Abstract

This is a tutorial and survey paper on kernels, kernel methods, and related fields. We start with reviewing the history of kernels in functional analysis and machine learning. Then, Mercer kernel, Hilbert and Banach spaces, Reproducing Kernel Hilbert Space (RKHS), Mercer’s theorem and its proof, frequently used kernels, kernel construction from distance metric, important classes of kernels (including bounded, integrally positive definite, universal, stationary, and characteristic kernels), kernel centering and normalization, and eigenfunctions are explained in detail. Then, we introduce types of use of kernels in machine learning including kernel methods (such as kernel support vector machines), kernel learning by semi-definite programming, Hilbert-Schmidt independence criterion, maximum mean discrepancy, kernel mean embedding, and kernel dimensionality reduction. We also cover rank and factorization of kernel matrix as well as the approximation of eigenfunctions and kernels using the Nyström method. This paper can be useful for various fields of science including machine learning, dimensionality reduction, functional analysis in mathematics, and mathematical physics in quantum mechanics.

1. Introduction

1.1. History of Kernels

It is 1904 when David Hilbert proposed his work on kernels and defined a definite kernel (Hilbert, 1904), and later, his and Erhard Schmidt’s works proposed integral equations such as Fredholm integral equations (Hilbert, 1904; Schmidt, 1908). This was the introduction of a new space which was named the Hilbert space. Later, the Hilbert space was found to be very useful for the formulations in quantum mechanics (Prugovecki, 1982). After the initial works on Hilbert space by Hilbert and Schmidt (Hilbert, 1904; Schmidt, 1908), James Mercer improved Hilbert’s work and proposed his theorem in 1909 (Mercer, 1909) which was named the Mercer’s theorem later. In the mean time, Stefan Banach, Hans Hahn, and Eduard Helly proposed the concepts of another new space in years 1920–1922 (Bourbaki, 1950) which was named the Banach space later by Maurice René Fréchet (Narici & Beckenstein, 2010). The Hilbert space is a subset of the Banach space.

Reproducing Kernel Hilbert Space (RKHS) is a special case of Hilbert space with some properties. It is a Hilbert space of functions with reproducing kernels (Berlinet &
The first work on RKHS was (Aronszajn, 1950). Later, the concepts of RKHS were improved further in (Aizerman et al., 1964). The RKHS remained in pure mathematics until this space was used for the first time in machine learning by introduction of kernel Support Vector Machine (SVM) (Boser et al., 1992; Vapnik, 1995). Eigenfunctions were also developed for eigenvalue problem applied on operators and functions (Williams & Seeger, 2000) and were used in machine learning (Bengio et al., 2003c) and physics (Kusse & Westwig, 2006). This is related to RKHS because it uses weighted inner product in Hilbert space (Williams & Seeger, 2000) and RKHS is a Hilbert space of functions with a reproducing kernel.

Using kernels was widely noticed when linear SVM (Vapnik & Chervonenkis, 1974) was kernelized (Boser et al., 1992; Vapnik, 1995). Kernel SVM showed off very successfully because of its merits. Two competing models, kernel SVM and neural network were the models which could handle nonlinear data (see Fausett, 1994 for history of neural networks). Kernel SVM transformed nonlinear data to RKHS to make the pattern of data linear hopefully and then applied linear SVM on it. However, the approach of neural network was different because the model itself was nonlinear (see Section 8 for more details). The success of kernel SVM plus the problem of vanishing gradients in neural networks (Goodfellow et al., 2016) resulted in the winter of neural network around years 2000 to 2006. However, the problems of training deep neural networks started to be resolved (Hinton & Salakhutdinov, 2006) and their success plus two problems of kernel SVM helped neural networks take over kernel SVM gradually. One problem of kernel SVM was not knowing the suitable kernel type for various learning problems. In other words, kernel SVM still required the user to choose the type of kernel but neural networks were end-to-end and almost robust to hyperparameters such as the number of layers or neurons. Another problem was that kernel SVM could not handle big data, although Nystrom method, first proposed in (Nyström, 1930), was used to resolve this problem of kernel methods by approximating kernels from a subset of data (Williams & Seeger, 2001). Note that kernels have been used widely in machine learning such as in SVM (Vapnik, 1995), Gaussian process classifiers (Williams & Barber, 1998), and spline methods (Wahba, 1990). The types of use of kernels in machine learning will be discussed in Section 9.

1.2. Useful Books on Kernels

There exist several books about use of kernels in machine learning. Some examples are (Smola & Schölkopf, 1998; Schölkopf et al., 1999a; Schölkopf & Smola, 2002; Shawe-Taylor & Cristianini, 2004; Camps-Valls, 2006; Steinwart & Christmann, 2008; Rojo-Álvarez et al., 2018; Kung, 2014). Some survey papers about kernel-based machine learning are (Hofmann et al., 2006; 2008; Müller et al., 2018). In addition to some of the above-mentioned books, there exist some other books/papers on kernel SVM such as (Schölkopf et al., 1997b; Burges, 1998; Hastie et al., 2009).

1.3. Kernel in Different Fields of Science

The term kernel has been used in different fields of science for various purposes. In the following, we briefly introduce the different uses of kernel in science to clarify which use of kernel we are focusing on in this paper.

1. Kernel of filter in signal processing: In signal processing, one can use filters to filter a price of signal, such as an image (Gonzalez & Woods, 2002). Digital filters have a kernel which determine the values of filter in the window of filter (Schlichtbarle, 2011). In convolutional neural networks, the filter kernels are learned in deep learning (Goodfellow et al., 2016).

2. Kernel smoothing for density estimation: Kernel density estimation can be used for fitting a mixture of distributions to some data instances (Scott, 1992). For this, a histogram with infinite number of bins is utilized. In limit, this histogram is converged to a kernel smoothing (Wand & Jones, 1994) where the kernel determines the type of distribution. For example, if a Radial Basis Function (RBF) kernel is used, a mixture of Gaussian distributions is fitted to data.

3. Kernelization in complexity theory: Kernelization is a pre-processing technique where the input to an algorithm is replaced by a part of the input named kernel. The output of the algorithm on kernel should either be the same as or be able to be transformed to the output of the algorithm for the whole input (Fomin et al., 2019). An example usage of kernelization is in vertex cover problem (Abu-Khzam et al., 2004).

4. Kernel in operating system: Kernel is the core of an operating system, such as Linux, which connects the hardware including CPU, memory, and peripheral devices to applications (Anderson & Dahlin, 2014).

5. Kernel in linear algebra and graphs: Consider a mapping from the vector space \( \mathcal{V} \) to the vector space \( \mathbb{R}^n \) as \( L: \mathcal{V} \rightarrow \mathbb{R}^n \). The kernel, also called the nullspace, of this mapping is defined as \( \ker(L) := \{ \mathbf{v} \in \mathcal{V} | L(\mathbf{v}) = 0 \} \). For example, for a matrix \( \mathbf{A} \in \mathbb{R}^{n \times k} \), the kernel of \( \mathbf{A} \) is \( \ker(\mathbf{A}) = \{ \mathbf{x} \in \mathbb{R}^n | \mathbf{Ax} = 0 \} \). The four fundamental subspaces of a matrix are its kernel, row space, column space, and left null space (Strang, 1993). Note that the kernel (nullspace) of adjacency matrix in graphs has also been well developed (Akbari et al., 2006).

6. Kernel in other domains of mathematics: There exist kernel concepts in other domains of mathematics and statistics such as geometry of polygon (Icking & Klein, 1995), set theory (Bergman, 2011, p. 14), etc.
7. Kernel in feature space for machine learning: In statistical machine learning, kernels pull data to a feature space for the sake of better discrimination of classes or simpler representation of data (Hofmann et al., 2006; 2008). In this paper, our focus is on this category which is kernels for machine learning.

1.4. Organization of Paper

This paper is a tutorial and survey paper on kernels and kernel methods. It can be useful for several fields of science including machine learning, functional analysis in mathematics, and mathematical physics in quantum mechanics. The remainder of this paper is organized as follows. Section 2 introduces the Mercer kernel, important spaces in functional analysis including the Hilbert and Banach spaces, and Reproducing Kernel Hilbert Space (RKHS). Mercer’s theorem and its proof are provided in Section 3. Characteristics of kernels are explained in Section 4. We introduce frequently used kernels, kernel construction from distance metric, and important classes of kernels in Section 5. Kernel centering and normalization are explained in Section 6. Eigenfunctions are then introduced in Section 7. We explain two techniques for kernelization in Section 8. Types of use of kernels in machine learning are reviewed in Section 9. Kernel factorization and Nyström approximation are introduced in Section 10. Finally, Section 11 concludes the paper.

Required Background for the Reader

This paper assumes that the reader has general knowledge of calculus, linear algebra, and basics of optimization. The required basics of functional analysis are explained in the paper.

2. Mercer Kernel and Spaces In Functional Analysis

2.1. Mercer Kernel and Gram Matrix

Definition 1 (Mercer Kernel (Mercer, 1909)). The function \( k : X^2 \to \mathbb{R} \) is a Mercer kernel function (also known as kernel function) where:

1. it is symmetric: \( k(x, y) = k(y, x) \),
2. and its corresponding kernel matrix \( K(i, j) = k(x_i, x_j) \) for \( i, j \in \{1, \ldots, n\} \) is positive semi-definite: \( K \succeq 0 \).

The corresponding kernel matrix of a Mercer kernel is a Mercer kernel matrix.

The two properties of a Mercer kernel will be proved in Section 4. By convention, unless otherwise stated, the term kernel refers to Mercer kernel. The effectiveness of Mercer kernel will be shown and proven in the Mercer’s theorem, i.e., Theorem 2.

Definition 2 (Gram Matrix or Kernel Matrix). The matrix \( K \in \mathbb{R}^{n \times n} \) is a Gram matrix, also known as a Gramian matrix or a kernel matrix, whose \((i, j)\)-th element is:

\[
K(i, j) := k(x_i, x_j), \quad \forall i, j \in \{1, \ldots, n\}.
\]

Here, we defined the square kernel matrix applied on a set of \( n \) data instances; hence, the kernel is a \( n \times n \) matrix. We may also have a kernel matrix between two sets of data instances. This will be explained more in Section 8. Moreover, note that the kernel matrix can be computed using the inner product between pulled data to the feature space. This will be explained in detail in Section 3.2.

2.2. Hilbert, Banach, \( L_p \), and Sobolev Spaces

Before defining the RKHS and details of kernels, we need to introduce Hilbert, Banach, \( L_p \), and Sobolev spaces, which are well-known spaces in functional analysis (Conway, 2007).

Definition 3 (Metric Space). A metric space is a set where a metric, for measuring the distance between instances of set, is defined on it.

Definition 4 (Vector Space). A vector space is a set of vectors equipped with some available operations such as addition and multiplication by scalars.

Definition 5 (Complete Space). A space \( F \) is complete if every Cauchy sequence converges to a member of this space \( f \in F \). Note that the Cauchy sequence is a sequence whose elements become arbitrarily close to one another as the sequence progresses (i.e., it converges in limit).

Definition 6 (Compact Space). A space is compact if it is closed (i.e., it contains all its limit points) and bounded (i.e., all its points lie within some fixed distance of one another).

Definition 7 (Hilbert Space (Reed & Simon, 1972)). A Hilbert space \( \mathcal{H} \) is an inner product space that is a complete metric space with respect to the norm or distance function induced by the inner product.

The Hilbert space generalizes the Euclidean space to a finite or infinite dimensional space. Usually, the Hilbert space is high dimensional. By convention in machine learning, unless otherwise stated, Hilbert space is also referred to as the feature space. By feature space, researchers often specifically mean the RKHS space which will be introduced in Section 2.3.

Definition 8 (Banach Space (Beauzamy, 1982)). A Banach space is a complete vector space equipped with a norm.

Remark 1 (Difference of Hilbert and Banach Spaces). Hilbert space is a special case of Banach space equipped with a norm defined using an inner product notion. All Hilbert spaces are Banach spaces but the converse is not true.
Suppose \( \mathbb{R}^n, \mathcal{H}, \mathcal{B}, \mathcal{M}_c, \mathcal{M}, \mathcal{T} \) denote the Euclidean space, Hilbert space, Banach space, complete metric space, metric space, and topological space (containing both open and closed sets), respectively. Then, we have:

\[
\mathbb{R}^n \subset \mathcal{H} \subset \mathcal{B} \subset \mathcal{M}_c \subset \mathcal{M} \subset \mathcal{T}.
\] (2)

**Definition 9 (L\(_p\) Space).** Consider a function \( f \) with domain \([a, b]\). For \( p > 0 \), let the \( L_p \) norm be defined as:

\[
\|f\|_p := \left( \int |f(x)|^p \, dx \right)^{\frac{1}{p}}.
\] (3)

The \( L_p \) space is defined as the set of functions with bounded \( L_p \) norm:

\[
L_p(a, b) := \{ f : [a, b] \to \mathbb{R} \mid \|f\|_p < \infty \}. \tag{4}
\]

**Definition 10 (Sobolev Space (Renardy & Rogers, 2006, Chapter 7)).** A Sobolev space is a vector space of functions equipped with \( L_p \) norms and derivatives:

\[
W_{m,p} := \{ f \in L_p(0, 1) \mid D^m f \in L_p(0, 1) \}, \tag{5}
\]

where \( D^m f \) denotes the \( m \)-th order derivative.

Note that the Sobolev spaces are RKHS with some specific kernels (Novak et al., 2018). RKHS will be explained in Section 2.3.

### 2.3. Reproducing Kernel Hilbert Space

#### 2.3.1. Definition of RKHS

Reproducing Kernel Hilbert Space (RKHS), first proposed in (Aronszajn, 1950), is a special case of Hilbert space with some properties. It is a Hilbert space of functions with reproducing kernels (Berlinet & Thomas-Agnan, 2011). After the initial work on RKHS (Aronszajn, 1950), another work (Aizerman et al., 1964) developed the RKHS concepts. In this section, we introduce this space.

**Definition 11 (RKHS (Aronszajn, 1950; Berlinet & Thomas-Agnan, 2011)).** A Reproducing Kernel Hilbert Space (RKHS) is a Hilbert space \( \mathcal{H} \) of functions \( f : \mathcal{X} \to \mathbb{R} \) with a reproducing kernel \( k : \mathcal{X}^2 \to \mathbb{R} \) where \( k(x, .) \in \mathcal{H} \) and \( f(x) = \langle k(x, .), f \rangle \).

