



HAL
open science

Characteristic and Universal Tensor Product Kernels

Zoltán Szabó, Bharath K Sriperumbudur

► **To cite this version:**

Zoltán Szabó, Bharath K Sriperumbudur. Characteristic and Universal Tensor Product Kernels. [Research Report] École Polytechnique; Pennsylvania State University. 2018. hal-01585727v2

HAL Id: hal-01585727

<https://hal.science/hal-01585727v2>

Submitted on 13 May 2018 (v2), last revised 2 Aug 2018 (v3)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Characteristic and Universal Tensor Product Kernels

Zoltán Szabó*

Bharath K. Sriperumbudur†

Abstract

Maximum mean discrepancy (MMD), also called energy distance or N-distance in statistics and Hilbert-Schmidt independence criterion (HSIC), specifically distance covariance in statistics, are among the most popular and successful approaches to quantify the difference and independence of random variables, respectively. Thanks to their kernel-based foundations, MMD and HSIC are applicable on a wide variety of domains. Despite their tremendous success, quite little is known about when HSIC characterizes independence and when MMD with tensor product kernel can discriminate probability distributions. In this paper, we answer these questions by studying various notions of characteristic property of the tensor product kernel.

Keywords: tensor product kernel, kernel mean embedding, characteristic kernel, \mathcal{I} -characteristic kernel, universality, maximum mean discrepancy, Hilbert-Schmidt independence criterion

1 Introduction

Kernel methods [Schölkopf and Smola, 2002] are among the most flexible and influential tools in machine learning and statistics, with superior performance demonstrated in a large number of areas and applications. The key idea in these methods is to map the data samples into a possibly infinite-dimensional feature space—precisely, a reproducing kernel Hilbert space (RKHS) [Aronszajn, 1950]—and apply linear methods in the feature space, without the explicit need to compute the map. A generalization of this idea to probability measures, i.e., mapping probability measures into an RKHS (Berlinet and Thomas-Agnan, 2004, Chapter 4; Smola et al., 2007) has found novel applications in nonparametric statistics and machine learning. Formally, given a probability measure \mathbb{P} defined on a measurable space \mathcal{X} and an RKHS \mathcal{H}_k with $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ as the reproducing kernel (which is symmetric and positive definite), \mathbb{P} is embedded into \mathcal{H}_k as

$$\mathbb{P} \mapsto \int_{\mathcal{X}} k(\cdot, x) d\mathbb{P}(x) =: \mu_k(\mathbb{P}), \quad (1)$$

where $\mu_k(\mathbb{P})$ is called the *mean element* or *kernel mean embedding* of \mathbb{P} . The *mean embedding* of \mathbb{P} has led to a new generation of solutions in two-sample testing [Baringhaus and Franz,

*Center for Applied Mathematics (CMAP), École Polytechnique, Route de Saclay, 91128 Palaiseau, France. E-mail: zoltan.szabo@polytechnique.edu

†Department of Statistics, Pennsylvania State University, 314 Thomas Building, University Park, PA 16802. E-mail: bks18@psu.edu

2004, Székely and Rizzo, 2004, 2005, Borgwardt et al., 2006, Harchaoui et al., 2007, Gretton et al., 2012], domain adaptation [Zhang et al., 2013] and generalization [Blanchard et al., 2017], kernel belief propagation [Song et al., 2011], kernel Bayes’ rule [Fukumizu et al., 2013], model criticism [Lloyd et al., 2014, Kim et al., 2016], approximate Bayesian computation [Park et al., 2016], probabilistic programming [Schölkopf et al., 2015], distribution classification [Muandet et al., 2011, Zaheer et al., 2017], distribution regression [Szabó et al., 2016, Law et al., 2018] and topological data analysis [Kusano et al., 2016]. For a recent survey on the topic, the reader is referred to [Muandet et al., 2017].

Crucial to the success of the mean embedding based representation is whether it encodes all the information about the distribution, in other words whether the map in (1) is injective in which case the kernel is referred to as *characteristic* [Fukumizu et al., 2008, Sriperumbudur et al., 2010]. Various characterizations for the characteristic property of k is known in the literature (e.g., see Fukumizu et al., 2008, 2009, Gretton et al., 2012, Sriperumbudur et al., 2010) using which the popular kernels on \mathbb{R}^d such as Gaussian, Laplacian, B-spline, inverse multi-quadratics, and the Matérn class are shown to be characteristic. The characteristic property is closely related to the notion of *universality* (Steinwart, 2001; Micchelli et al., 2006; Carmeli et al., 2010; Sriperumbudur et al., 2011)— k is said to be universal if the corresponding RKHS \mathcal{H}_k is dense in a certain target function class, for example, the class of continuous functions on compact domains—and the relation between these notions has recently been explored in [Sriperumbudur et al., 2011, Simon-Gabriel and Schölkopf, 2016].

Based on the mean embedding in (1), Smola et al. [2007] and Gretton et al. [2012] defined a semi-metric, called the maximum mean discrepancy (MMD) on the space of probability measures:

$$\text{MMD}_k(\mathbb{P}, \mathbb{Q}) := \|\mu_k(\mathbb{P}) - \mu_k(\mathbb{Q})\|_{\mathcal{H}_k},$$

which is a metric iff k is characteristic. A fundamental application of MMD is in non-parametric hypothesis testing that includes two-sample [Gretton et al., 2012] and independence tests [Gretton et al., 2008]. Particularly in independence testing, as a measure of independence, MMD measures the distance between the joint distribution \mathbb{P}_{XY} and the product of marginals $\mathbb{P}_X \otimes \mathbb{P}_Y$ of two random variables X and Y which are respectively defined on measurable spaces \mathcal{X} and \mathcal{Y} , with the kernel k being defined on $\mathcal{X} \times \mathcal{Y}$. As aforementioned, if k is characteristic, then $\text{MMD}_k(\mathbb{P}_{XY}, \mathbb{P}_X \otimes \mathbb{P}_Y) = 0$ implies $\mathbb{P}_{XY} = \mathbb{P}_X \otimes \mathbb{P}_Y$, i.e., X and Y are independent. A simple way to define a kernel on $\mathcal{X} \times \mathcal{Y}$ is through the tensor product of kernels k_X and k_Y defined on \mathcal{X} and \mathcal{Y} respectively: $k = k_X \otimes k_Y$, i.e., $k((x, y), (x', y')) = k_X(x, x')k_Y(y, y')$, $x, x' \in \mathcal{X}$, $y, y' \in \mathcal{Y}$, with the corresponding RKHS $\mathcal{H}_k = \mathcal{H}_{k_X} \otimes \mathcal{H}_{k_Y}$ being the tensor product space generated by \mathcal{H}_{k_X} and \mathcal{H}_{k_Y} . This means, when $k = k_X \otimes k_Y$,

$$\text{MMD}_k(\mathbb{P}_{XY}, \mathbb{P}_X \otimes \mathbb{P}_Y) = \|\mu_{k_X \otimes k_Y}(\mathbb{P}_{XY}) - \mu_{k_X \otimes k_Y}(\mathbb{P}_X \otimes \mathbb{P}_Y)\|_{\mathcal{H}_{k_X} \otimes \mathcal{H}_{k_Y}}. \quad (2)$$

In addition to the simplicity of defining a joint kernel k on $\mathcal{X} \times \mathcal{Y}$, the tensor product kernel offers a principled way of combining inner products (k_X and k_Y) on domains that can correspond to different modalities (say images, texts, audio). By exploiting the isomorphism between tensor product Hilbert spaces and the space of Hilbert-Schmidt operators¹, it follows

¹In the equivalence one assumes that \mathcal{H}_{k_X} , \mathcal{H}_{k_Y} are separable; this holds under mild conditions, for example if \mathcal{X} and \mathcal{Y} are separable topological domains and k_X , k_Y are continuous [Steinwart and Christmann, 2008, Lemma 4.33].

from (2) that

$$\text{MMD}_k(\mathbb{P}_{XY}, \mathbb{P}_X \otimes \mathbb{P}_Y) = \|C_{XY}\|_{\text{HS}} =: \text{HSIC}_k(\mathbb{P}_{XY}), \quad (3)$$

which is the Hilbert-Schmidt norm of the cross-covariance operator $C_{XY} := \mu_{k_X \otimes k_Y}(\mathbb{P}_{XY}) - \mu_{k_X}(\mathbb{P}_X) \otimes \mu_{k_Y}(\mathbb{P}_Y)$ and is known as the *Hilbert-Schmidt independence criterion* (HSIC) [Gretton et al., 2005]. HSIC has enjoyed tremendous success in a variety of applications such as independent component analysis [Gretton et al., 2005], feature selection [Song et al., 2012], independence testing [Gretton et al., 2008, Jitkrittum et al., 2017], post selection inference [Yamada et al., 2018] and causal detection [Mooij et al., 2016, Pfister et al., 2017, Strobl et al., 2017]. Recently, MMD and HSIC (as defined in (3) for two components) have been shown by Sejdinovic et al. [2013b] to be equivalent to other popular statistical measures such as the energy distance [Baringhaus and Franz, 2004, Székely and Rizzo, 2004, 2005]—also known as N-distance [Zinger et al., 1992, Klebanov, 2005]—and distance covariance [Székely et al., 2007, Székely and Rizzo, 2009, Lyons, 2013] respectively. HSIC has been generalized to $M \geq 2$ components [Quadrianto et al., 2009, Sejdinovic et al., 2013a] to measure the joint independence of M random variables

$$\text{HSIC}_k(\mathbb{P}) = \left\| \mu_{\otimes_{m=1}^M k_m}(\mathbb{P}) - \otimes_{m=1}^M \mu_{k_m}(\mathbb{P}_m) \right\|_{\otimes_{m=1}^M \mathcal{H}_{k_m}},$$

where \mathbb{P} is a joint measure on the product space $\mathcal{X} := \times_{m=1}^M \mathcal{X}_m$ and $(\mathbb{P}_m)_{m=1}^M$ are the marginal measures of \mathbb{P} defined on $(\mathcal{X}_m)_{m=1}^M$ respectively. The extended HSIC measure has recently been analyzed in the context of independence testing [Pfister et al., 2017]. In addition to testing, the extended HSIC measure is also useful in the problem of independent subspace analysis (ISA) [Cardoso, 1998], wherein the latent sources are separated by maximizing the degree of independence among them. In all the applications of HSIC, the key requirement is that $k = \otimes_{m=1}^M k_m$ captures the joint independence of M random variables (with joint distribution \mathbb{P})—we call this property as \mathcal{I} -characteristic—, which is guaranteed if k is characteristic. Since k is defined in terms of $(k_m)_{m=1}^M$, it is of fundamental importance to understand the characteristic and \mathcal{I} -characteristic properties of k in terms of the characteristic property of $(k_m)_{m=1}^M$, which is one of the main goals of this work.

For $M = 2$, the characterization of independence, i.e., the \mathcal{I} -characteristic property of k , is studied by Blanchard et al. [2011] and Gretton [2015] where it has been shown that if k_1 and k_2 are universal, then k is universal² and therefore HSIC captures independence. A stronger version of this result can be obtained by combining [Lyons, 2013, Theorem 3.11] and [Sejdinovic et al., 2013b, Proposition 29]: if k_1 and k_2 are characteristic, then the HSIC associated with $k = k_1 \otimes k_2$ characterizes independence. Apart from these results, not much is known about the characteristic/ \mathcal{I} -characteristic/universality properties of k in terms of the individual kernels. Our **goal** is to resolve this question and understand the characteristic, \mathcal{I} -characteristic and universal property of the product kernel $(\otimes_{m=1}^M k_m)$ in terms of the kernel components $((k_m)_{m=1}^M)$ for $M \geq 2$. Because of the relatedness of MMD and HSIC to energy distance and distance covariance, our results also contribute to the better understanding of these other measures that are popular in the statistical literature.

²Blanchard et al. [2011] deals with c -universal kernels while Gretton [2015] deals with c_0 -universal kernels. A brief description of these notions are provided in Section 3. We refer the reader to [Carmeli et al., 2010, Sriperumbudur et al., 2010] for more details on these notions of universality.

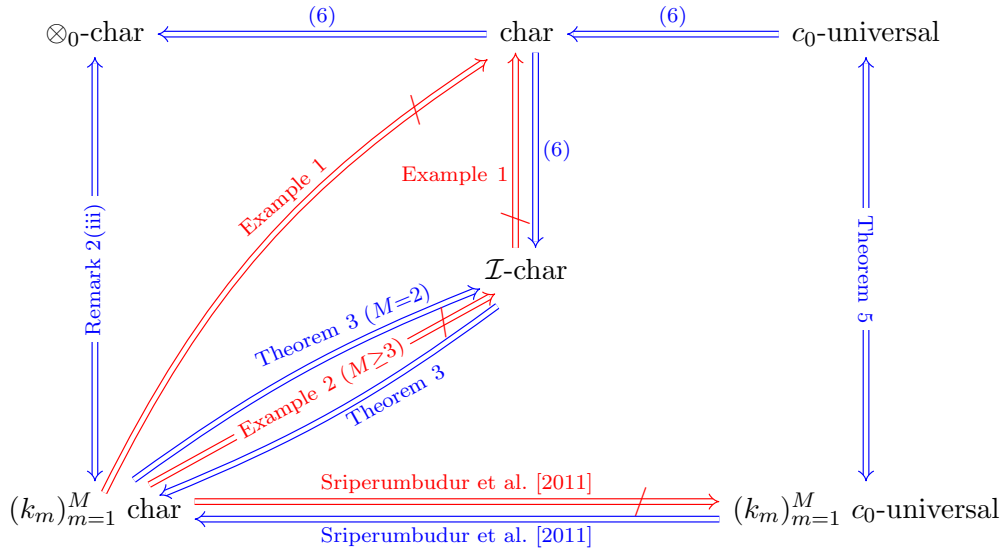


Figure 1: Summary of results: “char” denotes characteristic. In addition to the usual characteristic property, two new notions \otimes_0 -characteristic and \mathcal{I} -characteristic are introduced in Definition 1 which along with c_0 -universal (in the top right corner) correspond to the property of the tensor product kernel $\otimes_{m=1}^M k_m$, while the bottom part of the picture corresponds to the individual kernels $(k_m)_{m=1}^M$ being characteristic or c_0 -universal. If $(k_m)_{m=1}^M$ -s are continuous, bounded and translation invariant kernels on \mathbb{R}^{d_m} , $m \in [M]$, all the notions are equivalent (see Theorem 4).

