Compressed Empirical Measures
(in finite dimensions)

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Abstract
We study approaches for compressing the empirical measure in the context of finite dimensional reproducing kernel Hilbert spaces (RKHSs). In this context, the empirical measure is contained within a natural convex set and can be approximated using convex optimization methods. Such an approximation gives under certain conditions rise to a coreset of data points. A key quantity that controls how large such a coreset has to be is the size of the largest ball around the empirical measure that is contained within the empirical convex set. The bulk of our work is concerned with deriving high probability lower bounds on the size of such a ball under various conditions. We complement this derivation of the lower bound by developing techniques that allow us to apply the compression approach to concrete inference problems such as kernel ridge regression. We conclude with a construction of an infinite dimensional RKHS for which the compression is poor, highlighting some of the difficulties one faces when trying to move to infinite dimensional RKHSs.

1 Overview
Many methods in machine learning and statistics make use of the empirical measure which is effectively a representation of the data. Reducing the number of points on which the empirical measure is supported, while preserving most of the information that is necessary for inference, can result in a significant speed-up of algorithms without sacrificing accuracy. We study the question of how to compress the empirical measure while preserving information in the context of finite dimensional reproducing kernel Hilbert spaces (RKHSs). To give an overview of our results it is useful to introduce the key objects of our investigation. We are generally concerned with data taking values in some set $\mathcal{X}$. Often we will assume this set to be compact. We then look at a kernel function $k$ defined on $\mathcal{X}$ and the corresponding RKHS $\mathcal{H}$. For various results it is useful to assume that the functions in $\mathcal{H}$ are
continuous or even Lipschitz-continuous. Our main interest lies in the unknown distribution $P$ of data $X_1, \ldots, X_n$ where we assume throughout that $X_1, \ldots, X_n$ are independent and identically distributed. We adopt a common convention from the empirical process theory literature and will denote by $Pf$ the integral $\int f(x) \, dP(x)$ whenever $f \in \mathcal{L}^1(\mathcal{X}, P)$. Since $P$ is unknown it is common to use the empirical measure $P_n$ as a surrogate, where $P_n f = (1/n) \sum_{i=1}^n f(X_i)$. There is a very useful interplay between these measure $P$ and $P_n$ and RKHSs. Whenever $k(X_1, \cdot)$ is Bochner-integrable with respect to $P$ we can define $m = \int k(x, \cdot) \, dP(x) \in \mathcal{H}$ and it follows that

$$\langle m, h \rangle = Ph, \quad \text{for all } h \in \mathcal{H}.$$  

Similarly, by defining $m_n = (1/n) \sum_{i=1}^n k(X_i, \cdot)$ we have that $\langle m_n, h \rangle = P_n h$ for all $h \in \mathcal{H}$. Now we are ready to state the aim of this approach. We are interested in finding an element $\bar{m}_n$ such that

$$\|m_n - \bar{m}_n\| \approx \|m_n - m\|$$

to guarantee that $\|\bar{m}_n - m\|$ is of the same order as $\|m_n - m\|$ and $\bar{m}_n$ can be used in place of $m_n$ without sacrificing significant accuracy in applications.

To gain such an approximation $\bar{m}_n$ we make use of another fortunate circumstance. The element $m$ does not only lie in $\mathcal{H}$ but within the convex set

$$C = \text{cch} \{k(x, \cdot) : x \in \mathcal{X}\},$$

where cch denotes the closed convex hull. This is useful because the extremes of $C$ are contained within the set $\{k(x, \cdot) : x \in \mathcal{X}\}$ and often we can reduce the study of $C$ to the application of $k(x, \cdot)$ to a function $h \in \mathcal{H}$ which is just $h(x)$. For instance, the diameter of $C$ in a direction $h \in \mathcal{H}$, $\|h\| = 1$, is

$$\text{diam}_h(C) = \sup_{x \in \mathcal{X}} \langle k(x, \cdot), h \rangle - \inf_{x \in \mathcal{X}} \langle k(x, \cdot), h \rangle = \sup_{x \in \mathcal{X}} h(x) - \inf_{x \in \mathcal{X}} h(x).$$

The set $\{k(x, \cdot) : x \in \mathcal{X}\}$ is usually infinite and not directly useful for algorithms. However, when using $m_n$, we have another convex set in $\mathcal{H}$ that is usable, that is the empirical convex set $C_n = \text{ch} \{k(X_i, \cdot) : i \leq n\}$ which contains $m_n$. The extremes of $C_n$ are contained within the finite set $\{k(X_{i1}, \cdot) : i \leq n\}$.

Standard techniques like the conditional gradient method or the kernel herding algorithm are directly applicable to approximate $m_n$ by convex combinations of $\{k(X_i, \cdot) : i \leq n\}$. The kernel herding algorithm generates an approximation of the form $(1/l) \sum_{i=1}^l k(X_i, \cdot)$, where $l : \{1, \ldots, l\} \to \{1, \ldots, n\}$ is some selection of data points and $l \leq n$. The data points $X_{i(1)}, \ldots, X_{i(l)}$ themselves can be seen as a coreset for the data set. This approach is visualized in Figure [Figure 1](1). The conditional gradient method does not provide such an average but an arbitrary convex combination of the points $k(X_1, \cdot), \ldots, k(X_n, \cdot)$ and cannot be
Figure 1: (i) The figure depicts how a subset or coreset of the sample is selected: the data is embedded in $\mathcal{H}$ by using the kernel function of $\mathcal{H}$. An approximation algorithm is then applied to the convex polytope in $\mathcal{H}$ to find an approximation of $m$ that uses only few extremes of the convex polytope. The pre-images of these extremes are the sample points that are selected as the coreset. (ii) For most statistical problems approximating $m$ itself is insufficient and one has to approximate closely related quantities. In the case of least-squares regression one has to approximate the operator $C_{y,n} \in \mathcal{H} \otimes \mathcal{H}$, which is closely related to the empirical covariance operator, and a ‘weighted’ mean embedding $m_{y,n} \in \mathbb{R}' \otimes \mathcal{H}$. It is often of interest to approximate $C_{y,n}$ and $m_{y,n}$ simultaneously, for instance, when building a coreset for least-squares regression. This can be achieved by considering the direct sum $(\hat{\mathcal{H}} \otimes \mathcal{H}) \oplus (\mathbb{R}' \otimes \mathcal{H})$ and a ‘direct sum’ of the convex polytopes in the two spaces. The relation between the extremes of the convex polytopes are highlighted in the figure through the dotted lines.

used directly to find a coreset. That being said, a coreset is often not necessary and many algorithms can work directly with an approximation of $m$ or related quantities; we demonstrate this in Section 1.4 and Section 5. The advantage of the conditional gradient method over to the kernel herding algorithm is that it usually leads to a vastly superior compression of the data.

Crucially, the performance of these techniques depends on the size of the largest ball in $C_n$ that can be centered at $m_n$. The existence of such a ball is in itself already of major importance for the performance of the techniques and is known as Slater’s condition. In this paper our main focus lies in the derivation of high probability lower bounds on the size of such a ball around $m_n$ within $C_n$. Figure 2 outlines our approach. In (i) the setting is shown with $m_n \in C_n \subset C$ and the largest ball around $m_n$ in $C_n$. One of the main difficulties is that both $m_n$ and $C_n$ are stochastic and change with the sample. We sidestep this difficulty by analyzing $C$ and $m$, by lower bounding the size of the largest ball around $m$ in $C$, and
then by relating \( C_n \) and \( m_n \) to \( C \) and \( m \) through an application of some standard techniques from empirical process theory (Figure 2(iii)). Key steps for bounding the size of the ball within \( C \) are to lower bound the diameter of \( C \) uniformly over a range of ‘directions’ in \( \mathcal{H} \) (Figure 2(ii)) and by determining how centered \( m \) lies within \( C \) (Figure 2(iii)).

### 1.1 Lower bounding the diameter of \( C \)

When trying to control the diameter of \( C \) the first thing one notices is that we seem to know relatively little about \( C \). Even the RKHS \( \mathcal{H} \) itself is usually only accessed through \( k \) and we do not have easy access to a basis of \( \mathcal{H} \). So it might come as a surprise that there is a relatively simple way to access the diameter of \( C \). The key to bounding the diameter is that

\[
\text{diam}_h(C) = \frac{1}{2} \inf_{c \in \mathbb{R}} \|h - c1\|_{\infty},
\]

where \( h \in \mathcal{H}, \|h\| = 1 \), and \( 1 \) is the constant function that is equal to 1 everywhere. This relationship holds because

\[
\sup_{g \in C} \langle h, g \rangle - \inf_{g \in C} \langle h, g \rangle = \sup_{x \in \mathcal{X}} \langle h, k(x, \cdot) \rangle - \inf_{x \in \mathcal{X}} \langle h, k(x, \cdot) \rangle = \sup_{x \in \mathcal{X}} h(x) - \inf_{x \in \mathcal{X}} h(x).
\]

The relevance of this relation is that it reduces the problem of measuring the diameter to the problem of measuring how well constant functions can be approximated by functions in the RKHS. The question of how well certain functions can be approximated by RKHS functions is well understood when the RKHS is infinite dimensional. In particular, the K-functional is a common tool to control the approximation quality and results about the K-functional can be brought to bear to provide bounds on the diameter of \( C \). However, in the finite dimensional setting these results are of limited use. We develop for this case a simple approach to measure how well constant functions can be approximated: if the constant functions do not lie in the RKHS \( \mathcal{H} \) then we can construct a new RKHS \( \mathcal{H}^+ \) by introducing the kernel function \( k^+ = k + 1 \otimes 1 \), where \( k \) is the kernel of \( \mathcal{H} \). The RKHS \( \mathcal{H}^+ \) then contains the constant functions and \( \mathcal{H} \subset \mathcal{H}^+ \). In fact, we have an isometric embedding of \( \mathcal{H} \) into \( \mathcal{H}^+ \). Now, in \( \mathcal{H}^+ \) it is easy to measure how well constant functions can be approximated by functions in the unit sphere of \( \mathcal{H} \). In detail,

\[
\inf_{h \in \mathcal{H}, \|h\|=1} \inf_{c \in \mathbb{R}} \|h - c1\|_{\mathcal{H}^+} = 1.
\]

There are different ways to move from the norm of \( \mathcal{H}^+ \) to \( \|\cdot\|_{\infty} \) which we summarize in Lemma 1 on p. 27. One of these approaches applies if \( k^+ \) is a Mercer kernel and \( \lambda_{d+1} > 0 \) is the smallest eigenvalue in the series expansion. In this case

\[
\frac{\lambda_{d+1}^{1/2}}{2} \leq \text{diam}_h(C),
\]
Figure 2: The figure summarizes some of the key questions we address in this paper: (i) This is the central question in this paper; ‘how large a ball exists within the empirical convex set $C_n$ around $m_n$?’ (ii) We address this question by first controlling the diameter of $C$ itself. In this context we make use of functions $h \in \mathcal{H}$ and we measure the size of the projection of $C$ onto these functions. Lower bounds on the diameter of these projections that hold for all relevant $h$ translate to the existence of a ball in $C$. (iii) We need not just any ball in $C$ but one that is centered at $m$. Now, generally $m$ can lie close to the boundary and no large ball around it might exist. However, under certain natural conditions it can be ruled out that $m$ will lie too close to the boundary. In particular, under these conditions we can control the ratio of $a/b$ for the segments shown in the figure. Controlling this ratio then allows us to show that there exists a ball of a certain radius around $m$ in $C$. (iv) To translate this back to $C_n$ and $m_n$ we are making us of empirical process theory to control the convergence of $C_n \rightarrow C$ and $m_n \rightarrow m$ which allows us to lower bound the size of a ball around $m_n$ in $C_n$ with high probability. Similarly to (ii) we control the convergence per direction $h$ and then use high probability guarantees that hold simultaneously for all relevant $h$.

For all $h \in \mathcal{H}, \|h\| = 1$.

If the constant functions lie already in $\mathcal{H}$ then a different approach is necessary. Let us mention that we only need to control the diameter of $C$ within the affine subspace that is spanned by it. Since $\langle k(x, \cdot), 1 \rangle = 1$ for all $x \in \mathcal{X}$ we can observe that the space spanned by $1$ is perpendicular to the affine subspace of $C$. To get a lower bound on $\text{diam}_h(C)$ for functions $h$ in the affine subspace we can consider the kernel $k^- = k - \|1\|^2 1 \otimes 1$ and the corresponding RKHS $\mathcal{H}^-$. The constant functions do not lie in $\mathcal{H}^-$ and $\mathcal{H}^-$ can be isometrically embedded in $\mathcal{H}$. Most importantly the functions $h \in \mathcal{H}^-$ of norm $\|h\|_{\mathcal{H}^-} = 1$ are exactly the directions in which we need to bound the diameter of $C$. Now, with an approach analogous to the one involving $\mathcal{H}$ and $\mathcal{H}^+$ we get a lower bound of the form

$$\frac{\lambda_d^{1/2}}{2} \leq \text{diam}_h(C),$$

for all $h \in \mathcal{H}$. 

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for all $h \in \mathcal{H}^-, \|h\|_{\mathcal{H}^-} = 1$, and with $\lambda_d$ being the smallest eigenvalue of the Mercer decomposition of the kernel $k$.

Proposition 1 on p. 35 contains these results and results about related approaches to bound the diameter.

1.2 Locating $m$ within $C$

Controlling the diameter of $C$ alone is insufficient since $m$ might lie in the boundary of $C$. We therefore need to complement the lower bounds on the diameter with results that tell us how centered $m$ lies. This can be achieved by controlling the ratio $a/b$ and $b/a$ of the segments along any function $h$ from $m$ to the boundary (Figure 2.(iii)). Here is an observation that is useful in this context: if we have a probability measure on $\mathbb{R}$ which has a mean value of 0 and there exists some measurable set $B$ with $\inf B \geq \epsilon$ and $P(B) > 0$, then there will be probability mass on the negative axis since otherwise

$$0 = \int_{\mathbb{R}} x \, dP = \int_{(0,\infty)} x \, dP \geq \int_{B} x \, dP \geq \epsilon P(B) > 0.$$  

A similar argument applies to $C$ and $m$. For instance, say we have a uniform distribution on the boundary of the ellipse shown in Figure 2.(iii), then $m$ cannot lie in the boundary: otherwise, there would exist a function $h \in \mathcal{H}, \|h\| = 1$, such that $\langle h, k(x, \cdot) \rangle \geq \langle h, m \rangle$ for all $x \in X$ and an $\epsilon > 0$ such that $A = \{x : \langle h, k(x, \cdot) - m \rangle \geq \epsilon \}$ has non-zero measure. Consequently,

$$0 = \int \langle h, k(x, \cdot) - m \rangle \, dP(x) \geq \epsilon P(A) > 0.$$  

Combining this argument with a Lipschitz assumption on the kernel function and a lower bound on the density allows us to show that $m$ has to lie away from the boundary. How far away it has to lie is made precise in Proposition 2 on p. 40.

1.3 Convergence of $C_n$ to $C$

To transfer the results about $C$ and $m$ to $C_n$ and $m_n$ we use VC and Rademacher arguments to bound the difference between $C_n$ and $C$ and $m_n$ and $m$. For $\|m_n - m\|$ this is a standard argument that does not need new ideas. However, it is less clear how to best control the difference between $C_n$ and $C$. The approach that we are taking is the following. We consider indicators $\chi\{\langle k(X, \cdot) - m, h \rangle \leq -c \}$ where $X$ is a random variable with the same distribution as $X_1, \ldots, X_n$ and $c$ is a constant that we vary. Observe that whenever

$$P\chi\{\langle k(X, \cdot) - m, h \rangle \leq -c \} > 0$$
then there is a point \( x \in \mathcal{X} \), such that \( \langle k(x, \cdot) - m, h \rangle \leq -c \), or in other words, if there is a point which lies \( c \) away from \( m \) along \( h \). A VC argument allows us to control all these indicators simultaneously over all \( h \) in the unit ball of \( \mathcal{H} \) and to show that for any such \( h \),

\[
|P_n \chi\{\langle k(X, \cdot) - m, h \rangle \leq -c \} - P \chi\{\langle k(X, \cdot) - m, h \rangle \leq -c \}|,
\]

is small for sufficiently large \( n \). This allows us to show that \( C_n \) converges along \( h \) towards \( C \) with a certain rate and since we have guarantees that hold uniformly over the unit ball in \( \mathcal{H} \) we can derive a rate of convergence of \( C_n \) to \( C \).

A similar approach works for Rademacher complexities with the main difference being that we have to approximate the indicator functions with continuous functions. This approach underlies our first theorem in this paper, Theorem 1 on p. 42, which brings together some of the results on the diameter of \( C \), the location of \( m \) and the convergence results to show that for large enough \( n \) there is with high probability a ball of a certain radius around \( m_n \) in \( C_n \). In detail, there exists a ball of size \( \delta \) with the dominant term of \( \delta \) being

\[
\frac{\tilde{\lambda}_{d}^{l+1/2} \beta_l}{4(l + 1)(8L)^l}.
\]

where \( \mathcal{X} = [0, 1]^l \), \( L \) is the Lipschitz constant, \( \tilde{\lambda}_d \) the smallest eigenvalue of the Mercer decomposition of \( k \), \( \tilde{c} > 0 \) is a lower bound on the density of the law of \( X_1 \) on \( \mathcal{X} \) and \( \beta_l \) is the Lebesgue measure of the \( l \)-dimensional unit ball in \( \mathbb{R}^l \).

With probability \( q \in (0, 1) \) there then exists a ball of radius \( \delta/4 \) around \( m_n \) in \( C_n \) whenever \( n \) is greater than

\[
n \geq \left( \frac{\sqrt{2\log(1/q)} + 96\|k\|^{1/2}/\delta}{\tilde{c}\beta_l(\delta/8L)^l} \right)^2 \cdot \left( \frac{4\|k\|^{1/2} + 3\sqrt{2\log(1/q)}}{\delta/4} \right)^2.
\]

Interpreting these results, we can first observe that \( \delta \) is strongly dependent on the dimension \( l \) of the space \( \mathcal{X} \). This stems from our approach where we identify a point \( x_0 \in \mathcal{X} \) that corresponds to an element \( k(x_0, \cdot) \) that lies far away from \( m \). We then identify a point \( x_1 \) such that \( k(x_1, \cdot) \) lies in the opposite direction of \( k(x_0, \cdot) \) with respect to \( m \). If the space is low dimensional then \( k(x_1, \cdot) \) needs to lie far from \( m \) to counter the mass that is accumulated around \( k(x_0, \cdot) \). However, when the space is high dimensional then no single point \( k(x_1, \cdot) \) has to lie far away from \( m \) because the mass accumulated around \( k(x_0, \cdot) \) can be counter by ‘many points’ that lie close to \( m \).

To contrast this worst case bound with the best case, observe that there is a point in \( C \) such that a ball of radius \( \tilde{\lambda}_{d}^{l/2}/4 \) lies around it within \( C \). The factor \( \tilde{\lambda}_{d}^{l/2} \) itself is in all likelihood quite tight and reflects the fact that the convex set \( C \) is very small in certain directions.
1.4 Adapting the approach to concrete statistical problems

Most methods for inference do not use \( m \) itself but related quantities. For example, in the least squares problem where we try to fit observations \( Y_i \) through \( f(X_i) \) with some function \( f \) in an RKHS, we have

\[
\frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} \langle f \otimes f, k(X_i, \cdot) \otimes k(X_i, \cdot) \rangle - \frac{2}{n} \sum_{i=1}^{n} \langle f, Y_i k(X_i, \cdot) \rangle + \frac{1}{n} \sum_{i=1}^{n} Y_i^2
\]

where we denote by \( \mathcal{H} \otimes \mathcal{H} \) the tensor space \( \mathcal{H} \otimes \mathcal{H} \) when the functions are restricted to the diagonal \( \Delta = \{ (x, x) : x \in X \} \), \( C_n = (1/n) \sum_{i=1}^{n} k(X_i, \cdot) \otimes k(X_i, \cdot) \upharpoonright \Delta \) and \( m_{y,n} = (1/n) \sum_{i=1}^{n} Y_i k(X_i, \cdot) \).

There are significant similarities between the problem of compressing \( m_n \) and that of compressing \( C_n \) or \( m_{y,n} \). We discuss a variety of these in Section 4. Let us highlight a few results.

The empirical covariance operator \( C_n \) can quite easily be dealt with by associating it to the element \( (1/n) \sum_{i=1}^{n} \kappa(X_i, \cdot) \), where \( \kappa(x, y) = k^2(x, y) \). This way one can apply all the results we developed for \( m_n \) to \( C_n \), one only has to substitute \( \kappa \) for \( k \).

Dealing with the element \( m_{y,n} \) is more challenging and there is a certain degree of freedom of how to phrase the compression problem. A natural and simple choice is to consider \( Y_i k(X_i, \cdot) \) as the random elements which attain values in \( \mathcal{H} \). A first indicator that things are more complicated is that when \( Y_i \) is unbounded then we run into serious problems when trying to define a bounded convex set that contains \( (1/n) \sum_{i=1}^{n} Y_i k(X_i, \cdot) \). Things simplify if we assume boundedness and make some natural assumptions about how the data is generated. In particular, if we assume that \( X_1, \ldots, X_n \) are i.i.d. and \( Y_i = f_0(X_i) + \epsilon_i \), where the \( \epsilon_i \)'s are i.i.d., centered, independent of \( X_1, \ldots, X_n \) and bounded by \( |\epsilon_i| \leq b \) a.s., then \( m_{y,n} \) converges to

\[
m_y = \int f_0(X_1) k(X_1, \cdot) dP \in \mathcal{H}
\]

and \( m_y \) is contained in the convex set

\[
C_y = \text{cch} \{ (f_0(x) \pm b) k(x, \cdot) : x \in X \}.
\]

In this setting there is also a simple relationship between the diameter of \( C_y \) and \( C \): consider some \( h \in \mathcal{H}, \|h\| = 1 \), then

\[
diam_h(C_y) \geq b \diam_h(C)
\]

and results on \( \diam_h(C) \) are directly applicable.
Up to now we considered the approximation problems in isolation but it also makes sense to try to approximate $C_n$ simultaneously to $m_{y,n}$ by selecting elements $Y_i k(X_i, \cdot)$ that reduce the approximation error for both. Quite a different set of techniques are needed to deal with this simultaneous approximation problem. In Section 4.3 we develop an approach based on direct sums of Hilbert spaces to deal with this problem. The analysis is much more intricate and interesting than for the individual approximation problems. In Figure 1, the high level approach is visualized. The space $H \circledast H$ is the space of functions $H \circledast H$ when trivially extended from $X$ to $X \times \mathbb{R}$ and the space $\mathbb{R}' \otimes H$ is an RKHS with kernel function $((x_1, y_1), (x_2, y_2)) \mapsto \langle y_1, y_2 \rangle_{\mathbb{R}^k} (x_1, x_2)$ which is also defined on $X \times \mathbb{R}$. The convex sets we introduced above have natural analogues in $H \circledast H$ and in $\mathbb{R}' \times H$. By taking the direct sum of these spaces we also get a sort of direct sum of these convex sets and we are trying again to control quantities like the diameter of that set. The particular problem of approximating $C_n$ simultaneously to $m_{y,n}$ is benefiting from the fact that $H \circledast H \cap (\mathbb{R}' \otimes H) = \{0\}$. This allows us to define an RKHS that is isometrically isomorphic to the direct sum. Working with this RKHS allows us to relate quantities like the diameter of the convex set in the direct sum space back to the diameters of the individual convex sets (Proposition 3, p. 52).

The situation that the two Hilbert spaces that we combine through the direct sum are not overlapping is rather special. For instance, if we try to approximate $m$ and $C$ simultaneously then the Hilbert spaces overlap which adds another layer of difficulties. We are developing for this case a quotient space approach that factors out the intersection between the two Hilbert spaces. An interesting finding in this context is that the direct sum cannot be related directly to an RKHS but, like in the case of approximating $m$ and $C$ simultaneously, the affine subspace spanned by the convex set can be isometrically isomorphic to an RKHS which then allows us again to use results we developed for RKHSs (see Lemma 5, p. 54).

If we apply the conditional gradient method to the above RKHSs then we will not end up with a coreset of data points but with elements in $H \circledast H, \mathbb{R}' \otimes H$ or $H \circledast H \oplus (\mathbb{R}' \otimes H)$. However, that is not a major obstacle and it is for various problems quite easy to adapt the algorithms to deal with these approximations; we highlight that approach for kernel ridge regression in Section 5.

1.5 Slow rate of convergence in infinite dimensions

It was observed in [3] that the proof technique used to derive fast rates of convergence for the kernel herding algorithm and the conditional gradient method cannot be applied to compact sets in infinite dimensional RKHSs since compact sets in such spaces do not contain norm balls. Theorem 2 on p. 58 demonstrates that the problem lies deeper: there exist well behaved approximation problems in infinite dimensional spaces for which the kernel herding algorithm does not converge fast. We chose to construct the counter example for
Figure 3: The figure shows lower bounds on $|\langle e_n, w \rangle|$ in dependence of the first element $a_m$ that has not yet been chosen. The shaded area is a lower bound on $\|w\|$ when $m = 10^{20}$. The norm of $w$ goes to infinity in $m$ which implies that the kernel herding algorithm converges with a rate that is slower than $1/t$.

The kernel herding algorithm and not the conditional gradient methods since the behavior of the kernel herding algorithm is easier to control but we strongly suspect that similar problems will also occur with the conditional gradient method. In detail, we show that there exists a continuous kernel on $[0, 1]$, a Borel probability measure on $[0, 1]$ which assigns positive measure to open subsets of $[0, 1]$ and an initialization for which the kernel herding algorithm converges with a slower rate than $1/t$. Such a slow rate of convergence implies that the compression is poor and that too many data points have to be used to approximate $m_n$. Let use start by recalling the kernel herding algorithm [7]:

**Algorithm 1 (The Kernel Herding Algorithm)**

Initialise: let $w_0$ be some element in $C$, iterate through $t \geq 1$:

choose $x^* \in \arg \max_{x \in X} \langle w_i, k(x, \cdot) \rangle$,

set $x_i = x^*$, $w_{i+1} = w_i - (k(x^*, \cdot) - m_n)$, and $\hat{m}_t = (1/t) \sum_{i \leq t} k(x_i, \cdot)$.

Stop when $t = T$ and return the approximation $\hat{m}_T$.

The elements $w_t$ are measuring the error between $m_n$ and $\hat{m}_t$ as $\|w_t\| = t\|m_n - \hat{m}_t\|$. The algorithm converges with a rate of $1/t$ if, and only if, the sequence of weights $w_t$ is bounded. In other words, if the sequence diverges then the algorithm converges with a slow
Let us now move to the example. The construction of this example is somewhat involved since we need to gain control over the behaviour of the algorithm. The basic intuition, however, is rather simple. We start with some infinite dimensional Hilbert space $\mathcal{H}$ and an orthonormal sequence $\{e_n\}_{n \geq 1}$ in it. The construction is best explained when assuming that $m = 0$ (we cannot set it exactly to 0 and need a minor modification here). We then construct a compact convex set that contains elements $\{a_n\}_{n \geq 1}, \{b_n\}_{n \geq 1}$ where each $a_n$ is a positive multiple of $e_n$ and each $b_n$ a negative multiple of $e_n$. Furthermore, $b_n$ is of significantly smaller magnitude than $a_n$. Consider now an initialization of the algorithm with an element $c \in \mathcal{H}$ which is of small magnitude compared to the $a_n$ and has a positive inner product with each $a_n$. Because of this positive inner product the different $a_n$ will be chosen once by the algorithm and because the $b_n$ are of small magnitude compared to $a_n$ hardly any weight will be reduced in the directions $e_n$. This way the weight vector $w_t$, $t$ being the iteration index, builds up mass in the different directions $e_n$. The construction is more involved than this sketch, but, a suitably adapted version of this approach allows us to show that so much weight will be added to the approximation that its norm diverges to infinity. This effect is visualized in Figure 3. The figure shows four different weight vectors as inner products with $e_n$ ($n$ being shown on the $x$-axis). The shaded area continues past the right end of the plot (the limit of the shaded area is given in the legend: $10^5$ for the black line etc.). You can observe that the right limit of the shaded area grows significantly from the black line to the red line, i.e. from $10^5$ to $10^{20}$. While the right limit grows exponentially the left limit hardly changes. This is due to the small scale of the $b_n$’s. As a result the overall mass in the shaded area, which corresponds to the size $\|w_t\|$, goes off to infinity. This implies then directly that the algorithm cannot converge with the fast rate. All that then remains it to show that there exists a continuous kernel that gives rise to this setup. We construct first a continuous function $\phi : [0, 1] \to \mathcal{H}$ that goes over all $a_n$ and $b_n$ and we then use this Hilbert space and this continuous function to construct an RKHS with a continuous kernel.

### 1.6 Literature

The concept of a coreset is known for at least two decades and there is a wide range of literature on its application to machine learning, Bayesian statistics and geometric approximation problems (e.g. [4, 1, 16]). It is natural to apply the conditional gradient method [13] in that context (e.g. [16]).

The kernel herding algorithm and the conditional gradient method are greedy approximation algorithm as they choose at each stage $t$ an element that minimizes the remaining error. Greedy algorithms will generally not return the best possible approximation that can be achieved in $t$ steps but they are easy to compute. This is a big advantage since in the large data context computational efficiency is paramount. Greedy algorithms for approx-
imating functions have been popular at least since the late nineties. An overview of the
most popular approaches is provided in [25]. The approach is here to make use of a ba-
sis of a function space, say of a Sobolev or Besov space, to approximate elements inside
these function spaces in a greedy fashion. An important generalization is using so called
dictionaries which are families of functions that are not necessarily linearly independent,
i.e. there are redundancies in the representation of elements in the function space. These
approaches are very natural if one has access to a basis or related families of functions. In
contrast to this approach we are interested in approximating subsets of the function space
that are naturally described by point-evaluators, a kernel function or, more generally, a set
of extremes of a convex set. Instead of working then with linear subspaces of the func-
tion space we are working with convex subsets of the function spaces and we apply greedy
algorithms to approximate elements inside such convex sets.

The methods we are studying compress the sample into a potentially small subset of the
original sample while retaining optimal, or nearly optimal, rates of convergence. While our
approach is inspired by various optimization methods there are links to sample compres-
sion schemes as introduced in [18] [12]. Sample compression schemes are concerned with
the inference of 'concepts', which are indicators \( \chi_A \), \( A \) a Borel subset of some topological
space \( X \). In this setting one has given a set of concepts that contains the concept \( \chi_A \), or are
sufficient to approximate \( \chi_A \) in a suitable way, and one likes to infer \( \chi_A \) from observations
\((x_1, y_1), \ldots, (x_n, y_n)\), \( x_i \in X, y_i \in \{0, 1\} \). A sample compression scheme compresses
these observations into a subset that is sufficient to reconstruct the original labels \( y_i \) for all
\( x_i, i \leq n \), if the observations are consistent with some concept \( \chi_{A'} \), where \( \chi_{A'} \) is con-
tained in the predefined set of concepts. Compressibility is directly linked to VC-theory:
in [12] it is shown that under some technical conditions sets with VC-dimension \( d \) are \( d \)-
compressible, meaning that one can always reduce the sample to a sub-sample of size \( d \)
while still being able to reconstruct the sample in the above sense. Furthermore, it is not
possible to compress the sample to less than \( d \)-points without losing the reconstructability
property. Our aim is quite different in that we do not care about being able to reconstruct
the original labels. In that sense our approach is more closely related to sufficient statis-
tics which compress the data to facilitate inference. That being said, there are interesting
parallels. For instance, Radon’s theorem tells us that in our setting there is a compression
of the data down to \( d \)-points if we work with a \( d \)-dimensional RKHS; such an RKHS has
VC-dimension \( d \).

