

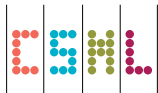
# A Kernel Test for Three Variable Interactions

Dino Sejdinovic<sup>1</sup>, Arthur Gretton<sup>1</sup>, Wicher Bergsma<sup>2</sup>

<sup>1</sup>Gatsby Unit, CSML, University College London

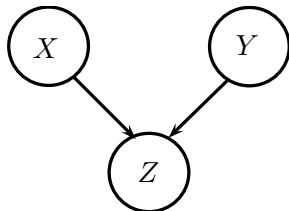
<sup>2</sup>Department of Statistics, London School of Economics

NIPS, 07 Dec 2013



## Detecting a higher order interaction

- How to detect V-structures with pairwise weak (or nonexistent) dependence?



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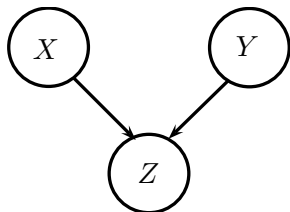
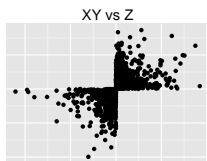
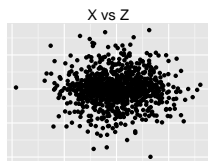
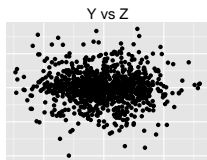
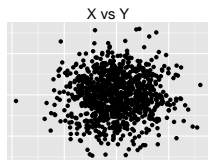
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## Detecting a higher order interaction

- How to detect V-structures with pairwise weak (or nonexistent) dependence?

- $X \perp\!\!\!\perp Y, Y \perp\!\!\!\perp Z, X \perp\!\!\!\perp Z$



- $X, Y \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1),$
- $Z | X, Y \sim \text{sign}(XY) \text{Exp}\left(\frac{1}{\sqrt{2}}\right)$

# Detecting pairwise dependence

- How to detect dependence in a **non-Euclidean / structured** domain?

$X_1$ : Honourable senators, I have a question for the Leader of the Government in the Senate with regard to the support funding to farmers that has been announced. Most farmers have not received any money yet.

$X_2$ : No doubt there is great pressure on provincial and municipal governments in relation to the issue of child care, but the reality is that there have been no cuts to child care funding from the federal government to the provinces. In fact, we have increased federal investments for early childhood development.

...

$Y_1$ : Honorables sénateurs, ma question s'adresse au leader du gouvernement au Sénat et concerne l'aide financière qu'on a annoncée pour les agriculteurs. La plupart des agriculteurs n'ont encore rien reçu de cet argent.

$Y_2$ : Il est évident que les ordres de gouvernements provinciaux et municipaux subissent de fortes pressions en ce qui concerne les services de garde, mais le gouvernement n'a pas réduit le financement qu'il verse aux provinces pour les services de garde. Au contraire, nous avons augmenté le financement fédéral pour le développement des jeunes enfants.

...

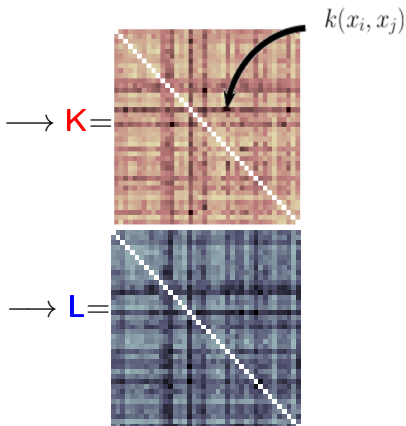


Are the French text extracts translations of the English ones?

