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

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- Informal goal: Construct a measure that can capture the

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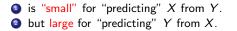
What are truly nonparametric analogs of the Pearson's correlation?

# Think of nonparametric regression

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

$$Y=f(X).$$

- If f(·) is a many-to-one function, predicting X from Y is not possible whereas predicting Y from X is immediate irrespective of f(·).
- 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



- 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 ⊥⊥ 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 X = Y = ℝ, authors propose measures that equal 0 iff Y ⊥⊥ X and 1 iff Y is a measurable function of X. Extended to the case X = ℝ<sup>d₁</sup> and Y = ℝ in Azadkia and Chatterjee, 2019.

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- Bottleneck: They rely on the canonical ordering of  $\mathbb{R}$ .

### Introduction

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- Bottleneck: They rely on the canonical ordering of  $\mathbb{R}$ .

### 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  $X \perp \!\!\!\perp Y$

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

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Define

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- When  $Y \perp X$ ,  $\mu_{Y|X} = \mu_Y$ . When Y is a measurable function of X,  $\mu_{Y|X}$  is a degenerate measure.

$$\mathcal{T} \equiv \mathcal{T}(\mu) := 1 - rac{\mathbb{E} \| Y' - \widetilde{Y}' \|_2}{\mathbb{E} \| Y_1 - Y_2 \|_2}.$$

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

# Some intuition

- Suppose  $d_2 = 1$ .
- Consider a slight modification:

$$T^* \equiv T^*(\mu) := 1 - rac{\mathbb{E} |Y' - ilde{Y}'|^2}{\mathbb{E} |Y_1 - Y_2|^2}.$$

- Plug-in  $\mathbb{E}|Y' \tilde{Y}'|^2 = \mathbb{E}|Y'|^2 + \mathbb{E}|\tilde{Y}'|^2 2\mathbb{E}Y'\tilde{Y}'.$
- Do the same for the denominator.
- Simplify  $T^*(\mu)$  to get:

$$T^*(\mu) = rac{\mathsf{Var}(\mathbb{E}[Y|X])}{\mathsf{Var}(Y)} \in [0,1].$$

• *T* can be interpreted as the proportion of the variance of *Y* explained by *X*.

# Back to $T(\mu)$ — More intuition

• Recall  $X' \sim \mu_X$  and  $Y'|X' \sim \mu_{Y|X'}$ ,  $\tilde{Y}'|X' \sim \mu_{Y|X'}$  such that Y' and  $\tilde{Y'}$  are conditionally independent given X'.

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

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• Suppose  $Y \perp X$ , then

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

$$Y' = \tilde{Y'} = h(X'), \quad ||Y' - \tilde{Y'}||_2 = 0$$

and so T = 1.

#### Theorem

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

- $T \in [0, 1].$
- T = 0 iff  $Y \perp X$ .
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- $T \in [0, 1].$
- 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,

$$1 - rac{\mathbb{E} \|Y' - ilde{Y}'\|_2^2}{\mathbb{E} \|Y_1 - Y_2\|_2^2}$$

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

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#### $\ensuremath{\mathcal{T}}$ 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

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

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

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Other examples: Let

$$Y = \lambda g(X) + \epsilon$$

where  $\lambda \geq 0$ ,  $\epsilon, X$  are independent,  $\epsilon' \stackrel{i.i.d.}{\sim} \epsilon$  such that  $\epsilon - \epsilon'$  is unimodal. Then  $T(\mu)$  is montonic in  $\lambda$ . What happens in the interval (0,1)?

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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  $\mathcal{Y} \to \mathbb{R}$ ; non-negative definite kernel; "reproducing property".
- Consider a non-negative definite kernel function on  $\mathcal{Y} \mathcal{K} : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$  satisfying

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

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

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

As a consequence of the reproducing property:

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• Using the above,

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

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

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

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$$\eta_{\mathcal{K}} := 1 - \frac{\mathbb{E} \|\mathcal{K}(\mathcal{Y}', \cdot) - \mathcal{K}(\tilde{\mathcal{Y}}', \cdot)\|_{\mathcal{H}}^2}{\mathbb{E} \|\mathcal{K}(\mathcal{Y}_1, \cdot) - \mathcal{K}(\mathcal{Y}_2, \cdot)\|_{\mathcal{H}}^2}$$