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2 Preliminaries

Throughout this paper we will be working with a set \( X \) in which covariates or features attain values and a kernel function \( k : X \times X \to \mathbb{R} \) (see [20, Def.2.12]). Recall that such a kernel function gives rise to an RKHS \( \mathcal{H} \) [20, Def.2.14]. While \( X \) does not need a particular structure to define a kernel on, we are interested in integrals involving \( k \) and we will assume for most of our results that \( X \) is a measurable space and \( k \) is a measurable in the sense that \( k(x, \cdot) : X \to \mathbb{R} \) is measurable for all \( x \in X \). This is equivalent to saying that any \( h \in H \) is a measurable function from \( X \) to \( \mathbb{R} \) (see [24, Lem.4.24]); we will state the assumptions that we are making in Lemmas, Propositions and Theorems etc. We need in various places vector valued integrals. In particular, we make use of Bochner integrals and Hilbert-space valued \( L^p \) spaces. Let \((\Omega, \mathcal{A}, P)\) be a probability space and \( X \) a random variable that attains values in \( X \) then by \( \int f(X) \, dP \), \( f : \Omega \to \mathcal{H} \) Bochner integrable, we mean the Bochner integral of the function \( f(X) : \Omega \to \mathcal{H} \) with respect to the measure \( P \). The Hilbert space valued \( L^p \) when \( 1 \leq p < \infty \) corresponding to this measure space are given by

\[
L^p(P; \mathcal{H}) = \{ f : \Omega \to \mathbb{R} : f \text{ Bochner measurable and } \int \| f(\omega) \|^p \, dP(\omega) < \infty \}.
\]

The seminorm on \( L^p(P; \mathcal{H}) \) is \( \| f \|^p_p = \int \| f \|^p \, dP \). We use bold fonts for the \( L^p(P; \mathcal{H}) \) seminorms throughout this paper. As usual there are corresponding spaces \( L^p \) of equivalence classes with norms \( \| \cdot \|_p \) under which these \( L^p \) spaces are complete. The space \( L^2(P; \mathcal{H}) \) is a Hilbert space with the inner product corresponding to the bi-linear function \( \langle \cdot, \cdot \rangle_2 \) on \( L^2(P; \mathcal{H}) \) given by \( \langle f, g \rangle_2 = \int \langle f(\omega), g(\omega) \rangle \, dP(\omega) \) whenever \( f, g \in L^2(P; \mathcal{H}) \). Of particular importance to us is the Bochner integral \( \int k(X, \cdot) \, dP \in \mathcal{H} \) which is well defined whenever \( k(X, \cdot) \in L^1(P; \mathcal{H}) \). We will denote this integral by \( m \). Finally, we have the following important relation between the inner product in \( \mathcal{H} \) and Bochner integrals: when \( f \in L^1(P; \mathcal{H}) \) and \( h \in \mathcal{H} \) then according to [9, Thm.6,p.47],

\[
\langle h, \int f \, dP \rangle = \int \langle h, f \rangle \, dP.
\]

In various parts of this paper we make use of the tensor product of two Hilbert spaces \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \). One way to define this tensor product is to first define an algebraic tensor product of the vector spaces \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \); given that we are only working with Hilbert spaces of functions it is natural to define the algebraic tensor product as

\[
\{ f : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} : f(x, y) = \sum_{i=1}^n g_i(x) h_i(y), g_i \in \mathcal{H}_1, h_i \in \mathcal{H}_2, n \in \mathbb{N} \},
\]

where we assume that functions in \( \mathcal{H}_1 \) map from \( \mathcal{X} \) to \( \mathbb{R} \) and functions in \( \mathcal{H}_2 \) from \( \mathcal{Y} \) to \( \mathbb{R} \). That this is a tensor product for \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) can be verified by applying Criterion 2.3 in [8].
Next, we equip the algebraic tensor product with the inner product \( \langle g_1 \otimes h_1, g_2 \otimes h_2 \rangle_\otimes = \langle g_1, h_1 \rangle_1 \langle g_2, h_2 \rangle_2 \), e.g. \cite{19} Thm.6.3.1, and complete the resulting pre-Hilbert space. In the case where \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) are RKHSs with kernels \( k_1 \) and \( k_2 \) we have bounded point evaluators for elements in the pre-Hilbert space, i.e. \( \langle h_1 \otimes h_2, k(x, \cdot) \otimes k(y, \cdot) \rangle_\otimes = h_1(x)h_2(y) \) for all \( x \in \mathcal{X}, y \in \mathcal{Y}, h_1 \in \mathcal{H}_1 \) and \( h_2 \in \mathcal{H}_2 \). Due to \cite{2} second theorem on p.347 there is then a unique functional completion of the algebraic tensor product and we will use this completion when working with RKHSs. We do not use the algebraic tensor product itself and, in the following, will reserve the notation \( (\mathcal{H}_1 \otimes \mathcal{H}_2, \langle \cdot, \cdot \rangle_\otimes) \) for the tensor product of the two Hilbert spaces, that is \( \mathcal{H}_1 \otimes \mathcal{H}_2 \) is a Hilbert space with inner product \( \langle \cdot, \cdot \rangle_\otimes \), and, whenever \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) are RKHSs, \( \mathcal{H}_1 \otimes \mathcal{H}_2 \) is a Hilbert space of functions. In fact, in the latter case \( \mathcal{H}_1 \otimes \mathcal{H}_2 \) is an RKHS with kernel \( \tilde{k}((x_1, y_1), (x_2, y_2)) = k_1(x_1, y_1)k_2(x_2, y_2) \). See also \cite{20} Thm.5.11.

When \( X, Y \) are independent random variables under the measure \( P \) attaining values in \( \mathcal{X}_1, \mathcal{X}_2 \), \( k_1, k_2 \) are kernel functions on \( \mathcal{X}_1 \) and \( \mathcal{X}_2 \) respectively, \( g \in \mathcal{H}_1, h \in \mathcal{H}_2 \), and the Bochner integrals \( \int k_1(X, \cdot) \, dP, \int k_2(Y, \cdot) \, dP, \int k_1(X, \cdot) \otimes k_2(Y, \cdot) \, dP \) are well defined then

\[
\langle g \otimes h, \int k_1(X, \cdot) \otimes k_2(Y, \cdot) \, dP \rangle_\otimes = \int g(X)h(Y) \, dP = \int g(X) \, dP \int h(Y) \, dP \\
= \langle g, \int k_1(X, \cdot) \, dP \rangle_1 \langle h, \int k_2(Y, \cdot) \, dP \rangle_2 = \langle g \otimes h, \int k_1(X, \cdot) \, dP \otimes \int k_2(Y, \cdot) \, dP \rangle_\otimes.
\]

Since this holds for all \( g \otimes h, g \in \mathcal{H}_1, h \in \mathcal{H}_2 \),

\[
\int k_1(X, \cdot) \otimes k_2(Y, \cdot) \, dP = \int k_1(X, \cdot) \, dP \otimes \int k_2(Y, \cdot) \, dP.
\] (1)

Another construction that we need is the direct sum of two Hilbert spaces \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \). The direct sum \( \mathcal{H}_1 \oplus \mathcal{H}_2 \) is the Cartesian product \( \{(g, h) : g \in \mathcal{H}_1, h \in \mathcal{H}_2\} \) equipped with the inner product \( \langle (g_1, h_1), (g_2, h_2) \rangle_\oplus = \langle g_1, g_2 \rangle_1 + \langle h_1, h_2 \rangle_2 \) \cite{21} p.40,Ex.5). We do not assume here that \( \mathcal{H}_1 \cap \mathcal{H}_2 = \{0\} \).

## 3 Approximating convex sets and locating \( m \) and \( m_n \)

We start this section with a discussion of a simple approach for approximating convex sets using \( \varepsilon \)-nets. We will find that such an approximation is of very limited use only which motivates the remainder of the paper. In this remainder we analyze a stochastic approach at length where we consider the random convex set which is induced by the sample. We conclude this section by analyzing where \( m \) and \( m_n \) lies within these convex approximations and we provide high probability bounds on the size of balls within the empirical convex set which are centered at \( m_n \).
3.1 Approximation based on \( \varepsilon \)-nets.

Let \( \mathcal{H} \) be an RKHS of real-valued functions acting on \( \mathcal{X} = [0, 1]^d \) with kernel function \( k \) being bounded by 1. Furthermore, let \( \phi : \mathcal{X} \to \mathcal{H} \) be the map \( \phi(x) = k(x, \cdot) \) and \( m_n = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i) \) for certain points \( x_1, \ldots, x_n \in \mathcal{X} \). For \( \varepsilon > 0 \) there exists an \( \varepsilon \)-net for \( [0, 1]^d \) that consists of \( N_{\varepsilon, d} = \lceil d^{d/2}/\varepsilon^d \rceil \) many closed balls that are centered at points \( y_1, \ldots, y_{N_{\varepsilon, d}} \) in \( [0, 1]^d \). This \( \varepsilon \)-cover of \( [0, 1]^d \) gives rise to a \( \varepsilon \varepsilon^\alpha \)-cover of \( \phi[\mathcal{X}] = S \) if \( \phi \) is \( \alpha \)-Hölder continuous with Lipschitz constant \( c \). Let \( s_i = \phi(x_i) \) for all \( i \leq n \) and \( s'_i \) the closest point to \( s_i \) in \( \phi[\{y_1, \ldots, y_{N_{\varepsilon, d}}\}] \). Then the approximation \( m'_n = \frac{1}{n} \sum_{i=1}^{n} s'_i \) of \( m_n \), which can be written as a sum over at most \( N_{\varepsilon, d} \) many terms, achieves an approximation error of

\[
\|m_n - m'_n\| \leq \frac{1}{n} \sum_{i=1}^{n} \|s_i - s'_i\| \leq c \varepsilon^\alpha.
\]

If we want to achieve an approximation error of at most \( n^{-1/2} \) then we need to include \( \lceil d^{d/2}(c^2 n)^{d/(2\alpha)} \rceil \) many balls in the cover. If \( \varepsilon \geq 1 \) then we can only represent \( m_n \) with less than \( n \)-points if \( d = 1 \) and \( \alpha > 1/2 \). The Lipschitz constant \( c \) is here only of limited help if we choose our kernel independent of \( n \).

We can also observe that a fine cover is necessary for good approximation if we do not impose assumptions on the measure and on \( m \). For instance, consider again \( \mathcal{X} = [0, 1]^d \) and a kernel \( k \) such that \( k(x, x) = 1 \) for all \( x \in \mathcal{X} \) and such that \( 1 - k(x, y) \leq c \|x - y\| \) for some constant \( c > 0 \) and any \( x, y \in \mathcal{X} \). Furthermore, assume that we have a cover centered at \( t^d \) points \( x_1, \ldots, x_t^d \) then there exists a point \( x_0 \) with \( \min_{i \leq t} \|x_0 - x_i\| \geq 1/2t \). If we consider now the measure with unit mass on \( x_0 \), i.e. \( m = k(x_0, \cdot) \), then the error, when approximating the expected value of the norm one function \( h = k(x_0, \cdot) \), is

\[
|\langle m, h \rangle - \langle m_n, h \rangle| = \|m\|^2 - \sum_{i=1}^{t} \alpha_i k(x_i, x_0) \geq \frac{c}{2t}.
\]

Hence, to attain an approximation error of order \( n^{-1/2} \) we need a cover consisting of at least \( n^{d/2} \) many points.

3.2 Empirical convex sets

In the following, let \( \mathcal{H} \) be a separable RKHS and let \( C_n = \text{ch} \{ \phi(X_i) : i \leq n \} \) be the set valued random variable determined by \( X_1, \ldots, X_n \). The variable \( C_n \) attains values in the closed convex subsets \( C(\mathcal{H}) \) of \( \mathcal{H} \). There exists various natural topologies on \( C(\mathcal{H}) \) (see [6]). We equip \( C(\mathcal{H}) \) with the Vietoris topology and the corresponding Borel-Effron \( \sigma \)-algebra. The random variable \( C_n \) is then well defined as a measurable map from \( \Omega \) to \( C(\mathcal{H}) \).
The random variable $C_n$ tends to $C = \text{ch} \{ \phi(x) : x \in X \}$ as $n$ tends to infinity. We aim to quantify how similar $C_n$ is to $C$. We do so by framing the question of convergence in the context of empirical process theory. In the following discussions we assume that $\mathcal{X}$ is compact, $\mathcal{H}$ is finite dimensional with dimension $d$, and the corresponding kernel function $k$ is continuous. In particular, $\|k\|_{\infty}^{1/2} =: b$ is finite.

Observe that we can reduce the question of convergence of $C_n$ to $C$ to the question of how fast the projection of $C_n$ on some direction $u \in \mathcal{H}$, $\|u\| = 1$, converge to the projection of $C$ on $u$. More specifically, if we can control the convergence uniformly over all such $u$ then we have control over the convergence of $C_n$ to $C$. Furthermore, since $C_n$ and $C$ are convex we only need to control the end points of the projections. To this end, let us introduce the functions $f_{u,c}(x) = \chi\{u(x) \leq c\}$, $f_{u,c} : \mathcal{X} \to \mathbb{R}$, for $u \in \mathcal{H}$, $\|u\| = 1$ and $c$ going through the interval $\{h, u\} = \{u(x) : x \in \mathcal{X}\}$ or a superset of this interval.

The importance of the functions $f_{u,c}$ is that $P f_{u,c} > 0$ if, and only if, there is an element $h \in C$ in direction $u$ such that $\langle h, u \rangle \leq c$ (given there is non-zero mass on that element or the mass of all elements whose projection falls below $c$ that lie strictly greater than zero). For instance, if $C$ contains the origin then we would vary negative $c$’s to explore the extension of the projection of $C$. Similarly, the empirical convex set will contain an element which lies $c$ away from the origin in direction $u$ if, and only if, $P_n(u(X) \leq c) > 0$. Notice that the condition $P_n(u(X) \leq c) > 0$ is equivalent to $\min_{i \leq n} u(X_i) \leq c$.

To make use of this approach to quantify the difference between $C$ and $C_n$ we need to control the convergence of $P_n f_{u,c}$ to $P f_{u,c}$ simultaneously over all these $f_{u,c}$. One simple approach to do that is to use VC theory. Since we are working here with finite dimensional RKHSs this is rather straightforward. In detail, whenever $u \in \mathcal{H}$, $\|u\| = 1$, then $|u(x)| \leq b$ and we can use $[-b, b]$ as the interval over which we vary $c$. Hence, let $\mathcal{F} = \{ f_{u,c} : u \in \mathcal{H}, \|u\| = 1, -b \leq c \leq b \}$.

We want to show that $\mathcal{F}$ is a VC-subgraph class of functions. In fact, it is convenient to work with a countable dense subset of $\mathcal{F}$ to sidestep measure theoretic complications relating to the empirical process. With this in mind, let $\mathcal{H}$ be a countable dense subset of $\mathcal{H}$ such that $\mathcal{H} \cap \{ u : \|u\| = 1, u \in \mathcal{H} \}$ lies dense in $\{ u : \|u\| = 1, u \in \mathcal{H} \}$ and define the countable set $\mathcal{F} = \{ f_{u,c} : u \in \mathcal{H}, \|u\| = 1, c \in \mathbb{Q} \cap [-b, b] \} \subset \mathcal{F}$.

The family $\mathcal{F}$ is a VC-subgraph class and its VC-dimension is upper bounded by $d + 1$: consider the family of function $\mathcal{G} = \text{span} \{ \mathcal{H} \cup \{ c1 : c \in \mathbb{R} \} \}$. The dimension of $\mathcal{G}$ is at most $d + 1$ and $c - u(x) \in \mathcal{G}$ for every $u \in \mathcal{H}$, $-b \leq c \leq b$. Applying [10], Theorem 4.6, shows that the VC dimension of $\text{Pos}(\mathcal{G}) = \{ \text{pos}(g) : g \in \mathcal{G} \}$, where $\text{pos}(g) = \{ x : g(x) \geq 0 \}$, is at most $d + 1$. Furthermore, the family $\mathcal{G}'$ of sets of the form $\{ (x, t) : x \in \text{pos}(g), t \leq 1 \}$, $g \in \mathcal{G}$, has the same VC-dimension. But $\mathcal{G}'$ is a family of subgraphs that contains all the subgraphs of functions in $\mathcal{F}$ and the claim follows. Since $\mathcal{F} \subset \mathcal{F}$ it also follows that $\mathcal{F}$ is a VC-subgraph class with VC-dimension at most $d + 1$. 

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The family $\tilde{F}$ has the measurable envelope $\chi_{\mathcal{X}}$ and, due to [15 Thm3.6.9], its covering numbers can be bounded by

$$N(\tilde{F}, L^2(Q), \varepsilon) \leq 4(8/\varepsilon^2)^{d+2} \vee \tilde{c},$$

where $\tilde{c}$ can be chosen as $\max\{m \in \mathbb{N}_+ : \log m \geq m^{1/(d+1)(d+2)}\}$ and whenever $Q$ is a probability measure on $\mathcal{X}$. Be aware that the $\nu$-index as defined in [15] is equal to one plus the VC-dimension when using the definition of [10] for the VC-dimension.

Now, applying Hölder’s inequality, $J(\delta) = \int_0^\delta \sup_Q \sqrt{\log 2N(\tilde{F}, L^2(Q), \varepsilon)} d\varepsilon \leq \delta (\log(2\tilde{c}) \vee (1 + 2(d+2)))^{1/2}$. In particular, $J(1) \leq \sqrt{\log 2\tilde{c} \vee 1 + 2(d+2)}$. By Remark 3.5.5 and Theorem 3.5.4 from [15] we can conclude that

$$E(\sup_{f \in \tilde{F}} |P_n f - Pf|) \leq 12J(1)n^{-1/2}.$$

We use now Bousquet’s version of Talagrand’s inequality to move to a high probability bound (e.g. [15], Theorem 3.3.9). For simplicity, we will denote the supremum over $u, c$, such that $f_{u,c} \in \tilde{F}$, by $\sup_{u,c}$ in the following. Let $S_n = \sup_{u,c} |\sum_{i=1}^n (f_{u,c}(X_i) - Pf_{u,c})| = n \sup_{u,c} |P_n f_{u,c} - Pf_{u,c}|$. Observe that $\|Pf_{u,c} - f_{u,c}\|_\infty \leq 1$ and $ES_n = nE(\sup_{u,c} |P_n f_{u,c} - Pf_{u,c}|)$. Applying Talagrand’s inequality yields

$$e^{-x} \geq \Pr\left(\max_{j \leq n} S_j \geq ES_n + \sqrt{2x(2ES_n + n)} + x/3\right)$$

for all $x \geq 0$. In particular, with probability at least $1 - \exp(-x)$,

$$\sup_{u,c} |P_n f_{u,c} - Pf_{u,c}| \leq 12J(1)n^{-1/2} + n^{-1/2} \sqrt{2x(24J(1)n^{-1/2} + 1)} + x/3n.$$  \hspace{1cm} (2)

As is usually the case with metric entropy based bounds, the constants are loose and $n$ needs to be large to gain useful results. Tighter bounds can often be attained by using Rademacher complexities (see [5, 15]). While bounds are generally tighter it is not possible to work directly with the indicator functions $f_{u,x}$ but we need a continuous approximation of these. Also, in the Rademacher approach that we develop it is beneficial to center the functions $h \in C$ by moving to $C_c = \{h - m : h \in C\}$.

In the following, let $F = \{(u, c) : u \in \mathcal{H}, \|u\| = 1, -b \leq c \leq b\}$ and $\tilde{F} = \{(u, c) : u \in \mathcal{H}, \|u\| = 1, c \in [-b, b] \cap \mathbb{Q}\}$. Furthermore, consider the function $\psi_\gamma : \mathbb{R} \to \mathbb{R}$, with $\gamma > 0$, defined by $\psi_\gamma(x) = 1$ for $x \leq -\gamma$, $\psi_\gamma(x) = 0$ for $x \geq 0$ and $\psi_\gamma(x) = -x/\gamma$.  \hspace{1cm} (2)
otherwise. Then \( f_{u,c}(h) = \chi\{|u,h| \leq c\} \geq \psi_\gamma(\langle u,h \rangle - c) \) for any \( u,h \in \mathcal{H} \). Furthermore, \( \psi(0) = 0 \) and \( |\psi_\gamma(x) - \psi_\gamma(y)| \leq |x-y|/\gamma \), that is \( \gamma \psi_\gamma(\cdot) \) is a contraction vanishing at zero (see [15] Thm3.2.1 or [17] Thm4.12).

We have that \( P_n f_{u,c+\langle u,m \rangle} \geq P_n \psi_\gamma(\langle u, \phi(\cdot) - m \rangle - c) \). Due to [15] Thm3.4.5, with probability \( p \), simultaneously for all \( u \in \mathcal{H}, \|u\| = 1 \) and \( c \in [-b,b] \cap \mathbb{Q} \), \( P_n \psi_\gamma(\langle u, \phi(\cdot) - m \rangle - c) \) is lower bounded by

\[
P\psi_\gamma(\langle u, \phi(\cdot) - m \rangle - c) - 2E\left( \sup_{(u',c') \in \tilde{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \psi_\gamma(\langle u', \phi(X_i) - m \rangle - c') \right| \right) - \sqrt{\frac{2 \log(1/p)}{n}},
\]

where \( \epsilon_i \) are i.i.d. Rademacher variables that are independent of \( X_1, \ldots, X_n \). Because \( \gamma \psi_\gamma \) is a contraction vanishing at zero

\[
E\left( \sup_{(u',c') \in \tilde{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \psi_\gamma(\langle u', \phi(X_i) - m \rangle - c') \right| \right) \leq \frac{2}{\gamma^2} E\left( \sup_{(u',c') \in \tilde{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i (\langle u', \phi(X_i) - m \rangle - c') \right| \right).
\]

Applying [5] Thm12.7 and Lem22] and using that the Rademacher complexity for the constant functions \( \langle u', m \rangle + c', (u', c') \in \tilde{F} \), where \( \|u', m\| + c' \leq b + |c'| \leq 2b \) is upper bounded by \( 4bn^{-1/2} \),

\[
E\left( \sup_{(u',c') \in \tilde{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i (\langle u', X_i \rangle - c') \right| \right) \leq 4bn^{-1/2} + E\left( \frac{2}{n} \left( \sum_{i=1}^{n} k(X_i,X_i) \right)^{1/2} \right) \leq 6bn^{-1/2}
\]

and for any \( (u,c) \in \tilde{F} \),

\[
P_n \psi_\gamma(\langle u, \phi(\cdot) - m \rangle - c) \geq P \psi_\gamma(\langle u, \phi(\cdot) - m \rangle - c) - (\sqrt{2 \log(1/p)} + 24b/\gamma)n^{-1/2}.
\]

The VC and Rademacher bounds allow us to control the size of the empirical convex set in terms of \( P f_{u,c} \) and \( P \psi_\gamma(\langle u, \phi(\cdot) - m \rangle - c) \). In either case we need to get a handle on \( P \) to move further. In particular, we need to understand how \( P \) concentrates around the extremes of \( C \). We are now looking at a few examples to get a better understanding of how \( P \) concentrates and what that implies for the convergence of the empirical convex set to \( C \). Of major importance is how smooth \( \phi : \mathcal{X} \to \mathcal{H} \) is and how the distribution of \( X_1, \ldots, X_n \) on \( \mathcal{X} \) looks like. We start with a couple of simple example before moving back to the machine learning setting.

### 3.2.1 Example 1: Unit circle

Consider the unit circle in \( \mathbb{R}^2 \) with the uniform distribution on it. What can we say about the interior of \( C_n \) as a function of \( n \)? In particular, what can be said about the size of \( C_n \) in direction \( u \in \mathbb{R}^2, \|u\| = 1 \)? Due to the symmetry of the unit sphere and because
the uniform distribution is used it is sufficient to consider the vector $u = (1,0)^\top$. The probability that a sample point, when we sample just once, lies to the right of $cu$ for $c \in [-1,1]$ is $(1/2\pi) \int_0^{2\pi} \chi\{\langle u, (\cos \theta, \sin \theta)^\top \rangle \geq c \} = \arccos(c)/\pi$, using that $\arccos$ is a monotonically decreasing function. Similarly, the probability that a sample point lies to the left of $cu$ is $1 - \arccos(c)/\pi$. Furthermore, if we draw $n$ independent samples then the probability to see at least one point on the right of $cu$ is $1 - (1 - \arccos(c)/\pi)^n$ and that at least one sample lies on the left of $cu$ is $1 - (\arccos(c)/\pi)^n$. Moving on to the distribution of the length of the interval, which corresponds to the projection of $C_n$ onto $u$, that is the distribution of $\text{diam} \ (u, C_n)$, we can observe that $\text{diam} \ (u, C_n)$ attains values in $[0, 2]$ and that $\text{diam} \ (u, C_n) = \max_i \cos \theta_i - \min_i \cos \theta_i$, where we denote with $\theta_i$ independent and uniformly distributed random variables on $[0, 2\pi)$. We could now try to calculate the distribution of $\text{diam} \ (u, C_n)$ by controlling the maximum and minimum. Since, we are interested in getting a better understanding of the VC and Rademacher approach we use instead the uniform guarantees on $P_{n, u,c}$ where we let $\mathcal{H}$ be $\mathbb{R}^2$ with the usual inner product and associate to $u \in \mathbb{R}^2$ the function $\tilde{u}(x) = \langle u, x \rangle$ on $\mathbb{R}^2$. As usual let $\tilde{\mathcal{H}}$ be countably dense subset of $\mathcal{H}$ and define $\mathcal{F} = \{ f_{\tilde{u},c} : u \in \mathcal{H}, \|u\| = 1, -1 \leq c \leq 1 \}$ and $\tilde{\mathcal{F}} = \{ f_{\tilde{u},c} : u \in \tilde{\mathcal{H}}, \|u\| = 1, -1 \leq c \leq 1 \}$, where $f_{\tilde{u},c}(x) = \chi\{\tilde{u}(x) \leq c\} = \chi\{\langle u, x \rangle \leq c\}$. The family of functions $\tilde{\mathcal{F}}$ is a VC-subgraph class and on an event of probability at least $p$ it holds simultaneously for all $f_{\tilde{u},c} \in \tilde{\mathcal{F}}$ that

$$P_{n} f_{\tilde{u},c} \geq P_{f_{\tilde{u},c}} - n^{-1/2}\xi_n = 1 - \arccos(c)/\pi - n^{-1/2}\xi_n,$$

where $\xi_n = 12J(1) + \sqrt{2\log(1/p)(24J(1)n^{-1/2} + 1)} + \log(1/p)n^{-1/2}/3$. We use here that the uniform distribution on the unit circle is invariant under rotations, i.e. for a given $u$ let $A$ be the rotation matrix for which $Au = (1,0)^\top$. Then,

$$P_{f_{\tilde{u},c}} = \frac{1}{2\pi} \int_0^{2\pi} \chi\{\langle A\cos(\theta), \sin(\theta) \rangle \leq c\} = \frac{1}{\pi} \int_0^{\pi} \chi\{\cos(\theta) \leq c\}.$$

In other words, on an event of probability $p$, whenever $n$ is such that $n^{-1/2}\xi_n < 1/2$, and for any $c > \cos((1 - n^{-1/2}\xi_n)\pi)$ there will be a sample such that the inner product between $u$ and the sample is smaller than $c$. To be exact, let $c_0 < 0$ be a real number strictly larger than $\cos((1 - n^{-1/2}\xi_n)\pi)$ and let the above event be denoted by $B$. It holds that $P(B) \geq p$ and for any $\omega \in B$, $\min_{i\leq n} \langle u, X_i(\omega) \rangle \leq c_0$. In fact, the VC-argument shows that $B$ can be chosen such that $P(B) \geq p$ and for all $\omega \in B$,

$$\sup_{u \in \mathcal{H}, \|u\| = 1} \min_{i\leq n} \langle u, X_i(\omega) \rangle \leq c_0.$$

From this we can infer that a ball centered at the origin and of radius $c_0$ is contained in the empirical convex set $C_n(\omega)$, whenever $\omega \in B$: consider without loss of generality the vector $v = (c_0, 0)^\top$ and an element $\omega \in B$. There exist elements $X_j$ such that $X_j(\omega)$ lies
on the unit circle and \( \langle -v, X_j(\omega) \rangle \leq \epsilon_0^2 \), that is \( \langle v, X_j(\omega) \rangle \geq \|v\|^2 \). Let \( X_i(\omega) \) be such an element which also attains the maximum of the map \( j \mapsto \langle v, X_j(\omega) \rangle \).

Assume that \( X_i(\omega) \) does not lie in span \( v \) and that \( X_i(\omega) \) lies north of span \( v \), i.e. \( \langle X_i(\omega), (0,1)^T \rangle > 0 \). Consider the lines between \( X_i(\omega) \) and the elements \( X_j(\omega), j \leq n, j \neq i \). There will be an index \( j_0 \leq n, j_0 \neq i \), such that the line between \( X_i(\omega) \) and \( X_{j_0}(\omega) \) intersects with span \( v \). Consider the vector \( w = (0,-c_0)^T \). There will be a sample point \( X_{j_1}(\omega) \) such that \( \langle w, X_{j_1}(\omega) \rangle \geq \|w\|^2 \) and the line between \( X_i(\omega) \) and \( X_{j_1}(\omega) \) crosses span \( v \). Order the samples according to how large the inner product between the point of intersection of the line between the sample and \( X_i(\omega) \) and \( v \) is. Let \( X_{j_2}(\omega) \) be the maximum in this ordering. Assume that \( \langle X_{j_2}(\omega), v \rangle < \|v\|^2 \), that is the intersection lies to the left of \( v \). Let \( \hat{v} \) be the point on the circle with radius \( c_0 \) for which the line between \( X_i(\omega) \) and \( X_{j_2}(\omega) \) is tangent and which lies to the right of the line. There is now a point \( X_{j_3}(\omega) \) on the sphere such that \( \langle X_{j_3}(\omega), \hat{v} \rangle \geq \|\hat{v}\|^2 \). The point \( X_{j_3}(\omega) \) cannot lie north of \( v \) since this would contradict the maximality of \( X_i(\omega) \). However, if \( X_{j_3}(\omega) \) lies south of \( v \) then the line between \( X_{j_3}(\omega) \) and \( X_i(\omega) \) crosses span \( v \) further to the right than the line between \( X_{j_2}(\omega) \) and \( X_i(\omega) \) which contradicts the maximality of \( X_{j_2}(\omega) \).

Hence, we have either two points to the right of \( v \), one on the north side and one on the south side of the sphere, or the point \((1,0)^T\) is contained in the sample. By the same argument, either \((-1,0)^T\) is contained in the sample or there are two points left of \(-v\), one on the north side and one on the south side. The convex hull of these points is a subset of \( C_n(\omega) \) and contains \( v \).

To provide a concrete example, let \( p = 0.9 \) and observe that \( \hat{c} \) can be chosen as \( 10^{21} \). Then \( J(1) \leq 8 \vee 3 = 8 \) and \( \xi_n \leq 96 + \sqrt{2\log(10)(192n^{-1/2} + 1)} + n^{-1/2}\log(10)/3 \). Hence, a ball of radius 0.2 exists around the origin inside the empirical convex set with probability \( p \) for \( n \) being about 52000 or larger.

As expected \( n \) needs to be large to guarantee the existence of the ball or radius 0.2. Using \textit{Rademacher complexities} we can attain significantly tighter bounds in this setting.

Building up on our discussion and using \( m = 0 \) we can see that

\[
P_n \psi_\gamma(\langle u, \cdot \rangle - c) \geq P \psi_\gamma(\langle u, \cdot \rangle - c) - (\sqrt{2\log(1/p)} + 12/\gamma)n^{-1/2}.
\]

Finally, by using a rotation of \( u \) and with \( c_\gamma = (c - \gamma) \vee -1 \) it follows that

\[
P \psi_\gamma(\langle u, \cdot \rangle - c) = \frac{1}{\pi} \int_0^\pi \psi_\gamma(\cos(\theta) - c) = 1 - \frac{\arccos(c_\gamma)}{\pi} + \frac{1}{\pi\gamma} \int_{\arccos(c)}^{\arccos(c_\gamma)} \left( c - \cos(\theta) \right) \text{d}\theta \]
\[= 1 - \frac{\arccos(c_\gamma)}{\pi} \left( 1 - c/\gamma \right) - c \frac{\arccos(c)}{\pi \gamma} + \frac{1}{\pi \gamma} (\sqrt{1 - c^2} - \sqrt{1 - c_\gamma^2}).
\]

For instance, with \( \gamma = 1 \) and \( c < 0 \) this leads to

\[
P_n \psi_\gamma(\langle u, \cdot \rangle - c) \geq c \frac{1 - \arccos(c)}{\pi} + \frac{\sqrt{1 - c^2}}{\pi} - (\sqrt{2\log(1/p)} + 12)n^{-1/2}.
\]
The bound guarantees in this case a ball of radius 0.2 around the origin inside the empirical convex set with probability at least 0.9 when \( n \) is about 5000, a 10-fold improvement in the constant over the VC-bound. That being said, even a number as small as \( n = 10 \) suffices in experiments for the empirical convex set to contains a ball of radius 0.2 with high probability.