# Detecting pairwise dependence

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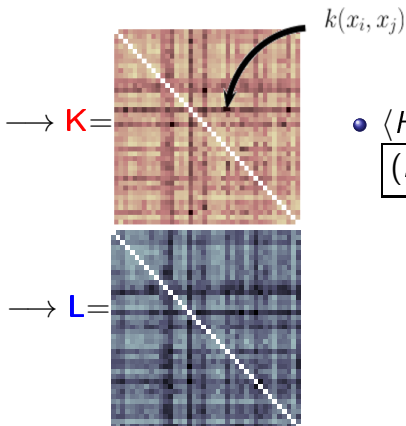
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- $\langle HKH, H LH \rangle = \boxed{(HKH \circ H LH)_{++}}$ 
  - $H = I - \frac{1}{n} \mathbf{1} \mathbf{1}^\top$   
(centering matrix)
  - $A_{++} = \sum_{i=1}^n \sum_{j=1}^n A_{ij}$

# Kernel Embedding

- feature map:  $z \mapsto k(\cdot, z) \in \mathcal{H}_k$   
instead of  $z \mapsto (\varphi_1(z), \dots, \varphi_s(z)) \in \mathbb{R}^s$
- $\langle k(\cdot, z), k(\cdot, w) \rangle_{\mathcal{H}_k} = k(z, w)$   
inner products easily **computed**



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- embedding:  $P \mapsto \mu_k(P) = \mathbb{E}_{Z \sim P} k(\cdot, Z) \in \mathcal{H}_k$   
instead of  $P \mapsto (\mathbb{E}\varphi_1(Z), \dots, \mathbb{E}\varphi_s(Z)) \in \mathbb{R}^s$
- $\langle \mu_k(P), \mu_k(Q) \rangle_{\mathcal{H}_k} = \mathbb{E}_{Z \sim P, W \sim Q} k(Z, W)$   
inner products easily **estimated**

# Independence test via embeddings

- **Maximum Mean Discrepancy (MMD)**

(Borgwardt et al, 2006; Gretton et al, 2007):

$$MMD_k(P, Q) = \|\mu_k(P) - \mu_k(Q)\|_{\mathcal{H}_k}$$

- **ISPD kernels:**  $\mu_k$  injective on **all signed measures** and  $MMD_k$  metric (Sriperumbudur, 2010)
  - Gaussian, Laplacian, inverse multiquadratics, Matérn etc.

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- **Hilbert-Schmidt Independence Criterion (HSIC)**

Gretton et al (2005, 2008); Smola et al (2007):

$$\|\mu_{\kappa}(P_{X,Y}) - \mu_{\kappa}(P_X P_Y)\|_{\mathcal{H}_{\kappa}}^2$$

$$k(\boxed{1}, \boxed{2}) \quad l(\boxed{1}, \boxed{2})$$

↓

$$\kappa(\boxed{1,1}, \boxed{2,2}) =$$
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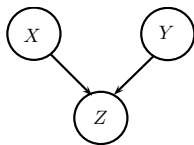
$$\|\mu_{\kappa}(P_{X,Y}) - \mu_{\kappa}(P_X P_Y)\|_{\mathcal{H}_{\kappa}}^2$$

- Empirical HSIC =  $\frac{1}{n^2} \boxed{(H\mathbf{K}H \circ H\mathbf{L}H)_{++}}$

Powerful independence tests that generalize dCov of Szekely et al (2007); DS et al (2013)

$$k(\boxed{1}, \boxed{2}) \quad l(\boxed{1}, \boxed{2})$$
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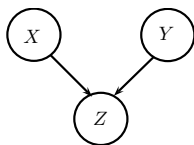
# V-structure Discovery



Assume  $X \perp\!\!\!\perp Y$  has been established. V-structure can then be detected by:

- CI test:  $H_0 : X \perp\!\!\!\perp Y | Z$  (Zhang et al 2011) or

## V-structure Discovery

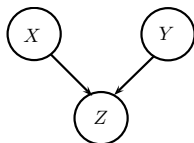
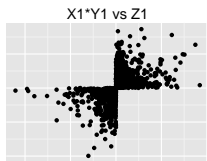
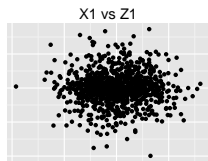
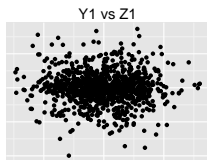
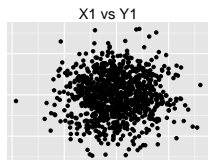


