

# Correlation and Independence

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## Correlation

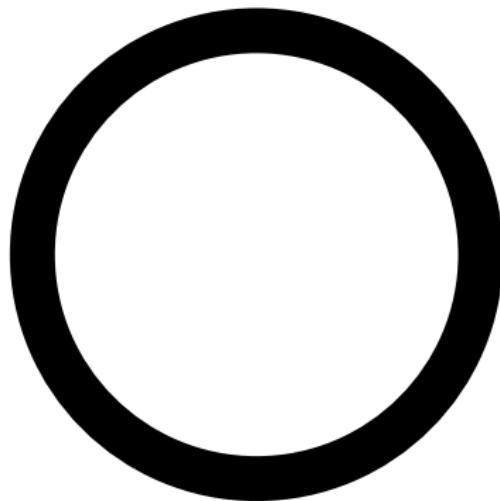
The Pearson's product-moment correlation is

$$\rho_{X,Y} := \frac{\mathbb{E}[(X - \mathbb{E}X)(Y - \mathbb{E}Y)]}{\sqrt{\mathbb{E}[(X - \mathbb{E}X)^2]\mathbb{E}[(Y - \mathbb{E}Y)^2]}}.$$

- ▶  $-1 \leq \rho_{X,Y} \leq 1$  and  $\rho_{X,Y} = \pm 1 \Leftrightarrow Y = cX + d$ , a.s. for some const.  $c, d$ .
- ▶  $X \perp\!\!\!\perp Y \Rightarrow \rho_{X,Y} = 0$ , but the reverse does not always hold.

We might want to reject  $X \perp\!\!\!\perp Y$ , possibly non-linear relationship.  
("association" is general but ambiguous.)

## Example



$$(X, Y) = (\cos(\Theta), \sin(\Theta)), \quad \Theta \sim (0, 2\pi].$$

$Y$  is non-linearly determined by  $X$ , but  $\rho_{X,Y} = 0$ .

## Classics: nonparametric methods

Let  $R_i$  and  $S_i$ ,  $1 \leq i \leq n$  be rank of the  $i$ -th sample point in  $X$  and  $Y$ , respectively.

Spearman's rank correlation (1904):

$$\rho_{Spearman} := 1 - \frac{6 \sum_i (R_i - S_i)^2}{n(n^2 - 1)}.$$

Kendall rank correlation (1938):

$$\tau := \frac{N_1 - N_2}{n(n - 1)/2},$$

where  $N_1$  is the number of concordant pairs in  $X$  and  $Y$ , and  $N_2$  is the number of discordant pairs.

# Independence

How to test independence?

Here, I will introduce methods based on

- ▶ divergence
- ▶ characteristic function
- ▶ kernel methods

# Divergence

Kullback-Leibler divergence between prob. measures  $\mathbf{P}$  and  $\mathbf{Q}$ :

$$D(\mathbf{P}||\mathbf{Q}) = \mathbb{E}_{\mathbf{P}} \left[ \log \frac{\mathbf{P}}{\mathbf{Q}} \right].$$

$$D(\mathbf{P}||\mathbf{Q}) = 0 \Leftrightarrow \mathbf{P} = \mathbf{Q}.$$

Let  $\mathbf{P} = \mathbf{P}(X, Y)$  and  $\mathbf{Q} = \mathbf{P}(X)\mathbf{P}(Y)$ , mutual information:

$$I(X, Y) := \mathbb{E}_{\mathbf{P}} \left[ \log \frac{\mathbf{P}(X, Y)}{\mathbf{P}(X)\mathbf{P}(Y)} \right].$$

$X \perp\!\!\!\perp Y \Leftrightarrow I(X, Y) = 0$ , so test  $I(X, Y) = 0$ .