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$$\begin{split} \eta_{\mathcal{K}} &:= 1 - \frac{\mathbb{E} \|\mathcal{K}(Y', \cdot) - \mathcal{K}(\tilde{Y}', \cdot)\|_{\mathcal{H}}^2}{\mathbb{E} \|\mathcal{K}(Y_1, \cdot) - \mathcal{K}(Y_2, \cdot)\|_{\mathcal{H}}^2} \\ &= 1 - \frac{\mathbb{E} \mathcal{K}(Y', Y') + \mathbb{E} \mathcal{K}(\tilde{Y}', \tilde{Y}') - 2\mathbb{E} \mathcal{K}(Y', \tilde{Y}')}{\mathbb{E} \mathcal{K}(Y_1, Y_1) + \mathbb{E} \mathcal{K}(Y_2, Y_2) - 2\mathbb{E} \mathcal{K}(Y_1, Y_2)} \end{split}$$

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#### Theorem (informal)

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

- $\eta_{K} \in [0, 1].$
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- $\eta_k = 0$  iff  $Y \perp X$ .
- $\eta_K = 1$  iff Y is a noiseless measurable function of X.
- 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.

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

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

 $\eta_{K} = T.$ 

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$$\eta_{\mathbf{K}} = \mathbf{T}.$$

- 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  $(X_1, Y_1), ..., (X_n, Y_n) \sim \mu$ .
- $\mathcal{X}$  is endowed with metric  $\rho_{\mathcal{X}}(\cdot, \cdot)$ .
- Recall

$$\eta_{\mathcal{K}} = \frac{\mathbb{E}\mathcal{K}(\mathcal{Y}', \tilde{\mathcal{Y}}') - \mathbb{E}\mathcal{K}(\mathcal{Y}_1, \mathcal{Y}_2)}{\mathbb{E}\mathcal{K}(\mathcal{Y}_1, \mathcal{Y}_1) - \mathbb{E}\mathcal{K}(\mathcal{Y}_1, \mathcal{Y}_2)}.$$

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- From standard U-Statistic theory,

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

and

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

• Hardest term to estimate is  $\mathbb{E}K(Y', \tilde{Y'})$ .

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

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

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

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

- If X is continuous, replace  $X_j = X_i$  with  $\rho_{\mathcal{X}}(X_i, X_j)$  being "small".
- Construct a graph  $G_n$  on  $\{X_1, \ldots, X_n\}$  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.

Replace

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

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  $E(G_n)$  — edge/neighbor set of  $G_n$  and  $d_i$  — degree of  $X_i$ .

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where  $E(G_n)$  — edge/neighbor set of  $G_n$  and  $d_i$  — degree of  $X_i$ .

Define

$$\hat{\eta}_{n} := \frac{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_{i}} \sum_{j:(i,j) \in E(G_{n})} K(Y_{i}, Y_{j}) - \frac{1}{n(n-1)} \sum_{i \neq j} K(Y_{i}, Y_{j})}{\frac{1}{n} \sum_{i=1}^{n} K(Y_{i}, Y_{i}) - \frac{1}{n(n-1)} \sum_{i \neq j} K(Y_{i}, Y_{j})}.$$

$$\hat{\eta}_n^{\mathsf{lin}} := \frac{\frac{1}{n} \sum_{i=1}^n \frac{1}{d_i} \sum_{j:(i,j) \in \mathsf{E}(\mathsf{G}_n)} \mathsf{K}(\mathsf{Y}_i, \mathsf{Y}_j) - \frac{1}{n} \sum_{i=1}^N \mathsf{K}(\mathsf{Y}_i, \mathsf{Y}_{i+1})}{\frac{1}{n} \sum_{i=1}^n \mathsf{K}(\mathsf{Y}_i, \mathsf{Y}_i) - \frac{1}{n} \sum_{i=1}^N \mathsf{K}(\mathsf{Y}_i, \mathsf{Y}_{i+1})}.$$

# Computational complexity

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

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

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Theorem (informal)

Suppose  $G_n$  satisfies the "close"-ness condition in the sense that:

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

and  $\mathbb{E} \mathcal{K}(Y_1,Y_1)^{2+\epsilon} < \infty$ , then

$$\hat{\eta}_n \stackrel{\mathbb{P}}{\longrightarrow} \eta_K, \qquad \hat{\eta}_n^{\text{lin}} \stackrel{\mathbb{P}}{\longrightarrow} \eta_K.$$

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$$\hat{\eta}_n \xrightarrow{\mathbb{P}} \eta_K, \qquad \hat{\eta}_n^{\text{lin}} \xrightarrow{\mathbb{P}} \eta_K.$$

- Under additional moments, convergence happens almost surely in μ (not required if bounded kernels are used).
- No smoothness assumption needed on  $\mathbb{E}K[(\cdot, Y)|X]$ .

