Independence and Conditional Independence with RKHS

Statistical Inference with Reproducing Kernel Hilbert Space

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Outline

1. Introduction
2. Covariance operators on RKHS
3. Independence with RKHS
4. Conditional independence with RKHS
5. Summary

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Covariance on RKHS

(X, Y): random variable taking values on $\mathcal{X} \times \mathcal{Y}$. resp.

$(H_{\mathcal{X}}, k_{\mathcal{X}})$, $(H_{\mathcal{Y}}, k_{\mathcal{Y}})$: RKHS with measurable kernels on $\mathcal{X}$ and $\mathcal{Y}$, resp.

Assume $E[k_{\mathcal{X}}(X,X)]E[k_{\mathcal{Y}}(Y,Y)] < \infty$

Cross-covariance operator: $\Sigma_{YX} : H_{\mathcal{X}} \to H_{\mathcal{Y}}$

$$\Sigma_{YX} \equiv E[\Phi_Y(Y) \otimes \Phi_X(X)] - m_Y \otimes m_X$$

$$= m_{P_{YX}} - m_{P_Y \otimes P_X} \qquad \in H_{\mathcal{Y}} \otimes H_{\mathcal{X}}$$

<u>Proposition</u>

$$\langle g, \Sigma_{YX} f \rangle = E[g(Y) f(X)] - E[g(Y)]E[f(X)] \quad (= \mathrm{Cov}[f(X), g(Y)])$$

for all $f \in H_{\mathcal{X}}, g \in H_{\mathcal{Y}}$

– *c.f.* Euclidean case

$V_{YX} = \mathrm{E}[YX^T] - \mathrm{E}[Y]\mathrm{E}[X]^T$: covariance matrix

$$(b, V_{YX} a) = Cov[(b,Y),(a,X)]$$

Characterization of independence

- Independence and Cross-covariance operator

Theorem

If the product kernel $k_{\mathcal{X}} k_{\mathcal{Y}}$ is characteristic on $\mathcal{X} \times \mathcal{Y}$, then

$$X \text{ and } Y \text{ are independent} \quad \Leftrightarrow \quad \Sigma_{XY} = O$$

proof)

$$\Sigma_{XY} = O \quad \Leftrightarrow \quad m_{P_{XY}} = m_{P_X \otimes P_Y}$$

$$\Leftrightarrow \quad P_{XY} = P_X \otimes P_Y \qquad \text{(by characteristic assumption)}$$

– *c.f.* for Gaussian variables

$$X \perp\!\!\!\perp Y \quad \Leftrightarrow \quad V_{XY} = O \qquad \textit{i.e.} \text{ uncorrelated}$$

– *c.f.* Characteristic function

$$X \perp\!\!\!\perp Y \quad \Leftrightarrow \quad E_{XY}[e^{\sqrt{-1}(uX+vY)}] = E_X[e^{\sqrt{-1}uX}]E_Y[e^{\sqrt{-1}vY}]$$

Estimation of cross-cov. operator

$(X_1, Y_1), \ldots, (X_N, Y_N)$: i.i.d. sample on $\mathcal{X} \times \mathcal{Y}$.

An estimator of Σ_{YX} is defined by

$$\hat{\Sigma}_{YX}^{(N)} = \frac{1}{N} \sum_{i=1}^{N} \left\{ k_{\mathcal{Y}}(\cdot, Y_i) - \hat{m}_Y \right\} \otimes \left\{ k_{\mathcal{X}}(\cdot, X_i) - \hat{m}_X \right\}$$

Theorem

$$\left\| \hat{\Sigma}_{YX}^{(N)} - \Sigma_{YX} \right\|_{HS} = O_p\left(1/\sqrt{N}\right) \qquad (N \to \infty)$$

Corollary to the $\sqrt{N}$ -consistency of the empirical mean, because the norm in $H_{\mathcal{X}} \otimes H_{\mathcal{Y}}$ is equal to the Hilbert-Schmidt norm of the corresponding operator $H_{\mathcal{X}} \to H_{\mathcal{Y}}$.

Hilbert-Schmidt Operator

– Hilbert-Schmidt operator

$A : H_1 \to H_2$: operator on a Hilbert space

A is called Hilbert-Schmidt if for complete orthonormal systems $\{\varphi_i\}$ of H_1 and $\{\psi_j\}$ of H_2

$$\sum_j \sum_i \langle \psi_j, A\varphi_i \rangle^2 < \infty.$$

Hilbert-Schmidt norm: $\|A\|_{HS}^2 = \sum_j \sum_i \langle \psi_j, A\varphi_i \rangle^2$

c.f. Frobenius norm of a matrix

– Fact: If $A : H_1 \to H_2$ is regarded as an element $F_A \in H_1 \otimes H_2$,

$$\| A \|_{HS} = \| F_A \|$$

$$\because) \quad \|A\|_{HS}^2 = \sum_j \sum_i \langle \psi_j, A\varphi_i \rangle_{H_2}^2 = \sum_j \sum_i \langle F_A, \underbrace{\varphi_i \otimes \psi_j}_{\text{CONS of } H_1 \otimes H_2} \rangle_{H_1 \otimes H_2}^2 = \| F_A \|^2 .$$

– Fact: $\|A\| \leq \|A\|_{HS}$

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Measuring Dependence

- Dependence measure

$$M_{YX} = \left\| \Sigma_{YX} \right\|_{HS}^{2}$$

$$M_{YX} = 0 \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y$$ with $k_{\mathcal{X}} k_{\mathcal{Y}}$ characteristic

- Empirical dependence measure

$$\hat{M}_{YX}^{(N)} = \left\| \hat{\Sigma}_{YX}^{(N)} \right\|_{HS}^{2}$$

M_{YX} and $\hat{M}_{YX}^{(N)}$ can be used as measures of dependence.

HS norm of cross-cov. operator I

- Integral expression

$$M_{YX} = \|\Sigma_{YX}\|_{HS}^2 = E[k_{\mathcal{X}}(X,\tilde{X})k_{\mathcal{Y}}(Y,\tilde{Y})] - 2E\left[E[k_{\mathcal{X}}(X,\tilde{X}) \mid \tilde{X}]E[k_{\mathcal{Y}}(Y,\tilde{Y}) \mid \tilde{Y}]\right]$$
$$+ E[k_{\mathcal{X}}(X,\tilde{X})]E[k_{\mathcal{Y}}(Y,\tilde{Y})]$$

where $(\tilde{X},\tilde{Y})$ is an independent copy of (X,Y).