Specifically, our results shed light on the following **surprising phenomena** of the \mathcal{I} -characteristic property of $\otimes_{m=1}^M k_m$ for $M \geq 3$:

1. characteristic property of $(k_m)_{m=1}^M$ is not sufficient but necessary for $\otimes_{m=1}^M k_m$ to be \mathcal{I} -characteristic;
2. universality of $(k_m)_{m=1}^M$ is sufficient for $\otimes_{m=1}^M k_m$ to be \mathcal{I} -characteristic, and
3. if at least one of $(k_m)_{m=1}^M$ is only characteristic and not universal, then $\otimes_{m=1}^M k_m$ need not be \mathcal{I} -characteristic.

The paper is organized as follows. In Section 3, we conduct a comprehensive analysis about the above mentioned properties of k and $(k_m)_{m=1}^M$ for any positive integer M . To this end, we define various notions of characteristic property on the product space \mathcal{X} (see Definition 1 and Figure 2(a) in Section 3) and explore the relation between them. In order to keep our presentation in this section to be non-technical, we relegate the problem formulation to Section 3, with the main results of the paper being presented in Section 4. A summary of the results is captured in Figure 1 while the proofs are provided in Section 5. Various definitions and notation that are used throughout the paper are collected in Section 2.

2 Definitions & Notation

$\mathbb{N} := \{1, 2, \dots\}$ and \mathbb{R} denotes the set of natural numbers and real numbers respectively. For $M \in \mathbb{N}$, $[M] := \{1, \dots, M\}$. $\mathbf{1}_d := (1, 1, \dots, 1) \in \mathbb{R}^d$ and $\mathbf{0}$ denotes the matrix of zeros. For $a := (a_1, \dots, a_d) \in \mathbb{R}^d$ and $b := (b_1, \dots, b_d) \in \mathbb{R}^d$, $\langle a, b \rangle = \sum_{i=1}^d a_i b_i$ is the Euclidean inner product. For sets A and B , $A \setminus B = \{a \in A : a \notin B\}$ is their difference, $|A|$ is the cardinality

of A and $\times_{m=1}^M A_m = \{(a_1, \dots, a_M) : a_m \in A_m, m \in [M]\}$ is the Descartes product of sets $(A_m)_{m=1}^M$. $\mathcal{P}(\mathcal{X})$ denotes the power set of a set \mathcal{X} , i.e., all subsets of \mathcal{X} (including the empty set and \mathcal{X}). The Kronecker delta is defined as $\delta_{a,b} = 1$ if $a = b$, and zero otherwise. χ_A is the indicator function of set A : $\chi_A(x) = 1$ if $x \in A$ and $\chi_A(x) = 0$ otherwise. $\mathbb{R}^{d_1 \times \dots \times d_M}$ is the set of $d_1 \times \dots \times d_M$ -sized tensors.

For a topological space $(\mathcal{X}, \tau_{\mathcal{X}})$, $\mathcal{B}(\mathcal{X}) := \mathcal{B}(\tau_{\mathcal{X}})$ is the Borel sigma-algebra on \mathcal{X} induced by the topology $\tau_{\mathcal{X}}$. Probability and finite signed measures in the paper are meant w.r.t. the measurable space $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$. Given $\{(\mathcal{X}_i, \tau_i)\}_{i \in I}$ topological spaces, their product $\times_{i \in I} \mathcal{X}_i$ is enriched with the product topology; it is the coarsest topology for which the canonical projections $\pi_i : \times_{i \in I} \mathcal{X}_i \rightarrow (\mathcal{X}_i, \tau_i)$ are continuous for all $i \in I$. A topological space $(\mathcal{X}, \tau_{\mathcal{X}})$ is called second-countable if $\tau_{\mathcal{X}}$ has a countable basis.³ $C(\mathcal{X})$ denotes the space of continuous functions on \mathcal{X} . $C_0(\mathcal{X})$ denotes the class of real-valued functions vanishing at infinity on a locally compact Hausdorff (LCH) space⁴ \mathcal{X} , i.e., for any $\epsilon > 0$, the set $\{x \in \mathcal{X} : |f(x)| \geq \epsilon\}$ is compact. $C_0(\mathcal{X})$ is endowed with the uniform norm $\|f\|_{\infty} = \sup_{x \in \mathcal{X}} |f(x)|$. $\mathcal{M}_b(\mathcal{X})$ and $\mathcal{M}_1^+(\mathcal{X})$ are the space of finite signed measures and probability measures on \mathcal{X} , respectively. For $\mathbb{P}_m \in \mathcal{M}_1^+(\mathcal{X}_m)$, $\otimes_{m=1}^M \mathbb{P}_m$ denotes the product probability measure on the product space $\times_{m=1}^M \mathcal{X}_m$, i.e., $\otimes_{m=1}^M \mathbb{P}_m \in \mathcal{M}_1^+(\times_{m=1}^M \mathcal{X}_m)$. δ_x is the Dirac measure supported on $x \in \mathcal{X}$. For $\mathbb{F} \in \mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m)$, the finite signed measure \mathbb{F}_m denotes its marginal on \mathcal{X}_m . \mathcal{H}_{k_m} is the reproducing kernel Hilbert space (RKHS) associated with the reproducing kernel $k_m : \mathcal{X}_m \times \mathcal{X}_m \rightarrow \mathbb{R}$, which in this paper is assumed to be measurable and bounded. The tensor product of $(k_m)_{m=1}^M$ is a kernel, defined as

$$\otimes_{m=1}^M k_m((x_1, \dots, x_M), (x'_1, \dots, x'_M)) = \prod_{m=1}^M k_m(x_m, x'_m), \quad x_m, x'_m \in \mathcal{X}_m,$$

whose associated RKHS is denoted as $\mathcal{H}_{\otimes_{m=1}^M k_m} = \otimes_{m=1}^M \mathcal{H}_{k_m}$ [Berlinet and Thomas-Agnan, 2004, Theorem 13], where the r.h.s. is the tensor product of RKHSs $(\mathcal{H}_{k_m})_{m=1}^M$. For $h_m \in \mathcal{H}_{k_m}$, $m \in [M]$, the multi-linear operator $\otimes_{m=1}^M h_m \in \otimes_{m=1}^M \mathcal{H}_{k_m}$ is defined as

$$(\otimes_{m=1}^M h_m)(v_1, \dots, v_M) = \prod_{m=1}^M \langle h_m, v_m \rangle_{\mathcal{H}_{k_m}}, \quad v_m \in \mathcal{H}_{k_m}.$$

A kernel $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ defined on a LCH space \mathcal{X} is called a c_0 -kernel if $k(\cdot, x) \in C_0(\mathcal{X})$ for all $x \in \mathcal{X}$. $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ is said to be a translation invariant kernel on \mathbb{R}^d if $k(x, y) = \psi(x - y)$, $x, y \in \mathbb{R}^d$ for a positive definite function $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$. $\mu_k(\mathbb{F})$ denotes the kernel mean embedding of $\mathbb{F} \in \mathcal{M}_b(\mathcal{X})$ to \mathcal{H}_k which is defined as $\mu_k(\mathbb{F}) = \int_{\mathcal{X}} k(\cdot, x) d\mathbb{F}(x)$, where the integral is meant in the Bochner sense.

3 Problem Formulation

In this section, we formally introduce the goal of the paper. To this end, we start with a definition. For simplicity, throughout the paper, we assume that all kernels are bounded. The

³Second-countability implies separability; in metric spaces the two notions coincide [Dudley, 2004, Proposition 2.1.4]. By the Urysohn's theorem, a topological space is separable and metrizable if and only if it is regular, Hausdorff and second-countable. Any uncountable discrete space is *not* second-countable.

⁴LCH spaces include \mathbb{R}^d , discrete spaces, and topological manifolds. Open or closed subsets, finite products of LCH spaces are LCH. Infinite-dimensional Hilbert spaces are *not* LCH.

definition is based on the observation [Sriperumbudur et al., 2010, Lemma 8] that a bounded kernel k on a topological space $(\mathcal{X}, \tau_{\mathcal{X}})$ is characteristic if and only if

$$\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, x') d\mathbb{F}(x) d\mathbb{F}(x') > 0, \quad \forall \mathbb{F} \in \mathcal{M}_b(\mathcal{X}) \setminus \{0\} \text{ such that } \mathbb{F}(\mathcal{X}) = 0.$$

In other words, characteristic kernels are integrally strictly positive definite (ispd) (see Sriperumbudur et al., 2010, p. 1523) w.r.t. the class of finite signed measures that assign zero measure to \mathcal{X} . The following definition extends this observation to tensor product kernels on product spaces.

Definition 1 (\mathcal{F} -ispd tensor product kernel) Suppose $k_m : \mathcal{X}_m \times \mathcal{X}_m \rightarrow \mathbb{R}$ is a bounded kernel on a topological space $(\mathcal{X}_m, \tau_{\mathcal{X}_m})$, $m \in [M]$. Let $\mathcal{F} \subseteq \mathcal{M}_b(\mathcal{X})$ be such that $0 \in \mathcal{F}$ where $\mathcal{X} := \times_{m=1}^M \mathcal{X}_m$. $k := \otimes_{m=1}^M k_m$ is said to be \mathcal{F} -ispd if

$$\begin{aligned} \mu_k(\mathbb{F}) = 0 &\Rightarrow \mathbb{F} = 0 \quad (\mathbb{F} \in \mathcal{F}), \text{ or equivalently} \\ \|\mu_k(\mathbb{F})\|_{\mathcal{H}_k}^2 &= \int_{\times_{m=1}^M \mathcal{X}_m} \int_{\times_{m=1}^M \mathcal{X}_m} (\otimes_{m=1}^M k_m)(x, x') d\mathbb{F}(x) d\mathbb{F}(x') > 0, \quad \forall \mathbb{F} \in \mathcal{F} \setminus \{0\}. \end{aligned} \quad (4)$$

Specifically,

- if k_m -s are c_0 -kernels on locally compact Polish (LCP)⁵ spaces \mathcal{X}_m -s and $\mathcal{F} = \mathcal{M}_b(\mathcal{X})$, then k is called c_0 -universal.
- if

$$\begin{aligned} \mathcal{F} &= [\mathcal{M}_b(\mathcal{X})]^0 && := \{\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) : \mathbb{F}(\mathcal{X}) = 0\}, \\ \mathcal{F} &= \mathcal{I} && := \{\mathbb{P} - \otimes_{m=1}^M \mathbb{P}_m : \mathbb{P} \in \mathcal{M}_1^+(\times_{m=1}^M \mathcal{X}_m)\}, \quad (M \geq 2) \\ \mathcal{F} &= \otimes_{m=1}^M \mathcal{M}_b^0(\mathcal{X}_m) && := \{\mathbb{F} = \otimes_{m=1}^M \mathbb{F}_m : \mathbb{F}_m \in \mathcal{M}_b(\mathcal{X}_m), \mathbb{F}_m(\mathcal{X}_m) = 0, \forall m \in [M]\}, \end{aligned}$$

then k is called characteristic, \mathcal{I} -characteristic and \otimes_0 -characteristic, respectively.

In Definition 1, k being characteristic matches the usual notion of characteristic kernels on a product space, i.e., there are no two distinct probability measures on $\mathcal{X} = \times_{m=1}^M \mathcal{X}_m$ such that the MMD between them is zero. The other notions such as \mathcal{I} -characteristic and \otimes_0 -characteristic are typically weaker than the usual characteristic property since

$$\begin{aligned} \otimes_{m=1}^M \mathcal{M}_b^0(\mathcal{X}_m) &\subseteq [\mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m)]^0 \subseteq \mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m). \\ &\cup \\ &\mathcal{I} \end{aligned} \quad (5)$$

Below we provide further intuition on the \mathcal{F} measure classes enlisted in Definition 1.

Remark 2 (i) $\mathcal{F} = \mathcal{M}_b(\mathcal{X})$: If k_m -s are c_0 -kernels on LCH spaces \mathcal{X}_m for all $m \in [M]$, then k is also a c_0 -kernel on LCH space \mathcal{X} implying that if k satisfies (4), then k is c_0 -universal (see Sriperumbudur et al., 2010, Proposition 2). It is well known that c_0 -universality

⁵A topological space is called Polish if it is complete, separable and metrizable. For example, \mathbb{R}^d and countable discrete spaces are Polish. Open and closed subsets, products and disjoint unions of countably many Polish spaces are Polish. Every second-countable LCH space is Polish.

reduces to c -universality (i.e., the notion of universality proposed by Steinwart, 2001) if \mathcal{X} is compact (see Sriperumbudur et al., 2010 for details) which is guaranteed if and only if each \mathcal{X}_m , $m \in [M]$ is compact.

- (ii) $\mathcal{F} = \mathcal{I}$: This family is useful to describe the joint independence of M random variables—hence the name \mathcal{I} -characteristic—defined on kernel-endowed domains $(\mathcal{X}_m)_{m=1}^M$: If \mathbb{P} denotes the joint distribution of random variables $(X_m)_{m=1}^M$ and $(\mathbb{P}_m)_{m=1}^M$ are the associated marginals on $(\mathcal{X}_m)_{m=1}^M$, then by definition $k = \otimes_{m=1}^M k_m$ is \mathcal{I} -characteristic iff

$$\text{HSIC}_k(\mathbb{P}) = 0 \iff \mathbb{P} = \otimes_{m=1}^M \mathbb{P}_m.$$

In other words, HSIC captures joint independence exactly with \mathcal{I} -characteristic kernels.

- (iii) $\mathcal{F} = \otimes_{m=1}^M \mathcal{M}_b^0(\mathcal{X}_m)$: In this case \mathcal{F} is chosen to be the product of finite signed measures on \mathcal{X} such that each marginal measure \mathbb{F}_m assigns zero to the corresponding space \mathcal{X}_m . This choice is relevant as the characteristic property of individual kernels $(k_m)_{m=1}^M$ need not imply the characteristic property of $\otimes_{m=1}^M k_m$, but is equivalent to the \otimes_0 -characteristic property of $\otimes_{m=1}^M k_m$. The equivalence holds for bounded kernels $k_m : \mathcal{X}_m \times \mathcal{X}_m \rightarrow \mathbb{R}$ on topological spaces \mathcal{X}_m ($m \in [M]$) since for any $\mathbb{F} = \otimes_{m=1}^M \mathbb{F}_m \in \otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m)$, $\mathbb{F}_m(\mathcal{X}_m) = 0$ ($\forall m \in [M]$)

$$\|\mu_k(\mathbb{F})\|_{\mathcal{H}_{\otimes_{m=1}^M k_m}}^2 = \prod_{m=1}^M \|\mu_{k_m}(\mathbb{F}_m)\|_{\mathcal{H}_{k_m}}^2,$$

and the l.h.s. is positive iff each term on the r.h.s. is positive.