Assume  $X \perp\!\!\!\perp Y$  has been established. V-structure can then be detected by:

- **CI test:**  $\mathbf{H}_0 : X \perp\!\!\!\perp Y|Z$  (Zhang et al 2011) or
- **Factorisation test:**  $\mathbf{H}_0 : (X, Y) \perp\!\!\!\perp Z \vee (X, Z) \perp\!\!\!\perp Y \vee (Y, Z) \perp\!\!\!\perp X$  (multiple standard two-variable tests)
  - compute  $p$ -values for each of the marginal tests for  $(Y, Z) \perp\!\!\!\perp X$ ,  $(X, Z) \perp\!\!\!\perp Y$ , or  $(X, Y) \perp\!\!\!\perp Z$
  - apply Holm-Bonferroni (**HB**) sequentially rejective correction (Holm 1979)

## V-structure Discovery (2)

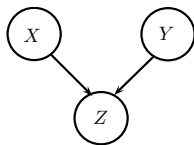
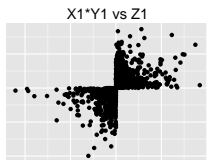
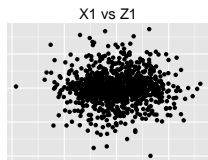
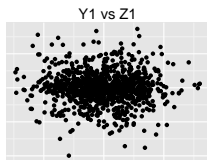
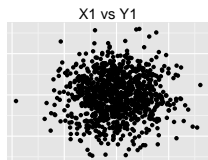
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- $X_{2:p}, Y_{2:p}, Z_{2:p} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, I_{p-1})$



## V-structure Discovery (3)

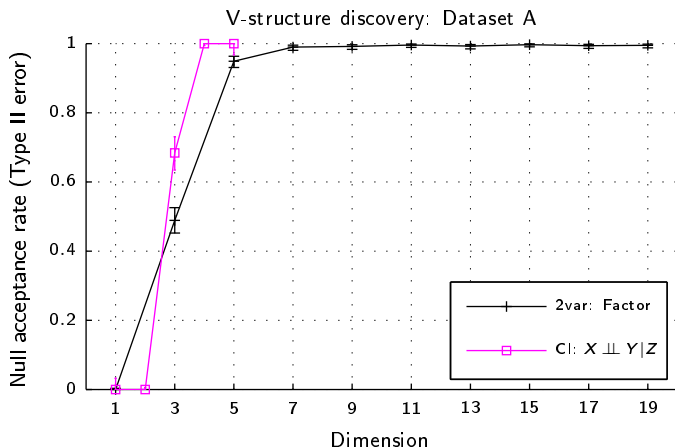


Figure: CI test for  $X \perp\!\!\!\perp Y|Z$  from Zhang et al (2011), and a factorisation test with a **HB** correction,  $n = 500$

# Lancaster Interaction Measure

**Definition** (Bahadur (1961); Lancaster (1969))

**Interaction measure** of  $(X_1, \dots, X_D) \sim P$  is a signed measure  $\Delta P$  that **vanishes** whenever  $P$  can be factorised in a non-trivial way as a product of its (possibly multivariate) marginal distributions.

