Robust Kernel (Cross-) Covariance Operators in Reproducing Kernel Hilbert Space toward Kernel Methods

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Abstract

To the best of our knowledge, there are no general well-founded robust methods for statistical unsupervised learning. Most of the unsupervised methods explicitly or implicitly depend on the kernel covariance operator (kernel CO) or kernel cross-covariance operator (kernel CCO). They are sensitive to contaminated data, even when using bounded positive definite kernels. First, we propose robust kernel covariance operator (robust kernel CO) and robust kernel cross-covariance operator (robust kernel CCO) based on a generalized loss function instead of the quadratic loss function. Second, we propose influence function of classical kernel canonical correlation analysis (classical kernel CCA). Third, using this influence function, we propose a visualization method to detect influential observations from two sets of data. Finally, we propose a method based on robust kernel CO and robust kernel CCO, called robust kernel CCA, which is designed for contaminated data and less sensitive to noise than classical kernel CCA. The principles we describe also apply to many kernel methods which must deal with the issue of kernel CO or kernel CCO. Experiments on synthesized and imaging genetics analysis demonstrate that the proposed visualization and robust kernel CCA can be applied effectively to both ideal data and contaminated data. The robust methods show the superior performance over the state-of-the-art methods.

1 Introduction

The incorporation of various unsupervised learning methods for multiple data sources into genomic analysis is a rather recent topic. Using the dual representations, the task of learning with multiple
data sources is related to the kernel-based data fusion, which has been actively studied in the last
decade Bach (2008), Steinwart and Christmann (2008), Hofmann et al. (2008). Kernel fusion in
unsupervised learning has a close connection with unsupervised kernel methods. As unsupervised
kernel methods, kernel principal component analysis (Schölkopf et al., 1998, Alam and Fukumizu,
2014, kernel PCA), kernel canonical correlation analysis (Akaho, 2001, Bach and Jordan, 2002,
classical kernel CCA), weighted multiple kernel CCA and others have been extensively studied
in unsupervised kernel fusion for decades (S. Yu and Moreau, 2011). But these methods are not
robust; these are sensitive to contaminated data. Even though a number of researches has been done
on robustness issue for supervised learning, especially support vector machine for classification and
regression (Christmann and Steinwart, 2004, 2007, Debruyne et al., 2008), there are no general
well-founded robust methods for unsupervised learning.

Robustness is an essential and challenging issue in statistical machine learning for multiple
sources data analysis. Because outliers, data that cause surprise in relation to the majority of the
data, are often occur in the real data. Outliers may be right, but we need to examine for transcription
errors. They can play havoc with classical statistical methods or statistical machine learning meth-

dods. To overcome this problem, since 1960 many robust methods have been developed, which are
less sensitive to outliers. The goals of robust statistics are to use the methods from the bulk of the
data and indicate the points deviating from the original pattern for further investment (Huber and
Ronchetti, 2009, Hampel et al., 2011). In recent years, a robust kernel density estimation (robust
kernel DE) has been proposed Kim and Scott (2012), which is less sensitive than the kernel den-
sity estimation. To the best of our knowledge, two spacial robust kernel PCA methods have been
proposed based on weighted eigenvalues decomposition Huang et al. (2009b) and spherical kernel
PCA (Debruyne et al., 2010). They show that the influence function (IF), a well-known measure of
robustness, of kernel PCA can be arbitrary large for unbounded kernels.

During the last ten years, a number of papers have been about the properties of kernel CCA,
CCA using positive definite kernels, called classical kernel CCA and its variants have been pro-
posed Fukumizu et al. 2007, Hardoon and Shawe-Taylor, 2009, Otopal, 2012, Alam and Fuku-
mizu, 2015. Due to the properties of eigen decomposition it is still a well applied methods for
multiple sources data analysis. In recent years, two canonical correlation analysis (CCA) methods
based on Hilbert-Schmidt independence criterion (hsicCCA) and centered kernel target alignment
(ktacCCA) have been proposed by Chang et al. (2013). These methods are able to extract nonlinear
structure of the data as well. Due to the gradient based optimization, these methods are not able
to extract all canonical variates using the same initial value and do not work for high dimensional
datasets. For more details, see Section 5.3. An empirical comparison and sensitivity analysis for robust linear CCA and classical kernel CCA is also discussed, and gives similar interpretation as kernel PCA for kernel CCA without any theoretical results (Alam et al., 2010).

Most of the kernel methods explicitly or implicitly depend on kernel covariance operator (kernel CO) or kernel cross-covariance operator (kernel CCO). Among others, these are most useful tools of unsupervised kernel methods but have not been robust yet. They can be formulated as an empirical optimization problem to achieve robustness by combining empirical optimization problem with ideas of Huber or Hampels M-estimation model (Huber and Ronchetti, 2009, Hampel et al., 2011). The robust kernel CO and robust kernel CCO can be computed efficiently via a kernelized iteratively re-weighted least square (KIRWLS) problem. In robust kernel DE based on robust kernel mean elements (robust kernel ME) is used KIRWLS in reproducing kernel Hilbert space (RKHS) (Kim and Scott, 2012). Debruyne et al. (2010) have proposed a visualization methods for detecting influential observations from one set of the data using IF of kernel PCA. In addition, Romanazzi (1992) has proposed the IF of canonical correlation and canonical vectors of linear CCA but the IF of classical kernel CCA and any robust kernel CCA have not been proposed, yet. All of these considerations motivate us to conduct studies on robust kernel CCO toward kernel unsupervised methods.

Contribution of this paper is fourfold. First, we propose robust kernel CO and robust kernel CCO based on generalized loss function instead of the quadratic loss function. Second, we propose IF of classical kernel CCA: kernel canonical correlation (kernel CC) and kernel canonical variates (kernel CV). Third, to detect influential observations from multiple sets of data, we propose a visualization method using the inflection function of kernel CCA. Finally, we propose a method based on robust kernel CO and robust kernel CCO, called robust kernel CCA, which is less sensitive than classical kernel CCA. Experiments on synthesized and imaging genetics analysis demonstrate that the proposed visualization and robust kernel CCA can be applied effectively to both ideal data (ID) and contaminated data (CD).

The remainder of this paper is organized as follows. In the next Section, we provide a brief review of kernel ME, kernel CCO, robust kernel ME, robust kernel CO, robust kernel CCO and robust Gram matrices with algorithms. In Section 3, we discuss in brief the IF, IF of kernel ME and IF of kernel CO and kernel CCO. After a brief review of classical kernel CCA in Section 4.1, we propose the IF of classical kernel CCA: kernel CC and kernel CV in Section 4.1.1. The robust kernel CCA is proposed in Section 4.2. In Section 5, we describe experiments conducted on both synthesized data and the imaging genetics analysis with a visualizing method. In Appendix, we
discuss the results in detail.

2 Classical and robust kernel (cross-) covariance operator in RKHS

Kernel ME, kernel CO and kernel CCO with positive definite kernel have been extensively applied to nonparametric statistical inference through representing distribution in the form of means and covariance in RKHS (Gretton et al., 2008, Fukumizu et al., 2008, Song et al., 2008, Kim and Scott, 2012, Gretton et al., 2012). Basic notion of kernel MEs, kernel CO and kernel CCO with its robustness through IF are briefly discussed below.

2.1 Classical kernel (cross-) covariance operator

Let $F_X$, $F_Y$ and $F_{XY}$ be the probability measure on $X$, $Y$ and $X \times Y$, respectively. Also let $X_1, X_2, \ldots, X_n; Y_1, Y_2, \ldots, Y_n$ and $(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n)$ be the random sample from the distribution $F_X$, $F_Y$ and $F_{XY}$, respectively. A symmetric kernel $k(\cdot, \cdot)$ defined on a space is called positive definite kernel if the Gram matrix $(k(X_i, X_j))_{ij}$ is positive semi-definite (Aronszajn, 1950).

By the reproduction properties and kernel trick, the kernel can evaluate the inner product of any two feature vectors efficiently without knowing an explicit form of either the feature map $(\Phi(\cdot) = k(\cdot, X), \forall X \in X)$ or feature spaces ($\mathcal{H}$). In addition, the computational cost does not depend on dimension of the original space after computing the Gram matrices (Fukumizu and Leng, 2014, Alam and Fukumizu, 2014).

A mapping $M_X := \mathbb{E}_X[\Phi(X)] = \mathbb{E}_X[k(\cdot, X)]$ with $\mathbb{E}_X[k(X, X)] < \infty$ is an element of the RKHS $\mathcal{H}_X$. By the reproducing property with $X \in X$, kernel mean elements is defined as

$$\langle M_X, f \rangle_{\mathcal{H}_X} = \langle \mathbb{E}_X[k(\cdot, X)], f \rangle = \mathbb{E}_X\langle k(\cdot, X), f \rangle_{\mathcal{H}_X} = \mathbb{E}_X[f(X)], \text{ for all } f \in \mathcal{H}_X.$$

Given an independent and identically distributed sample, the mapping $m_X = \frac{1}{n} \sum_{i=1}^n \Phi(X_i) = \frac{1}{n} \sum_{i=1}^n k(\cdot, X_i)$ is an empirical element of the RKHS, $\mathcal{H}_X$, $\langle m_X, f \rangle_{\mathcal{H}_X} = \langle \frac{1}{n} \sum_{i=1}^n k(\cdot, X_i), f \rangle = \frac{1}{n} \sum_{i=1}^n f(X_i)$. The sample kernel ME of the feature vectors $\Phi(X_i)$ can be regraded as a solution to the empirical risk optimization problem (Kim and Scott, 2012)

$$\argmin_{f \in \mathcal{H}_X} \frac{1}{n} \sum_{i=1}^n \|\Phi(X_i) - f\|_{\mathcal{H}_X}^2. \quad (1)$$

Similarly, we can define kernel CCO as an empirical risk optimization problem. An operator, $\Sigma_{XY} := \mathcal{H}_X \rightarrow Y$ with $\mathbb{E}_X[k_X(X, X)] < \infty$, and $\mathbb{E}_Y[k_Y(Y, Y)] < \infty$, by the reproducing property which is
defined as
\[
\langle f_X, \Sigma_{YX} f_X \rangle_{\mathcal{H}_Y} = \mathbb{E}_{XY} \left[ \langle f_X, k_X(\cdot, X) - M_X \rangle_{\mathcal{H}_X} \langle f_Y, k_Y(\cdot, Y) - M_Y \rangle_{\mathcal{H}_Y} \right]
\]
\[
= \mathbb{E}_{XY} \left[ (f_X(X) - E_X[f(X)])(f_Y(Y) - E_Y[f(Y)]) \right]
\]
and called kernel CCO. Given the pair of independent and identically distributed sample, \((X_i, Y_i)_{i=1}^n\), the kernel CCO is an operator of the RKHS, \(\mathcal{H}_X \otimes \mathcal{H}_Y\), Eq. (1) becomes
\[
\argmin_{\Sigma_{XY} \in \mathcal{H}_X \otimes \mathcal{H}_Y} \frac{1}{n} \sum_{i=1}^{n} \| \Phi_c(X_i) \otimes \Phi_c(Y_i) - \Sigma_{XY} \|^2,
\]
where \(\Phi_c(X_i) = \Phi(X_i) - \frac{1}{n} \sum_{b=1}^{n} \Phi(X_b)\). and the kernel covariance operator at point \((X_i, Y_i)\) is then
\[
\hat{\Sigma}_{XY}(X_i, Y_i) = (k_X(X_i, X_b) - \frac{1}{n} \sum_{b=1}^{n} k_X(\cdot, X_b)) \otimes (k_Y(Y_i, Y_d) - \frac{1}{n} \sum_{d=1}^{n} k_Y(Y_i, Y_d)).
\]
Special case, if \(Y\) is equal to \(X\), gives kernel CO.