The RKHS is explained in more detail in the following. Consider the kernel function \( k(x, y) \) which is a function of two variables. Suppose, for \( n \) points, we fix one of the variables to have \( k(x_1, y), k(x_2, y), \ldots, k(x_n, y) \). These are all functions of the variable \( y \). RKHS is a function space which is the set of all possible linear combinations of these functions (Kimeldorf & Wahba, 1971), (Aizerman et al., 1964, p. 834), (Mercer, 1909):

\[
\mathcal{H} := \left\{ f(\cdot) = \sum_{i=1}^{n} \alpha_i k(x_i, \cdot) \right\} \overset{(a)}{=} \left\{ f(\cdot) = \sum_{i=1}^{n} \alpha_i k_{x_i}(\cdot) \right\}, \tag{6}
\]

where \((a)\) is because we define \( k_{\nu}(\cdot) := k(x, .) \). This equation shows that the bases of an RKHS are kernels. The proof of this equation is obtained by considering both Eqs. (21) and (34) together (n.b. for better organization, it is better that we provide those equations later). It is also noteworthy that this equation will also appear in Theorem 1.

According to Eq. (6), every function in the RKHS can be written as a linear combination. Consider two functions in this space represented as \( f = \sum_{i=1}^{n} \alpha_i k(x_i, y) \) and \( g = \sum_{j=1}^{n} \beta_j k(x, y_j) \). Hence, the inner product in RKHS is calculated as:

\[
\langle f, g \rangle_k \overset{(a)}{=} \left\{ \sum_{i=1}^{n} \alpha_i k(x_i, \cdot), \sum_{j=1}^{n} \beta_j k(\cdot, y_j) \right\}_k
\]

\[
= \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \beta_j k(x_i, y_j), \tag{7}
\]

where \((a)\) is because kernel is symmetric (it will be proved in Section 4). Hence, the norm in RKHS is calculated as:

\[
\|f\|_k := \sqrt{\langle f, f \rangle_k}. \tag{8}
\]

The subscript of norm and inner product in RKHS has various notations in the research papers. Some most famous notations are \( \langle f, g \rangle_k \), \( \langle f, g \rangle_{\mathcal{H}} \), \( \langle f, g \rangle_{\mathcal{H}_k} \), \( \langle f, g \rangle_F \) where \( \mathcal{H}_k \) denotes the Hilbert space associated with kernel \( k \) and \( F \) stands for the feature space because RKHS is sometimes referred to as the feature space.

**Remark 2 (RKHS Being Unique for a Kernel).** Given a kernel, the corresponding RKHS is unique (up to isometric isomorphisms). Given an RKHS, the corresponding kernel is unique. In other words, each kernel generates a new RKHS.

**Remark 3.** As we also saw in Mercer’s theorem, the bases of RKHS space is the eigenfunctions \( \{ \psi_i(\cdot) \}_{i=1}^{\infty} \) which are functions themselves. This, along with Eq. (6), show that the RKHS space is a space of functions and not a space of vectors. In other words, the basis vectors of RKHS are basis functions named eigenfunctions. Because the RKHS is a space of functions rather than a space of vectors, we usually do not know the exact location of pulled points to the RKHS but we know the relation of them as a function. This will be explained more in Section 3.2 and Fig. 1.

#### 2.3.2. Reproducing Property

In Eq. (7), consider only one component for \( g \) to have \( g(x) = \sum_{j=1}^{n} \beta_j k(x, x_j) = \beta k(x, x) \) where we take \( \beta = 1 \) to have \( g(x) = k(x, x) = k_x(\cdot) \). In other words, assume the function \( g(x) \) is a kernel in the RKHS space. Also consider the function \( f(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x) \) in
the space. According to Eq. (7), the inner product of these functions is:
\[
\langle f(x), g(x) \rangle_k = \langle f, k_x(\cdot) \rangle_k \\
= \left\langle \sum_{i=1}^{n} \alpha_i k(x_i, x), k(x, x) \right\rangle_k \\
= \sum_{i=1}^{n} \alpha_i k(x_i, x) \overset{(a)}{=} f(x),
\]
where \((a)\) is because the term before equation is the previously considered function \(f\). As Eq. (9) shows, the function \(f\) is reproduced from the inner product of that function with one of the kernels in the space. This shows the reproducing property of the RKHS space. A special case of Eq. (9) is \(\langle k_x, k_x \rangle_k = k(x, x)\).

The name of RKHS consists of several parts because of the following justifications:

1. “Reproducing”: because if the reproducing property of RKHS which was proved above.
2. “Kernel”: because of the kernels associated to RKHS as stated in Definition 11 and Eq. (6).
3. “Hilbert Space”: because RKHS is a Hilbert space of functions with a reproducing kernel, as stated in Definition 11.

2.3.3. REPRESENTATION IN RKHS
In the following, we provide a proof for Eq. (6) and explain why that equation defines the RKHS.

**Theorem 1** (Representer Theorem (Kimeldorf & Wahba, 1971), simplified in (Rudin, 2012)). For a set of data \(\mathcal{X} = \{x_i\}_{i=1}^{n}\), consider a RKHS \(\mathcal{H}\) of functions \(f : \mathcal{X} \rightarrow \mathbb{R}\) with kernel function \(k\). For any function \(\ell : \mathbb{R}^2 \rightarrow \mathbb{R}\) (usually called the loss function), consider the optimization problem:

\[
f^* \in \arg \min_{f \in \mathcal{H}} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \eta \Omega(\|f\|_k),
\]
where \(\eta \geq 0\) is the regularization parameter and \(\Omega(\|f\|_k)\) is a penalty term such as \(\|f\|_k^2\). The solution of this optimization can be expressed as:

\[
f^* = \sum_{i=1}^{n} \alpha_i k(x_i, \cdot) = \sum_{i=1}^{n} \alpha_i k_x(\cdot).
\]

**Proof.** Proof is inspired by (Rudin, 2012). Assume we project the function \(f\) onto a subspace spanned by \(\{k(x_i, \cdot)\}_{i=1}^{n}\). The function \(f\) can be decomposed into components along and orthogonal to this subspace, respectively denoted by \(f_{\parallel}\) and \(f_{\perp}\):

\[
f = f_{\parallel} + f_{\perp} \\
\Rightarrow \|f\|_{\mathcal{H}}^2 = \|f_{\parallel}\|_{\mathcal{H}}^2 + \|f_{\perp}\|_{\mathcal{H}}^2 \geq \|f_{\parallel}\|_{\mathcal{H}}^2.
\]
Moreover, using the reproducing property of the RKHS, we have:

\[
f(x_i) = \langle f, k(x_i, \cdot) \rangle_k \\
= \sum_{i=1}^{n} \alpha_i k(x_i, x) \overset{(a)}{=} f(x),
\]
where \((a)\) is because the orthogonal component has zero inner product with the bases of subspace. According to Eq. (14), we have:

\[
\sum_{i=1}^{n} \ell(f(x_i), y_i) = \sum_{i=1}^{n} \ell(f_{\parallel}(x_i), y_i).
\]
Using Eqs. (13) and (15), we can say:

\[
\min_{f \in \mathcal{H}} \sum_{i=1}^{n} \ell(f(x_i), y_i) + \eta \|f\|_{\mathcal{H}}^2 \\
= \min_{f \in \mathcal{H}} \sum_{i=1}^{n} \ell(f_{\parallel}(x_i), y_i) + \eta \|f_{\parallel}\|_{\mathcal{H}}^2.
\]

Hence, for this minimization, we only require the component lying in the space spanned by the kernels of RKHS. Therefore, we can represent the function (solution of optimization) to lie in the space as linear combination of basis vectors \(\{k(x_i, \cdot)\}_{i=1}^{n}\). Q.E.D.

**Corollary 1.** In Section 2.2, we mentioned that Hilbert space can be infinite dimensional. According to Definition 11, RKHS is a Hilbert space so it may be infinite dimensional. The representer theorem states that, in practice, we only need to deal with a finite-dimensional space; although, that finite number of dimensions is usually a large number.

Note that the representer theorem has been used in kernel SVM where \(\alpha_i\)’s are the dual variables which are non-zero for support vectors (Boser et al., 1992; Vapnik, 1995). According to this theorem, kernel SVM only requires to learn the dual variables, \(\alpha_i\)’s, to find the optimal boundary between classes.

3. Mercer’s Theorem and Feature Map
3.1. Mercer’s Theorem

**Definition 12** (Definite Kernel (Hilbert, 1904)). A kernel \(k : [a, b] \times [a, b] \rightarrow \mathbb{R}\) is a definite kernel where the following double integral:

\[
J(f) = \int_{a}^{b} \int_{a}^{b} k(x, y) f(x) f(y) \, dx \, dy,
\]


satisfies $J(f) > 0$ for all $f(x) \neq 0$.

Mercer improved over Hilbert’s work (Hilbert, 1904) to prove his theorem, the Mercer’s theorem (Mercer, 1909), introduced in the following.

**Theorem 2** (Mercer’s Theorem (Mercer, 1909)). Suppose $k : [a, b] \times [a, b] \rightarrow \mathbb{R}$ is a continuous symmetric positive semi-definite kernel which is bounded:

$$\sup_{x,y} k(x, y) < \infty. \quad (17)$$

Assume the operator $T_k$ takes a function $f(x)$ as its argument and outputs a new function as:

$$T_k f(x) := \int_a^b k(x, y) f(y) \, dy,$$  \quad (18)

which is a Fredholm integral equation (Schmidt, 1908). The operator $T_k$ is called the Hilbert–Schmidt integral operator (Renardy & Rogers, 2006, Chapter 8). This output function is positive semi-definite:

$$\int \int k(x, y) f(y) \, dx \, dy \geq 0. \quad (19)$$

Then, there is a set of orthonormal bases $\{\psi_i(.)\}_{i=1}^{\infty}$ of $L_2(a, b)$ consisting of eigenfunctions of $T_k$ such that the corresponding sequence of eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$ are non-negative:

$$\int k(x, y) \psi_i(y) \, dy = \lambda_i \psi_i(x). \quad (20)$$

The eigenfunctions corresponding to the non-zero eigenvalues are continuous on $[a, b]$ and $k$ can be represented as (Alzerman et al., 1964):

$$k(x, y) = \sum_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(y), \quad (21)$$

where the convergence is absolute and uniform.

**Proof.** A roughly high-level proof for the Mercer’s theorem is as follows.

**Step 1 of proof:** According to assumptions of theorem, the Hilbert-Schmidt integral operator $T_k$ is a symmetric operator on $L_2(a, b)$ space. Consider a unit ball in $L_2(a, b)$ as input to the operator. As the kernel is bounded, $\sup_{x,y} k(x, y) < \infty$, the sequence $f_1, f_2, \ldots$ converges in norm, i.e. $\|f_n - f\| \rightarrow 0$ as $n \rightarrow 0$. Therefore, according to the Arzelà-Ascoli theorem (Arzelà, 1895), the image of the unit ball after applying the operator is compact. In other words, the operator $T_k$ is compact.

**Step 2 of proof:** According to the spectral theorem (Hawkins, 1975), there exist several orthonormal bases $\{\psi_i(.)\}_{i=1}^{\infty}$ in $L_2(a, b)$ for the compact operator $T_k$. This provides a spectral (or eigenvalue) decomposition for the operator $T_k$ (Ghojogh et al., 2019a):

$$T_k \psi_i(x) = \lambda_i \psi_i(x), \quad (22)$$

where $\{\psi_i(.)\}_{i=1}^{\infty}$ and $\{\lambda_i\}_{i=1}^{\infty}$ are the eigenvectors and eigenvalues of the operator $T_k$, respectively. Noticing the defined Eq. (18) and the eigenvalue decomposition, Eq. (22), we have:

$$\int k(x, y) \psi_i(y) \, dy = T_k \psi_i(x) = \lambda_i \psi_i(x). \quad (23)$$

This proves the Eq. (20) which is the eigenfunction decomposition of the operator $T_k$. Note that the eigenvectors $\{\psi_i(.)\}_{i=1}^{\infty}$ are referred to as the eigenfunctions because the decomposition is applied on a function or operator rather than a matrix. Note that eigenfunctions will be explained more in Section 7.

**Step 3 of proof:** According to Parseval’s theorem (Parseval des Chenes, 1806), the Bessel’s inequality can be converted to equality (Saxe, 2002). For the orthonormal bases $\{\psi_i(.)\}_{i=1}^{\infty}$ in the Hilbert space $H$ associated with kernel $k$, we have for any function $f \in L_2(a, b)$:

$$f = \sum_{i=1}^{\infty} (f, \psi_i)_k \psi_i. \quad (24)$$

If we replace $\psi_i$ with $f$ in Eq. (22) and consider Eq. (24), we will have:

$$T_k f = \sum_{i=1}^{\infty} \lambda_i (f, \psi_i)_k \psi_i. \quad (25)$$

One can consider Eq. (18) as $T_k f = kf$. Noticing this and Eq. (25) results in:

$$kf = \sum_{i=1}^{\infty} \lambda_i (f, \psi_i)_k \psi_i. \quad (26)$$

Ignoring $f$ from Eq. (26) gives:

$$k(x, y) = \sum_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(y), \quad (27)$$

which is Eq. (21); hence, that is proved.

**Step 4 of proof:** We define the truncated kernel $r_n$ (with parameter $n$) as:

$$r_n(x, y) := k(x, y) \sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(y)$$

$$= \sum_{i=n+1}^{\infty} \lambda_i \psi_i(x) \psi_i(y). \quad (28)$$
As $T_k$ is an integral operator, this truncated kernel has positive kernel, i.e., for every $x \in [a, b]$, we have:
\[
 r_n(x, x) = k(x, x) - \sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(x) \geq 0
\]
\[
 \implies \sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(x) \leq k(x, x) \leq \sup_{x \in [a, b]} k(x, x).
\]
(29)

By Cauchy-Schwartz inequality, we have:
\[
 \left| \sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(y) \right|^2 \leq \left( \sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(x) \right) \left( \sum_{i=1}^{n} \lambda_i \psi_i(y) \psi_i(y) \right)
\]
\[
 \leq \left( \sup_{x \in [a, b]} (k(x, x)) \right)^2.
\]
Taking second root from the sides of inequality gives:
\[
 \sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(x) \leq \sup_{x \in [a, b]} |k(x, x)| \leq \infty.
\]
(30)

This shows that the sequence $\sum_{i=1}^{n} \lambda_i \psi_i(x) \psi_i(x)$ converges absolutely and uniformly. Q.E.D.

The Mercer’s theorem is very important. Many of its equations, such as Eqs. (18), (20), and (21) are used in theory of kernels and kernel methods.

### 3.2. Feature Map and Pulling Function

Let $X := \{x_i\}_{i=1}^{n}$ be the set of data in the input space (note that the input space is the original space of data). The $t$-dimensional (perhaps infinite dimensional) feature space (or Hilbert space) is denoted by $\mathcal{H}$.