### 3.2.2 Example 2: Polytopes with finitely many extremes

Let us consider next a simple example of a polytope. Let \( C = \text{ch}\{x_i : i \leq m\} \) with \( x_1, \ldots, x_m \in \mathbb{R}^d \) and such that the random variable \( X \) attains values in \( x_1, \ldots, x_m \) and \( \Pr(X = x_i) \geq \alpha > 0 \) for all \( i \leq m \). Then for all \( u \in \mathcal{H}, \|u\| = 1, |c| \leq b \) either \( Pf_u,c = 0 \) or \( Pf_{u,c} \geq \alpha \). Hence, on \( A_x \), where \( x = n^{1/2} \), we have that \( Pf_{u,c} > 0 \) whenever

\[
n \geq \left( 12J(1) + \sqrt{2(24J(1) + 1)} + 1/3 \right)^2/\alpha^2.
\]

In other words, for \( n \) that large the empirical convex set equals \( C \) on an event of probability at least \( 1 - e^{-\sqrt{n}} \).

If each of the \( x_i \) is an extreme then we can compare this probability to the probability that in \( n \) independent trials all \( m \) extremes are drawn: the probability that element \( i \) is not drawn in \( n \) independent trials is \( 1 - \Pr(X = x_i)^n \) and the probability that at least one element \( i \) is not drawn is upper bounded by

\[
\Pr(\bigcup_{i \leq m} \{X_j \neq x_i\}) \leq \sum_{i \leq m} (1 - \Pr(X = x_i))^n \leq m(1 - \alpha)^n = m \exp(-\beta n).
\]

where \( \beta = -\log(1 - \alpha) \).

Consider now the special case of the \( d \)-dimensional simplex \( \text{ch} S \), with \( S = \{0, e_1, \ldots, e_d\} \) and \( e_1, \ldots, e_d \) being an orthonormal basis in \( \mathbb{R}^d \). Furthermore, assume that each \( x \in S \) has probability \( 1/(d + 1) \) to be sampled. The interior of the empirical convex set \( C_n \) is empty unless all points have been sampled. Hence, in this example either \( \text{int} C_n = \emptyset \) or \( C_n = C \) and the interior of \( n \) does not grow slowly in size as \( n \) increases but changes abruptly.

Let us now consider a rhombus given by \( C = \text{ch}\{e_1, -e_1, re_2, -re_2\} \) where \( e_1, e_2 \) are orthonormal vectors in \( \mathbb{R}^2 \) and \( r \in (0, 1) \). Furthermore, let \( X \) be uniformly distributed on the boundary of \( C \). We can again consider the functions \( f_{u,c} \) to measure the interior of the empirical convex set. However, in contrast to the unit circle the measure in direction \( u \) that lies \( c \) apart from the origin is not the same for all \( u \) but depends strongly on the direction. For instance, for direction \( -e_1 \) and \( c \in (0, 1) \) it holds that \( Pf_{-e_1,-c} = 2p(1-c)\sqrt{1+r^2} \), where \( p \) denotes here the density of the uniform distribution on the boundary, while for \( -e_2 \) we get \( Pf_{-e_2,-c'} = 2p(1-c'/r)\sqrt{1+r^2} \), for \( c' \in (0, r) \). In particular, for \( c = 0.9, c' = 0.9r \) the probabilities \( Pf_{-e_1,-c} \) and \( Pf_{-e_2,-c'} \) are equal and the probability \( Pf_{-e_1,-c} \), which is spread out over an interval of length 0.1 in direction \( e_1 \), is contained in an interval of length 0.1r in direction \( e_2 \) irrespective of how small \( r \) is.
3.2.3 Example 3: Image of a Lipschitz-continuous kernel function

Let us go back to the setting that we discussed at the beginning of the section. In detail, let \( k \) be a continuous kernel function on compact set \( \mathcal{X} \) that is upper bounded by \( b \). Furthermore, let us assume that the corresponding feature map \( \phi(x) = k(x, \cdot) \) is \( L \)-Lipschitz continuous with Lipschitz constant \( L > 0 \) and the law of \( X_1, \ldots, X_n \) has a density on \( \mathcal{X} \) which is lower bounded by \( b' > 0 \). We want to measure the size of the convex set relative to \( m \). For \( u \in \mathcal{H}, \|u\| = 1 \), let \( x_u \in \mathcal{X} \) be a point at which \( c_u := \langle u, \phi(x_u) - m \rangle = \max_{x \in \mathcal{X}} \langle u, \phi(x) - m \rangle \). And, as before, for \( c \in \mathbb{R} \) let \( f_{u,c} = \chi \{ \langle u, \phi(\cdot) - m \rangle \geq c \} \) and observe that \( \| \langle u, \phi(x_u) - \phi(x) \rangle \| \leq L \| x_u - x \| \). Therefore, with \( r_u = (c_u - c)/L \) and whenever \( c_u > c \),

\[
P_{f_{u,c}} \geq \int_{\mathcal{X}} b' \times \chi\{\langle u, \phi(x) - m \rangle \geq c\} dx \geq \int_{B(x_u, r_u) \cap \mathcal{X}} b' = b' \text{vol}(B(x_u, r_u) \cap \mathcal{X}).
\]

For example, when \( \mathcal{X} = [0, 1] \), \( u \) any element in \( \mathcal{H} \) with \( \|u\| = 1 \) and \( c < c_u \) such that \( x_u - (c_u - c)/L \geq 0 \), it follows that \( \text{vol}(B(x_u, r_u) \cap \mathcal{X}) \geq r_u \) and \( P_{f_{u,c}} \geq b'r_u = b'(c_u - c)/L \).

The bound on \( P_{f_{u,c}} \) is useful in conjunction with a metric entropy bound. If we want to rely instead on a Rademacher bound then applying \( \psi_{\gamma} \) to \( \langle u, \phi(\cdot) - m \rangle - c \) serves as an alternative to \( f_{u,c} \). Under the above Lipschitz assumption and for any \( u, \|u\| = 1 \), and whenever \( c_u \geq \gamma + c \),

\[
1 = \psi_{\gamma}(\langle u, \phi(x) - m \rangle - c) \\
\leq 0 \leq \langle u, \phi(x) - m \rangle - c - \gamma \\
\leq c_u - \gamma - c \geq \langle u, \phi(x_u) - \phi(x) \rangle \\
\leq c_u - \gamma - c \geq L \| x_u - x \|.
\]

Similarly, \( \psi_{\gamma}(\langle u, \phi(x) - m \rangle - c) > 0 \) whenever \( L \| x_u - x \| \leq c_u - c \). Let \( r_{u,1} = (c_u - c - \gamma)/L \) and \( r_{u,2} = (c_u - c)/L \). For \( x \in (B(x_u, r_{u,1}) \setminus B(x_u, r_{u,1})) \cap \{ x' : \langle u, \phi(x') - m \rangle \geq c + \gamma \} \) we have that \( \psi_{\gamma}(\langle u, \phi(x) - m \rangle - c) = 1 \geq (c_u - c - L \| x_u - x \|)/\gamma \). Similarly, for \( x \in (B(x_u, r_{u,2}) \setminus B(x_u, r_{u,1})) \cap \{ x' : \langle u, \phi(x') - m \rangle < c + \gamma \} \), \( \psi_{\gamma}(\langle u, \phi(x) - m \rangle - c) \geq (c_u - c - L \| x_u - x \|)/\gamma \). Hence, \( \psi_{\gamma}(\langle u, \phi(x) - m \rangle - c) \) is lower bounded by

\[
\chi\{x \in B(x_u, r_{u,1})\} + ((c_u - c - L \| x_u - x \|)/\gamma) \times \chi\{x \in B(x_u, r_{u,2}) \setminus B(x_u, r_{u,1})\}
\]

and

\[
\begin{align*}
P_{\psi_{\gamma}}(\langle u, \phi(\cdot) - m \rangle - c) & \geq b' \text{vol}(\mathcal{X} \cap B(x_u, r_{u,1})) \\
& \quad + b'(c_u - c)/\gamma (\text{vol}(\mathcal{X} \cap B(x_u, r_{u,2})) - \text{vol}(\mathcal{X} \cap B(x_u, r_{u,1}))) \\
& \quad - (Lb'/\gamma) \int_{\mathcal{X} \cap B(x_u, r_{u,2}) \setminus B(x_u, r_{u,1})} \| x_u - x \|.
\end{align*}
\]

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Furthermore, the following simple bound holds:

\[ P_{\gamma}(\langle u, \phi(\cdot) - m \rangle - c) \geq b' \text{vol}(X \cap B(x_u, r_{u,1})). \]

For example, when \( X = [0, 1] \), \( u \) any element in \( \mathcal{H} \) with \( \|u\| = 1 \), \( c + \gamma < c^*_u \), and such that \( x_u - (c^*_u - c)/L \geq 0 \), then

\[
P_{\gamma}(\langle u, \phi(\cdot) \rangle - m) \geq b' r_{u,1} + (b'/\gamma)(c^*_u - c)(r_{u,2} - r_{u,1}) - (Lb'/\gamma) \int_{r_{u,1}}^{r_{u,2}} x \]

These results can now be combined with the Rademacher bounds. However, to say anything concrete about the size of the empirical convex set some knowledge of \( c^*_u \) is required.

In the next section we will derive methods to measure the diameter of \( C \) in any direction, then we will derive lower bounds on \( c^*_u \) and we will combine these bounds in Section 3.5 with the bounds from this section.

### 3.3 Diameter of the convex set \( C \)

The diameter of a convex set plays an important role when trying to control the convergence behavior of various convex approximation algorithms. By the diameter of the convex set \( C = \text{cch} \{ \phi(x) : x \in X \} \), where \( X \) is as usual a measurable space and \( \phi \) is a feature map, we mean the size of the projection of \( C \) on a function of norm one within the RKHS corresponding to \( \phi \),

\[
\text{diam}_h(C) := \sup_{x \in X} \langle h, \phi(x) \rangle - \inf_{x \in X} \langle h, \phi(x) \rangle = \sup_{x \in X} h(x) - \inf_{x \in X} h(x),
\]

where \( h \in \mathcal{H}, \|h\| = 1 \).

There is a simple relationship between the diameter of the convex \( C \) in direction \( h \) and how close \( h \) is to a constant function. In the following, let \( 1 \) denote the function that is equal to one for all \( x \in X \) and let \( \|f\|_{\infty} = \sup_{x \in X} |f(x)| \) for any function \( f : X \to \mathbb{R} \), allowing for \( \|f\|_{\infty} = \infty \). For any \( h \in \mathcal{H}, \|h\| = 1 \),

\[
\text{diam}_h(C) = \frac{1}{2} \inf_{c \in \mathbb{R}} \|h - c1\|_{\infty},
\]

In particular, \( h \) is a constant function if, and only if, \( \text{diam}_h(C) = 0 \).

Small diameters of \( C \) in any direction \( h \) are a concern when trying to approximate \( m \) because various performance bounds of algorithms discussed in later sections depend on a lower bound on the diameter; the higher this lower bound the faster the convergence. To
be precise, the set $C$ can lie in an affine subspace that is not all of $H$ and the algorithms we study depend only on the affine subspace. Denote the closure of the affine span of $C$ by $\text{aff } C$. In other words, $\text{aff } C$ is the closure of $\{\alpha_1 h_1 + \ldots + \alpha_n h_n : n \in \mathbb{N}, h_i \in C, \alpha_i \in \mathbb{R} \text{ for all } i \leq n\}$ which is a closed affine subspace. Furthermore, let $U_C = \text{aff } C - f$, where $f$ is any element of $C$, then $U_C$ is a closed subspace of $H$. Observe that the dimension of $U_C^\perp$ is at most one since for $h \in U_C^\perp$ it holds that $h(x) = \langle h, \phi(x) \rangle = \langle h, \phi(y) \rangle = h(y)$ for all $x, y \in X$, and, hence, only constant functions can lie in $U_C^\perp$.

The key quantity which influences the behavior of the algorithms is now

$$\inf_{h \in U_C, \|h\| = 1} \text{diam}_h(C).$$

If $1$ lies in the RKHS then $1$, and all constant functions, lie in $U_C^\perp$ and we do not have to worry about them. The important question is now, how closely can an $h \in U_C, \|h\| = 1$, approximate a constant function.

Before leveraging Equation (3) for controlling the diameter of $C$ we recall some topological properties. If $X$ is compact and $\phi$ is continuous then $\phi[X]$ is compact [11, Thm. 3.1.10]. Due to Mazur’s Theorem $C = \text{cch } \phi[X]$ is then also compact [9, Thm. 12, p.51]. This implies, in particular, that there exists no norm ball inside $\phi[X]$, $\text{ch } \phi[X]$ or $\text{cch } \phi[X]$ whenever $H$ is infinite dimensional because a closed norm ball inside the compact set $\text{cch } \phi[X]$ would be compact [11, Thm. 3.1.2]. However, closed norm balls in infinite dimensional Hilbert spaces are not compact [26, S. 1.2.7]. Similarly, there exist no norm ball $B$ such that $B \cap \text{aff } C$ lies inside $C$.

Furthermore, whenever $H$ is infinite dimensional, $C$ is compact, $(e_n)_{n \geq 1}$ is an orthonormal sequence in $H$ and $\epsilon > 0$, it holds that for only finite many of the $e_n$ the diameter $\text{diam}_{e_n}(C)$ can be greater than $\epsilon$. Assume otherwise and let $I : \mathbb{N} \rightarrow \mathbb{N}$ be an enumeration of all the elements $e_n$ for which the diameter is greater than $\epsilon$. Furthermore, assume w.l.o.g. that $C$ is centered in the sense that for all $n \in \mathbb{N}$, $\sup_{u \in C} \langle u, e_I(n) \rangle + \inf_{u \in C} \langle u, e_I(n) \rangle = 0$. Since $C$ is compact $\sup_{u \in C} \langle u, e_I(1) \rangle$ is attained at some point $u_1 \in C$.

Inductively, we can select a countably infinite sequence of points $(u_n)_{n \geq 1} \in C$ such that $\|u_n - u_m\| \geq \epsilon/4 > 0$ whenever $n \neq m$: given points $u_1, \ldots, u_n$ there exists $m \in \mathbb{N}$ such that $\max_{i \leq n} \|\{u_i, e_I(m')\}\| \leq \epsilon/4$ for all $m' \geq m$. Let $u_{n+1}$ be a point in $C$ such that $\epsilon/2 \leq \sup_{u \in C} \langle u, e_I(m') \rangle = \langle u_{n+1}, e_I(m') \rangle$. Then $\|u_{n+1} - u_i\| \geq \epsilon/4$ for all $i \leq n$. Hence, we have countably infinitely many points with distance at least $\epsilon/4$ between them. These points give rise to an open cover of $C$ that does not contain a finite sub-cover, contradicting the compactness of $C$.

This last statement implies that whenever $H$ is infinite dimensional, $C$ is compact and $\|k\|_{\infty} < \infty$ then for any $\epsilon > 0$ there are infinitely many orthonormal elements $h_1, h_2, \ldots$ in $H$ such that for each $i$, $\sup_{x \in X} h_i(x) - \inf_{x \in X} h_i(x) \leq \epsilon$. Furthermore, at most one of the $h_i$’s can be constant, because if $h_i$ and $h_j$, $i \neq j$, were both constants then they clearly would not be orthogonal.
3.3.1 Interpolation spaces

Interpolation spaces are useful when trying to quantify the diameter of \( C \) because we can use them to measure how well the constant functions can be approximated. Consider 1 as an element of \( C(\mathcal{X}) \) and let \( \mathcal{H} \) be an RKHS that is continuously embedded in \( C(\mathcal{X}) \); for simplicity we will treat \( \mathcal{H} \) as a subset of \( C(\mathcal{X}) \). Furthermore, define for \( \theta \in (0,1) \) the interpolation space \( \mathcal{H}_\theta := (C(\mathcal{X}), \mathcal{H})_\theta = \{ f : \| f \|_\theta < \infty \} \), where \( \| f \|_\theta = \sup_{t>0} K(f,t)/t^\theta \) and \( K : C(\mathcal{X}) \times (0,\infty) \to \mathbb{R} \) is the K-functional defined by \( K(f,t) = \inf_{h \in \mathcal{H}}(\| f - h \|_\infty + t\| h \|). \) If 1 \( \in \mathcal{H}_\theta \) then for any \( r > 0 \) there exists an element \( h \in \mathcal{H}, \| h \| \leq r \), such that \( \| 1 - h \|_\infty \leq \| 1 \|^{1/(1-\theta)} r^{-2\theta/(1-\theta)} \). In particular, for any \( \epsilon > 0 \) there exists an \( r \) and \( h \in \mathcal{H}, \| h \| \leq r \), such that \( \| 1 - h \|_\infty < \epsilon \). Therefore, with \( c = 1/\| h \| \) and \( h^* = h/\| h \| \), i.e. \( \| h^* \| = 1 \), it holds that \( \| c1 - h^* \|_\infty < \epsilon \) and \( \text{diam}_h(C) \leq (1/\epsilon) \). If 1 itself does not lie in \( \mathcal{H} \) then \( h^* \) lies in the affine span of \( C \) and is a problematic direction.

In the finite dimensional case the situation is simpler. If \( \mathcal{H} \) is finite dimensional and if the constant function is not in \( \mathcal{H} \) then it is also not in any of the interpolation spaces since \( \mathcal{H}_\theta \) is a subset of the closure of \( \mathcal{H} \) in \( C(\mathcal{X}) \). But because \( \mathcal{H} \) is finite dimensional the closure of \( \mathcal{H} \) is equal to \( \mathcal{H} \), i.e. \( \mathcal{H}_\theta = \mathcal{H} \) for all \( \theta \in (0,1) \). The K-functional can be used in this case to quantify how well 1 can be approximated.

The K-functional has a few useful properties with regard to the constant function. Observe that \( K(1,1) \leq \| 1 - 0 \|_\infty = 1 \), which does not need any conditions on the kernel function. When \( \| k \|_\infty \leq 1 \) then we also have for any \( h \in \mathcal{H} \) that

\[
\| h - 1 \|_\infty + \| h \| \geq (1 - \| h \|) + \| h \| = 1
\]

since \( \| h \|_\infty \leq \| k \|_\infty^{1/2} \| h \| \leq \| h \|. \) Hence, \( K(1,1) = 1 \) whenever \( \| k \|_\infty \leq 1 \). It is straightforward to generalize this to any \( c \in \mathbb{R} \) whenever \( \| k \|_\infty < 1 \), i.e.

\[
K(c1, \| k \|_\infty^{1/2}) = c.
\]

(4)

Also, for any \( c \in \mathbb{R}, t > 0 \) we have the trivial bound \( K(c1,t) \leq c \). For \( t < \| k \|_\infty^{1/2} \) the value \( K(c1,t) \) can be smaller than \( c \). If \( K(c1,t) < c \) then for any \( \epsilon > 0 \) there exists a function \( h \in \mathcal{H}, h \neq 0 \), such that

\[
K(c1,t) + \epsilon \geq \| c1 - h \|_\infty + t\| h \|,
\]

and the norm of such an element \( h \) is bounded by

\[
\frac{c - K(c1,t) - \epsilon}{\| k \|_\infty^{1/2}} \leq \| h \| \leq \frac{K(c1,t) + \epsilon}{t}.
\]

Furthermore,

\[
K(c1,t) = |c| \inf_{h \in \mathcal{H}}(\| 1 - h/c \|_\infty + t\| h/c \|) = |c|K(1,t)
\]

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and a minimizer exists for $K(1, t)$ if, and only if, there exists a minimizer for $K(c1, t)$. The relation between these minimizers is straightforward: $h^*$ is a minimizer of $K(1, t)$ if, and only if, $ch^*$ is a minimizer of $K(c1, t)$.

When $\mathcal{H}$ is finite dimensional and $\|k\|_\infty < \infty$ then there exists a minimizer of the $K$-functional. For any $c \in \mathbb{R}, t > 0$,

$$K(c1, t) = \inf_{h \in \mathcal{H}} \|c1 - h\|_\infty + t\|h\| = \min_{h \in A} \|c1 - h\|_\infty + t\|h\|,$$

where $A = \{h : h \in \mathcal{H}, \|h\| \leq (c/t) \wedge (1 + K(c1, t)/t)\}$. This holds because $A$ is compact and $h \to \|c1 - h\|_\infty + t\|h\|$ is continuous whenever $\|k\|_\infty < \infty$. The norm of such a minimizer $h^*_{t,c}$ is bounded by $(c \wedge K(c1, t))/t$ (the additional one in the definition of $A$ is, in fact, unnecessary as the above argument shows that the infimum is attained). Hence, we have that

$$\frac{1 - K(1, t)}{\|k\|_\infty^{1/2}} \leq \frac{\|h^*_{t,c}\|}{c} \leq \frac{1 \wedge K(1, t)}{t}.$$

In fact, we can say more about the norm of $h^*_{t,c}$ in the finite dimensional case. Notice first that $\|h^*_{t,c}\|_\infty \leq 2c$ since otherwise 0 would be a better approximation of $c1$. Since the RKHS is finite dimensional this implies an upper bound on the RKHS-norm of $h^*_{t,c}$ as the next lemma shows. The lemma is actually of major importance in this paper and we develop it further than what is needed for the current discussion. In particular, the second part of the Lemma is concerned with the relation between $\|h\|_\infty$ and $\|h\|$ when Mercer’s theorem (e.g. [24 Thm.4.49]) applies. Recall that Mercer’s theorem provides us under certain conditions with orthonormal elements $e^*_1, \ldots, e^*_d$ in $L^2(\mathcal{X}, \mu)$, $\mu$ being a Borel measure on $\mathcal{X}$, where $e_1, \ldots, e_d$ are continuous functions and such that $\tilde{e}_i = \tilde{\lambda}_i e_i$ for all $i \leq d$, where $\tilde{\lambda}_1 \geq \ldots \geq \tilde{\lambda}_d > 0$, lie in the RKHS $\mathcal{H}$ and are an orthonormal basis of $\mathcal{H}$. The kernel function has to be continuous for Mercer’s theorem to hold. There are various forms of Mercer’s theorem together with a variety of assumptions for the theorems to hold. Instead of making such assumptions the following lemma assumes directly in its second part that the $e_1, \ldots, e_d$ exist and have the above properties.

**Lemma 1.** Let $\mathcal{X}$ be a set, $k$ a kernel on $\mathcal{X}$ such that the corresponding RKHS $\mathcal{H}$ is $d$-dimensional. For any $c \in \mathbb{R}$, $\{h : \|h\|_\infty \leq c\}$ is a compact subset of $\mathcal{H}$. Furthermore, for $h \in \mathcal{H}$ and any points $x_1, \ldots, x_d$ for which $k(x_1, \cdot), \ldots, k(x_d, \cdot)$ are linearly independent,

$$((\lambda_d/d)^{1/2} \|h\| \leq \|h\|_\infty,$$

where $\lambda_d$ is the minimal eigenvalue of the kernel matrix for the points $x_1, \ldots, x_d$.

Whenever $\mathcal{X}$ is a topological space, $k$ is a continuous kernel function on $\mathcal{X}$ and there exist continuous functions $e_i : \mathcal{X} \to \mathbb{R}, i \leq d$, and a Borel probability measure $\mu$ on $\mathcal{X}$ such that $e^*_i, \ldots, e^*_d$ are orthonormal in $L^2(\mathcal{X}, \mu)$, and $\{e_i\}_{i \leq d}$ is an orthonormal basis of $\mathcal{H}$ where $\tilde{e}_i = (\tilde{\lambda}_i)^{1/2} e_i$, for all $i \leq d$, and $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \ldots \geq \tilde{\lambda}_d > 0$, then

$$((\tilde{\lambda}_d)^{1/2} \|h\| \leq \|h\|_\infty.$$

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Proof. (a) For the first statement let $x_1, \ldots, x_d$ be such that $k(x_1, \cdot), \ldots, k(x_d, \cdot)$ are linearly independent. Observe that such points always exist: assume that $d' < d$ points $x_1, \ldots, x_{d'}$ exist such that any $k(x, \cdot)$ lies in the span of $k(x_1, \cdot), \ldots, k(x_{d'}, \cdot)$. Now any $h \in \mathcal{H}$ of the form $\sum_{j=1}^{N} \alpha_j k(z_j, \cdot)$ with coefficients $\alpha_j$ and $z_j \in \mathcal{X}$ can be written as a sum $\sum_{i=1}^{d'} \beta_i k(x_i, \cdot)$ with suitable coefficients $\beta_i$. The family of functions $h$ that can be written this way lies dense in $\mathcal{H}$, that is, span $\{k(x_i, \cdot) : i \leq d'\}$ is a dense subspace of $\mathcal{H}$. But this subspace is closed and therefore equal to $\mathcal{H}$. Hence, $\mathcal{H}$ is $d'$-dimensional contradicting our assumption about $\mathcal{H}$.

Consider the linear operator $A : \mathcal{H} \to \mathbb{R}^d$, defined for any $f \in \mathcal{H}$ by

$$Af = (f(x_1), \ldots, f(x_d))^\top = ((f, k(x_1, \cdot)), \ldots, (f, k(x_d, \cdot)))^\top.$$

The operator is bounded since $\|Af\|_{\mathbb{R}^d}^2 = \|f\|_2^2 \sum_{i=1}^{d} k(x_i, x_i)$ and $\|A\|_{op}^2 = \sum_{i=1}^{d} k(x_i, x_i)$.

$A$ is also injective. One way to see this is by means of Gram-Schmidt orthogonalization through which we gain an orthonormal basis $e_1, \ldots, e_d$ of $\mathcal{H}$ from $k(x_1, \cdot), \ldots, k(x_d, \cdot)$ and for any $f, g \in \mathcal{H}$ it holds that $f = g$ if, and only if, $\langle e_i, f \rangle = \langle e_i, g \rangle$ for all $i \leq d$ if, and only if, $\langle k(x_i, \cdot), f \rangle = \langle k(x_i, \cdot), g \rangle$ for all $i \leq d$.

Since $A$ is injective and the dimension of $\mathcal{H}$ is $d$ it follows that $A$ is surjective and invertible. By the open mapping theorem $A^{-1}$ is continuous and $A^{-1}([v : v \in \mathbb{R}^d, \|v\|_\infty \leq c])$ is a compact subset of $\mathcal{H}$.

(b) Let $K$ be the kernel matrix corresponding to the points $x_1, \ldots, x_d$. The rows of the kernel matrix are linearly independent since they are the images of the linearly independent elements $k(x_1, \cdot), \ldots, k(x_d, \cdot)$ under the isomorphism $A$. Hence, $K$ is invertible and for any $y \in \mathbb{R}^d$, with $\alpha = K^{-1}y$,

$$A(\sum_{i=1}^{d} \alpha_i k(x_i, \cdot)) = \sum_{i=1}^{d} \alpha_i (k(x_i, x_1), \ldots, k(x_i, x_d)) = \alpha^\top K = y.$$

In particular, for $f = \sum_{i=1}^{d} \alpha_i k(x_i, \cdot)$, with $\alpha_i \in \mathbb{R}$, it follows that $\alpha = K^{-1}A(f)$. We have a useful inner product on $\mathbb{R}^d$ given by $\langle x, y \rangle_{K^{-1}} = x^\top K^{-1}y$. For arbitrary $f, g \in \mathcal{H}$ with $f = \sum_{i=1}^{d} \beta_i k(x_i, \cdot)$ and $g = \sum_{i=1}^{d} \alpha_i k(x_i, \cdot)$,

$$\langle f, g \rangle = \beta^\top K \alpha = (K^{-1}A)^\top K(K^{-1}A) = (Af, Ag)_{K^{-1}}.$$

Applying this to $h$,

$$\|h\|^2 = (Ah)^\top K^{-1}(Ah) = \text{tr} (K^{-1}(Ah)(Ah)^\top) \leq \|K^{-1}\|_{op} (Ah)^\top (Ah) \leq d\|K^{-1}\|_{op} \|h\|_\infty^2.$$

(c) Now assuming that $k$ is continuous and the $e_1, \ldots, e_d$ have the assumed properties, we can write any $h \in \mathcal{H}$ as $h = \sum_{i=1}^{d} \alpha_i \tilde{e}_i$, $\sum_{i=1}^{d} \alpha_i^2 = \|h\|^2$, and

$$\|h\|_2^2 = \sum_{i=1}^{d} \alpha_i^2 \tilde{\lambda}_i \geq \tilde{\lambda}_d \|h\|^2.$$
Since \( \|h\|_2 \geq \hat{\lambda}_d \|h\| \) and \( \mu \) is a probability measure there has to be some point \( x \in \mathcal{X} \) at which \( |h(x)| \geq \hat{\lambda}_d \|h\| \).

\[ \square \]

**Example 1.** Consider the space \( \mathcal{X} = \{1, \ldots, d\} \) with kernel function \( k(x, y) = 1 \) if \( x = y \) and zero otherwise. Then \( \|h\|^2 = \sum_{i=1}^d |h(i)|^2 \) and if \( h(i) = c > 0 \) for all \( i \leq d \) then \( \|h\| = \sqrt{d} \|h\|_\infty \) which matches the bound if \( x_1 = 1, \ldots, x_d = d \).

Coming back to the case of \( \mathcal{H} \) being \( d \)-dimensional, \( \|k\|_\infty < \infty \) and \( x_1, \ldots, x_d \in \mathcal{X} \) be any points such that \( k(x_1, \cdot), \ldots, k(x_d, \cdot) \) are linearly independent and the kernel matrix is full rank. Furthermore, let \( \lambda_d \) be the smallest eigenvalue of the kernel matrix. Consider the map \( \psi(h) = \|1 - h\|_\infty \). By a similar argument as above we can infer that there exists a minimizer of \( \psi \). However, there is usually not a unique minimizer. Consider, for example, \( \mathcal{X} = [-1, 1] \) and the RKHS consisting of linear and quadratic functions such that \( x \mapsto x \) and \( x \mapsto x^2 \) both have norm 1. Then both of these functions minimize the distance to 1 as does 0. Any minimizer \( h \) of \( \psi \) has norm \( \|h\|_\infty \leq 2 \) and therefore, according to Lemma 1 it has a RKHS norm \( \|h\| \leq (Ad/\lambda_d)^{1/2} = r \). In particular, all minimizers of \( \psi \) are included in the compact ball \( B = \{h : h \in \mathcal{H}, \|h\| \leq r\} \). Let \( A \) be the set of all minimizers of \( \psi \) then \( A \) is itself a compact set: if \( A \) is finite then this follows right away. Otherwise, take a convergent sequence \( \{h_n\}_{n \in \mathbb{N}} \) in \( A \) and denote the limit by \( h \). Since for all \( x \in \mathcal{X}, |h(x) - 1| = \lim_{n \to \infty} |h_n(x) - 1| \leq \inf_{h \in \mathcal{H}} \|1 - h\|_\infty \) and \( h \in \mathcal{A} \). Finally, consider the norm as a function on \( A \). The norm is continuous and the image of the compact set \( A \) under the norm is a compact subset in \( \mathbb{R} \). Hence, there exists an element \( h^* \in A \) of maximal norm. Let us assume first that \( h^* \neq 0 \). For such an element \( h^* \) let \( b = 1/\|h^*\| \) and note that \( \|b1 - bh^*\|_\infty = \inf_{c \in \mathbb{R}} \min_{\|h\|=1} \|c1 - h\|_\infty \). Otherwise, there is an element \( \tilde{h}, \|\tilde{h}\| = 1 \) and \( c \) such that \( \|c1 - \tilde{h}\|_\infty < \|b1 - bh^*\| \). The constant \( c \) cannot be equal to \( b \) since then \( \|1 - \tilde{h}/b\|_\infty < \|1 - h^*\| \) in contradiction to our assumption on \( h^* \). It also cannot be larger than \( b \) because then \( \|1 - \tilde{h}/c\|_\infty < (b/c) \|1 - h^*\|_\infty < \|1 - h^*\|_\infty \) which is again in contradiction to \( h^* \) being a best approximation of 1. But \( c \) can also not be smaller than \( b \); whenever \( \|c1 - \tilde{h}\|_\infty \) is minimal it follows that \( \|1 - \tilde{h}/c\|_\infty \) is minimal and equal to \( \|1 - h^*\|_\infty \). But \( \|\tilde{h}/c\| = 1/c > 1/b = \|h^*\| \) in contradiction to the assumption that \( \|h^*\| \) has maximal norm within \( A \).