Note: a Hilbert-Schmidt norm always has an integral expression

Proof.

$$\begin{aligned}
\|\Sigma_{YX}\|_{HS}^2 &= \|E[k_{\mathcal{X}}(X,\cdot) \otimes k_{\mathcal{Y}}(Y,\cdot)] - m_X \otimes m_Y\|^2 \\
&= \langle E[k_{\mathcal{X}}(X,\cdot) \otimes k_{\mathcal{Y}}(Y,\cdot)], E[k_{\mathcal{X}}(\tilde{X},\cdot) \otimes k_{\mathcal{Y}}(\tilde{Y},\cdot)]\rangle \\
&\quad -2\langle E[k_{\mathcal{X}}(X,\cdot) \otimes k_{\mathcal{Y}}(Y,\cdot)], m_{\tilde{X}} \otimes m_{\tilde{Y}}\rangle + \langle m_X \otimes m_Y, m_{\tilde{X}} \otimes m_{\tilde{Y}}\rangle \\
&= E[k_{\mathcal{X}}(X,\tilde{X})k_{\mathcal{Y}}(Y,\tilde{Y})] - 2E[E[k_{\mathcal{X}}(X,\tilde{X})|\tilde{X}]E[k_{\mathcal{Y}}(Y,\tilde{Y})|\tilde{Y}]] \\
&\quad +E[k_{\mathcal{X}}(X,\tilde{X})]E[k_{\mathcal{Y}}(Y,\tilde{Y})].
\end{aligned}$$

HS norm of cross-cov. operator II

- Empirical estimator

  Gram matrix expression

  HS-norm can be evaluated only in the subspaces $\mathrm{Span}\{k_{\mathcal{X}}(\cdot, X_i) - \hat{m}_X^{(N)}\}_{i=1}^N$ and $\mathrm{Span}\{k_{\mathcal{Y}}(\cdot, Y_i) - \hat{m}_Y^{(N)}\}$.

$$\Rightarrow \quad \hat{M}_{YX}^{(N)} = \frac{1}{N^2} \mathrm{Tr}\left[G_X G_Y \right]$$

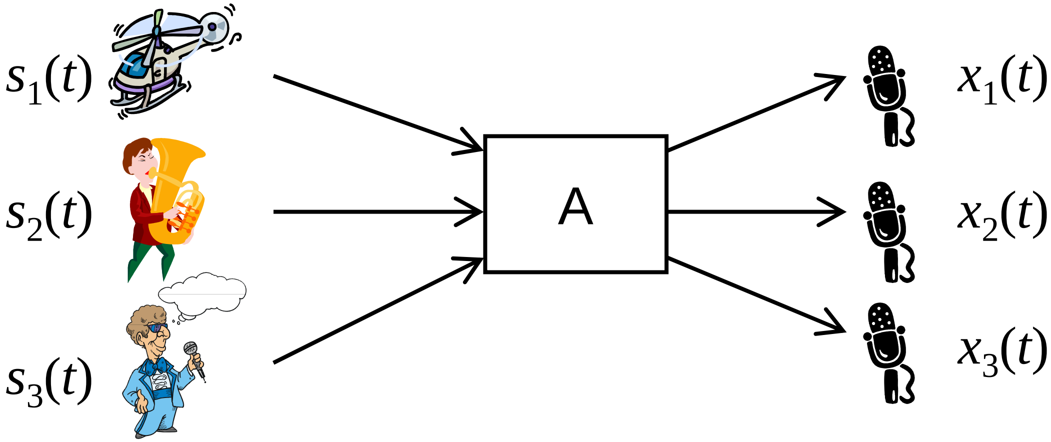
where $G_X = Q_N K_X Q_N$, $\quad Q_N = I_N - \frac{1}{N} \mathbf{1}_N \mathbf{1}_N^T$

Or equivalently,

$$\hat{M}_{YX}^{(N)} = \left\| \hat{\Sigma}_{YX}^{(N)} \right\|_{HS}^2 = \frac{1}{N^2} \sum_{i,j=1}^N k_{\mathcal{X}}(X_i, X_j) k_{\mathcal{Y}}(Y_i, Y_j) - \frac{2}{N^3} \sum_{i,j,k=1}^N k_{\mathcal{X}}(X_i, X_j) k_{\mathcal{Y}}(Y_i, Y_k) + \frac{1}{N^4} \sum_{i,j=1}^N k_{\mathcal{X}}(X_i, X_j) \sum_{k,\ell=1}^N k_{\mathcal{Y}}(Y_k, Y_\ell)$$

Application: ICA

- Independent Component Analysis (ICA)
  - Assumption
    - m independent source signals
    - m observations of linearly mixed signals



$$X(t) = AS(t)$$

A: m x m invertible matrix

  - Problem
    - Restore the independent signals S from observations X.

$$\hat{S} = BX$$

B: m x m orthogonal matrix

ICA with HSIC

$X^{(1)},\ldots,X^{(N)}$: i.i.d. observation (m-dimensional)

Pairwise-independence criterion is applicable.

Minimize $$L(B) = \sum_{a=1}^{m} \sum_{b>a} HSIC(Y_a, Y_b) \qquad Y = BX$$

Objective function is non-convex. Optimization is not easy.

→ Approximate Newton method has been proposed

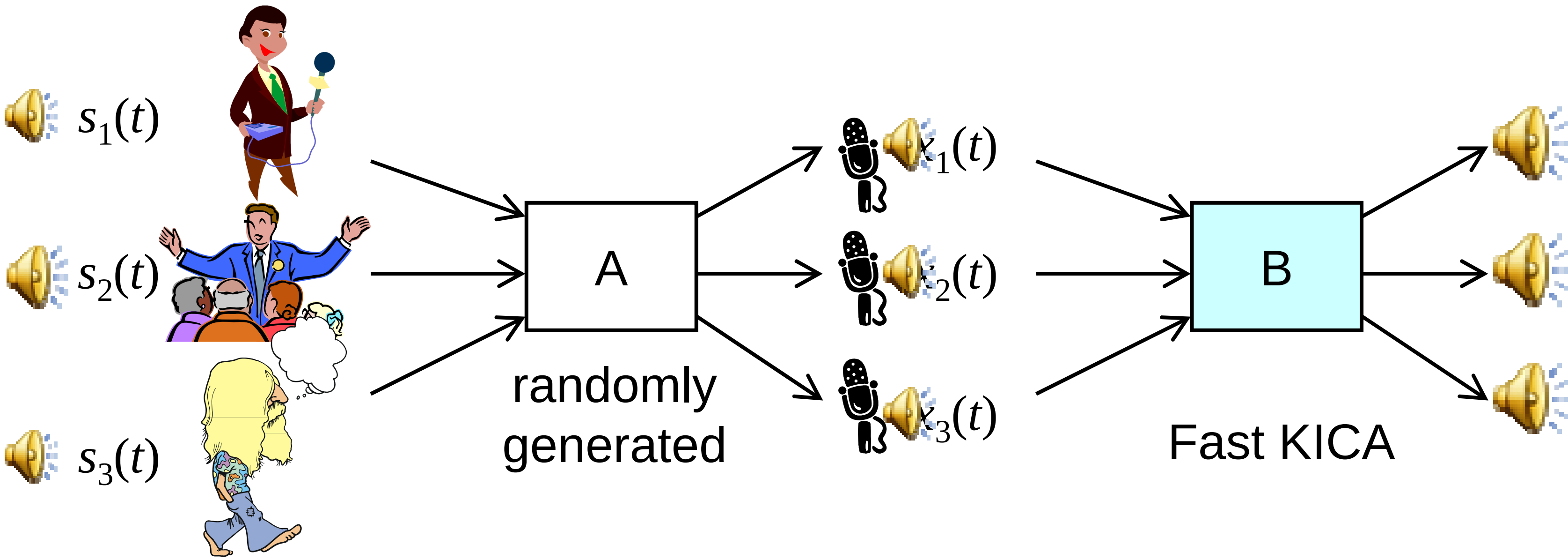
Fast Kernel ICA (FastKICA, Shen et al 07)

(Software downloadable at Arthur Gretton's homepage)

Other methods for ICA

See, for example, Hyvärinen et al. (2001).