**Definition 13** (Feature Map or Pulling Function). We define the mapping:
\[
 \phi : X \rightarrow \mathcal{H},
\]
(31)
to transform data from the input space to the feature space, i.e. Hilbert space. In other words, this mapping pulls data to the feature space:
\[
 x \mapsto \phi(x).
\]
(32)

The function $\phi(x)$ is called the feature map or pulling function. The feature map is a (possibly infinite-dimensional) vector whose elements are (Minh et al., 2006):
\[
 \phi(x) = [\phi_1(x), \phi_2(x), \ldots]^{\top}
\]
\[
 := [\sqrt{\lambda_1} \psi_1(x), \sqrt{\lambda_2} \psi_2(x), \ldots]^{\top},
\]
where $\{\psi_i\}$ and $\{\lambda_i\}$ are eigenfunctions and eigenvalues of the kernel operator (see Eq. (20)). Note that eigenfunctions will be explained more in Section 7.

Let $t$ denote the dimensionality of $\phi(x)$. The feature map may be infinite or finite dimensional, i.e. $t$ can be infinity; it is usually a very large number (recall Definition 7 where we said Hilbert space may have infinite number of dimensions).

Considering both Eqs. (21) and (33) shows that:
\[
 k(x, y) = \left\langle \phi(x), \phi(y) \right\rangle_k = \phi(x)^{\top}\phi(y).
\]
(34)

Hence, the kernel between two points is the inner product of pulled data points to the feature space. Suppose we stack the feature maps of all points $X \in \mathbb{R}^{d \times n}$ column-wise in:
\[
 \Phi(X) := [\phi(x_1), \phi(x_2), \ldots, \phi(x_n)],
\]
(35)
which is $t \times n$ dimensional and $t$ may be infinity or a large number. The kernel matrix defined in Definition 2 can be calculated as:
\[
 \mathbb{R}^{n \times n} \ni K = \langle \Phi(X), \Phi(X) \rangle_k = \Phi(X)^{\top}\Phi(X).
\]
(36)

Eqs. (34) and (36) show that there is no need to compute kernel using eigenfunctions but a simple inner product suffices for kernel computation. This is the beauty of kernel methods which are simple to compute.

**Definition 14** (Input Space and Feature Space (Schölkopf et al., 1999b)). The space in which data $X$ exist is called the input space, also known as the original space. This space is denoted by $\mathcal{X}$ and is usually an $\mathbb{R}^d$ Euclidean space. The RKHS to which the data have been pulled is called the feature space. Data can be pulled from the input to feature space using kernels.

**Remark 4** (Kernel is a Measure of Similarity). Inner product is a measure of similarity in terms of angles of vectors or in terms of location of points with respect to origin. According to Eq. (34), kernel can be seen as inner product between feature maps of points; hence, kernel is a measure of similarity between points and this similarity is computed in the feature space rather than input space.

Pulling data to the feature space is performed using kernels which is the inner product of points in RKHS according to Eq. (34). Hence, the relative similarity (inner product) of pulled data points is known by the kernel. However, in most of kernels, we cannot find an explicit expression for the pulled data points. Therefore, the exact location of pulled data points to RKHS is not necessarily known but the relative similarity of pulled points, which is the kernel, is known. An exceptional kernel is the linear kernel in which we have $\phi(x) = x$. Figure 1 illustrates what we mean by not knowing the explicit location of pulled points to RKHS.
4. Characteristics of Kernels

In this section, we review some of the characteristics of kernels including the symmetry and positive semi-definiteness properties of Mercer kernel (recall Definition 1).

Lemma 1 (Symmetry of Kernel). A square Mercer kernel matrix is symmetric, so we have:

\[ (f, g)_k = (g, f)_k, \quad \text{or} \quad K \in S^n, \quad \text{i.e.,} \quad k(x, y) = k(y, x). \]  (37)

Proof.

\[ k(x, y) = \langle \phi(x), \phi(y) \rangle_k = \phi(x)^\top \phi(y) \]

\[ = \langle \phi(y)^\top \phi(x) \rangle_k = k(y, x), \]

where \( \langle \cdot, \cdot \rangle \) is because \( \phi(x)^\top \phi(y) \) and \( \phi(y)^\top \phi(x) \) are scalars and are equivalent according to the definition of dot product between vectors. Q.E.D.

Lemma 2 (Zero Kernel). We have:

\[ (f, f)_k = 0 \quad \text{iff} \quad f = 0. \]  (39)

Proof.

\[ 0 \leq f^2(x) = \langle f, f \rangle_k \leq \|f\|_k \|k_x\|_k = \|f\|_k \|k_x\|_k^2 \]

\[ = \|f\|_k^2 \|k_x\|_k^2 \quad \text{iff} \quad \|f\|_k = 0, \]

where \( \langle \cdot, \cdot \rangle \) is because Cauchy-Schwarz inequality and \( b \) is because we had assumed \( \langle f, f \rangle_k = \|f\|_k = 0 \). Hence:

\[ 0 \leq f^2(x) = 0 \implies f(x) = 0. \]

\[ \Box \]

Lemma 3 (Positive Semi-definiteness of Kernel). The Mercer kernel matrix is positive semi-definite:

\[ K \in S^n_+, \quad \text{i.e.,} \quad K \succeq 0. \]  (40)

Proof. Let \( v(i) \) denote the \( i \)-th element of vector \( v \).

\[ v^\top K v \]

\[ \overset{(\text{7})}{=} \sum_{i=1}^n \sum_{j=1}^n v(i) v(j) \langle \phi(x(i)), \phi(x(j)) \rangle_k \]

\[ = \sum_{i=1}^n \sum_{j=1}^n \langle v(i) \phi(x(i)), v(j) \phi(x(j)) \rangle_k \]

\[ = \sum_{i=1}^n \langle v(i) \phi(x(i)) \rangle^2_k \geq 0, \quad \forall v \in \mathbb{R}^n. \]

Hence, according to the definition of positive semi-definiteness (Bhatia, 2009), we have \( K \succeq 0 \). Q.E.D. \( \Box \)

5. Well-known Kernel Functions

5.1. Frequently Used Kernels

There exist many different kernel functions which are widely used in machine learning (Rojo-Álvarez et al., 2018). In the following, we list some of the most well-known kernels.

\[- Linear Kernel:\]

Linear kernel is the simplest kernel which is the inner product of points:

\[ k(x, y) := x^\top y. \]  (41)

Comparing this with Eq. (34) shows that in linear kernel we have \( \phi(x) = x \). Hence, in this kernel, the feature map is explicitly known. Note that \( \phi(x) = x \) shows that data are not pulled to any other space in linear kernel but in the input space, the inner products of points are calculated to obtain the feature space. Moreover, recall Remark 9 which states that, depending on the kernelization approach, using lin-
– **Radial Basis Function (RBF) or Gaussian Kernel:**

RBF kernel has a scaled Gaussian (or normal) distribution where the normalization factor of distribution is usually ignored. Hence, it is also called the Gaussian kernel. The RBF kernel is formulated as:

\[ k(x, y) := \exp(-\gamma \|x - y\|_2^2) = \exp\left(-\frac{\|x - y\|_2^2}{\sigma^2}\right), \]

(42)

where \( \gamma := 1/\sigma^2 \) and \( \sigma^2 \) is the variance of kernel. A proper value for this parameter is \( \gamma = 1/d \) where \( d \) is the dimensionality of data. Note that RBF kernel has also been widely used in RBF networks (Orr, 1996) and kernel density estimation (Scott, 1992).

– **Laplacian Kernel:**

The Laplacian kernel, also called the Laplace kernel, is similar to the RBF kernel but with \( \ell_1 \) norm rather than squared \( \ell_2 \) norm. The Laplacian kernel is:

\[ k(x, y) := \exp(-\gamma \|x - y\|_1) = \exp\left(-\frac{\|x - y\|_1}{\sigma^2}\right), \]

(43)

where \( \|x - y\|_1 \) is also called the Manhattan distance. A proper value for this parameter is \( \gamma = 1/d \) where \( d \) is the dimensionality of data. In some specific fields of science, the Laplacian kernel has been found to perform better than Gaussian kernel (Rupp, 2015). This makes sense because of betting on sparsity principal (Hastie et al., 2009) since \( \ell_1 \) norm makes algorithm sparse. Note that the \( \ell_1 \) computation and derivative of \( \ell_1 \) norm is more difficult than \( \ell_2 \) norm.

– **Sigmoid Kernel:**

Sigmoid kernel is a hyperbolic tangent function applied on inner product of points. It is formulated as:

\[ k(x, y) := \tanh(\gamma x^\top y + c), \]

(44)

where \( \gamma > 0 \) is the slope and \( c \) is the intercept. Some proper values for these parameters are \( \gamma = 1/d \) and \( c = 1 \) where \( d \) is the dimensionality of data. Note that the hyperbolic tangent function is also used widely for activation functions in neural networks (Goodfellow et al., 2016).

– **Polynomial Kernel:**

Polynomial kernel applies a polynomial function with degree \( \delta \) (a positive integer) on inner product of points:

\[ k(x, y) := (\gamma x^\top y + c)^\delta, \]

(45)

where \( \gamma > 0 \) is the slope and \( c \) is the intercept. Some proper values for these parameters are \( \gamma = 1/d \) and \( c = 1 \) where \( d \) is the dimensionality of data.

– **Cosine Kernel:**

According to Remark 4, kernel is a measure of similarity and computes the inner product between points in the feature space. Cosine kernel computes the similarity between points. It is obtained from the formula of cosine and inner product:

\[ k(x, y) := \cos(x, y) = \frac{x^\top y}{\|x\|_2 \|y\|_2}. \]

(46)

The normalization in the denominator projects the points onto a unit hyper-sphere so that the inner product measures the similarity of their angles regardless of their lengths. Note that angle-based measures such as cosine are found to work better for face recognition compared to Euclidean distances (Perlbakas, 2004).

– **Chi-squared Kernel:**

Assume \( x(j) \) denotes the \( j \)-th dimension of the \( d \)-dimensional point \( x \). The Chi-squared (\( \chi^2 \)) kernel is (Zhang et al., 2007):

\[ k(x, y) := \exp\left(-\gamma \sum_{j=1}^{d} \frac{(x(j) - y(j))^2}{x(j) + y(j)}\right), \]

(47)

where \( \gamma > 0 \) is a parameter (a proper value is \( \gamma = 1 \)). Note that the summation term inside exponential (without the minus) is the Chi-squared distance which is related to the Chi-squared test in statistics.

### 5.2. Kernel Construction from Distance Metric

Consider \( d_{ij}^2 = \|x_i - x_j\|_2^2 \) as the squared Euclidean distance between \( x_i \) and \( x_j \). We have:

\[
    d_{ij}^2 = \|x_i - x_j\|_2^2 = (x_i - x_j)^\top (x_i - x_j) \\
    = x_i^\top x_i - x_j^\top x_j - x_j^\top x_i + x_j^\top x_j \\
    = x_i^\top x_i - 2x_i^\top x_j + x_j^\top x_j = G_{ii} - 2G_{ij} + G_{jj},
\]

where \( \mathbb{R}^{n \times n} \ni G := X^\top X \) is the linear Gram matrix. If \( \mathbb{R}^n \ni g := [g_1, \ldots, g_n] = [G_{11}, \ldots, G_{nn}] = \text{diag}(G) \), we have:

\[
    d_{ij}^2 = g_i - 2G_{ij} + g_j, \\
    D = g1^\top - 2G + g1^\top = 1g^\top - 2G + g1^\top,
\]

where \( 1 \) is the vector of ones and \( D \) is the distance matrix with squared Euclidean distance (\( d_{ij}^2 \) as its elements). Let \( H \) denote the centering matrix:

\[
    \mathbb{R}^{n \times n} \ni H := I - \frac{1}{n}1_n1_n^\top,
\]

(48)

and \( I \) is the identity matrix, \( 1_n := [1, \ldots, 1]^\top \in \mathbb{R}^n \) and \( 1_{n \times n} := 1_n1_n^\top \in \mathbb{R}^{n \times n} \). Refer to (Ghojogh & Crowley, 2019, Appendix A) for more details about the centering
matrix. We double-center the matrix $D$ as follows (Oldford, 2018):

$$HDH = (I - \frac{1}{n}11^\top)D(I - \frac{1}{n}11^\top)$$

$$= (I - \frac{1}{n}11^\top)(1g^\top - 2G + g1^\top)(I - \frac{1}{n}11^\top)$$

$$= [(I - \frac{1}{n}11^\top)1g^\top - 2(I - \frac{1}{n}11^\top)G$$

$$+ (I - \frac{1}{n}11^\top)g1^\top](I - \frac{1}{n}11^\top)$$

$$= -2(I - \frac{1}{n}11^\top)G(I - \frac{1}{n}11^\top)$$

$$+ (I - \frac{1}{n}11^\top)g1^\top(I - \frac{1}{n}11^\top)$$

$$= -2(I - \frac{1}{n}11^\top)G(I - \frac{1}{n}11^\top) = -2HGH.$$  

$$\therefore HGH = XX^\top XH = -\frac{1}{2}HDH. \quad (49)$$

Note that $(I - \frac{1}{n}11^\top)1 = 0$ and $1^\top(I - \frac{1}{n}11^\top) = 0$ because removing the row mean of 1 and column mean of $1^\top$ results in the zero vectors, respectively.

If data $X$ are already centered, i.e., the mean has been removed ($X ← XH$), Eq. (49) becomes:

$$X^\top X = -\frac{1}{2}HDH. \quad (50)$$

According to the kernel trick, Eq. (104), we can write a general kernel matrix rather than the linear Gram matrix in Eq. (50), to have (Cox & Cox, 2008):

$$\mathbb{R}^{n \times n} \ni K = \Phi(X)^\top \Phi(X) = -\frac{1}{2}HDH. \quad (51)$$

This kernel is double-centered because of $HDH$. It is also noteworthy that Eq. (51) can be used for unifying the spectral dimensionality reduction methods as special cases of kernel principal component analysis with different kernels. See (Ham et al., 2004; Bengio et al., 2004) and (Strange & Zwiggelaar, 2014, Table 2.1) for more details.

**Lemma 4** (Distance-based Kernel is a Mercer Kernel). The kernel constructed from a valid distance metric, i.e. Eq. (51), is a Mercer kernel.

**Proof.** The kernel is symmetric because:

$$K^\top = -\frac{1}{2}H^\top D^\top H^\top (a) \equiv -\frac{1}{2}HDH = K,$$

where $(a)$ is because $H$ and $D$ are symmetric matrices. Moreover, the kernel is positive semi-definite because:

$$K = -\frac{1}{2}HDH = \Phi(X)^\top \Phi(X)$$

$$\Rightarrow v^\top K v = v^\top \Phi(X)^\top \Phi(X) v$$

$$= ||\Phi(X)v||^2_2 \geq 0, \quad \forall v \in \mathbb{R}^n.$$

Hence, according to Definition 1, this kernel is a Mercer kernel. Q.E.D.