Hence,

\[ \lim_{t \to 0} K(b1, t) = \|b1 - bh^*\|_\infty = \inf_{c \in \mathbb{R}} \min_{\|h\|=1} \|c1 - h\|_\infty = 2 \inf_{\|h\|=1} \text{diam}_h(C) \]

and, since \( K(b1, t) = bK(1, t) \geq (1/r)K(1, t) \), it follows that

\[ \frac{1}{4} \left( \frac{\lambda_d}{d} \right)^{1/2} \lim_{t \to 0} K(1, t) \leq \inf_{\|h\|=1} \text{diam}_h(C). \]

(5)

If \( h^* = 0 \) then \( \lim_{t \to 0} K(1, t) = \|1\|_\infty = 1 \) but also for any \( c \in \mathbb{R}, h \in \mathcal{H}, \|c1 - h\|_\infty > \|c1\|_\infty \) since otherwise \( h/c \) would be a minimizer of norm greater zero contradicting the
assumption that \( h^* = 0 \) is the minimizer with largest norm. Hence, in this case,
\[
1 = \lim_{t \to 0} K(1, t) = 2 \inf_{\|h\| = 1} \text{diam}_h(C)
\]
and whenever \( \lambda_d \leq 4d \) this lower bound is larger then the left hand side of (5).

We can set in the above derivation \( r \) to \((4/\tilde{\lambda}_d)^{1/2}\) when Mercer’s theorem applies, where \( \tilde{\lambda}_d \) is the \( d \)-th eigenvalue of \( T_k \). The bound, when \( h^* \neq 0 \), then becomes
\[
(\tilde{\lambda}_d^{1/2}/4) \lim_{t \to 0} K(1, t) \leq \inf_{\|h\| = 1} \text{diam}_h(C)
\]
and lies below the bound for the case when \( h^* = 0 \) whenever \( \tilde{\lambda}_d \leq 4 \).

These results are only meaningful if \( 1 \) is not in the RKHS. In the next section we discuss an approach to remove constants from an RKHS which allows us, among other things, to extend these results to RKHSs that contain constants.

### 3.3.2 Adding and removing constants

It is sometimes useful to be able to remove constant functions from an RKHS or to add constant functions to an RKHS. There is an efficient way to do that by manipulating the kernel function.

In the following let \( \mathcal{X} \) be some topological space and consider the p.s.d. functions \( k : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) that lie in \( L^2(\mathcal{X} \times \mathcal{X}) \) and denote these by \( \mathcal{K} \). Furthermore, consider the partial order on \( \mathcal{K} \) given by \( k \succeq l \) if, and only if, \( k - l \) is p.s.d. where \( k, l \in \mathcal{K} \). Also note that \( \mathcal{K} \) is not a lattice, i.e. for \( k, l \in \mathcal{K} \) the infimum \( k \land l \) and the supremum \( k \lor l \) will generally not be defined.

For a function \( f : \mathcal{X} \to \mathbb{R} \) we let \( f \otimes f \) be the function that maps \((x, y)\) to \( f(x)f(y) \) for any \( x, y \in \mathcal{X} \). There is a simple criterion which tells us if \( f \in \mathcal{H}_k \) for a kernel function \( k \in \mathcal{K} \). Assume that \( f \otimes f \in L^2(\mathcal{X} \times \mathcal{X}) \), then \( f \in \mathcal{H}_k \) if, and only if, there exists a \( c > 0 \) with \( c^2 k \succeq f \otimes f \). In case that \( f \in \mathcal{H}_k \) it holds that \( \|f\|_k = \inf\{c : c^2 k \succeq f \otimes f\} \).

This observation motivates the following definitions. For an RKHS \( \mathcal{H} \) with kernel \( k \) that does not contain \( 1 \) let
\[
k^+ := k + 1 \otimes 1 \quad \text{and} \quad \mathcal{H}^+ := \mathcal{H}_{k^+}.
\]

The function \( k^+ \) is kernel function being the sum of the kernel functions \( k \) and \( 1 \otimes 1 \) and \( \mathcal{H}^+ \) is well defined. We denote the norm of \( \mathcal{H}^+ \) by \( \|\cdot\|_+ \) and we can observe that
\[
\|1\|_+ = \inf\{c : c^2 (k + 1 \otimes 1) \succeq 1 \otimes 1\} \leq 1.
\]

In fact, \( \|1\|_+ = 1 \) because otherwise there exists a \( c < 1 \) such that
\[
c^2 k \succeq (1 - c^2)1 \otimes 1 \quad \Rightarrow \quad \left(\frac{c}{\sqrt{1 - c^2}}\right)^2 k \succeq 1 \otimes 1 \quad \Rightarrow \quad 1 \in \mathcal{H}.
\]
We also have that $\mathcal{H} \subset \mathcal{H}^+$, since $k \leq k^+$, and for $h \in \mathcal{H}$,

$$\|h\|_+ \leq \|h\|. \quad (7)$$

When the RKHS $\mathcal{H}$ is finite dimensional then $\|h\|_+$ is actually equal to $\|h\|$. To show this we make use of the following lemma which is a simple extension of [20, Sec5.3].

**Lemma 2.** Let $h_1, \ldots, h_d$ be linearly independent functions mapping from some topological space $X$ to $\mathbb{R}$ and let $a_1, \ldots, a_d > 0$ then $\kappa = \sum_{i=1}^d a_i h_i \otimes h_i$ is a kernel function, the functions $h_i$ lie in $\mathcal{H}_\kappa$ and are orthogonal in $\mathcal{H}_\kappa$. Furthermore, the dimension of $\mathcal{H}_\kappa$ is $d$ and $\|h_i\|_\kappa = 1/\sqrt{a_i}$. 

Now, let $d < \infty$ be the dimension of $\mathcal{H}$, choose orthogonal functions $h_1, \ldots, h_d \in \mathcal{H}$, $h_1, \ldots, h_d \neq 0$, and define the kernel $\kappa = \sum_{i=1}^d (1/\|h_i\|^2) h_i \otimes h_i$. Then $k = \kappa$. This follows because, according to the above lemma, both spaces consist of span $\{h_1, \ldots, h_d\}$, $\|h_i\|_\kappa = \|h_i\|_k$, for all $i \leq d$, and the $h_i$’s are orthogonal in both spaces, i.e. $H_k = H_\kappa$ which implies that $k = \kappa$. The importance of this statement is that it shows that we can write the kernel as a finite sum of weighted tensor products.

From this description of $\kappa$ we also gain that $k^+ = \sum_{i=1}^d a_i h_i \otimes h_i + 1 \otimes 1$ and, because 1 is not in the original RKHS $\mathcal{H}$, it follows that 1 is linearly independent of $h_1, \ldots, h_d$ which implies that 1 is orthogonal to $h_1, \ldots, h_d$ in $\mathcal{H}^+$.

Consider now one of the $h_i$’s. We like to show that $\|h_i\|_+ \geq \|h_i\|$ which then implies, together with (7), that $\|h_i\|_+ = \|h_i\|$ and $\|h\|_+ = \|h\|$ for all $h \in \mathcal{H}$: the $h_i$’s are orthogonal in both $\mathcal{H}$ and $\mathcal{H}^+$. Let $l = k^+ - (1/\|h_i\|^2) h_i \otimes h_i$ so that $h_i \notin \mathcal{H}_l$. Furthermore, consider any $c$ such that $0 < c < \|h_i\|$. If $\|h_i\|_+ = c$ then

$$c^2 k^+ \geq h_i \otimes h_i \Rightarrow c^2 l \geq (1 - c^2/\|h_i\|^2) h_i \otimes h_i \Rightarrow \frac{c^2 \|h_i\|^2}{\|h_i\|^2 - c^2} \geq h_i \otimes h_i \Rightarrow h_i \in \mathcal{H}_l,$$

which is impossible and, therefore, $\|h_i\|_+ \geq \|h_i\|$.

Similarly, for an RKHS $\mathcal{H}$ that does contain 1 and is not of dimension 1 let

$$k^- = k - c^2 1 \otimes 1,$$

where $c = \inf \{\tilde{c} : c^2 k \geq 1 \otimes 1\}$, and $\mathcal{H}^- := \mathcal{H}_{k^-}$. \quad (8)

It follows right away that $1 \notin \mathcal{H}_-$ and because, $k^- \preceq k$ we know that $\mathcal{H}^- \subset \mathcal{H}$ and $\|h\|_- \leq \|h\|$ for all $h \in \mathcal{H}^-$. Next, notice that we can write $k = \sum_{i=1}^{d-1} a_i h_i \otimes h_i + c^2 1 \otimes 1$ where $h_1, \ldots, h_{d-1}, 1$ are orthogonal in $\mathcal{H}$ and $a_1, \ldots, a_{d-1} > 0$. Due to the orthogonality it follows that the $h_1, \ldots, h_{d-1}$ are linearly independent elements in $\mathcal{H}^-$ and $\mathcal{H}^-$ is $d-1$ dimensional. Lemma 2 tells us furthermore that $h_1, \ldots, h_{d-1}$ are orthogonal in $\mathcal{H}^-$. Finally, for all $i \leq d - 1$ we have that $\|h_i\|_- = \|h_i\|$; assume $c = 1$ and observe that in this case $(\mathcal{H}^-)^+ = \mathcal{H}$ and due to the above results for $\mathcal{H}^+$ we can conclude that $\|h_i\|_- = \|h_i\|_+ = \|h_i\|$. The above argument for $\mathcal{H}^+$ does not rely on $\|1\| = c = 1$ and we can generalize
then the best approximation error of \( f \) is

\[
\| f \| - \| h \| \text{ for all } h \in H.\]

We summarize these results for the case when \( H \) is finite dimensional in the following lemma.

**Lemma 3.** If \( H \) is a finite dimensional RKHS with dimension \( d \), kernel \( k \in K \), and which does not contain \( 1 \) then \( H^+ \), as defined in (6), is \( d + 1 \) dimensional, \( H \subset H^+ \), \( 1 \in H^+ \) with \( \| 1 \| = 1 \), \( \langle g, h \rangle = \langle g, h \rangle \) for all \( g, h \in H \), and \( 1 \) is orthogonal to all \( h \in H \). Similarly, if \( H \) is a finite dimensional RKHS with dimension \( d > 1 \), kernel \( k \in K \), and which does contain \( 1 \) then \( H^- \), as defined in (8), is \( d - 1 \) dimensional, \( H^- \subset H \), \( 1 \notin H^- \), \( \langle g, h \rangle = \langle g, h \rangle \) for all \( g, h \in H \) which are orthogonal to \( 1 \).

### 3.3.3 Lower bounds on the approximation error in finite dimensions

In finite dimensions we can now provide lower bounds on the approximation error of any function \( f : X \to \mathbb{R} \). Before specializing to constant functions we take a short detour and discuss the general technique. The approach to get lower bounds is the following: let \( k = \sum_{i=1}^{d} a_i h_i \otimes h_i \) for linearly independent \( h_1, \ldots, h_d \) and \( a_i > 0 \). If \( f \) is linearly dependent on the \( h_i \)'s then \( f \in H \). Otherwise, we can move to the kernel function \( k' = \sum_{i=1}^{d} a_i h_i \otimes h_i + f \otimes f \) and the corresponding RKHS \( H' \). The function \( f \) is orthogonal to \( h_1, \ldots, h_d \) in \( H' \). That means that the lowest approximation error, when approximating \( f \) by functions in the subspace corresponding to \( H' \), is given by the projection onto this subspace. Due to the orthogonality the projection of \( f \) onto this subspace is just the origin and the approximation error is \( \| f \|_{H'} = 1 \) when measured in the RKHS norm of \( H' \). If we consider the constraint that the approximation has to lie in \( H \) and has to have norm \( \| h \| = 1 \) then the best approximation error of \( f \) is \( \sqrt{2} \), i.e.

\[
\inf_{h \in H, \| h \|=1} \| f - h \|_{H'} = \sqrt{2}.
\]

To gain a lower bound on the approximation error in \( \| \cdot \|_\infty \) we use Lemma 1 which shows that

\[
\inf_{h \in H, \| h \|=1} \| f - h \|_\infty \geq \sqrt{2} \left( \frac{\lambda_{d+1}}{d + 1} \right)^{1/2},
\]

where we have \( d + 1 \) since we use the RKHS \( H' \). The constant \( \lambda_{d+1} \) is the smallest eigenvalue of a kernel matrix corresponding to points \( x_1, \ldots, x_{d+1} \) such that \( k'(x_1, \cdot), \ldots, k'(x_{d+1}, \cdot) \) are linearly independent. Notice, that this approximation error depends implicitly on the particular function \( f \) through the kernel matrix and the smallest eigenvalue. The bound can become loose when \( \| f \|_\infty \) is significantly larger than \( \| h_i \|_\infty \), but observe that we can always replace \( f \) by \( c f \) for some constant \( c < 1 \) to rescale the infinity norm. In the following, let \( k'' = \sum_{i=1}^{d} a_i h_i \otimes h_i + (c f) \otimes (c f) \) and treat \( H \) as a subset of \( H'' := H_{k''} \). Such a
rescaling leads to a problem in the constraint $\|h\| = 1$ because

$$\inf_{h \in \mathcal{H}, \|h\| = 1} \|cf - h\|_\infty = c \inf_{h \in \mathcal{H}, \|h\| = 1/c} \|f - h\|_\infty.$$  

We can compensate for this by using the constraint $\|h\| = c$. Since $\|cf\|_{\mathcal{H}'} = 1$,

$$\inf_{h \in \mathcal{H}, \|h\| = 1} \|f - h\|_\infty = \frac{1}{c} \inf_{h \in \mathcal{H}, \|h\| = c} \|cf - h\|_\infty \geq \frac{\sqrt{1 + c^2}}{c} \left(\frac{\lambda_{d+1}}{d + 1}\right)^{1/2},$$

where $\lambda_{d+1}$ is again the smallest eigenvalue of a kernel matrix but now for the kernel $k''$.

**Example 2.** Let $\mathcal{X} = \{0, 1\}$ and $h : \mathcal{X} \rightarrow \mathbb{R}$ be given by $h(0) = 1, h(1) = 0$, and let $f : \mathcal{X} \rightarrow \mathbb{R}$ be defined by $f(0) = 0, f(1) = r$ for $r > 0$. Let $\mathcal{H}$ be the RKHS with kernel $h \otimes h$ which consists of span \{h\}. The smallest approximation error of $f$ by elements in $\mathcal{H}$ which have norm $1$ is attained by $-h$ and $h$ and is equal to $\|f - h\|_\infty = r \vee 1$. Considering now the bound: let the kernel of the RKHS $\mathcal{H}'$ be $k = h \otimes h + f \otimes f$. Consider $x_1 = 0, x_2 = 1$ and the corresponding kernel matrix

$$K = \begin{pmatrix} h(0)^2 & 0 \\ 0 & f(1)^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & r^2 \end{pmatrix}$$

which has minimal eigenvalue $1 \wedge r^2$. The corresponding lower bound is

$$\inf_{g \in \mathcal{H}, \|g\| = 1} \|g - f\|_\infty \geq \sqrt{2} \left(\frac{1 \wedge r^2}{2}\right)^{1/2} = 1 \wedge r$$

which is exact when $\|f\|_\infty = 1$ but degrades for $r$ away from $1$.

Scaling $f$ by $c = 1/\|f\|_\infty = 1/r$ gives us the kernel $k' = h \otimes h + (1/r)^2 f \otimes f$ and a kernel matrix

$$K' = \begin{pmatrix} h(0)^2 & 0 \\ 0 & (1/r)^2 f(1)^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which has minimal eigenvalue $1$. The bound becomes

$$\inf_{g \in \mathcal{H}, \|g\| = 1} \|g - f\|_\infty \geq \sqrt{\frac{1 + r^2}{2}} \geq 1 \wedge r.$$

Coming now back to the approximation of constant functions. When $\mathcal{H}$ does not contain the constant functions then an approach to calculate lower bounds is to use the kernel $k_+$ and the corresponding RKHS $\mathcal{H}^+$. The norm of $c1$ in this RKHS, where $c \in \mathbb{R}$, is $|c|$ and for any such $c$,

$$\inf_{h \in \mathcal{H}, \|h\| = 1} \|h - c1\|_\infty \geq \frac{\sqrt{1 + |c|^2}}{|c|} \left(\frac{\lambda_{d+1}}{d + 1}\right)^{1/2} \geq \left(\frac{\lambda_{d+1}}{d + 1}\right)^{1/2}$$

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with \(d\) being the dimension of \(H\) and \(\lambda_{d+1}\) the lowest eigenvalue of a kernel matrix corresponding to points \(x_1, \ldots, x_{d+1}\) for the kernel \(k^+\). Using the right hand side as the lower bound has the advantage that we only deal with one RKHS, i.e. with \(H^+\), and we only need \(\lambda_{d+1}\) for that kernel. Scaling of the function \(1\) in dependence of which constant \(c\) we want to approximate might improve the lower bounds but then \(\lambda_{d+1}\) has to be calculated for the individual scalings.

When Mercer’s theorem applies we gain the bound

\[
\inf_{c \in \mathbb{R}} \inf_{h \in H, \|h\| = 1} \|h - c1\|_\infty \geq \hat{\lambda}_{d+1}^{1/2},
\]

where \(\lambda_{d+1}\) is the \((d+1)\)-th eigenvalue of \(T_{k^+}\). For Mercer’s theorem to apply it is important that \(k^+\) is continuous. But when \(k\) is continuous then so is \(k^+\).

If \(H\) already contains the constant functions then we are interested in determining the diameter of the convex set in the affine subspace spanned by \(C\). In particular, because \(\langle k(x, \cdot), 1 \rangle = 1\) for all \(x \in \mathcal{X}\), there exists a subspace \(S\) of \(H\) that is orthogonal to \(1\) and a \(c \neq 0\) such that \(\text{aff } C = \text{aff } \{k(x, \cdot) : x \in \mathcal{X}\} = c1 + S\). In fact, \(c = \arg \min_{c \in \mathbb{R}} \|k(x, \cdot) - c'1\|\), where we can use an arbitrary \(x \in \mathcal{X}\) and \(S = H^\perp\). This is exactly the same situation that we faced above with \(H^+\) and a lower bound on the diameter of the convex set in the affine space spanned by it can be gained through

\[
\inf_{c \in \mathbb{R}} \inf_{\|h\| = 1} \|h - c1\|_\infty \geq \left(\frac{\lambda_d}{d}\right)^{1/2},
\]

where \(d\) is the dimension of \(H\) and \(\lambda_d\) the smallest eigenvalue of any kernel matrix for kernel \(k\). If we can use Mercer’s theorem then we also gain the lower bound

\[
\inf_{c \in \mathbb{R}} \inf_{\|h\| = 1} \|h - c1\|_\infty \geq \hat{\lambda}_d^{1/2},
\]

where \(\hat{\lambda}_d\) is the \(d\)-th eigenvalue of \(T_k\).

We can now also extend the results from Section 3.3.1 on the application of K-functionals. We summarize in the following proposition these results together with a variety of results on the diameter of \(C\) that we derived up to now. We use the notation \(K_-(1, t)\) for the \(K\)-functional corresponding to \(H_\perp\). We hope that the use of the letter \(K\) for both the \(K\)-functional and the kernel matrix does not lead to confusion. To streamline the statement of the following proposition let us say that \(k\) has a \textit{Mercer decomposition with lowest eigenvalue} \(\hat{\lambda}_d\) if \(k\) is a continuous kernel function on \(\mathcal{X}\) and there exist continuous functions \(e_i : \mathcal{X} \to \mathbb{R}, i \leq d\), and a Borel probability measure \(\mu\) on \(\mathcal{X}\) such that \(e_1^*, \ldots, e_d^*\) are orthonormal in \(L^2(\mathcal{X}, \mu)\), \(\{\hat{e}_i\}_{i \leq d}\) is an orthonormal basis of \(H\), where \(\hat{e}_i = (\hat{\lambda}_i)^{1/2} e_i\), for all \(i \leq d\), and \(\hat{\lambda}_1 \geq \hat{\lambda}_2 \ldots \geq \hat{\lambda}_d > 0\).
Proposition 1. Let $\mathcal{X}$ be a measurable set and $k \in \mathcal{K}$ a kernel function defined on $\mathcal{X}$. The following holds.

1. If $\mathcal{H}$ is infinite dimensional, $\mathcal{X}$ is compact and $k$ is continuous, then for every $\epsilon > 0$ there exist infinitely many orthonormal elements $(e_n)_{n \geq 1}$ in $\mathcal{H}$ such that $\sup_{n \geq 1} \text{diam } e_n(C) < \epsilon$.

If $\mathcal{H}$ is finite dimensional with dimension $1 \leq d$ then the following hold.

2. If $1 \in \mathcal{H}$ for some $\theta \in (0, 1)$ then there exists $h \in \mathcal{H}$, $\|h\| = 1$, such that $\text{diam } h(C) = 0$.

3. If $1 \not\in \mathcal{H}$ then for any $x_1, \ldots, x_{d+1} \in \mathcal{X}$ and corresponding kernel matrix $K^+ = (k^+(x_i, x_j))_{i,j \leq d+1}$ with smallest eigenvalue $\lambda_{d+1}$,

$$\inf_{\|h\| = 1} \text{diam } h(C) \geq \frac{1}{2} \left( \frac{\lambda_{d+1}}{d+1} \right)^{1/2}.$$

4. If $1 \not\in \mathcal{H}$, $\|k\|_{\infty} < \infty$, then for any $x_1, \ldots, x_d \in \mathcal{X}$ and corresponding kernel matrix $K = (k(x_i, x_j))_{i,j \leq d}$ with smallest eigenvalue $\lambda_d \leq 4d$,

$$\inf_{\|h\| = 1} \text{diam } h(C) \geq \frac{1}{4} \left( \frac{\lambda_d}{d} \right)^{1/2} \lim_{t \to 0} K(1, t).$$

5. If $1 \in \mathcal{H}$ and $2 \leq d$, then for any $x_1, \ldots, x_d \in \mathcal{X}$ with corresponding kernel matrix $K = (k(x_i, x_j))_{i,j \leq d}$ and with the smallest eigenvalue of $K$ being $\lambda_d$,

$$\inf_{\|h\| = 1} \text{diam } h(C) \geq \frac{1}{2} \left( \frac{\lambda_d}{d} \right)^{1/2}.$$

6. If $1 \in \mathcal{H}$, $2 \leq d$, then for any $x_1, \ldots, x_{d-1} \in \mathcal{X}$ with corresponding kernel matrix $K^- = (k(x_i, x_j))_{i,j \leq d-1}$ and with the smallest eigenvalue of $K^-$ being $\lambda_{d-1} \leq 4(d-1)$,

$$\inf_{\|h\| = 1} \text{diam } h(C) \geq \frac{1}{4} \left( \frac{\lambda_{d-1}}{d-1} \right)^{1/2} \lim_{t \to 0} K^-(1, t).$$

In the following, let $\mathcal{X}$ be a compact space and $k$ a continuous kernel function on $\mathcal{X}$. The following hold.

7. If $k^+$ has a Mercer decomposition with lowest eigenvalue $\tilde{\lambda}_{d+1} \leq 4$ and $1 \not\in \mathcal{H}$ then

$$\inf_{\|h\| = 1} \text{diam } h(C) \geq (\tilde{\lambda}_{d+1}^{1/2}/2).$$
8. If \( k \) has a Mercer decomposition with lowest eigenvalue \( \tilde{\lambda}_d \leq 4 \) and \( 1 \not\in \mathcal{H} \) then
\[
\inf_{\|h\| = 1} \text{diam}_h(C) \geq (\tilde{\lambda}_d^{1/2}/4) \lim_{t \to 0} K(1, t).
\]

9. If \( k \) has a Mercer decomposition with lowest eigenvalue \( \tilde{\lambda}_d \leq 4 \) and \( 1 \in \mathcal{H} \) then
\[
\inf_{\|h\| = 1} \text{diam}_h(C) \geq (\tilde{\lambda}_d^{1/2}/2).
\]

10. If \( \mathcal{H} \) is \( d \geq 2 \) dimensional, \( k^- \) has a Mercer decomposition with lowest eigenvalue \( \tilde{\lambda}_{d-1} \leq 4 \) and \( 1 \not\in \mathcal{H} \) then
\[
\inf_{\|h\| = 1} \text{diam}_h(C) \geq (\tilde{\lambda}_{d-1}^{1/2}/4) \lim_{t \to 0} K_-(1, t).
\]

Example 3. Consider the kernels \( k_d(x, y) = \sum_{u=1}^{d} x^u y^u \), with \( x, y \in [-1, 1] \), which corresponds to polynomials of order 1 to 4 but without the constant functions. To test the kernel matrix based lower bound in a simple experiment we are calculating upper bounds on \( \inf_{c \in \mathbb{R}} \inf_{h \in \mathcal{H}} \|h - c1\|_{\infty} \) in the following way: the functions \( x^u \) and \( x^v \) are orthogonal in the corresponding RKHSs whenever \( u \neq v \) and have norm 1. Therefore, functions of the form \( (1/\sqrt{d}) \sum_{u=1}^{d} x^u \) have norm 1. To get a good approximation of constant functions we use such functions for \( d = 3, 4 \), with signs adjusted so that the different terms cancel each other as well as possible. In detail, for \( d = 1 \) we use the function \( h_1(x) = x \) which has approximation error 1 when approximating the (constant) function 0; for \( d = 2 \) we use \( h_2(x) = x^2 \); for \( d = 3 \) we use \( h_3(x) = (1/\sqrt{3})(x + x^2 - x^3) \); and for \( d = 4 \), \( h_4(x) = (1/\sqrt{4})(-x + x^2 + x^3 - x^4) \). The functions for \( d = 2, 3 \) and 4 are shown in Figure 4 in the left three plots in blue. The constant that are best approximated by these functions are shown in orange. In the right plot the corresponding approximation error in \( \| \cdot \|_{\infty} \) norm is plotted against \( d \) (top curve; orange). The blue curve in the right plot corresponds to the lower bound where we use \( -1 = x_1 < \ldots < x_d = 1 \) with equidistant spacing to get full rank kernel matrices.

3.3.4 Quantifying the diameter of the empirical convex set \( C_n \)

The subspace spanned by the empirical convex set \( C_n \) can be identified with an RKHS with kernel \( k' \) in such a way that \( C_n = C' := \text{ch} \{ k'(x, \cdot) : x \in \mathcal{X} \} \). This equivalence allows us to apply the techniques we developed for measuring the size of sets like \( C' \) to the empirical convex set \( C' \). We discuss this approach for the simplified case where the images of the data points are linearly independent and the constant functions do not lie in the RKHS \( \mathcal{H} \).
Assume that for $x_1, \ldots, x_n \in \mathcal{X}$ the elements $k(x_1, \cdot), \ldots, k(x_n, \cdot)$ are linearly independent and consider the map $A : \mathcal{H} \to \mathbb{R}^n$ from the proof of Lemma 1 for which $\langle g, h \rangle = \langle Ag, Ah \rangle_{K^{-1}}$ for all $g, h \in \text{span} \{ k(x_1, \cdot), \ldots, k(x_n, \cdot) \}$. Write the eigendecomposition of $K$ as $UDU^\top$ and observe that $K_{ij} = (KK^{-1}K)_{ij} = \langle Ak(x_i, \cdot), Ak(x_j, \cdot) \rangle_{K^{-1}}$. Hence, for $a_i = D^{-1/2}U^\top Ak(x_i, \cdot)$ and $h_i = A^{-1}a_i$,

$$\langle h_i, h_j \rangle = a_i^\top K^{-1}a_j = (D^{-1/2}U^\top KUD^{-1/2})_{ij} = \begin{cases} 1 \text{ if } i = j, \\ 0 \text{ otherwise,} \end{cases}$$

and the functions $h_1, \ldots, h_n$ are an orthonormal basis of the subspace of $\mathcal{H}$ that is spanned by $k(x_1, \cdot), \ldots, k(x_n, \cdot)$. Consider the kernel $k' = \sum_{i=1}^n h_i \otimes h_i$ which induces an RKHS $\mathcal{H}' \subset \mathcal{H}$ which is equivalent to the subspace and

$$\langle h_i, h_j \rangle_{\mathcal{H}'} = \delta_{ij} = \langle h_i, h_j \rangle$$

since $k'$ is a sum of tensor products $h_i \otimes h_i$. Therefore, for any $g, h$ in the subspace,

$$\langle g, h \rangle = \langle g, h \rangle_{\mathcal{H}'}.$$

This mean that the kernel $k'$ induces the subspace spanned by $k(x_1, \cdot), \ldots, k(x_n, \cdot)$ which is an RKHS in its own right. Whenever $k(x, \cdot) \in \mathcal{H}'$ it holds for all $h \in \mathcal{H}'$ that

$$\langle h, k(x, \cdot) \rangle_{\mathcal{H}'} = \langle h, k(x, \cdot) \rangle = h(x) = \langle h, k'(x, \cdot) \rangle_{\mathcal{H}'}.$$
and \( k(x, \cdot) = k'(x, \cdot) \). If \( \mathcal{H}' \neq \mathcal{H} \) then there are points \( x \in \mathcal{X} \) such that \( k(x, \cdot) \not\in \mathcal{H}' \). For such a point there exists an element in \( \mathcal{H}' \) that corresponds to the point-evaluator at \( x \) for elements in the subspace. That element is \( k'(x, \cdot) \) and for \( h \in \mathcal{H}' \)
\[
\langle k(x, \cdot), h \rangle = h(x) = \langle k'(x, \cdot), h \rangle_{\mathcal{H}'} = \langle k'(x, \cdot), h \rangle
\]
but \( k(x, \cdot) \neq k'(x, \cdot) \).

If \( \mathcal{H} \) does not contain constant functions then using the kernel \( (k')^+ \) with RKHS \( \mathcal{H}'^+ \), we can lower bound the diameter of \( C' \). The elements \((k')^+(x_1, \cdot), \ldots, (k')^+(x_n, \cdot)\) are linearly independent since
\[
a_1(k')^+(x_1, \cdot) + \ldots + a_n(k')^+(x_n, \cdot) = \sum_{i=1}^n a_i 1(\cdot) + \sum_{i=1}^n k'(x_i, \cdot)
\]
for \( a_1, \ldots, a_n \in \mathbb{R} \) is different from zero unless \( a_1 = \ldots = a_n = 0 \) since by assumption \( 1(\cdot), k'(x_1, \cdot), \ldots, k'(x_n, \cdot) \) are linearly independent. In particular, there is some \( x_{n+1} \in \mathcal{X} \) such that the kernel matrix \( ((k')^+(x_i, x_j))_{i,j \leq n+1} \) has full rank and the smallest eigenvalue of that matrix allows us to bound the diameter of the \( C' \).

In practice this approach is only applicable in the small sample regime since we need the smallest eigenvalue of the kernel matrix to control the diameter. This eigenvalue can be computed by applying the power iteration method. The power iteration returns the largest absolute value of a matrix. A standard way to find \( \lambda_0 \) is the following: apply the power iteration to \( K \) to find \( \lambda_1 \); then move to matrix \( B = K - \lambda_1 I \), which is negative definite, and apply the power iteration to get \( \lambda_d - \lambda_1 \). Each iteration of the power iteration relies on a multiplication of an \( n \times n \) matrix with a vector. This makes this method prohibitively costly to apply in the large sample regime.