## Remark

- ▶ c.f. Independent Component Analysis
- ▶ Power divergence:

$$\mathbb{E}_{\mathbf{P}} \left\{ \left[ \frac{\mathbf{P}(X, Y)}{\mathbf{P}(X)\mathbf{P}(Y)} \right]^\lambda - 1 \right\}.$$

## Characteristic Function

Let  $\phi_{X,Y}$ ,  $\phi_X$  and  $\phi_Y$  be characteristic func. of  $(X, Y)$ ,  $X \in \mathbb{R}^p$  and  $Y \in \mathbb{R}^q$ .

$X \perp\!\!\!\perp Y \Leftrightarrow \phi_{X,Y} = \phi_X \phi_Y$ , so test  $\|\phi_{X,Y} - \phi_X \phi_Y\|^2 = 0$ , where  $\|\cdot\|$  is a distance.

Székely et al. (2007, Ann. Stat. 35: 2769) proposal:

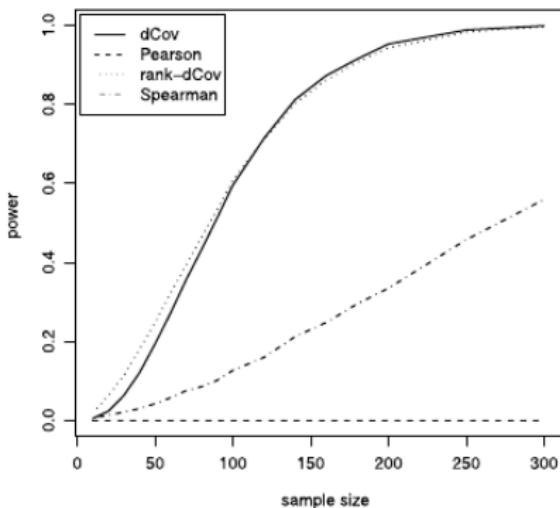
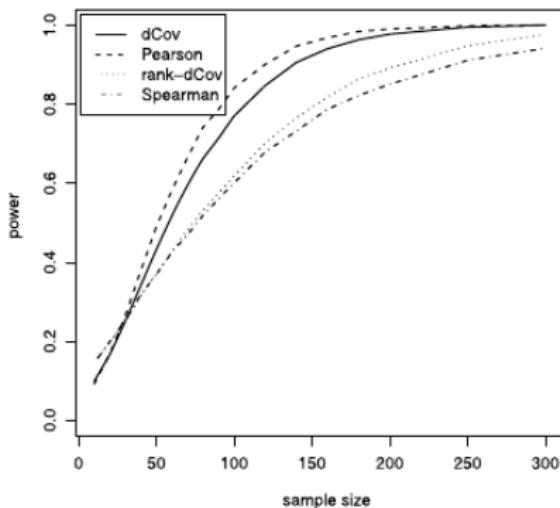
$$\mathcal{V}^2(X, Y) := \|\phi_{X,Y} - \phi_X \phi_Y\|_w^2 = \int |\phi_{X,Y}(t, s) - \phi_X(t) \phi_Y(s)|^2 w(t, s) dt ds,$$

with  $w(t, s) \propto t^{-1-p} s^{-1-q}$ .

Distance correlation:

$$R^2(X, Y) := \frac{\mathcal{V}^2(X, Y)}{\sqrt{\mathcal{V}^2(X) \mathcal{V}^2(Y)}}.$$

# Experiments



$$f(x, y) = [(1 + \theta x)(1 + \theta y)] \exp(-x - y - \theta xy), \quad x, y > 0, \quad 0 \leq \theta \leq 1.$$

Székely & Rizzo (2009) Ann. Appl. Stat. 3: 1236.