**Remark 5** (Kernel Construction from Metric). One can use any valid distance metric, satisfying the following properties:

1. non-negativity: $D(x, y) \geq 0$,
2. equal points: $D(x, y) = 0 \iff x = y$,
3. symmetry: $D(x, y) = D(y, x)$,
4. triangular inequality: $D(x, y) \leq D(x, z) + D(z, y)$.

to calculate elements of distance matrix $D$ in Eq. (50). It is important that the used distance matrix should be a valid distance matrix. Using various distance metrics in Eq. (50) results in various useful kernels.

Some examples are the geodesic kernel and Structural Similarity Index (SSIM) kernel, used in Isomap (Tenenbaum et al., 2000) and image structure subspace learning (Ghojogh et al., 2019c), respectively. The geodesic kernel is defined as (Tenenbaum et al., 2000; Ghojogh et al., 2020b):

$$K = -\frac{1}{2}HD^{(g)}H, \quad (52)$$

where the approximation of geodesic distances using piecewise Euclidean distances is used in calculating the geodesic distance matrix $D^{(g)}$. The SSIM kernel is defined as (Ghojogh et al., 2019c):

$$K = -\frac{1}{2}HD^{(s)}H, \quad (53)$$

where the distance matrix $D^{(a)}$ is calculated using the SSIM distance (Brunet et al., 2011).

### 5.3. Important Classes of Kernels

In the following, we introduce some of the important classes of kernels which are widely used in statistics and machine learning. A good survey on the classes of kernels is (Genton, 2001).

#### 5.3.1. Bounded Kernels

**Definition 15** (Bounded Kernel). A kernel function $k$ is bounded if:

$$\sup_{x, y \in X} k(x, y) < \infty, \quad (54)$$

where $X$ is the input space. Likewise, the kernel matrix $K$ is bounded if $\sup_{x, y \in X} K(x, y) < \infty$. 


5.3.2. Integrally Positive Definite Kernels

**Definition 16** (Integrally Positive Definite Kernel). A kernel matrix $K$ is integrally positive definite ($\int$ p.d.) on $\Omega \times \Omega$ if:

$$\int_\Omega \int_\Omega K(x, y) f(x) f(y) \geq 0, \forall f \in L^2(\Omega).$$ (55)

A kernel matrix $K$ is integrally strictly positive definite ($\int$ s.p.d.) on $\Omega \times \Omega$ if:

$$\int_\Omega \int_\Omega K(x, y) f(x) f(y) > 0, \forall f \in L^2(\Omega).$$ (56)

5.3.3. Universal Kernels

**Definition 17** (Universal Kernel (Steinwart, 2001, Definition 4), (Steinwart, 2002, Definition 2)). Let $C(X)$ denote the space of all continuous functions on space $X$. A continuous kernel $k$ on a compact metric space $X$ is called universal if the RKHS $H$, with kernel function $k$, is dense in $C(X)$. In other words, for every function $g \in C(X)$ and all $\epsilon > 0$, there exists a function $f \in H$ such that $\|f - g\|_{\infty} \leq \epsilon$.

**Remark 6.** We can approximate any function, including continuous functions and functions which can be approximated by continuous functions, using a universal kernel.

**Lemma 5** ((Steinwart, 2001, Corollary 10)). Consider a function $f : (-r, r) \rightarrow \mathbb{R}$ where $0 < r \leq \infty$ and $f \in C^\infty$ ($C^\infty$ denotes the differentiable space for all degrees of differentiation). Let $\mathcal{X} := \{x \in \mathbb{R}^d | \|x\|_2 < \sqrt{r}\}$. If the function $f$ can be expanded by Taylor expansion in $0$ as:

$$f(x) = \sum_{j=0}^{\infty} a_j x^j, \quad \forall x \in (-r,r),$$ (57)

and $a_j > 0$ for all $j \geq 0$, then $k(x,y) = f(|x - y|)$ is a universal kernel on every compact subset of $\mathcal{X}$.

**Proof.** For proof, see (Steinwart, 2001, proof of Corollary 10). Note that the Stone-Weierstrass theorem (De Branges, 1959) is used for the proof of this lemma.

An example for universal kernel is RBF kernel (Steinwart, 2001, Example 1) because its Taylor series expansion is:

$$\exp(-\gamma r) \approx 1 - \gamma r + \frac{\gamma^2}{2} r^2 - \frac{\gamma^3}{6} r^3 + \ldots,$$

where $r := \|x - y\|_2$. Considering Eq. (34) and noticing that this Taylor series expansion has infinite number of terms, we see that the RKHS for RBF kernel is infinite dimensional because $\phi(x)$, although cannot be calculated explicitly for this kernel, will have infinite dimensions. Another example for universal kernel is the SSIM kernel (Ghojogh et al., 2020d), denoted by $K_s$, whose Taylor series expansion is (Ghojogh et al., 2019c):

$$K_s \approx -\frac{5}{16} - \frac{15}{16} r + \frac{5}{16} r^2 - \frac{1}{16} r^3 + \ldots,$$

where $r$ is the squared SSIM distance (Brunet et al., 2011) between images. Note that polynomial kernels are not universal. Universal kernels have been widely used for kernel SVM. More detailed discussion and proofs for use of universal kernels in kernel SVM can be found in (Steinwart & Christmann, 2008).

**Lemma 6** ((Borgwardt et al., 2006), (Song, 2008, Theorem 10)). A kernel is universal if for arbitrary sets of distinct points, it induces strictly positive definite kernel matrices (Borgwardt et al., 2006; Song, 2008). Conversely, if a kernel matrix can be written as $K = K' + \epsilon I$ where $K' \succeq 0$, $\epsilon > 0$, and $I$ is the identity matrix, the kernel function corresponding to $K$ is universal (Pan et al., 2008).

5.3.4. Stationary Kernels

**Definition 18** (Stationary Kernel (Genton, 2001; Noack & Sethian, 2021)). A kernel $k$ is stationary if it is a positive definite function of the form:

$$k(x, y) = k(||x - y||),$$ (58)

where $\|\cdot\|$ is some norm defined on the input space.

An example for stationary kernel is the RBF kernel defined in Eq. (42) which has the form of Eq. (58). Stationary kernels are used for Gaussian processes (Noack & Sethian, 2021).

5.3.5. Characteristic Kernels

The characteristic kernels, which are widely used for distribution embedding in the Hilbert space, will be defined and explained in Section 9.4. Examples for characteristic kernels are RBF and Laplacian kernels. Polynomial kernels, however, are not characteristic. Note that the relation between universal kernels, characteristic kernels, and integrally strictly positive definite kernels has been studied in (Striperumbudur et al., 2011).

6. Kernel Centering and Normalization

6.1. Kernel Centering

In some cases, there is a need to center the pulled data in the feature space. For this, the kernel matrix should be centered in a way that the mean of pulled dataset becomes zero. Note that this will restrict the place of pulled points in the feature space further (see Fig. 2); however, because of different possible rotations of pulled points around origin, the exact positions of pulled points are still unknown.

For kernel centering, one should follow the following theory, which is based on (Schölkopf et al., 1997a) and
The kernel matrix becomes:

\[ K = C + \frac{1}{n} 1_{n \times n} K + \frac{1}{n} K 1_{n \times n} + \frac{1}{n^2} 1_{n \times n} K 1_{n \times n}, \]  

where \( H \) is the centering matrix (see Eq. (48)). The Eq. (61) is called the double-centered kernel. This equation is the kernel matrix when the pulled training data in the feature space are centered. Also, double-centered kernel has zero row-wise and column-wise mean (so its row and column summations are zero). Therefore, after this kernel centering, we will have:

\[
\frac{1}{n} \sum_{i=1}^{n} \tilde{\phi}(x_i) = 0, \\
\sum_{i=1}^{n} \sum_{j=1}^{n} \tilde{K}(i, j) = 0.
\]  

6.1.2. Centering the Kernel Between Training and Out-of-Sample Data

Now, consider the kernel matrix between the training data and the out-of-sample data \( \mathbb{R}^{n \times n_t} \ni K_t := \Phi(X)^\top \Phi(X_t) \), whose \((i, j)\)-th element is \( \mathbb{R} \ni K_t(i, j) = \phi(x_i)^\top \phi(x_{t,j}) \). We want to center the pulled training data in the feature space, i.e., Eq. (59). Moreover, the out-of-sample data should be centered using the mean of training (and not out-of-sample) data:

\[
\tilde{\phi}(x_{i,t}) := \phi(x_{i,t}) - \frac{1}{n} \sum_{k=1}^{n} \phi(x_k).
\]  

If we center the pulled training and out-of-sample data, the \((i, j)\)-th element of kernel matrix becomes:

\[
\tilde{K}_t(i, j) := \phi(x_i)^\top \phi(x_{t,j})
\]

\[
\tilde{x}_i := \phi(x_i) - \frac{1}{n} \sum_{k=1}^{n} \phi(x_k).
\]  

Figure 2. Centered pulled data the feature space (RKHS). This happens after kernel centering where the mean of cloud of pulled data becomes zero in RKHS. Even by kernel centering, the explicit locations of pulled points are not necessarily known because of not knowing the rotation of pulled data in that space.

(Schölkopf et al., 1998, Appendix A). An example of use of kernel centering in machine learning is kernel principal component analysis (see (Ghojogh & Crowley, 2019) for more details).
where:

\[ \mathbb{R}^n \ni k_i = k_i(X, x_i) := \Phi(X)^\top \phi(x_i) \] (67)

\[ = \langle \phi(x_1), \ldots, \phi(x_n) \rangle \top, \]

\[ \mathbb{R}^n \ni \tilde{k}_i = \tilde{k}_i(X, x_i) := \tilde{\Phi}(X)^\top \tilde{\phi}(x_i), \] (68)

\[ = \langle \tilde{\phi}(x_1), \ldots, \tilde{\phi}(x_n) \rangle \top, \]

where \( \tilde{\Phi}(X) \) and \( \tilde{\phi}(x_i) \) are according to Eqs. (59) and (64), respectively.

Note that Eq. (61) or (65) can be restated as the following lemma.

**Lemma 7** (Kernel Centering (Bengio et al., 2003b)). The pulled data to the feature space can be centered by kernel centering. The kernel matrix \( K(x, y) \) is centered as:

\[ \tilde{K}(x, y) = \langle \phi(x) - \mathbb{E}_x[\phi(x)], \phi(y) - \mathbb{E}_y[\phi(y)] \rangle \]

\[ = K(x, y) - \mathbb{E}_x[K(x, y)] - \mathbb{E}_y[K(x, y)] + \mathbb{E}_x[\mathbb{E}_y[K(x, y)]] \]. (69)

**Proof.** The explained derivations for Eqs. (59) and (64) and definition of expectation complete the proof. \( \square \)

Note that in Eq. (69), \( \mathbb{E}_x[K(x, y)], \mathbb{E}_y[K(x, y)], \) and \( \mathbb{E}_x[\mathbb{E}_y[K(x, y)]] \) are average of rows, average of columns, and total average of rows and columns of the kernel matrix, respectively.

### 6.2. Kernel Normalization

According to Eq. (34), kernel value can be large if the pulled vectors to the feature map have large length. Hence, in practical computations and optimization, it is sometimes required to normalize the kernel matrix.

**Lemma 8** (Cosine Normalization of Kernel (Rennie, 2005; Ah-Pine, 2010)). The kernel matrix \( K \in \mathbb{R}^{n \times n} \) can be normalized as:

\[ K(i, j) \leftarrow \frac{K(i, j)}{\sqrt{K(i, i)K(j, j)}}, \quad \forall i, j \in \{1, \ldots, n\}. \] (70)

**Proof.** Cosine normalizes points onto a unit hyper-sphere and then computes the similarity of points using inner product. Cosine is computed by Eq. (46) and according to the relation of norm and inner product, it is:

\[ \cos(x_i, x_j) = \frac{x_i^\top x_j}{\|x_i\|_2 \|x_j\|_2} = \frac{x_i^\top x_j}{\sqrt{\|x_i\|^2 \|x_j\|^2}} = \frac{\|x_i\|_2 \|x_j\|_2}{\sqrt{\|x_i\|^2 \|x_j\|^2}}. \]

According to Remark 4, kernel is also a measure of similarity. Using kernel trick, Eq. (103) (which is already normalized) is kernelized as:

\[ K(i, j) = \frac{\phi(x_i)^\top \phi(x_j)}{\sqrt{\langle \phi(x_i), x_i \rangle \langle \phi(x_j), x_j \rangle}} \]

\[ \overset{(103)}{=} \frac{K(i, j)}{\sqrt{K(i, i)K(j, j)}}. \]

Q.E.D.

**Definition 19** (generalized mean with exponent \( t \) (Ah-Pine, 2010)). The generalized mean with exponent \( t \) as:

\[ m_t(a_1, \ldots, a_n) := \left( \frac{1}{p} \sum_{i=1}^{p} a_i^t \right)^{1/t}. \] (71)

The generalized mean becomes the harmonic, geometric, and arithmetic mean for \( t = -1, t \to 0, \) and \( t = 1, \) respectively.

**Definition 20** (Generalized Kernel Normalization of order \( t \) (Ah-Pine, 2010)). The generalized kernel normalization of order \( t > 0 \) normalizes the kernel \( K \in \mathbb{R}^{n \times n} \) as:

\[ K(i, j) \leftarrow \frac{K(i, j)}{m_t(K(i, i), K(j, j))}, \quad \forall i, j \in \{1, \ldots, n\}. \] (72)

Both cosine normalization and generalized normalization make the kernel of every point with itself one. In other words, after normalization, we have:

\[ k(x, x) = 1, \quad \forall x \in X. \] (73)

As the most similar point to a point is itself, the values of a normalized kernel will be less than or equal to one. In other words, after normalization, we have:

\[ k(x_i, x_j) \leq 1, \quad \forall i, j \in \{1, \ldots, n\}. \] (74)

This helps the values not explode to large values in algorithms, especially in the iterative algorithms (e.g., algorithms which use gradient descent for optimization).

### 7. Eigenfunctions

#### 7.1. Inner Product in Hilbert Space

**Lemma 9** (Inner Product in Hilbert Space). If the domain of functions in a Hilbert space \( \mathcal{H} \) is \([a, b] \), the inner product of two functions in the Hilbert space is calculated as:

\[ \langle f(x), g(x) \rangle_{\mathcal{H}} = \int_a^b f(x) g(x) dx \overset{(37)}{=} \int_a^b f^*(x) g(x) dx, \] (75)

where \( g^* \) is the complex conjugate of function \( g \). If functions are real, the inner product is simplified to \( \int_a^b f(x) g(x) dx \).