### 3.3.5 Extremes of \( C \)

For the convex set \( C = \text{cch} \{ \phi(x) : x \in \mathcal{X} \} \) the extremes of \( C \) which are close to \( m \) are images under \( \phi \) of points \( x \) which lie close to each other. In detail, consider a kernel function with \( k(x, x) = 1 \) for all \( x \in \mathcal{X} \). Whenever \( \| \phi(x) - m \| < \epsilon \) and \( \| \phi(y) - m \| < \epsilon \) for some \( \epsilon > 0 \) then \( 4\epsilon^2 \geq \| \phi(x) - \phi(y) \| ^2 = 2(1 - k(x, y)) \). In other words, if there exists an extreme \( \phi(x_0) \) of \( C \) that lies \( \epsilon \) close to \( m \) then all the extremes of \( C \) that are \( \epsilon \) close to \( m \) are contained in
\[
\phi[\{ y : k(x_0, y) \geq 1 - 2\epsilon^2 \}].
\]

### 3.4 Locating \( m \)

For various convex approximation methods the “distance” from \( m \) to the boundary of the convex set characterizes the rate of convergence: the larger the distance the faster the rate
of convergence. A crude way to measure the distance is to consider the largest ball that fits within the convex set around \(m\) and, for the approximation methods that we consider, rates of convergence are known which depend on the size of this ball. Having a closed ball of size \(\delta > 0\) around \(m\) in \(C\) is equivalent to

\[
\inf_{\|h\|=1} \sup_{x \in X} \langle h, k(x, \cdot) - m \rangle \geq \delta.
\]

This can be seen in the following way: clearly when there exists a closed ball around \(m\) with the stated properties then for any \(h, \|h\| = 1\), some extreme of the convex set must fulfill (9). On the other hand, \(C - m\) is equal to the intersection of the closed half-spaces tangent to it [22, Thm18.8]. To each of these half-spaces there exists a normal \(h \in H, h \neq 0\), and an \(\alpha_h \in \mathbb{R}\) such that \(\langle g, h \rangle \leq \alpha_h\) whenever \(g \in C - m\). Without loss of generality we can assume that the normals have norm one and by assuming that (9) holds we know that for any such normal \(h, \alpha_h \geq \delta\). If there would not exist a ball of size \(\delta\) around \(m\) in \(C\) then there would be an element \(g \notin C - m, \|g\| \leq \delta\). But then \(\langle h, g \rangle \leq \delta\) for all \(h \in H, \|h\| = 1\), and \(g\) would lie in the intersection of the half-spaces and then also in \(C - m\) due to [22, Thm18.8] which cannot be.

In the previous section we quantified the diameter of the set \(C\) in direction \(h\), i.e. \(\text{diam}_h(C) = \sup_{x \in X, h(x)} h(x) - \inf_{x \in X} h(x)\). The diameter tells us how large a ball around \(m\) can be in the ideal case where \(m\) lies centered within \(C\), however, we do not know how centered \(m\) lies within \(C\). In [3] it was observed that when the probability measure corresponding to \(m\) has a density on \(X\) which is bounded away from 0 and \(H\) is finite dimensional then it is at least guaranteed that some open ball exists around \(m\) in \(C\). This result can be strengthened and turned into a quantitative statement by using a simple observation.

Consider first the Lebesgue integral on \(\mathbb{R}\). If we have a (non-atomic) probability measure on \(\mathbb{R}\) which has a mean value of 0 and there exists some measurable set \(B\) with \(\inf B \geq \epsilon\) and \(P(B) > 0\), then there will be probability mass on the negative axis to counter the “pull” from \(B\) since otherwise

\[
0 = \int_{\mathbb{R}} x \, dP = \int_{(0, \infty)} x \, dP \geq \int_{B} x \, dP \geq \epsilon P(B) > 0.
\]

This argument can also be applied to \(m\). Consider the set \(X = [0, 1]\), an RKHS \(H\) with continuous kernel function \(k(x, y)\) and assume that \(k(x, \cdot) \in L^1(P; H)\) with Bochner-integral \(m\) and the probability measure \(P\) has a density function that is bounded away from 0. For every \(y \in X\) with \((k(y, \cdot) - m, k(x, \cdot) - m) < 0\) there exists an \(x \in X\) such that \(\langle k(y, \cdot) - m, k(x, \cdot) - m \rangle < 0\). Otherwise, let \(\epsilon = \|k(y, \cdot) - m\|^2/2\) then \(B = \{x : \langle k(y, \cdot) - m, k(x, \cdot) - m \rangle > \epsilon\}\) is non-empty as \(y \in B\) and contains an open interval \(I\) of
$X$, with $P(I) > 0$. Hence, $P(B) > 0$ and because $\|m\|^2 = \int_X \langle m, k(x, \cdot) \rangle \, dP(x)$,

$$0 = \int_X \langle k(y, \cdot) - m, k(x, \cdot) - m \rangle \, dP(x) \geq \int_B \langle k(y, \cdot) - m, k(x, \cdot) - m \rangle \, dP(x)$$

$$\geq \epsilon P(B) > 0.$$ 

This implies that we have on both sides of $m$ (with respect to the direction $k(y, \cdot) - m$) elements of $\text{cch} \{k(x, \cdot) : x \in X\} = C$.

To provide lower bounds on the radius of a ball around $m$ in $C$ we need more. Ideally, we like to have assumptions on the kernel function and the measure which guarantee the existence of some strictly positive function $\psi : (0, \infty) \rightarrow (0, \infty)$ such that for any $h \in \mathcal{H}$, $\|h\| \leq 1$, $x \in X$, if $\langle h, k(x, \cdot) - m \rangle > 0$ then

$$\inf_{y \in X} \langle h, k(y, \cdot) - m \rangle \leq -\psi(\langle h, k(x, \cdot) - m \rangle).$$

Under a Lipschitz assumption on the functions in $\mathcal{H}$ we can provide such a function $\psi$. The Lipschitz assumption we are using is that any $h \in \mathcal{H}$ fulfills

$$\sup_{x \neq x'} \frac{|h(x) - h(x')|}{\|x - x'\|} \leq \|h\|L,$$

where $L > 0$ is the Lipschitz-constant. When the space $X$ is a compact subset of $\mathbb{R}$ this Lipschitz assumption is often fulfilled. For instance, when a polynomial or Gaussian kernel is used. In fact, whenever we have a well behaved domain $X$ this Lipschitz assumption is often fulfilled. For instance, when a polynomial or Gaussian kernel is used. In fact, whenever we have a well behaved domain $X$ like $[0, 1]^d$, $h \, | \, \text{int} \, X \in C^1(\text{int} \, X), h \in C(X)$ and $\|D_x h\|_{op} \leq \|h\|L$ (compare to [24, Cor.4.36]) then the condition is fulfilled.

In the following, $\beta_d$ denotes $d$-dimensional Lebesgue measure of the unit ball in $\mathbb{R}^d$ and $\lambda_d$ denotes Lebesgue measure.

**Proposition 2.** Let $X = \{0, 1\}^d$ and let $\mathcal{H}$ be an RKHS such that for all $h \in \mathcal{H}$ and $x, x' \in X$, $|h(x) - h(x')| \leq L\|h\||x - x'|$. Furthermore, $P$ be a probability measure on $X$ and assume that $P$ has a density $p$ with $\inf_{x \in X} p(x) \geq c > 0$. Then for any $h \in \mathcal{H}$, $\|h\| \leq 1$,

$$\max_{y \in X} \langle -h, k(y, \cdot) - m \rangle \geq \frac{c \gamma^{d+1}}{(d + 1)(2L)^d} \beta_d,$$

whenever there exists an $x \in X$ such that $\langle h, k(x, \cdot) - m \rangle \geq \gamma > 0$ and $\gamma/L \leq 1$.

**Proof.** Fix any $h$ in the unit ball of $\mathcal{H}$ and let $f(x) = \langle h, k(x, \cdot) - m \rangle$. Let $x^* \in X$ be a point at which $f(x^*) = \langle h, k(x^*, \cdot) - m \rangle \geq \gamma$. The function $f$ is also Lipschitz continuous with Lipschitz-constant $\|h\|L \leq L$ and $f$ is therefore non-negative on the set $A = \{y : \|y - x^*\| \leq \gamma/L, y \in X\}$. Let $B = \{y : \|y\| \leq \gamma/L, y \in X\}$ then $P(A) \geq \frac{c \gamma^{d+1}}{(d + 1)(2L)^d} \beta_d$. 

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\[ c \lambda_d(A) \geq c \lambda_d(B) \] because \( B \) minimizes the volume of the intersection of \( \mathcal{X} \) with a ball of radius \( \gamma/L \). Furthermore, \( \lambda_d(B) = (\gamma/2L)^d \beta_d \); this is the volume of a \( d \)-dimensional ball of radius \( \gamma/L \) scaled by \( 2^{-d} \). Now, integrating over \( A \) and using (14, 265G, 265H) again

\[
\int_A f(x) \, dP(x) \geq \int_{A-x^*} c(f(x^*) - L\|x\|) \, dx \geq c \int_B f(x^*) - L\|x\| \, dx
\]

\[
\geq \frac{c \gamma^{d+1}}{(2L)^d \beta_d} - c L 2^{-d} \frac{d}{d+1} \frac{\gamma^{d+1}}{L^{d+1} \beta_d} = \frac{c \gamma^{d+1}}{(2L)^d \beta_d} \left(1 - \frac{d}{d+1}\right).
\]

Since \( \int_X f(x) \, dP(x) = 0 \) there must be a point \( y \in \mathcal{X} \) such that

\[
f(y) \leq -\frac{c \gamma^{d+1}}{(2L)^d \beta_d} \left(\frac{1}{d+1}\right).
\]

Under the conditions of the proposition we can state a lower bound on the size of a ball included in \( C \) around \( m \). Let \( h \in \mathcal{H} \), \( \|h\| = 1 \), and assume w.l.o.g. that \( s := \sup_{x \in \mathcal{X}} \langle h, k(x, \cdot) - m \rangle \geq -\inf_{x \in \mathcal{X}} \langle h, k(x, \cdot) - m \rangle =: i \). Then \( s \geq (1/2) \text{diam}_h(C) \) and

\[
i \geq \frac{c s^{d+1}}{(d+1)(2L)^d \beta_d} \geq \frac{c ((1/2) \text{diam}_h(C))^{d+1}}{(d+1)(2L)^d \beta_d} \beta_d.
\]

If we have a lower bound \( b \) on \( \text{diam}_h(C) \) for all such \( h \) then we can conclude that there exists a ball of radius

\[
\delta = \min \{ (b/2), \frac{c (b/2)^{d+1} \beta_d}{(d+1)(2L)^d} \}
\]

around \( m \) in \( C \).

### 3.5 Locating \( m_n \) within the empirical convex set

We are now combining the various results we have derived. Section 3.4 allows us to refer the size of a ball within \( C \) around \( m \) back to the question of the diameter of \( C \). In Section 3.3 we derived various ways to lower bound the diameter of \( C \). We also know that \( C_n \) converges to \( C \). Section 3.2 contains various results on that. These results combine Rademacher or VC bounds with lower bounds on \( \text{P}_\psi, \langle \langle u, \phi(\cdot) - m \rangle \rangle - c \) and \( \text{P}_f u, c \). These lower bounds are closely related to the bounds in Section 3.4 since in both settings we need to measure how much probability mass lies in various directions behind some threshold. To get now high probability bounds for the existence of ball of a certain size around \( m_n \) within \( C_n \) we also need to control the convergence of \( m_n \) to \( m \). But that is easy to do with another VC or Rademacher argument. The following theorem combines now all these findings in
one statement under some natural conditions; in particular, that $\mathcal{X} = [0, 1]^l$, $\mathcal{H}$ is finite dimensional, that functions in $\mathcal{H}$ are Lipschitz continuous and that we have lower bound on the density of the law of $X_1, \ldots, X_n$ on $\mathcal{X}$. We also assume that $1 \in \mathcal{H}$ but the result can easily be adapted to the case of $1 \notin \mathcal{H}$.

**Theorem 1.** Let $\mathcal{X} = [0, 1]^l, l \geq 1$, and $k$ a continuous kernel function on $\mathcal{X}$ such that the corresponding RKHS $\mathcal{H}$ is $d$-dimensional, $1 \leq d < \infty$, functions $h \in \mathcal{H}$ are Lipschitz continuous in the sense of $(10)$ with Lipschitz constant $L > 0$, and $1 \in \mathcal{H}$. Furthermore, let $X_1, \ldots, X_n$ be i.i.d. random variables on some probability space $(\Omega, \mathcal{A}, P)$ such that the law of $X_1$ has a density $p$ on $\mathcal{X}$ and $\inf_{x \in \mathcal{X}} p(x) \geq c > 0$ for some constant $c$. Mercer’s theorem applies to $k$ and let $\tilde{\lambda}_d$ be the lowest eigenvalue of the Mercer decomposition and assume that $\tilde{\lambda}_d \leq 4$. Also, let $b = \tilde{\lambda}_d^{1/2} / 2$. There exists a ball of radius

$$\delta = (b/2) \wedge \frac{c(b/2)^{l+1} \beta_l}{(l+1)(2L)^l}$$

around $m$ in $C$ in the affine subspace spanned by $C$. Furthermore, for any $q \in (0, 1)$ and whenever

$$n > \left( \frac{\sqrt{2\log(1/q)} + 96\|k\|_\infty^{1/2}}{c\beta_l(\delta/8L)^l} \right)^2 \vee \left( \frac{4\|k\|_\infty^{1/2} + 3\sqrt{2\log(1/q)}}{\delta/4} \right)^2$$

then with probability $q$ there exists a ball of radius $\delta/4$ around $m_n$ in $C_n$ within the affine subspace spanned by $C$.

**Proof.** The existence of the ball around $m$ in $C$ has already been derived in earlier section and so has the bound on diameter in terms of the lowest eigenvalue of the Mercer decomposition.

(a) We start with high probability bounds for $\|m_n - m\|$ being small using Rademacher complexities. Let $\tilde{\mathcal{F}}$ be a dense subset of the unit ball of $\mathcal{H}$. Then for any $\alpha \in \mathbb{R}$,

$$\Pr \left( \|m_n - m\| \geq \alpha \right) = \Pr \left( \sup_{h \in \tilde{\mathcal{F}}} \left| \frac{1}{n} \sum_{i=1}^{n} f(X_i) - Pf \right| \geq \alpha \right)$$

since, $\|m_n - m\| = \sup_{h \in \tilde{\mathcal{F}}} \langle h, m_n - m \rangle$. In particular, for $\alpha = 4n^{-1/2}\|k\|_\infty$ we can infer from [5 Lem.22] and [15 Thm.3.4.5] that for any $q > 0$,

$$\Pr \left( \|m_n - m\| \geq (4\|k\|_\infty^{1/2} + 3\sqrt{2\log(1/q)})n^{-1/2} \right) \leq q. \quad (11)$$

(b) Next, we expand the argument from Section 3.2.3 to control the difference between $C_n$ and $C$. For any $\gamma > 0$ and with probability $q > 0$ simultaneously for all
\(c' \in [-\|k\|_{\infty}^{1/2}, \|k\|_{\infty}^{1/2}] \cap \mathbb{Q}\) and \(u \in \tilde{F}\),

\[
P_n \psi_\gamma((u, \phi(\cdot) - m) - c') \geq P \psi_\gamma((u, \phi(\cdot) - m) - c') - (\sqrt{2\log(1/q)} + 24\|k\|_{\infty}^{1/2}/\gamma)n^{-1/2}.
\]

We know that there is a ball of size \(\delta\) around \(m\) in \(C\). A simple way to use that fact is to let \(c' = \delta/2\) and \(\gamma = \delta/4\) and let \(x_0 \in \mathcal{X}\) be a point such that \(\langle u, \phi(x_0) - m \rangle \leq -\delta\). Then,

\[
P \psi_\gamma((u, \phi(\cdot) - m) - c') \geq P((u, \phi(X_1) - m) \leq -\gamma - c').
\]

As in the proof of Proposition 2 let \(A = \{y : \|y - x_0\| \leq \delta/4L, y \in \mathcal{X}\}\) and \(B\) the translation of \(A\) to the origin, \(B = \{y : \|y\| \leq \delta/4\}\). Then \(\lambda(A) = (\delta/8L)^l \beta_l\) and \(P(X_1 \in A) \geq c\lambda(A)\). Hence,

\[
P((u, \phi(X_1) - m) \leq -\gamma - c') \geq P(X_1 \in B) \geq c\beta_l(\delta/8L)^l.
\]

For a given \(q\) let

\[
N_q = \left(\frac{\sqrt{2\log(1/q)} + 96\|k\|_{\infty}^{1/2}/\delta}{c\beta_l(\delta/8L)^l}\right)^2
\]

then whenever \(n > N_q\) with probability \(q\) there is a ball of radius \(\delta/2\) around \(m\) in \(C_n\).

(c) Finally, we transfer the lower bound that we have for a ball within \(C_n\) around \(m\) to \(m_n\). For \(q \in (0, 1)\) let

\[
\tilde{N}_q = \left(\frac{4\|k\|_{\infty}^{1/2} + 3\sqrt{2\log(1/q)}}{\delta/4}\right)^2.
\]

Then for any \(n > \tilde{N}_q\) with probability at least \(q\), \(\|m_n - m\| \leq \delta/4\).

Bringing this together, with probability \(q\) there is ball of size \(\delta/4\) in \(C_n\) around \(m_n\) whenever \(n > \tilde{N}_{(1-q)/2} \vee \tilde{N}_{(1-q)/2}\).

The convergence of the empirical mean embedding and empirical convex set are both unproblematic in the large sample case. The bottleneck of the approach is rather the size of the convex set \(C\) itself.

### 4 Related approximation problems

When confronted with a concrete statistical problem it is typically insufficient to only approximate \(m\). For example, the least-squares error, when a regressor \(f\) from an RKHS \(\mathcal{H}\)
with kernel $k$ is used, is
\[
\frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} \langle f \otimes f, k(X_i, \cdot) \otimes k(X_i, \cdot) \rangle_\otimes - \frac{2}{n} \sum_{i=1}^{n} \langle f, Y_i k(X_i, \cdot) \rangle_\otimes + \frac{1}{n} \sum_{i=1}^{n} Y_i^2.
\]

The \textit{third term} in this sum is unproblematic since it does not depend on $f$ and can be summarized by a single real number. The \textit{first term} corresponds to an empirical covariance and can be treated in a similar way to the empirical measure, i.e.
\[
\frac{1}{n} \sum_{i=1}^{n} k(X_i, \cdot) \otimes k(X_i, \cdot)
\]
attains values in $\mathcal{H} \otimes \mathcal{H}$. It fact, since we are only interested in the terms $f^2(X_i)$, there is an RKHS that is better suited than $\mathcal{H} \otimes \mathcal{H}$. Due to [20, Thm.5.16] there exists a function $g \in \mathcal{H} \otimes \mathcal{H}$ such that $f^2(X_i) = g(X_i)$, where $\mathcal{H} \otimes \mathcal{H}$ is the RKHS that corresponds to the kernel function $\kappa(x, y) = k^2(x, y)$. The empirical covariance, when restricted to $\{(h, h) : h \in \mathcal{H}\}$, can be identified with
\[
\mathcal{C}_n = \frac{1}{n} \sum_{i=1}^{n} \kappa(X_i, \cdot) \in \mathcal{H} \otimes \mathcal{H},
\]
i.e. for any $h \in \mathcal{H}$,
\[
\langle \mathcal{C}_n, h^2 \rangle_{\mathcal{H} \otimes \mathcal{H}} = \frac{1}{n} \sum_{i=1}^{n} h^2(X_i) = \frac{1}{n} \sum_{i=1}^{n} \langle k(X_i, \cdot) \otimes k(X_i, \cdot), h \otimes h \rangle_\otimes.
\]

The random element $\mathcal{C}_n$ attains values within the empirical convex set
\[
C_{\otimes, n} := \text{cch} \{ \kappa(X_i, \cdot) : i \leq n \}.
\]
The corresponding population covariance operator is given by
\[
\mathcal{C} = \int_X \kappa(x, \cdot) \: dP(x)
\]
which is contained in the convex set
\[
C_\otimes = \text{cch} \{ \kappa(x, \cdot) : x \in \mathcal{X} \}.
\]
The \textit{second term} in the above sum is more difficult to deal with than the other two due to the elements $Y_i$. We are looking at two approaches in Section 4.2. In the first approach we consider $m_{y,n} = (1/n) \sum_{i=1}^{n} Y_i k(X_i, \cdot)$ as a subset of $\text{cch} \{ Y_i k(X_i, \cdot) : i \leq n \}$. That

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approach works well when we consider the approximation problem in isolation, but it does lead to complications when trying to approximate \( m_{y,n} \) simultaneously to \( C_n \). In the second approach we incorporate the \( Y_i \)'s into the kernel by using \( \langle Y_i, \cdot \rangle_H \otimes k(X_i, \cdot) \) and mapping \( f \in \mathcal{H} \) to \( \langle 1, \cdot \rangle_R \otimes f(\cdot) \in \mathbb{R}^n \otimes \mathcal{H} \), i.e. for \( i \leq n \),

\[
\langle 1, \cdot \rangle_R \otimes f(\cdot), \langle Y_i, \cdot \rangle_R \otimes k(X_i, \cdot) \rangle_{\mathbb{R}^n \otimes \mathcal{H}} = Y_i f(X_i) = \langle f, Y_i k(X_i, \cdot) \rangle.
\]

In this approach we are aiming to approximate

\[
m_{y,n}^\odot = \frac{1}{n} \sum_{i=1}^n \langle Y_i, \cdot \rangle_R \otimes k(X_i, \cdot) = \langle 1, \cdot \rangle_R \otimes m_{y,n}.
\]

In various settings we have to deal with multiple approximation problems. There are two high level approaches to that. We can either solve each approximation problem individually or we can solve them simultaneously. For example, in the least-squares problem we might like to use the same points \( X_i \) with the same weights \( w_i \) to approximate \( \mathcal{G}_n \) and \( m_{y,n} \) simultaneously. As we mentioned above this approach is facilitated by incorporating the \( Y_i \)'s into the kernel by using

\[
\langle \hat{h}, \kappa_g((y,x), (y,x)) \rangle_{\mathcal{H}^\odot \mathcal{H}} = \hat{h}(y,x).
\]

The empirical covariance operator now becomes

\[
\mathcal{C}_{y,n} = \frac{1}{n} \sum_{i=1}^n \kappa_g((Y_i, X_i), \cdot).
\]

One way to achieve a simultaneous approximation of \( \mathcal{C}_{y,n} \) and \( m_{y,n}^\odot \) is to use a direct sum \( \mathcal{G} = (\mathcal{H} \otimes \mathcal{H}) \oplus (\mathbb{R}^I \otimes \mathcal{H}) \) and consider the convex set

\[
C_{\odot,n} = \text{cch} \{ (\kappa((Y_i, X_i), \cdot), \langle Y_i, \cdot \rangle_R \otimes k(X_i, \cdot) : i \leq n \} \subset \mathcal{G}.
\]

The element that we like to approximate is in this context \( (\mathcal{C}_{y,n}, m_{y,n}^\odot) \) which lies in \( C_{\odot,n} \). Let \( (\tilde{\mathcal{C}}_{y,n}, \tilde{m}_{y,n}^\odot) \) be some element in \( \mathcal{G} \), then

\[
\| (\tilde{\mathcal{C}}_{y,n}, \tilde{m}_{y,n}^\odot) - (\mathcal{C}_{y,n}, m_{y,n}^\odot) \|^2_{\mathcal{H}^\odot \mathcal{H}} = \| \tilde{\mathcal{C}}_{y,n} - \mathcal{C}_{y,n} \|^2_{\mathcal{H}^\odot \mathcal{H}} + \| \tilde{m}_{y,n}^\odot - m_{y,n}^\odot \|^2_{\mathcal{H}^\odot \mathcal{H}}
\]

and a good approximation in \( \mathcal{G} \) guarantees good approximations of \( \mathcal{C}_{y,n} \) and \( m_{y,n}^\odot \) simultaneously.

There are some minimal assumptions that we need to impose on \( \mathcal{C}, m_y \) and variations thereof to be well defined. Generally, we assume that we have independent pairs of random variables \( (X, Y), (X_1, Y_1), \ldots \) defined on some probability space \( (\Omega, \mathcal{A}, \mathbb{P}) \). For \( \mathcal{C} \) to be well-defined it suffices to assume that \( \kappa(Y, \cdot) \in L^1(\mathbb{P} ; \mathcal{H} \otimes \mathcal{H}) \) and, similarly, for \( m_y \) it
suffices to assume that \( Y \in \mathcal{L}^2(\mathcal{P}) \) and \( k(X, \cdot) \in \mathcal{L}^2(\mathcal{P}; \mathcal{H}) \) since then \( \int \| Yk(X, \cdot) \| d\mathcal{P} \leq \| Y \|_2 \| k(X, \cdot) \|_2 < \infty \) and \( m_y = \int Yk(X, \cdot) d\mathcal{P} \in \mathcal{H} \).

Some further assumptions are useful to facilitate the following analyses. In particular, it is natural to assume that \( Y = f_0(X) + \epsilon \), where \( f_0 \) is a suitable function, \( \epsilon \) is a zero mean real-valued random variable representing measurement noise, and \( X \) and \( \epsilon \) are independent. When making this assumption we are assuming that \( \epsilon \) is a bounded random variable. We will highlight in the following discussions which of these assumptions we are making.

4.1 Covariance operators

The space \( \mathcal{H} \otimes \mathcal{H} \) is not just the RKHS corresponding to the kernel \( \kappa(x, y) = k^2(x, y) \) but it is also closely associated with the tensor product \( \mathcal{H} \otimes \mathcal{H} \). In particular, \( h \in \mathcal{H} \otimes \mathcal{H} \) if, and only if, \( h(x) = u(x, x) \) for some \( u \in \mathcal{H} \otimes \mathcal{H} \) and \( \| h \|_{\mathcal{H} \otimes \mathcal{H}} = \inf \{ \| u \|_{\mathcal{H} \otimes \mathcal{H}} : h(x) = u(x, x) \} \) [20, Thm.5.16]. Observe that for any \( h \in \mathcal{H} \otimes \mathcal{H} \) the set \( A_h := \{ u \in \mathcal{H} \otimes \mathcal{H} : h(x) = u(x, x) \} \) is a convex subset of \( \mathcal{H} \otimes \mathcal{H} \). Define the linear operator \( T : \mathcal{H} \otimes \mathcal{H} \to \mathcal{H} \otimes \mathcal{H} \) by \( Tu = u \circ \phi \) where \( \phi : \mathcal{X} \to \mathcal{X} \times \mathcal{X}, \phi(x) = (x, x) \), and observe that \( T \) is bounded since \( \| Tu \|_{\mathcal{H} \otimes \mathcal{H}} \leq \| u \|_{\mathcal{H} \otimes \mathcal{H}} \). Hence, \( A_h = T^{-1}(\{ h \}) \) is closed.

**Diameter of \( C_\circ \)** To determine the diameter of \( C_\circ \) we can either try to exploit the link to the tensor product or the characterization of \( \mathcal{H} \otimes \mathcal{H} \) as the RKHS with kernel \( \kappa \).

If we exploit the characterization of \( \mathcal{H} \otimes \mathcal{H} \) as the RKHS with kernel \( \kappa \) then we can use directly the approaches we developed for \( m \). For instance, if we have access to a Mercer decomposition of \( \kappa \) then we can use this to lower bound the diameter of the convex set \( C_\circ \).

On the other hand, making use of the tensor product characterization is, in fact, not straightforward. For instance, if \( h(x) = (f \otimes g)(x, x) \) for all \( x \) with \( f, g \in \mathcal{H} \) then

\[
\sup_{x \in \mathcal{X}} h(x) - \inf_{x \in \mathcal{X}} h(x) = \sup_{x \in \mathcal{X}} f(x)g(x) - \inf_{x \in \mathcal{X}} f(x)g(x)
\]

measures how constant \( f \times g \) is. In particular, the difference is small for a \( f, g \) if there is a constant \( c \) such that \( f \approx c/g \).

Furthermore, the elements in \( \mathcal{H} \otimes \mathcal{H} \) are limits of linear combinations \( \sum_{i=1}^n \alpha_i f_i \otimes g_i \), where \( n \in \mathbb{N}, \alpha_i \in \mathbb{R} \) and \( f_i, g_i \in \mathcal{H} \) for all \( i \leq n \), and not just simple tensors \( f \otimes g \). This complicates the situation further since terms \( \alpha_i f_i \otimes g_i \) might cancel with \( \alpha_j f_j \otimes g_j \) terms, \( j \neq i \), at some \( x \in \mathcal{X} \).

The situation simplifies if we consider tensors of the form \( f \otimes f, f \in \mathcal{H}, \| f \otimes f \| =...
1 = \|f\|. The diameter of \( C_\oplus \) in direction \( h \), where \( h(x) = (f \otimes f)(x,x) \) for all \( x \in \mathcal{X} \), is
\[
\text{diam}_h C_\oplus = \sup_{x \in \mathcal{X}} h(x) - \inf_{x \in \mathcal{X}} h(x) \\
= \sup_{x \in \mathcal{X}} (f \otimes f, k(x,\cdot) \otimes k(x,\cdot))_\oplus - \inf_{x \in \mathcal{X}} (f \otimes f, k(x,\cdot) \otimes k(x,\cdot))_\oplus \\
= \sup_{x \in \mathcal{X}} f^2(x) - \inf_{x \in \mathcal{X}} f^2(x).
\]

If \( \mathcal{X} \) is convex, \( k \) is continuous and, hence, \( f \) is continuous, then we can relate \( \text{diam}_h C_\oplus \) to \( \text{diam}_f(C) \): whenever there exist \( x, x' \in \mathcal{X} \) such that \( f(x) > 0 > f(x') \), then there also exists an \( \tilde{x} \in \mathcal{X} \) with \( f(\tilde{x}) = 0 \) due to the mean value theorem. In this case,
\[
\text{diam}_h C_\oplus \geq (\sup_{x \in \mathcal{X}} f(x) \vee - \inf_{x \in \mathcal{X}} f(x))^2 \geq ((1/2)\text{diam}_f(C))^2.
\]

If there is no \( x \) such that \( f(x) = 0 \), that is \( f \) attains only positive or only negative values, then we can argue in the following way. W.l.o.g. assume that \( f \) attains only positive values. Since for \( a, b \geq 0, a \geq b \), it holds that \( a^2 - b^2 \geq ((1/2)(a-b))^2 \), it follows that
\[
\text{diam}_h C_\oplus \geq ((1/2)\text{diam}_f(C))^2.
\]

This lower bound can fail to hold when the assumptions about \( k \) and \( \mathcal{X} \) are not fulfilled. Consider \( \mathcal{X} = \{-1, 1\} \) with \( k(x,y) = \delta_{x,y} \) and \( f = k(1,\cdot) \circ k(-1,\cdot) \) which lies in the RKHS. For this \( f \) we have that
\[
\sup_{x \in \mathcal{X}} f^2(x) - \inf_{x \in \mathcal{X}} f^2(x) = 0 < 1 = ((1/2)(\sup_{x \in \mathcal{X}} f(x) - \inf_{x \in \mathcal{X}} f(x)))^2.
\]

The factor \( 1/2 \) in the lower bound is redundant when \( f \) attains only positive or negative values since \( a^2 - b^2 \geq (a-b)^2 \) whenever \( a \) and \( b \) have the same sign. More importantly, the bound becomes loose when \( \inf_{x \in \mathcal{X}} f^2(x) \) is large since \( a^2 - b^2 - (a-b)^2 = 2b(a-b) \) whenever \( a \geq b > 0 \).

### 4.2 Weighted mean embedding

We discuss two closely related approaches to deal with \( Y_i k(X_i,\cdot), i \leq n \). In each of the two approaches we first look at the general situation where the \( Y_i \) do not have a particular structure before specializing to the case where we have observations \( Y_i = f_0(X_i) + \epsilon_i \), \( i \leq n \), the \( X_i \)'s and \( \epsilon_i \)'s are i.i.d. and independent of each other. Furthermore, we assume that the \( \epsilon_i \)'s have mean zero, that \( f_0(X_i) \in \mathcal{L}^2(P) \) and \( k(X_i,\cdot) \in \mathcal{L}^2(P; \mathcal{H}) \).
4.2.1 First approach

A simple approach to deal with the empirical version \( m_{y,n} = (1/n) \sum_{i=1}^{n} Y_i k(X_i, \cdot) \) is to consider the empirical convex set

\[
C_{y,n} = \text{cch} \{ Y_i k(X_i, \cdot) : i \leq n \}.
\]

We controlled the rate of convergence for the empirical measure \( m_n \) by linking it to \( m \) and by comparing the empirical convex set \( C_n \) to a limiting set \( C \). The limit of \( m_{y,n} \) is easy to define whenever \((X_i, Y_i)\) are i.i.d., \( Y_i \in L^2(P) \) and \( m_y \) is the limit of \( m_{y,n} \).