## Examples of graphs (Euclidean)

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

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- For k-NNG,  $\hat{\eta}_n$  is consistent provided  $k = o(n/\log n)$ .
- Recall

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

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

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

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

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

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When Y ⊥⊥ 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

$$\frac{\sqrt{n}\hat{\eta}_n^{\mathsf{lin}}}{V_n^{\mathsf{lin}}} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1), \qquad \frac{\sqrt{n}\hat{\eta}_n}{V_n} \stackrel{d}{\longrightarrow} \mathcal{N}(0,1).$$

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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.,

$$\sup_{G_n\in\mathcal{G}_n}\sup_{x\in\mathbb{R}}\left|\mathbb{P}(\sqrt{n}\hat{\eta}_n^{\mathsf{lin}}/V_n\leq x)-\Phi(x)\right|\overset{n\to\infty}{\longrightarrow}0.$$

• Theorem holds for data driven choices  $\hat{G}_n$  provided  $\mathbb{P}(\hat{G}_n \in \mathcal{G}_n) \xrightarrow{n \to \infty} 1.$ 

### Independence testing

• Consider the testing problem:

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

• Recall  $\eta_{\mathcal{K}} = 0$  iff  $\mu = \mu_{\mathcal{X}} \otimes \mu_{\mathcal{Y}}, \eta_{\mathcal{K}} > 0$  otherwise,  $\hat{\eta}_n \stackrel{\mathbb{P}}{\longrightarrow} \eta_{\mathcal{K}}$ .

A natural test:

Reject if  $\sqrt{n}\hat{\eta}_n^{\text{lin}}/V_n \ge z_{\alpha}$ .

• Consistent and maintains level, i.e.,

$$\lim_{n\to\infty}\mathbb{P}_{\mathrm{H}_0}(\mathsf{Reject}\ \mathrm{H}_0)=\alpha,\quad \lim_{n\to\infty}\mathbb{P}_{\mathrm{H}_1}(\mathsf{Reject}\ \mathrm{H}_0)=1.$$

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• Near linear complexity.

- Class of kernel measures of association (KMAc) when  $\mathcal Y$  admits a non-negative definite kernel.
- Class of graph-based, consistent estimators (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 μ<sub>X</sub>.
- 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.



# Simulations (choice of k)

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

• (W-shaped)

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

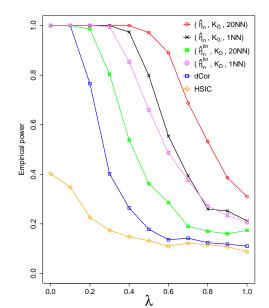
 $\epsilon \sim \mathcal{N}(0,1)$  with varying  $\lambda$ .

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

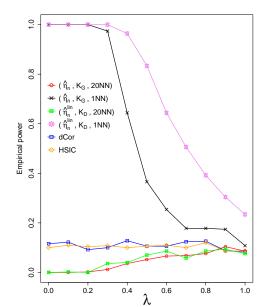
 $\epsilon \sim \mathcal{N}(0,1)$  with varying  $\lambda$ .

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

$$\eta_{\mathcal{K}} = \frac{\underbrace{\mathbb{E}\mathcal{K}(Y', \tilde{Y'})}_{*\mu_{Y|X}} - \underbrace{\mathbb{E}\mathcal{K}(Y_1, Y_2)}_{*\mu_{Y}}}_{\mathbb{E}\mathcal{K}(Y_1, Y_1) - \mathbb{E}\mathcal{K}(Y_1, Y_2)}$$

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

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

### Conditional association

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

$$\tilde{\eta}_{\mathcal{K}} := \frac{\underbrace{\mathbb{E}\mathcal{K}(Y'_{2}, \tilde{Y}'_{2})}_{*\mu_{Y|X,Z}} - \underbrace{\mathbb{E}\mathcal{K}(Y', \tilde{Y}')}_{*\mu_{Y|X}}}{\mathbb{E}\mathcal{K}(Y_{1}, Y_{1}) - \mathbb{E}\mathcal{K}(Y', \tilde{Y}')}$$

where  $(X', Z') \sim \mu_{XZ}$  and  $Y'_2, \tilde{Y'_2}$  are drawn independently from  $\mu_{Y|(X',Z')}$ .