Proof. If we discretize the domain $[a, b]$, for example by sampling, with step $\Delta x$, the function values become vectors as $f(x) = [f(x_1), f(x_2), \ldots, f(x_n)]^\top$ and $g(x) = [g(x_1), g(x_2), \ldots, g(x_n)]^\top$. According to the inner product of two vectors, we have:

$$
(f(x), g(x)) = g^H f = \sum_{i=1}^{n} f(x_i)g(x_i),
$$

where $g^H$ denotes the conjugate transpose of $g$ (it is transpose if functions are real). Multiplying the sides of this equation by the setp $\Delta x$ gives:

$$
(f(x), g(x)) \Delta x = g^H f = \sum_{i=1}^{n} f(x_i)g(x_i)\Delta x,
$$

which is a Riemann sum. This is the Riemann approximation of the Eq. (75). This approximation gets more accurate by $\Delta x \to 0$ or $n \to \infty$. Hence, that equation is a valid inner product in the Hilbert space. Q.E.D.

Remark 7 (Interpretation of Inner Product of Functions in Hilbert Space). The inner product of two functions, i.e. Eq. (75), measures how similar two functions are. The more similar they are in their domain $[a, b]$, the larger inner product they have. Note that this similarity is more about the pattern (or changes) of functions and not the exact value of functions. If the pattern of functions is very similar, they will have a large inner product.

Corollary 2 (Weighted Inner Product in Hilbert Space (Williams & Seeger, 2000), (Bengio et al., 2003c, Section 2)). The Eq. (75) is the inner product with uniform weighting. With density function $p(x)$, one can weight the inner product in the Hilbert space as (assuming the functions are real):

$$
(f(x), g(x))_H = \int_a^b f(x)g(x)p(x)\,dx. \quad (76)
$$

7.2. Eigenfunctions

Recall eigenvalue problem for a matrix $A$ (Ghojogh et al., 2019a):

$$
A\phi_i = \lambda_i\phi_i, \quad \forall i \in \{1, \ldots, d\}, \quad (77)
$$

where $\phi_i$ and $\lambda_i$ are the $i$-th eigenvector and eigenvalue of $A$, respectively. In the following, we introduce the Eigenfunction problem which has a similar form but for an operator rather than a matrix.

Definition 21 (Eigenfunction (Kusse & Westwig, 2006, Chapter 11.2)). Consider a linear operator $O$ which can be applied on a function $f$. If applying this operator on the function results in a multiplication of function to a constant:

$$
O f = \lambda f, \quad (78)
$$

then the function $f$ is an eigenfunction for the operator $O$ and the constant $\lambda$ is the corresponding eigenvalue. Note that the form of eigenfunction problem is:

$$
O f = \lambda f. \quad (79)
$$

Some examples of operator are derivative, kernel function, etc. For example, $e^{\lambda x}$ is an eigenfunction of derivative because $\frac{d}{dx}e^{\lambda x} = \lambda e^{\lambda x}$. Note that eigenfunctions have application in many fields of science including machine learning (Bengio et al., 2003c) and quantum mechanics (Reed & Simon, 1972).

Recall that in eigenvalue problem, the eigenvectors show the most important or informative directions of matrix and the corresponding eigenvalue shows the amount of importance (Ghojogh et al., 2019a). Likewise, in eigenfunction problem of an operator, the eigenfunction is the most important function of the operator and the corresponding eigenvalue shows the amount of this importance. This connection between eigenfunction and eigenvalue problems is proved in the following theorem.

Theorem 3 (Connection of Eigenfunction and Eigenvalue Problems). If we assume that the operator and the function are a matrix and a vector, eigenfunction problem is converted to an eigenvalue problem where the vector is the eigenvector of the matrix.

Proof. Consider any function space such as a Hilbert space. Let $\{e_j\}_{j=1}^n$ be the bases (basis functions) of this function space where $n$ may be infinite. The function $f$ in this space can be represented as a linear combination bases:

$$
f(x) = \sum_{j=1}^{n} \alpha_j e_j(x). \quad (80)
$$

An example of this linear combination is Eq. (6) in RKHS where the bases are kernels. Consider the operator $O$ which can be applied on the functions in this function space. Applying this operator on Eq. (80) gives:

$$
O f(x) = \sum_{j=1}^{n} \alpha_j e_j(x) = O \sum_{j=1}^{n} \alpha_j O e_j(x), \quad (81)
$$

where $(a)$ is because the operator $O$ is a linear operator according to Definition 21. Also, we have:

$$
O f(x) \overset{(78)}{=} \lambda f(x) \overset{(a)}{=} \sum_{j=1}^{n} \lambda \alpha_j e_j(x), \quad (82)
$$

where $(a)$ is because $\lambda$ is a scalar.

On the other hand, the output function from applying the operator on a function can also be written as a linear combination of the bases:

$$
O f(x) = \sum_{j=1}^{n} \beta_j e_j(x). \quad (83)
$$
From Eqs. (81) and (83), we have:

\[ \sum_{j=1}^{n} \alpha_j Oe_j(x) = \sum_{j=1}^{n} \beta_j e_j(x). \quad (84) \]

In parentheses, consider an \( n \times n \) matrix \( A \) whose \( (i, j) \)-th element is the inner product of \( e_i \) and \( Oe_j \):

\[ A(i, j) := \langle e_i, Oe_j \rangle_k \overset{(75)}{=} \int e_i^*(x) Oe_j(x)dx, \quad (85) \]

where integral is over the domain of functions in the function space.

Using Eq. (75), we take the inner product of sides of Eq. (84) with an arbitrary basis function \( e_i \):

\[ \sum_{j=1}^{n} \alpha_j \int e_i^*(x) Oe_j(x)dx = \sum_{j=1}^{n} \beta_j \int e_i^*(x) e_j(x)dx. \]

According to Eq. (85), this equation is simplified to:

\[ \sum_{j=1}^{n} \alpha_j A(i, j) = \sum_{j=1}^{n} \beta_j \int e_i^*(x) e_j(x)dx \overset{(a)}{=} \beta_i, \quad (86) \]

which is true for \( \forall i \in \{1, \ldots, n\} \) and \((a)\) is because the bases are orthonormal, so:

\[ \langle e_i, e_j \rangle_k \overset{(75)}{=} \int e_i^*(x) e_j(x)dx = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{Otherwise}. \end{cases} \]

The Eq. (86) can be written in matrix form:

\[ A\alpha = \beta, \quad (87) \]

where \( \alpha := [\alpha_1, \ldots, \alpha_n]^T \) and \( \beta := [\beta_1, \ldots, \beta_n]^T \).

From Eqs. (82) and (83), we have:

\[ \sum_{j=1}^{n} \lambda \alpha_j e_j(x) = \sum_{j=1}^{n} \beta_j e_j(x) \implies \lambda \alpha = \beta. \quad (88) \]

Comparing Eqs. (87) and (88) shows:

\[ A\alpha = \lambda \alpha, \]

which is an eigenvalue problem for matrix \( A \) with eigenvector \( \alpha \) and eigenvalue \( \lambda \) (Ghojogh et al., 2019a). Note that, according to Eq. (80), the information of function \( f \) is in the coefficients \( \alpha_j \)'s of the basis functions of space. Therefore, the function is converted to the eigenvector (vector of coefficients) and the operator \( O \) is converted to the matrix \( A \). Q.E.D.

### 7.3. Use of Eigenfunctions for Spectral Embedding

Consider a Hilbert space \( \mathcal{H} \) of functions with the inner product defined by Eq. (76). Let the data in the input space be \( \mathcal{X} = \{ x_i \in \mathbb{R}^d \}_{i=1}^{n} \). In this space, we can consider an operator for the kernel function \( K_p \) as (Williams & Seeger, 2000), (Bengio et al., 2003a, Section 3):

\[ (K_p f)(x) := \int k(x, y) f(y) dy, \quad (89) \]

where \( f \in \mathcal{H} \) and the density function \( p(y) \) can be approximated empirically. A discrete approximation of this operator is (Williams & Seeger, 2000):

\[ (K_{p,n} f)(x) := \frac{1}{n} \sum_{i=1}^{n} k(x, x_i) f(x_i), \quad (90) \]

which converges to Eq. (89) if \( n \to \infty \). Note that this equation is also mentioned in (Bengio et al., 2003c, Section 2), (Bengio et al., 2004, Section 4), (Bengio et al., 2006, Section 3.2).

**Lemma 10** (Relation of Eigenvalues of Eigenvalue Problem and Eigenfunction Problem for Kernel (Bengio et al., 2003a, Proposition 1), (Bengio et al., 2003c, Theorem 1), (Bengio et al., 2004, Section 4)). Assume \( \lambda_k \) denotes the \( k \)-th eigenvalue for eigenvalue decomposition of the operator \( K_p \) and \( \delta_k \) denotes the \( k \)-th eigenvalue for eigenvalue problem of the matrix \( K \in \mathbb{R}^{n \times n} \). We have:

\[ \delta_k = n \lambda_k. \quad (91) \]

**Proof.** This proof gets help from (Bengio et al., 2003b, proof of Proposition 3). According to Eq. (78), the eigenfunction problems for the operators \( K_p \) and \( K_{p,n} \) (discrete version) are:

\[ (K_p f_k)(x) = \lambda_k f_k(x), \quad \forall k \in \{1, \ldots, n\}, \]
\[ (K_{p,n} f_k)(x) = \lambda_k f_k(x), \quad \forall k \in \{1, \ldots, n\}, \quad (92) \]

where \( f_k(\cdot) \) is the \( k \)-th eigenfunction and \( \lambda_k \) is the corresponding eigenvalue. Consider the kernel matrix defined by Definition 2. The eigenvalue problem for the kernel matrix is (Ghojogh et al., 2019a):

\[ Kv_k = \delta_k v_k, \quad \forall k \in \{1, \ldots, n\}, \quad (93) \]

where \( v_k \) is the \( k \)-th eigenvector and \( \delta_k \) is the corresponding eigenvalue. According to Eqs. (90) and (92), we have:

\[ \frac{1}{n} \sum_{i=1}^{n} k(x, x_i) f(x_i) = \lambda_k f_k(x), \quad \forall k \in \{1, \ldots, n\}. \]

When this equation is evaluated only at \( x_i \in \mathcal{X} \), we have (Bengio et al., 2004, Section 4), (Bengio et al., 2006, Section 3.2):

\[ \frac{1}{n} K f_k = \lambda_k f_k, \quad \forall k \in \{1, \ldots, n\}, \]
\[ \implies K f_k = n \lambda_k f_k. \]
According to Theorem 3, eigenfunction can be seen as an eigenvector. If so, we can say:

\[ K f_k = n \lambda_k f_k \implies K v_k = n \lambda_k v_k, \quad (94) \]

Comparing Eqs. (93) and (94) results in Eq. (91). Q.E.D.

**Lemma 11** (Relation of Eigenvalues of Kernel and Covariance in the Feature Space (Schölkopf et al., 1998)). Consider the covariance of pulled data to the feature space:

\[ C_H := \frac{1}{n} \sum_{i=1}^{n} \phi(x_i) \phi(x_i)^\top, \quad (95) \]

where \( \phi(x_i) \) is the centered pulled data defined by Eq. (64). which is \( t \times d \) dimensional where \( t \) may be infinite. Assume \( \eta_k \) denotes the \( k \)-th eigenvalue \( C_H \) and \( \delta_k \) denotes the \( k \)-th eigenvalue of centered kernel \( K \). We have:

\[ \delta_k = n \eta_k, \quad (96) \]

**Proof.** This proof is based on (Schölkopf et al., 1998, Section 2). The eigenvalue problem for this covariance matrix is:

\[ \eta_k u_k = C_H u_k, \quad \forall k \in \{1, \ldots, n\}, \]

where \( u_k \) is the \( k \)-th eigenvector and \( \eta_k \) is its corresponding eigenvalue (Ghojogh et al., 2019a). Left multiplying this equation with \( \phi(x_j)^\top \) gives:

\[ \eta_k \phi(x_j)^\top u_k = \phi(x_j)^\top C_H u_k, \quad \forall k \in \{1, \ldots, n\}. \quad (97) \]

As \( u_k \) is the eigenvector of the covariance matrix in the feature space, it lies in the feature space; hence, according to Lemma 13 which will come later, we can represent it as:

\[ u_k = \frac{1}{\sqrt{\delta_k}} \sum_{\ell=1}^{n} v_\ell \tilde{\phi}(x_\ell), \quad (98) \]

where pulled data to feature space are assumed to be centered, \( v_\ell \)'s are the coefficients in representation, and the normalization by \( 1/\sqrt{\delta_k} \) is because of a normalization used in (Bengio et al., 2003c, Section 4). Substituting Eq. (98) and Eq. (95) in Eq. (97) results in:

\[ \eta_k \tilde{\phi}(x_j)^\top \sum_{\ell=1}^{n} v_\ell \tilde{\phi}(x_\ell) = \tilde{\phi}(x_j)^\top \frac{1}{n} \sum_{i=1}^{n} \phi(x_i) \phi(x_i)^\top \sum_{\ell=1}^{n} v_\ell \tilde{\phi}(x_\ell), \]

where normalization factors are simplified from sides. In the right-hand side, as the summations are finite, we are allowed to re-arrange them. Re-arranging the terms in this equation gives:

\[ \eta_k \sum_{\ell=1}^{n} v_\ell \tilde{\phi}(x_j)^\top \tilde{\phi}(x_\ell) = \frac{1}{n} \sum_{\ell=1}^{n} v_\ell \left( \tilde{\phi}(x_j)^\top \sum_{i=1}^{n} \phi(x_i) \right) \left( \tilde{\phi}(x_\ell)^\top \tilde{\phi}(x_\ell) \right). \]

Considering Eqs. (36) and (60), we can write this equation in matrix form \( \eta_k \tilde{K} v_k = \frac{1}{n} \tilde{K}^2 v_k \) where \( v_k := [v_1, \ldots, v_n]^\top \). As \( \tilde{K} \) is positive semi-definite (see Lemma 3), it is often non-singular. For non-zero eigenvalues, we can left multiply this equation to \( \tilde{K}^{-1} \) to have:

\[ n \eta_k v_k = \tilde{K} v_k, \]

which is the eigenvalue problem for \( \tilde{K} \) where \( v \) is the eigenvector and \( \delta_k = n \eta_k \) is the eigenvalue (cf. Eq. (93)). Q.E.D.