■ Experiments (speech signal)



Three speech signals

Independence test with kernels I

- Independence test with positive definite kernels
  - Null hypothesis H0: X and Y are independent
  - Alternative H1: X and Y are not independent

$\hat{M}_{YX}^{(N)}$ can be used for a test statistics.

$$\hat{M}_{YX}^{(N)} = \left\|\hat{\Sigma}_{YX}^{(N)}\right\|_{HS}^{2} = \frac{1}{N^2}\sum_{i,j=1}^{N} k_{\mathcal{X}}(X_i, X_j) k_{\mathcal{Y}}(Y_i, Y_j) - \frac{2}{N^3}\sum_{i,j,k=1}^{N} k_{\mathcal{X}}(X_i, X_j) k_{\mathcal{Y}}(Y_i, Y_k)$$

$$+ \frac{1}{N^4}\sum_{i,j=1}^{N} k_{\mathcal{X}}(X_i, X_j) \sum_{k,\ell=1}^{N} k_{\mathcal{Y}}(Y_k, Y_\ell)$$

Independence test with kernels II

- Asymptotic distribution under null-hypothesis

Theorem (Gretton et al. 2008)

If X and Y are independent, then

$$N\,\hat{M}_{YX}^{(N)} \quad \Rightarrow \quad \sum_{i=1}^{\infty} \lambda_i Z_i^2 \qquad \text{in law} \quad (N \to \infty)$$

where

Z_i : i.i.d. ~ $N(0,1)$,

$\{\lambda_i\}_{i=1}^{\infty}$ is the eigenvalues of the following integral operator

$$\int h(u_a, u_b, u_c, u_d)\varphi_i(u_b)\,dP_{U_b}\,dP_{U_c}\,dP_{U_d} = \lambda_i \varphi_i(u_a)$$

$$h(U_a, U_b, U_c, U_d) = \tfrac{1}{4!}\sum_{(a,b,c,d)} k_{a,b}^{\mathcal{X}} k_{a,b}^{\mathcal{Y}} - 2k_{a,b}^{\mathcal{X}} k_{a,c}^{\mathcal{Y}} + k_{a,b}^{\mathcal{X}} k_{c,d}^{\mathcal{Y}}$$

$$k_{a,b}^{\mathcal{X}} = k_{\mathcal{X}}(X_a, X_b), \quad U_a = (X_a, Y_a)$$

– The proof is easy by the theory of U (or V)-statistics (see e.g. Serfling 1980, Chapter 5).

Independence test with kernels III

- Consistency of test

Theorem (Gretton et al. 2008)

If M_{YX} is not zero, then

$$\sqrt{N}\left(\hat{M}_{YX}^{(N)} - M_{YX}\right) \Rightarrow N(0,\sigma^2) \quad \text{in law} \quad (N \to \infty)$$

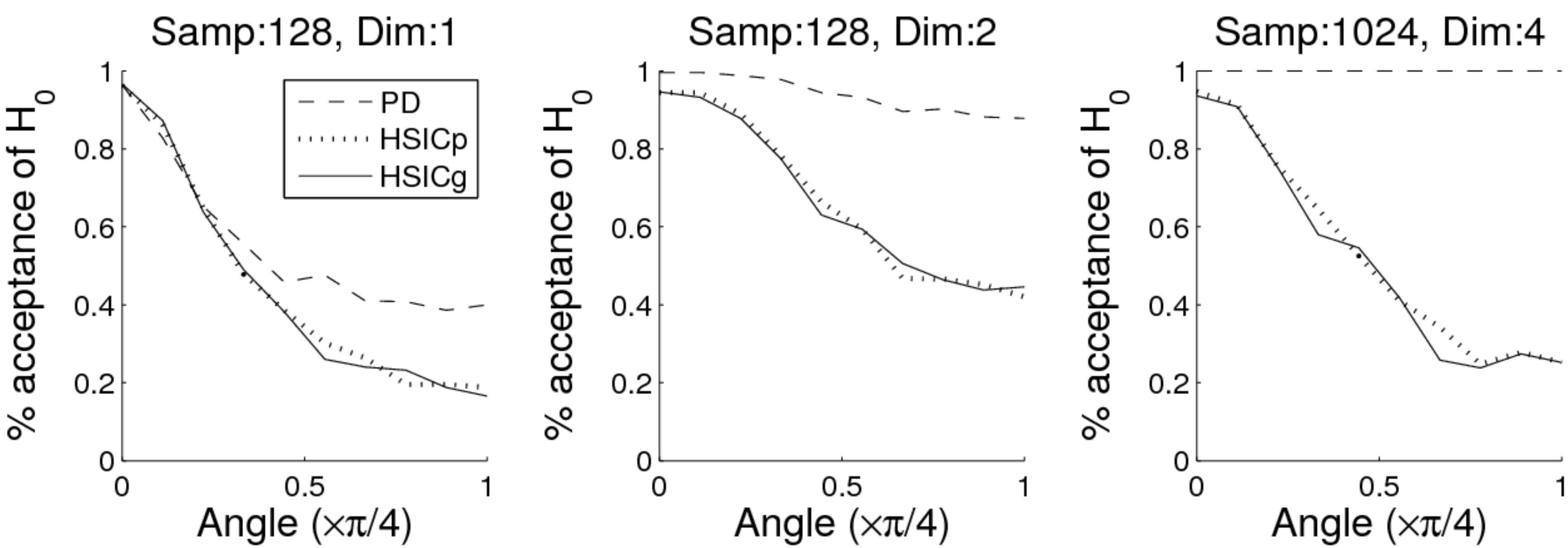
where

$$\sigma^2 = 16\left(E_a\left[E_{b,c,d}[h(U_a,U_b,U_c,U_d)]^2\right] - M_{YX}\right)$$

Example of Independent Test

- Synthesized data
  - Data: two d-dimensional samples

$$(X_1^{(1)},\dots,X_d^{(1)}),\dots,(X_1^{(N)},\dots,X_d^{(N)}) \qquad (Y_1^{(1)},\dots,Y_d^{(1)}),\dots,(Y_1^{(N)},\dots,Y_d^{(N)})$$



strength of dependence

Power Divergence (Ku&Fine05, Read&Cressie)

- Make partition $\{A_j\}_{j \in J}$: Each dimension is divided into q parts so that each bin contains almost the same number of data.

- Power-divergence

$$T_N = 2I^{\lambda}(X, m) = N \frac{2}{\lambda(\lambda+2)} \sum_{j \in J} \hat{p}_j \left\{ \left(\hat{p}_j \Big/ \prod_{k=1}^{N} \hat{p}_{j_k}^{(k)} \right)^{\lambda} - 1 \right\}$$

I^0 = MI

I^2 = Mean Square Conting.

$\hat{p}_j$: frequency in A_j

$\hat{p}_r^{(k)}$: marginal freq. in r-th interval

- Null distribution under independence

$$T_N \quad \Rightarrow \quad \chi^2_{q^N - qN + N - 1}$$

Limitations

- All the standard tests assume vector (numerical / discrete) data.
- They are often weak for high-dimensional data.