- (iv) **\mathcal{F} -ispd relations:** Given the relations in (5), it immediately follows that $k = \otimes_{m=1}^M k_m$ satisfies

$$\begin{aligned} \otimes_0\text{-characteristic} &\iff \text{characteristic} \iff c_0\text{-universal} & (6) \\ &\Downarrow \\ &\mathcal{I}\text{-characteristic} \end{aligned}$$

when \mathcal{X}_m for all $m \in [M]$ are LCP. A visual illustration of (5) and (6) is provided in Figure 2.

Having defined the \mathcal{F} -ispd property, our **goal** is to investigate whether the characteristic or c_0 -universal property of k_m -s ($m \in [M]$) imply different \mathcal{F} -ispd properties of $\otimes_{m=1}^M k_m$, and vice versa.

4 Main Results

In this section, we present our main results related to the \mathcal{F} -ispd property of tensor product kernels, which are summarized in Figure 1. The results in this section will deal with various assumptions on \mathcal{X}_m , such as second-countability, Hausdorff, locally compact Hausdorff (LCH) and locally compact Polish (LCP), so that they are presented in more generality. However, for simplicity, all these assumptions can be unified by simply assuming a stronger condition that \mathcal{X}_m 's are LCP.

Our first example illustrates that the characteristic property of k_m -s does not imply the characteristic property of the tensor product kernel. In light of Remark 2(iv) of Section 3, it

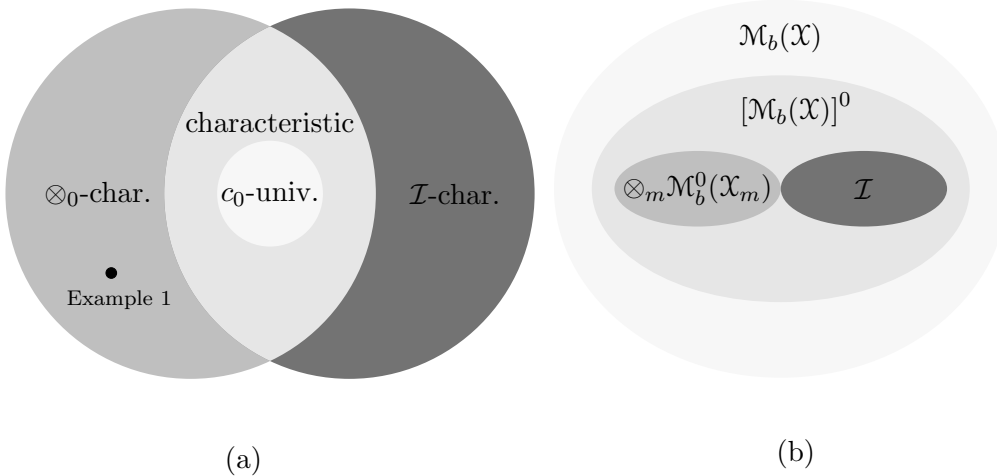


Figure 2: (a) \mathcal{F} -ispd $\otimes_{m=1}^M k_m$ kernels (see (6)), (b) $\mathcal{F} \subseteq \mathcal{M}_b(\mathcal{X})$, $\mathcal{X} = \times_{m=1}^M \mathcal{X}_m$. Example 1: $\otimes_{m=1}^M k_m$ is \otimes_0 -characteristic but not characteristic.

follows that the class of \otimes_0 -characteristic tensor product kernels form a *strictly* larger class than characteristic tensor product kernels; see also Figure 2.

Example 1 Let $\mathcal{X}_1 = \mathcal{X}_2 = \{1, 2\}$, $\tau_{\mathcal{X}_1} = \tau_{\mathcal{X}_2} = \mathcal{P}(\{1, 2\})$, $k_1(x, x') = k_2(x, x') = 2\delta_{x, x'} - 1$. It is easy to verify that k_1 and k_2 are characteristic. However, it can be proved that $k_1 \otimes k_2$ is not characteristic. On the hand, interestingly, $k_1 \otimes k_2$ is \mathcal{I} -characteristic. We refer the reader to Section 5.1 for details.

In the above example, we showed that the tensor product of k_1 and k_2 (which are characteristic kernels) is \mathcal{I} -characteristic. The following result generalizes this behavior for any bounded characteristic kernels. In addition, under a mild assumption, it shows the converse to be true for any M .

Theorem 3 Let $k_m : \mathcal{X}_m \times \mathcal{X}_m \rightarrow \mathbb{R}$ be bounded kernels on topological spaces \mathcal{X}_m for all $m \in [M]$, $M \geq 2$. Then the following holds.

- (i) Suppose \mathcal{X}_m is second-countable for all $m \in [M]$ with $M = 2$. If k_1 and k_2 are characteristic, then $k_1 \otimes k_2$ is \mathcal{I} -characteristic.
- (ii) Suppose \mathcal{X}_m is Hausdorff and $|\mathcal{X}_m| \geq 2$ for all $m \in [M]$. If $\otimes_{m=1}^M k_m$ is \mathcal{I} -characteristic, then k_1, \dots, k_M are characteristic.

Lyons [2013] has showed an analogous result to Theorem 3(i) for distance covariances ($M = 2$) on metric spaces of negative type (see Theorem 3.11 in Lyons, 2013), which via Sejdinovic et al. [2013b, Proposition 29] holds for HSIC yielding the \mathcal{I} -characteristic property of $k_1 \otimes k_2$. Recently, Gretton [2015] presented a direct proof showing that HSIC corresponding to $k_1 \otimes k_2$ captures independence if k_1 and k_2 are translation invariant characteristic kernels on \mathbb{R}^d (which is equivalent to c_0 -universality). Blanchard et al. [2011] proved a result similar to Theorem 3(i) assuming that \mathcal{X}_m 's are compact and k_1, k_2 being c -universal. In contrast, Theorem 3(i) establishes the result for bounded kernels on general second-countable topological spaces. In fact, the results of [Gretton, 2015, Blanchard et al., 2011] are special cases of Theorems 4 and 5 below. Theorem 3(i) raises a pertinent question: whether $\otimes_{m=1}^M k_m$ is \mathcal{I} -characteristic if k_m -s

are characteristic for all $m \in [M]$ where $M > 2$? The following example provides a negative answer to this question. On a positive side, however, we will see in Theorem 5 that the \mathcal{I} -characteristic property of $\otimes_{m=1}^M k_m$ can be guaranteed for any $M \geq 2$ if a stronger condition is imposed on k_m -s (and \mathcal{X}_m -s). Theorem 3(ii) generalizes Proposition 3.15 of [Lyons, 2013] for any $M > 2$, which states that every kernel k_m , $m \in [M]$ being characteristic is necessary for the tensor kernel $\otimes_{m=1}^M k_m$ to be \mathcal{I} -characteristic.

Example 2 Let $M = 3$ and $\mathcal{X}_m := \{1, 2\}$, $\tau_{\mathcal{X}_m} = \mathcal{P}(\mathcal{X}_m)$, $k_m(x, x') = 2\delta_{x, x'} - 1$ ($m = 1, 2, 3$). As mentioned in Example 1, $(k_m)_{m=1}^3$ are characteristic. However, it can be shown that $\otimes_{m=1}^3 k_m$ is not \mathcal{I} -characteristic. See Section 5.3 for details.

In Remark 2(iii) and Example 1, we showed that in general, only the \otimes_0 -characteristic property of $\otimes_{m=1}^M k_m$ is equivalent to the characteristic property of k_m -s. Our next result shows that all the various notions of characteristic property of $\otimes_{m=1}^M k_m$ coincide if k_m -s are translation-invariant, continuous bounded kernels on \mathbb{R}^d .

Theorem 4 Suppose $k_m : \mathbb{R}^{d_m} \times \mathbb{R}^{d_m} \rightarrow \mathbb{R}$ are continuous, bounded and translation-invariant kernels for all $m \in [M]$. Then the following statements are equivalent:

- (i) k_m -s are characteristic for all $m \in [M]$;
- (ii) $\otimes_{m=1}^M k_m$ is \otimes_0 -characteristic;
- (iii) $\otimes_{m=1}^M k_m$ is \mathcal{I} -characteristic;
- (iv) $\otimes_{m=1}^M k_m$ is characteristic.

The following result shows that on LCP spaces, the tensor product of $M \geq 2$ c_0 -universal kernels is also c_0 -universal, and vice versa.

Theorem 5 Suppose $k_m : \mathcal{X}_m \times \mathcal{X}_m \rightarrow \mathbb{R}$ are c_0 -kernels on LCP spaces \mathcal{X}_m ($m \in [M]$). Then $\otimes_{m=1}^M k_m$ is c_0 -universal iff k_m -s are c_0 -universal for all $m \in [M]$.

Remark 6 (i) A special case of Theorem 5 for $M = 2$ is proved by Lyons [2013, Lemma 3.8] in the context of distance covariance which reduces to Theorem 5 through the equivalence established by Sejdinovic et al. [2013b]. Another special case of Theorem 5 is proved by Blanchard et al. [2011, Lemma 5.2] for c -universality with $M = 2$ using the Stone-Weierstrass theorem: if k_1 and k_2 are c -universal then $k_1 \otimes k_2$ is c -universal.

(ii) Since the notions of c_0 -universality and characteristic property are equivalent for translation invariant c_0 -kernels on \mathbb{R}^d (see Carmeli et al., 2010, Proposition 5.16 and Sriperumbudur et al., 2010, Theorem 9), Theorem 4 can be considered as a special case of Theorem 5. In other words, requiring $(k_m)_{m=1}^M$ to be also c_0 -kernels in Theorem 4(i)-(iv) is equivalent to

- (v) k_m -s are c_0 -universal for all $m \in [M]$;
- (vi) $\otimes_{m=1}^M k_m$ is c_0 -universal.

(iii) Since the c_0 -universality of $\otimes_{m=1}^M k_m$ implies its \mathcal{I} -characteristic property (see (6)), Theorem 5 also provides a generalization of Theorem 3(i) to $M \geq 2$ under additional assumptions on k_m -s, while constraining \mathcal{X}_m -s to LCP-s instead of second-countable topological spaces.

In Example 2 and Theorem 5, we showed that for $M \geq 3$ components while the characteristic property of $(k_m)_{m=1}^M$ is not sufficient, their universality is enough to guarantee the \mathcal{I} -characteristic property of $\otimes_{m=1}^M k_m$. The next example demonstrates that these results are tight: If at least one k_m is not universal but only characteristic, then $\otimes_{m=1}^M k_m$ might not be \mathcal{I} -characteristic.

Example 3 Let $M = 3$ and $\mathcal{X}_m := \{1, 2\}$, $\tau_{\mathcal{X}_m} = \mathcal{P}(\mathcal{X}_m)$, for all $m \in [3]$, $k_1(x, x') = 2\delta_{x, x'} - 1$, and $k_m(x, x') = \delta_{x, x'}$ ($m = 2, 3$). k_1 is characteristic (Example 1), k_2 and k_3 are universal since the associated Gram matrix $\mathbf{G} = [k_m(x, x')]_{x, x' \in \mathcal{X}_m}$ is an identity matrix, which is strictly positive definite ($m = 2, 3$). However, $\otimes_{m=1}^3 k_m$ is not \mathcal{I} -characteristic. See Section 5.6 for details.

5 Proofs

In this section, we provide the proofs of our results presented in Section 4.

5.1 Proof of Example 1

The proof is structured as follows.

1. First we show that $k := k_1 = k_2$ is a kernel and it is characteristic.
2. Next it is proved that $k_1 \otimes k_2$ is not characteristic.
3. Finally, the \mathcal{I} -characteristic property of $k_1 \otimes k_2$ is established.

The individual steps are as follows:

k is a kernel. Assume w.l.o.g. that $x_1 = \dots = x_N = 1$, $x_{N+1} = \dots = x_n = 2$. Then it is easy to verify that the Gram matrix $\mathbf{G} = [k(x_i, x_j)]_{i, j=1}^n = \mathbf{a}\mathbf{a}^\top$ where $\mathbf{a} := (\mathbf{1}_N^\top, -\mathbf{1}_{n-N}^\top)^\top$ and \mathbf{a}^\top is the transpose of \mathbf{a} . Clearly \mathbf{G} is positive semidefinite and so k is a kernel.

k is characteristic. We will show that k satisfies (4). On $\mathcal{X} = \{1, 2\}$ a finite signed measure \mathbb{F} takes the form $\mathbb{F} = a_1\delta_1 + a_2\delta_2$ for some $a_1, a_2 \in \mathbb{R}$. Thus,

$$\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) \setminus \{0\} \Leftrightarrow (a_1, a_2) \neq \mathbf{0} \quad \text{and} \quad \mathbb{F}(\mathcal{X}) = 0 \Leftrightarrow a_1 + a_2 = 0. \quad (7)$$

Consider

$$\begin{aligned} \int_{\mathcal{X}} \int_{\mathcal{X}} k(x, x') \, d\mathbb{F}(x) \, d\mathbb{F}(x') &= a_1^2 k(1, 1) + a_2^2 k(2, 2) + 2a_1 a_2 k(1, 2) \\ &= a_1^2 + a_2^2 - 2a_1 a_2 = (a_1 - a_2)^2 = 4a_1^2 > 0, \end{aligned} \quad (8)$$

where we used (7) and the facts that $k(1, 1) = k(2, 2) = 1$, $k(1, 2) = -1$.