Dealing with \( C_{y,n} \) is more difficult mainly because it is not directly obvious what a natural characterization of the limiting set is. For example, if the \( Y_i \) are unbounded then the limiting set will be unbounded in certain directions. Even when the \( Y_i \) are bounded there is another difficulty in that \( Y_i \) might attain very different values depending on \( X_i \).

The problem simplifies if the \( Y_i \)'s are of the form \( f_0(X_i) + \epsilon_i \) where \( f_0 \in L^2(P) \), \( \epsilon_i \) is independent of \( X_i \) and \( E(\epsilon_i) = 0 \) since then \( m_y \in H \) and

\[
m_y = \int f_0(X_1) k(X_1, \cdot) dP.
\]

Furthermore, if \( f_0 \) and the random variables \( \epsilon_i \) are bounded then we can characterize the limit of \( C_{y,n} \). Let \( \bar{b} = \inf \{ b : b \in \mathbb{R}, \epsilon_i \leq b \text{ a.s.} \} \), \( \underline{b} = -\sup \{ b : b \in \mathbb{R}, \epsilon_i \geq b \text{ a.s.} \} \) and

\[
C_y = \text{cch} \{ (f_0(x) + \bar{b}) k(x, \cdot) : x \in \mathcal{X} \} \cup \{ (f_0(x) - \underline{b}) k(x, \cdot) : x \in \mathcal{X} \}
\]

with \( \mathcal{X} \) being the support of push-forward measure \( P \circ X^{-1} \). Furthermore, \( C_y \supset C_{y,n} \supset m_{y,n} \) almost surely as well as \( m_y \in C_y \).

**Diameter of \( C_y \).** The diameter of the convex set \( C_y \) can be lower bounded by observing that

\[
\text{diam}_h(C_y) = \sup_{x \in \mathcal{X}} \langle h, (f_0(x) + \bar{b}) k(x, \cdot) \rangle - \inf_{x \in \mathcal{X}} \langle h, (f_0(x) + \bar{b}) k(x, \cdot) \rangle
\]

\[
= \sup_{x \in \mathcal{X}} (f_0(x) + \bar{b}) h(x) - \inf_{x \in \mathcal{X}} (f_0(x) + \bar{b}) h(x) \geq (\bar{b} - \underline{b}) \sup_{x \in \mathcal{X}} |h(x)|
\]

and lower bounds on \( \text{diam}_h(C) \) provide lower bounds on \( \text{diam}_h(C_y) \) since

\[
\sup_{x \in \mathcal{X}} |h(x)| \geq (1/2) \text{diam}_h(C).
\]

Observe that if there is no noise then \( \bar{b} = \underline{b} \) and the lower bound is zero. In fact, there are functions \( f_0 \) for which this is the true diameter in direction \( h \). In particular, if \( h \) is invertible then for \( f_0 = h^{-1} \) it follows that \( \text{diam}_h(C_y) = 0 \).
4.2.2 Second Approach

When mapping $f \in \mathcal{H}$ to $\langle 1, \cdot \rangle \otimes f(\cdot)$ then

$$m_y \otimes y = \int \langle Y, \cdot \rangle \otimes k(X, \cdot) \, dP = \langle 1, \cdot \rangle \otimes \int Y k(X, \cdot) \, dP = \langle 1, \cdot \rangle \otimes m_y$$

due to (1). The element $m_y \otimes y$ lies in $\mathbb{R}' \otimes \mathcal{H}$ whenever $Y^2k(X, X) \in L^1(P)$.

Under the additional assumption that $Y = f_0(X) + \epsilon$ and $X, \epsilon$ are independent random variables the representation of $m_y \otimes y$ simplifies to

$$m_y \otimes y = \int \langle f_0(X) + \epsilon, \cdot \rangle \otimes k(X, \cdot) \, dP$$

where we used (1) in the second and in the last equality.

The natural convex set that contains $m_y$ is now $C^\otimes_y = \text{cch} \{ \langle f_0(x) + z, \cdot \rangle \otimes k(x, \cdot) : x \in X, \bar{b} \leq z \leq \bar{b} \}$.

Diameter of $C^\otimes_y$. The diameter of $C^\otimes_y$ in direction $u = \langle 1, \cdot \rangle \otimes h \in \mathbb{R}' \otimes \mathcal{H}$, $h \in \mathcal{H}$, $\|h\| = 1$, is now

$$\sup_{x \in X, z \in E} \langle u, \langle f_0(x) + z, \cdot \rangle \otimes k(x, \cdot) \rangle \otimes - \inf_{x \in X, z \in E} \langle u, \langle f_0(x) + z, \cdot \rangle \otimes k(x, \cdot) \rangle \otimes$$

$$= \sup_{x \in X, z \in E} (f_0(x) + z) h(x) - \inf_{x \in X, z \in E} (f_0(x) + z) h(x) \geq (\bar{b} - \bar{b}) \sup_{x \in X} |h(x)|$$

as in the first approach. Hence, $\text{diam}_u(C^\otimes_y) \geq (1/2)(\bar{b} - \bar{b}) \text{diam}_h(C)$.

4.3 Simultaneous approximation

One of the main challenges when trying to control the approximation error of $c_n$ and $m_{y,n}$ simultaneously is to determine the size of the convex set that contains $(c_n, m_{y,n})$ and to locate $(c_n, m_{y,n})$ within the convex set. The problem would be easier if we could identify the direct sum space with an RKHS and apply the techniques that we have developed for RKHSs. When using the first approach for $m_{y,n}$ we face directly a problem in that we will gain some weighted sum of $(\kappa(X_i, \cdot), k(X_i, \cdot))$ as an approximation, but we need a
weighted sum of \((\kappa(X_i, \cdot), Y_i k(X_i, \cdot))\). This problem can be circumvented by incorporating the \(Y_i\)'s into the kernel as we have done in the second approach, i.e. let

\[
k_y((y_1, x_1), (y_2, x_2)) = y_1y_2k(x_1, x_2) = \langle \langle y_1, \cdot \rangle_\mathbb{R} \otimes k(x_1, \cdot), \langle y_2, \cdot \rangle_\mathbb{R} \otimes k(x_2, \cdot) \rangle \otimes
\]

then \(k_y\) is a kernel function on \(\mathbb{R} \times \mathcal{X}\). It helps to also extend \(\kappa\) to \(\mathbb{R} \times \mathcal{X}\) by setting

\[
\kappa_y((y_1, x_1), (y_2, x_2)) = \kappa(x_1, x_2).
\]

When \(\hat{h}\) is the extension of \(h \in \mathcal{H}_\kappa\) to \(\mathbb{R} \times \mathcal{X}\) then \(\|\hat{h}\|_{\mathcal{H}_\kappa} = \|h\|_{\kappa}\). For finite linear combinations this follows from \(\| \sum_{i=1}^n \alpha_i \kappa_y((y_i, x_i), \cdot) \|_{\kappa_y}^2 = \sum_{i,j=1}^n \alpha_i \alpha_j \kappa_y((y_i, x_i), (y_j, x_j)) = \| \sum_{i=1}^n \alpha_i \kappa(x_i, \cdot) \|_{\kappa}^2\), where \(n \in \mathbb{N}, \alpha_i \in \mathbb{R}, x_i \in \mathcal{X}, y_i \in \mathbb{R}\) for all \(i \leq n\) and extends to all of \(\mathcal{H}_\kappa\) by a denseness argument. By a similar argument we can see that the extension map is also surjective.

Observe that \(\mathcal{H} \odot \mathcal{H}\) and \(\mathcal{H}' \otimes \mathcal{H}\) are linearly independent, i.e. \((\mathcal{H} \odot \mathcal{H}) \cap (\mathcal{H}' \otimes \mathcal{H}) = \{0\}\), because \(\kappa_y((x_1, y_1), (x_2, y_2))\) does not depend on the values \(y_1, y_2\) while \(k_y\) does. Due to this linear independence we have that \(\mathcal{K} := (\mathcal{H} \odot \mathcal{H}) \oplus (\mathcal{H}' \otimes \mathcal{H})\) is isometrically isomorphic to \(\mathcal{H}_{\kappa_y+k_y}\). Let \(\mathcal{G} = \{g + h : (g, h) \in \mathcal{K}\}\) with norm \(\|f\|_{\mathcal{G}} = \inf\{\|\langle g, h \rangle\|_{\kappa} : g + h = f, (g, h) \in \mathcal{K}\}\). There exists a surjective isometry between \(\mathcal{K}\) and \(\mathcal{G}\). Because \(\mathcal{H} \odot \mathcal{H}\) and \(\mathcal{H}' \otimes \mathcal{H}\) are linearly independent there is for every \(f \in \mathcal{G}\) exactly one pair \((g, h) \in \mathcal{K}\) such that \(g + h = f\) and \(\|f\|_{\mathcal{G}} = \|(g, h)\|_{\kappa}\). Furthermore, we have an inner product on \(\mathcal{G}\) which is given by \(\langle f_1, f_2 \rangle_{\mathcal{G}} = \langle (g_1, h_1), (g_2, h_2) \rangle_{\kappa}\) whenever \(f_1 = g_1 + h_1\) and \(f_2 = g_2 + h_2\). For \((g, h) \in \mathcal{K}\) we have that \(g \in \mathcal{H}_{\kappa_y}\) and \(h \in \mathcal{H}_{k_y}\). By \([2] Thm.,p.353\) the kernel \(\kappa_y + k_y\) is the kernel of \(\mathcal{G}\) and, therefore, \(\mathcal{H}_{\kappa_y+k_y}\) is isometrically isomorphic to \(\mathcal{K}\). We summarize this finding in the following lemma.

**Lemma 4.** Let \(\mathcal{X}\) be a measurable space and \(k\) a measurable kernel function on \(\mathcal{X}\) with corresponding RKHS \(\mathcal{H}\) then

\[
\mathcal{H} \odot \mathcal{H} \oplus (\mathcal{H}' \otimes \mathcal{H}) \cong \mathcal{H}_{\kappa_y+k_y}.
\]

When \(Y = f_0(X) + \epsilon\) with bounded \(f_0\) and \(\epsilon\) it is natural to define \(C_{\beta}\) as

\[
C_{\beta} = \text{cch} \left( \{ (\kappa_y((x, f_0(x) + \bar{b}), \cdot), \langle f_0(x) + \bar{b}, \cdot \rangle_{\mathbb{R}'} \otimes k(x, \cdot) : x \in \mathcal{X} \} \right.
\]

\[
\cup \{ (\kappa_y((x, f_0(x) - \bar{b}), \cdot), \langle f_0(x) - \bar{b}, \cdot \rangle_{\mathbb{R}'} \otimes k(x, \cdot) : x \in \mathcal{X} \})
\]

and \(c_y\) as \(\int \kappa_y((X,Y), \cdot) dP\).

**Diameter of \(C_{\beta}\)** We measure the diameter of \(C_{\beta}\) with regard to elements \(u \in \mathcal{K}, \|u\| = 1\). We can write \(u\) as \((\hat{g}, v)\), where \(g \in \mathcal{H} \odot \mathcal{H}, \hat{g}\) is the extension of \(g\) to \(\mathbb{R} \times \mathcal{X}\), and
$v \in \mathbb{R}' \otimes \mathcal{H}$. Observe that if $v$ is given by a finite linear combination of elements $\langle y_i, \cdot \rangle_\mathbb{R} \otimes h_i$, $y_i \in \mathbb{R}$, $h_i \in \mathcal{H}$, then

$$v = \sum_{i=1}^{n} \alpha_i(\langle y_i, \cdot \rangle_\mathbb{R} \otimes h_i) = \langle 1, \cdot \rangle_\mathbb{R} \otimes (\sum_{i=1}^{n} y_i \alpha_i h_i). \quad (13)$$

For such finite linear combinations let $\psi : \mathbb{R}' \otimes \mathcal{H} \to \mathcal{H}$ be $\psi(v) = \sum_{i=1}^{n} y_i \alpha_i h_i$. The map $\psi$ is independent of the particular representation of $v$ because if

$$\sum_{i=1}^{n} \alpha_i(\langle y_i, \cdot \rangle_\mathbb{R} \otimes h_i) = \sum_{i=1}^{m} \beta_i(\langle z_i, \cdot \rangle_\mathbb{R} \otimes g_i)$$

for a suitable $m \in \mathbb{N}$ and corresponding $\beta_i, z_i \in \mathbb{R}$, $g_i \in \mathcal{H}$ for all $i \leq m$, then

$$0 = \| \langle 1, \cdot \rangle_\mathbb{R} \otimes (\sum_{i=1}^{n} y_i \alpha_i h_i - \sum_{i=1}^{m} z_i \beta_i g_i) \|^2 = \sum_{i=1}^{n} y_i \alpha_i h_i - \sum_{i=1}^{m} z_i \beta_i g_i \|^2$$

We can also observe that $\|v\|_{\otimes}^2 = \| \sum_{i=1}^{n} y_i \alpha_i h_i \|^2 = \|\psi(v)\|^2$. Furthermore, $\psi$ is linear and therefore an isometry. Since the finite linear combinations lie dense in $\mathbb{R}' \otimes \mathcal{H}$ and $\mathcal{H}$, and both $\mathbb{R}' \otimes \mathcal{H}$ and $\mathcal{H}$ are complete, we can extend $\psi$ to a surjective isometry between $\mathbb{R}' \otimes \mathcal{H}$ and $\mathcal{H}$ [II Cor.4.3.18]. In particular, any $v \in \mathbb{R}' \otimes \mathcal{H}$ can be represented as $\psi^{-1}(h)$ with a unique $h \in \mathcal{H}$.

The diameter of $C_\oplus$ can be lower bounded in the following way: let $I = [-\bar{b}, \bar{b}]$ then

$$\text{diam}_{(\hat{g}, \psi^{-1}(h))} C_\oplus = \sup_{x \in \mathcal{X}, y \in I} (g(x) + (f_0(x) + y)h(x)) - \inf_{x \in \mathcal{X}, y \in I} (g(x) + (f_0(x) + y)h(x))$$

whenever $\|(\hat{g}, \psi^{-1}(h))\|_{\oplus} = 1$, $g \in \mathcal{H} \otimes \mathcal{H}$ and $h \in \mathcal{H}$. In particular, when choosing the same point $x$ and using $y$ to move to absolute values, we gain

$$\text{diam}_{(\hat{g}, \psi^{-1}(h))} C_\oplus \geq \|h\|(\bar{b} + \bar{b}) \sup_{x \in \mathcal{X}} \|h(x)\| \geq \|h\|(\bar{b} + \bar{b}) \frac{2}{2} \text{diam}_{\|h\|}(C_\oplus) \quad (14)$$

where $C$ is the usual convex set in $\mathcal{H}$. We need to complement this bound with a bound that is based on $g$ since when $\|h\|$ is small this lower bound is of no use.

When $-\bar{b} \leq \inf_{x \in \mathcal{X}} f_0(x) \leq \sup_{x \in \mathcal{X}} f_0(x) \leq \bar{b}$ there is a simple way to get a lower bound that involves $g$. For two points $x_1, x_2 \in \mathcal{X}$ we can choose $y_1 = -f_0(x_1)$ and $y_2 = -f_0(x_2)$. Hence, under this assumption,

$$\text{diam}_{(\hat{g}, \psi^{-1}(h))} C_\oplus \geq \sup_{x \in \mathcal{X}} g(x) - \inf_{x \in \mathcal{X}} g(x) \geq \|g\|_{\mathcal{H} \otimes \mathcal{H}} \text{diam}_{\|g\|_{\mathcal{H} \otimes \mathcal{H}}} C_\oplus \quad (15)$$

We can combine (14) and (15) to gain a lower bound on the the diameter of $C_\oplus$ in terms of the diameters of $C$ and $C_\oplus$. We summarize this bound in the following proposition.
Proposition 3. Let $(\Omega, \mathcal{A}, P)$ be probability space on which i.i.d. random variables $X, X_1, X_2, \ldots$ are defined that attain values in the measurable space $\mathcal{X}$. Furthermore, let $\epsilon, \epsilon_1, \epsilon_2, \ldots$ be a sequence of i.i.d. zero mean real value random that are independent of $X$ and the $X_i$’s and such that $\bar{b} = \inf \{b : \epsilon \leq b \ a.s.\}$ and $\bar{b} = -\sup \{b : \epsilon \geq b \ a.s.\}$ are finite. Finally, let $f_0: \mathcal{X} \to \mathbb{R}, f_0 \in L^2(P)$, be such that $-\bar{b} \leq f_0(x) \leq \bar{b}$ for all $x \in \mathcal{X}$ and $k$ a kernel function on $\mathcal{X}$ such that $k(x, \cdot) \in L^2(P; \mathcal{H})$, then for any $g \in \mathcal{H} \otimes \mathcal{H}, h \in \mathcal{H}, \|\langle \hat{g}, \phi^{-1}(h) \rangle\|_\oplus = 1$, we have the following lower bound

$$\text{diam}_{\langle \hat{g}, \psi^{-1}(h) \rangle} C_\oplus \geq (\|h\| (\bar{b} + \bar{b})/2) \text{diam}_{\mathcal{H}/\|h\|}(C) \lor (\|g\|_{\mathcal{H} \otimes \mathcal{H}} \text{diam}_{\mathcal{H}/\|g\|_{\mathcal{H} \otimes \mathcal{H}}}(C_\oplus)).$$

The low noise setting. The situation gets more complicated when $|f_0|$ attains values that are significantly larger than $\bar{b}$. For instance, when $\bar{b} = \bar{b} = 0$, $h(x) \neq 0$ and $f_0(x) = -g(x)/h(x)$, it holds that $\text{diam}_{\langle \hat{g}, \psi^{-1}(h) \rangle} C_\oplus = 0$. For $f_0$ to be equal or close to $-g/h$ it is necessary that $f_0$ attains large values when $\|h\|$ is small. For example, in the context of Lemma 4 where $\mathcal{H} \otimes \mathcal{H}$ is finite dimensional with dimension $d$, $\lambda_d > 0$ is the smallest eigenvalue of a suitable kernel matrix based on the kernel $\kappa$, and $k$ is a bounded kernel, we have the following lower bound

$$\sup_{x \in \mathcal{X}} |f_0(x)| \geq \frac{\|g\|_{\infty}}{\|h\|_{\infty}} \geq \frac{\|g\|_{\mathcal{H}} \lambda_d^{1/2}}{d^{1/2} \|h\|_{\mathcal{H}} \|k\|_{\mathcal{H}}^{1/2}}.$$ 

For a small value of $\|h\|$ this implies that $\|g\|$ will be close to 1 and $|f_0|$ has to attain a large value at at least some locations $x \in \mathcal{X}$.

4.3.1 Linearly dependent spaces

We are taking a digression and consider the problem of approximating $\mathcal{C}$ and $\mathcal{m}$ simultaneously to highlight how linearly dependent spaces can be addressed. When the spaces over which we want to optimize are linearly dependent then the RKHS is not isometrically isomorphic to the direct product space. This can happen, for example, when we try to approximate $\mathcal{C}$ simultaneously to $\mathcal{m}$. In this context the corresponding spaces $\mathcal{H} \otimes \mathcal{H}$ and $\mathcal{H}$ can overlap. For instance, when $k$ is a polynomial kernel of order two then $\mathcal{H}$ and $\mathcal{H} \otimes \mathcal{H}$ are not linearly independent.

Whenever $\mathcal{H} \otimes \mathcal{H}$ and $\mathcal{H}$ are not linearly independent it is natural to identify elements like $(h, 0)$ and $(0, h)$, $h \in (\mathcal{H} \otimes \mathcal{H}) \cap \mathcal{H}$. One way to do this is to consider the subspace $U = \{(h, h) : h \in (\mathcal{H} \otimes \mathcal{H}) \cap \mathcal{H}\}$ of $\mathcal{K} := (\mathcal{H} \otimes \mathcal{H}) \oplus \mathcal{H}$. The subspace is closed: let $\{(h_n, h_m)\}_{n \in \mathbb{N}}$ be a convergent sequence in $U$. This sequence is also a Cauchy sequence and for any $\epsilon > 0$ there exists an $N \in \mathbb{N}$ such that for all $n, m \geq N$,

$$\epsilon > \|(-h_n, h_n) - (-h_m, h_m)\|_{\oplus}^2 = \|h_m - h_n\|^2 + \|h_n - h_m\|^2_{\mathcal{H} \otimes \mathcal{H}}.$$ 

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and \( \{h_n\}_{n \in \mathbb{N}} \) is a Cauchy sequence both in \( \mathcal{H} \) and \( \mathcal{H} \oplus \mathcal{H} \). Hence, it converges in both spaces. Let \( f \) be its limit in \( \mathcal{H} \oplus \mathcal{H} \) and \( g \) its limit in \( \mathcal{H} \) then for any \( x \in \mathcal{X} \) there exists an \( n \in \mathbb{N} \) such that \(|f(x) - g(x)| \leq \epsilon + |h_n(x) - h_n(x)| = \epsilon \) and \( f = g \). It also follows right away that \( \lim_{n \to \infty} \|(-h_n, h_n) - (-f, g)\|_\mathcal{B} = 0 \) and the sequence has its limit in \( U \).

Consider the quotient space \( \mathcal{K}/U \) with co-sets \( f^* = f + U, f \in \mathcal{K} \), and the quotient norm \( \|f^*\|_{\mathcal{K}/U} = \inf\{\|f + h\|_\mathcal{K} : h \in U\} \). The space \( \mathcal{K}/U \) is again a Hilbert space since \( U \) is closed (e.g. [21, Sec.III.4]), and it is isometrically isomorphic to the Hilbert space \( \mathcal{H} \oplus \mathcal{H} + \mathcal{H} \) when the latter is equipped with the norm \( \|f\|_+^2 = \inf\{\|g\|_{\mathcal{H} \oplus \mathcal{H}}^2 + \|h\|^2 : f = g + h, g \in \mathcal{H} \oplus \mathcal{H}, h \in \mathcal{H}\} \); in particular, a co-set \((g, h) + U \in \mathcal{K}/U \) is mapped to the function \( f = g + h \). This map is well defined since if \((g_1, h_1) \in (g, h)^* \) then there is some \( h_2 \) such that \( g_1 + h_1 = g - h_2 + h + h_2 = f \). Furthermore, by the choice of \( U \), there are no two elements \( u^*, v^* \in \mathcal{K}/U, u^* \neq v^* \), that are mapped to the same function \( f \). Assume otherwise, then there is some \( f \) such that \( f = g_1 + h_1 = g_2 + h_2 \) and, therefore, \((g_2 + g_1 - g_2, h_2 - g_1 + g_2) = (g_1, h_1) \). Since \( g_1 - g_2 \in \mathcal{H} \oplus \mathcal{H} \) and \( g_1 - g_2 = h_1 - h_2 \in \mathcal{H} \) it follows that \((g_2, h_2)^* = (g_1, h_1)^* \) which contradicts the assumption. Finally, any element in \( \mathcal{H} \oplus \mathcal{H} + \mathcal{H} \) can be represented this way since if \( f = g + h, g \in \mathcal{H} \oplus \mathcal{H}, h \in \mathcal{H} \) then \((g, h)^* \) is mapped to \( f \). Using again [2 Thm.,p.353] we can conclude that \( \mathcal{K}/U \) and \( \mathcal{H}_{\kappa + k} \) are isometrically isomorphic.

While \( \mathcal{K}/U \) and \( \mathcal{H}_{\kappa + k} \) are isometrically isomorphic it does not hold in general that \( \mathcal{K} \) and \( \mathcal{K}/U \) are isometrically isomorphic to \( \mathcal{H}_{\kappa + k} \). Hence, when mapping an element \( u \in \mathcal{K} \) to \( u^* \in \mathcal{K}/U \), then finding an approximation \( v^* \) of \( u^* \) in \( \mathcal{K}/U \), we generally cannot invert the \( \bullet \) operation to gain an approximation of \( u \). Selecting an arbitrary element in \( v^* \) does not work either since a small value of \( \|u^* - v^*\|_{\mathcal{K}/U} \) does not imply that all elements in the corresponding co-sets have small distances, i.e. there is no reason why \( \sup_{w \in v^*} \|u - w\|_{\mathcal{K}} \) should be small.

Fortunately we are not trying to approximate arbitrary elements but only

\[
(\mathcal{C}, m) = \frac{1}{n} \sum_{i=1}^{n} \langle \kappa(X_i, \cdot), k(X_i, \cdot) \rangle
\]

and we are optimizing the approximation over \( \tilde{C} = \text{cch} \{(\kappa(x, \cdot), k(x, \cdot)) : x \in \mathcal{X}\} \subset \mathcal{K} \). The important observation is that for any non-zero element \((-h, h) \in U\), that is \( h \in (\mathcal{H} \oplus \mathcal{H}) \cap \mathcal{H} \), we have

\[
\langle (-h, h), (\kappa(x, \cdot), k(x, \cdot)) \rangle_{\mathcal{K}} = -h(x) + h(x) = 0,
\]

and \( \tilde{C} \) is a subset of \( U^\perp \).

The subspace \( U^\perp \) together with the inner product inherited from \( \mathcal{K} \) is isometrically isomorphic to \( \mathcal{H}_{\kappa + k} \). This follows since \( \mathcal{K}/U \) and \( \mathcal{H}_{\kappa + k} \) are isometrically isomorphic and \( U^\perp \) and \( \mathcal{K}/U \) are isometrically isomorphic. The latter holds since every co-set corresponds to exactly one element in \( U^\perp \), and for \( u \in U^\perp \), \( \|u^*\|_{\mathcal{K}/U} = \inf\{\|u + v\|_{\mathcal{K}} : v \in U\} = \|u\|_{\mathcal{K}} \).
Also, \( \text{span} \, C = U^\perp \). We know already that \( \text{span} \, C \subset U^\perp \). To show that they are equal let \( K = \text{span} \left( \text{span} \, C \cup U \right) \). Observe that this space is closed since \( \text{span} \, C \) and \( U \) are, and because they are orthogonal. It is sufficient to show that \( (f, 0) \in K \), \( (0, g) \in K \) for all \( f \in H \otimes \mathcal{H} \) and \( g \in \mathcal{H} \) since the smallest closed subspace that contains all these elements is \((H \otimes \mathcal{H}) \oplus \mathcal{H}\).

For \( f = \sum_{i=1}^{n} \beta_i (\kappa(x_i, \cdot) + k(x_i, \cdot)) \in H_{n+k} \) define \( \psi(f) = \sum_{i=1}^{n} \beta_i (\kappa(x_i, \cdot), k(x_i, \cdot)) \in \text{span} \, C \subset (H \otimes \mathcal{H}) \oplus \mathcal{H} \). The operator \( \psi : H_{n+k} \to \text{span} \, C \) is linear and defined on a dense subset of \( H_{n+k} \). It is furthermore norm preserving since

\[
\|\psi(f)\|^2 = \sum_{i,j=1}^{n} \beta_i \beta_j \kappa(x_i, x_j) + \sum_{i,j=1}^{n} \beta_i \beta_j k(x_i, x_j) = \|f\|^2_{n+k}.
\]

Hence, it can be extended to a linear isometry, which we will also denote by \( \psi \), between \( H_{n+k} \) and \( \text{span} \, C \) with the norm inherited from \( (H \otimes \mathcal{H}) \oplus \mathcal{H} \).

For any \( h \in (H \otimes \mathcal{H}) \cap \mathcal{H} \) we can infer that it lies in the RKHS with kernel \( \kappa + k \) due to \([2]\) Thm.,p.353] and \( \psi(h) \) lies in \( \text{span} \, C \). Write \( \psi(h) \) as \((h_1, h_2), h_1 \in H \otimes \mathcal{H}, h_2 \in \mathcal{H}, \) then for all \( x \in X \),

\[
h_1(x) + h_2(x) = ((h_1, h_2), (\kappa(x, \cdot), k(x, \cdot)))_{\oplus} = \langle \psi(h), \psi(\kappa(x, \cdot) + k(x, \cdot)) \rangle_{\rho} = \langle h, \kappa(x, \cdot) + k(x, \cdot) \rangle_{n+k} = h(x).
\]

In other words, for any \( h \in (H \otimes \mathcal{H}) \cap \mathcal{H} \) we have \( h_1 \in H \otimes \mathcal{H}, h_2 \in \mathcal{H} \) such that \( h = h_1 + h_2 \) and \((h_1, h_2) \in \text{span} \, C \). Since \( h, h_1 \in H \otimes \mathcal{H} \) it follows that \( h_2 = h - h_1 \in (H \otimes \mathcal{H}) \cap \mathcal{H} \) and \((h_2, -h_2) \in U \). Thus, \((h, 0) = (h_1, h_2) + (h_2, -h_2) \in K \). Similarly, we can observe that \((0, h) \in K \).

For \( f \in H \otimes \mathcal{H} \) let \( \psi(f) = (f_1, f_2) \) with \( f_1 \in H \otimes \mathcal{H} \) and \( f_2 \in \mathcal{H} \). In other words, \( f = f_1 + f_2 \) and since \( H \otimes \mathcal{H} \) is a linear space, we know that \( f_2 = f - f_1 \in (H \otimes \mathcal{H}) \cap \mathcal{H} \).

And, as above, we can conclude that \((f, 0)\) also lies in \( K \). The same argument also shows that for any \( g \in \mathcal{H} \) we have \((0, g) \in K \). Hence, \( K = (H \otimes \mathcal{H}) \oplus \mathcal{H} \) and \( \text{span} \, C = U^\perp \).

**Lemma 5.** Let \( X \) be a measurable space and \( k \) a measurable kernel function on \( X \) with corresponding RKHS \( \mathcal{H} \) then \( \text{span} \{ (\kappa(x, \cdot), k(x, \cdot)) : x \in X \} \subset (H \otimes \mathcal{H}) \oplus \mathcal{H} \) equipped with the inner product of \((H \otimes \mathcal{H}) \oplus \mathcal{H}\) is isometrically isomorphic to \( H_{n+k} \).

### 4.3.2 Interpolation and another look at the low noise setting

We are revisiting now the low noise setting. In fact, assume in the following that there is no noise, that is \( Y = f_0(X), C_\oplus = \text{cch} \{ (\kappa_Y((x, f_0(x)), \cdot), (f_0(x), \cdot)_{R^\vee} \otimes k(x, \cdot)) : x \in X \} \) and we are interested in interpolating \( f_0 \). We are first assuming that \( f_0 \) is available to us and we are controlling the diameter of \( C_\oplus \) depending on how \( f_0 \) is related to \( \mathcal{H} \) and \( H \otimes \mathcal{H} \). The direct sum and quotient space approach are useful again to gain a deeper understanding of
how well \((\mathcal{C}_y, m_y^\otimes)\) can be approximated. The diameter of \(C_{\otimes}\) in this interpolation setting has a simpler form. For \(g \in \mathcal{H} \otimes \mathcal{H}, h \in \mathcal{H},\)

\[
\text{diam}_{(g,\psi^{-1}(h))}C_{\otimes} = \sup_{x \in \mathcal{X}} (g(x) + f_0(x)h(x)) - \inf_{x \in \mathcal{X}} (g(x) + f_0(x)h(x))
\]

The functions \(f_0 \times h\) lie in the RKHS \(\mathcal{H}_{f_0}\) which has the kernel function \(k_0(x,y) = f_0(x)k(x,y)f_0(y)\). According to [20, Prop.5.20] the RKHS \(\mathcal{H}_{f_0}\) is equal to \(\{f_0 \times h : h \in \mathcal{H}\}\) and the inner product on \(\mathcal{H}_{f_0}\) is given by \(\langle f_0 \times h_1, f_0 \times h_2 \rangle_{f_0} = \langle h_1, h_2 \rangle\) whenever \(h_1, h_2 \in \mathcal{H}\). We can now compare \(\mathcal{H}_{f_0}\) with \(\mathcal{H} \otimes \mathcal{H}\). If \(\mathcal{H}_{f_0} \cap (\mathcal{H} \otimes \mathcal{H}) = \{0\}\) then we can embed both \(\mathcal{H}_{f_0}\) and \(\mathcal{H} \otimes \mathcal{H}\) in the direct sum \(G = (\mathcal{H} \otimes \mathcal{H}) \oplus \mathcal{H}_{f_0}\) such that for any \(f \in \mathcal{H}_{f_0}, h \in \mathcal{H} \otimes \mathcal{H}\) it holds that \(\|f\|_{\mathcal{H}_{f_0}} = \|(0, f)\|_G\) and \(\|h\|_{\mathcal{H} \otimes \mathcal{H}} = \|(h, 0)\|_G\). As in Lemma 4 it holds that \(G \cong \mathcal{H}_{k_0+\kappa}\) and, therefore, it also holds that \(\|f\|_{k_0} = \|f\|_{k_0+\kappa}\) and \(\|h\|_{\mathcal{H} \otimes \mathcal{H}} = \|h\|_{k_0+\kappa}\). In this case,

\[
\text{diam}_{(g,\psi^{-1}(h))}C_G = \text{diam}_{(g,f_0 \times h)}C_{G}
\]

whenever \(g \in \mathcal{H} \otimes \mathcal{H}, h \in \mathcal{H}\), where \(C_G = \text{cch}\{(\kappa(x,\cdot), k_0(x,\cdot)) : x \in \mathcal{X}\} \subset G\). This follows directly from

\[
g(x) + f_0(x)h(x) = \langle (g, f_0 \times h), (\kappa(x,\cdot), k_0(x,\cdot)) \rangle_G.
\]

We can now follow the approach from Section 3.3.3 and, in particular, apply Proposition 1 to the RKHS with kernel \(k_{f_0} + \kappa\). In this context and whenever the constant function is not in \(\mathcal{H}_{k_0+\kappa}\), the approach effectively constructs

\[(\mathcal{H} \otimes \mathcal{H}) \oplus \mathcal{H}_{f_0} \oplus \mathcal{H}_1,
\]

where \(\mathcal{H}_1\) is the one dimensional RKHS corresponding to the constant functions and with the kernel function \(1 \otimes 1\).

