

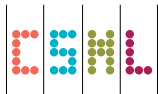
# Hypothesis Testing with Pairwise Distances and Associated Kernels

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## Two-sample and independence tests

- **Two-sample test:** Given  $\{Z^{(i)}\}_{i=1}^{n_z} \stackrel{i.i.d.}{\sim} P$ , and  $\{W^{(i)}\}_{i=1}^{n_w} \stackrel{i.i.d.}{\sim} Q$ ,
  - $H_0: P = Q$
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  - $H_0: P = Q$
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- **Independence test:** Given  $\{(X^{(i)}, Y^{(i)})\}_{i=1}^m \stackrel{i.i.d.}{\sim} P_{XY}$ ,
  - $H_0: P_{XY} = P_X P_Y$
  - $H_A: P_{XY} \neq P_X P_Y$

# Energy distance and distance covariance

- **Energy distance:**

$$D_E(P, Q) = 2\mathbb{E}_{ZW} \|Z - W\|_2 - \mathbb{E}_{ZZ'} \|Z - Z'\|_2 - \mathbb{E}_{WW'} \|W - W'\|_2,$$

where  $Z, Z' \stackrel{i.i.d.}{\sim} P$  and  $W, W' \stackrel{i.i.d.}{\sim} Q$ .

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- **Distance covariance** (weighted  $L_2$ -distance between characteristic functions):

$$\begin{aligned} \mathcal{V}^2(X, Y) &= \mathbb{E}_{XY} \mathbb{E}_{X'Y'} \|X - X'\|_2 \|Y - Y'\|_2 \\ &\quad + \mathbb{E}_X \mathbb{E}_{X'} \|X - X'\|_2 \mathbb{E}_Y \mathbb{E}_{Y'} \|Y - Y'\|_2 \\ &\quad - 2\mathbb{E}_{XY} [\mathbb{E}_{X'} \|X - X'\|_2 \mathbb{E}_{Y'} \|Y - Y'\|_2], \end{aligned}$$

where  $(X, Y)$  and  $(X', Y')$  are  $\stackrel{i.i.d.}{\sim} P_{XY}$ .

- Székely and Rizzo (2004, 2005); Székely, Rizzo and Bakirov (2007); Székely and Rizzo (2009), Lyons (2011)

# MMD & HSIC

- $k : \mathcal{Z} \times \mathcal{Z} \rightarrow \mathbb{R}$  a kernel on  $\mathcal{Z}$ , with RKHS  $\mathcal{H}_k$ ;  $P$  a probability measure on  $\mathcal{Z}$ ; mean embedding of  $P$  is  $\mu_P = \int k(\cdot, z)dP(z)$
- **Maximum Mean Discrepancy** between  $P$  and  $Q$ :

$$\begin{aligned}\gamma_k(P, Q) &= \|\mu_k(P) - \mu_k(Q)\|_{\mathcal{H}_k} \\ &= [\mathbb{E}_{ZZ'} k(Z, Z') + \mathbb{E}_{WW'} k(W, W') - 2\mathbb{E}_{ZW} k(Z, W)]^{1/2}\end{aligned}$$

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- $k_X$  a kernel on  $\mathcal{X}$ ,  $k_Y$  a kernel on  $\mathcal{Y}$ , and  $k = k_X k_Y$
- **Hilbert-Schmidt Independence Criterion** between  $X$  and  $Y$ :

$$HSIC(X, Y; k_X, k_Y) = \|\mu_k(P_{XY}) - \mu_k(P_X P_Y)\|_{\mathcal{H}_k}$$

- Gretton et al (2005, 2008); Smola et al (2007); Zhang et al (2011); Gretton et al (2012)

## Beyond Euclidean metrics

- Lyons (2011) generalized energy distance and distance covariance to *metric spaces of negative type*  $(\mathcal{Z}, \rho)$ , s.t.

$$\sum_{i=1}^n \alpha_i = 0 \Rightarrow \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \rho(z_i, z_j) \leq 0.$$



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- If  $\rho$  is a (semi)metric of negative type, then  $k(z, z') = \frac{1}{2} [\rho(z, z_0) + \rho(z', z_0) - \rho(z, z')]$  is a valid kernel (**distance kernel**)

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- If  $k$  is a kernel, then  $\rho(z, z') = \|k(\cdot, z) - k(\cdot, z')\|_{\mathcal{H}_k}^2$  is a semimetric of negative type (*generated by  $k$* )

# Main results

## Theorem

Let  $(\mathcal{Z}, \rho)$  be a semimetric space of negative type and let  $k$  be any kernel that generates  $\rho$ . Then,

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### Theorem

Let  $(\mathcal{X}, \rho_X)$  and  $(\mathcal{Y}, \rho_Y)$  be semimetric spaces of negative type, and let  $k_X$  and  $k_Y$  be any two kernels on  $\mathcal{X}$  and  $\mathcal{Y}$  that generate  $\rho_X$  and  $\rho_Y$ , respectively. Then,

$$\mathcal{V}_{\rho_X, \rho_Y}^2(X, Y) = 4\text{HSIC}^2(X, Y; k_X, k_Y).$$

# Conclusions

- Distance-based statistics of Szekely et al are a special case of the RKHS framework.
- Conversely, RKHS-based statistics have a clear interpretation in terms of implicitly imposing a (semi)metric onto the original space.
- For problem settings defined most naturally in terms of some given distances, and where these distances are of negative type, RKHS machinery can be brought to bear.