eta}}_{K} \xrightarrow{P} \tilde{\eta}_{K} .
$$

Also $\tilde{\eta}_{K} \in[0,1]$ and $\tilde{\eta}_{K}=0$ iff $Y \Perp Z \mid X$ and $\tilde{\eta}_{K}=1$ if $Y$ is a measurable function of $X, Z$.

## Local power in independence testing

- Consider the family of alternatives (Farlie):

$$
f_{X, Y}(x, y)=\left(1-r_{n}\right) f_{1}(x) f_{2}(y)+r_{n} g(x, y) .
$$

- What happens to test based on $\hat{\eta}_{n}^{\text {lin }}$ as $r_{n} \rightarrow 0$ ?


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- What happens to test based on $\hat{\eta}_{n}^{\text {lin }}$ as $r_{n} \rightarrow 0$ ?
- For $d_{1} \leq 7$, power converges to 1 if $r_{n} \gg n^{-1 / 4}$ and to 0 if $r_{n} \ll n^{-1 / 4}$.
- (Blessing of dimensionality?): For $d_{1} \geq 9$, power converges to 1 if $r_{n} \gg n^{-\left(\frac{1}{2}-\frac{2}{d_{1}}\right)}$ and power converges to 0 if $r_{n} \ll n^{-\left(\frac{1}{2}-\frac{2}{d_{1}}\right)}$.
- For $d=8$, the power depends on a rather complicated tradeoff.


## Illustration of monotonicity

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

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\end{aligned}
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## W-shaped (noiseless)



## W-shaped (noisy)



## W-shaped (monotonicity)



## Galton Peas dataset

- Mean diameters of sweet peas in mother plants and daughter plants $(700 \times 2)$



## Galton Peas (continued)

- 7 unique values for the mother $(X)$ and 52 for the daughter $(Y)$.
- $X$ and $Y$ seem to be associated.
- Pearson's correlation $=0.35, p$-value $\ll 0.05$.


## Galton Peas (continued)

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- $X$ and $Y$ seem to be associated.
- Pearson's correlation $=0.35, p$-value $\ll 0.05$.
- Can we say something more?


## A curious observation (Chatterjee, 2020)

|  | Parent |  |  |  |  |  |  |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| Child | 15 | 16 | 17 | 18 | 19 | 20 | 21 |
| 13.77 | 46 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13.92 | 0 | 0 | 37 | 0 | 0 | 0 | 0 |
| 14.07 | 0 | 0 | 0 | 0 | 35 | 0 | 0 |
| 14.28 | 0 | 34 | 0 | 0 | 0 | 0 | 0 |
| 14.35 | 0 | 0 | 0 | 34 | 0 | 0 | 0 |
| 14.66 | 0 | 0 | 0 | 0 | 0 | 23 | 0 |
| 14.67 | 0 | 0 | 0 | 0 | 0 | 0 | 22 |
| 14.77 | 14 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14.92 | 0 | 0 | 16 | 0 | 0 | 0 | 0 |
| 15.07 | 0 | 0 | 0 | 0 | 16 | 0 | 0 |
| 15.28 | 0 | 15 | 0 | 0 | 0 | 0 | 0 |
| 15.35 | 0 | 0 | 0 | 12 | 0 | 0 | 0 |
| 15.66 | 0 | 0 | 0 | 0 | 0 | 10 | 0 |
| 15.67 | 0 | 0 | 0 | 0 | 0 | 0 | 8 |
| 15.77 | 9 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15.92 | 0 | 0 | 13 | 0 | 0 | 0 | 0 |
| 16.07 | 0 | 0 | 0 | 0 | 12 | 0 | 0 |
| 16.28 | 0 | 18 | 0 | 0 | 0 | 0 | 0 |
| 16.35 | 0 | 0 | 0 | 13 | 0 | 0 | 0 |
| 16.66 | 0 | 0 | 0 | 0 | 0 | 12 | 0 |
| 16.67 | 0 | 0 | 0 | 0 | 0 | 0 | 10 |
| 16.77 | 11 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16.92 | 0 | 0 | 16 | 0 | 0 | 0 | 0 |
| 17.07 | 0 | 0 | 0 | 0 | 13 | 0 | 0 |
| 17.28 | 0 | 16 | 0 | 0 | 0 | 0 | 0 |
| 17.35 | 0 | 0 | 0 | 17 | 0 | 0 | 0 |