### 4.3.3 Including \(Y_i\)'s in the simultaneous approximation

Often it is unnecessary to include the \((1/n) \sum_{i=1}^n Y_i^2\) term in the simultaneous approximation since many methods only rely on the terms that include \(f\) (e.g., the ridge regressor) and also \((1/n) \sum_{i=1}^n Y_i^2 \in \mathbb{R}\) itself is obviously the best compression of the average \(Y_i^2\). However, when selecting points \((X_{i(1)}, Y_{i(m)}), m \ll n,\) for a coreset then

\[
\frac{1}{m} \sum_{i=1}^m (f^2(X_{i(i)}) - 2Y_{i(i)}f(X_{i(i)})) + \frac{1}{n} \sum_{i=1}^n Y_i^2
\]

is not the mean squared error of \(f\) given the sample \(X_{i(1)}, Y_{i(1)}, \ldots, X_{i(m)}, Y_{i(m)}\) and might even be negative. An easy way to remedy this problem is to move to \((1/m) \sum_{i=1}^m Y_{i(i)}^2\)
but then we do not have any guarantee that this is close to \((1/n) \sum_{i=1}^{n} Y_i^2\). An alternative is to include the \(Y_i\)’s in the simultaneous approximation problem. This can be done by, for instance, defining a kernel on \(\mathbb{R} \times \mathcal{X}\) through \(l((y_1, x_1), (y_2, x_2)) = \langle y_1, y_2 \rangle_{\mathbb{R}}\) and by considering the direct sum
\[
\mathcal{H} \otimes \mathcal{H} \oplus (\mathbb{R}' \otimes \mathcal{H}) \oplus \mathcal{H}_t.
\]

5 Applications

In the following we look at how these techniques can be combined with machine learning methods. In particular, we are looking at mean embeddings and the two sample problem, and at kernel ridge regression.

5.1 Two Sample Test

In the two sample test problem i.i.d. data \(X_1, \ldots, X_n\) and \(Y_1, \ldots, Y_m\) attaining values in \(\mathcal{X}\) are given, the \(X_i\)’s are furthermore independent from the \(Y_i\)’s but it is unknown if the \(X_i\)’s have the same distribution as the \(Y_i\)’s. The null-hypothesis is that the distributions are equal. One way to build a test statistic for this hypothesis testing problem is to consider
\[
\|m_{X,n} - m_{Y,m}\| \quad \text{where } k \text{ is a kernel function on } \mathcal{X}, k(X, \cdot), k(Y, \cdot) \in \mathcal{L}^1(P), m_{X,n} = (1/n) \sum_{i=1}^{n} k(X_i, \cdot) \text{ and } m_{Y,m} = (1/m) \sum_{i=1}^{m} k(Y_i, \cdot).\]
Calculating the norm can be done in \(O((n \lor m)^2)\) by using that
\[
\|m_{X,n} - m_{Y,m}\|^2 = \frac{1}{n^2} \sum_{i,j=1}^{n} k(X_i, X_j) - \frac{2}{nm} \sum_{i=1}^{n} \sum_{j=1}^{m} k(X_i, Y_j) + \frac{1}{m^2} \sum_{i,j=1}^{m} k(Y_i, Y_j).
\]
Under the conditions of Theorem 1 and when using the conditional gradient method we can reduce this run-time to \(O((n \log(n)) \lor (m \log(m)))\) whenever \(n\) is large enough and without increasing the rate of convergence towards \(\|m_X - m_Y\|\), where \(m_X = \int k(X, \cdot) \, dP\) and \(m_Y = \int k(Y, \cdot) \, dP\), under the condition that we have access to the vectors \((m_{X,n}, k(X_1, \ldots)), \ldots, m_{X,n}, k(X_n, \ldots))\) and \((m_{Y,m}, k(Y_1, \ldots)), \ldots, m_{Y,m}, k(Y_m, \ldots))\). A naive computation of these vectors takes of order \(O((n \lor m)^2)\) steps and to gain significant run-time savings it is necessary to also study ways to compute these efficiently; a natural approach to do so is to consider of order \(n^{1/2}\) many batches of size \(n^{1/2}\), compress each batch down to \(\log(n)\) by using the conditional gradient method, and then apply the conditional gradient method again to the \(n^{1/2}\) many elements to approximate \(m_{X,n}\) and \(m_{Y,m}\) respectively. The analysis of this last step of this approach is more involved and beyond the scope of this paper.
5.2 Tikhonov regularized regression

When the conditional gradient method is used to approximate \( \mathcal{C}_y \) and \( m_y \) simultaneously there is an index function \( \iota : \{1, \ldots, l\} \rightarrow \{1, \ldots, n\} \) and the approximations are \( \hat{\mathcal{C}}_{y,l} = \sum_{i=1}^{l} w_i k(X_{\iota(i)}, \cdot) \) and \( \hat{m}_{y,l} = \sum_{i=1}^{l} w_i \langle Y_{\iota(i)}, \cdot \rangle \otimes k(X_{\iota(i)}, \cdot) \) with strictly positive \( w_i \)'s such that \( w_1 + \ldots + w_l = 1 \), then the approximation of the least-squares error for a function \( h \in \mathcal{H} \) is

\[
\sum_{i=1}^{l} w_i (Y_{\iota(i)} - h(X_{\iota(i)}))^2 = \langle \hat{\mathcal{C}}_{y,l}, \tilde{h} \rangle_{\mathcal{H} \otimes \mathcal{H}} - 2 \langle \hat{m}^\otimes_{y,l}, \tilde{h} \rangle_{\mathbb{R} \otimes \mathcal{H}} + \sum_{i=1}^{l} w_i Y_{\iota(i)}^2,
\]

where \( \tilde{h} \) is the extension of \( h \) to \( \mathcal{X} \times \mathbb{R} \) and where we denote the function \( (x, y) \mapsto h^2(x) \) by \( \tilde{h} \). Due to the representer theorem we can write the solution to the ridge regression problem in the form \( \tilde{h} = \sum_{i=1}^{l} \alpha_i k(X_{\iota(i)}, \cdot) \) for suitable \( \alpha_i \in \mathbb{R} \). Substituting this into the equation for the least-squares error and ignoring the last term, which is irrelevant for finding the solution, we gain

\[
\langle \hat{\mathcal{C}}_{y,l}, \tilde{h} \rangle_{\mathcal{H} \otimes \mathcal{H}} = \alpha^\top C_l \alpha.
\]

Let \( C_l \) be an \( l \times l \) matrix with the entry in row \( i \) and column \( j \) being

\[
\sum_{u=1}^{l} w_u \langle k(X_{\iota(u)}, \cdot) \otimes k(X_{\iota(u)}, \cdot), k(X_{\iota(i)}, \cdot) \otimes k(X_{\iota(j)}, \cdot) \rangle_{\otimes} = \sum_{u=1}^{l} w_u k(X_{\iota(u)}, X_{\iota(i)}) k(X_{\iota(u)}, X_{\iota(j)}).
\]

Then

\[
\langle \hat{\mathcal{C}}_{y,l}, \tilde{h} \rangle_{\mathcal{H} \otimes \mathcal{H}} = \alpha^\top C_l \alpha.
\]

Also, let \( K_l \) be the kernel matrix for samples \( X_{i(1)}, \ldots, X_{i(l)} \) and let \( m_l \) be an \( l \)-dimensional vector with entry \( i \) being

\[
\langle \hat{m}^\otimes_{y,l}, \tilde{h} \rangle_{\mathbb{R} \otimes \mathcal{H}} = \sum_{u=1}^{l} w_u Y_{\iota(u)} k(X_{\iota(i)}, X_{\iota(u)}).
\]

With these in place the solution of the ridge-regression problem with regularization parameter \( \lambda > 0 \) is found by minimizing

\[
\alpha^\top C_l \alpha - 2 \alpha^\top m_l + \lambda \alpha^\top K_l \alpha.
\]
with respect to \( \alpha \in \mathbb{R}^l \). Taking the gradient with respect to \( \alpha \) and setting it to zero yields

\[
2C_l \alpha - 2m_l + 2\lambda K_l \alpha = 0.
\]

(16)

Observe that \( C_l = K_l W K_l \), where \( W \) is a diagonal matrix with \( W_{uu} = w_u \) for all \( u \leq l \). Similarly, \( m_l = K_l W y = K_l W (K_l W)^\dagger K_l W y \), where \( y \) is a vector with entries \( y_u = Y_{i(u)} \) for all \( u \leq l \). Hence, we can rewrite (16) as

\[
K_l ((W K_l + \lambda I_l) \alpha - W (K_l W)^\dagger K_l W y) = 0,
\]

where \( I_l \) is the \( l \times l \) identity matrix. Since \( W \) has strictly positive entries on the diagonal we can rewrite this as

\[
K_l W ((K_l + \lambda W^{-1}) \alpha - (K_l W)^\dagger K_l W y) = 0,
\]

(17)

for which a solution is given by

\[
\alpha = (K_l + \lambda W^{-1})^{-1} (K_l W)^\dagger K_l W y.
\]

(18)

The inverse is well defined because \( K_l \) is p.s.d. and \( W^{-1} \) is (strictly) positive definite; the sum of a p.s.d. and strictly positive definite matrix is strictly positive definite and, therefore, has an inverse. Also \((K_l W)^\dagger = (K_l W)^{-1}\) whenever \( K_l \) is of full rank and in this case

\[
\alpha = (K_l + \lambda W^{-1})^{-1} y.
\]

(19)

This \( \alpha \) is also a solution to (17) in the general case when \( K_l \) is not full rank since \((K_l W)^\dagger K_l W y\) can be replaced by \( y \) in this equation. The solution in (18) has the additional property that \( \|\alpha\|_2 \) is minimal among all the solutions to the ridge-regression optimization problem.

Because the entries in \( W \) are upper bounded by one it follows that the ‘regularization’ by adding \( \lambda W^{-1} \) is stronger than when adding \( \lambda I_l \), which would correspond to standard ridge regression for the samples \((X_{i(1)}, Y_{i(1)}), \ldots, (X_{i(l)}, Y_{i(l)})\).

### 6 Example: Slow rate of convergence in infinite dimensions

Our final result it summarize in the theorem below and highlights difficulties of the approach in infinite dimensions.

**Theorem 2.** There exists an initialization, a continuous kernel and a Borel probability measure, which assigns non-zero probability to open intervals, on \([0, 1]\), for which the kernel herding algorithm does not converge fast, i.e. there exists no constant \( b \) such that \( \|m_t - m\| \leq b/t \) for all \( t \geq 1 \).
We split the proof of Proposition 2 into two parts. In the first part, we construct a Hilbert space, a map \( \phi \), and an element \( m \) such that the algorithm does not converge fast. We then use this Hilbert space to construct an RKHS for which the algorithm behaves in exactly the same way as in the Hilbert space and the algorithm does not converge fast either.

The construction idea. Before going into the technical details we like to outline the basic intuition of the construction. First, we let the mean element \( m = 0 \). Then we choose an orthonormal sequence \( \{ e_n \}_{n \geq 1} \) and elements \( \{ a_n \}_{n \geq 1} \) in \( \mathcal{H} \) such that each \( a_n \) is a multiple of \( e_n \). Furthermore, we use an initialization of the algorithm with an element \( c \in \mathcal{H} \) which is of small magnitude compared to the \( a_n \) and has a positive inner product with each \( a_n \). The idea is that the different \( a_n \)'s will be chosen at one point by the algorithm and will add weight to the approximation error \( w_t \) of \( m \) (\( t \) is the iteration number of the algorithm). In fact, we like to show that eventually so much weight will be added to the approximation that its norm will diverge to infinity.

This initial construction has a few problems which have to be addressed to make it work. The first problem with this construction is that \( \langle a_n, c \rangle \) is positive. In fact, \( \langle a_n, e_n \rangle, \langle c, e_n \rangle > 0 \) for all \( n \geq 1 \). But, we want the mean element \( m \) to be 0. So we will need probability mass on the negative side to counter the mass accumulated by the \( a_n \) and the \( c \). We do this by introducing another set of elements \( \{ b_n \}_{n \geq 1} \) which are lying opposite to the \( a_n \). Therefore, each \( b_n \) is a negative multiple of \( e_n \). These \( b_n \) need to be further constraint in magnitude. If they are of a similar order like the \( a_n \) then they can cancel the weight added to \( w_t \) by the \( a_n \). We are using here sequences with values in the order of \( 1/\ln(n+1) \) for the \( a_n \) and \( -2^{-n} \) for the \( b_n \).

Even though the \( b_n \)'s are of small magnitude compared to the \( a_n \)'s it is not directly obvious why these \( b_n \)'s should not be chosen many times by the algorithm to cancel step-by-step the weight accumulated by the \( a_n \)'s. Here is an argument why this does not happen: the \( a_n \)'s are constructed such that each \( a_n \) is chosen exactly once and they are selected in order by the algorithm. At a given iteration there is then an element \( a_m \) which has not yet been chosen and our construction assures that in this case \( \langle a_m, w_t \rangle \) equals the initial value \( \langle a_m, c \rangle \), which is of magnitude \( 1/(m \ln(m+1)) \). Since the algorithm chooses the element \( h \in \phi[\mathcal{X}] \) that maximizes the inner product with \( w_t \) we can infer that this inner product must be larger than \( 1/(m \ln(m+1)) \). Or put differently, an element \( b_n \) will only be chosen if \( \langle b_n, w_t \rangle \geq 1/(m \ln(m+1)) \), that is \( \langle e_n, w_t \rangle \geq 2^n/(m \ln(m+1)) \). If, in fact, the algorithm chooses in this case \( b_n \) then we are at least assured that \( \langle e_n, w_{t+1} \rangle \geq 2^n/(m \ln(m+1)) - 2^{-m} \) which will be for many dimensions \( e_n \) significant in scale (Figure 3 visualizes these bounds for different \( m \) ). We actually do not need this extra scaling of \( 2^n \) and we use in the proof only that there are sufficiently many \( e_n \) for which \( |\langle e_n, w_t \rangle| \) is larger than \( 1/\ln(m+1) \). The number of elements which fulfills this grows in \( m \) and summing the weight over these elements gives us a diverging number which approaches infinity in \( m \). This is then sufficient.
to show that the norm of the weight vector diverges.

**Interlacing.** In the above discussion we assume \( m = 0 \). However, there exists no probability measure on \([0, 1]\) which can enforce this. The problem is that the scaling on the positive side (the \( a_n \)'s and the \( c \)) is exponentially larger than the scaling on the negative side (the \( b_n \)'s). To get \( m = 0 \) we would need that the probability mass corresponding to the \( a_n \)'s and \( c \) scaled by the magnitude of these elements equals the probability mass of the \( b_n \)'s times the scale of the \( b_n \)'s. The exponential difference in scale implies that the probability mass of the \( b_n \)'s needs to grow exponentially in \( n \) and the sum of all this ‘probability mass’ adds up to infinity.

By closer inspection one can observe that the \( a_n \)'s pose no serious problem since one can just downscale the probability assigned to them by an exponential factor. However, the \( c \) poses a more serious problem. Let \( p > 0 \) be the probability on \( c \). We use \( c = \sum_{n=1}^{\infty} n^{-1} e_n \) and we thus have a factor of \( p/n \) pulling the mean element towards the positive direction in dimension \( n \). Hence, we will need a weight \( p_n = p2^n/n \) for the \( b_n \) elements to counter this pull. The \( p \) does not change with \( n \) and we are left with weights \( p_n \) which grow rapidly in \( n \).

The approach with the initialization \( c \) is in a way to rigid and does not allow us to assign lower probability mass in \( n \). One way to overcome this problem is to break up the initialization and add probability mass to the different dimensions while the algorithm is running. We do this by replacing the single \( c \) with elements for each dimension \( n \). Since we do not want to alter the overall behavior of the algorithm these different elements will need to be of a low scale and we need multiple elements to regain the \( 1/n \) value that \( c \) would assign. So for each dimension \( e_n \) we are left with a finite sequence of elements \( c_{n,1}, c_{n,2}, \ldots \) which takes the role of the original \( c \).

The question is then how we can guarantee that all these \( c_{n,i} \) elements are chosen to simulate the initialization through \( c \) before the algorithm proceeds as usual. We guarantee this by introducing dimensions \( \tilde{e}_{n,i} \) which are orthogonal to all the \( e_n \). These dimensions are used to force the algorithm to choose \( c_{n,i+1} \) after \( c_{n,i} \) until the final element of the sequence is chosen and we have a weight of \( 1/n \) in dimension \( e_n \).

We still have not addressed the problem of assigning different weights to the different dimensions. But, since the \( c \) is broken into many small pieces, it is now easy to ‘lose’ weight in \( n \). We do this by introducing elements \( d_n \) which lie in the span of \( \tilde{e}_{n,1} \). These elements serve the single purpose of canceling weight of the \( c_{n,i} \) elements and thus to enforce \( m = 0 \).

**Proposition 4.** For any infinite dimensional Hilbert space \( \mathcal{H} \) there exists a continuous function \( \phi : X \to \mathcal{H}, X := [0, 1] \), a probability measure \( P \) on \( \mathcal{B}[0,1] \) which assigns positive measure to any open subset of \( X \). There exists and initialization \( w_1 \in \phi[X] \) such that the kernel herding algorithm when applied to \( \int \phi(x) dP(x) \) generates a sequence
\{w_t\}_{t \geq 1} \text{ that is unbounded and the algorithm does not converge with the fast } 1/t \text{ rate to } m = \int \phi(x) \, dP(x) \in \mathcal{H}.

\textbf{Proof.} \textbf{(a) Definition of the convex set:} Let \( \{N_i\}_{i=1}^\infty \) be a set of natural numbers to be defined below, pick a countable infinite orthonormal sequence \( \{e'_n\}_{n \geq 1} \) in \( \mathcal{H} \) and split this sequence into \( \{e_n\}_{n \geq 1} \) and the sequences \( \tilde{e}_{n,1}, \ldots, \tilde{e}_{n,N_n} \) where \( n \) goes through 2, 3, \ldots. This can be done since these are countable many sequences of \( N_n + 1 \) elements and since countable unions of countable sets are again countable. Furthermore, define the sequences \( \{a_n\}_{n \geq 1}, \{b_n\}_{n \geq 1}, \{c_{n,m} : 1 \leq n, 1 \leq m \leq N_n\}, \{d_n : 2 \leq n\} \subseteq \mathcal{H} \) by

\[
a_n := \left( a'_n + \frac{1}{n} \right) e_n \text{ with } a'_n := C \left[ \frac{2^n}{\ln(n + 1)} \right] 2^{-n} \quad \text{and} \quad C = 4 \left[ 3 + \frac{4 \ln(9)}{\ln(2)} \right] = 64,
\]

\[
b_n := -2^{-n} e_n,
\]

\[
N_1 := 1 \text{ and for } n \geq 2, \quad N_n := \left\lceil \frac{2}{n \langle -b_n, e_n \rangle} \right\rceil,
\]

\[
c_{1,1} := e_1 + \alpha_2,1 \tilde{e}_{2,1}, \quad \text{and for } n \geq 2 :
\]

\[
c_{n,1} := \beta_n e_n + \alpha_{n,1} \tilde{e}_{n-1} - \alpha_{n,2} \tilde{e}_{n,2}, \quad \ldots
\]

\[
c_{n,N_n-1} := \beta_n e_n + \alpha_{n,N_n-1} \tilde{e}_{n,N_n-1} - \alpha_{n,N_n} \tilde{e}_{n,N_n},
\]

\[
c_{n,N_n} := \beta_n e_n + \alpha_{n,N_n} \tilde{e}_{n,N_n} - \alpha_{n+1,1} \tilde{e}_{n+1,1},
\]

\[
d_2 := -(1/2)\alpha_{2,1} \tilde{e}_{2,1} \text{ and for all } 2 \leq n \text{ let}
\]

\[
d_n := (1/2)\alpha_{n,1} \tilde{e}_{n,1},
\]

\[
\beta_n := -\frac{1}{nN_n}, \text{ for which } -\beta_n < \langle -b_n, e_n \rangle \text{ holds},
\]

\[
\alpha_{n,1} := \sqrt{\frac{\langle e_n, a_n \rangle}{n}}, \quad \text{and } \alpha_{n,i} := \sqrt{\alpha_{n,1}^2 + (i - 1)\beta_n^2} \text{ for } 2 \leq i \leq N_n.
\]

\(-\beta_n\) is smaller than \( \langle -b_n, e_n \rangle \) because \(-\beta_n = 1/(nN_n) \leq \langle -b_n, e_n \rangle /2\). Also observe that the sequence \( a'_n \) is non-increasing in \( n \) since

\[
\left\lceil \frac{2^n}{\ln(n + 2)} \right\rceil \frac{1}{2^{n+1}} \leq \left\lceil \frac{2^n}{\ln(n + 1)} \right\rceil \frac{1}{2^n} \leq 2 \left\lceil \frac{2^n}{\ln(n + 1)} \right\rceil \frac{1}{2^{n+1}} = \left\lceil \frac{2^n}{\ln(n + 1)} \right\rceil \frac{1}{2^n},
\]

where we used that the function \([\cdot]\) is monotonically increasing.

\textbf{(b) Construction of a continuous map } \phi: \text{ We construct a continuous function } \phi: [0,1] \to \mathcal{H} \text{ which goes through the points } \{a_n\}_{n \in \mathbb{N}}, \{b_n\}_{n \in \mathbb{N}}, \{c_{n,i} : 1 \leq n, 1 \leq i \leq N_n\} \text{ and } \{d_n : 2 \leq n\}. \text{ We split the construction into three separate functions, } \phi_1 \text{ for the } a_n, b_n \text{ elements, } \phi_2 \text{ for the } c_{n,i} \text{ and } \phi_3 \text{ for the } d_n \text{ elements.}

\text{For ease of reading let } y_n = 1/(n + 1) \text{ and } z_n = (y_n + y_{n+1})/2 \text{ for all } n \geq 1. \text{ Define}
\[ \phi_1 : [0, 1] \to \mathcal{H}, \text{ with } n \text{ going through } 1, 2, 3 \ldots, \text{ by} \]

\[ \phi_1(x) := \begin{cases} 
\frac{1-x}{1-y_1} a_1 & \text{if } y_1 < x \leq 1, \\
\frac{x-\xi}{y_{n-\xi}} a_n & \text{if } \xi := \frac{y_{n+\xi}}{2} < x \leq y_n, \\
\frac{\xi-z_n}{z_n-\xi} b_n & \text{if } z_n < x \leq \frac{y_{n+\xi} + z_n}{2} := \xi, \\
\frac{z_n-y_{n+1}}{z_n-\xi} a_{n+1} & \text{if } y_{n+1} < x \leq \frac{y_{n+1} + z_n}{2} := \xi, \\
0 & \text{if } x = 0. 
\end{cases} \]

The function is continuous on \((0, 1]\) as it is piecewise linear and the end points of the lines are connected. The only critical point is 0. For continuity at 0 it suffices that for any \(\epsilon > 0\) we can pick a \(\delta\) such that \(x < \delta\) implies \(\|\phi(x)\| < \epsilon\). We restrict the search for a \(\delta\) to points \(1/n, n \in \mathbb{N}\). For such a \(\delta\) the maximum of \(\phi(x)\) in an interval \([0, \delta]\) is either attained on an \(a_n\) or a \(b_n\). As we have that \(\lim_{n \to \infty} \|a_n\| = \lim_{n \to \infty} \|b_n\| = 0\) there is for every \(\epsilon > 0\) an \(N \in \mathbb{N}\) such that for all \(n > N\) we have that \(\max(\|a_n\|, \|b_n\|) < \epsilon\) and, consequently for \(\delta = 1/(N+1)\) we have that \(\|\phi(x)\| < \epsilon\) for any \(0 \leq x \leq \delta\).

In the following let \(N_1 := 1\). Furthermore, let \(\tilde{y}_n := 1/n, \Delta_n := (\tilde{y}_n - \tilde{y}_{n+1})/N_n, u_{n,m} := \tilde{y}_n - m\Delta_n, u_{n,0} := \tilde{y}_n\), and let \(\tilde{z}_{n,m} := (u_{n,m-1} + u_{n,m})/2\), for all \(n \geq 1\) and \(1 \leq m \leq N_n - 1\). With \(n\) going through all of 1, 2, \ldots, define \(\phi_2 : [0, 1] \to \mathcal{H}\) by

\[ \phi_2(x) := \begin{cases} 
\frac{\tilde{y}_n-x}{\tilde{y}_n-\tilde{z}_{n,1}} c_{n,1} & \text{if } \tilde{z}_{n,1} < x \leq \tilde{y}_n, \\
\frac{x-u_{n,m}}{u_{n,m}-\tilde{z}_{n,m}} c_{n,m} & \text{if } u_{n,m} < x \leq \tilde{z}_{n,m}, 1 \leq m \leq N_n - 1, \\
\frac{x-y_{n+1}}{y_{n+1}-\tilde{z}_{n,m+1}} c_{n,m+1} & \text{if } \tilde{z}_{n,m+1} < x \leq u_{n,m}, 1 \leq m \leq N_n - 1, \\
\frac{y_{n+1}-x}{y_{n+1}-\tilde{z}_{n,1}} c_{n,N_n} & \text{if } \tilde{z}_{n,1} < x \leq y_{n+1}, \\
0 & \text{if } x = 0. 
\end{cases} \]

Similarly, by going through all \(n \geq 2\) define \(\phi_3 : [0, 1] \to \mathcal{H}\) by

\[ \phi_3(x) := \begin{cases} 
0 & \text{if } 1/2 < x \leq 1, \\
\frac{y_n-x}{y_n-\tilde{z}_{n,1}} d_n & \text{if } \tilde{z}_{n,1} < x \leq \tilde{y}_n, \\
\frac{x-u_{n,1}}{u_{n,1}-\tilde{z}_{n,1}} d_n & \text{if } u_{n,1} < x \leq \tilde{z}_{n,1}, \\
0 & \text{if } \tilde{y}_{n+1} < x \leq u_{n,1}, \\
0 & \text{if } x = 0. 
\end{cases} \]

With the same reasoning as for \(\phi_1\) one can infer that \(\phi_2\) and \(\phi_3\) are continuous. Define

\[ \phi(x) := \begin{cases} 
\phi_1(3x - 2) & \text{if } 2/3 < x \leq 1, \\
\phi_2(3x - 1) & \text{if } 1/3 < x \leq 2/3, \\
\phi_3(3x) & \text{if } 0 \leq x \leq 1/3. 
\end{cases} \]
The function \( \phi \) is continuous since \( \phi_1, \phi_2, \phi_3 \) are continuous and \( \phi_1(0) = \phi_2(1) = \phi_2(0) = \phi_3(1) = 0 \). This implies also that \( \phi : [0, 1] \to \mathcal{H} \) is measurable. It is also Bochner integrable with respect to any probability measure defined on the Borel sets of \( \mathbb{R} \) as \( \| \phi(\cdot) \| : [0, 1] \to \mathbb{R} \) is continuous and, hence, bounded, i.e. \( \int \| \phi(x) \| \ dP(x) < \infty \).

(c) **Definition of the probability measure:** We construct a Borel measure by defining a density \( p \) on \([0, 1]\). Using the variables defined for \( \phi_1, \phi_2, \phi_3 \), constants \( a_1, b_1, \ldots \) and \( n \) going through \( 1, 2, \ldots \) we set

\[
p_1(x) = \begin{cases} a_1 & \text{if } y_1 < x \leq 1, \\ a_n & \text{if } \frac{y_n + z_n}{2} < x \leq y_n, \\ b_n & \text{if } \frac{y_n + z_n}{2} < x \leq \frac{y_n + z_n}{2}, \\ a_{n+1} & \text{if } y_{n+1} < x \leq \frac{y_{n+1} + z_n}{2}, \\ 0 & \text{if } x = 0. \\
\end{cases}
\]

and using constants \( c_n \) we furthermore define

\[
p_2(x) := \begin{cases} c_n & \text{if } \tilde{y}_{n+1} < x \leq \tilde{y}_n, \\ 0 & \text{if } x = 0. \\
\end{cases}
\]

Finally, going through all \( n \geq 2, 1 \leq m \leq N_n \) and with the constants \( d_{n,m} \) let

\[
p_3(x) := \begin{cases} 1 & \text{if } 1/2 < x \leq 1, \\ d_n & \text{if } u_{n,1} \leq x \leq \tilde{y}_n, \\ 1 & \text{if } \tilde{y}_{n+1} \leq x \leq u_{n,1} \\ 0 & \text{if } x = 0 \\
\end{cases}
\]

and combine these to define the density \( p \) by

\[
p(x) := \begin{cases} p_1(3x - 2) & \text{if } 2/3 < x \leq 1, \\ p_2(3x - 1) & \text{if } 1/3 < x \leq 2/3, \\ p_3(3x) & \text{if } 0 \leq x \leq 1/3. \\
\end{cases}
\]

Now, \( m = 0 \) iff \( \langle e_n, m \rangle = E \langle e_n, \phi \rangle = 0 = \langle e'_{n,i}, m \rangle = E \langle e'_{n,i}, \phi \rangle \) for all \( n \geq 1, 1 \leq i \leq N_n \).