2.2 Robust kernel (cross-) covariance operator

It is known that (as in Section 2.1) the kernel ME is the solution to the empirical risk optimization problem, which are the least square type estimators. This type of estimators are sensitive to the presence of outliers in the features, \(\Phi(X_i)\). In recent years, the robust kernel ME has been proposed for density estimation (Kim and Scott, 2012). Our goal is to extend this notion to kernel CO and kernel CCO. To do these, we estimates kernel CO and kernel CCO based on robust loss functions, M-estimator, and called, robust kernel CO and robust kernel CCO, respectively. Most common example of robust loss functions, \(\zeta(t)\) on \(t \geq 0\), are Huber’s or Hampel’s loss function. Unlike the quadratic loss function, the derivative of these loss functions is bounded (Huber and Ronchetti, 2009, Hampel et al., 1986). The Huber’s function is defined as
\[
\zeta(t) = \begin{cases} 
\frac{t^2}{2}, & 0 \leq t \leq c \\
ct - \frac{c^2}{2}, & c \leq t
\end{cases}
\]
and Hampel’s function is defined as

\[
\zeta(t) = \begin{cases} 
\frac{t^2}{2}, & 0 \leq t \leq c_1 \\
\frac{c_1 t - c_1^2}{2}, & c_1 \leq t < c_2 \\
\frac{c_1 (t - c_2)^2}{2(c_2 - c_3)} + \frac{c_1 (c_2 + c_3 - c_1)}{2}, & c_2 \leq t < c_3 \\
\frac{c_1 (c_2 + c_3 - c_1)}{2}, & c_3 \leq t.
\end{cases}
\]

The basic assumptions are: (i) \( \zeta \) is non-decreasing, \( \zeta(0) = 0 \) and \( \zeta(t)/t \to 0 \) as \( t \to 0 \) (ii) \( \varphi(t) = \frac{\zeta(t)}{t} \) exists and is finite, where \( \zeta'(t) \) is derivative of \( \zeta(t) \). (iii) \( \zeta'(t) \) and \( \varphi(t) \) are continuous and bounded (iv) \( \varphi(t) \) is Lipschitz continuous. Huber’s loss function as well as others hold for all of these assumptions (Kim and Scott, 2012).

Given weights of robust kernel ME, \( w = [w_1, w_2, \cdots, w_n]^T \), of a set of observations, the points \( \Phi_c(X_i) := \Phi(X_i) - \sum_{a=1}^{n} w_a \Phi(X_a) \) are centered and the centered Gram matrix is \( \tilde{K}_{ij} = (H K H^T)_{ij} \), where \( 1_n = [1, 1, \cdots, 1]^T \) and \( H = I - 1_n w^T \).

Eq. (2) can be written as

\[
\arg\min_{f \in H_k} \frac{1}{n} \sum_{i=1}^{n} \zeta(||\Phi_c(X_i) \otimes \Phi_c(Y_i) - \Sigma_{XY}||).
\]

As in (Kim and Scott, 2012), Eq. (3) does not has a closed form solution, but using the kernel trick the classical re-weighted least squares (IRWLS) can be extended to a RKHS. The solution is then,

\[
\tilde{\Sigma}^{(h)}_{XY} = \sum_{i=1}^{n} w_i^{(h-1)} k(X_i) k(Y_i),
\]

where \( w_i^{(h)} = \frac{\varphi(||\Phi_c(X_i) \otimes \Phi_c(Y_i) - \Sigma_{XY}||)_{H_k \otimes H_k}}{\sum_{i=1}^{n} \varphi(||\Phi_c(X_i) \otimes \Phi_c(Y_i) - \Sigma_{XY}||)_{H_k \otimes H_k}} \), and \( \varphi(x) = \frac{\zeta'(x)}{x} \).

The algorithms of estimating robust Gram matrix and robust kernel CCO are given in Figure 1 and in Figure 2, respectively.

### 3 Influence function of kernel (cross-) covariance operator

To define the notion of robustness in statistics, different approaches have been proposed science 70’s decay for examples, the minimax approach (Huber, 1964), the sensitivity curve (Tukey, 1977), the influence functions (Hampel, 1974, Hampel et al., 1986) and in the finite sample emb breakdown point (Donoho and Huber, 1983). Due to simplicity, IF is the most useful approach in statistics and in statistical supervised learning (Christmann and Steinwart, 2007, 2004). In this section, we
Input: $D = \{X_1, X_2, \ldots, X_n\}$ in $\mathbb{R}^m$. The kernel matrix $K$ with kernel $k$ and $K_X = k(\cdot, X_i)$. Threshold $TH$, (e.g., $10^{-8}$). The objective function of robust mean element is

$$M_R = \arg \min_{f \in H} J(f), \quad \text{where } J(f) = \frac{1}{n} \sum_{i=1}^{n} \rho(||K_{X_i} - f||_H)$$

Do the following steps until:

$$\left| \frac{J(M_R^{(h+1)}) - J(M_R^{(h)})}{J(M_R^{(h)})} \right| < TH,$$

where $M_R^{(h)} = \sum_{i=1}^{n} w_i K_{X_i}$, $w_i^{(h)} = \frac{\varphi(||K_{X_i} - M_R^{(h)}||_H)}{\sum_{i=1}^{n} \varphi(||K_{X_i} - M_R^{(h)}||_H)}$, and $\varphi(x) = \frac{\xi'(x)}{x}$

1. Set $h = 1$ and $w_i^{(0)} = \frac{1}{n}$.
2. Solve $w_i^{(h)} = \frac{\varphi(||K_{X_i} - M_R^{(h)}||_H)}{\sum_{i=1}^{n} \varphi(||K_{X_i} - M_R^{(h)}||_H)}$ and make a vector $w$ for $i = 1, 2, \ldots, n$.
3. Update the mean element, $M_R^{(h+1)} = [w^{(h)}]^T K$.
4. Update error, $e^{(h+1)} = (\text{diag}(K) - 2[w^{(h)}]^T K + [w^{(h)}]^T K[w^{(h)}]^T I_n)^{1/2}$.
5. Update $h$ as $h + 1$.

Output: the centered robust kernel matrix, $\tilde{K}_R = HKH^T$ where $H = I_n - \frac{1}{n} w^T$

Figure 1: The algorithm of estimating centered kernel matrix using robust kernel mean element.

briefly discuss the notion of IF, IF of kernel ME, IF of kernel CO and kernel CCO. (For details see in Appendix).

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space and $(\mathcal{X}, \mathcal{B})$ a measure space. We want to estimate the parameter $\theta \in \Theta$ of a distribution $F$ in $\mathcal{A}$. We assume that exists a functional $R : D(R) \to \mathbb{R}$, where $D(R)$ is the set of all probability distribution in $\mathcal{A}$. Let $G$ be some distribution in $\mathcal{A}$. If data do not fallow the model $F$ exactly but slightly going toward $G$, the Gâteaux Derivative at $F$ is given by

$$\lim_{\epsilon \to 0} \frac{R((1 - \epsilon)F + \epsilon G) - R(F)}{\epsilon}$$ (4)

Suppose $x \in \mathcal{X}$ and $G = \Delta_x$ is the probability measure which gives mass 1 to $\{x\}$. The influence function (special case of Gâteaux Derivative) of $R$ at $F$ is defined by

$$IF(x, R, F) = \lim_{\epsilon \to 0} \frac{R((1 - \epsilon)F + \epsilon \Delta_x) - R(F)}{\epsilon}$$ (5)

provided that the limit exists. It can be intuitively interpreted as a suitably normalized asymptotic influence of outliers on the value of an estimate or test statistic.

There are three properties of IF: gross error sensitivity, local shift sensitivity and rejection point.
Input: $D = \{(X_1, Y_1), (X_2, Y_2), \ldots (X_n, Y_n)\}$. The robust centered kernel matrix $\tilde{K}_X$ and $\tilde{K}_Y$ with kernel $k_X$ and $k_Y$, $\tilde{K}_{X_i}$ and, $\tilde{K}_{Y_i}$ are the $i$th column of the $\tilde{K}_X$ and $\tilde{K}_Y$, respectively. Also define $\tilde{K}_{X_i} = k_X(\cdot, X_i)$ and $\tilde{K}_{Y_i} = k_Y(\cdot, Y_i)$. Threshold $TH$ (e.g., $10^{-8}$). The objective function of robust cross-covariance operator is

$$\hat{\Sigma}_R = \arg \min_{A \in H_X \otimes H_Y} J(A), \quad \text{where } J(A) = \frac{1}{n} \sum_{i=1}^{n} \rho(||B_i - A||_{H_X \otimes H_Y}),$$

$$B_i = \tilde{\Phi}(X_i) \otimes \tilde{\Phi}(Y_i)^T = \tilde{K}_X \otimes \tilde{K}_Y.$$

Do the following steps until:

$$\left| \frac{J(\Sigma_R^{(h+1)}) - J(\Sigma_R^{(h)})}{J(\Sigma_R^{(h)})} \right| < TH,$$

where $\Sigma_R^{(h)} = \sum_{i=1}^{n} w_i^{(h-1)} B_i$, $w_i^{(h)} = \frac{\varphi(||B_i - \Sigma_R^{(h)}||_{H_X \otimes H_Y})}{\sum_{i=1}^{n} \varphi(||B_i - \Sigma_R^{(h)}||_{H_X \otimes H_Y})}$ and $\varphi(x) = \frac{\xi(x)}{x}$

1. Set $h = 1$, and $w_i^{(0)} = \frac{1}{n}$
2. Solve $w_i^{(h)} = \frac{\varphi(e_i^{(h)})}{\sum_i \varphi(e_i^{(h)})}$ and make a vector $w$ for $i = 1, 2, \ldots n$.
3. Calculate a $n^2 \times 1$ vector, $v^{(h)} = B w^{(h)}$ and make a $n \times n$ matrix $V^{(h)}$, where $B$ is $n^2 \times n$ matrix that $i$th column consists of all elements of the $n \times n$ matrix $B_i$.
4. Update the robust covariance, $\Sigma_R^{(h+1)} = \sum_i w_i^{(h)} B_i = V^{(h)}$.
5. Update error, $e^{[h+1]} = \text{diag} (\tilde{K}_X \tilde{K}_Y) - 2[w^{(h)}]^T \tilde{K}_X \tilde{K}_Y + [w^{(h)}]^T \tilde{K}_Y [w^{(h)}]^T 1_n$. 
6. Update $h$ as $h + 1$.

Output: the robust cross-covariance operator.

Figure 2: The algorithm of estimating robust cross-covariance operator.
They measured the worst effect of gross error, the worst effect of rounding error and rejection point. For a scalar, we just define influence function (IF) at a fixed point. But if the estimate is a function, we are able to express the change of the function value at every points (Kim and Scott, 2012).

3.1 Influence function of kernel mean element and kernel cross-raw moment

For a scalar we just define IF at a fixed point. But if the estimate is a function, we are able to express the change of the function value at every point.

Let the cross-raw moments

\[ R(F_{XY}) = \mathbb{E}_{XY}[\langle k_X(\cdot, X), f\rangle_{\mathcal{H}_X} \langle k_Y(\cdot, Y), g\rangle_{\mathcal{H}_Y}] = \mathbb{E}_{XY}[f(X)g(Y)] = \int f(X)g(Y)dF_{XY}. \]

The IF of \( R(F_X) \) at \( Z' = (X', Y') \) for every points (\( \cdot \)) is given by

\[ IF(\cdot, Z', R, F_{XY}) = k_X(\cdot, X')k_Y(\cdot, Y') - \mathbb{E}_{XY}[\langle k_X(\cdot, X), f\rangle_{\mathcal{H}_X} \langle k_Y(\cdot, Y), g\rangle_{\mathcal{H}_Y}], \]

\[ \forall k_X(\cdot, X) \in \mathcal{H}_X, \ k_Y(\cdot, Y) \in \mathcal{H}_Y, \] which is estimated with the pairs of data points \((X_1, Y_1), (X_2, Y_2), \cdots, (X_n, Y_n) \in X \times Y\) at any evaluated point \((X_i, Y_i) \in X \times Y\)

\[ k_X(X_i, X')k_Y(Y_i, Y') - \frac{1}{n} \sum_{a=1}^{n} k_X(X_i, X_a)k_Y(Y_i, Y_a) \quad \forall k_X(\cdot, X_a) \in \mathcal{H}_X, \ k_Y(\cdot, Y_a) \in \mathcal{H}_Y. \]

3.2 Influence function of complicated statistics

The IF of complicated statistics, which are functions of simple statistics, can be calculated with the chain rule. Say \( R(F) = a[R_1(F), \ldots, R_s(F)] \), then

\[ IF_R(\zeta) = \sum_{i=1}^{s} \frac{\partial a}{\partial R_i} IF_{R_i}(\zeta). \]

It can also be used to find the IF for a transformed statistic, given the influence function for the statistic itself.