$k_1 \otimes k_2$ is not characteristic. We show a slightly stronger statement: $k_1 \otimes k_2$ is not even \mathcal{F} -ispd with $\mathcal{F} = [\otimes_{m=1}^2 \mathcal{M}_b(\mathcal{X}_m)]^0 := \{\mathbb{F} \in \otimes_{m=1}^2 \mathcal{M}_b(\mathcal{X}_m) : \mathbb{F}(\mathcal{X}) = 0\} \subset [\mathcal{M}_b(\mathcal{X})]^0$, in other words we construct a witness $\mathbb{F} = \mathbb{F}_1 \otimes \mathbb{F}_2 \in \otimes_{m=1}^2 \mathcal{M}_b(\mathcal{X}_m) \setminus \{0\}$ such that

$$\mathbb{F}(\mathcal{X}_1 \times \mathcal{X}_2) = \mathbb{F}_1(\mathcal{X}_1)\mathbb{F}_2(\mathcal{X}_2) = 0, \quad (9)$$

and

$$\begin{aligned}
0 &= \int_{\mathcal{X}_1 \times \mathcal{X}_2} \int_{\mathcal{X}_1 \times \mathcal{X}_2} \underbrace{(k_1 \otimes k_2)((i_1, i_2), (i'_1, i'_2))}_{k_1(i_1, i'_1)k_2(i_2, i'_2)} d\mathbb{F}(i_1, i_2) d\mathbb{F}(i'_1, i'_2) \\
&= \prod_{m=1}^2 \int_{\mathcal{X}_m} \int_{\mathcal{X}_m} k_m(i_m, i'_m) d\mathbb{F}_m(i_m) d\mathbb{F}_m(i'_m). \tag{10}
\end{aligned}$$

Finite signed measures on $\{1, 2\}$ take the form $\mathbb{F}_1 = \mathbb{F}_1(\mathbf{a}) = a_1\delta_1 + a_2\delta_2$, $\mathbb{F}_2 = \mathbb{F}_2(\mathbf{b}) = b_1\delta_1 + b_2\delta_2$ form, where $\mathbf{a} = (a_1, a_2) \in \mathbb{R}^2$, $\mathbf{b} = (b_1, b_2) \in \mathbb{R}^2$. With these notations, (9) and (10) can be rewritten as

$$\begin{aligned}
0 &= (a_1 + a_2)(b_1 + b_2), \\
0 &= \left[\sum_{i, i'=1}^2 k_1(i, i')a_i a_{i'} \right] \left[\sum_{j, j'=1}^2 k_2(j, j')b_j b_{j'} \right] = (a_1 - a_2)^2(b_1 - b_2)^2.
\end{aligned}$$

Keeping the solutions where neither \mathbf{a} nor \mathbf{b} is the zero vector, there are 2 (symmetric) possibilities: (i) $a_1 + a_2 = 0$, $b_1 = b_2$ and (ii) $a_1 = a_2$, $b_1 + b_2 = 0$. In other words, for any $a, b \neq 0$, the possibilities are (i) $\mathbf{a} = (a, -a)$, $\mathbf{b} = (b, b)$ and (ii) $\mathbf{a} = (a, a)$, $\mathbf{b} = (b, -b)$. This establishes the non- $[\boxtimes_{m=1}^2 \mathcal{M}_b(\mathcal{X}_m)]^0$ -ispd property of $k_1 \otimes k_2$.

$k_1 \otimes k_2$ is \mathcal{I} -characteristic. Our goal is to show that $k_1 \otimes k_2$ is \mathcal{I} -characteristic, i.e., for any $\mathbb{P} \in \mathcal{M}_1^+(\mathcal{X}_1 \times \mathcal{X}_2)$, $\mu_{k_1 \otimes k_2}(\mathbb{F}) = 0$ implies $\mathbb{F} = 0$, where $\mathbb{F} = \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2$. We divide the proof into two parts:

1. First we derive the equations of

$$\mathbb{F}(\mathcal{X}_1 \times \mathcal{X}_2) = 0 \quad \text{and} \quad \int \int_{(\mathcal{X}_1 \times \mathcal{X}_2)^2} (k_1 \otimes k_2)((i, j), (r, s)) d\mathbb{F}(i, j) d\mathbb{F}(r, s) = 0 \tag{11}$$

for general finite signed measures $\mathbb{F} = \sum_{i, j=1}^2 a_{ij}\delta_{(i, j)}$ on $\mathcal{X}_1 \times \mathcal{X}_2$.

2. Then, we apply the $\mathbb{F} = \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2$ parameterization and solve for \mathbb{P} that satisfies (11) to conclude that $\mathbb{P} = \mathbb{P}_1 \otimes \mathbb{P}_2$, i.e., $\mathbb{F} = 0$. Note that in the chosen parametrization for \mathbb{F} , $\mathbb{F}(\mathcal{X}_1 \times \mathcal{X}_2) = 0$ holds automatically.

The details are as follows.

Step 1.

$$\begin{aligned}
0 &= \mathbb{F}(\mathcal{X}_1 \times \mathcal{X}_2) \Leftrightarrow 0 = a_{11} + a_{12} + a_{21} + a_{22}, \tag{12} \\
0 &= \int_{\mathcal{X}_1 \times \mathcal{X}_2} \int_{\mathcal{X}_1 \times \mathcal{X}_2} \underbrace{(k_1 \otimes k_2)((i, j), (r, s))}_{k_1(i, r)k_2(j, s)} d\mathbb{F}(i, j) d\mathbb{F}(r, s) \\
&= \sum_{i, j=1}^2 \sum_{r, s=1}^2 k_1(i, r)k_2(j, s)a_{ij}a_{rs} = \sum_{i, r=1}^2 k_1(i, r) \sum_{j, s=1}^2 k_2(j, s)a_{ij}a_{rs} \\
&= k_1(1, 1) [k_2(1, 1)a_{11}a_{11} + k_2(1, 2)a_{11}a_{12} + k_2(2, 1)a_{12}a_{11} + k_2(2, 2)a_{12}a_{12}] \\
&\quad + k_1(1, 2) [k_2(1, 1)a_{11}a_{21} + k_2(1, 2)a_{11}a_{22} + k_2(2, 1)a_{12}a_{21} + k_2(2, 2)a_{12}a_{22}]
\end{aligned}$$

$\mathbb{P}: y \setminus x$	1	2	\mathbb{P}_2	
1	p_{11}	p_{21}	$q_1 = p_{11} + p_{21}$	\Rightarrow
2	p_{12}	p_{22}	$q_2 = p_{12} + p_{22}$	
\mathbb{P}_1	$p_1 = p_{11} + p_{12}$ $p_2 = p_{21} + p_{22}$			

$\mathbb{F} := \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2$	1	2	
1	$a_{11} = p_{11} - (p_{11} + p_{12})(p_{11} + p_{21})$	$a_{21} = p_{21} - (p_{21} + p_{22})(p_{11} + p_{21})$	
2	$a_{12} = p_{12} - (p_{11} + p_{12})(p_{12} + p_{22})$	$a_{22} = p_{22} - (p_{21} + p_{22})(p_{12} + p_{22})$	

Table 1: Joint (\mathbb{P}), joint minus product of the marginals ($\mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2$).

$$\begin{aligned}
& + k_1(2, 1) [k_2(1, 1)a_{21}a_{11} + k_2(1, 2)a_{21}a_{12} + k_2(2, 1)a_{22}a_{11} + k_2(2, 2)a_{22}a_{12}] \\
& + k_1(2, 2) [k_2(1, 1)a_{21}a_{21} + k_2(1, 2)a_{21}a_{22} + k_2(2, 1)a_{22}a_{21} + k_2(2, 2)a_{22}a_{22}] \\
= & \underbrace{(a_{11}^2 - 2a_{11}a_{12} + a_{12}^2)}_{(a_{11}-a_{12})^2} + \underbrace{(a_{21}^2 - 2a_{21}a_{22} + a_{22}^2)}_{(a_{21}-a_{22})^2} - 2 \underbrace{(a_{11}a_{21} - a_{11}a_{22} - a_{12}a_{21} + a_{12}a_{22})}_{(a_{11}-a_{12})(a_{21}-a_{22})} \\
= & (a_{11} - a_{12} - a_{21} + a_{22})^2. \tag{13}
\end{aligned}$$

Solving (12) and (13) yields

$$a_{11} + a_{22} = 0 \quad \text{and} \quad a_{12} + a_{21} = 0. \tag{14}$$

Step 2. Any $\mathbb{P} \in \mathcal{M}_1^+(\mathcal{X}_1 \times \mathcal{X}_2)$ can be parametrized as

$$\mathbb{P} = \sum_{i,j=1}^2 p_{ij} \delta_{(i,j)}, \quad p_{ij} \geq 0, \forall (i, j) \quad \text{and} \quad \sum_{i,j=1}^2 p_{ij} = 1. \tag{15}$$

Let $\mathbb{F} = \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2 = \sum_{i,j=1}^2 a_{ij} \delta_{(i,j)}$; for illustration see Table 1. It follows from step 1 that \mathbb{F} satisfying (14) is equivalent to satisfying (11). Therefore, for the choice of $\mathbb{F} := \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2$, we obtain

$$p_{11} - (p_{11} + p_{12})(p_{11} + p_{21}) + p_{22} - (p_{21} + p_{22})(p_{12} + p_{22}) = 0, \tag{16}$$

$$p_{12} - (p_{11} + p_{12})(p_{12} + p_{22}) + p_{21} - (p_{21} + p_{22})(p_{11} + p_{21}) = 0, \tag{17}$$

where $(p_{ij})_{i,j \in [2]}$ satisfy (15). Solving (15)–(17), we obtain

$$p_{11} = \frac{a[1 - (a + b)]}{a + b}, \quad p_{12} = \frac{b[1 - (a + b)]}{a + b}, \quad p_{21} = a \quad \text{and} \quad p_{22} = b,$$

with $0 \leq a, b \leq 1$, $a + b \leq 1$ and $(a, b) \neq \mathbf{0}$. The resulting distribution family with its marginals is summarized in Table 2. It can be seen that each member of this family (any a, b in the constraint set) factorizes: $\mathbb{P} = \mathbb{P}_1 \otimes \mathbb{P}_2$. In other words, $\mathbb{F} = \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2 = \mathbf{0}$; hence $k_1 \otimes k_2$ is \mathcal{I} -characteristic.

Remark. We would like to mention that while k_1 and k_2 are characteristic, they are not

$\mathbb{P}: y \setminus x$	1	2	\mathbb{P}_2
1	$p_{11} = \frac{a[1-(a+b)]}{a+b}$	$p_{21} = a$	$q_1 = \frac{a}{a+b}$
2	$p_{12} = \frac{b[1-(a+b)]}{a+b}$	$p_{22} = b$	$q_2 = \frac{b}{a+b}$
\mathbb{P}_1	$p_1 = 1 - (a + b)$	$p_2 = a + b$	

Table 2: Family of probability distributions solving (15)–(17).

universal. Since \mathcal{X} is finite, the usual notion of universality (also called c -universality) matches with c_0 -universality. Therefore, from (8), we have $\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, x') d\mathbb{F}(x) d\mathbb{F}(x) = (a_1 - a_2)^2$ where $\mathbb{F} = a_1\delta_1 + a_2\delta_2$ for some $a_1, a_2 \in \mathbb{R} \setminus \{0\}$. Clearly, the choice of $a_1 = a_2$ establishes that there exists $\mathbb{F} \in \mathcal{M}_b(\mathcal{X}) \setminus \{0\}$ such that $\int_{\mathcal{X}} \int_{\mathcal{X}} k(x, x') d\mathbb{F}(x) d\mathbb{F}(x) = 0$. Hence k is not universal. Note that the constraint in (7), which is needed to verify the characteristic property of k is not needed to verify its universality.

5.2 Proof of Theorem 3

Define $\mathcal{H}_m := \mathcal{H}_{k_m}$.

(i) Suppose k_1 and k_2 are characteristic and that for some $\mathbb{F} = \mathbb{P} - \mathbb{P}_1 \otimes \mathbb{P}_2 \in \mathcal{I}$,

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \ni \int_{\mathcal{X}_1 \times \mathcal{X}_2} (k_1 \otimes k_2)(\cdot, x) d\mathbb{F}(x) = \int_{\mathcal{X}_1 \times \mathcal{X}_2} k_1(\cdot, x_1) \otimes k_2(\cdot, x_2) d\mathbb{F}(x) = 0, \quad (18)$$

where $x = (x_1, x_2)$. We want to show that $\mathbb{F} = 0$. By the second-countability of $\mathcal{X}_{m\text{-s}}$, the product σ -field, i.e., $\otimes_{m=1}^2 \mathcal{B}(\mathcal{X}_m)$ generated by the cylinder sets $B_1 \times \mathcal{X}_2$ and $\mathcal{X}_1 \times B_2$ ($B_m \in \mathcal{B}(\mathcal{X}_m), m = 1, 2$), coincides with the Borel σ -field $\mathcal{B}(\mathcal{X}_1 \times \mathcal{X}_2)$ on the product space [Dudley, 2004, Lemma 4.1.7]:

$$\otimes_{m=1}^2 \mathcal{B}(\mathcal{X}_m) = \mathcal{B}(\mathcal{X}_1 \times \mathcal{X}_2).$$

Hence, it is sufficient to prove that $\mathbb{F}(B_1 \times B_2) = 0, \forall B_m \in \mathcal{B}(\mathcal{X}_m), m = 1, 2$. To this end, it follows from (18) that for all $h_2 \in \mathcal{H}_2$,

$$\mathcal{H}_1 \ni \int_{\mathcal{X}_1 \times \mathcal{X}_2} k_1(\cdot, x_1) h_2(x_2) d\mathbb{F}(x) = \int_{\mathcal{X}_1} k_1(\cdot, x_1) d\nu(x_1) = 0, \quad (19)$$

where

$$\nu(B_1) := \nu_{h_2}(B_1) = \int_{\mathcal{X}_1 \times \mathcal{X}_2} \chi_{B_1}(x_1) h_2(x_2) d\mathbb{F}(x), \quad B_1 \in \mathcal{B}(\mathcal{X}_1).$$