Independent Test on Text

– Data: Official records of Canadian Parliament in English and French.
  - Dependent data: 5 line-long parts from English texts and their French translations.
  - Independent data: 5 line-long parts from English texts and random 5 line-parts from French texts.
– Kernel: Bag-of-words and spectral kernel

Topic	Match	BOW(N=10)		Spec(N=10)		BOW(N=50)		Spec(N=50)	
		$HSIC_g$	$HSIC_p$	$HSIC_g$	$HSIC_p$	$HSIC_g$	$HSIC_p$	$HSIC_g$	$HSIC_p$
Agri-culture	Random	1.00	0.94	1.00	0.95	1.00	0.93	1.00	0.95
	Same	0.99	0.18	1.00	0.00	0.00	0.00	0.00	0.00
Fishery	Random	1.00	0.94	1.00	0.94	1.00	0.93	1.00	0.95
	Same	1.00	0.20	1.00	0.00	0.00	0.00	0.00	0.00
Immig-ration	Random	1.00	0.96	1.00	0.91	0.99	0.94	1.00	0.95
	Same	1.00	0.09	1.00	0.00	0.00	0.00	0.00	0.00

Acceptance rate (α = 5%)

(Gretton et al. 07)

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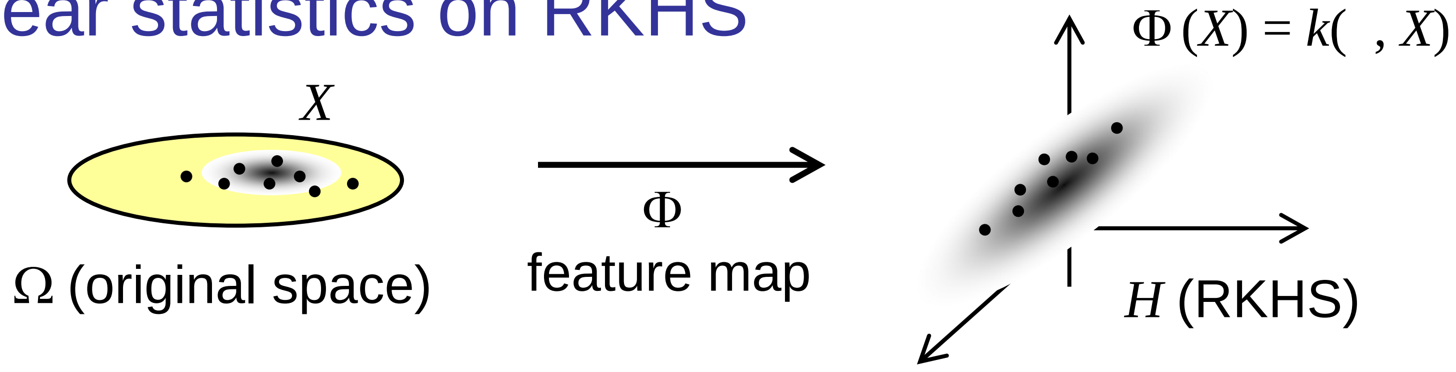
Re: Statistics on RKHS

- Linear statistics on RKHS



– Basic statistics on Euclidean space → Basic statistics on RKHS

Basic statistics on Euclidean space		Basic statistics on RKHS
Mean	$\longrightarrow$	Mean element
Covariance	$\longrightarrow$	Cross-covariance operator Σ_{YX}
Conditional covariance	$\longrightarrow$	Cond. cross-covariance operator

– Plan: define the basic statistics on RKHS and derive nonlinear/ nonparametric statistical methods in the original space.

Conditional Independence

- Definition

  X, Y, Z: random variables with joint p.d.f. $p_{XYZ}(x, y, z)$

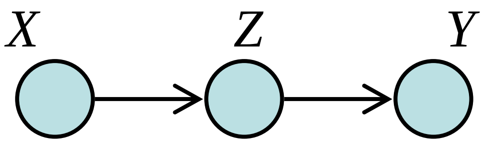
  X and Y are conditionally independent given Z, if

$$p_{Y|ZX}(y \mid z, x) = p_{Y|Z}(y \mid z) \qquad \text{(A)}$$

or

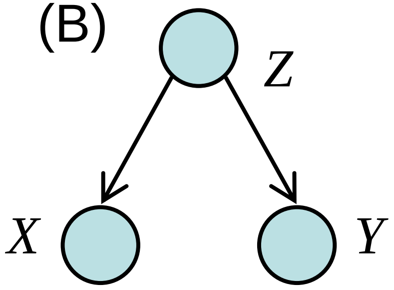
$$p_{XY|Z}(x, y \mid z) = p_{X|Z}(x \mid z)\, p_{Y|Z}(y \mid z) \qquad \text{(B)}$$

(A)



With Z known, the information of X
is unnecessary for the inference on Y

(B)



Review: Conditional Covariance

- Conditional covariance of Gaussian variables
  - Jointly Gaussian variable

    $X = (X_1, \ldots, X_p), Y = (Y_1, \ldots, Y_q)$

    $Z = (X, Y)$: m ($= p + q$) dimensional Gaussian variable

    $$Z \sim N(\mu, V) \qquad \mu = \begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \qquad V = \begin{pmatrix} V_{XX} & V_{XY} \\ V_{YX} & V_{YY} \end{pmatrix}$$

  - Conditional probability of Y given X is again Gaussian

    $\sim N(\mu_{Y|X}, V_{YY|X})$

    Cond. mean $\quad \mu_{Y|X} \equiv E[Y \mid X = x] = \mu_Y + V_{YX} V_{XX}^{-1} (x - \mu_X)$

    Cond. covariance $\quad V_{YY|X} \equiv Var[Y \mid X = x] = \underline{V_{YY} - V_{YX} V_{XX}^{-1} V_{XY}}$

    Schur complement of V_{XX} in V

    Note: $V_{YY|X}$ does not depend on x

Conditional Independence for Gaussian Variables

- Two characterizations

X,Y,Z are Gaussian.