The IF of kernel CCO, \( R(F_{XY}) \), with joint distribution, \( F_{XY} \), using complicated statistics at
\[ Z' = (X', Y') \] is given by

\[
\text{IF}(\cdot, Z', R, F_{XY}) = \langle k_X(\cdot, X') - M(F_X), f \rangle_{\mathcal{H}_X} \langle k_Y(\cdot, Y') - M(F_Y), g \rangle_{\mathcal{H}_Y} - \mathbb{E}_{XY} [\langle k_X(\cdot, X) - M(F_X), f \rangle_{\mathcal{H}_X} \langle k_Y(\cdot, Y) - M(F_Y), g \rangle_{\mathcal{H}_Y}].
\]

which is estimated with the data points \((X_1, Y_1), (X_2, Y_2), \cdots, (X_n, Y_n) \in \mathcal{X} \times \mathcal{Y}\) for every \(Z_i = (X_i, Y_i)\) as

\[
\hat{\text{IF}}(Z_i, Z', R, F_{XY}) = \left[ k_X(X_i, X') - \frac{1}{n} \sum_{b=1}^{n} k_X(X_i, X_b) \right] \left[ k_Y(Y_i, Y') - \frac{1}{n} \sum_{b=1}^{n} k_Y(Y_i, Y_b) \right] - \frac{1}{n} \sum_{b=1}^{n} k_X(X_i, X_b) - \frac{1}{n} \sum_{d=1}^{n} k_Y(Y_i, Y_d) - \frac{1}{n} \sum_{b=1}^{n} k_Y(Y_i, Y_b).
\]

For the bounded kernels, the above IFs have three properties: gross error sensitivity, local shift sensitivity and rejection point. It is not true for the unbounded kernels, for example, liner and polynomial kernels. We can make similar conclusion for the kernel covariance operator.

## 4 Classical and robust kernel canonical correlation analysis

In this Section, we review classical kernel CCA and propose the IF and empirical IF (EIF) of kernel CCA. After that we propose a robust kernel CCA method based on robust kernel CO and robust kernel CCO.

### 4.1 Classical kernel CCA

Classical kernel CCA has been proposed as a nonlinear extension of linear CCA (Akaho, 2001, Lai and Fyfe, 2000, Bach and Jordan, 2002) has extended the classical kernel CCA with efficient computational algorithm, incomplete Cholesky factorization. Over the last decade, classical kernel CCA has been used for various purposes including preprocessing for classification, contrast function of independent component analysis, test of independence between two sets of variables, which has been applied in many domains such as genomics, computer graphics and computer-aided drug discovery and computational biology (Alzate and Suykens, 2008, Hardoon et al., 2004, Huang et al., 2009a). Theoretical results on the convergence of kernel CCA have also been obtained (Fukumizu
et al., 2007, Hardoon and Shawe-Taylor, 2009).

The aim of classical kernel CCA is to seek the sets of functions in the RKHS for which the correlation (Corr) of random variables is maximized. The simplest case, given two sets of random variables $X$ and $Y$ with two functions in the RKHS, $f_X(\cdot) \in \mathcal{H}_X$ and $f_Y(\cdot) \in \mathcal{H}_Y$, the optimization problem of the random variables $f_X(X)$ and $f_Y(Y)$ is

$$
\max_{f_X \in \mathcal{H}_X, f_Y \in \mathcal{H}_Y \atop f_X \neq 0, f_Y \neq 0} \text{Corr}(f_X(X), f_Y(Y)). \tag{6}
$$

The optimizing functions $f_X(\cdot)$ and $f_Y(\cdot)$ are determined up to scale.

Using a finite sample, we are able to estimate the desired functions. Given an i.i.d sample, $(X_i, Y_i)_{i=1}^n$ from a joint distribution $F_{XY}$, by taking the inner products with elements or “parameters” in the RKHS, we have features $f_X(\cdot) = \langle f_X, \Phi_X(X) \rangle_{\mathcal{H}_X} = \sum_{i=1}^n a_i^X k_X(\cdot, X_i)$ and $f_Y(\cdot) = \langle f_Y, \Phi_Y(Y) \rangle_{\mathcal{H}_Y} = \sum_{i=1}^n a_i^Y k_Y(\cdot, Y_i)$, where $k_X(\cdot, X)$ and $k_Y(\cdot, Y)$ are the associated kernel functions for $\mathcal{H}_X$ and $\mathcal{H}_Y$, respectively. The kernel Gram matrices are defined as $K_X := (k_X(X_i, X_j))_{i,j=1}^n$ and $K_Y := (k_Y(Y_i, Y_j))_{i,j=1}^n$. We need the centered kernel Gram matrices $M_X = CK_X C$ and $M_Y = CK_Y C$, where $C = I_n - \frac{1}{n} B_n$ with $B_n = 1_n 1_n^T$ and $1_n$ is the vector with $n$ ones. The empirical estimate of Eq. (6) is then given by

$$
\max_{f_X \in \mathcal{H}_X, f_Y \in \mathcal{H}_Y \atop f_X \neq 0, f_Y \neq 0} \frac{\widehat{\text{Cov}}(f_X(X), f_Y(Y))}{[\widehat{\text{Var}}(f_X(X)) + \kappa \|f_X\|_{\mathcal{H}_X}]^{1/2} [\widehat{\text{Var}}(f_Y(Y)) + \kappa \|f_Y\|_{\mathcal{H}_Y}]^{1/2}}
$$

where

$$
\widehat{\text{Cov}}(f_X(X), f_Y(Y)) = \frac{1}{n} a_X^T M_X M_Y a_Y = a_X^T M_X W M_Y a_Y,
$$

$$
\widehat{\text{Var}}(f_X(X)) = \frac{1}{n} a_X^T M_X^2 a_X = a_X^T M_X W M_X a_X,
$$

$$
\widehat{\text{Var}}(f_Y(Y)) = \frac{1}{n} a_Y^T M_Y^2 a_Y = a_Y^T M_Y W M_Y a_Y,
$$

and $W$ is a diagonal matrix with elements $\frac{1}{n}$, and $a_X$ and $a_Y$ are the directions of $X$ and $Y$, respectively. The regularized coefficient $\kappa > 0$.

### 4.1.1 Influence function of classical kernel CCA

By using the IF results of kernel PCA, linear PCA and of linear CCA, we can derive the IF of kernel CCA: kernel CC and kernel CVs,
Theorem 4.1 Given two sets of random variables \((X, Y)\) having distribution \(F_{XY}\), the influence function of kernel canonical correlation and canonical variate at \(Z' = (X', Y')\) are given by

\[
\text{IF}(Z', \rho^2_j) = -\rho^2_j \tilde{f}_{jX}(X') + 2\rho_j \tilde{f}_{jX}(X') \tilde{f}_{jY}(Y') - \rho^2_j \tilde{f}_{jY}(Y'),
\]

\[
\text{IF}(\cdot, Z', f_{jX}) = -\rho_j (\tilde{f}_{jY}(Y') - \rho_j \tilde{f}_{jX}(X')) \tilde{L} \tilde{k}_X(\cdot, X') - (\tilde{f}_{jX}(X'))
\]

\[
-\rho_j \tilde{f}_{jX}(X')) \tilde{L} \Sigma_{XY} \Sigma_{YX}^{-1} \tilde{k}_Y(\cdot, Y') + \frac{1}{2} [1 - \tilde{f}^2_{jX}(X')] f_{jX},
\]

\[
\text{IF}(\cdot, Z', f_{jY}) = -\rho_j (\tilde{f}_{jX}(X') - \rho_j \tilde{f}_{jY}(Y')) \tilde{L} \tilde{k}_Y(\cdot, Y') - (\tilde{f}_{jY}(Y'))
\]

\[
-\rho_j \tilde{f}_{jX}(X')) \tilde{L} \Sigma_{XY} \Sigma_{YX}^{-1} \tilde{k}_Y(\cdot, Y') + \frac{1}{2} [1 - \tilde{f}^2_{jY}(Y')] f_{jY},
\]

where \(L = \Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{YX}^{-1} \Sigma_{XX}^{-1} - \rho^2 I - \Sigma_{XX}^{-1} \Sigma_{XX}^{-1}\).

To prove Theorem 4.1 we need to find the IF of \(L\). All notations and proof are explained in Appendix.

It is known that the inverse of an operator may not exist even exist it may not be continuous operator in general (Fukumizu et al., 2007). While we can derive kernel canonical correlation using correlation operator \(V_{XY} = \Sigma_{XY} \Sigma_{YX} \Sigma_{XX}^{-1}\), even when \(\Sigma_{XX}^{-1}\) and \(\Sigma_{XY}^{-1}\) are not proper operators, the IF of covariance operator is true only for the finite dimensional RKHSs. For infinite dimensional RKHSs, we can find IF of \(\Sigma_{XX}^{-1}\) by introducing a regularization term as follows

\[
\text{IF}(\cdot, X', (\Sigma_{XX} + \kappa I)^{-\frac{1}{2}}) = \frac{1}{2} [((\Sigma_{XX} + \kappa I)^{-\frac{1}{2}} - (\Sigma_{XX} + \kappa I)^{-\frac{1}{2}} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') (\Sigma_{XX} + \kappa I)^{-\frac{1}{2}}],
\]

where \(\kappa > 0\) is a regularization coefficient, which gives empirical estimator.

Let \((X_i, Y_i)_{i=1}^n\) be a sample from the distribution \(F_{XY}\). The EIF of kernel CC and kernel CV at \(Z' = (X', Y')\) for all points \(Z_i = (X_i, Y_i)\) are \(\text{EIF}(Z_i, Z', \rho^2_j) = \tilde{IF}(Z', \rho^2_j)\), \(\text{EIF}(Z_i, Z', f_{jX}) = \tilde{IF}(Z', f_{jX})\), \(\text{EIF}(Z_i, Z', f_{jY}) = \tilde{IF}(Z', f_{jY})\), respectively.

For the bounded kernels the IFs or EIFs, which are stated in Theorem 4.1 and after that, have the three properties: gross error sensitivity, local shift sensitivity and rejection point. But for unbounded kernels, say a linear, polynomial, the IFs are not bounded. In this consequence, the results of classical kernel CCA using the bounded kernels are less sensitive than the results of classical kernel CCA using the unbounded kernels. In practice, classical kernel CCA affected by the contaminated data even using the bounded kernels (Alam et al., 2010).
Input: \( D = \{(X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n)\} \) in \( \mathbb{R}^{m_1 \times m_2} \).

1. Calculate the robust cross-covariance operator, \( \hat{\Sigma}_{YX} \) using algorithm in Figure 2.

2. Calculate the robust covariance operator \( \hat{\Sigma}_{XX} \) and \( \hat{\Sigma}_{YY} \) using the same weight of cross-covariance operator (for simplicity).

3. Find \( B_{YX} = (\hat{\Sigma}_{YY} + \kappa I)^{-\frac{1}{2}} \hat{\Sigma}_{YX} (\hat{\Sigma}_{XX} + \kappa I)^{-\frac{1}{2}} \).

4. For \( \kappa > 0 \), we have \( \rho^2_j \) the largest eigenvalue of \( B_{YX} \) for \( j = 1, 2, \ldots, n \).

5. The unit eigenfunctions of \( B_{YX} \) corresponding to the \( j \)th eigenvalues are \( \hat{\xi}_{jX} \in H_X \) and \( \hat{\xi}_{jY} \in H_Y \).

6. The \( j \)th \( (j = 1, 2, \ldots, n) \) kernel canonical variates are given by
   \[
   \hat{f}_{jX}(X) = \langle \hat{f}_{jX}, \hat{\xi}_{jX}(\cdot, X) \rangle \quad \text{and} \quad \hat{f}_{jY}(X) = \langle \hat{f}_{jY}, \hat{\xi}_{jY}(\cdot, Y) \rangle
   \]
   where \( \hat{f}_{jX} = (\hat{\Sigma}_{XX} + \kappa I)^{-\frac{1}{2}} \hat{\xi}_{jX} \) and \( f_{jY} = (\hat{\Sigma}_{YY} + \kappa I)^{-\frac{1}{2}} \hat{\xi}_{jY} \).