Since k_1 is characteristic, (19) implies $\nu = 0$, provided that $|\nu|(\mathcal{X}_1) < \infty$ and $\nu(\mathcal{X}_1) = 0$. These two requirements hold:

$$\begin{aligned} \nu(\mathcal{X}_1) &= \int_{\mathcal{X}_1 \times \mathcal{X}_2} h_2(x_2) d\mathbb{F}(x) = \int_{\mathcal{X}_2} h_2(x_2) d[\mathbb{P}_2 - \mathbb{P}_2](x_2) = 0; \\ |\nu|(\mathcal{X}_1) &\leq \int_{\mathcal{X}_1 \times \mathcal{X}_2} \underbrace{|h_2(x_2)|}_{|\langle h_2, k_2(\cdot, x_2) \rangle_{\mathcal{H}_2}|} d[\mathbb{P} + \mathbb{P}_1 \otimes \mathbb{P}_2](x_1, x_2) \end{aligned}$$

$$\begin{aligned}
&\leq \|h_2\|_{\mathcal{H}_2} \int_{\mathcal{X}_1 \times \mathcal{X}_2} \sqrt{k_2(x_2, x_2)} \, d[\mathbb{P} + \mathbb{P}_1 \otimes \mathbb{P}_2](x_1, x_2) \\
&\leq 2 \|h_2\|_{\mathcal{H}_2} \int_{\mathcal{X}_2} \sqrt{k_2(x_2, x_2)} \, d\mathbb{P}_2(x_2) < \infty,
\end{aligned}$$

where the last inequality follows from the boundedness of k_2 . The established $\nu = 0$ implies that for $\forall B_1 \in \mathcal{B}(\mathcal{X}_1)$ and $\forall h_2 \in \mathcal{H}_2$,

$$0 = \nu(B_1) = \left\langle h_2, \int_{\mathcal{X}_1 \times \mathcal{X}_2} \chi_{B_1}(x_1) k_2(\cdot, x_2) \, d\mathbb{F}(x) \right\rangle_{\mathcal{H}_2},$$

and hence

$$0 = \int_{\mathcal{X}_1 \times \mathcal{X}_2} \chi_{B_1}(x_1) k_2(\cdot, x_2) \, d\mathbb{F}(x) = \int_{\mathcal{X}_2} k_2(\cdot, x_2) \, d\theta_{B_1}(x_2), \quad (20)$$

where

$$\theta_{B_1}(B_2) = \int_{\mathcal{X}_1 \times \mathcal{X}_2} \chi_{B_1}(x_1) \chi_{B_2}(x_2) \, d\mathbb{F}(x), \quad B_2 \in \mathcal{B}(\mathcal{X}_2).$$

Using the characteristic property of k_2 , it follows from (20) that $\theta_{B_1} = 0$ for $\forall B_1 \in \mathcal{B}(\mathcal{X}_1)$, i.e.,

$$0 = \theta_{B_1}(B_2) = \mathbb{F}(B_1 \times B_2), \quad \forall B_1 \in \mathcal{B}(\mathcal{X}_1), \forall B_2 \in \mathcal{B}(\mathcal{X}_2)$$

provided that $\theta_{B_1}(\mathcal{X}_2) = 0$ and $|\theta_{B_1}|(\mathcal{X}_2) < \infty$. Indeed, both these conditions hold:

$$\begin{aligned}
\theta_{B_1}(\mathcal{X}_2) &= \int_{\mathcal{X}_1 \times \mathcal{X}_2} \chi_{B_1}(x_1) \, d\mathbb{F}(x) = \int_{\mathcal{X}_1} \chi_{B_1}(x_1) \, d[\mathbb{P}_1 - \mathbb{P}_1](x_1) = 0; \\
|\theta_{B_1}|(\mathcal{X}_2) &\leq \int_{\mathcal{X}_1 \times \mathcal{X}_2} d[\mathbb{P} + \mathbb{P}_1 \otimes \mathbb{P}_2](x) = 2.
\end{aligned}$$

(ii) Assume w.l.o.g. that k_1 is not characteristic. This means there exists $\mathbb{P}_1 \neq \mathbb{P}'_1 \in \mathcal{M}_1^+(\mathcal{X}_1)$ such that $\mu_{k_1}(\mathbb{P}_1) = \mu_{k_1}(\mathbb{P}'_1)$. Our goal is to construct an $\mathbb{F} \in \mathcal{M}_1^+(\times_{m=1}^M \mathcal{X}_m)$ such that

$$\mu_{\otimes_{m=1}^M k_m}(\mathbb{F} - \otimes_{m=1}^M \mathbb{F}_m) = \int_{\times_{m=1}^M} \otimes_{m=1}^M k_m(\cdot, x_m) \, d[\mathbb{F} - \otimes_{m=1}^M \mathbb{F}_m] = 0, \text{ but } \mathbb{F} \neq \otimes_{m=1}^M \mathbb{F}_m.$$

Define $\mathbb{I} := \mathbb{F} - \otimes_{m=1}^M \mathbb{F}_m \in \mathcal{I}$. In other words we want to get a witness $\mathbb{I} \in \mathcal{I}$ proving that $\otimes_{m=1}^M k_m$ is not \mathcal{I} -characteristic. Let us take $z \neq z' \in \mathcal{X}_2$, which is possible since $|\mathcal{X}_2| \geq 2$. Let us define \mathbb{F} as⁶

$$\mathbb{F} = \frac{\mathbb{P}_1 \otimes \delta_z \otimes (\otimes_{m=3}^M \mathbb{Q}_m) + \mathbb{P}'_1 \otimes \delta_{z'} \otimes (\otimes_{m=3}^M \mathbb{Q}_m)}{2} \in \mathcal{M}_1^+(\times_{m=1}^M \mathcal{X}_m).$$

It is easy to verify that

$$\mathbb{F}_1 = \frac{\mathbb{P}_1 + \mathbb{P}'_1}{2}, \mathbb{F}_2 = \frac{\delta_z + \delta_{z'}}{2} \text{ and } \mathbb{F}_m = \mathbb{Q}_m \quad (m = 3, \dots, M),$$

where $\mathbb{Q}_3, \dots, \mathbb{Q}_M$ are arbitrary probability measures on $\mathcal{X}_3, \dots, \mathcal{X}_M$, respectively. First we check that $\mathbb{I} \neq 0$. Indeed it is the case since

⁶The \mathbb{F} construction specializes to that of Lyons [2013, Proposition 3.15] in the $M = 2$ case; Lyons used it for distance covariances, which is known to be equivalent to HSIC [Sejdinovic et al., 2013b].

- $z \neq z'$ and \mathcal{X}_2 is a Hausdorff space, there exists $B_2 \in \mathcal{B}(\mathcal{X}_2)$ such that $z \in B_2, z' \notin B_2$.
- $\mathbb{P}_1 \neq \mathbb{P}'_1, \mathbb{P}_1(B_1) \neq \mathbb{P}'_1(B_1)$ for some $B_1 \in \mathcal{B}(\mathcal{X}_1)$.

Let $S = B_1 \times B_2 \times (\times_{m=3}^M \mathcal{X}_m)$, and compare its measure under \mathbb{F} and $\otimes_{m=1}^M \mathbb{F}_m$:

$$\begin{aligned} \mathbb{F}(S) &= \frac{\overbrace{\mathbb{P}_1(B_1)}^{=1(z \in B_2)} \overbrace{\delta_z(B_2)}^{=1} \prod_{m=3}^M \overbrace{\mathbb{Q}_m(\mathcal{X}_m)}^{=1} + \overbrace{\mathbb{P}'_1(B_1)}^{=0(z' \notin B_2)} \overbrace{\delta_{z'}(B_2)}^{=0} \prod_{m=3}^M \overbrace{\mathbb{Q}_m(\mathcal{X}_m)}^{=1}}{2} \\ &= \frac{\mathbb{P}_1(B_1)}{2}, \end{aligned}$$

$$\begin{aligned} (\otimes_{m=1}^M \mathbb{F}_m)(S) &= \prod_{m=1}^M \mathbb{F}_m(B_m) = \frac{\mathbb{P}_1(B_1) + \overbrace{\mathbb{P}'_1(B_1)}^{=1} \overbrace{\delta_z(B_2)}^{=1} + \overbrace{\mathbb{P}'_1(B_1)}^{=0} \overbrace{\delta_{z'}(B_2)}^{=0}}{2} \prod_{m=3}^M \overbrace{\mathbb{Q}_m(\mathcal{X}_m)}^{=1} \\ &= \frac{\mathbb{P}_1(B_1) + \mathbb{P}'_1(B_1)}{4} \neq \frac{\mathbb{P}_1(B_1)}{2}, \end{aligned}$$

where the last equality holds since $\mathbb{P}_1(B_1) \neq \mathbb{P}'_1(B_1)$. This shows that $\mathbb{I} = \mathbb{F} - \otimes_{m=1}^M \mathbb{F}_m \neq 0$ since $\mathbb{I}(S) \neq 0$.

Next we prove that $\mu_{\otimes_{m=1}^M k_m}(\mathbb{F} - \otimes_{m=1}^M \mathbb{F}_m) = 0$. Indeed,

$$\begin{aligned} \mu_{\otimes_{m=1}^M k_m}(\mathbb{I}) &= \int_{\times_{m=1}^M \mathcal{X}_m} \otimes_{m=1}^M k_m(\cdot, x_m) d[\mathbb{F} - \otimes_{m=1}^M \mathbb{F}_m](x_1, \dots, x_M) \\ &= \int_{\times_{m=1}^M \mathcal{X}_m} \otimes_{m=1}^M k_m(\cdot, x_m) d\left(\left[\frac{\mathbb{P}_1 \otimes \delta_z + \mathbb{P}'_1 \otimes \delta_{z'}}{2} - \frac{\mathbb{P}_1 + \mathbb{P}'_1}{2} \otimes \frac{\delta_z + \delta_{z'}}{2} \right] \right. \\ &\quad \left. \otimes (\otimes_{m=3}^M \mathbb{Q}_m) \right)(x_1, \dots, x_M) \\ &= \int_{\times_{m=1}^M \mathcal{X}_m} \otimes_{m=1}^M k_m(\cdot, x_m) d\left(\left[\frac{\mathbb{P}_1(x_1) \otimes \delta_z(x_2) + \mathbb{P}'_1(x_1) \otimes \delta_{z'}(x_2)}{2} \right. \right. \\ &\quad \left. \left. - \frac{\mathbb{P}_1(x_1) \otimes \delta_z(x_2) + \mathbb{P}_1(x_1) \otimes \delta_{z'}(x_2)}{4} \right. \right. \\ &\quad \left. \left. - \frac{\mathbb{P}'_1(x_1) \otimes \delta_z(x_2) + \mathbb{P}'_1(x_1) \otimes \delta_{z'}(x_2)}{4} \right] \otimes (\otimes_{m=3}^M \mathbb{Q}_m(x_m)) \right) \\ &\stackrel{(*)}{=} \left[\frac{\mu_{k_1}(\mathbb{P}_1) \otimes k_2(\cdot, z) + \mu_{k_1}(\mathbb{P}'_1) \otimes k_2(\cdot, z')}{2} \right. \\ &\quad \left. - \frac{\mu_{k_1}(\mathbb{P}_1) \otimes k_2(\cdot, z) + \mu_{k_1}(\mathbb{P}_1) \otimes k_2(\cdot, z')}{4} \right. \\ &\quad \left. - \frac{\mu_{k_1}(\mathbb{P}'_1) \otimes k_2(\cdot, z) + \mu_{k_1}(\mathbb{P}'_1) \otimes k_2(\cdot, z')}{4} \right] \otimes [\otimes_{m=3}^M \mu_{k_m}(\mathbb{Q}_m)] \\ &= \underbrace{0}_{\in \mathcal{H}_{k_1 \otimes k_2}} \otimes [\otimes_{m=3}^M \mu_{k_m}(\mathbb{Q}_m)] = 0, \end{aligned}$$

where we used $\mu_{k_1}(\mathbb{P}_1) = \mu_{k_1}(\mathbb{P}'_1)$ in (*).

5.3 Proof of Example 2

Let $M = 3, \times_{m=1}^M \mathcal{X}_m = \{(i_1, i_2, i_3) : i_m \in \{1, 2\}, m \in [3]\}, k_m(x, x') = 2\delta_{x,x'} - 1$. Our goal is to show that $\otimes_{m=1}^3 k_m$ is *not* \mathcal{I} -characteristic. The structure of the proof is as follows:

1. First we describe the equations of the non-characteristic property of $\otimes_{m=1}^3 k_m$ with a general finite signed measure $\mathbb{F} = \sum_{i_1, i_2, i_3=1}^2 a_{i_1, i_2, i_3} \delta_{(i_1, i_2, i_3)}$ on $\times_{m=1}^3 \mathcal{X}_m$ where $a_{i_1, i_2, i_3} \in \mathbb{R}$ ($\forall i_1, i_2, i_3$).
2. Next, we apply the $\mathbb{F} = \mathbb{P} - \otimes_{m=1}^3 \mathbb{P}_m$ parameterization and show that there exists \mathbb{P} that satisfies the equations of step 1 to conclude that $\otimes_{m=1}^3 k_m$ is not \mathcal{I} -characteristic.

The details are as follows.

Step 1. The equations of non-characteristic property in terms of $\mathbf{A} = [a_{i_1, i_2, i_3}]_{(i_m)_{m=1}^3 \in [2]^3} \in \mathbb{R}^{2 \times 2 \times 2}$ are

$$\begin{aligned} \mathbb{F} \in \mathcal{M}_b(\times_{m=1}^3 \mathcal{X}_m) \setminus \{0\} &\Leftrightarrow \mathbf{A} \neq \mathbf{0}, \\ 0 = \mathbb{F}(\times_{m=1}^3 \mathcal{X}_m) &\Leftrightarrow 0 = \sum_{i_1, i_2, i_3=1}^2 a_{i_1, i_2, i_3}, \end{aligned} \quad (21)$$

$$\begin{aligned} 0 &= \int_{\times_{m=1}^3 \mathcal{X}_m} \int_{\times_{m=1}^3 \mathcal{X}_m} \underbrace{(\otimes_{m=1}^3 k_m)((i_1, i_2, i_3), (i'_1, i'_2, i'_3))}_{\prod_{m=1}^3 k_m(i_m, i'_m)} d\mathbb{F}(i_1, i_2, i_3) d\mathbb{F}(i'_1, i'_2, i'_3) \\ &= \sum_{i_1, i_2, i_3=1}^2 \sum_{i'_1, i'_2, i'_3=1}^2 \prod_{m=1}^3 k_m(i_m, i'_m) a_{i_1, i_2, i_3} a_{i'_1, i'_2, i'_3}. \end{aligned} \quad (22)$$

Solving (21) and (22) yields

$$a_{1,1,1} + a_{1,2,2} + a_{2,1,2} + a_{2,2,1} = 0 \quad \text{and} \quad a_{1,1,2} + a_{1,2,1} + a_{2,1,1} + a_{2,2,2} = 0.$$

Step 2. The equations of non \mathcal{I} -characteristic property can be obtained from step 1 by choosing $\mathbb{F} = \mathbb{P} - \otimes_{m=1}^M \mathbb{P}_m$, where

$$\mathbb{P} = \sum_{i_1, i_2, i_3=1}^2 p_{i_1, i_2, i_3} \delta_{(i_1, i_2, i_3)} \quad \text{and} \quad \mathbf{P} = [p_{i_1, i_2, i_3}]_{(i_m)_{m=1}^3 \in [2]^3} \in \mathbb{R}^{2 \times 2 \times 2}.$$

In other words, it is sufficient to obtain a \mathbf{P} that solves the following system of equations for which $\mathbf{A} = \mathbf{A}(\mathbf{P}) \neq \mathbf{0}$:

$$\sum_{i_1, i_2, i_3=1}^2 p_{i_1, i_2, i_3} = 1, \quad (23)$$

$$p_{i_1, i_2, i_3} \geq 0, \quad \forall (i_1, i_2, i_3) \in [2]^3, \quad (24)$$

$$a_{1,1,1} + a_{1,2,2} + a_{2,1,2} + a_{2,2,1} = 0, \quad (25)$$

$$a_{1,1,2} + a_{1,2,1} + a_{2,1,1} + a_{2,2,2} = 0, \quad (26)$$

where

$$a_{i_1, i_2, i_3} = p_{i_1, i_2, i_3} - p_{1, i_1} p_{2, i_2} p_{3, i_3}, \quad (27)$$

and

$$p_{1, i_1} = \sum_{i_2, i_3=1}^2 p_{i_1, i_2, i_3}, \quad p_{2, i_2} = \sum_{i_1, i_3=1}^2 p_{i_1, i_2, i_3}, \quad p_{3, i_3} = \sum_{i_1, i_2=1}^2 p_{i_1, i_2, i_3}. \quad (28)$$

One can get an analytical description for the solution of (23)–(28), where the solution $\mathbf{P}(\mathbf{z})$ is parameterized by $\mathbf{z} = (z_0, \dots, z_5) \in \mathbb{R}^6$. For explicit expressions, we refer the reader to Appendix A. In the following, we present two examples of \mathbf{P} that satisfy (23)–(28) such that $\mathbf{A} \neq \mathbf{0}$, thereby establishing the non \mathcal{I} -characteristic property of $\otimes_{m=1}^3 k_m$.