## Kernel Methods

Reproducing Kernel Hilbert Space: A positive definite kernel  $\mathbf{k}$  uniquely determine a Hilbert space  $\mathcal{H}_k$  with

- ▶  $\mathbf{k}(\cdot, \mathbf{x}) \in \mathcal{H}_k, \forall \mathbf{x} \in \mathcal{X}$ .
- ▶ Reproducing property:

$$\langle \mathbf{f}(\cdot), \mathbf{k}(\cdot, \mathbf{x}) \rangle_{\mathcal{H}_k} = \mathbf{f}(\mathbf{x}), \quad \forall \mathbf{x} \in \mathcal{X}, \forall \mathbf{f} \in \mathcal{H}_k.$$

### Remark

- ▶ Let  $\mathbf{x} \mapsto \Phi(\mathbf{x}) = \mathbf{k}(\cdot, \mathbf{x})$ . Inner product in  $\mathcal{H}_k$  is a Grammian:

$$\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}_j) \rangle_{\mathcal{H}_k} = \mathbf{k}(\mathbf{x}_i, \mathbf{x}_j),$$

so we do not know explicit form of mapping, possibly non-linear.

- ▶ c.f. Support Vector Machine

# Cross-Covariance Operator

Expectation operator:

$$\mathbf{m}_X := \mathbb{E}[\Phi(X)] = \mathbb{E}[k(\cdot, X)].$$

- ▶  $\langle \mathbf{m}_X, f \rangle = \mathbb{E}[f(X)]$ . (c.f. characteristic func.).
- ▶ Estimator:  $\hat{\mathbf{m}}_X^{(n)} = \frac{1}{n} \sum_{i=1}^n k(\cdot, X_i)$ .

Cross-Covariance operator:

- ▶  $\forall f \in \mathcal{H}_X, \forall g \in \mathcal{H}_Y,$

$$\langle \Sigma_{Y,X} f, g \rangle = \mathbb{E}[f(X)g(Y)] - \mathbb{E}[f(X)]\mathbb{E}[g(Y)],$$

- ▶  $X \perp\!\!\!\perp Y \Leftrightarrow \Sigma_{Y,X} = \mathbf{0}$ , so test  $\|\hat{\Sigma}_{Y,X}\|_{Hilbert-Schmidt}^2 = 0$  (Gretton et al. 2005 16th ALT).

# Randomized Dependence Coefficient

Hirschfeld-Gebelein-Rényi maximum correlation coefficient:

$$\rho_{X,Y}^{HGR} = \sup_{f,g} \rho_{f(X),g(Y)}$$

with  $X \perp\!\!\!\perp Y \Leftrightarrow \rho_{X,Y}^{HGR} = 0$ . DRC is an “approximation” of  $\rho_{X,Y}^{HGR}$  (Lopez-Paz et al. NIPS 2013):

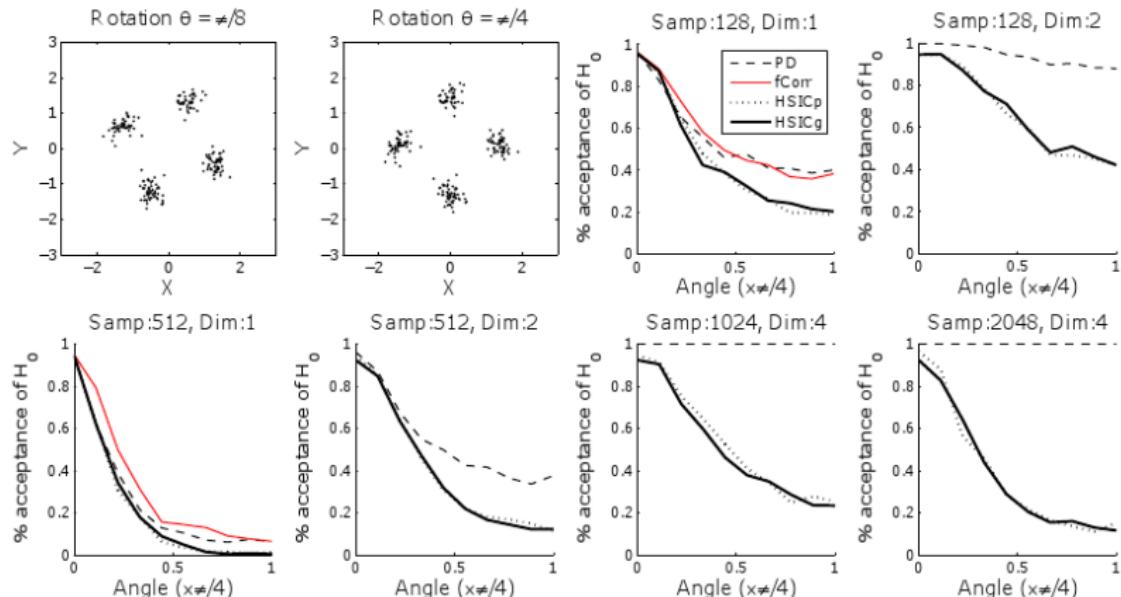
$$\max_{a,b} \rho_{a'\Phi(F_X(X)), b'\Phi(F_Y(Y))},$$