Output: the robust kernel CCA

Figure 3: The algorithm of estimating robust kernel CCA

### 4.2 Robust kernel CCA

In this Section, we propose a robust kernel CCA methods based on robust kernel CO and robust kernel CCO. While many robust linear CCA methods have proposed to emphasize on the linear CCA methods that they fit the bulk of the data well and indicate the points deviating from the original pattern for further investment (Adrover and Donato, 2015, Alam et al., 2010), there is no general well-founded robust methods of kernel CCA. The classical kernel CCA considers the same weights for each data point, \( \frac{1}{n} \), to estimate kernel CO and kernel CCO, which is the solution of an empirical risk optimization problem using the quadratic loss function. It is known that the least square loss function is a no robust loss function. Instead of, we can solve empirical risk optimization problem using the robust least square loss function and the weights are determined based on data via KIRWLS. After getting robust kernel CO and kernel CCO, they are used in classical kernel CCA, which we called a robust kernel CCA method. Figure 3 presents detailed algorithm of the proposed methods (except first two steps, all steps are similar as classical kernel CCA). This method is designed for contaminated data as well, and the principles we describe apply also to the kernel methods, which must deal with the issue of kernel CO and kernel CCO.
5 Experiments

We generate two types of simulated data, original data and those with 5% of contamination, which are called ideal data (ID) and contaminated data (CD), respectively. We conduct experiments on the synthetic data as well as real data sets. The description of 7 real data sets are in Sections 5.2 and 5.3 respectively. The 5 synthetic data sets are as follows:

**Three circles structural data (TCSD):** Data are generated along three circles of different radii with small noise:

\[
X_i = r_i \begin{pmatrix} \cos(Z_{i1}) \\ \sin(Z_{i1}) \end{pmatrix} + \epsilon_i,
\]

where \( r_i = 1, 0.5 \) and 0.25, for \( i = 1, \ldots, n_1, i = n_1 + 1, \ldots, n_2, \) and \( i = n_2 + 1, \ldots, n_3, \) respectively, \( Z_{i1} \sim U[-\pi, \pi] \) and \( \epsilon_i \sim N(0, 0.01 I_{10}) \) independently for an ID and \( Z_{i1} \sim U[-10, 10] \) for the CD.

**Sign function structural data (SFSD):** 1500 data are generated along sine function with small noise:

\[
X_i = \begin{pmatrix} Z_{i1} \\ 2 \sin(2Z_{i1}) \\ \vdots \\ 10 \sin(10Z_{i1}) \end{pmatrix} + \epsilon_i,
\]

where \( Z_{i1} \sim U[-2\pi, 0] \) and \( \epsilon_i \sim N(0, 0.01 I_{10}) \) independently for the ID and \( \epsilon_i \sim N(0, 10 I_{10}) \) for the CD.

**Multivariate Gaussian structural data (MGSD):** Given multivariate normal data, \( Z_{i} \in \mathbb{R}^{12} \sim N(0, \Sigma) \) \( (i = 1, 2, \ldots, n) \) where \( \Sigma \) is the same as in Alam and Fukumizu (2015). We divide \( Z_{i} \) into two sets of variables \( (Z_{i1}, Z_{i2}) \), and use the first six variables of \( Z_{i} \) as \( X \) and perform log transformation of the absolute value of the remaining variables \( (\log_{e}(|Z_{i2}|)) \) as \( Y \). For the CD \( Z_{i} \in \mathbb{R}^{12} \sim N(1, \Sigma) \) \( (i = 1, 2, \ldots, n) \).

**Sign and cosine function structural data (SCSD):** We use uniform marginal distribution, and transform the data by two periodic sin and cos functions to make two sets \( X \) and \( Y \), respectively, with additive Gaussian noise: \( Z_i \sim U[-\pi, \pi], \eta_i \sim N(0, 10^{-2}), \) \( i = 1, 2, \ldots, n, X_{ij} = \sin(j \ast Z_{i1}) + \eta_j, Y_{ij} = \cos(j \ast Z_{i1}) + \eta_j, j = 1, 2, \ldots, 100. \) For the CD \( \eta_i \sim N(1, 10^{-2}) \).

**SNP and fMRI structural data (SMSD):** Two data sets of SNP data \( X \) with 1000 SNPs and fMRI data \( Y \) with 1000 voxels were simulated. To correlate the SNPs with the voxels, a latent model
is used as in Parkhomenko et al. (2009)). For contamination, we consider the signal level, 0.5 and noise level, 1 to 10 and 20, respectively.

In our experiments, first we compare classical and robust kernel covariance operators. After that the robust kernel CCA is compared with the classical kernel CCA, hsicCCA and ktaCCA. In all experiments, for the Gaussian kernel we use median of the pairwise distance as a bandwidth and for the Laplacain kernel the bandwidth is equal to 1. The regularized parameters of classical kernel CCA and robust kernel CCA is \( \kappa = 10^{-5} \). In robust methods, we consider Hubuer’s loss function with the constant, \( c \), equals to the median.

5.1 Kernel covariance operator and robust kernel operator covariance

We evaluate the performance of kernel CO and robust kernel CO in two different settings. First, we check the accuracy of both operators by considering the kernel CO with large data (say a population kernel CO). The measure of the kernel CO and robust kernel CO estimators are defined as

\[
\eta_{kco} = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} k(X_i, X_j)^2 - 2 \frac{1}{Nn} \sum_{i=1}^{n} \sum_{J=1}^{N} k(X_i, X_J)^2 + \frac{1}{N^2} \sum_{I=1}^{N} \sum_{J=1}^{N} k(X_I, X_J)^2,
\]

\[
\eta_{rkco} = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j k(X_i, X_j)^2 - 2 \frac{1}{N} \sum_{i=1}^{n} w_i \sum_{J=1}^{N} k(X_i, X_J)^2 + \frac{1}{N^2} \sum_{I=1}^{N} \sum_{J=1}^{N} k(X_I, X_J)^2,
\]

respectively.

In theory, the above two equations become to zero for large population size, \( N \), with the sample size, \( n \to N \). To do this, we consider the synthetic data, TCSD with \( N \in \{1500, 3000, 6000, 9000\} \) and \( n \in \{15, 30, 45, 60, 90, 120, 150, 180, 210, 240, 270, 300\} \) \( (n = n_1 + n_2 + n_3) \). For each \( n \) with 5% CD, we consider 100 samples and the results (mean with standard error) are plotted in Figure 4. Figures show that the both estimators give similar performance in small sample size but for large sample sizes the robust estimator, robust kernel CO shows much better results than kernel CO estimate at all population sizes.

Second, we compare kernel CO and robust kernel CO estimators using 5 kernels: linear (Poly-1), polynomial with degree 2 (Poly-2) and polynomial with degree 3 (Poly-3), Gaussian and Laplacian on two synthetic data sets: TCSD and SFSD. To measure the performance, we use 4 matrix norms: maximum of absolute column sum (O), Frobenius norm (F), maximum modulus of all the elements (M) and spectral (S) (Sequeira et al., 2011). We calculate the ratio between ID and CD for the kernel
Figure 4: Accuracy measure of kernel covariance operator (Classical, $\eta_{kco}$) and robust kernel covariance operator (Robust, $\eta_{rkco}$).

CO and robust kernel CO. For both estimators, we consider the following measure,

$$
\eta_{kco} = \left| 1 - \frac{\|C_{XX}^{ID}\|}{\|C_{XX}^{CD}\|} \right|
$$

We repeat the experiment for 100 samples with sample size, $n = 1500$. The results (mean ± standard deviation) of $\eta_{kco}$ for kernel CO (Classical) and robust kernel CO (Robust) are tabulated in Table I. From this table, it is clear that the robust estimator performs better than the classical estimator in all cases. Moreover, both estimators using Gaussian and Lapalasian kernels are less sensitive than all polynomial kernels.

5.2 Visualizing influential subject using classical kernel CCA and robust kernel CCA

We evaluate the performance of the propose methods, robust kernel CCA, in three different settings. First, we compare robust kernel CCA with the classical kernel CCA using Gaussian kernel (same
Table 1: Mean and standard deviation of the measure, $\eta_{cov}$, of kernel covariance operator (Classical) and robust kernel covariance operator (Robust).

| Measure | Data | TCSD | SFSD |
|---------|------|------|------|
|         | Kernel | Classical | Robust | Classical | Robust |
| $\|\hat{C}_{XX}\|_O$ | Poly-1 | 0.9947 ± 0.0007 | 0.9546 ± 0.0026 | 0.5692 ± 0.1426 | 0.4175 ± 0.1482 |
|         | Poly-2 | 1.0000 ± 0.0000 | 0.9909 ± 0.0013 | 0.9652 ± 0.0494 | 0.6703 ± 0.1722 |
|         | Poly-3 | 1.0000 ± 0.0000 | 0.9997 ± 0.0001 | 0.9971 ± 0.0095 | 0.8754 ± 0.1104 |
|         | Gaussian | 0.0844 ± 0.0054 | 0.0756 ± 0.0051 | 0.1167 ± 0.0459 | 0.09640.0424 |
|         | Laplacian | 0.1133 ± 0.0054 | 0.0980 ± 0.0128 | 0.1332 ± 0.0830 | 0.1420 ± 0.0745 |
| $\|\hat{C}_{XX}\|_F$ | Poly-1 | 0.9874 ± 0.0017 | 0.8963 ± 0.0069 | 0.3067 ± 0.1026 | 0.1669 ± 0.0626 |
|         | Poly-2 | 1.0000 ± 0.0000 | 0.9863 ± 0.0020 | 0.9559 ± 0.0622 | 0.5917 ± 0.1598 |
|         | Poly-3 | 1.0000 ± 0.0000 | 0.9996 ± 0.0001 | 0.9973 ± 0.0094 | 0.8793 ± 0.1067 |
|         | Gaussian | 0.1153 ± 0.0034 | 0.1181 ± 0.0039 | 0.1174 ± 0.0266 | 0.1059 ± 0.0258 |
|         | Laplacian | 0.1420 ± 0.0032 | 0.1392 ± 0.0035 | 0.1351 ± 0.0459 | 0.1580 ± 0.0366 |
| $\|\hat{C}_{XX}\|_M$ | Poly-1 | 0.9993 ± 0.0001 | 0.9940 ± 0.0005 | 0.8074 ± 0.0838 | 0.6944 ± 0.1118 |
|         | Poly-2 | 1.0000 ± 0.0000 | 0.9996 ± 0.0001 | 0.9921 ± 0.0122 | 0.9070 ± 0.0703 |
|         | Poly-3 | 1.0000 ± 0.0000 | 1.0000 ± 0.0000 | 0.9994 ± 0.0020 | 0.9709 ± 0.0344 |
|         | Gaussian | 0.1300 ± 0.0133 | 0.1028 ± 0.0038 | 0.1065 ± 0.0583 | 0.0735 ± 0.0370 |
|         | Laplacian | 0.1877 ± 0.0053 | 0.1474 ± 0.0042 | 0.1065 ± 0.0583 | 0.0735 ± 0.0370 |
| $\|\hat{C}_{XX}\|_S$ | Poly-1 | 0.9886 ± 0.0019 | 0.9007 ± 0.0091 | 0.2897 ± 0.1412 | 0.1538 ± 0.0877 |
|         | Poly-2 | 1.0000 ± 0.0000 | 0.9887 ± 0.0017 | 0.9591 ± 0.0660 | 0.5927 ± 0.2002 |
|         | Poly-3 | 1.0000 ± 0.0000 | 0.9997 ± 0.0001 | 0.9975 ± 0.0090 | 0.8846 ± 0.1225 |
|         | Gaussian | 0.1281 ± 0.0051 | 0.1227 ± 0.0048 | 0.1333 ± 0.0475 | 0.1091 ± 0.0459 |
|         | Laplacian | 0.1716 ± 0.0050 | 0.1499 ± 0.0045 | 0.1614 ± 0.0759 | 0.1696 ± 0.0613 |

The method, which does not depend on the contaminated data, the above measures, $\eta_p$ and $\eta_f$, should be approximately zero. In other words, the best methods should give small values. To compare, we consider 3 simulated data sets: MGSD, SCSD, SMSD with 3 sample sizes, $n \in \{100, 500, 1000\}$. For each sample size, we repeat the experiment for 100 samples. Table 2 presents the results (mean ± standard deviation) of classical kernel CCA and robust kernel CCA. From this table, we observe that robust kernel CCA outperforms than the classical kernel CCA in all cases.
Second, we propose a simple graphical display based on EIF of kernel CCA, the index plots (the subject on x-axis and the influence, $\eta_\rho$, on y-axis), to assess the related influence data points in data fusion with respect to EIF based on kernel CCA, $\eta_\rho$. To do this, we consider simulated SNP and fMRI data (SMSD) and real SNP and fMRI, Mind Clinical Imaging Consortium (MCIC) Data.

**Mind Clinical Imaging Consortium (MCIC) Data:** The Mind Clinical Imaging Consortium (MCIC) has collected two types of data (SNPs and fMRI) from 208 subjects including 92 schizophrenia patients and 116 healthy controls. Without missing data the number of subjects is 184 (81 schizophrenia patients and 103 healthy controls) [Lin et al., 2014]. After prepossessing we select 19872 voxels and 39770 loci for fMRI data and SNP data, respectively.