1. \mathbf{P} :

$$\begin{aligned} p_{1,1,1} &= \frac{1}{5}, & p_{1,1,2} &= \frac{1}{10}, & p_{1,2,1} &= \frac{1}{10}, & p_{1,2,2} &= \frac{1}{10}, \\ p_{2,1,1} &= \frac{1}{5}, & p_{2,1,2} &= \frac{1}{10}, & p_{2,2,1} &= \frac{1}{10}, & p_{2,2,2} &= \frac{1}{10}, \end{aligned}$$

and \mathbf{A} :

$$a_{1,1,1} = \frac{1}{50}, \quad a_{1,1,2} = -\frac{1}{50}, \quad a_{1,2,1} = -\frac{1}{50}, \quad a_{1,2,2} = \frac{1}{50}, \quad (29)$$

$$a_{2,1,1} = \frac{1}{50}, \quad a_{2,1,2} = -\frac{1}{50}, \quad a_{2,2,1} = -\frac{1}{50}, \quad a_{2,2,2} = \frac{1}{50}. \quad (30)$$

2. \mathbf{P} :

$$\begin{aligned} p_{1,1,1} &= 0, & p_{1,1,2} &= \frac{1}{10}, & p_{1,2,1} &= \frac{1}{10}, & p_{1,2,2} &= \frac{1}{10}, \\ p_{2,1,1} &= \frac{1}{10}, & p_{2,1,2} &= \frac{1}{10}, & p_{2,2,1} &= \frac{3}{10}, & p_{2,2,2} &= \frac{1}{5}, \end{aligned}$$

and \mathbf{A} :

$$\begin{aligned} a_{1,1,1} &= -\frac{9}{200}, & a_{1,1,2} &= \frac{11}{200}, & a_{1,2,1} &= -\frac{1}{200}, & a_{1,2,2} &= -\frac{1}{200}, \\ a_{2,1,1} &= -\frac{1}{200}, & a_{2,1,2} &= -\frac{1}{200}, & a_{2,2,1} &= \frac{11}{200}, & a_{2,2,2} &= -\frac{9}{200}. \end{aligned}$$

In fact these examples are obtained with the choices $\mathbf{z} = (\frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10})$ and $\mathbf{z} = (\frac{3}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{1}{10}, \frac{2}{10})$ respectively. See Appendix A for details.

5.4 Proof of Theorem 4

It follows from (6) and Remark 2(iii) that $(iv) \Rightarrow (ii) \Leftrightarrow (i)$. It also follows from (6) and Theorem 3(ii) that $(iv) \Rightarrow (iii) \Rightarrow (i)$. We now show that $(i) \Rightarrow (iv)$ which establishes the equivalence of (i) – (iv) . Suppose (i) holds. Then by Bochner's theorem [Wendland, 2005, Theorem 6.6], we have that for all $m \in [M]$,

$$k_m(x_m, y_m) = \int_{\mathbb{R}^{d_m}} e^{-\sqrt{-1}\langle \omega_m, x_m - y_m \rangle} d\Lambda_m(\omega_m), \quad x_m, y_m \in \mathbb{R}^{d_m},$$

where $(\Lambda_m)_{m=1}^M$ are finite non-negative Borel measures on $(\mathbb{R}^{d_m})_{m=1}^M$ respectively. This implies

$$\otimes_{m=1}^M k_m(x_m, y_m) = \otimes_{m=1}^M \int_{\mathbb{R}^{d_m}} e^{-\sqrt{-1}\langle \omega_m, x_m - y_m \rangle} d\Lambda_m(\omega_m) = \int_{\mathbb{R}^d} e^{-\sqrt{-1}\langle \omega, x - y \rangle} d\Lambda(\omega),$$

where $x = (x_1, \dots, x_M) \in \mathbb{R}^d$, $y = (y_1, \dots, y_M) \in \mathbb{R}^d$, $\omega = (\omega_1, \dots, \omega_M) \in \mathbb{R}^d$, $d = \sum_{m=1}^M d_m$ and $\Lambda := \otimes_{m=1}^M \Lambda_m$. Sriperumbudur et al. [2010, Theorem 9] showed that k_m is characteristic iff $\text{supp}(\Lambda_m) = \mathbb{R}^{d_m}$, where $\text{supp}(\cdot)$ denotes the support of its argument. Since $\text{supp}(\Lambda) = \text{supp}(\otimes_{m=1}^M \Lambda_m) = \times_{m=1}^M \text{supp}(\Lambda_m) = \times_{m=1}^M \mathbb{R}^{d_m} = \mathbb{R}^d$, it follows that $\otimes_{m=1}^M k_m$ is characteristic.

5.5 Proof of Theorem 5

The c_0 -kernel property of k_m -s ($m = 1, \dots, M$) implies that of $\otimes_{m=1}^M k_m$. Moreover, \mathcal{X}_m -s are LCP spaces, hence $\times_{m=1}^M \mathcal{X}_m$ is also LCP.

(\Leftarrow) Assume that $\otimes_{m=1}^M k_m$ is c_0 -universal. Since $\otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m) \subseteq \mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m)$, we have that for all $\mathbb{F} = \otimes_{m=1}^M \mathbb{F}_m \in \otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m) \setminus \{0\}$,

$$\begin{aligned} 0 &< \int_{\times_{m=1}^M \mathcal{X}_m} \int_{\times_{m=1}^M \mathcal{X}_m} \underbrace{(\otimes_{m=1}^M k_m)(x, x')}_{\prod_{m=1}^M k_m(x_m, x'_m)} d\mathbb{F}(x) d\mathbb{F}(x') \\ &= \prod_{m=1}^M \int_{\mathcal{X}_m \times \mathcal{X}_m} k_m(x_m, x'_m) d\mathbb{F}_m(x_m) d\mathbb{F}_m(x'_m), \end{aligned}$$

where $x = (x_1, \dots, x_M)$ and $x' = (x'_1, \dots, x'_M)$. The above inequality implies

$$\int_{\mathcal{X}_m \times \mathcal{X}_m} k_m(x_m, x'_m) d\mathbb{F}_m(x_m) d\mathbb{F}_m(x'_m) > 0, \quad \forall m \in [M].$$

Since $\mathbb{F} \in \otimes_{m=1}^M \mathcal{M}_b(\mathcal{X}_m) \setminus \{0\}$ iff $\mathbb{F}_m \in \mathcal{M}_b(\mathcal{X}_m) \setminus \{0\}$ for all $m \in [M]$, the result follows.

(\Rightarrow) Assume that k_m -s are c_0 -universal. By the note above $\otimes_{m=1}^M k_m$ is c_0 -kernel; its c_0 -universality is equivalent to the injectivity of $\mu = \mu_{\otimes_{m=1}^M k_m}$ on $\mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m)$. In other words, we want to prove that $\mu(\mathbb{F}) = 0$ implies $\mathbb{F} = 0$, where $\mathbb{F} \in \mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m)$. We will use the shorthand $\mathcal{H}_m = \mathcal{H}_{k_m}$ below.

Suppose there exists $\mathbb{F} \in \mathcal{M}_b(\times_{m=1}^M \mathcal{X}_m)$ such that

$$\mu_{\mathbb{F}} = \int_{\times_{m=1}^M \mathcal{X}_m} \underbrace{(\otimes_{m=1}^M k_m)(\cdot, x)}_{\otimes_{m=1}^M k_m(\cdot, x_m)} d\mathbb{F}(x) = 0 \quad (\in \otimes_{m=1}^M \mathcal{H}_m). \quad (31)$$

Since \mathcal{X}_m -s are LCP, $\otimes_{m=1}^M \mathcal{B}(\mathcal{X}_m) = \mathcal{B}(\times_{m=1}^M \mathcal{X}_m)$ [Steinwart and Christmann, 2008, page 480]. Hence, in order to get $\mathbb{F} = 0$ it is sufficient to prove that

$$\mathbb{F}(\times_{m=1}^M B_m) = 0, \quad \forall B_m \in \mathcal{B}(\mathcal{X}_m), m \in [M].$$

We will prove by induction that for $m = 0, \dots, M$

$$\begin{aligned} (\otimes_{j=m+1}^M \mathcal{H}_j \ni) 0 &= \int_{\times_{j=1}^M \mathcal{X}_j} \prod_{j=1}^m \chi_{B_j}(x_j) \otimes_{j=m+1}^M k_j(\cdot, x_j) d\mathbb{F}(x) \\ &=: o(B_1, \dots, B_m, k_{m+1}, \dots, k_M), \forall B_j \in \mathcal{B}(\mathcal{X}_j), j \in [m], \end{aligned} \quad (32)$$

which

(*) reduces to (31) when $m = 0$ by defining $\prod_{j=1}^0 \chi_{B_j}(x_j) := 1$;

(†) for $m = M$, $\otimes_{m=M+1}^M \mathcal{H}_m$ is defined to be equal to \mathbb{R} and $\otimes_{m=M+1}^M k_m(\cdot, x_m) := 1$, in which case $o(B_1, \dots, B_M) = \mathbb{F}(\times_{j=1}^M B_j) = 0 \Rightarrow \mathbb{F} = 0$, the result we want to prove.

From the above, it is clear that (32) holds for $m = 0$. Assuming (32) holds for some m , we now prove that it holds for $m+1$. To this end, it follows from (32) that $\forall h_{m+2} \in \mathcal{H}_{m+2}, \dots, \forall h_M \in \mathcal{H}_M$,

$$\begin{aligned}
(\mathcal{H}_{m+1} \ni) 0 &= o(B_1, \dots, B_m, k_{m+1}, \dots, k_M) (h_{m+2}, \dots, h_M) \\
&= \left[\int_{\times_{j=1}^M \mathcal{X}_j} \left(\prod_{j=1}^m \chi_{B_j}(x_j) \right) \otimes_{j=m+1}^M k_j(\cdot, x_j) d\mathbb{F}(x) \right] (h_{m+2}, \dots, h_M) \\
&= \int_{\times_{j=1}^M \mathcal{X}_j} k_{m+1}(\cdot, x_{m+1}) \prod_{j=1}^m \chi_{B_j}(x_j) \prod_{j=m+2}^M h_j(x_j) d\mathbb{F}(x) \\
&= \int_{\mathcal{X}_{m+1}} k_{m+1}(\cdot, x_{m+1}) d\nu(x_{m+1}),
\end{aligned}$$

where

$$\begin{aligned}
\nu(B) &:= \nu_{B_1, \dots, B_m, h_{m+2}, \dots, h_M}(B) \\
&= \int_{\times_{j=1}^M \mathcal{X}_j} \left[\prod_{j=1}^m \chi_{B_j}(x_j) \right] \chi_B(x_{m+1}) \left[\prod_{j=m+2}^M h_j(x_j) \right] d\mathbb{F}(x), \quad B \in \mathcal{B}(\mathcal{X}_{m+1}).
\end{aligned}$$

By the c_0 -universality of k_{m+1} ,

$$\nu = 0 \text{ for } \forall h_{m+2} \in \mathcal{H}_{m+2}, \dots, \forall h_M \in \mathcal{H}_M \quad (33)$$

provided that $\nu \in \mathcal{M}_b(\mathcal{X}_{m+1})$, in other words if $|\nu|(\mathcal{X}_{m+1}) < \infty$. This condition is met:

$$\begin{aligned}
|\nu|(\mathcal{X}_{m+1}) &\leq \int_{\times_{j=1}^M \mathcal{X}_j} \prod_{j=m+2}^M \underbrace{\left| \langle h_j, k_j(\cdot, x_j) \rangle_{\mathcal{H}_j} \right|}_{\leq \|h_j\|_{\mathcal{H}_j} \sqrt{k_j(x_j, x_j)}} d|\mathbb{F}|(x) \\
&\leq |\mathbb{F}| \left(\times_{m=1}^M \mathcal{X}_m \right) \prod_{j=m+2}^M \|h_j\|_{\mathcal{H}_j} \sup_{x \in \mathcal{X}_j, x' \in \mathcal{X}_j} \sqrt{k_j(x, x')} < \infty,
\end{aligned}$$

where we used the boundedness of k_m -s in the last inequality. (33) implies that for $\forall B_1 \in \mathcal{B}(\mathcal{X}_1), \dots, \forall B_{m+1} \in \mathcal{B}(\mathcal{X}_{m+1})$ and $\forall h_{m+2} \in \mathcal{H}_{m+2}, \dots, \forall h_M \in \mathcal{H}_M$

$$\begin{aligned}
0 &= \nu(B_{m+1}) = \int_{\times_{j=1}^M \mathcal{X}_j} \left[\prod_{j=1}^{m+1} \chi_{B_j}(x_j) \right] \left[\prod_{j=m+2}^M h_j(x_j) \right] d\mathbb{F}(x) \\
&= \left\langle \otimes_{j=m+2}^M h_j, \int_{\times_{j=1}^M \mathcal{X}_j} \left[\prod_{j=1}^{m+1} \chi_{B_j}(x_j) \right] \otimes_{j=m+2}^M k_j(\cdot, x_j) d\mathbb{F}(x) \right\rangle_{\otimes_{j=m+2}^M \mathcal{H}_j},
\end{aligned}$$

and therefore

$$o(B_1, \dots, B_{m+1}, k_{m+2}, \dots, k_M) = \int_{\times_{j=1}^M \mathcal{X}_j} \left[\prod_{j=1}^{m+1} \chi_{B_j}(x_j) \right] \otimes_{j=m+2}^M k(\cdot, x_j) d\mathbb{F}(x)$$

$$= 0 \left(\in \otimes_{j=m+2}^M \mathcal{H}_j \right)$$

for $\forall B_1 \in \mathcal{B}(\mathcal{X}_1), \dots, \forall B_{m+1} \in \mathcal{B}(\mathcal{X}_{m+1})$, i.e., (32) holds for $m+1$. Therefore, by induction, (32) holds for $m=M$ and the result follows from (†). To justify the convention in (†), consider the case of $m=M-1$ in which case (32) can be written as

$$\int_{\mathcal{X}_M} k_M(\cdot, x_M) d\nu(x_M) = 0,$$

where

$$\nu(B) = \int_{\times_{j=1}^M \mathcal{X}_j} \left[\prod_{j=1}^{M-1} \chi_{B_j}(x_j) \right] \chi_B(x_M) d\mathbb{F}(x), \quad B \in \mathcal{B}(\mathcal{X}_M).$$