**Lemma 12** (Relation of Eigenfunctions and Eigenvectors for Kernel (Bengio et al., 2003a, Proposition 1), (Bengio et al., 2003c, Theorem 1)). Consider a training dataset \( \{x_i \in \mathbb{R}^d\}_{i=1}^{n} \) and the eigenvalue problem (93) where \( v_k \in \mathbb{R}^n \) and \( \delta_k \) are the \( k \)-th eigenvector and eigenvalue of matrix \( K \in \mathbb{R}^{n \times n} \). If \( v_{ki} \) is the \( i \)-th element of vector \( v_k \), the eigenfunction for the point \( x \) and the \( i \)-th training point \( x_i \) are:

\[ f_k(x) = \sqrt{n} \sum_{i=1}^{n} v_{ki} \hat{k}(x_i, x), \quad (99) \]

\[ f_k(x_i) = \sqrt{n} v_{ki}, \quad (100) \]

respectively, where \( \hat{k}(x_i, x) \) is the centered kernel. If \( x \) is a training point, \( \hat{k}(x_i, x) \) is the centered kernel over training data and if \( x \) is an out-of-sample point, then \( \hat{k}(x_i, x) = \hat{k}_t(x_i, x) \) is between training set and the out-of-sample point (n.b. kernel centering is explained in Section 6.1).

**Proof.** For proof of Eq. (99), see (Bengio et al., 2003c, proof of Theorem 1) or (Williams & Seeger, 2001, Section 1.1). The Eq. (100) is claimed in (Bengio et al., 2003c, Proposition 1). For proof of this equation, see (Bengio et al., 2003c, proof of Theorem 1, Eq. 7).

It is noteworthy that Eq. (99) is similar and related to the Nyström approximation of eigenfunctions of kernel operator which will be explained in Lemma 16.

**Theorem 4** (Embedding from Eigenfunctions of Kernel Operator (Bengio et al., 2003a, Proposition 1), (Bengio et al., 2003c, Section 4)). Consider a dimensionality reduction algorithm which embeds data into a low-dimensional
embedding space. Let the embedding of the point \( x \) be
\[\mathbb{R}^p \ni y(x) = [y_1(x), \ldots, y_p(x)]^\top \text{ where } p \leq n. \]
The \( k \)-th dimension of this embedding is:
\[y_k(x) = \sqrt{\delta_k} \frac{f_k(x)}{\sqrt{n}} = \frac{1}{\sqrt{\delta_k}} \sum_{i=1}^{n} v_{ki} \tilde{k}(x_i, x), \quad (101)\]
where \( \tilde{k}(x_i, x) \) is the centered training or out-of-sample kernel depending on whether \( x \) is a training or an out-of-sample point (n.b. kernel centering will be explained in Section 6.1).

**Proof.** We can embed data point \( x \) by pulling it to the feature space and centering the pulled dataset to have \( \tilde{\phi}(x) \) and then projecting it onto the eigenvector of covariance matrix in the feature space (Schölkopf et al., 1998, Section 2), (Bengio et al., 2003c, Section 4):
\[
y_k(x) = u_k^\top \tilde{\phi}(x) = \left( \frac{1}{\sqrt{\delta_k}} \sum_{i=1}^{n} v_i \phi(x_i)^\top \phi(x) \right)_{v_k} = \frac{1}{\sqrt{\delta_k}} \sum_{i=1}^{n} v_{ki} \tilde{k}(x_i, x).
\]
Q.E.D.

The Theorem 4 has been widely used for out-of-sample (test data) embedding in many spectral dimensionality reduction algorithms (Bengio et al., 2003a).

**Corollary 3** (Embedding from Eigenvectors of Kernel Matrix). Consider the eigenvalue problem for the kernel matrix, i.e. Eq. (93), where \( \psi_k = [v_{k1}, \ldots, v_{kn}]^\top \) and \( \delta_k \) are the \( k \)-th eigenvector and eigenvalue of kernel, respectively. According to Eqs. (100) and (101), we can compute the embedding of point \( x \), denoted by \( y(x) = [y_1(x), \ldots, y_p(x)]^\top \) (where \( p \leq n \)) using the eigenvector of kernel as:
\[y_k(x) = \sqrt{\delta_k} \frac{1}{\sqrt{n}} v_{ki} = \sqrt{\delta_k} v_{ki}. \quad (102)\]
The Eq. (102) is used in several dimensionality reduction methods such as maximum variance unfolding (or semidefinite embedding) (Weinberger et al., 2005; Weinberger & Saul, 2006b,a). We will introduce this method in Section 9.2.

8. Kernelization Techniques
Linear algorithms cannot properly handle nonlinear patterns of data obviously. When dealing with nonlinear data, if the algorithm is linear, two solutions exist to have acceptable performance:
1. Either the linear method should be modified to become nonlinear or a completely new nonlinear algo-

![Figure 3](image_url)

Figure 3. Transforming data to RKHS using kernels to make the nonlinear pattern of data more linear. For example, here the classes have become linearly separable (by a linear hyperplane) after kernelization.

2. Or the nonlinear data should be modified in a way to become more linear in pattern. In other words, a transformation should be applied on data so that the pattern of data becomes roughly linear or easier to process by the linear algorithm. Some examples of this category are nonlinear dimensionality methods such as locally linear embedding (Ghojogh et al., 2020a) and Isomap (Ghojogh et al., 2020b).

The second approach is called kernelization in machine learning which we define in the following. Figure 3 shows how kernelization for transforming data can help separate classes for better classification.

**Definition 22** (Kernelization). In machine learning and data science, kernelization means a slight change in algorithm formulation (without any modification in the idea of algorithm) so that the pulled data to the RKHS, rather than the raw data, are used as input of algorithm.

Note that kernelization can be useful for enabling linear algorithms to handle nonlinear data better. Nevertheless, it should be noted that nonlinear algorithms can also be kernelized to be able to handle nonlinear data perhaps better by transforming data.

Generally, there exist two main approaches for kernelization in machine learning. These two approaches are related in theory but have two ways for kernelization. In the following, we explain these methods which are kernel trick and kernelization using representation theory.
8.1. Kernelization by Kernel Trick

Recall Eqs. (34) and (36) where kernel can be computed by inner product between pulled data instances to the RKHS. One technique to kernelize an algorithm is kernel trick. In this technique, we first try to formulate the algorithm formulas or optimization in a way that data always appear as inner product of data instances and not a data instance alone. In other words, the formulation of algorithm should only have \( x^\top x \), \( x^\top X \), \( X^\top x \), or \( X^\top X \) and not a lonely \( x \) or \( X \). In this way, kernel trick replaces \( x^\top x \) with \( \phi(x)^\top \phi(x) \) and uses Eq. (34) or (36). To better explain, kernel trick applies the following mapping (Burges, 1998):

\[
x^\top x \mapsto \phi(x)^\top \phi(x) \quad \text{(34)}
\]

Therefore, the inner products of points are all replaced with the kernel between points. The matrix form of kernel trick is:

\[
X^\top X \mapsto \Phi(X)^\top \Phi(X) = K(X, X) \in \mathbb{R}^{n \times n}. \quad \text{(36)}
\]

Most often, kernel matrix is computed over one dataset; hence, its dimensionality is \( n \times n \). However, in some cases, the kernel matrix is computed between two sets of data instances with sample sizes \( n_1 \) and \( n_2 \) for example, i.e., datasets \( X_1 := [x_{1,1}, \ldots, x_{1,n_1}] \) and \( X_2 := [x_{2,1}, \ldots, x_{2,n_2}] \). In this case, the kernel matrix has size \( n_1 \times n_2 \) and the kernel trick is:

\[
x_{1,i,j}^\top \mapsto \phi(x_{1,i})^\top \phi(x_{1,j}) = k(x_{1,i}, x_{1,j}), \quad \text{(105)}
\]

\[
X_1^\top X_2 \mapsto \Phi(X_1)^\top \Phi(X_2) = K(X_1, X_2) \in \mathbb{R}^{n_1 \times n_2}. \quad \text{(36)}
\]

An example for kernel between two sets of data is the kernel between training data and out-of-sample (test) data. As stated in (Schölkopf, 2001), the kernel trick is proved to work for Mercer kernels in (Boser et al., 1992; Vapnik, 1995) or equivalently for the positive definite kernels (Berg et al., 1984; Wahba, 1990).

Some examples of using kernel trick in machine learning are kernel PCA (Schölkopf et al., 1997a; 1998; Ghojogh & Crowley, 2019) and kernel SVM (Boser et al., 1992; Vapnik, 1995). More examples will be provided in Section 9.

Note that in some algorithms, data do not not appear only by inner product which is required for the kernel trick. In these cases, if possible, a “dual” method for the algorithm is proposed which only uses the inner product of data. Then, the dual algorithm is kernelized using kernel trick. Some examples for this are kernelization of dual PCA (Ghojogh & Crowley, 2019) and dual SVM (Burges, 1998). As an additional point, it is noteworthy that it is possible to replace kernel trick with function replacement (see (Ma, 2003) for more details on this).

8.2. Kernelization by Representation Theory

As was explained in Section 8.1, if the formulation of algorithm has data only as inner products of points, kernel trick can be used. In some cases, a dual version of algorithm is used to have only inner products. Some algorithms, however, cannot be formulated in a way to have data only in inner product form, nor does their dual have this form. An example is Fisher Discriminant Analysis (FDA) (Ghojogh et al., 2019b) which uses another technique for kernelization (Mika et al., 1999). In the following, we explain this technique.

Lemma 13 (Representation of Function Using Bases (Mika et al., 1999)). Consider a RKHS denoted by \( \mathcal{H} \). Any function \( f \in \mathcal{H} \) lies in the span of all points in the RKHS, i.e.,

\[
f = \sum_{i=1}^{n} \alpha_i \phi(x_i). \quad \text{(107)}
\]

**Proof.** Consider Eq. (6) which can be restated as:

\[
f(y) = \sum_{i=1}^{n} \alpha_i k(x_i, y) \quad \text{(34)}
\]

\[
\implies f(\cdot) = \sum_{i=1}^{n} \alpha_i \phi(x_i). \quad \text{Q.E.D.}
\]

**Remark 8** (Justification by Representation Theory). According to representation theory (Alperin, 1993), any function in the space can be represented as a linear combination of bases of the space. This makes sense because the function is in the space and the space is spanned by the bases. Now, assume the space is RKHS. Hence, any function should lie in the RKHS spanned by the pulled data points to the feature space. This justifies Lemma 13 using representation theory.

8.2.1. Kernelization for Vector Solution

Now, consider an algorithm whose optimization variable or solution is the vector/direction \( u \in \mathbb{R}^d \) in the input space. For kernelization, we pull this solution to RKHS by Eq. (32) to have \( \phi(u) \). According to Lemma 13, this pulled solution must lie in the span of all pulled training points \( \{\phi(x_i)\}_{i=1}^{n} \) as:

\[
\phi(u) = \sum_{i=1}^{n} \alpha_i \phi(x_i) = \Phi(X) \alpha, \quad \text{(108)}
\]

which is \( t \) dimensional and \( t \) may be infinite. Note that \( \Phi(X) \) is defined by Eq. (35) and is \( t \times n \) dimensional. The vector \( \alpha := [\alpha_1, \ldots, \alpha_n]^\top \in \mathbb{R}^n \) contains the coefficients. According to Eq. (32), we can replace \( u \) with \( \phi(u) \) in the algorithm. If, by this replacement, the terms \( \phi(x_i)^\top \phi(x_i) \)
The steps of kernelization by representation theory are summarized below:

- Step 1: \( u \rightarrow \phi(u) \)
- Step 2: Replace \( \phi(u) \) with Eq. (108) in the algorithm formulation
- Step 3: Some \( \phi(x_i)^\top \phi(x_i) \) or \( \Phi(X)^\top \Phi(X) \) terms appear in the formulation
- Step 4: Use Eq. (34) or (36)
- Step 5: Solve (optimize) the algorithm where the variable to find is \( \alpha \) rather than \( u \)

Usually, the goal of algorithm results in kernel. For example, if \( u \) is a projection direction, the desired projected data are obtained as:

\[
u^\top x_i \overset{(32)}{\mapsto} \phi(u)^\top \phi(x_i) = \alpha^\top k(x_i, x_i), \tag{109}\]

where \( k(X, x_i) \in \mathbb{R}^n \) is the kernel between all \( n \) training points with the point \( x_i \). As this equation shows, the desired goal is based on kernel.

### 8.2.2. Kernelization for Matrix Solution

Usually, the algorithm has multiple directions/vectors as its solution. In other words, its solution is a matrix \( U = [u_1, \ldots, u_p] \in \mathbb{R}^{d \times p} \). In this case, Eq. (108) is used for all \( p \) vectors and in a matrix form, we have:

\[
\Phi(U) = \Phi(X) A, \tag{110}
\]

where \( \mathbb{R}^{n \times p} \ni A := [\alpha_1, \ldots, \alpha_p]^\top \) and \( \Phi(U) \) is \( t \times p \)-dimensional where \( t \) may be infinite. Similarly, the following steps should be performed to kernelize the algorithm:

- Step 1: \( U \rightarrow \phi(U) \)
- Step 2: Replace \( \phi(U) \) with Eq. (110) in the algorithm formulation
- Step 3: Some \( \Phi(X)^\top \Phi(X) \) terms appear in the formulation
- Step 4: Use Eq. (36)
- Step 5: Solve (optimize) the algorithm where the variable to find is \( A \) rather than \( U \)

Again the goal of algorithm usually results in kernel. For example, if \( U \) is a projection matrix onto its column space, we have:

\[
U^\top x_i \overset{(32)}{\mapsto} \phi(U)^\top \phi(x_i) = A^\top k(X, x_i), \tag{111}\]

where \( k(X, x_i) \in \mathbb{R}^n \) is the kernel between all \( n \) training points with the point \( x_i \). As this equation shows, the desired goal is based on kernel.

As was mentioned, in many machine learning algorithms, the solution \( U \in \mathbb{R}^{d \times p} \) is a projection matrix for projecting \( d \)-dimensional data onto a \( p \)-dimensional subspace. Some example methods which have used kernelization by representation theory are kernel Fisher discriminant analysis (FDA) (Mika et al., 1999; Ghojogh et al., 2019), kernel supervised principal component analysis (PCA) (Barshan et al., 2011; Ghojogh & Crowley, 2019), and direct kernel Roweis discriminant analysis (RDA) (Ghojogh et al., 2020c).