The index plots of classical kernel CCA and robust kernel CCA using the SMSD are presented in Figure 5. The 1st and 2nd rows, and columns of this figure are for ID and CD, and classical kernel CCA (Classical KCCA) and robust kernel CCA (Robust KCCA), respectively. These plots show that both methods have almost similar results of the ID. But for CD, it is clear that the classical kernel CCA is affected by the CD in significantly. We can easily identify influence of observation using this visualization. On the other hand, the robust kernel CCA has almost similar results of both data sets, ID and CD.

To detect influential subjects (in schizophrenia patients and healthy controls), we use the EIF of kernel CC of classical and robust kernel CCA methods. For robust kernel CCA, we use robust kernel CC and kernel CVs in Theorem 4.1. The values of $\eta_\rho$ are plotted separately in Figure 6. The schizophrenia patients and healthy controls are in 1st and 2nd rows, respectively. These plots show that healthy controls have less influence than the schizophrenia patients group. The subject 59

### Table 2: Mean and standard deviation of the measures, $\eta_\rho$ and $\eta_f$ of classical kernel CCA (Classical) and robust kernel CCA (Robust).

| Data  | Measure  | $\eta_\rho$ Classical | $\eta_\rho$ Robust | $\eta_f$ Classical | $\eta_f$ Robust |
|-------|----------|-----------------------|--------------------|--------------------|-----------------|
| MGSD  | 100      | 1.9114 ± 3.5945       | 1.2445 ± 3.1262    | 1.3379 ± 3.5092    | 1.3043 ± 2.1842 |
|       | 500      | 1.1365 ± 1.9545       | 1.0864 ± 1.5963    | 0.8631 ± 1.3324    | 0.7096 ± 0.7463 |
|       | 1000     | 1.1695 ± 1.6264       | 1.0831 ± 1.8842    | 0.6193 ± 0.7838    | 0.5886 ± 0.6212 |
| SCSD  | 100      | 0.4945 ± 0.5750       | 0.3963 ± 0.4642    | 1.6855 ± 2.1862    | 0.9953 ± 1.3497 |
|       | 500      | 0.2581 ± 0.2101       | 0.2786 ± 0.4315    | 1.3933 ± 1.9546    | 1.1606 ± 1.3400 |
|       | 1000     | 0.1537 ± 0.1272       | 0.1501 ± 0.1252    | 1.6822 ± 2.2284    | 1.2715 ± 1.7100 |
| SMSD  | 100      | 0.6455 ± 0.0532       | 0.1485 ± 0.1020    | 0.6507 ± 0.2589    | 2.6174 ± 3.3295 |
|       | 500      | 0.6449 ± 0.0223       | 0.0551 ± 0.0463    | 3.7345 ± 2.2394    | 1.3733 ± 1.3765 |
|       | 1000     | 0.6425 ± 0.0134       | 0.0350 ± 0.0312    | 7.7497 ± 1.2857    | 0.3811 ± 0.3846 |
in Schizophrenia patients has the largest influence over all data and the subject 119 has the largest influence over healthy controls only. However, both classical and robust kernel CCA have identified similar subject but robust kernel CCA is less sensitive than classical kernel CCA.

5.3 Extraction of low-dimensional space for classification

Finally, we use 6 well-known real datasets for classification from the UCI repository (Bache and Lichman, 2013): Wine, BUPA liver disorders, Breast tissue, Diabetes, Sona, and Lymphoma to test the significance of low dimensional canonical features of the input space. We use the features for the classification task. To specify the classes, for an $\ell$-class classification problem, the $\ell$ dimensional binary vectors $(1, 0, \ldots, 0), (0, 1, \ldots, 0), \ldots, (0, 0, \ldots, 1)$ are used for $Y$.

Using the low-dimensional canonical features (only 2, 5 and 10) obtained by CCA, we evaluate the classification errors by the kNN classifier ($k = 5$) with 10-fold cross-validation. In comparison, we use the canonical features given by the classical kernel CCA, robust kernel CCA, hsicCCA and
ktaCCA methods. For hsicCCA and ktaCCA methods we use "hsicCCA" R-package. The Table 3 presents the results with the number of data and dimensions. By this table, we see that the hsicCCA and ktaCCA methods are not able to extract all of the canonical variates. On top of that, these methods do not work for the high dimensional dataset. In Table 3 these situation are noted by * and ** respectively. On the other hand, classical kernel CCA and robust kernel CCA can extract all canonical variates as well as for all data sets. In fact, the kernel CCA methods are more faster than the hsicCCA and ktaCCA methods.

6 Concluding remark and future research

The robust estimator employs robust loss function instead of quadratic loss function to achieve robustness for the contamination of the training sample. The robust estimators are weighted estimators, where smaller weights are given more outlying data points. The weights can be estimated efficiently using a KIRLS approach. In terms of the accuracy and sensitivity, it is clear that the ro-
Table 3: Classification errors by the kNN classifier ($k = 5$) with 10-fold cross-validation

| Dataset    | # of Data | Dim | Methods    | # of canonical variates |
|------------|-----------|-----|------------|-------------------------|
|            | X         | Y   |            | 2 | 5 | 10 |
| Classical KCCA | 2.81 | 0.56 | 0.56 |
| Robust KCCA  | 2.81 | 0.56 | 0.56 |
| hsicCCA     | 2.47 | *   | *          |
| ktaCCA      | 2.47 | *   | *          |
| Wine        | 178       | 13  | 3          | Classical KCCA           | 36.79 | 20.76 | 17.92 |
| Breast Tisu | 106       | 10  | 6          | Robust KCCA              | 38.68 | 19.81 | 18.81 |
|             |           |     |            | hsicCCA                  | 24.53 | 20.75 | * |
|             |           |     |            | ktaCCA                   | 22.64 | 20.75 | * |
| Diabetes    | 145       | 5   | 3          | Classical KCCA           | 12.41 | 5.52  | 4.14  |
|             |           |     |            | Robust KCCA              | 12.41 | 5.52  | 4.14  |
|             |           |     |            | hsicCCA                  | 11.03 | *     | *     |
|             |           |     |            | ktaCCA                   | 11.03 | *     | *     |
| Sona        | 208       | 60  | 2          | Classical KCCA           | 14.90 | 14.90 | 13.94 |
|             |           |     |            | Robust KCCA              | 13.94 | 13.94 | 13.94 |
|             |           |     |            | hsicCCA                  | **    | **    | **    |
|             |           |     |            | ktaCCA                   | **    | **    | **    |
| Lymphoma    | 64        | 4026| 3          | Classical KCCA           | 1.61  | 0.00  | 0.00  |
|             |           |     |            | Robust KCCA              | 1.61  | 0.00  | 0.00  |
|             |           |     |            | hsicCCA                  | **    | **    | **    |
|             |           |     |            | ktaCCA                   | **    | **    | **    |

*Functions cannot be evaluated at initial parameters
**Curse of dimensionality

Robust estimators (robust kernel CO and robust kernel CCO) perform better than classical estimators (kernel CO and kernel CCO). We propose the IF of kernel CCA: kernel CC and kernel CVs and robust kernel CCA based on robust kernel CO and robust kernel CCO. The proposed IF measures the sensitivity of kernel CCA, which shows that classical kernel CCA is sensitive to contamination. But the proposed, robust kernel CCA is less sensitive to contamination. The visualization methods can identify influential (outlier) data in both synthesized and real imaging genetics analysis data. We also obtain low dimensional subspace for classification by CCA. We evaluate the classification errors by the kNN classifier ($k = 5$) with 10-fold cross-validation. The proposed robust CCA shows the best performance over hsicCCA and ktaCCA methods.

For the EIF of robust kernel CCA, we use robust kernel CC and kernel CVs in Theorem 4.1. The theoretical IF of robust kernel CCA is an expected future direction of research. Although our focus was on kernel CCA but we can robustify other kernel methods, which must deal with the issue of kernel CO and kernel CCO. In future work, it would be also interesting to develop robust multiple kernel PCA and robust multiple weighted kernel CCA to apply in genomic analysis.
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7 Appendix

We present, derivation of robust centering Gram matrix, robust kernel cross-covariance operator, influence function (IF) of kernel mean elements and kernel cross-covariance operator and proofs which were omitted from the paper.

7.1 Derivation of centering Gram matrix using robust kernel mean element

Given weight of robust kernel mean element $w = [w_1, w_2, \cdots, w_n]^T$ of a set of observations $X_1, \cdots, X_n$, the points

$$\Phi_c(X_i) := \Phi(X_i) - \sum_{b=1}^{n} w_b \Phi(X_b)$$
are centered. Thus

\[
\tilde{K}_{ij} = \langle \Phi_c(X_i), \Phi_c(X_j) \rangle
\]

\[
= \langle \Phi(X_i) - \sum_{b=1}^{n} w_b \Phi(X_b), \Phi(X_j) - \sum_{d=1}^{n} w_d \Phi(X_d) \rangle
\]

\[
= \langle \Phi(X_i), \Phi(X_j) \rangle - \sum_{b=1}^{n} w_b \langle \Phi(X_b), \Phi(X_j) \rangle - \sum_{d=1}^{n} w_d \langle \Phi(X_i), \Phi(X_d) \rangle + \sum_{b=1}^{n} \sum_{d=1}^{n} w_b w_d \langle \Phi(X_b), \Phi(X_d) \rangle
\]

\[
= K_{ij} - \sum_{b=1}^{n} w_b K_{bj} - \sum_{d=1}^{n} K_{id} w_d + \sum_{b=1}^{n} \sum_{d=1}^{n} w_b K_{bd} w_d
\]

\[
= (K - 1_n w^T K - Kw1_n^T + 1_n w^T K w1_n^T)_{ij}
\]

\[
= ((I - 1_n w^T)K(I - 1_n w^T)^T)_{ij}
\]

\[
= (HKH^T)_{ij},
\]

(8)

where \(1_n = [1, 1, \ldots, 1]^T\) and \(H = I - 1_n w^T\). For a set of test points \(X_1^t, X_2^t, \ldots, X_p^t\), we define two matrices of order \(T \times n\) as \(K^\text{test}_{ij} = \langle \Phi(X_i^t), \Phi(X_j) \rangle\) and \(\tilde{K}^\text{test}_{ij} = \langle \Phi(X_i^t) - \sum_{b=1}^{n} w_b \Phi(X_b), \Phi(X_j) - \sum_{d=1}^{n} w_d \Phi(X_d) \rangle\) As in Eq. 8, the robust centered Gram matrix of test points, \(K^\text{test}_{ij}\), in terms of robust Gram matrix is defined as,

\[
\tilde{K}_{ij} = K_{ij} - 1_f w^T K - K^\text{test}_n w^T 1_f + 1_f w^T K w1_n^T
\]

### 7.2 Derivation of centering Gram matrix using robust kernel mean element

Similarly, we can define higher-order moment elements of the feature vector as an empirical risk optimization problem.

**Definition 7.1 (Kernel rth raw moment element)** A mapping \(M^{(r)} := \mathbb{E}_X[\Phi(X) \otimes \Phi(X) \otimes \cdots \otimes \Phi(X)] = \otimes^r \Phi(X) = \mathbb{E}_X[k(X, \cdot)k(X, \cdot) \cdots k(X, \cdot)] = \mathbb{E}_X[k^{(r)}(\cdot, X)]\) with \(\mathbb{E}_X[k^{(r)}(X, X)] < \infty\) is an element of the RKHS, \(\otimes^r \mathcal{H}_X\). By the reproducing property with \(X \in X\)

\[
\langle M^{(r)}, f \rangle_{\otimes^r \mathcal{H}_X} = \mathbb{E}_X[\langle M, f \rangle_{\mathcal{H}_X} \langle M, f \rangle_{\mathcal{H}_X} \cdots \langle M, f \rangle_{\mathcal{H}_X}] = \mathbb{E}_X[f(X)f(X) \cdots f(X)] = \mathbb{E}_X[f^{(r)}(X)],
\]

(9)

for all \(f \in \mathcal{H}_X\). The mapping \(m^{(r)} = \frac{1}{n} \sum_{i=1}^{n} \otimes^r \Phi(X_i)\) is an empirical rth row moment element of the RKHS, \(\otimes^r \mathcal{H}_X\).

\[
\langle m^{(r)}, f \rangle_{\otimes^r \mathcal{H}_X} = \frac{1}{n} \sum_{i=1}^{n} f^{(r)}(X_i),
\]
where $\otimes^r f = f \otimes f \otimes \cdots \otimes f$ is the tensor product of $r$ functions, $f \in \mathcal{H}_X$. The sample $r$th row moment element of the $\Phi(X_i)$ is a solution of an empirical risk optimization problem

$$
\arg\min_{g \in \otimes^r \mathcal{H}_X} \frac{1}{n} \sum_{i=1}^{n} \| \otimes^r_j \Phi_i^{(r)}(X_i) - g \|_{\otimes^r \mathcal{H}_X}^2, \quad (10)
$$

at the point $X$. $g(X, X, \cdots X) \in \otimes^r \mathcal{H}_X$.