Then by the c_0 -universal property of k_M , since

$$|\nu|(\mathcal{X}_M) \leq \int_{\times_{j=1}^M \mathcal{X}_j} 1 d|\mathbb{F}|(x) = |\mathbb{F}|(\times_{j=1}^M \mathcal{X}_j) < \infty$$

we obtain

$$\int_{\times_{j=1}^M \mathcal{X}_j} \prod_{j=1}^M \chi_{B_j}(x_j) d\mathbb{F}(x) = \mathbb{F}(\times_{j=1}^M B_j) = 0, \quad \forall B_1 \in \mathcal{B}(\mathcal{X}_1), \dots, \forall B_M \in \mathcal{B}(\mathcal{X}_M).$$

5.6 Proof of Example 3

The proof follows by a simple modification of that of Example 2 (Section 5.3). The equations of a witness $\mathbf{A} = [a_{i_1, i_2, i_3}]_{(i_m)_{m=1}^3 \in [2]^3}$ (and corresponding $\mathbf{P} = [p_{i_1, i_2, i_3}]_{(i_m)_{m=1}^3 \in [2]^3}$) for the non- \mathcal{I} -characteristic property of $\otimes_{m=1}^3 k_m$ take the form:

$$\mathbf{A} \neq \mathbf{0},$$

$$0 = \sum_{i_1, i_2, i_3=1}^2 a_{i_1, i_2, i_3}, \quad (34)$$

$$\begin{aligned} 0 &= \sum_{i_1, i_2, i_3=1}^2 \sum_{i'_1, i'_2, i'_3=1}^2 \prod_{m=1}^3 k_m(i_m, i'_m) a_{i_1, i_2, i_3} a_{i'_1, i'_2, i'_3} \\ &= (a_{1,1,1} - a_{2,1,1})^2 + (a_{1,1,2} - a_{2,1,2})^2 + (a_{1,2,1} - a_{2,2,1})^2 + (a_{1,2,2} - a_{2,2,2})^2, \end{aligned} \quad (35)$$

where (34) and (35) are equivalent to

$$0 = \sum_{i_1, i_2, i_3=1}^2 a_{i_1, i_2, i_3}, \quad a_{1,1,1} = a_{2,1,1}, \quad a_{1,1,2} = a_{2,1,2}, \quad a_{1,2,1} = a_{2,2,1}, \quad a_{1,2,2} = a_{2,2,2}. \quad (36)$$

While (36) is more restrictive than (25) and (26) (hence its solution set might even be empty), one can immediately see that the example of $\mathbf{A} \neq \mathbf{0}$ given in (29) and (30) fulfills (36) proving the non- \mathcal{I} -characteristic property of $\otimes_{m=1}^3 k_m$.

Acknowledgments

We would like to thank the anonymous reviewers for their constructive comments that improved the manuscript. A part of the work was carried out while BKS was visiting ZS at CMAP, École Polytechnique. BKS is supported by NSF-DMS-1713011 and also thanks CMAP and DSI for their generous support. ZS is highly grateful for the Greek hospitality around the Aegean Sea; it greatly contributed to the development of the induction arguments.

A Analytical Solution to (23)–(28) in Example 2

The solution of (23)–(28) takes the form

$$\begin{aligned}
& z_2 + z_1 + z_4 + z_5 - 3z_2z_1 - 4z_2z_4 - 4z_1z_4 - z_2z_3 - 2z_2z_0 - 2z_1z_3 - 3z_2z_5 \\
& - 2z_4z_3 - z_1z_0 - 3z_1z_5 - 2z_4z_0 - 4z_4z_5 - z_3z_0 - z_3z_5 - z_0z_5 + 2z_2z_1^2 + 2z_2^2z_1 \\
& + 4z_2z_4^2 + 2z_2^2z_4 + 4z_1z_4^2 + 2z_1^2z_4 + 2z_2^2z_0 + 2z_1^2z_3 + 2z_2z_5^2 + 2z_2^2z_5 + 2z_4^2z_3 \\
& + 2z_1z_5^2 + 2z_1^2z_5 + 2z_4^2z_0 + 2z_4z_5^2 + 4z_4^2z_5 - z_2^2 - z_1^2 - 3z_4^2 + 2z_4^3 - z_5^2 \\
& + 6z_2z_1z_4 + 2z_2z_1z_3 + 2z_2z_4z_3 + 2z_2z_1z_0 + 4z_2z_1z_5 + 4z_2z_4z_0 + 4z_1z_4z_3 \\
& + 6z_2z_4z_5 + 2z_1z_4z_0 + 6z_1z_4z_5 + 2z_2z_3z_0 + 2z_2z_3z_5 + 2z_1z_3z_0 + 2z_2z_0z_5 \\
& + 2z_1z_3z_5 + 2z_4z_3z_0 + 2z_4z_3z_5 + 2z_1z_0z_5 + 2z_4z_0z_5 \\
p_{1,1,1} = & - \frac{2z_2z_1 - z_1 - 2z_4 - z_3 - z_0 - 2z_5 - z_2 + 2z_2z_4 + 2z_1z_4 + 2z_2z_0 + 2z_1z_3 + 2z_2z_5}{2z_4z_3 + 2z_1z_5 + 2z_4z_0 + 4z_4z_5 + 2z_3z_0 + 2z_3z_5 + 2z_0z_5 + 2z_4^2 + 2z_5^2}, \\
& + 2z_4z_3 + 2z_1z_5 + 2z_4z_0 + 4z_4z_5 + 2z_3z_0 + 2z_3z_5 + 2z_0z_5 + 2z_4^2 + 2z_5^2
\end{aligned}$$

$$p_{1,1,2} = z_2,$$

$$p_{1,2,1} = z_1,$$

$$p_{1,2,2} = z_4,$$

$$\begin{aligned}
& z_4 + z_3 + z_0 + z_5 - z_2z_1 - z_2z_4 - z_1z_4 - z_2z_3 - 2z_2z_0 - 2z_1z_3 - 2z_2z_5 \\
& - 3z_4z_3 - z_1z_0 - 2z_1z_5 - 3z_4z_0 - 4z_4z_5 - 3z_3z_0 - 4z_3z_5 - 4z_0z_5 + 2z_2z_0^2 \\
& + 2z_1z_3^2 + 2z_2z_5^2 + 2z_4z_3^2 + 2z_4^2z_3 + 2z_1z_5^2 + 2z_4z_0^2 + 2z_4^2z_0 + 4z_4z_5^2 + 2z_4^2z_5 \\
& + 2z_3z_0^2 + 2z_3^2z_0 + 4z_3z_5^2 + 2z_3^2z_5 + 4z_0z_5^2 + 2z_0^2z_5 - z_4^2 - z_3^2 - z_0^2 - 3z_5^2 \\
& + 2z_5^3 + 2z_2z_1z_3 + 2z_2z_4z_3 + 2z_2z_1z_0 + 2z_2z_1z_5 + 2z_2z_4z_0 + 2z_1z_4z_3 \\
& + 2z_2z_4z_5 + 2z_1z_4z_0 + 2z_1z_4z_5 + 2z_2z_3z_0 + 2z_2z_3z_5 + 2z_1z_3z_0 + 4z_2z_0z_5 \\
& + 4z_1z_3z_5 + 4z_4z_3z_0 + 6z_4z_3z_5 + 2z_1z_0z_5 + 6z_4z_0z_5 + 6z_3z_0z_5 \\
p_{2,1,1} = & - \frac{2z_2z_1 - z_1 - 2z_4 - z_3 - z_0 - 2z_5 - z_2 + 2z_2z_4 + 2z_1z_4 + 2z_2z_0 + 2z_1z_3 + 2z_2z_5}{2z_4z_3 + 2z_1z_5 + 2z_4z_0 + 4z_4z_5 + 2z_3z_0 + 2z_3z_5 + 2z_0z_5 + 2z_4^2 + 2z_5^2}, \\
& + 2z_4z_3 + 2z_1z_5 + 2z_4z_0 + 4z_4z_5 + 2z_3z_0 + 2z_3z_5 + 2z_0z_5 + 2z_4^2 + 2z_5^2
\end{aligned}$$

$$p_{2,1,2} = z_3,$$

$$p_{2,2,1} = z_0,$$

$$p_{2,2,2} = z_5,$$

form, where $\mathbf{z} = (z_0, z_1, \dots, z_5) \in \mathbb{R}^6$ satisfies

$$0 \leq (2z_0z_2 - z_1 - z_2 - z_3 - 2z_4 - 2z_5 - z_0 + 2z_0z_3 + 2z_1z_2 + 2z_0z_4 + 2z_1z_3 + 2z_0z_5$$

$$\begin{aligned}
& +2z_1z_4 + 2z_1z_5 + 2z_2z_4 + 2z_2z_5 + 2z_3z_4 + 2z_3z_5 + 4z_4z_5 + 2z_4^2 + 2z_5^2) \times \\
& (z_0z_3 - z_3 - z_4 - z_5 - z_0z_1 - z_0 - z_1z_2 + z_0z_5 - 2z_1z_4 - z_2z_3 - z_1z_5 - 2z_2z_4 - z_2z_5 \\
& + z_3z_5 + 2z_0z_2^2 + 2z_1z_2^2 + 2z_1^2z_2 + 2z_0z_4^2 + 2z_1^2z_3 + 4z_1z_4^2 + 2z_1^2z_4 + 2z_1z_5^2 + 4z_2z_4^2 \\
& + 2z_1^2z_5 + 2z_2^2z_4 + 2z_2z_5^2 + 2z_3z_4^2 + 2z_2^2z_5 + 2z_4z_5^2 + 4z_4^2z_5 - z_1^2 - z_2^2 - z_4^2 + 2z_4^3 + z_5^2 \\
& + 2z_0z_1z_2 + 2z_0z_1z_3 + 2z_0z_1z_4 + 2z_0z_2z_3 + 2z_0z_1z_5 + 4z_0z_2z_4 + 2z_1z_2z_3 + 2z_0z_2z_5 \\
& + 2z_0z_3z_4 + 6z_1z_2z_4 + 4z_1z_2z_5 + 4z_1z_3z_4 + 2z_0z_4z_5 + 2z_1z_3z_5 + 2z_2z_3z_4 + 6z_1z_4z_5 \\
& + 2z_2z_3z_5 + 6z_2z_4z_5 + 2z_3z_4z_5),
\end{aligned}$$

$$\begin{aligned}
0 \leq & (2z_0z_2 - z_1 - z_2 - z_3 - 2z_4 - 2z_5 - z_0 + 2z_0z_3 + 2z_1z_2 + 2z_0z_4 + 2z_1z_3 + 2z_0z_5 \\
& + 2z_1z_4 + 2z_1z_5 + 2z_2z_4 + 2z_2z_5 + 2z_3z_4 + 2z_3z_5 + 4z_4z_5 + 2z_4^2 + 2z_5^2) \times \\
& (z_1z_2 - z_2 - z_4 - z_5 - z_0z_1 - z_0z_3 - z_1 - z_0z_4 - 2z_0z_5 + z_1z_4 - z_2z_3 + z_2z_4 \\
& - z_3z_4 - 2z_3z_5 + 2z_0^2z_2 + 2z_0z_3^2 + 2z_0^2z_3 + 2z_0z_4^2 + 2z_1z_3^2 + 2z_0^2z_4 + 4z_0z_5^2 + 2z_0^2z_5 \\
& + 2z_1z_5^2 + 2z_2z_5^2 + 2z_3z_4^2 + 2z_3^2z_4 + 4z_3z_5^2 + 2z_3^2z_5 + 4z_4z_5^2 + 2z_4^2z_5 - z_0^2 - z_3^2 + z_4^2 \\
& - z_5^2 + 2z_5^3 + 2z_0z_1z_2 + 2z_0z_1z_3 + 2z_0z_1z_4 + 2z_0z_2z_3 + 2z_0z_1z_5 + 2z_0z_2z_4 + 2z_1z_2z_3 \\
& + 4z_0z_2z_5 + 4z_0z_3z_4 + 6z_0z_3z_5 + 2z_1z_2z_5 + 2z_1z_3z_4 + 6z_0z_4z_5 + 4z_1z_3z_5 + 2z_2z_3z_4 \\
& + 2z_1z_4z_5 + 2z_2z_3z_5 + 2z_2z_4z_5 + 6z_3z_4z_5),
\end{aligned}$$

$$\begin{aligned}
& 2z_0z_2 + 2z_0z_3 + 2z_1z_2 + 2z_0z_4 + 2z_1z_3 + 2z_0z_5 + 2z_1z_4 + 2z_1z_5 + 2z_2z_4 + 2z_2z_5 \\
& + 2z_3z_4 + 2z_3z_5 + 4z_4z_5 + 2z_4^2 + 2z_5^2 \neq z_0 + z_1 + z_2 + z_3 + 2z_4 + 2z_5,
\end{aligned}$$