(c.f. canonical correlation), with

$$(\Phi(X))_{i,j} = \Phi(w'_i x_j + b_i), \quad 1 \leq i \leq k, 1 \leq j \leq n,$$

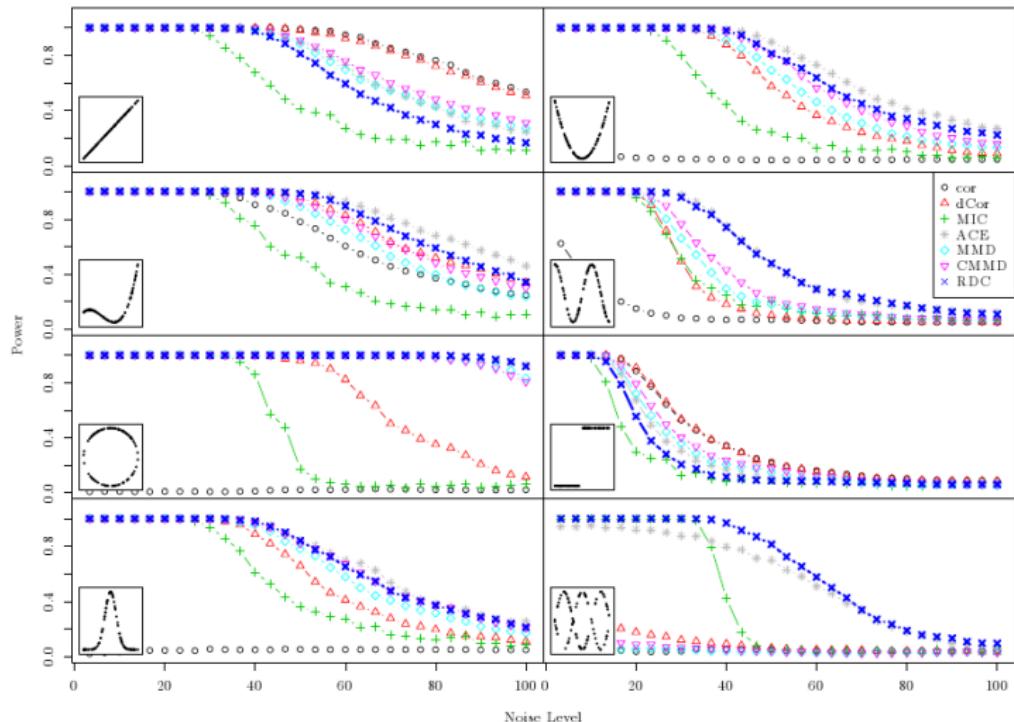
where  $w_i$  and  $b_i$  are random variables.

# Experiments



Gretton et al. 2008, Advances in NIPS 20, 585.

# Experiments



Lopez-Paz et al. NIPS 2013.