– Conditional covariance

$$X \perp\!\!\!\perp Y \mid Z \quad \Leftrightarrow \quad V_{XY|Z} = O \qquad \text{i.e.} \quad V_{YX} - V_{YZ}V_{ZZ}^{-1}V_{ZX} = O$$

– Comparison of conditional variance

$$X \perp\!\!\!\perp Y \mid Z \quad \Leftrightarrow \quad V_{YY|[X,Z]} = V_{YY|Z}$$

$$\because) \quad V_{YY} - V_{Y[X,Z]}V_{[X,Z][X,Z]}^{-1}V_{[Z,X]Y} = V_{YY} - (V_{YX}, V_{YZ})\begin{pmatrix} V_{XX} & V_{XZ} \\ V_{ZX} & V_{ZZ} \end{pmatrix}^{-1}\begin{pmatrix} V_{XY} \\ V_{ZY} \end{pmatrix}$$

$$= V_{YY} - (V_{YX}, V_{YZ})\begin{pmatrix} I & O \\ -V_{ZZ}^{-1}V_{ZX} & I \end{pmatrix}\begin{pmatrix} V_{XX|Z}^{-1} & O \\ O & V_{ZZ}^{-1} \end{pmatrix}\begin{pmatrix} I & -V_{XZ}V_{ZZ}^{-1} \\ O & I \end{pmatrix}\begin{pmatrix} V_{XY} \\ V_{ZY} \end{pmatrix}$$

$$= V_{YY|Z} - V_{YX|Z}V_{XX|Z}^{-1}V_{XY|Z}$$

Linear Regression and Conditional Covariance

Review: linear regression

– X, Y: random vector (not necessarily Gaussian) of dim p and q (resp.)

$$\tilde{X} = X - E[X], \quad \tilde{Y} = Y - E[Y]$$

– Linear regression: predict Y using the linear combination of X.
Minimize the mean square error:

$$\min_{A: q \times p \text{ matrix}} E\left\|\tilde{Y} - A\tilde{X}\right\|^2$$

– The residual error is given by the conditional covariance matrix.

$$\min_{A: q \times p \text{ matrix}} E\left\|\tilde{Y} - A\tilde{X}\right\|^2 = \mathrm{Tr}\left[V_{YY|X}\right]$$

– For Gaussian variables,

$$V_{YY|[X,Z]} = V_{YY|Z} \qquad (\Leftrightarrow \;\; X \perp\!\!\!\perp Y \mid Z \;)$$

can be interpreted as

"If Z is known, X is not necessary for linear prediction of Y."

Conditional Covariance on RKHS

- Conditional Cross-covariance operator

  X, Y, Z : random variables on Ω_X, Ω_Y, Ω_Z (resp.).

  (H_X, k_X), (H_Y, k_Y), (H_Z, k_Z) : RKHS defined on Ω_X, Ω_Y, Ω_Z (resp.).

  – Conditional cross-covariance operator $H_X \to H_Y$

  $$\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZX}$$

  – Conditional covariance operator $H_Y \to H_Y$

  $$\Sigma_{YY|Z} \equiv \Sigma_{YY} - \Sigma_{YZ}\Sigma_{ZZ}^{-1}\Sigma_{ZY}$$

  – Σ_{ZZ}^{-1} may not exist as a bounded operator. But, we can justify the definions.

Decomposition of covariance operator

$$\Sigma_{YX} = \Sigma_{YY}^{1/2} W_{YX} \Sigma_{XX}^{1/2}$$

such that W_{YX} is a bounded operator with $\| W_{YX} \| \leq 1$ and

$$\overline{Range(W_{YX})} = \overline{Range(\Sigma_{YY})}, \quad Ker(W_{YX}) \perp \overline{Range(\Sigma_{XX})}.$$

Rigorous definition of conditional covariance operators

$$\Sigma_{YX|Z} \equiv \Sigma_{YX} - \Sigma_{YY}^{1/2} W_{YZ} W_{ZX} \Sigma_{XX}^{1/2}$$

$$\Sigma_{YY|Z} \equiv \Sigma_{YY} - \Sigma_{YY}^{1/2} W_{YZ} W_{ZY} \Sigma_{YY}^{1/2}$$

Two Characterizations of Conditional Independence with Kernels

(1) Conditional covariance operator (FBJ04, 08)

- Conditional variance (k_Z is characteristic)

$$\left\langle g, \Sigma_{YY|Z}\, g \right\rangle = E\big[Var[g(Y) \mid Z]\big] = \inf_{f \in H_Z} E\left|\tilde{g}(Y) - \tilde{f}(Z)\right|^2$$

- Conditional independence (all the kernels are characteristic)

$$X \perp\!\!\!\perp Y \mid Z \qquad \Leftrightarrow \qquad \Sigma_{YY|[XZ]} = \Sigma_{YY|Z}$$

X is not necessary for predicting $g(Y)$

- *c.f.* Gaussian variables

$$b^T V_{YY|Z}\, b = Var[b^T Y \mid Z] = \min_a \left| b^T \tilde{Y} - a^T \tilde{Z} \right|^2$$

$$X \perp\!\!\!\perp Y \mid Z \qquad \Leftrightarrow \qquad V_{YY|[X,Z]} = V_{YY|Z}$$

(2) Cond. cross-covariance operator (FBJ04)

– Conditional Covariance (k_Z is characteristic)

$$\langle g, \Sigma_{YX|Z} f \rangle = E\big[\mathrm{Cov}[g(Y), f(X) \mid Z]\big]$$

– Conditional independence

$$X \perp\!\!\!\perp Y \mid Z \quad \Leftrightarrow \quad \Sigma_{Y\ddot{X}|Z} = O \quad \left(\Leftrightarrow \quad \Sigma_{\ddot{Y}X|Z} = O\right)$$

where $\ddot{X} = (X, Z),\ \ddot{Y} = (Y, Z)$

– *c.f.* Gaussian variables

$$a^T V_{XY|Z} b = \mathrm{Cov}[a^T X, b^T Y \mid Z]$$

$$X \perp\!\!\!\perp Y \mid Z \quad \Leftrightarrow \quad V_{XY|Z} = O$$

– Proof of (1) (partial) : relation between residual error and operator

$$E\left|\left(g(Y)-E[g(Y)]\right)-\left(f(Z)-E[f(Z)]\right)\right|^2$$

$$=\langle f,\Sigma_{ZZ} f\rangle-2\langle f,\Sigma_{ZY} g\rangle+\langle g,\Sigma_{YY} g\rangle$$

$$=\left\|\Sigma_{ZZ}^{1/2} f\right\|^2-2\left\langle f,\Sigma_{ZZ}^{1/2}W_{ZY}\Sigma_{YY}^{1/2} g\right\rangle+\left\|\Sigma_{YY}^{1/2} g\right\|^2$$

$$=\left\|\Sigma_{ZZ}^{1/2} f-W_{ZY}\Sigma_{YY}^{1/2} g\right\|^2+\left\|\Sigma_{YY}^{1/2} g\right\|^2-\left\|W_{ZY}\Sigma_{YY}^{1/2} g\right\|^2$$

$$=\underbrace{\left\|\Sigma_{ZZ}^{1/2} f-W_{ZY}\Sigma_{YY}^{1/2} g\right\|^2}+\left\langle g,\underbrace{\left(\Sigma_{YY}-\Sigma_{YY}^{1/2}W_{YZ}W_{ZY}\Sigma_{YY}^{1/2}\right)}_{\Sigma_{YY|Z}}g\right\rangle$$

This part can be arbitrary small by choosing *f* because of $\overline{Range(W_{ZY})}=\overline{Range(\Sigma_{ZZ})}$.