## A curious observation (Chatterjee, 2020)

|  |  |  | Parent |  |  |  |  |  |  |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | :---: |
| Child | 15 | 16 | 17 | 18 | 19 | 20 | 21 |  |  |
| 13.77 | 46 | 0 | 0 | 0 | 0 | 0 | 0 |  |  |
| 13.92 | 0 | 0 | 37 | 0 | 0 | 0 | 0 |  |  |
| 14.07 | 0 | 0 | 0 | 0 | 35 | 0 | 0 |  |  |
| 14.28 | 0 | 34 | 0 | 0 | 0 | 0 | 0 |  |  |
| 14.35 | 0 | 0 | 0 | 34 | 0 | 0 | 0 |  |  |
| 14.66 | 0 | 0 | 0 | 0 | 0 | 23 | 0 |  |  |
| 14.67 | 0 | 0 | 0 | 0 | 0 | 0 | 22 |  |  |
| 14.77 | 14 | 0 | 0 | 0 | 0 | 0 | 0 |  |  |
| 14.92 | 0 | 0 | 16 | 0 | 0 | 0 | 0 |  |  |
| 1.5 .07 | 0 | 0 | 0 | 0 | 16 | 0 | 0 |  |  |
| 15.28 | 0 | 15 | 0 | 0 | 0 | 0 | 0 |  |  |
| 15.35 | 0 | 0 | 0 | 12 | 0 | 0 | 0 |  |  |
| 15.66 | 0 | 0 | 0 | 0 | 0 | 10 | 0 |  |  |
| 15.67 | 0 | 0 | 0 | 0 | 0 | 0 | 8 |  |  |
| 15.77 | 9 | 0 | 0 | 0 | 0 | 0 | 0 |  |  |
| 15.92 | 0 | 0 | 13 | 0 | 0 | 0 | 0 |  |  |
| 16.07 | 0 | 0 | 0 | 0 | 12 | 0 | 0 |  |  |
| 16.28 | 0 | 18 | 0 | 0 | 0 | 0 | 0 |  |  |
| 16.35 | 0 | 0 | 0 | 13 | 0 | 0 | 0 |  |  |
| 16.66 | 0 | 0 | 0 | 0 | 0 | 12 | 0 |  |  |
| 16.67 | 0 | 0 | 0 | 0 | 0 | 0 | 10 |  |  |
| 16.77 | 11 | 0 | 0 | 0 | 0 | 0 | 0 |  |  |
| 16.92 | 0 | 0 | 16 | 0 | 0 | 0 | 0 |  |  |
| 17.07 | 0 | 0 | 0 | 0 | 13 | 0 | 0 |  |  |
| 17.28 | 0 | 16 | 0 | 0 | 0 | 0 | 0 |  |  |
| 17.35 | 0 | 0 | 0 | 17 | 0 | 0 | 0 |  |  |

- Every row has exactly one non-zero element.


## Galton Peas (continued)

- Recall $X$-mother, $Y$-daughter.
- It is more convenient to predict $X$ from $Y$ (Parent from daughter) than the other way round.
- Pearson's correlation being symmetric cannot distinguish between the two problems - same is the case for most measures of dependence.


## Galton Peas (continued)

- Recall $X$-mother, $Y$-daughter.
- It is more convenient to predict $X$ from $Y$ (Parent from daughter) than the other way round.
- Pearson's correlation being symmetric cannot distinguish between the two problems - same is the case for most measures of dependence.
- How to design a measure that captures this asymmetry?