### Estimating Conditional association

Recall

$$T_{1,n} := \frac{1}{n} \sum_{i=1}^{n} \frac{1}{d_i} \sum_{j:(i,j) \in E(G_n)} K(Y_i, Y_j) \approx \mathbb{E}K(Y', \tilde{Y}')$$

where  $E(G_n)$  — edge/neighbor set of  $G_n$ , the nearest neighbor graph on  $(X_1, \ldots, X_n)$  and  $d_i$  — degree of  $X_i$ .

Use the estimator

$$\hat{\tilde{\eta}}_{\mathcal{K}} := \frac{\frac{1}{n} \sum_{i=1}^{n} \frac{1}{\tilde{d}_{i}} \sum_{j:(i,j) \in \boldsymbol{E}(\tilde{G}_{n})} \boldsymbol{K}(\boldsymbol{Y}_{i}, \boldsymbol{Y}_{j}) - \boldsymbol{T}_{1,n}}{\frac{1}{n} \sum_{i=1}^{n} \boldsymbol{K}(\boldsymbol{Y}_{i}, \boldsymbol{Y}_{i}) - \boldsymbol{T}_{1,n}},$$

 $\hat{G}_n$  — edge/neighbor set of  $G_n$ , the nearest neighbor graph on  $(X_1, Z_1), \ldots, (X_n, Z_n)$  and  $\tilde{d}_i$  — degree of  $(X_i, Z_i)$ .

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Then

$$\hat{\tilde{\eta}}_K \xrightarrow{P} \tilde{\eta}_K.$$

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

• Consider the family of alternatives (Farlie):

 $f_{X,Y}(x,y) = (1-r_n)f_1(x)f_2(y) + r_ng(x,y).$ 

• What happens to test based on  $\hat{\eta}_n^{\text{lin}}$  as  $r_n \to 0$ ?

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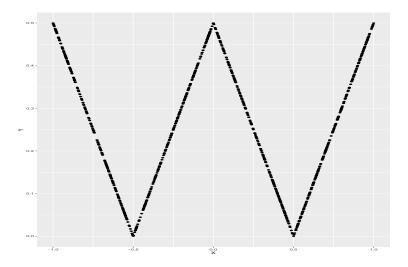
- What happens to test based on  $\hat{\eta}_n^{\sf lin}$  as  $r_n \to 0$ ?
- For  $d_1 \leq 7$ , power converges to 1 if  $r_n \gg n^{-1/4}$  and to 0 if  $r_n \ll n^{-1/4}$ .
- (Blessing of dimensionality?): For  $d_1 \ge 9$ , power converges to 1 if  $r_n \gg n^{-\left(\frac{1}{2} \frac{2}{d_1}\right)}$  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.

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

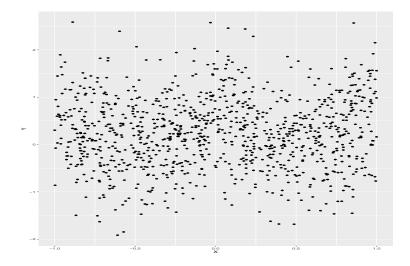
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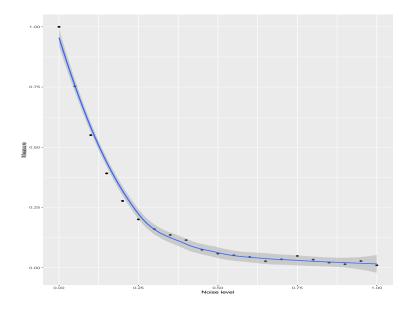
# W-shaped (noiseless)



# W-shaped (noisy)

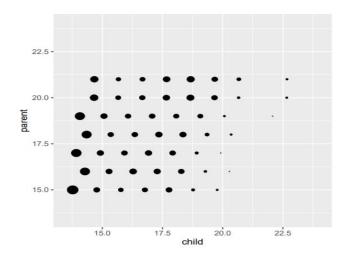


# W-shaped (monotonicity)



### Galton Peas dataset

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



- 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  $\ll 0.05$ .

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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			
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• Every row has exactly one non-zero element.

- 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.

- 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?