Proof of (1): conditional independence

Lemma $$Var[Y] = Var_X\left[E_{Y|X}[Y \mid X]\right] + E_X\left[Var_{Y|X}[Y \mid X]\right]$$

From the above lemma

$$Var[g(Y) \mid Z] = E_{X|Z}\left[Var[g(Y) \mid X, Z] \mid Z\right] + Var_{X|Z}\left[E[g(Y) \mid X, Z] \mid Z\right]$$

Take $E_Z[\cdot]$

$$E\left[Var[g(Y) \mid Z]\right] - E\left[Var[g(Y) \mid X, Z]\right] = E_Z\left[Var_{X|Z}\left[E[g(Y) \mid X, Z] \mid Z\right]\right]$$

L.H.S = 0 from $\Sigma_{YY|[XZ]} = \Sigma_{YY|Z}$

$\Rightarrow$ $$Var_{X|Z}\left[E[g(Y) \mid X, Z] \mid Z\right] = 0 \quad P_z - \text{almost every } z$$

$\Rightarrow$ $$E[g(Y) \mid X, Z] = E[g(Y) \mid Z] \quad P_{XZ} - \text{almost every } (x, z)$$

$\Rightarrow$ $$P_{Y|XZ} = P_{Y|Z}$$ (k_Y characteristic)

– Why is the “extended variable” needed in (2)?

$$\left\langle g, \Sigma_{YX|Z} f \right\rangle = E\left[Cov[g(Y), f(X) \mid Z]\right]$$

$$\left\langle g, \Sigma_{YX|Z} f \right\rangle \neq Cov[g(Y), f(X) \mid Z = z]$$

The l.h.s is not a funciton of z. *c.f.* Gaussian case

$$\Sigma_{YX|Z} = O \quad \Rightarrow \quad p(x, y) = \int p(x \mid z) p(y \mid z) p(z) dz$$

$$\Sigma_{YX|Z} = O \quad \not\Rightarrow \quad p(x, y \mid z) = p(x \mid z) p(y \mid z)$$

However, if X is replaced by $[X, Z]$

$$\Sigma_{Y[X,Z]|Z} = O \quad \Rightarrow \quad p(x, y, z') = \int p(x, z' \mid z) p(y \mid z) p(z) dz$$

where $p(x, z' \mid z) = p(x \mid z) \delta(z' - z)$

$$\Rightarrow \quad p(x, y, z') = p(x \mid z') p(y \mid z') p(z')$$

i.e. $p(x, y \mid z') = p(x \mid z') p(y \mid z')$

Empirical Estimator of Cond. Cov. Operator

$(X_1, Y_1, Z_1), \ldots, (X_N, Y_N, Z_N)$

$\Sigma_{YZ} \quad \to \quad \hat{\Sigma}_{YZ}^{(N)}$ etc. finite rank operators

$\Sigma_{ZZ}^{-1} \quad \to \quad \left(\hat{\Sigma}_{ZZ}^{(N)} + \varepsilon_N I\right)^{-1}$ regularization for inversion

– Empirical conditional covariance operator

$$\hat{\Sigma}_{YX|Z}^{(N)} := \hat{\Sigma}_{YX}^{(N)} - \hat{\Sigma}_{YZ}^{(N)}\left(\hat{\Sigma}_{ZZ}^{(N)} + \varepsilon_N I\right)^{-1}\hat{\Sigma}_{ZX}^{(N)}$$

– Estimator of Hilbert-Schmidt norm

$$\left\|\hat{\Sigma}_{YX|Z}^{(N)}\right\|_{HS}^{2} = \mathrm{Tr}\left[G_X S_Z G_Y S_Z\right]$$

$$G_X = Q_N K_X Q_N, \quad Q_N = I_N - \frac{1}{N}\mathbf{1}_N \mathbf{1}_N^{\,T}$$ centered Gram matrix

$$S_Z = I_N - (G_Z + N\varepsilon_N I_N)^{-1} G_Z = \left(I_N + \tfrac{1}{N\varepsilon_N} G_Z\right)^{-1}$$

Statistical Consistency

- Consistency on conditional covariance operator

<u>Theorem (FBJ08, Sun et al. 07)</u>

Assume $\varepsilon_N \to 0$ and $\sqrt{N}\varepsilon_N \to \infty$

$$\left\| \hat{\Sigma}_{YX|Z}^{(N)} - \Sigma_{YX|Z} \right\|_{HS} \to 0 \qquad (N \to \infty)$$

In particular,

$$\left\| \hat{\Sigma}_{YX|Z}^{(N)} \right\|_{HS} \to \left\| \Sigma_{YX|Z} \right\|_{HS} \qquad (N \to \infty)$$

Normalized Covariance Operator

- Normalized Cross-Covariance Operator

NOCCO $\quad W_{YX} = \Sigma_{YY}^{-1/2} \Sigma_{YX} \Sigma_{XX}^{-1/2}$ $\quad$ Recall: $\Sigma_{YX} = \Sigma_{YY}^{1/2} W_{YX} \Sigma_{XX}^{1/2}$

- Normalized Conditional cross-covariance operator

NOC³O

$$W_{YX|Z} = \Sigma_{YY}^{-1/2} \Sigma_{YX|Z} \Sigma_{XX}^{-1/2} = \Sigma_{YY}^{-1/2} \left(\Sigma_{YX} - \Sigma_{YZ} \Sigma_{ZZ}^{-1} \Sigma_{ZX} \right) \Sigma_{XX}^{-1/2}$$
$$= W_{YX} - W_{YZ} W_{ZX}$$

- Characterization of conditional independence

With characteristic kernels,

$$W_{YX} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y$$

$$W_{Y\tilde{X}|Z} = O \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid Z$$

Measures for Conditional Independence

Assume W_{XY} etc. are Hilbert-Schmidt.

– Dependence measure

$$\mathrm{NOCCO} = \left\| W_{YX} \right\|_{HS}^2$$

– Conditional dependence measure

$$\mathrm{NOC^3O} = \left\| W_{\tilde{X}\tilde{Y}|Z} \right\|_{HS}^2$$

(X and Y augmented)

– Independence / conditional independence

$$\mathrm{NOCCO} = 0 \Leftrightarrow X \perp\!\!\!\perp Y \qquad \mathrm{NOC^3O} = 0 \Leftrightarrow X \perp\!\!\!\perp Y \mid Z$$

Kernel-free Integral Expression

<u>Theorem</u>

Let $E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right](B \times A) = \int P_{Y|Z}(B \mid Z=z) P_{X|Z}(A \mid Z=z) dP_Z(z)$

probability on $\Omega_X \times \Omega_Y$.

Assume

P_{XY} and $E_Z\left[P_{Y|Z} \otimes P_{X|Z}\right]$ have density $p_{XY}(x,y)$ and $p_{X\perp Y|Z}(x,y)$, resp.

H_Z and $H_X \otimes H_Y$ are characteristic.

W_{YX} and $W_{YZ}W_{ZX}$ are Hilbert-Schmidt.

Then,

$$\| W_{YX|Z} \|_{HS}^2 = \iint \left(\frac{p_{XY}(x,y) - p_{X\perp Y|Z}(x,y)}{p_X(x)p_Y(y)} \right)^2 p_X(x)p_Y(y)dxdy$$

In the unconditional case

$$\| W_{YX} \|_{HS}^2 = \iint \left(\frac{p_{XY}(x,y)}{p_X(x)p_Y(y)} - 1 \right)^2 p_X(x)p_Y(y)dxdy$$

- Kernel-free expression, though the definitions are given by kernels!

– Kernel-free value is desired as a “measure” of dependence.
c.f. If unnormalized operators are used, the measures depend on the choice of kernel.