**Remark 9** (Linear Kernel in Kernelization). If we use kernel trick, the kernelized algorithm with a linear kernel is equivalent to the non-kernelized algorithm. This is because in linear kernel, we have \( \phi(x) = x \) and \( k(x, y) = x^\top y \) according to Eq. (41). So, the kernel trick, which is Eq. (105), maps data as \( x^\top y \rightarrow \phi(x)^\top \phi(y) = x^\top y \) for linear kernel. Therefore, linear kernel does not have any effect when using kernel trick. Examples for this are kernel PCA (Schölkopf et al., 1997a; 1998; Ghojogh & Crowley, 2019) and kernel SVM (Boser et al., 1992; Vapnik, 1995) which are equivalent to PCA and SVM, respectively, if linear kernel is used.

However, kernel trick does have impact when using kernelization by representation theory because it finds the inner products of pulled data points after pulling the solution and representation as a span of bases. Hence, kernelized algorithm using representation theory with linear kernel is not equivalent to non-kernelized algorithm. Examples of this are kernel FDA (Mika et al., 1999; Ghojogh et al., 2019) and kernel supervised PCA (Barshan et al., 2011; Ghojogh & Crowley, 2019) which are different from FDA and supervised PCA, respectively, even if linear kernel is used.

### 9. Types of Use of Kernels in Machine Learning

There are several types of using kernels in machine learning. In the following, we explain these types of usage of kernels.

#### 9.1. Kernel Methods

The first type of using kernels in machine learning is kernelization of algorithms using either kernel trick or representation theory. As was discussed in Section 8, linear methods can be kernelized to handle nonlinear data better. Even nonlinear algorithms can be kernelized to perform in the feature space rather than the input space. In machine learning both kernel trick and kernelization by representation theory have been used. We provide some examples for each of these categories:

- Examples for kernelization by kernel trick: kernel Principal Component Analysis (PCA) (Schölkopf et al., 1997a; 1998; Ghojogh & Crowley, 2019), kernel Support Vector Machine (SVM) (Boser et al., 1992;
discussions on kernel SVM can be found in (Schölkopf, 1995). More noticed when linear SVM (Vapnik & Chervonenkis, 1974) was kernelized in (Boser et al., 1992; Vapnik, 1995). More discussions on kernel SVM can be found in (Schölkopf et al., 1997b; Hastie et al., 2009). A tutorial on kernel SVM is (Burges, 1998). Universal kernels, introduced in Section 8.1, many machine learning methods in machine learning, it was found out that kernel learning by SDP has also been used for labeling a not completely labeled dataset and is also used for kernel SVM (Lanckriet et al., 2004; Karimi, 2017). Our focus here is on MVU. In the following, we briefly introduce the MVU (or SDE) algorithm.

**Lemma 14** (Distance in RKHS (Schölkopf, 2001)). The squared Euclidean distance between points in the feature space is:

\[
\|\phi(x_i) - \phi(x_j)\|^2 = k(x_i, x_i) + k(x_j, x_j) - 2k(x_i, x_j).
\]

**Proof.**

\[
\|\phi(x_i) - \phi(x_j)\|^2 = (\phi(x_i) - \phi(x_j))^\top (\phi(x_i) - \phi(x_j)) = \phi(x_i)^\top \phi(x_i) + \phi(x_j)^\top \phi(x_j) - \phi(x_i)^\top \phi(x_j) - \phi(x_j)^\top \phi(x_i) = k(x_i, x_i) + k(x_j, x_j) - 2k(x_i, x_j).
\]

Q.E.D.

MVU desires to unfolds the manifold of data in its maximum variance direction. For example, consider a Swiss roll which can be unrolled to have maximum variance after being unrolled. As trace of matrix is the summation of eigenvalues and kernel matrix is a measure of similarity between points (see Remark 4), the trace of kernel can be used to show the summation of variance of data. Hence, we should maximize \(\text{tr}(K)\) where \(\text{tr}(\cdot)\) denotes the trace of matrix. MVU pulls data to the RKHS and then unfolds the manifold. This unfolding should not ruin the local distances between points after pulling data to the feature space. Hence, we should preserve the local distances as:

\[
\|x_i - x_j\|^2 = \|\phi(x_i) - \phi(x_j)\|^2 = k(x_i, x_i) + k(x_j, x_j) - 2k(x_i, x_j).
\]

Moreover, according to Lemma 3, the kernel should be positive semidefinite, i.e. \(K \succeq 0\). MVU also centers kernel to have zero mean for the pulled dataset in the feature space (see Section 6.1). According to Eq. (63), we will have

\[
\sum_{i=1}^{n} \sum_{j=1}^{n} K(i, j) = 0.
\]

In summary, the optimization of MVU is (Weinberger et al., 2005; Weinberger & Saul, 2006b;a):

\[
\begin{align*}
\text{maximize} & \quad \text{tr}(K) \\
\text{subject to} & \quad \|x_i - x_j\|^2 = K(i, i) + K(j, j) - 2K(i, j), \\
& \quad \forall i, j \in \{1, \ldots, n\}, \\
& \quad \sum_{i=1}^{n} \sum_{j=1}^{n} K(i, j) = 0, \\
& \quad K \succeq 0.
\end{align*}
\]
which is a SDP problem (Vandenberghe & Boyd, 1996). Solving this optimization gives the best kernel for maximum variance unfolding of manifold. Then, MVU considers the eigenvalue problem for kernel, i.e. Eq. (102), and finds the embedding using Eq. (102).

9.3. Use of Kernels for Difference of Distributions

There exist several different measures for difference of distributions (i.e., PDFs). Some of them make use of kernels and some do not. A measure of difference of distributions. One of the measures without kernels and then introduce the this measure better in Corollary 5.

For the information of reader, we first enumerate some of the measures without kernels and then introduce the kernel-based measures for difference of distributions. One of methods which do not use kernels is the Kullback-Leibler (KL) divergence (Kullback & Leibler, 1951). KL-divergence, which is a relative entropy from one distribution to the other one and has been widely used in deep divergence, which is a relative entropy from one distribution to another reference distribution using optimization. We will explain the second use of this measure better in Corollary 5.

In the following, we introduce some well-known measures for difference of distributions, using kernels.

9.3.1. Hilbert-Schmidt Independence Criterion (HSIC)

Suppose we want to measure the dependence of two random variables. Measuring the correlation between them is easier because correlation is just “linear” dependence.

According to (Hein & Bousquet, 2004), two random variables X and Y are independent if and only if any bounded continuous functions of them are uncorrelated. Therefore, if we map the samples of two random variables \{x_i\}_{i=1}^n and \{y_i\}_{i=1}^n to two different (“separable”) RKHSs and have \(\phi(x)\) and \(\phi(y)\), we can measure the correlation of \(\phi(x)\) and \(\phi(y)\) in Hilbert space to have an estimation of dependence of \(x\) and \(y\) in the input space.

The correlation of \(\phi(x)\) and \(\phi(y)\) can be computed by the Hilbert-Schmidt norm of the cross-covariance of them (Gretton et al., 2005). Note that the squared Hilbert-Schmidt norm of a matrix \(A\) is (Bell, 2016):

\[
||A||_{HS}^2 := \text{tr}(A^\top A),
\]

and the cross-covariance matrix of two vectors \(x\) and \(y\) is (Gubner, 2006; Gretton et al., 2005):

\[
\text{Cov}(x, y) := \mathbb{E}\left[ (x - \mathbb{E}(x))(y - \mathbb{E}(y)) \right].
\]

Using the explained intuition, an empirical estimation of the Hilbert-Schmidt Independence Criterion (HSIC) is introduced (Gretton et al., 2005):

\[
\text{HSIC}(X, Y) := \frac{1}{(n - 1)^2} \text{tr}(K_x H K_y H),
\]

where \(K_x := \phi(x)^\top \phi(x)\) and \(K_y := \phi(y)^\top \phi(y)\) are the kernels over \(x\) and \(y\), respectively. The term \(1/(n - 1)^2\) is used for normalization. The matrix \(H\) is the centering matrix (see Eq. (48)). Note that HSIC double-centers one of the kernels and then computes the Hilbert-Schmidt norm between kernels.

HSIC measures the dependence of two random variable vectors \(x\) and \(y\). Note that HSIC = 0 and HSIC > 0 mean that \(x\) and \(y\) are independent and dependent, respectively. The greater the HSIC, the greater dependence they have.

**Lemma 15** (Independence of Random Variables Using Cross-Covariance (Gretton & Györfi, 2010, Theorem 5)). Two random variables \(X\) and \(Y\) are independent if and only if \(\text{Cov}(f(x), f(y)) = 0\) for any pair of bounded continuous functions \((f, g)\). Because of relation of HSIC with the cross-covariance of variables, two random variables are independent if and only if \(\text{HSIC}(X, Y) = 0\).

9.3.2. Maximum Mean Discrepancy (MMD)

MMD, also known as the kernel two sample test and proposed in (Gretton et al., 2006; 2012), is a measure for difference of distributions. For comparison of two distributions, one can find the difference of all moments of the two distributions. However, as the number of moments is infinite, it is intractable to calculate the difference of all moments. One idea to do this tractably is to pull both distributions to the feature space and then compute the distance of all pulled data points from distributions in RKHS. This difference is a suitable estimate for the difference of all moments in the input space. This is the idea behind MMD.

MMD is a semi-metric (Simon-Gabriel et al., 2020) and uses distance in the RKHS (Schölkopf, 2001) (see Lemma 14). Consider PDFs \(P\) and \(Q\) and samples \(\{x_i\}_{i=1}^n \sim P\) and \(\{y_i\}_{i=1}^n \sim Q\). The squared MMD between these PDFs is:

\[
\text{MMD}^2(P, Q) := \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \phi(x_i) - \frac{1}{n^2} \sum_{i=1}^n \phi(y_i) \right\|_k^2
\]

\[
= \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(x_i, x_j) + \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(y_i, y_j)
\]

\[
- \frac{2}{n^2} \sum_{i=1}^n \sum_{j=1}^n k(x_i, y_j)
\]

\[
= \mathbb{E}_x[K(x, y)] + \mathbb{E}_y[K(x, y)] - 2\mathbb{E}_x[\mathbb{E}_y[K(x, y)]],
\]

where \(\mathbb{E}_x[K(x, y)]\), \(\mathbb{E}_y[K(x, y)]\), and \(\mathbb{E}_x[\mathbb{E}_y[K(x, y)]]\) are average of rows, average of columns, and total aver-
age of rows and columns of the kernel matrix, respectively. Note that MMD $\geq 0$ where MMD $= 0$ means the two distributions are equivalent if the used kernel is characteristic (see Corollary 5 which will be provided later). MMD has been widely used in machine learning such as generative moment matching networks (Li et al., 2015).

**Remark 10** (Equivalence of HSIC and MMD (Sejdinovic et al., 2013)). After development of HSIC and MMD measures, it was found out that they are equivalent.

### 9.4. Kernel Embedding of Distributions (Kernel Mean Embedding)

**Definition 23** (Kernel Embedding of Distributions (Smola et al., 2007)). Kernel embedding of distributions, also called the Kernel Mean Embedding (KME) or mean map, represents (or embeds) Probability Density Functions (PDFs) in a RKHS.

**Corollary 4** (Distribution Embedding in Hilbert Space). Inspired by Eq. (6) or (11), if we map a PDF $\mathcal{P}$ from its space $\mathcal{X}$ to the Hilbert space $\mathcal{H}$, its mapped PDF, denoted by $\phi(\mathcal{P})$, can be represented as:

$$
\mathcal{P} \mapsto \phi(\mathcal{P}) = \int_{\mathcal{X}} k(x, \cdot) \, d\mathcal{P}(x). \tag{119}
$$

This integral is called the Bochner integral.

KME and MMD were first proposed in the field of pure mathematics (Guilbart, 1978). Later on, KME and MMD were used in machine learning, first in (Smola et al., 2007). KME is a family on methods which use Eq. (119) for embedding PDFs in RKHS. This family of methods is more discussed in (Sriperumbudur et al., 2010). A survey on KME is (Muandet et al., 2016).

Universal kernels, introduced in Section 5.3.3, can be used for KME (Sriperumbudur et al., 2011; Simon-Gabriel & Schölkopf, 2018). In addition to universal kernels, characteristic kernels and integrally strictly positive definite are useful for KME (Sriperumbudur et al., 2011; Simon-Gabriel & Schölkopf, 2018). The integrally strictly positive definite kernel was introduced in Section 5.3.2. In the following, we introduce the characteristic kernels.

**Definition 24** (Characteristic Kernel (Fukumizu et al., 2008)). A kernel is characteristic if the mapping (119) is injective. In other words, for a characteristic kernel $k$, we have:

$$
E_{X \sim \mathcal{P}}[k(\cdot, X)] = E_{Y \sim \mathcal{Q}}[k(\cdot, Y)] \iff \mathcal{P} = \mathcal{Q}, \tag{120}
$$

where $\mathcal{P}$ and $\mathcal{Q}$ are two PDFs and $X$ and $Y$ are random variables from these distributions, respectively.

Some examples for characteristic kernels are RBF and Laplacian kernels. Polynomial kernels are not characteristic kernels.

**Corollary 5** (Convergence of Distributions to Each Other Using Characteristic Kernels (Simon-Gabriel et al., 2020)). Let $\mathcal{Q}$ be the PDF for a theoretical or sample reference distribution. Following Definition 24, if the kernel used in measures for difference of distributions is characteristic, the measure can be used in an optimization framework to converge a PDF $\mathcal{P}$ to the reference distribution $\mathcal{Q}$ as:

$$
d_k(\mathcal{P}, \mathcal{Q}) = 0 \iff \mathcal{P} = \mathcal{Q}. \tag{121}
$$

where $d_k(\cdot, \cdot)$ denotes a measure for difference of distributions such as MMD.

Characteristic kernels have been used for dimensionality reduction in machine learning. For example, see (Fukumizu et al., 2004; 2009).

So far, we have introduced three different types of embedding in RKHS. In the following, we summarize these three types available in the literature of kernels.

**Remark 11** (Types of Embedding in Hilbert Space). There are three types of embeddings in Hilbert space:

1. **Embedding of points in the Hilbert space**: This embedding maps $x \mapsto k(x, \cdot)$ as stated in Sections 2.3 and 8.
2. **Embedding of functions in the Hilbert space**: This embedding maps $f(x) \mapsto \int K(x, y) f(y) \, dy$ as stated in Section 7.
3. **Embedding of distributions (PDF's) in the Hilbert space**: This embedding maps $\mathcal{P} \mapsto \int k(x, \cdot) \, d\mathcal{P}(x)$ as stated in Section 9.4.

Researchers are expecting that a combination of these types of embedding might appear in the future.