**Definition 7.2 (Kernel $r$th central moment element)** A mapping $\mathcal{M}^{(r)} := \mathbb{E}_X[\tilde{k}(\cdot, X)\tilde{k}(\cdot, X)\cdots \tilde{k}(\cdot, X)]$ with $\mathbb{E}_X[\tilde{k}^{(r)}(X, X)] < \infty$ is an element of the RKHS, $\otimes^r \mathcal{H}_X$. By the reproducing property $\forall k(\cdot, X), f \in \mathcal{H}_X$, and $X \in X \forall f \in \mathcal{H}_X$,

$$
\langle \mathcal{M}^{(r)}_c, \otimes^r f_c \rangle_{\otimes^r \mathcal{H}_X} = \langle \mathcal{M}_c, f_c \rangle_{\mathcal{H}_X} \langle \mathcal{M}_c, f_c \rangle_{\mathcal{H}_X} \cdots \langle \mathcal{M}_c[F_X], f_c \rangle_{\mathcal{H}_X} = \mathbb{E}_X[k_c^{(r)}(\cdot, X)]
$$

and the empirical $r$th central moment element at every point $X_i$ is defined by

$$
\langle \mathcal{M}^{(r)}_c, \otimes^r f_c \rangle_{\otimes^r \mathcal{H}_X} = \frac{1}{n} \sum_{b=1}^{n} f_c^{(r)}(X_b) = \frac{1}{n} \sum_{b=1}^{n} k_c^{(r)}(X_i, X_b).
$$

The sample $r$th kernel moment element of the $\Phi(X_i)$ is a solution of

$$
\arg\min_{\otimes^r f_c \in \otimes^r \mathcal{H}_X} \frac{1}{n} \sum_{i=1}^{n} \| \otimes^r_j \Phi_c^{(r)}(X_i) - \otimes^r f_c \|_{\otimes^r \mathcal{H}_X}^2 = \arg\min_{\otimes^r f_c \in \otimes^r \mathcal{H}_X} \frac{1}{n} \sum_{i=1}^{n} \| \otimes^r_j \Phi_c^{(r)}(X_i) - g \|_{\otimes^r \mathcal{H}_X}^2, \quad (11)
$$

where $\Phi_c^{(r)}(X_i) = \Phi^{(r)}(X_i) - \frac{1}{n} \sum_{i=1}^{n} \Phi^{(r)}(X_i)$, at point $X$, $g_c(X, X, \cdots X) = f_c(X)f_c(X) \cdots f_c(X) = f_c^{(r)}(X)$ and $\otimes^r f_c = f_c \otimes f_c \otimes \cdots \otimes f_c$ is the tensor product of $r$ functions $f_c \in \mathcal{H}_X$.

### 7.3 Influence function and cross-raw moment

**Definition 7.3 (Influence function).** Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space and $(X, \mathcal{B})$ a measure space. We want to estimate the parameter $\theta \in \Theta$ of a distribution $F$ in $\mathcal{A}$. We assume that exists a functional $R : \mathcal{D}(R) \to \mathbb{R}$, where $\mathcal{D}(R)$ is the set of all probability distribution in $\mathcal{A}$. Let $G$ be some distribution in $\mathcal{A}$. If data do not follow the model $F$ exactly but slightly going toward $G$, the Gâteaux Derivative at $F$ is given by

$$
\lim_{\epsilon \to 0} \frac{R((1-\epsilon)F + \epsilon G) - R(F)}{\epsilon}, \quad (12)
$$

27
Suppose $x \in X$ and $G = \Delta_x$ is the probability measure which gives mass 1 to $\{x\}$. The influence function (special case of Gâteaux Derivative) of $R$ at $F$ is defined by

$$IF(x, R, F) = \lim_{\epsilon \to 0} \frac{R[(1 - \epsilon)F + \epsilon \Delta_x] - R(F)}{\epsilon}$$  \hspace{1cm} (13)$$

provided that the limit exists. It can be intuitively interpreted as a suitably normalized asymptotic influence of outliers on the value of an estimate or test statistic.

The equivalent definition can also be defined using the perturbation theory. Consider the case where $R(\epsilon) = R[(1 - \epsilon)F + \epsilon G] - R(F)$ is expanded as a convergent power series of $\epsilon$ as

$$R(\epsilon) = R + \epsilon R^{(1)} + \epsilon^2 R^{(2)} + O(\epsilon^3)$$

Due to the properties of convergent power series $R(\epsilon)$ is differentiable in a neighborhood of $\epsilon = 0$.

The IF, $IF(x, R)$ equals to $R^{(1)}$, the first order term of $\epsilon$. There are three properties of IF: gross error sensitivity, local shift sensitivity and rejection point. They measured the worst effect of gross error, the worst effect of rounding error and rejection point.

For a scalar, we just define influence function (IF) at a fixed point. But if the estimate is a function, we are able to express the change of the function value at every points (Kim and Scott, 2012).

**Example 7.1 (Kernel mean element)** Let $R(F_X) = \langle M, f \rangle_{H_X} = \mathbb{E}_X[f(X)] = \int f(X)dF_X = \int k(\cdot, X)dF_X$.

The value of parameter at the contamination model, $W^\epsilon = (1 - \epsilon)F_X + \epsilon \Delta X'$, is given by

$$R[W^\epsilon] = R[(1 - \epsilon)F_X + \epsilon \Delta X'] = \int f(\tilde{X})d[(1 - \epsilon)F_X + \epsilon \Delta X'] = (1 - \epsilon) \int f(\tilde{X})dF_X + \epsilon \int f(\tilde{X})d\Delta_{X'}$$

$$= (1 - \epsilon) \int k(\tilde{X}, X)dF_X + \epsilon \int k(\tilde{X}, X)d\Delta_{X'}$$

$$= (1 - \epsilon) \int k(X, X)dF_X + \epsilon R(F_X) + \epsilon k(\tilde{X}, X')$$

$$= (1 - \epsilon)R(F_X) + \epsilon k(\tilde{X}, X')$$
Thus the IF of $R(F_X)$ at point $X'$ for every point $\hat{X}$ is given by

$$\text{IF}(X', \hat{X}, R, F_X) = \lim_{\epsilon \to 0} \frac{R[W_X^\epsilon] - R(F_X)}{\epsilon} = \lim_{\epsilon \to 0} \frac{(1 - \epsilon)RF_X + \epsilon k(\hat{X}, X') - R(F_X)}{\epsilon} = \lim_{\epsilon \to 0} \left[ k(\hat{X}, X') - R(F_X) \right] = k(\hat{X}, X') - \mathbb{E}_X[k\hat{X}, X], \quad \forall k(\cdot, X) \in \mathcal{H}_X.$$

Which is estimated with the data points $X_1, X_2, \ldots, X_n \in X$ as

$$k(\hat{X}, X') - \frac{1}{n} \sum_{i=1}^n k(\hat{X}, X_i), \quad \forall k(\cdot, X) \in \mathcal{H}_X, \ \hat{X}, X' \in X.$$

Example 7.2 (Kernel cross-raw moment) Let $R(F_{XY}) = \mathbb{E}_{XY}[(k_X(\cdot, X), f_X)_{\mathcal{H}_X}(k_Y(\cdot, Y), f_Y)_{\mathcal{H}_Y}] = \mathbb{E}_{XY}[f_X(X)f_Y(Y)] = \int f_X(x)f_Y(y)dF_{XY}$. The value of parameter at at $Z' = (X', Y')$ the contamination data, for every point $\tilde{Z} = (\tilde{X}, \tilde{Y}) W_{X'}^\epsilon = (1 - \epsilon)F_{XY} + \epsilon \Delta Z'$ is given by

$$R[W_{X'}^\epsilon] = R[(1 - \epsilon)F_{XY} + \epsilon \Delta Z'] = \int f_X(\tilde{X})f_Y(\tilde{Y})d[(1 - \epsilon)F_{XY} + \epsilon \Delta Z'] = (1 - \epsilon) \int f_X(\tilde{X})f_Y(\tilde{Y})dF_{XY} + \epsilon \int f_X(\tilde{X})f_Y(\tilde{Y})d\Delta Z' = (1 - \epsilon) \int f_X(\tilde{X})f_Y(\tilde{Y})dF_{XY} + \epsilon f_X(X')f_Y(Y') = (1 - \epsilon)R(F_{XY}) + \epsilon f_X(X')f_Y(Y')$$

Thus the IF of $R(F_{XY})$ is given by

$$\text{IF}(\cdot, Z', R, F_{XY}) = \lim_{\epsilon \to 0} \frac{R[W_{X'}^\epsilon] - R(F_{XY})}{\epsilon} = \lim_{\epsilon \to 0} \frac{(1 - \epsilon)RF_{XY} + \epsilon f_X(X')f_Y(Y') - R(F_{XY})}{\epsilon} = \lim_{\epsilon \to 0} \left[ f_X(X')f_Y(Y') - R(F_{XY}) \right] = f_X(X')f_Y(Y') - R(F_{XY}) = k_X(\tilde{X}, X')k_Y(\tilde{Y}, Y') - \mathbb{E}_{XY}[(k_X(\tilde{X}, X), f_X)_{\mathcal{H}_X}(k_Y(\tilde{Y}, Y), f_Y)_{\mathcal{H}_Y}].$$
Which is estimated as
\[ k_X(X_i, X')k_Y(Y, Y') - \frac{1}{n} \sum_{b=1}^{n} k_X(X_i, X_b)k_Y(Y, Y_b) \]

**Example 7.3 (Kernel cross-covariance operator)** An cross-covariance operator of \((X, Y), \Sigma_{XY}: \mathcal{H}_X \to \mathcal{H}_Y\) is defined as
\[
R(F_X Y) = \langle f_X, \Sigma_{XY} f_Y \rangle_{\mathcal{H}_F} = \mathbb{E}_{XY}[k_X(\cdot, X) - \mathcal{M}(F_X), f_X \rangle_{\mathcal{H}_F} \langle k_Y(\cdot, Y) - \mathcal{M}(F_Y), f_Y \rangle_{\mathcal{H}_F}
\]
\[
= \mathbb{E}_{XY}[(f_X(X) - \mathbb{E}[f_X])](f_Y(Y) - \mathbb{E}[f_Y])
\]
\[
= \mathbb{E}_{XY}[f_X(X)g_Y(Y)] - \mathbb{E}[f_X(X)]\mathbb{E}[g_Y(Y)]
\]
for \(f_X \in \mathcal{H}_X\) and \(f_Y \in \mathcal{H}_Y\). The IF of \(R(F_X Y)\) at \(Z' = (X', Y')\) using the rule of IF of complicated statistics is given by
\[
\text{IF}(\cdot, Z', R, F_X Y) = f_X(X')f_Y(Y') - \mathbb{E}_{XY}[f_X(X)f_Y(Y)] - \mathbb{E}[f_Y(Y)][f(X) - \mathbb{E}[f_X(X)]]
\]
\[
= \mathbb{E}[f_X(X)][f_Y(Y)] - \mathbb{E}[f_Y(Y)]
\]
\[
= [f_Y(X) - \mathbb{E}[f_Y]](f_Y(Y) - \mathbb{E}[f_Y]) - R(F_X Y)
\]
\[
= \langle k_X(\cdot, X) - \mathcal{M}(F_X), f_X \rangle_{\mathcal{H}_F} \langle k_Y(\cdot, Y) - \mathcal{M}(F_Y), f_Y \rangle_{\mathcal{H}_F}
\]
\[
- \mathbb{E}_{XY}[(k_X(\cdot, X) - \mathcal{M}(F_X), f_X \rangle_{\mathcal{H}_F} \langle k_Y(\cdot, Y) - \mathcal{M}(F_Y), f_Y \rangle_{\mathcal{H}_F}]
\]
Which is estimated with the data points \((X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n) \in X \times Y\) as
\[
\left[ k_X(X_i, X') - \frac{1}{n} \sum_{b=1}^{n} k_X(X_i, X_b) \right] \left[ k_Y(Y, Y') - \frac{1}{n} \sum_{b=1}^{n} k_Y(Y_b, Y') \right] -
\]
\[
\frac{1}{n} \sum_{b=1}^{n} k_X(X_i, X_b) - \frac{1}{n} \sum_{b=1}^{n} k_X(X_i, X_b)\left[ k_Y(Y, Y_j) - \frac{1}{n} \sum_{d=1}^{n} k_Y(Y_d, Y_j) \right]
\]