– In the unconditional case,

$$\text{NOCCO} = \| W_{YX} \|_{HS}^2$$

is equal to the mean square contingency, which is a very popular measure of dependence for discrete variables.

– In the conditional case, if the augmented variables are used,

$$\| W_{\ddot{Y}\ddot{X}|Z} \|_{HS}^2$$

$$= \iint \left(\frac{p_{XYZ}(x,y,z) - p_{X|Z}(x \mid z) p_{Y|Z}(y \mid z) p_Z(z)}{p_{XZ}(x,z) p_{YZ}(y,z)} \right)^2 p_{XZ}(x,z) p_{YZ}(y,z) dxdydz$$

(conditional mean square contingency)

Empirical Estimators

- Empirical estimation is straightforward with the empirical cross-covariance operator $\hat{\Sigma}_{YX}^{(N)}$.
- Inversion → regularization: $\Sigma_{XX}^{-1} \to \left(\hat{\Sigma}_{XX}^{(N)} + \varepsilon I\right)^{-1}$
- Replace the covariances in $W_{YX} = \Sigma_{YY}^{-1/2}\Sigma_{YX}\Sigma_{XX}^{-1/2}$ by the empirical ones given by the data $\Phi_X(X_1),\ldots,\Phi_X(X_N)$ and $\Phi_Y(Y_1),\ldots,\Phi_Y(Y_N)$

$$\mathrm{NOCCO}_{emp} = \mathrm{Tr}\left[R_X R_Y\right]$$ (dependence measure)

$$\mathrm{NOC^3O}_{emp} = \mathrm{Tr}\left[R_{\tilde{X}} R_{\tilde{Y}} - 2R_{\tilde{X}} R_{\tilde{Y}} R_Z + R_{\tilde{X}} R_Z R_{\tilde{Y}} R_Z\right]$$

(conditional dependence measure)

where $R_X \equiv G_X\left(G_X + N\varepsilon_N I_N\right)^{-1}$

$$G_X = \left(I_N - \tfrac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right)K_X\left(I_N - \tfrac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right) \qquad K_X = \left(k(X_i, X_j)\right)_{i,j=1}^N$$

- NOCCO_{emp} and $\mathrm{NOC^3O}_{emp}$ give kernel estimates for the mean square contingency and conditional mean square contingency, resp.

Consistency

Theorem (Fukumizu et al. 2008)

Assume that $W_{YX|Z}$ is Hilbert-Schmidt, and the regularization coefficient satisfies

$$\varepsilon_N \to 0 \qquad N^{1/3}\varepsilon_N \to \infty.$$

Then,

$$\left\| \hat{W}_{YX|Z}^{(N)} - W_{YX|Z} \right\|_{HS} \to 0 \qquad (N \to \infty)$$

In particular,

$$\left\| \hat{W}_{YX|Z}^{(N)} \right\|_{HS} \to \left\| W_{YX|Z} \right\|_{HS} \qquad (N \to \infty)$$

i.e. NOC^{3}O$_{emp}$ (NOCCO$_{emp}$) converges to the population value NOC^{3}O (NOCCO, resp).

Choice of Kernel

- How to choose a kernel?
  - No definitive solutions have been proposed yet.
  - For statistical tests, comparison of power or efficiency will be desirable.
  - Other suggestions:
    - Make a relevant supervised problem, and use cross-validation.
    - Some heuristics
      - Heuristics for Gaussian kernels (Gretton et al 2007)

$$\sigma \;=\; \text{median}\left\{ \left\| X_i - X_j \right\| \;|\; i \neq j \right\}$$

      - Speed of asymptotic convergence (Fukumizu et al. 2008)

$$\lim_{N\to\infty} Var\left[N \times HSIC_{emp}^{(N)} \right] = 2\left\|\Sigma_{XX}\right\|_{HS}^2 \left\|\Sigma_{YY}\right\|_{HS}^2 \quad \text{under independence}$$

Compare the bootstrapped variance and the theoretical one, and choose the parameter to give the minimum discrepancy.

Conditional Independence Test

- Permutation test

$$T_N = \left\| \hat{\Sigma}^{(N)}_{YX|Z} \right\|^2_{HS} \qquad \text{or} \qquad T_N = \left\| \hat{W}^{(N)}_{YX|Z} \right\|^2_{HS}$$

  – If Z takes values in a finite set $\{1, \ldots, L\}$,

  set $A_\ell = \{ i \mid Z_i = \ell \} \;\; (\ell = 1, \ldots, L)$,

  otherwise, partition the values of Z into L subsets $C_1, \ldots, C_L$, and set

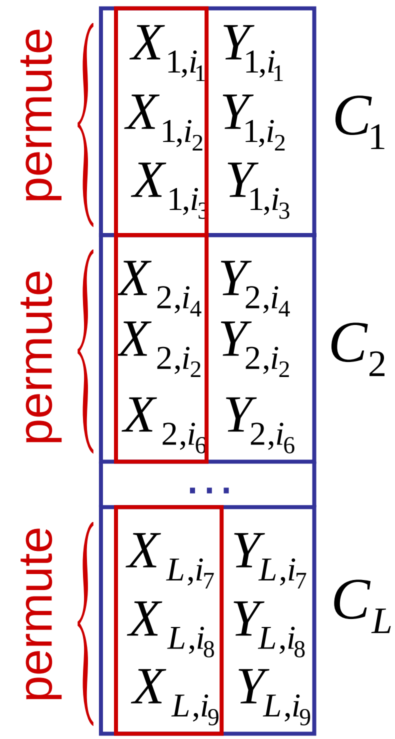
  $$A_\ell = \{ i \mid Z_i \in C_\ell \} \quad (\ell = 1, \ldots, L).$$

  – Repeat the following process B times: ($b = 1, \ldots, B$)

  1. Generate pseudo cond. independent data $D^{(b)}$ by permuting X data within each A_ℓ.
  2. Compute $T_N^{(b)}$ for the data $D^{(b)}$.

     $\longrightarrow$ Approximate null distribution under cond. indep. assumption

  – Set the threshold by the $(1\text{-}\alpha)$-percentile of the empirical distributions of $T_N^{(b)}$.



Causality of Time Series

- Granger causality (Granger 1969)

  $X(t)$, $Y(t)$: two time series $t = 1, 2, 3, \ldots$

  – Problem:

  Is $\{X(1), \ldots, X(t)\}$ a cause of $Y(t+1)$?

  (No inverse causal relation)

  – Granger causality

  Model: AR

  $$Y(t) = c + \sum_{i=1}^{p} a_i Y(t-i) + \sum_{j=1}^{p} b_j X(t-j) + U_t$$

  Test

  $$H_0:\ b_1 = b_2 = \ldots = b_p = 0$$

  X is called a Granger cause of Y if H_0 is rejected.