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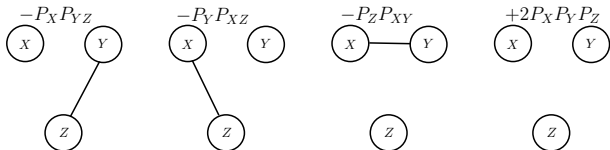
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$$\Delta_L P = P_{XYZ}$$



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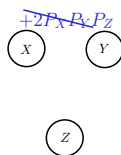
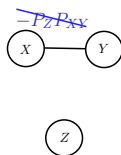
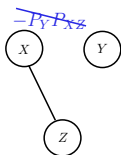
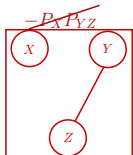
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$$\Delta_L P = 0$$

~~$P_{XYZ}$~~



## A Test using Lancaster Measure

- Construct a test by estimating  $\|\mu_\kappa(\Delta_L P)\|_{\mathcal{H}_\kappa}^2$ , where  $\kappa = k \otimes l \otimes m$ :

$$\begin{aligned} & \|\mu_\kappa(P_{XYZ} - P_{XY}P_Z - \dots)\|_{\mathcal{H}_\kappa}^2 = \\ & \langle \mu_\kappa P_{XYZ}, \mu_\kappa P_{XYZ} \rangle_{\mathcal{H}_\kappa} - 2 \langle \mu_\kappa P_{XYZ}, \mu_\kappa P_{XY}P_Z \rangle_{\mathcal{H}_\kappa} \dots \end{aligned}$$

# Inner Product Estimators

$\nu \setminus \nu'$	$P_{XYZ}$	$P_{XY}P_Z$	$P_{XZ}P_Y$	$P_{YZ}P_X$	$P_XP_YP_Z$
$P_{XYZ}$	$(K \circ L \circ M)_{++}$	$((K \circ L)M)_{++}$	$((K \circ M)L)_{++}$	$((M \circ L)K)_{++}$	$tr(K_+ \circ L_+ \circ M_+)$
$P_{XY}P_Z$		$(K \circ L)_{++} M_{++}$	$(MKL)_{++}$	$(KLM)_{++}$	$(KL)_{++} M_{++}$
$P_{XZ}P_Y$			$(K \circ M)_{++} L_{++}$	$(KML)_{++}$	$(KM)_{++} L_{++}$
$P_{YZ}P_X$				$(L \circ M)_{++} K_{++}$	$(LM)_{++} K_{++}$
$P_XP_YP_Z$					$K_{++}L_{++}M_{++}$

Table:  $V$ -statistic estimators of  $\langle \mu_{\kappa} \nu, \mu_{\kappa} \nu' \rangle_{\mathcal{H}_{\kappa}}$



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$P_{XYZ}$	$(K \circ L \circ M)_{++}$	$((K \circ L)M)_{++}$	$((K \circ M)L)_{++}$	$((M \circ L)K)_{++}$	$\text{tr}(K_{++} \circ L_{++} \circ M_{++})$
$P_{XY}P_Z$		$(K \circ L)_{++} M_{++}$	$(MKL)_{++}$	$(KLM)_{++}$	$(KL)_{++} M_{++}$
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Proposition (Lancaster interaction statistic)

$$\|\mu_{\kappa}(\Delta_L P)\|_{\mathcal{H}_{\kappa}}^2 = \frac{1}{n^2} \boxed{(HKH \circ H L H \circ H M H)_{++}}$$

Empirical joint central moment in the feature space

## Example A: factorisation tests

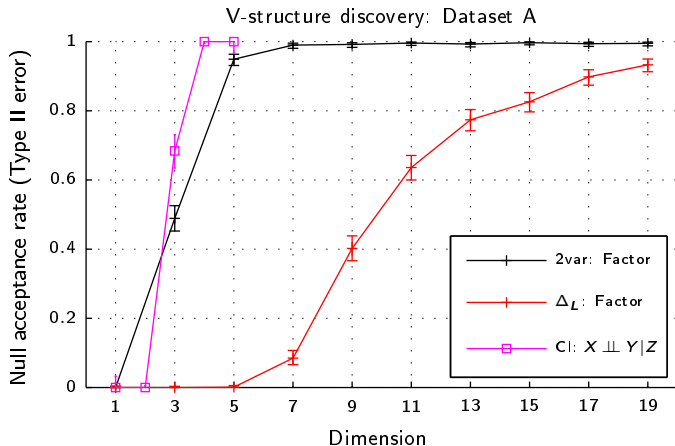


Figure: Factorisation hypothesis: Lancaster statistic vs. a two-variable based test (both with **HB** correction); Test for  $X \perp\!\!\!\perp Y|Z$  from Zhang et al (2011),  $n = 500$