**7.4 Robust kernel cross-covariance operator**

**Lemma 7.1** Under the assumptions (i) and (ii) the Gâteaux differential of the objective function \(J\) at \(g_1 \in \mathcal{S}'\mathcal{H}\) and incremental \(g_2 \in \mathcal{S}'\mathcal{H}\) is
\[
\delta J(g_1, g_2) = -\langle G(g_1), g_2 \rangle_{\mathcal{S}'\mathcal{H}}.
\]
where $G : \mathcal{G}'\mathcal{H} \rightarrow \mathcal{G}'\mathcal{H}$ is defined as

$$G(g_1) = \frac{1}{n} \sum_{i=1}^{n} \phi(||\otimes\Phi_c(X_i) - g_1||_{\mathcal{G}'\mathcal{H}} \cdot (\otimes\Phi_c(X_i) - g_1)).$$

The necessary condition for $g_1 = \hat{f}(r)$, the kernel central moment element is $G(g_1) = 0$

**Lemma 7.2** Under the same assumption of Lemma 7.1, $r$th robust kernel central moment element (robust kernel CME) at $X$ is given as

$$f_c^{(r)}(X, X, \cdots, X)^{(h)} = \sum_{i=1}^{n} w_i^{(h-1)} k(X, X_i) \tilde{k}(X, X_i) \cdots \tilde{k}(X, X_i)$$

where $w_i^{(h)} = \frac{\varphi(||\otimes\Phi_c^{(h)}(X_i) - g_c||_{\mathcal{G}'\mathcal{H}})}{\sum_{i=1}^{n} \varphi(||\otimes\Phi_c^{(h)}(X_i) - g_c||_{\mathcal{G}'\mathcal{H}})}$, and $\varphi(x) = \frac{\zeta'(x)}{x}$. Putting the different value of $r$, we get the different robust kernel moment estimates.

**Corollary 7.1** Under the same assumption of Lemma 7.1 kernel CO at $(X, X)$ and kernel CCO at $(X, Y)$ are estimated as

$$\hat{\Sigma}_{XX}^{(h)} = \sum_{i=1}^{n} w_i^{(h-1)} \tilde{k}(X, X_i) \tilde{k}(X, X_i), \quad \hat{\Sigma}_{XY}^{(h)} = \sum_{b=1}^{n} w_b^{(h-1)} \tilde{k}(X, X_b) \tilde{k}(Y, Y_i),$$

respectively and $w_b^{(h)}$ is the same as in Lemma Eq. (7.1) with $r = 2$.

### 7.4.1 Proof of Theorem 4.1: Influence function of kernel CCA

As in Fukumizu et al. (2007), using the cross-covariance operator of $(X, Y)$, $\Sigma_{XY} : \mathcal{H}_Y \rightarrow \mathcal{H}_X$ we can reformulate the optimization problem of classical kernel canonical correlation (classical kernel CCA) as follows:

$$\sup_{f_X \in \mathcal{H}_X, f_Y \in \mathcal{H}_Y \atop f_X \neq 0, f_Y \neq 0} \langle f_X, \Sigma_{XY} f_Y \rangle_{\mathcal{H}_X} \quad \text{subject to} \quad \langle f_X, \Sigma_{XX} f_X \rangle_{\mathcal{H}_X} = 1, \quad \langle f_Y, \Sigma_{YY} f_Y \rangle_{\mathcal{H}_Y} = 1. \quad (14)$$

Using generalized eigenvalue problem, we can derive the solution of Eq. (14) as with liner CCA (Anderson, 2003).

$$\begin{cases}
\Sigma_{XY} f_X - \rho \Sigma_{YY} f_Y = 0, \\
\Sigma_{XY} f_Y - \rho \Sigma_{XX} f_X = 0.
\end{cases}$$
After some simple calculation, we can reset the solution as a single matrix equation for \( f_X \) or \( f_Y \).

\[
\begin{align*}
(\Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{XY} - \rho^2 \Sigma_{XX}) f_X = 0, \\
(\Sigma_{XY} \Sigma_{XX}^{-1} \Sigma_{XY} - \rho^2 \Sigma_{YY}) f_Y = 0.
\end{align*}
\] (15)

The generalized eigenvalue problem in Eq. (15) (for simplicity we use first equation only) can be formulated as a simple eigenvalue problem using \( j \)th eigenfunction.

\[
(\Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{XY} \Sigma_{XX}^{-1} - \rho^2 I) \Sigma_{XX}^{-1} f_X = 0
\]

\[
\Rightarrow (\Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{XY} \Sigma_{XX}^{-1} - \rho^2 I) f_X = 0
\] (16)

To use the results of IF of liner principle components analysis (Tanaka, 1988), IF of liner canonical correlation analysis (Romanazzi, 1992) and IF of kernel principle component analysis (Huang et al., 2009b) for the finite dimension and for the infinite dimension, respectively, we convert generalized eigenvalue problem of kernel canonical correlation analysis into a simple eigenvalue problem. Thus, we need to find, the IF of \( \Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{XY} \Sigma_{XX}^{-1} \) and henceforth IF of \( \Sigma_{YY}^{-1}, \Sigma_{XX}^{-1} \) and \( \Sigma_{XY} \). Let \( \Sigma_{XY} \) be the covariance of the random vectors \( k_X(\cdot, X) \) and \( k_Y(\cdot, Y) \) on RKHS i.e., kernel covariance operator, \( \Sigma_{XX} : \mathcal{H}_X \rightarrow \mathcal{H}_X \), for all \( f_X \in \mathcal{H} \) and \( f_Y \in \mathcal{H}_Y \) we have

\[
\mathbb{E}_{XY}\{\langle f_X, k_X(\cdot, X) - M_X \rangle_{\mathcal{H}_X} \langle k_Y(\cdot, Y) - M_Y, f_Y \rangle_{\mathcal{H}_Y}\}
= \mathbb{E}_{XY}\{f_Y, (k_X(\cdot, X) - M_X) \otimes (k_Y(\cdot, Y) - M_Y) f_X\}_{\mathcal{H}_Y}
= \langle f_Y, \mathbb{E}_{XY}(k_X(\cdot, X) - M_X) \otimes (k_Y(\cdot, Y) - M_Y) f_X\rangle_{\mathcal{H}_Y}
= \langle f_Y, \Sigma_{XX}^{-1} f_X\rangle_{\mathcal{H}_Y}
\] (17)

where \( M_X \) is kernel mean elements in \( \mathcal{H}_X \) and \( \Sigma_{XX} = (k_X(\cdot, X) - M_X) \otimes (k_Y(\cdot, Y) - M_Y) \), since \((T_1 \otimes T_2)(x) = (x, T_2)T_1\). Using simple algebra we have at \( Z' = (X', Y') \)

\[
\text{IF}(X', X' \otimes \Sigma_{XX}) = (k_X(\cdot, X') - M_X) \otimes (k_X(\cdot, X') - M_X) - \Sigma_{XX},
\]

\[
\text{IF}(Y', Y' \otimes \Sigma_{YY}) = (k_Y(\cdot, Y') - M_Y) \otimes (k_Y(\cdot, Y') - M_Y) - \Sigma_{YY},
\]

\[
\text{IF}(Z', X' \otimes \Sigma_{XY}) = (k_X(\cdot, X') - M_X) \otimes (k_Y(\cdot, Y') - M_Y) - \Sigma_{XY}
\]

and

\[
\text{IF}(Z', X' \otimes \Sigma_{XX}^{-1} \Sigma_{XY}) = \frac{1}{2} [\Sigma_{XX}^{-1} - \Sigma_{XX}^{-1} (k_X(\cdot, X') - M_X) \otimes (k_X(\cdot, X') - M_X) \Sigma_{XX}^{-1} ].
\]
For simplicity, let us define \( \tilde{k}_Y(\cdot, X') := k_Y(\cdot, X') - \mathcal{M}_X \), \( \tilde{k}_Y(\cdot, Y') := k_Y(\cdot, Y') - \mathcal{M}_Y \) and \( A := \Sigma_{XY}^{-1} \Sigma_{YY} \), \( B := \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XX}^{-\frac{1}{2}} \), and \( L = \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YX} \Sigma_{XX}^{-\frac{1}{2}} - \rho^2 \mathbf{I} \). Now,

\[
\begin{align*}
\text{IF}(\cdot, Z', A) &= \text{IF}(\cdot, Y', \Sigma_{YY}^{-1} \Sigma_{XXX}) + \Sigma_{XY} \Sigma_{YY}^{-1} \text{IF}(X', Y', \Sigma_{YY}^{-1}) + \Sigma_{XY} \Sigma_{YY}^{-1} \text{IF}(X', Y', \Sigma_{YY}^{-1}) \\
&= \left[ \tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') - \Sigma_{XY} \right] \Sigma_{YY}^{-1} \Sigma_{YX} + \Sigma_{XY} \left[ \Sigma_{YY}^{-1} - \Sigma_{YY}^{-1} \tilde{k}_Y(\cdot, Y') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{YY}^{-1} \right] \Sigma_{YX} \\
&\quad + \Sigma_{XY} \Sigma_{YY}^{-1} \left[ \tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') - \Sigma_{YX} \right] \\
&= 2 \Sigma_{XY} \Sigma_{YY}^{-1} \left[ \tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') - \Sigma_{YX} \right] + \Sigma_{XY} \left[ \Sigma_{YY}^{-1} - \Sigma_{YY}^{-1} \tilde{k}_Y(\cdot, Y') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{YY}^{-1} \right] \Sigma_{YX}
\end{align*}
\]

Then,

\[
\Sigma_{XX}^{-\frac{1}{2}} \text{IF}(Z', A) \Sigma_{XX}^{-\frac{1}{2}} = 2 \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YX} \Sigma_{XX}^{-\frac{1}{2}} [\tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') - \Sigma_{YX}] \Sigma_{XX}^{-\frac{1}{2}} \\
\quad + \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} [\Sigma_{YY}^{-1} - \Sigma_{YY}^{-1} \tilde{k}_Y(\cdot, Y') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{YY}^{-1}] \Sigma_{YX} \Sigma_{XX}^{-\frac{1}{2}}
\]

and

\[
\text{IF}(X', \Sigma_{XX}^{-\frac{1}{2}} A \Sigma_{XX}^{-\frac{1}{2}}) = 2 \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} + \Sigma_{XX}^{-\frac{1}{2}} \text{IF}(X', \Sigma_{XX}^{-\frac{1}{2}}) A \Sigma_{XX}^{-\frac{1}{2}} = [\Sigma_{XX}^{-\frac{1}{2}} - \Sigma_{XX}^{-\frac{1}{2}} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \Sigma_{XX}^{-\frac{1}{2}}] A \Sigma_{XX}^{-\frac{1}{2}}
\]

The influence of \( B \) is given by

\[
\begin{align*}
\text{IF}(X', Y', B) &= 2 \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} + \Sigma_{XX}^{-\frac{1}{2}} \text{IF}(X', Y', A) \Sigma_{XX}^{-\frac{1}{2}} \\
&= [\Sigma_{XX}^{-\frac{1}{2}} - \Sigma_{XX}^{-\frac{1}{2}} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \Sigma_{XX}^{-\frac{1}{2}}] \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \\
&\quad + 2 \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} [\tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, Y') - \Sigma_{XX}] \Sigma_{XX}^{-\frac{1}{2}} \\
&\quad + \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} [\Sigma_{YY}^{-1} - \Sigma_{YY}^{-1} \tilde{k}_Y(\cdot, Y') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{YY}^{-1}] \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \\
&= -\Sigma_{XX}^{-\frac{1}{2}} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \\
&\quad + 2 \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, Y') \Sigma_{XX}^{-\frac{1}{2}} \\
&\quad - \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \tilde{k}_X(\cdot, Y') \otimes \tilde{k}_X(\cdot, Y') \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{YY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} \\
&= 2 \Sigma_{XX}^{-\frac{1}{2}} \Sigma_{XY} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma_{XX}^{-\frac{1}{2}} + \Sigma_{XX}^{-\frac{1}{2}} \text{IF}(X', Y', A) \Sigma_{XX}^{-\frac{1}{2}}
\end{align*}
\]