– *F*-test

- Linear estimation

$$Y(t) = c + \sum_{i=1}^{p} a_i Y(t-i) + \sum_{j=1}^{p} b_j X(t-j) + U_t \quad \longrightarrow \quad \hat{c}, \hat{a}_i, \hat{b}_j$$

H$_0$: $$Y(t) = c + \sum_{i=1}^{p} a_i Y(t-i) + W_t \quad \longrightarrow \quad \hat{\hat{c}}, \hat{\hat{a}}_i$$

$$ERR_1 = \sum_{t=p+1}^{N} \left(\hat{Y}(t) - Y(t) \right) \qquad ERR_0 = \sum_{t=p+1}^{N} \left(\hat{\hat{Y}}(t) - Y(t) \right)^2$$

- Test statistics

$$T_N \equiv \frac{\left(ERR_0 - ERR_1 \right) / p}{ERR_1 / (N - 2p + 1)} \quad \overset{\text{under } H_0}{\Rightarrow} \quad F_{p, N-2p+1} \quad (N \to \infty)$$

p.d.f of $$F_{d_1,d_2} = \frac{1}{B(d_1/2, d_2/2)} \left(\frac{d_1 x}{d_1 x + d_2} \right)^{d_1} \left(1 - \frac{d_1 x}{d_1 x + d_2} \right)^{d_2} \frac{1}{x}$$

– Software

- Matlab: Econometrics toolbox (www.spatial-econometrics.com)
- R: lmtest package

- Granger causality is widely used and influential in econometrics.

  Clive Granger received Nobel Prize in 2003.

- Limitations
  - Linearity: linear AR model is used.
    No nonlinear dependence is considered.
  - Stationarity: stationary time series are assumed.
  - Hidden cause: hidden common causes (other time series) cannot be considered.

  "Granger causality" is not necessarily "causality" in general sense.

- There are many extensions.

- With kernel dependence measures, it is easily extended to incorporate nonlinear dependence.

  Remark: There are few good conditional independence tests
  for continuous variables.

Kernel Method for Causality of Time Series

- Causality by conditional independence
  - Extended notion of Granger causality

    X is NOT a cause of Y if

$$p(Y_t \mid Y_{t-1},\ldots,Y_{t-p}, X_{t-1},\ldots,X_{t-p}) = p(Y_t \mid Y_{t-1},\ldots,Y_{t-p})$$

$$\Leftrightarrow$$

$$Y_t \perp\!\!\!\perp X_{t-1},\ldots,X_{t-p} \mid Y_{t-1},\ldots,Y_{t-p}$$

  - Kernel measures for causality

$$HSCIC = \left\| \hat{\Sigma}^{(N-p+1)}_{\ddot{Y}\mathbf{X_p}|\mathbf{Y_p}} \right\|^2_{HS}$$

$$HSNCIC = \left\| \hat{W}^{(N-p+1)}_{\ddot{Y}\mathbf{X_p}|\mathbf{Y_p}} \right\|^2_{HS}$$

$$\mathbf{X}_{\mathrm{p}} = \{(X_{t-1,}X_{t-2},\cdots,X_{t-p}) \in \mathbf{R}^p \mid t = p+1,\ldots,N\}$$

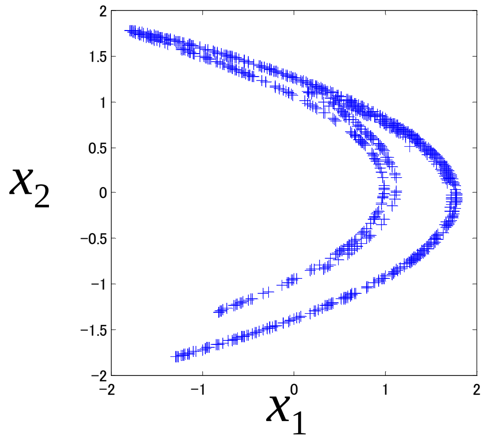
$$\mathbf{Y}_{\mathrm{p}} = \{(Y_{t-1,}Y_{t-2},\cdots,Y_{t-p}) \in \mathbf{R}^p \mid t = p+1,\ldots,N\}$$

Example

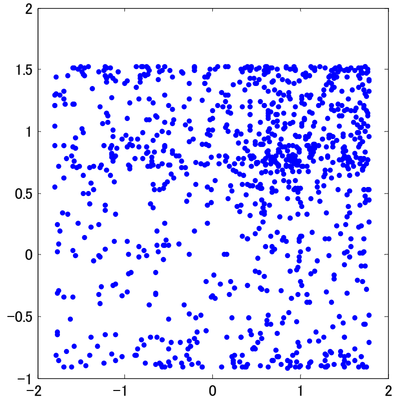
- Coupled Hénon map
  - X, Y:

$$\begin{cases} x_1(t+1) = 1.4 - x_1(t)^2 + 0.3x_2(t) \\ x_2(t+1) = x_1(t) \end{cases}$$

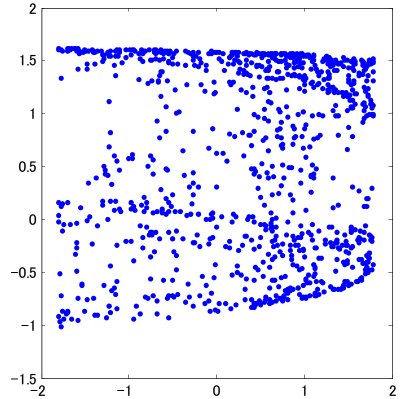
$$\begin{cases} y_1(t+1) = 1.4 - \left\{\underline{\gamma x_1(t)}\, y_1(t) + (1-\gamma) y_1(t)^2\right\} + 0.1y_2(t) \\ y_2(t+1) = y_1(t) \end{cases}$$



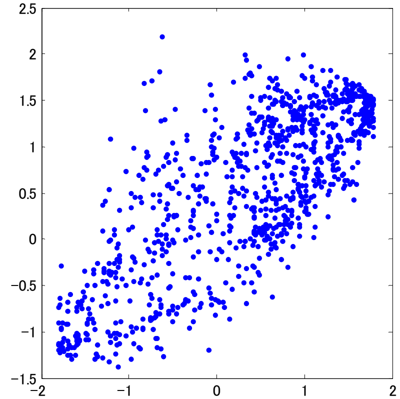
x_1-y_1



$\gamma = 0$



$\gamma = 0.25$



$\gamma = 0.8$

Causality in coupled Hénon map

- X is a cause of Y if $\gamma > 0$. $Y_{t+1} \not\perp\!\!\!\perp X_t \mid Y_t$
- Y is not a cause of X for all γ. $X_{t+1} \perp\!\!\!\perp Y_t \mid X_t$
- Permutation tests for non-causality with NOC^{3}O

N = 100 $x_1 - y_1$	H$_0$: Y_t is not a cause of X_{t+1}							H$_0$: X_t is not a cause of Y_{t+1}						
γ	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.0	0.1	0.2	0.3	0.4	0.5	0.6
NOC^{3}O	94	88	81	63	86	77	62	97	0	0	0	0	0	0
Granger	92	96	95	90	90	94	93	96	92	85	45	13	2	3

Number of times accepting H$_0$ among 100 datasets (α = 5%)

Summary

- Dependence analysis with RKHS
  - Covariance and conditional covariance on RKHS can capture the (in)dependence and conditional (in)dependence of random variables.
  - Easy estimators can be obtained for the Hilbert-Schmidt norm of the operators.
  - Statistical tests of independence and conditional independence are possible with kernel measures.
    - Applications: dimension reduction for regression (FBJ04, FBJ08), causal inference (Sun et al. 2007).
  - Further studies are required for kernel choice.

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