### 9.5. Kernel Dimensionality Reduction for Sufficient Dimensionality Reduction

Kernels can also be used directly for dimensionality reduction. Assume $X$ is the random variable of data and $Y$ is the random variables of labels of data. The labels can be discrete finite for classification or continuous for regression. Sufficient Dimensionality Reduction (SDR) (Adragni & Cook, 2009) is a family of methods which find a transformation of data to a lower dimensional space, denoted by $R(x)$, which does not change the conditional of labels given data:

$$
\mathcal{P}_{Y \mid X}(y \mid x) = \mathcal{P}_{Y \mid R(X)}(y \mid R(x)). \tag{122}
$$

Kernel Dimensionality Reduction (KDR) (Fukumizu et al., 2004; 2009; Wang et al., 2010b) is a SDR method with linear projection for transformation, i.e. $R(x) : x \mapsto U^\top x$ which projects data onto the column space of $U$. The goal of KDR is:

$$
\mathcal{P}_{Y \mid X}(y \mid x) = \mathcal{P}_{Y \mid U, X}(y \mid U, x). \tag{123}
$$
Definition 25 (Dual Space). A dual space of a vector space $\mathcal{V}$, denoted by $\mathcal{V}^*$, is the set of all linear functionals $\phi: \mathcal{V} \to \mathbb{F}$ where $\mathbb{F}$ is the field on which vector space is defined.

Theorem 5 (Riesz (or Riesz–Fréchet) representation theorem (Garling, 1973)). Let $\mathcal{H}$ be a Hilbert space with norm $\langle \cdot,\cdot \rangle_{\mathcal{H}}$. Suppose $\phi \in \mathcal{H}^*$ (e.g., $\phi: f \to \mathbb{R}$). Then, there exists a unique $f \in \mathcal{H}$ such that for any $x \in \mathcal{H}$, we have $\phi(x) = \langle f, g \rangle_{\mathcal{H}}$:

$$\forall f \in \mathcal{H} : \phi \in \mathcal{H}^*, \forall x \in \mathcal{H}, \quad \phi(x) = \langle f, x \rangle_{\mathcal{H}}. \quad (124)$$

Corollary 6. According to Theorem 5, we have:

$$\mathbb{E}_X[f(x)] = \langle f, \phi(P) \rangle_{\mathcal{H}}, \quad \forall f \in \mathcal{H}, \quad (125)$$

where $\phi(P)$ is defined by Eq. (119).

KDR uses Theorem 5 and Corollary 6 in its formulations. Note that characteristic kernels (Fukumizu et al., 2008), introduced in Definition 24, are used in KDR.

10. Rank and Factorization of Kernel and the Nyström Method

10.1. Rank and Factorization of Kernel Matrix

Usually, the rank of kernel is small. This is because the manifold hypothesis which states that data points often do not cover the whole space but lie on a sub-manifold. Nyström approximation of the kernel matrix also works well because kernels are often low-rank matrices (we will discuss it in Corollary 7). Because of low rank of kernels, they can be approximated (Kishore Kumar & Schneider, 2017), learned (Kulis et al., 2006; 2009), and factorized. Kernel factorization has also be used for the sake of clustering (Wang et al., 2010a). In the following, we introduce some of the most well-known decompositions for the kernel matrix.

10.1.1. SINGULAR VALUE AND EIGENVALUE DECOMPOSITIONS

The Singular Value Decomposition (SVD) of the pulled data to the feature space is:

$$\mathbb{R}^{t \times n} \ni \Phi(X) = U \Sigma V^\top, \quad (126)$$

where $U \in \mathbb{R}^{t \times n}$ and $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices and contain the left and right singular vectors, respectively, and $\Sigma \in \mathbb{R}^{n \times n}$ is a diagonal matrix with singular values. Note that here, we are using notations such as $\mathbb{R}^{t \times n}$ for showing the dimensionality of matrices and this notation does not imply a Euclidean space.

As mentioned before, the pulled data are not necessarily available so Eq. (126) cannot necessarily be done. The kernel, however, is available. Using the SVD of pulled data in the formulation of kernel gives:

$$K^{(36)} = \Phi(X)\top \Phi(X)^{(126)} = (U \Sigma V^\top)^\top (U \Sigma V^\top)$$

$$= V \Sigma U^\top U \Sigma V = \Sigma^2 V^\top = \Sigma^2 V = K V = \Sigma^2. \quad (127)$$

If we take $\Delta = \text{diag}(\delta_1, \ldots, \delta_n)^\top : = \Sigma^2$, this equation becomes:

$$KV = V \Delta, \quad (128)$$

which is the matrix of Eq. (93), i.e. the eigenvalue problem (Ghojogh et al., 2019a) for the kernel matrix with $V$ and $\Delta$ as eigenvectors and eigenvalues, respectively. Hence, for SVD on the pulled dataset, one can apply Eigenvalue Decomposition (EVD) on the kernel where the eigenvectors of kernel are equal to right singular vectors of pulled dataset and the eigenvalues of kernel are the squared singular values of pulled dataset. This technique has been used in kernel PCA (Ghojogh & Crowley, 2019).

10.1.2. CHOLESKY AND QR DECOMPOSITIONS

The kernel matrix can be factorized using LU decomposition; however, as the kernel matrix is symmetric positive semi-definite matrix (see Lemmas 1 and 3), it can be decomposed using Cholesky decomposition which is much faster than LU decomposition. The Cholesky decomposition of kernel is in the form $\mathbb{R}^{n \times n} \ni K = LL^\top$ where $L \in \mathbb{R}^{n \times n}$ is a lower-triangular matrix. The kernel matrix can also be factorized using QR decomposition as $\mathbb{R}^{n \times n} \ni K = QR$ where $Q \in \mathbb{R}^{n \times n}$ is an orthogonal matrix and $R \in \mathbb{R}^{n \times n}$ is an upper-triangular matrix. The paper (Bach & Jordan, 2005) has incorporated side information, such as class labels, in the Cholesky and QR decompositions of kernel matrix.

10.2. Nyström Method for Approximation of Eigenfunctions

Nyström method, first proposed in (Nyström, 1930), was initially used for approximating the eigenfunctions of an operator (or of a matrix corresponding to an operator). The following lemma provides the Nyström approximation for the eigenfunctions of the kernel operator defined by Eq. (89). For more discussion on this, reader can refer to (Baker, 1978), (Williams & Seeger, 2001, Section 1.1), and (Williams & Seeger, 2000).

Lemma 16 (Nyström Approximation of Eigenfunction (Baker, 1978, Chapter 3), (Williams & Seeger, 2001, Section 1.1)). Consider a training dataset $\{x_i \in \mathbb{R}^d\}_{i=1}^n$ and the eigenfunction problem (78) where $f_k \in \mathcal{H}$ and $\lambda_k$ are the $k$-th eigenfunction and eigenvalue of kernel operator defined by Eq. (89) or (90). The eigenfunction can be ap-
proximated by Nyström method as:

\[ f_k(x) \approx \frac{1}{n\lambda_k} \sum_{i=1}^{n} k(x_i, x) f_k(x_i), \]  

(129)

where \( k(x_i, x) \) is the kernel (or centered kernel) corresponding to the kernel operator.

**Proof.** This Lemma is somewhat similar and related to Lemma 12. Consider the kernel operator, defined by Eq. (89), in Eq. (78): \( Kf = \lambda f \). Combining this with the discrete version of operator, Eq. (90), gives \( \lambda_k f_k(x) = \frac{1}{n} \sum_{i=1}^{n} k(x_i, x) f_k(x_i) \). Dividing the sides of this equation by \( \lambda_k \) brings Eq. (129). Q.E.D.

10.3. Nyström Method for Kernel Completion and Approximation

As explained before, the kernel matrix has a low rank often. Because of its low rank, it can be approximated (Kishore Kumar & Schneider, 2017). This is important because in big data when \( n \gg 1 \), constructing the kernel matrix is both time-consuming and also intractable to store in computer; i.e., its computation will run forever and will raise a memory error finally. Hence, it is desired to compute the kernel function between a subset of data points (called landmarks) and then approximate the rest of kernel matrix using this subset of kernel matrix. Nyström approximation can be used for this goal.

The Nyström method can be used for kernel approximation. It is a technique used to approximate a positive semi-definite matrix using merely a subset of its columns (or rows) (Williams & Seeger, 2001, Section 1.2), (Drineas et al., 2005). Hence, it can be used for kernel completion in big data where computation of the entire kernel matrix is time consuming and intractable. One can compute some of the important important columns or rows of a kernel matrix, called landmarks, and approximate the rest of columns or rows by Nyström approximation.

Consider a positive semi-definite matrix \( \mathbb{R}^{n \times n} \ni K \succeq 0 \) whose parts are:

\[ \mathbb{R}^{n \times n} \ni K = \begin{bmatrix} A & B \\ B^{\top} & C \end{bmatrix}, \]  

(130)

where \( A \in \mathbb{R}^{m \times m} \), \( B \in \mathbb{R}^{m \times (n-m)} \), and \( C \in \mathbb{R}^{(n-m) \times (n-m)} \) in which \( m \ll n \). This positive semi-definite matrix can be a kernel (or Gram) matrix.

The Nyström approximation says if we have the small parts of this matrix, i.e. \( A \) and \( B \), we can approximate \( C \) and thus the whole matrix \( K \). The intuition is as follows. Assume \( m = 2 \) (containing two points, a and b) and \( n = 5 \) (containing three other points, c, d, and e). If we know the similarity (or distance) of points a and b from one another, resulting in matrix \( A \), as well as the similarity (or distance) of points c, d, and e from a and b, resulting in matrix \( B \), we cannot have much freedom on the location of c, d, and e, which is the matrix \( C \). This is because of the positive semi-definiteness of the matrix \( K \). The points selected in submatrix \( A \) are named landmarks. Note that the landmarks can be selected randomly from the columns/rows of matrix \( K \) and, without loss of generality, they can be put together to form a submatrix at the top-left corner of matrix. For Nyström approximation, some methods have been proposed for sampling more important columns/rows of matrix more wisely rather than randomly. We will mention some of these sampling methods in Section 10.5.

As the matrix \( K \) is positive semi-definite, by definition, it can be written as \( K = O^\top O \). If we take \( O = [R, S] \) where \( R \) are the selected columns (landmarks) of \( O \) and \( S \) are the other columns of \( O \). We have:

\[ K = O^\top O = \begin{bmatrix} R^\top \\ S^\top \end{bmatrix} \begin{bmatrix} R & S \end{bmatrix} \]  

(131)

\[ \Rightarrow R^\top R = U \Sigma U^\top \Rightarrow R = \Sigma^{(1/2)} U^\top. \]  

(132)

Hence, we have \( A = R^\top R \). The eigenvalue decomposition (Ghojogh et al., 2019a) of \( A \) gives:

\[ A = U \Sigma U^\top \]  

(133)

\[ \Rightarrow R^\top R = U \Sigma U^\top \]  

(134)

Moreover, we have \( B = R^\top S \) so we have:

\[ B = (\Sigma^{(1/2)} U^\top) S = U \Sigma^{(1/2)} S \]  

\[ \Rightarrow U^\top B = \Sigma^{(1/2)} S \Rightarrow S = \Sigma^{(-1/2)} U^\top B, \]  

(135)

where (a) is because \( U \) is orthogonal (in the eigenvalue decomposition). Finally, we have:

\[ C = S^\top S = B^\top U \Sigma^{(-1/2)} \Sigma^{(-1/2)} U^\top B \]  

\[ = B^\top U \Sigma^{-1} U^\top B \]  

(136)

Therefore, Eq. (130) becomes:

\[ K \approx \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix} \]  

(137)

**Lemma 17** (Impact of Size of sub-matrix \( A \) on Nyström approximation). By increasing \( m \), the approximation of Eq. (137) becomes more accurate. If rank of \( K \) is at most \( m \), this approximation is exact.

**Proof.** In Eq. (136), we have the inverse of \( A \). In order to have this inverse, the matrix \( A \) must not be singular. For having a full-rank \( A \in \mathbb{R}^{m \times m} \), the rank of \( A \) should be \( m \). This results in \( m \) to be an upper bound on the rank of \( K \)
and a lower bound on the number of landmarks. In practice, it is recommended to use more number of landmarks for more accurate approximation but there is a trade-off with the speed.

**Corollary 7.** As we usually have \( m \ll n \), the Nyström approximation works well especially for the low-rank matrices (Kishore Kumar & Schneider, 2017) because we will need a small \( A \) (so small number of landmarks) for approximation. Usually, because of the manifold hypothesis, data fall on a submanifold; hence, usually, the kernel (similarity) matrix or the distance matrix has a low rank. Therefore, the Nyström approximation works well for many kernel-based or distance-based manifold learning methods.

### 10.4. Use of Nyström Approximation for Landmark Spectral Embedding

The spectral dimensionality reduction methods (Saul et al., 2006) are based on geometry of data and their solutions often follow an eigenvalue problem (Ghojogh et al., 2019a). Therefore, they cannot handle big data where \( n \gg 1 \). To tackle this issue, there exist some landmark methods which approximate the embedding of all points using the embedding of some landmarks. Big data, i.e. \( n \gg 1 \), results in large kernel matrices. Selecting some most informative columns or rows of the kernel matrix, called landmarks, can reduce computations. This technique is named the Nyström approximation which is used for kernel approximation and completion.

Nyström approximation, introduced below, can be used to make the spectral methods such as locally linear embedding (Ghojogh et al., 2020a) and Multidimensional Scaling (MDS) (Ghojogh et al., 2020b) scalable and suitable for big data embedding. It is shown in (Platt, 2005) that all the landmark MDS methods are Nyström approximations. For more details on usage of Nyström approximation in spectral embedding, refer to (Ghojogh et al., 2020a,b).

### 10.5. Other Improvements over Nyström Approximation of Kernels

The Nyström method has been improved for kernel approximation in a line of research. For example, it has been used for clustering (Fowlkes et al., 2004) and regularization (Rudi et al., 2015). Greedy Nyström (Farahat et al., 2011; 2015) and large scale Nyström (Li et al., 2010) are other examples. There is a trade-off between the approximation accuracy and computational efficiency and they are balanced in (Lim et al., 2015; 2018). The error analysis of Nyström method can be found in (Zhang et al., 2008; Zhang & Kwok, 2010). It is better to sample the landmarks wisely rather than randomly. This field of research is named “column subset selection” or “landmark selection” for Nyström approximation. Some of these methods are (Kumar et al., 2009; 2012) and landmark selection on a sparse manifold (Silva et al., 2006).

### 11. Conclusion

This paper was a tutorial and survey paper on kernels and kernel methods. We covered various topics including Mercer kernels, Mercer’s theorem, RKHS, eigenfunctions, Nyström methods, kernelization techniques, and use of kernels in machine learning. This paper can be useful for different fields of science such as machine learning, functional analysis, and quantum mechanics.

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