$$\begin{aligned}
& (2z_0z_2 - z_1 - z_2 - z_3 - 2z_4 - 2z_5 - z_0 + 2z_0z_3 + 2z_1z_2 + 2z_0z_4 + 2z_1z_3 + 2z_0z_5 \\
& + 2z_1z_4 + 2z_1z_5 + 2z_2z_4 + 2z_2z_5 + 2z_3z_4 + 2z_3z_5 + 4z_4z_5 + 2z_4^2 + 2z_5^2) \times \\
& (z_1 + z_2 + z_4 + z_5 - z_0z_1 - 2z_0z_2 - z_0z_3 - 3z_1z_2 - 2z_0z_4 - 2z_1z_3 - z_0z_5 - 4z_1z_4 \\
& - z_2z_3 - 3z_1z_5 - 4z_2z_4 - 3z_2z_5 - 2z_3z_4 - z_3z_5 - 4z_4z_5 + 2z_0z_2^2 + 2z_1z_2^2 + 2z_1^2z_2 \\
& + 2z_0z_4^2 + 2z_1^2z_3 + 4z_1z_4^2 + 2z_1^2z_4 + 2z_1z_5^2 + 4z_2z_4^2 + 2z_1^2z_5 + 2z_2^2z_4 + 2z_2z_5^2 \\
& + 2z_3z_4^2 + 2z_2^2z_5 + 2z_4z_5^2 + 4z_4^2z_5 - z_1^2 - z_2^2 - 3z_4^2 + 2z_4^3 - z_5^2 + 2z_0z_1z_2 \\
& + 2z_0z_1z_3 + 2z_0z_1z_4 + 2z_0z_2z_3 + 2z_0z_1z_5 + 4z_0z_2z_4 + 2z_1z_2z_3 + 2z_0z_2z_5 \\
& + 2z_0z_3z_4 + 6z_1z_2z_4 + 4z_1z_2z_5 + 4z_1z_3z_4 + 2z_0z_4z_5 + 2z_1z_3z_5 + 2z_2z_3z_4 + 6z_1z_4z_5 \\
& + 2z_2z_3z_5 + 6z_2z_4z_5 + 2z_3z_4z_5) \leq 0,
\end{aligned}$$

$$\begin{aligned}
& (2z_0z_2 - z_1 - z_2 - z_3 - 2z_4 - 2z_5 - z_0 + 2z_0z_3 + 2z_1z_2 + 2z_0z_4 + 2z_1z_3 + 2z_0z_5 \\
& + 2z_1z_4 + 2z_1z_5 + 2z_2z_4 + 2z_2z_5 + 2z_3z_4 + 2z_3z_5 + 4z_4z_5 + 2z_4^2 + 2z_5^2) \times \\
& (z_0 + z_3 + z_4 + z_5 - z_0z_1 - 2z_0z_2 - 3z_0z_3 - z_1z_2 - 3z_0z_4 - 2z_1z_3 - 4z_0z_5 \\
& - z_1z_4 - z_2z_3 - 2z_1z_5 - z_2z_4 - 2z_2z_5 - 3z_3z_4 - 4z_3z_5 - 4z_4z_5 + 2z_0^2z_2 \\
& + 2z_0z_3^2 + 2z_0^2z_3 + 2z_0z_4^2 + 2z_1z_3^2 + 2z_0^2z_4 + 4z_0z_5^2 + 2z_0^2z_5 + 2z_1z_5^2 + 2z_2z_5^2 \\
& + 2z_3z_4^2 + 2z_3^2z_4 + 4z_3z_5^2 + 2z_3^2z_5 + 4z_4z_5^2 + 2z_4^2z_5 - z_0^2 - z_3^2 - z_4^2 - 3z_5^2 + 2z_5^3)
\end{aligned}$$

$$\begin{aligned}
&+2z_0z_1z_2 + 2z_0z_1z_3 + 2z_0z_1z_4 + 2z_0z_2z_3 + 2z_0z_1z_5 + 2z_0z_2z_4 + 2z_1z_2z_3 \\
&+4z_0z_2z_5 + 4z_0z_3z_4 + 6z_0z_3z_5 + 2z_1z_2z_5 + 2z_1z_3z_4 + 6z_0z_4z_5 + 4z_1z_3z_5 \\
&+2z_2z_3z_4 + 2z_1z_4z_5 + 2z_2z_3z_5 + 2z_2z_4z_5 + 6z_3z_4z_5) \leq 0,
\end{aligned}$$

and $0 \leq z_0, z_1, z_2, z_3, z_4, z_5 \leq 1$.

The above analytic solution to (23)–(28) is obtained by symbolic math programming in MATLAB.

References

- N. Aronszajn. Theory of reproducing kernels. *Transactions of the American Mathematical Society*, 68:337–404, 1950.
- L. Baringhaus and C. Franz. On a new multivariate two-sample test. *Journal of Multivariate Analysis*, 88:190–206, 2004.
- A. Berlinet and C. Thomas-Agnan. *Reproducing Kernel Hilbert Spaces in Probability and Statistics*. Kluwer, 2004.
- G. Blanchard, G. Lee, and C. Scott. Generalizing from several related classification tasks to a new unlabeled sample. In *Advances in Neural Information Processing Systems (NIPS)*, pages 2178–2186, 2011.
- G. Blanchard, A. A. Deshmukh, U. Dogan, G. Lee, and C. Scott. Domain generalization by marginal transfer learning. Technical report, 2017. (<https://arxiv.org/abs/1711.07910>).
- K. Borgwardt, A. Gretton, M. J. Rasch, H.-P. Kriegel, B. Schölkopf, and A. J. Smola. Integrating structured biological data by kernel maximum mean discrepancy. *Bioinformatics*, 22:e49–e57, 2006.
- J.-F. Cardoso. Multidimensional independent component analysis. In *International Conference on Acoustics, Speech, and Signal Processing (ICASSP)*, pages 1941–1944, 1998.
- C. Carmeli, E. De Vito, A. Toigo, and V. Umanitá. Vector valued reproducing kernel Hilbert spaces and universality. *Analysis and Applications*, 8:19–61, 2010.
- R. M. Dudley. *Real Analysis and Probability*. Cambridge University Press, 2004.
- K. Fukumizu, A. Gretton, X. Sun, and B. Schölkopf. Kernel measures of conditional dependence. In *Advances in Neural Information Processing Systems (NIPS)*, pages 498–496, 2008.
- K. Fukumizu, F. Bach, and M. Jordan. Kernel dimension reduction in regression. *The Annals of Statistics*, 37(4):1871–1905, 2009.
- K. Fukumizu, L. Song, and A. Gretton. Kernel Bayes’ rule: Bayesian inference with positive definite kernels. *Journal of Machine Learning Research*, 14:3753–3783, 2013.

- A. Gretton. A simpler condition for consistency of a kernel independence test. Technical report, University College London, 2015. (<http://arxiv.org/abs/1501.06103>).
- A. Gretton, O. Bousquet, A. Smola, and B. Schölkopf. Measuring statistical dependence with Hilbert-Schmidt norms. In *Algorithmic Learning Theory (ALT)*, pages 63–78, 2005.
- A. Gretton, K. Fukumizu, C. H. Teo, L. Song, B. Schölkopf, and A. J. Smola. A kernel statistical test of independence. In *Advances in Neural Information Processing Systems (NIPS)*, pages 585–592, 2008.
- A. Gretton, K. M. Borgwardt, M. J. Rasch, B. Schölkopf, and A. Smola. A kernel two-sample test. *Journal of Machine Learning Research*, 13:723–773, 2012.
- Z. Harchaoui, F. Bach, and E. Moulines. Testing for homogeneity with kernel Fisher discriminant analysis. In *Advances in Neural Information Processing Systems (NIPS)*, pages 609–616, 2007.
- W. Jitkrittum, Z. Szabó, and A. Gretton. An adaptive test of independence with analytic kernel embeddings. In *International Conference on Machine Learning (ICML; PMLR)*, volume 70, pages 1742–1751, 2017.
- B. Kim, R. Khanna, and O. O. Koyejo. Examples are not enough, learn to criticize! criticism for interpretability. In *Advances in Neural Information Processing Systems (NIPS)*, pages 2280–2288, 2016.
- L. Klebanov. *N-Distances and Their Applications*. Charles University, Prague, 2005.
- G. Kusano, K. Fukumizu, and Y. Hiraoka. Persistence weighted Gaussian kernel for topological data analysis. In *International Conference on Machine Learning (ICML)*, pages 2004–2013, 2016.
- H. C. L. Law, D. J. Sutherland, D. Sejdinovic, and S. Flaxman. Bayesian approaches to distribution regression. In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, volume 84, pages 1167–1176, 2018.
- J. R. Lloyd, D. Duvenaud, R. Grosse, J. B. Tenenbaum, and Z. Ghahramani. Automatic construction and natural-language description of nonparametric regression models. In *AAAI Conference on Artificial Intelligence*, pages 1242–1250, 2014.
- R. Lyons. Distance covariance in metric spaces. *The Annals of Probability*, 41:3284–3305, 2013.
- C. A. Micchelli, Y. Xu, and H. Zhang. Universal kernels. *Journal of Machine Learning Research*, 7:2651–2667, 2006.
- J. M. Mooij, J. Peters, D. Janzing, J. Zscheischler, and B. Schölkopf. Distinguishing cause from effect using observational data: Methods and benchmarks. *Journal of Machine Learning Research*, 17:1–102, 2016.
- K. Muandet, K. Fukumizu, F. Dinuzzo, and B. Schölkopf. Learning from distributions via support measure machines. In *Advances in Neural Information Processing Systems (NIPS)*, pages 10–18, 2011.

- K. Muandet, K. Fukumizu, B. Sriperumbudur, and B. Schölkopf. Kernel mean embedding of distributions: A review and beyond. *Foundations and Trends in Machine Learning*, 10(1-2):1–141, 2017.
- M. Park, W. Jitkrittum, and D. Sejdinovic. K2-ABC: Approximate Bayesian computation with kernel embeddings. In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, volume 51, pages 51:398–407, 2016.
- N. Pfister, P. Bühlmann, B. Schölkopf, and J. Peters. Kernel-based tests for joint independence. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 80(1):5–31, 2017.
- N. Quadrianto, L. Song, and A. Smola. Kernelized sorting. In *Advances in Neural Information Processing Systems (NIPS)*, pages 1289–1296, 2009.
- B. Schölkopf and A. J. Smola. *Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond*. MIT Press, 2002.
- B. Schölkopf, K. Muandet, K. Fukumizu, S. Harmeling, and J. Peters. Computing functions of random variables via reproducing kernel Hilbert space representations. *Statistics and Computing*, 25(4):755–766, 2015.
- D. Sejdinovic, A. Gretton, and W. Bergsma. A kernel test for three-variable interactions. In *Advances in Neural Information Processing Systems (NIPS)*, pages 1124–1132, 2013a.
- D. Sejdinovic, B. K. Sriperumbudur, A. Gretton, and K. Fukumizu. Equivalence of distance-based and RKHS-based statistics in hypothesis testing. *Annals of Statistics*, 41:2263–2291, 2013b.
- C.-J. Simon-Gabriel and B. Schölkopf. Kernel distribution embeddings: Universal kernels, characteristic kernels and kernel metrics on distributions. Technical report, Max Planck Institute for Intelligent Systems, 2016. (<https://arxiv.org/abs/1604.05251>).
- A. Smola, A. Gretton, L. Song, and B. Schölkopf. A Hilbert space embedding for distributions. In *Algorithmic Learning Theory (ALT)*, pages 13–31, 2007.
- L. Song, A. Gretton, D. Bickson, Y. Low, and C. Guestrin. Kernel belief propagation. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, pages 707–715, 2011.
- L. Song, A. Smola, A. Gretton, J. Bedo, and K. Borgwardt. Feature selection via dependence maximization. *Journal of Machine Learning Research*, 13:1393–1434, 2012.
- B. K. Sriperumbudur, A. Gretton, K. Fukumizu, B. Schölkopf, and G. R. G. Lanckriet. Hilbert space embeddings and metrics on probability measures. *Journal of Machine Learning Research*, 11:1517–1561, 2010.
- B. K. Sriperumbudur, K. Fukumizu, and G. R. G. Lanckriet. Universality, characteristic kernels and RKHS embedding of measures. *Journal of Machine Learning Research*, 12:2389–2410, 2011.

- I. Steinwart. On the influence of the kernel on the consistency of support vector machines. *Journal of Machine Learning Research*, 6(3):67–93, 2001.
- I. Steinwart and A. Christmann. *Support Vector Machines*. Springer, 2008.
- E. V. Strobl, S. Visweswaran, and K. Zhang. Approximate kernel-based conditional independence tests for fast non-parametric causal discovery. Technical report, 2017. (<https://arxiv.org/abs/1702.03877>).
- Z. Szabó, B. Sriperumbudur, B. Póczos, and A. Gretton. Learning theory for distribution regression. *Journal of Machine Learning Research*, 17(152):1–40, 2016.
- G. J. Székely and M. L. Rizzo. Testing for equal distributions in high dimension. *InterStat*, 5, 2004.
- G. J. Székely and M. L. Rizzo. A new test for multivariate normality. *Journal of Multivariate Analysis*, 93:58–80, 2005.
- G. J. Székely and M. L. Rizzo. Brownian distance covariance. *The Annals of Applied Statistics*, 3:1236–1265, 2009.
- G. J. Székely, M. L. Rizzo, and N. K. Bakirov. Measuring and testing dependence by correlation of distances. *The Annals of Statistics*, 35:2769–2794, 2007.
- H. Wendland. *Scattered Data Approximation*. Cambridge Monographs on Applied and Computational Mathematics. Cambridge University Press, 2005.
- M. Yamada, Y. Umezū, K. Fukumizu, and I. Takeuchi. Post selection inference with kernels. In *International Conference on Artificial Intelligence and Statistics (AISTATS; PMLR)*, volume 84, pages 152–160, 2018.
- M. Zaheer, S. Kottur, S. Ravanbakhsh, B. Póczos, R. R. Salakhutdinov, and A. J. Smola. Deep sets. In *Advances in Neural Information Processing Systems (NIPS)*, pages 3394–3404, 2017.
- K. Zhang, B. Schölkopf, K. Muandet, and Z. Wang. Domain adaptation under target and conditional shift. *Journal of Machine Learning Research*, 28(3):819–827, 2013.
- A. A. Zinger, A. V. Kakosyan, and L. B. Klebanov. A characterization of distributions by mean values of statistics and certain probabilistic metrics. *Journal of Soviet Mathematics*, 1992.