We convert generalized eigenvalue problem as a eigenvalue problem and use the Lemma 1 of Huang et al. (2009b) to define the IF of kernel CC, \( \rho^2_f \) and kernel CVs, \( f_X(X) \) and, \( f_Y(Y) \). Then the IF of
kernel $\rho^2_j$ is defined as

$$\text{IF}(Z', \rho^2_j) = \langle \tilde{f}_X, \text{IF}(Z', \mathbb{B}) \tilde{f}_X \rangle_{H_x \otimes H_y}$$

$$= -(f_{jX}, \sum_{XX}^{1} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \Sigma_{XX}^{-1} \Sigma_{XY} \Sigma_{XX}^{-1} \Sigma_{X} f_{jX})_{H_x \otimes H_y}$$

$$+ 2(\tilde{f}_{jX}, \sum_{XX}^{1} \sum_{XY} \Sigma_{XX}^{-1} \sum_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX})_{H_x \otimes H_y}$$

$$- \langle \tilde{f}_{jX}, \sum_{XX}^{1} \sum_{XY} \sum_{YY} \tilde{k}_X(\cdot, Y') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{XY} \Sigma_{XX}^{-1} - \sum_{XX} f_{jX})_{H_x \otimes H_y}$$

$$= -(f_{jX}, \sum_{XX}^{1} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \sum_{XX} \tilde{\Sigma}_{XX} \Sigma_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX})_{H_x \otimes H_y}$$

$$+ 2(\tilde{f}_{jX}, \sum_{XX}^{1} \sum_{XY} \sum_{YY} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') \sum_{XY} \sum_{XX} f_{jX})_{H_x \otimes H_y}$$

$$- \langle \tilde{f}_{jX}, \sum_{XX}^{1} \sum_{XY} \sum_{YY} \tilde{k}_Y(\cdot, Y') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{YY} \sum_{XX} f_{jX})_{H_x \otimes H_y}$$

For simplicity we calculate in parts of Eq. (19). The first part derive as

$$\langle f_{jX}, \sum_{XX}^{1} \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \sum_{XX} \tilde{\Sigma}_{XX} \Sigma_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y}$$

$$= (\sum_{XX} f_{jX}, \tilde{k}_X(\cdot, X') \otimes \tilde{k}_X(\cdot, X') \sum_{XX} \tilde{\Sigma}_{XX} \Sigma_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y}$$

$$= (f_{jX}, \tilde{k}_X(\cdot, X'))_{H_x} (\tilde{k}_X(\cdot, X'), \sum_{XX} \tilde{\Sigma}_{XX} \Sigma_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y}$$

$$= \rho^2_j f_{jX}(X'),$$

in the last equality, we use Eq. (16). The 2nd part of the Eq. (19) derive as

$$\langle f_{jX}, \sum_{XX}^{1} \sum_{XY} \Sigma_{XX}^{-1} \sum_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y}$$

$$= (\sum_{XX} f_{jX}, \tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') \sum_{XY} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y}$$

$$= (f_{jX}, \tilde{k}_X(\cdot, X') \otimes \tilde{k}_Y(\cdot, Y') \Sigma_{XY} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y}$$

$$= \rho^2_j f_{jX}(X') f_{jY}(Y'),$$

in the last second equality, we use Eq. (15). Similarly, we can write the 3rd term as

$$\langle f_{jX}, \sum_{XX}^{1} \sum_{XY} \Sigma_{XX}^{-1} \sum_{XY} \Sigma_{XX}^{-1} \sum_{XX} f_{jX} \rangle_{H_x \otimes H_y} = \rho^2_j f_{jX}(Y')$$

where $\tilde{f}_{jX} = f_{jX}(X') = \langle f_{jX}, \tilde{k}_X(\cdot, X') \rangle$ and similar for $\tilde{f}_{jY}$. Therefore, substituting Eq. (20), (21) and (22) into Eq. (19) the IF of kernel CC is given by

$$\text{IF}(X', Y', \rho_j) = -\rho^2_j f_{jX}(Y') + 2\rho_j f_{jX}(X') \tilde{f}_{jY}(Y') - \rho^2_j f_{jY}(Y')$$

(23)
Now we derive the IF of kernel Cvs. To this end first we need to derive

\[ IF(X', f_{jX}) = IF(X', \Sigma^{-\frac{1}{2}}_{XX} f_{jX}) = \Sigma^{-\frac{1}{2}}_{XX} IF(X', f_{jX}) + IF(X', \Sigma^{-\frac{1}{2}}_{XX}) f_{jX} \] (24)

By the first term of Eq. (24) we have

\[
\Sigma^{-\frac{1}{2}}_{XX} IF(X', Y', f_{jX}) = \Sigma^{-\frac{1}{2}}_{XX} (\mathbb{B} - \rho^2 \mathbf{I})^{-1} IF(X', Y', \mathbb{B}) f_{jX} \\
= -\Sigma^{-\frac{1}{2}}_{XX} (\mathbb{B}) - \rho^2 \mathbf{I}^{-1} [\Sigma^{-\frac{1}{2}}_{XX} \hat{k}_X(\cdot, X') \odot \hat{k}_Y(\cdot, Y') \Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma^{-\frac{1}{2}}_{XX}]
+ 2 \Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \hat{k}_X(\cdot, X') \odot \hat{k}_Y(\cdot, Y') \Sigma^{-\frac{1}{2}}_{XX} - \Sigma^{-\frac{1}{2}}_{XX} \Sigma_{XX} \Sigma_{YY}^{-1} \Sigma_{XX} \Sigma^{-\frac{1}{2}}_{XX} f_{jX} \] (25)

We derive each terms of Eq. (25), respectively. The first term of Eq. (25) is given by

\[
\Sigma^{-\frac{1}{2}}_{XX} (\mathbb{B}) - \rho^2 \mathbf{I}^{-1} [\Sigma^{-\frac{1}{2}}_{XX} \hat{k}_X(\cdot, X') \odot \hat{k}_X(\cdot, X') \Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma^{-\frac{1}{2}}_{XX} f_{jX}]
= \mathbb{L}(\hat{k}_X(\cdot, X') \odot \hat{k}_X(\cdot, X') \Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \Sigma_{YY} \Sigma^{-\frac{1}{2}}_{XX} f_{jX})
= \mathbb{L}(\rho_j^2(\hat{k}_X(\cdot, X') \odot \hat{k}_X(\cdot, X') f_{jX}))
= \mathbb{L}(\rho_j^2(\hat{k}_X(\cdot, X') \odot \hat{k}_X(\cdot, X') f_{jX}))
= \mathbb{L}(\rho_j^2(\hat{k}(\cdot, X') f_{jX}))
= \mathbb{L}(\rho_j^2(\hat{k}(\cdot, X')))
\]

(26)

2nd term of Eq. (25) is

\[
2 \mathbb{L}(\Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \hat{k}_X(\cdot, X') \hat{k}_Y(\cdot, Y') \Sigma^{-\frac{1}{2}}_{XX} f_{jX})
= \mathbb{L}(\Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \hat{k}_X(\cdot, X') \hat{k}_Y(\cdot, Y') f_{jX})
+ \mathbb{L}(\Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \hat{k}_X(\cdot, X') f_{jX}) \hat{k}_Y(\cdot, Y')
= \mathbb{L}(\rho_j^2(\hat{k}_Y(\cdot, Y') f_{jX}))
+ \mathbb{L}(\Sigma^{-\frac{1}{2}}_{XX} \Sigma_{YY}^{-1} \hat{k}_X(\cdot, X') \hat{k}_Y(\cdot, Y') f_{jX})
\]

and the 3rd term of Eq. (25) is

\[
\mathbb{L}(\Sigma_{YY}^{-1} \hat{k}_Y(\cdot, Y') \odot \hat{k}_Y(\cdot, Y') \Sigma^{-\frac{1}{2}}_{XX} f_{jX})
= \mathbb{L}(\Sigma_{YY}^{-1} \hat{k}_Y(\cdot, Y') \Sigma^{-\frac{1}{2}}_{XX} f_{jX} \hat{k}_Y(\cdot, Y'))
= \mathbb{L}(\Sigma_{YY}^{-1} \hat{k}_Y(\cdot, Y') \rho_j f_{jX} \hat{k}_Y(\cdot, Y'))
= \mathbb{L}(\rho_j \Sigma_{YY}^{-1} \hat{k}_Y(\cdot, Y') \rho_j f_{jX} \hat{k}_Y(\cdot, Y'))
\]

35
By substituting the above three equations into Eq. (25) we have

\[
\Sigma_{XX}^{-\frac{1}{2}} \text{IF}(\cdot, Z', f_{jX}) = \Sigma_{XX}^{-\frac{1}{2}}(\mathbb{E} - \rho^2 I)^{-1} \text{IF}(\cdot, Z', \mathbb{E}) f_{jX}
\]

\[
= -\rho_j \bar{f}_j(Y') - \rho_j \bar{f}_j(X') L \bar{k}(\cdot, X') - (\bar{f}_j(X') - \rho_j \bar{f}_j(Y')) \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}} \bar{k}(\cdot, Y')
\]

(27)

The 2nd term of the Eq. (24) is give by

\[
\text{IF}(X', \Sigma_{XX}^{-\frac{1}{2}} f_{jX})
\]

\[
= -\langle f_{jX}, \Sigma_{XX}^{-\frac{1}{2}} f_{jX} \rangle \Sigma_{XX}^{-\frac{1}{2}} \text{IF}(X', \Sigma_{XX}^{-\frac{1}{2}} f_{jX}) f_{jX}
\]

\[
= -\frac{1}{2} \langle f_{jX}, \Sigma_{XX}^{-\frac{1}{2}} \text{IF}(X', \Sigma_{XX}^{-\frac{1}{2}} f_{jX}) \rangle + \langle f_{jX}, \text{IF}(X', \Sigma_{XX}^{-\frac{1}{2}} f_{jX}) \rangle f_{jX}
\]

\[
= -\frac{1}{2} \langle f_{jX}, (\bar{k}(\cdot, X') - \Sigma_{XX} f_{jX}) \rangle f_{jX}
\]

\[
= -\frac{1}{2} \bar{f}_j(X') \langle f_{jX}, \Sigma_{XX} f_{jX} \rangle f_{jX}
\]

\[
= \frac{1}{2} \langle f_{jX}, \Sigma_{XX} f_{jX} \rangle f_{jX}
\]

(28)

Therefore, substituting Eq. (27) and Eq. (28) into Eq. (24) we get the IF of kernel canonical variate (CV) of

\[
\text{IF}(\cdots, X', Y', f_{jX}) = -\rho_j \bar{f}_j(Y') - \rho_j \bar{f}_j(X') L \bar{k}(\cdot, X') - (\bar{f}_j(X') - \rho_j \bar{f}_j(Y')) \Sigma_{XY} \Sigma_{YY}^{-\frac{1}{2}} \bar{k}(\cdot, Y')
\]

\[
+ \frac{1}{2} [1 - \bar{f}_j^2(Y')] f_{jX}
\]

Similarly, we can derive \(\text{IF}(\cdot, X', Y', f_{jY})\).

Let \((X_i, Y_i)_{i=1}^n\) be a sample from the distribution \(F_{XY}\). The empirical estimator of Eq. (14) and Eq. (15) are

\[
\sup_{f_X \in H_\alpha, f_Y \in H_\beta \atop f_X \neq 0, f_Y \neq 0} \langle f_Y, \hat{\Sigma}_{YY} f_Y \rangle_{H_\beta} \quad \text{subject to} \quad \begin{cases} 
\langle f_X, (\hat{\Sigma}_{XX} + \alpha I) f_X \rangle_{H_\alpha} = 1, \\
\langle f_Y, (\hat{\Sigma}_{YY} + \alpha I) f_Y \rangle_{H_\beta} = 1,
\end{cases}
\]

(29)
\[
\begin{align*}
(\hat{\Sigma}_{XY}(\hat{\Sigma}_{YY} + \kappa I)^{-1} - \rho^2(\hat{\Sigma}_{XX} + \kappa I))f_x &= 0, \\
(\hat{\Sigma}_{YX}(\hat{\Sigma}_{XX} + \kappa I)^{-1} - \rho^2(\hat{\Sigma}_{YY} + \kappa I))f_y &= 0,
\end{align*}
\]

respectively.

Using the above equations, the empirical IF (EIF) of kernel CC and kernel CVs at \(Z' = (X', Y')\) for all points \(Z_i = (X_i, Y_i)\) are
\[
\text{EIF}(Z_i, \hat{\rho}^2_j) = \hat{\text{EIF}}(Z', \hat{\rho}^2_j), \quad \text{EIF}(\cdot, Z', f_{X}) = \hat{\text{EIF}}(Z_i, Z', f_{X}), \quad \text{EIF}(\cdot, Z', f_{Y}) = \hat{\text{EIF}}(Z_i, Z', \hat{f}_{Y}),
\]
respectively.