## Example B: Joint dependence can be easier to detect

- $X_1, Y_1 \stackrel{i.i.d.}{\sim} \mathcal{N}(0, 1)$
- $Z_1 = \begin{cases} X_1^2 + \epsilon, & w.p. 1/3, \\ Y_1^2 + \epsilon, & w.p. 1/3, \\ X_1 Y_1 + \epsilon, & w.p. 1/3, \end{cases}$  where  $\epsilon \sim \mathcal{N}(0, 0.1^2)$ .
- $X_{2:p}, Y_{2:p}, Z_{2:p} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, I_{p-1})$
- dependence of  $Z$  on pair  $(X, Y)$  is stronger than on  $X$  and  $Y$  individually

## Example B: factorisation tests

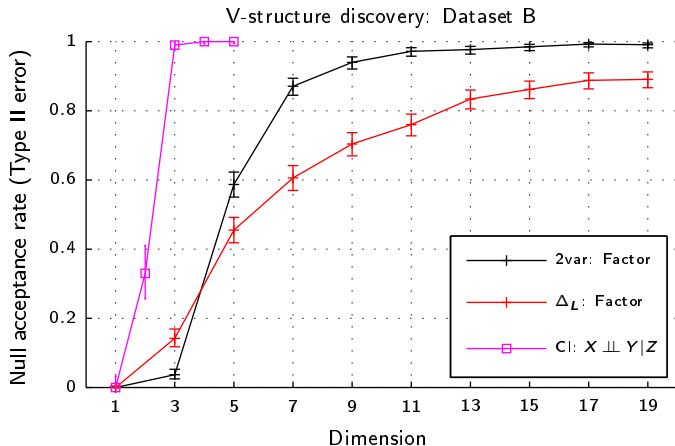


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## Interaction for $D \geq 4$

- Interaction measure valid for all  $D$   
(Streitberg, 1990):

$$\Delta_S P = \sum_{\pi} (-1)^{|\pi|-1} (|\pi| - 1)! J_{\pi} P$$

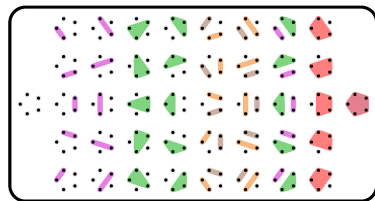
- For a partition  $\pi$ ,  $J_{\pi}$  associates to the joint the corresponding factorisation, e.g.,  $J_{13|2|4} P = P_{X_1 X_3} P_{X_2} P_{X_4}$ .

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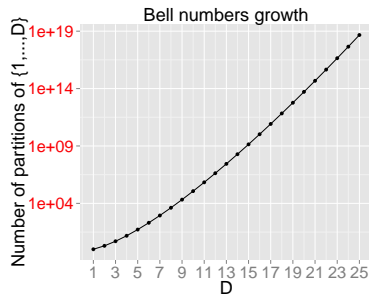


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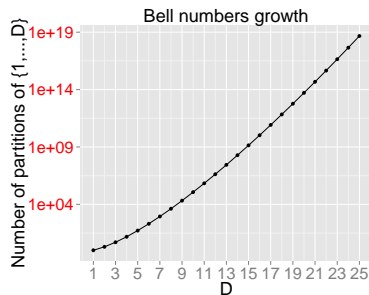
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**joint central moments** (Lancaster interaction)

vs.

**joint cumulants** (Streitberg interaction)





# Summary

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Thank You!

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