Observe that in general, if \( a, b \in [0, 1], a \leq b \), the density \( p \) is constant on \([a, b]\) with value \( \mu \in [0, \infty) \), \( h \in \mathcal{H} \) and \( \psi : [0, 1] \to \mathcal{H} \) is defined by

\[
\psi(x) = \begin{cases} (x - a)/(b - a)\mu h & \text{if } x \in [a, b], \\ 0 & \text{otherwise.} \\
\end{cases}
\]
then for any $e_n$ (and $e'_{n,i}$):
\[
\langle e_n, E\psi \rangle = E \langle e_n, \psi \rangle = \int_{[a,b]} \frac{x - a}{b - a} \mu \langle e_n, h \rangle = \frac{1}{2}\mu \langle e_n, h \rangle (b - a)
\]
and if
\[
\psi(x) = \begin{cases} 
(b - x)/(b - a)\mu h & x \in [a, b], \\
0 & \text{otherwise}
\end{cases}
\]
then
\[
\langle e_n, E\psi \rangle = \frac{1}{2}\mu \langle e_n, h \rangle (b - a).
\]

So,
\[
\langle e_1, m \rangle = \frac{1}{6} \left( e_1, \left(1 - \frac{y_1 + z_1}{2}\right) a_1 a_1 + \left(\frac{y_1 - y_2}{2}\right) b_1 b_1 + (\tilde{y}_1 - \tilde{y}_2)c_1c_1,1 \right)
\]
will be zero by setting
\[
b_1 := 2 \cdot 6 \left(1 - \frac{y_1 + z_1}{2}\right) a_1 \frac{\langle a_1, e_1 \rangle}{\langle -b_1, e_1 \rangle} + \left(1 - \frac{1}{2}\right) c_1 \frac{\langle c_{1,1}, e_1 \rangle}{\langle -b_1, e_1 \rangle}
\]
and $\langle e_n, m \rangle = 0$ by setting
\[
b_n = 2(n + 1)(n + 2) \left(\frac{1}{4} \left(\frac{1}{n} - \frac{1}{n + 2}\right) a_n \frac{\langle a_n, e_n \rangle}{\langle -b_n, e_n \rangle} + \left(\frac{1}{n} - \frac{1}{n + 1}\right) c_n \frac{\langle c_n, e_n \rangle}{\langle -b_n, e_n \rangle} \right).
\]

Also, for any $n \geq 1$ we have that $b_n > 0$ if $a_n, c_n > 0$. Let, $\mathcal{N}$ be a normalising constant to be defined below and let
\[
a_1 := \frac{\mathcal{N} \langle -b_1, e_1 \rangle}{24 \langle a_1, e_1 \rangle} / \left(1 - \frac{y_1 + z_1}{2}\right) > 0 \quad \text{and} \quad c_1 := \frac{\mathcal{N} \langle -b_1, e_1 \rangle}{12 \langle c_{1,1}, e_1 \rangle} > 0
\]
such that $b_1 = \mathcal{N}$. Also set for all $n \geq 2$
\[
a_n := \frac{n}{n + 1} \frac{\mathcal{N} \langle -b_n, e_n \rangle}{\langle a_n, e_n \rangle} > 0 \quad \text{and} \quad c_n := \frac{n}{2(n + 2)} \frac{\mathcal{N} \langle b_n, e_n \rangle \Delta_{n+1}}{\beta_n \Delta_n} \frac{\Delta_{n+1}}{\Delta_n} > 0
\]
which makes $b_n = \mathcal{N}(1 - \Delta_{n+1}/\Delta_n)$ and all $\langle e_n, m \rangle = 0$. For the elements $\tilde{c}_{n,i}$ we have that
\[
6 \langle \tilde{c}_{2,1}, m \rangle = \Delta_1 c_1 \langle c_{1,1}, \tilde{e}_{2,1} \rangle + \Delta_2 c_2 \langle c_{2,1}, \tilde{e}_{2,1} \rangle + \Delta_2 \tilde{d}_2 \langle d_{2, \tilde{e}_{2,1}} \rangle
\]
and we set
\[
\tilde{d}_2 := \Delta_1 \frac{\langle c_{1,1}, \tilde{e}_{2,1} \rangle}{\Delta_2} + \frac{\langle c_{2,1}, \tilde{e}_{2,1} \rangle}{\langle -d_2, \tilde{e}_{2,1} \rangle} > 0.
\]
Furthermore, for all $n > 2$ let
\[
\delta_n := \frac{\Delta_{n-1} c_{n-1}}{\Delta_n} \frac{-c_{n-1,N_{n-1},\tilde{e}_{n,1}}}{\langle d_n, \tilde{e}_{n,1} \rangle} - c_n \frac{\langle c_{n,1}, \tilde{e}_{n,1} \rangle}{\langle d_n, \tilde{e}_{n,1} \rangle}.
\]

$\delta_n > 0$ for $n > 2$ since
\[
\frac{2 \langle -d_n, \tilde{e}_{n,1} \rangle}{\alpha_{n,1} N} \delta_n = \frac{(n-1)^2}{n+1} \langle -b_{n-1}, e_{n-1} \rangle \left[ \frac{2}{(n-1) \langle -b_{n-1}, e_{n-1} \rangle} \right]
- \frac{\Delta_{n+1}}{\Delta_n} \frac{n^2}{n+2} \langle -b_n, e_n \rangle \left[ \frac{2}{n \langle -b_n, e_n \rangle} \right]
\geq 2 \frac{n-1}{n+1} - 3 \frac{n}{n+2} \frac{\Delta_{n+1}}{\Delta_n} = 2 \frac{n-1}{n+1} - 3 \frac{n^2}{(n+2)^2} \frac{N_n}{N_{n+1}}
\geq 2 \frac{n-1}{n+1} - 3 \frac{n^2(n+1)}{2(n+2)^2} \left( \frac{1}{n} + \frac{1}{2n+1} \right)
\]
which is strictly greater zero if
\[
4(n-1)(n+2)^2 - 4n(n+1)^2 = 4(n^2 + n - 4)
\]
is. But this is obvious for $n \geq 3$. For all remaining $n, i \geq 2$ we can observe that
\[
\langle \tilde{e}_{n,i}, m \rangle = (1/6) \Delta_n c_n \langle c_{n,i-1} - c_{n,i}, \tilde{e}_{n,i} \rangle = 0
\]
for all $m \geq 2$. Hence, $m = 0$ and the density is strictly greater 0 on all but three points. It remains to set $N$ such that the density integrates to one. We have for any $N > 0$ that
\[
0 < \int_{[0,1]} p = a_1 (1 - (y_1 + z_1)/2)/3 + (1/3) \sum_{n=2}^{\infty} a_n ((y_n - z_{n-1}) - (y_n - z_n))/2
+ \frac{1}{3n(n+1)} \sum_{n=2}^{\infty} b_n ((y_n - z_n) - (y_{n+1} - z_n))/2
+ \sum_{n=1}^{\infty} \Delta_n \delta_n + \frac{1}{3n(n+1)} \sum_{n=1}^{\infty} \Delta_n (u_{n,1} - \tilde{y}_{n+1}).
\]

The first sum is a finite multiple of $N$ since $a_n \approx 2^{-n}$ and the sum over $((y_n - z_{n-1}) - (y_n - z_n))/2$ is bounded by 1. Similarly, the $c_n$ sum is bounded since $c_n$ itself is upper bounded by $N$ and the rest is quadratic in $n$. Furthermore, $b_n$ is upper bounded by $N$ and the sum of the intervals cannot exceed 1. Finally, $\delta_n$ is upper bounded since
\[
\frac{2 \langle -d_n, \tilde{e}_{n,1} \rangle}{\alpha_{n,1} N} \delta_n \leq \frac{2(n-1)}{n+1}
\]
\(\alpha_{n,1}\) is bounded and so is \(\langle -d_n, \hat{e}_{n,1}\rangle\). Hence, the sum is a finite multiple of \(N\) and we have in total a term that is a finite multiple of \(N\) plus a constant that is smaller than 1/2. Therefore, we can choose \(N\) such that \(\int p = 1\).

**d) Behaviour of the algorithm:** Initialize the algorithm with \(w_1 := c_{1,1} \in \phi[X]\) and let \(x_t\) be the element which is chosen at stage \(t\). The algorithm behaves as follows:

1. For any \(t \geq 1\), if \(w_t \neq 0\) then \(x_t \in \{a_n\}_{n \geq 1} \cup \{b_n\}_{n \geq 1} \cup \{c_{n,m}: 1 \leq n, 1 \leq m \leq N_n\} \cup \{d_{n,m}: 2 \leq n, 1 \leq m \leq N_n\}\).

2. Let \(n = \min\{m: a_m\) has not been chosen in steps \(1 \ldots t - 1\}\). If \(t \geq 2\) then either the smallest element of \(\{m, j\}: c_{m,j}\) has not been chosen in steps \(1 \ldots t - 1\}\{c_{1,1}\}\) in the lexicographic order is \((n, i)\) with \(1 \leq i \leq N_n\) and
\[
w_t = -\gamma_1 e_1 - \ldots - \gamma_{n-1} e_{n-1} + \gamma_n e_n + \alpha_{n,i} \hat{e}_{n,i},
\]
where
\[
\gamma_j = (2^{j} a'_j - l)2^{-j}, l \in \mathbb{N} \quad \text{and} \quad a'_j \geq \gamma_j \geq \min\left\{a'_j, \max\left\{\frac{2^{j} \langle a_n, e_n\rangle}{n} - 2^{-j}, 0\right\}\right\}
\]
for \(1 \leq j \leq n - 1\) and \(\gamma_n = -(i - 1)\beta_n\) (first case), or the smallest element is \((n + 1, 1)\) and
\[
w_t = -\gamma_1 e_1 - \ldots - \gamma_{n-1} e_{n-1} + \gamma_n e_n + \alpha_{n+1,1} \hat{e}_{n+1,1},
\]
with \(\gamma_1, \ldots, \gamma_{n-1}\) like above and \(\gamma_n = 1/n\) (second case). In particular \(w_t \neq 0\).

3. Let \(N(n) := \lfloor 1 + \log_2(n \ln(n + 1))\rfloor\) then \(n - 1 \geq N(n)\) for all \(n \geq 7\). If \(n\) is the smallest index of an \(a_n\) which has not been chosen yet and if this \(n \geq 7\) then for any \(i\) with \(n - 1 \geq i \geq N(n)\)
\[
\langle e_i, w_t \rangle \leq -\frac{1}{\ln(n + 1)}.
\]

4. For each \(n \geq 1\) there exists a step \(t \geq 1\) with \(x_t = a_n\).

\(\phi\) (1) is saying that no point on the line from 0 to an \(a_n, b_n, c_{n,m}\) or \(d_{n,m}\) is chosen that differs from \(a_n, b_n, c_{n,m}\) and \(d_{n,m}\). To see this first observe that only points \(\phi(x)\) will be chosen at any stage \(t\) for which \(\langle w_t, \phi(x)\rangle > 0\): By assumption \(w_t \neq 0\). If there exists an \(e_n\) with \(\langle e_n, w_t \rangle \neq 0\) then either \(\langle a_n, w_t \rangle\) or \(\langle b_n, w_t \rangle\) is strictly positive. Also, if there is an \(\hat{e}_{n,m}, (n, m) \neq (2, 1),\) such that \(\langle \hat{e}_{n,m}, w_t \rangle > 0\) then \(\langle d_{n,m}, w_t \rangle\) is strictly positive. Similarly, if \(\langle \hat{e}_{2,1}, w_t \rangle < 0\) then \(\langle d_{2,1}, w_t \rangle > 0\). Assuming that none of these cases apply we have that
either $\langle e_{2,1}, w_i \rangle > 0$ or there is an $\tilde{e}_{n,m}$, $(n,m) \neq (2,1)$, with $\langle \tilde{e}_{n,m}, w_i \rangle < 0$. In the first case $\langle e_{1,1}, w_i \rangle > 0$. In the latter case and with $\langle \tilde{e}_{2,1}, w_i \rangle = 0$ let $(n', m') := \min \{ (n,m) : \langle \tilde{e}_{n,m}, w_i \rangle < 0 \}$ where the minimum is taken wrt. the lexicographic ordering. We have $\langle c_{n',m'} - 1, w_i \rangle = \alpha_{n',m'} - 1 \langle \tilde{e}_{n',m'} - 1, w_i \rangle - \alpha_{n',m'} \langle \tilde{e}_{n',m'}, w_i \rangle > -\alpha_{n',m'} \langle \tilde{e}_{n',m'}, w_i \rangle > 0$, if $m' > 1$, and if $m' = 1$ then

$$\langle c_{n'-1,N_{n'-1}}, w_i \rangle = \alpha_{n'-1,N_{n'-1}} \langle \tilde{e}_{n'-1,N_{n'-1}}, w_i \rangle - \alpha_{n',1} \langle \tilde{e}_{n',1}, w_i \rangle > -\alpha_{n',1} \langle \tilde{e}_{n',1}, w_i \rangle > 0.$$  

If the chosen $\phi(x)$ is on the line from 0 to $a_n$ then $a_n = \xi \phi(x)$ with $\xi \geq 1$ and $0 < \langle \phi(x), w_i \rangle \leq \xi \langle \phi(x), w_i \rangle = \langle a_n, w_i \rangle$ and $\phi(x) = a_n$. The same argument applies to $b_n, c_{n,m}$ and $d_{n,m}$.

(β) We prove by induction over $t \geq 2$ that (2) holds. We start with the induction basis.  

$w_1 = c_{1,1} = c_1 + \alpha_{2,1} \tilde{e}_{2,1}$ and we have $\langle w_1, b_n \rangle \leq 0, \langle w_1, d_n \rangle \leq 0$ for all $n$, $\langle w_1, a_n \rangle = 0$ for all $n \geq 2$, $\langle w_1, c_{n,1} \rangle = 0$ if either $n > 2$ or $(n = 2$ and $i > 2)$. Furthermore,

$$\langle w_1, c_{1,1} \rangle = \| c_{1,1} \|^2 = 1 + \alpha_{2,1}^2 = 1 + \frac{\langle e_{2,1}, a_{1,1} \rangle}{2} = 1 + \frac{C}{8} \left[ \frac{4}{\ln(3)} \right] + \frac{1}{4} \leq 1 + \frac{C}{4} \left[ \frac{2}{\ln(2)} \right] + \frac{1}{4} < 1 + \frac{C}{2} \left[ \frac{2}{\ln(2)} \right] = \langle w_1, a_1 \rangle$$

since $C \geq 1$, $[2/\ln(2)] = 3$ and hence

$$\frac{C}{4} \left[ \frac{2}{\ln(2)} \right] > \frac{1}{4}.$$  

Also, $\langle w_1, c_{2,1} \rangle = \alpha_{2,1}^2 < \langle w_1, c_{1,1} \rangle < \langle w_1, a_1 \rangle$ and $x_1 = a_1$. Therefore,

$$w_2 = w_1 - a_1 = c_1 + \alpha_{2,1} \tilde{e}_{2,1} - (a_1' + 1)c_1 = -a_1'c_1 + \alpha_{2,1} \tilde{e}_{2,1}$$

and $w_2$ has the promised form.

(γ) Next, we address the induction step. (i) Assuming $w_t$ has the given form in step $t$ we can observe that

$$\langle x_t, w_t \rangle \geq \frac{\langle a_n, c_n \rangle}{n} > 0$$

since in the first case

$$\langle c_{n,i}, w_t \rangle = \beta_n \gamma_n + \alpha_{n,i}^2 = -(i-1) \beta_n^2 + (\alpha_{n,1}^2 + (i-1) \beta_n^2) = \frac{\langle c_n, a_n \rangle}{n}$$

in case that $i > 1$ or, for $i = 1$,

$$\langle c_{n,1}, w_t \rangle = \alpha_{n,1}^2 = \frac{\langle c_n, a_n \rangle}{n}.$$
In the second case,
\[ \langle a_n, w_t \rangle \geq \gamma_n \langle e_n, a_n \rangle = \frac{\langle e_n, a_n \rangle}{n}. \]

**ii** For the \( b_j \) (i) implies that, first, no \( j \geq n \) will have been chosen in \( t \) since for these \( \langle b_j, w_t \rangle \leq 0 \) holds in both cases. Also, if for a \( j, 1 \leq j \leq n - 1 \), \( \gamma_j < 2^j \langle a_n, e_n \rangle / n \) then \( \langle b_j, w_t \rangle = \gamma_j 2^{-j} < \langle a_n, e_n \rangle / n \) \( b_j \neq x_t \). On the other hand, if \( \gamma_j \geq 2^j \langle a_n, e_n \rangle / n \) and \( x_t = b_j \) then the coefficient changes by \(-2^{-j}\), i.e. the new coefficient is
\[ \gamma_j - 2^{-j} \geq 2^j \frac{\langle a_n, e_n \rangle}{n} - 2^{-j}. \]

The coefficient is also always non-negative since \( \gamma_j \) is a multiple of \( 2^{-j} \) and \( b_j \) will not be selected if \( \gamma_j = 0 \). In total, all cases are consistent with our induction hypothesis and we are safe against any application of \( b_j \).

**iii** In terms of \( a_j \), we can directly observe that \( \langle a_j, w_t \rangle = 0 \) if \( j > n \) and \( \langle a_j, w_t \rangle = -\gamma_j \langle e_j, a_j \rangle \leq 0 \) if \( j < n \). So only \( a_n \) might have been chosen at time \( t \). However, in the first case we have that
\[ \langle a_n, w_t \rangle = \gamma_n \langle a_n, e_n \rangle = -(i - 1)\beta_n \langle a_n, e_n \rangle \leq \frac{N_n - 1}{nN_n} \langle a_n, e_n \rangle < \frac{\langle a_n, e_n \rangle}{n} \]
and \( x_t \neq a_n \). In the second case, if \( \gamma_n = 1/n \), then
\[ \langle a_n, w_t \rangle = \frac{\langle a_n, e_n \rangle}{n}. \]

Thus \( a_n \) might be chosen, and, in case it is, then the new coefficient is \( \gamma_n - a_n' - 1/n = -a_n' \)
which is consistent with the induction hypothesis.

**iv** Turning to the \( c_{n',i'} \) elements we can observe that for \( (n, i) > (2, 1) \) we have \( \langle w_t, c_{1,1} \rangle \leq 0 \). For \( (n, i) = (2, 1) \) we are in the first case since \( N_2 = 4 \) and
\[ \langle w_t, c_{1,1} \rangle = (\langle -\gamma_1 e_1 + \gamma_2 e_2 + \alpha_2 \tilde{e}_{2,1}, e_1 + \alpha_2 \tilde{e}_{2,1} \rangle = -\gamma_1 + (1/2) \langle e_2, a_2 \rangle \leq -(1/2) \langle e_2, a_2 \rangle + 1/2 + (1/2) \langle e_2, a_2 \rangle. \]

But, \( 1/2 < (1/2) \langle a_2, e_2 \rangle \) and \( c_{1,1} \) will never be chosen. For the remaining \( c_{n',i'} \) elements we have in the first case in step \( t \) that no \( c_{n',i'} \) will be chosen if \( n' \neq n \) or \( i' \neq i \) since in these cases
\[ \begin{aligned}
\langle w_t, c_{n',i'} \rangle &= \begin{cases}
0 & \text{if } n' > n, \\
\gamma_n \beta_n = -(i - 1)\beta_n^2 & \text{if } n' = n \text{ and } (i' > i \text{ or } i' < i - 1), \\
\gamma_n \beta_n - \alpha_{n,i}^2 & \text{if } n' = n \text{ and } i' + 1 = i, \\
0 & \text{if } 2 \leq n' = n - 1 \text{ and } i' = N_n' \text{ and } i = 1, \quad (*) \\
-\gamma_{n'} \beta_{n'} < \langle w_t, b_{n'} \rangle & \text{if } n' < n \text{ and } (*) \text{ does not apply.}
\end{cases}
\end{aligned} \]
(*) follows for $n \geq 3$ from

$$\langle w_t, c_{n-1,N_{n-1}} \rangle = \langle w_t, \beta_{n-1}e_{n-1} + \alpha_{n-1,N_{n-1}} \tilde{e}_{n-1,N_{n-1}} - \alpha_{n,1} \tilde{e}_{n,1} \rangle$$

$$= -\gamma_{n-1} \beta_{n-1} - \alpha_{n,1}^2 = \frac{\gamma_{n-1}}{(n-1)N_{n-1}} - \alpha_{n,1}^2$$

$$\leq \gamma_{n-1} 2^{-n} - \frac{\langle e_n, a_n \rangle}{n} \leq 2^{-n} \alpha_{n-1}' - \frac{\alpha_n'}{n}$$

$$= C \left( 2^{-n} \left[ \frac{2^{n-1}}{\ln(n)} \right] 2^{-(n-1)} - \frac{1}{n} \left[ \frac{2^n}{\ln(n+1)} \right] 2^{-n} \right)$$

$$\leq C n^{-1} 2^{-2n-1} \left( n \left[ \frac{2^n}{\ln(n^2)} \right] - 2^{n-1} \left[ \frac{2^n}{\ln(n+1)} \right] \right) \leq 0.$$ 

If now $x_t = c_{n,i}$ then, in case $i < N_n$,

$$w_{t+1} = w_t - c_{n,i} = -\sum_{i=1}^{n-1} \gamma_i e_i - (i-1) \beta_n e_n + \alpha_{n,i} \tilde{e}_{n,i} - \beta_n e_n - \alpha_{n,i} \tilde{e}_{n,i} + \alpha_{n,i+1} \tilde{e}_{n,i+1}$$

$$= -\sum_{i=1}^{n-1} \gamma_i e_i - i \beta_n e_n + \alpha_{n,i+1} \tilde{e}_{n,i+1}$$

which has the desired form. Similarly, in case that $i = N_n$

$$w_{t+1} = w_t - c_{n,N_n}$$

$$= -\sum_{i=1}^{n-1} \gamma_i e_i - (N_n - 1) \beta_n e_n + \alpha_{n,N_n} \tilde{e}_{n,N_n} - \beta_n e_n - \alpha_{n,N_n} \tilde{e}_{n,N_n} + \alpha_{n+1,1} \tilde{e}_{n+1,1}$$

$$= -\sum_{i=1}^{n-1} \gamma_i e_i - N_n \beta_n e_n + \alpha_{n+1,1} \tilde{e}_{n+1,1}$$

which has the form of the second case since $-N_n \beta_n = 1/n$.

In the second case no element $c_{n',i'}$ will be chosen since

$$\langle w_t, c_{n',i'} \rangle = \begin{cases} 
0 & \text{if } n' > n + 1 \text{ or } (n' = n + 1 \text{ and } i' > 1), \\
\alpha_{n+1,1}^2 < \langle e_n, a_n \rangle / n & \text{if } n' = n + 1 \text{ and } i' = 1, \\
\beta_n / n - \alpha_{n+1,1}^2 < 0 & \text{if } n' = n \text{ and } i' = N_n, \\
\beta_n / n < 0 & \text{if } n' = n \text{ and } i' < N_n, \\
-\gamma_{n'} \beta_{n'} < \langle w_t, b_{n'} \rangle & \text{or } = 0 \text{ if } n' < n.
\end{cases}$$

(v) We turn to the $d$ elements. First case: If $(n, i) = (2, 1)$ then $\langle w_t, d_2 \rangle = -(1/2) \alpha_{2,1}^2 < 0$ and otherwise $\langle w_t, d_2 \rangle = 0$. In either way $d_2$ will not be chosen. For any other $n'$ we have
that \(\langle w_t, d_{n'} \rangle = 0\) if \((n, i) \neq (n', 1)\). Otherwise

\[
\langle w_t, d_{n'} \rangle = (1/2)\alpha_{n,1}^2 = \frac{1}{2} \frac{\langle e_n, a_n \rangle}{n}
\]

and \(\langle w_t, d_{n'} \rangle < \langle a_n, e_n \rangle / n\) and \(d_{n'}\) will never be chosen.

Second case: \(\langle w_t, d_{2} \rangle \leq 0\) and all \(d_{n'}\) with \(n' \neq n + 1\) are zero. Finally

\[
\langle w_t, d_{n+1} \rangle = (1/2)\alpha_{n+1,1}^2 = \frac{\langle e_{n+1}, a_{n+1} \rangle}{n+1} < \frac{\langle e_n, a_n \rangle}{n}
\]

since the sequence \(\langle e_n, a_n \rangle\) is non-increasing.

So in step \(t+1\) the element \(w_{t+1}\) will have the right form, and, certainly, \(w_{t+1} \neq 0\).

(\(\delta\)) Next we prove (3). Since the smallest index \(n\) for which \(a_n\) has not been chosen in rounds 1 to \(t\) is assumed to be larger than 7 we can assume that \(t \geq 2\).

For each \(m\), \(\langle a_m, e_m \rangle / m \geq \frac{a'_m}{m} \geq \frac{1}{m \ln(m + 1)}\). Hence, from (2) we conclude for all \(i\) with \(n - 1 \geq i \geq N(n)\)

\[
-\langle e_i, w_{t+1} \rangle = \gamma_i \geq \min \left\{ a'_i, \max \left\{ 2^i \frac{\langle a_n, e_n \rangle}{n} - 2^{-i}, 0 \right\} \right\}
\]

\[
\geq \min \left\{ \frac{1}{\ln(i + 1)}, \max \left\{ \frac{2^i}{n \ln(n + 1)} - 2^{-i}, 0 \right\} \right\}.
\]

Using the assumption \(i \geq N(n)\) we observe that

\[
i \geq 1 + \log_2(n \ln(n + 1)) = \log_2(2n \ln(n + 1)) \Rightarrow 2^i \geq 2n \ln(n + 1) \Rightarrow \frac{2^i}{n \ln(n + 1)} - 1 \geq 1
\]

and since \(i > 1\)

\[
\frac{2^i}{n \ln(n + 1)} - 2^{-i} \geq \frac{2^i}{n \ln(n + 1)} - 1 \geq \frac{1}{\ln(i + 1)} \geq \frac{1}{\ln(n + 1)}.
\]

So, for \(n - 1 \geq i \geq N(n), \)

\[
-\langle e_i, w_{t+1} \rangle \geq \frac{1}{\ln(n + 1)}.
\]

(e) (4) also follows from (2). First, if \(a_n\) has been chosen in any step \(t\) then for all \(t' > t\) (2) tells us that \(\langle a_n, w_{t'} \rangle \leq 0\). Consequently, \(x_{t'} \neq a_n\) and \(a_n\) will be chosen at most ones. Also, if \(a_n\) is the element with minimal index which has not been chosen yet in time \(t\) then either \(\langle w_t, a_n \rangle = \langle w_t, a_m \rangle = 0\) or \(\langle w_t, a_n \rangle > \langle w_t, a_m \rangle\) for all \(m > n\). In the first case no element \(a_{n'}\) will be chosen and in the second case, if an \(a_{n'}\) will be chosen it will be the one with the smallest index in the set of elements which have not been chosen yet. So the elements \(a_n\) will be chosen in order and no element will be skipped.
Let us now assume that \( \{a_m : a_m \neq x_t \text{ for all } t \geq 1\} \) is not empty and let \( a_n \) be the element with the smallest index in this set.

The argument in (\( \gamma \)) shows us that no \( c_{m,j} \) with \( m > n \) will be chosen. Also, if \( c_{m,j} \) with \( m \leq n \) has been chosen in any step \( t \) then for all \( t' > t \) we again infer from (2) and the argument in (\( \gamma \)) that \( c_{m,j} \) will not be chosen in \( t' \) and, hence, each \( c_{m,j} \) is not chosen more than ones. Also none of the \( d_{n,j} \) elements will be ever chosen.

So the only way that an \( a_n \) is never chosen is that infinite many \( b_m \) elements are selected. Yet, no \( b_m \) with \( m \geq n \) will be chosen since the inner product with the weight vector is less or equal to zero. Also each \( b_m \), \( m < n \) can only be chosen finite many times before the weight vector in direction \( e_m \) becomes 0 and the inner product with \( b_m \) becomes 0 too (at which point it will certainly not be chosen any more). So only finite many applications of \( b_m \)’s are possible with a contradiction that \( a_n \) will not be chosen. 

(e) Unboundedness: d.3 and d.4 allow us now to show that the sequence \( \{\|w_t\|\}_{t \geq 1} \) is unbounded. Assume that at stage \( t \) the element \( n \) is the smallest index such that \( \langle a_n, w_t \rangle \) is positive.

For \( n \geq 7 \) we know from d.3 that \( |\langle e_i, w_t \rangle| \geq 1/\ln(n+1) \) for all \( i, N(n) \leq i < n \)

Hence, for \( n \geq 7 \),

\[
\|w_t\|^2 = \sum_{i=1}^{\infty} |\langle e_i, w_t \rangle|^2 \geq \sum_{i=N(n)}^{n-1} \frac{1}{(\ln(n+1))^2} \geq \frac{n - 1 - N(n)}{(\ln(n+1))^2} 
\]

\[
= \frac{n - 1 - \left[1 + \log_2(n \ln(n+1))\right]}{(\ln(n+1))^2} \geq \frac{n - 3 - \log_2(n \ln(n+1))}{(\ln(n+1))^2}.
\]

Furthermore,

\[
\frac{\log_2(n \ln(n+1))}{(\ln(n+1))^2} = \frac{\ln(n) + \ln(\ln(n+1))}{\ln(2)(\ln(n+1))^2} \leq \frac{2}{\ln(2)},
\]

since \( \ln(x) \leq x \) for all \( x > 0 \) and \( \ln(n+1) > 0 \). Hence,

\[
\|w_t\|^2 \geq \frac{n - 3}{(\ln(n+1))^2} - \frac{2}{\ln(2)}.
\]

The right side goes to infinity in \( n \) and, since for every \( n \) there is a \( t \) at which \( a_n \) is chosen due to d.4, the norm of \( w_t \) crosses any boundary at one time \( t \).

**Corollary 1.** There exists a continuous kernel on \([0, 1]\), a Borel probability measure on \([0, 1]\) which assigns positive measure to open subsets of \([0, 1]\) and an initialization for which the algorithm does not converge fast to \( m \).

**Proof.** We consider the Hilbert space \( (\mathcal{H}, \langle \cdot, \cdot \rangle) \) from Proposition 4 with the corresponding feature map \( \phi : [0, 1] \to \mathcal{H} \). Define the continuous kernel function \( k(x, y) := \langle \phi(x), \phi(y) \rangle \)
on $[0, 1]$ and let the corresponding RKHS be $(\mathcal{K}, (\cdot, \cdot))$. The geometry of the two spaces is closely related. We have for scalars $a_i, b_j$ and $x_i, y_j \in [0, 1]$, $i = 1, \ldots, n$, $j = 1, \ldots, m$, that

$$\left( \sum_{i=1}^{n} a_i \phi(x_i), \sum_{j=1}^{m} b_j \phi(y_j) \right) = \sum_{i=1}^{n} \sum_{j=1}^{m} k(x_i, y_j) = \left( \sum_{i=1}^{n} a_i k(x_i, \cdot), \sum_{j=1}^{m} b_j k(y_j, \cdot) \right).$$

Furthermore, we know that the Bochner-integral $m \in \mathcal{H}$ lies in $\text{cch} \phi[\mathcal{X}]$ which equals the closure of $\text{ch} \phi[\mathcal{X}]$ [23][Thm. 5.2, p.71] and there exists a sequence $\{n_i\}_{i \in \mathbb{N}}$, $n_i \in \mathbb{N}$, elements $x_{ij} \in [0, 1]$, and non-negative weights $a_{ij}$ with $\sum_{j=1}^{n_i} a_{ij} = 1$ such that the sequence $\{s_i = \sum_{j=1}^{n_i} a_{ij} \phi(x_{ij})\}_{i \in \mathbb{N}}$ converges to $m$ in norm, i.e. $\|m - s_i\| \to 0$ for $i \to \infty$.

The corresponding sequence $\{\bar{s}_i = \sum_{j=1}^{n_i} a_{ij} k(x_{ij}, \cdot)\}_{i \in \mathbb{N}}$ is a Cauchy sequence in $\mathcal{K}$ since

$$\|\bar{s}_i - s_j\|_{\mathcal{K}} = \|s_i - s_j\|_{\mathcal{H}}$$

and has a limit $n \in \mathcal{K}$ because $\mathcal{K}$ is complete. In particular, for any $x \in \mathcal{X}$

$$|(n, k(x, \cdot)) - \langle m, \phi(x) \rangle| = |(n - \bar{s}_i, k(x, \cdot)) + (\bar{s}_i, k(x, \cdot)) - \langle s_i, \phi(x) \rangle + \langle s_i - m, \phi(x) \rangle| \leq k(x, x) \|n - \bar{s}_i\|_{\mathcal{K}} + \|\phi(x)\|_{\mathcal{H}} \|m - s_i\|_{\mathcal{H}} \to 0 \text{ (in i)}$$

and $(n, k(x, \cdot)) = \langle m, \phi(x) \rangle$ for every $x \in X$. Furthermore, for arbitrary $l$ points $x_1, \ldots, x_l \in X$ and scalars $a_1, \ldots, a_l$ it holds that $(n, \sum_{i=1}^{l} a_i k(x_i, \cdot)) = \langle m, \sum_{i=1}^{l} a_i \phi(x_i) \rangle$ and

$$\|n\|_{\mathcal{K}} - \|m\|_{\mathcal{H}} \leq \|n\|_{\mathcal{K}} - \|\bar{s}_i\|_{\mathcal{K}} + \|\bar{s}_i\|_{\mathcal{K}} - \|s_i\|_{\mathcal{H}} + \|s_i\|_{\mathcal{H}} - \|m\|_{\mathcal{H}}$$

which also goes to 0 in $i$ and therefore $\|n\|_{\mathcal{K}} = \|m\|_{\mathcal{H}}$.

The function $k(x, \cdot) : X \to \mathcal{H}$ is continuous and therefore Bochner-integrable with respect to $\mathcal{P}$. Denote the Bochner integral with $n' = \int k(x, \cdot) \, d\mathcal{P}$. For any $x \in X$

$$n(x) = (n, k(x, \cdot)) = \langle m, \phi(x) \rangle = E \langle \phi(\cdot), \phi(x) \rangle = Ek(x, \cdot) = (n', k(x, \cdot)) = n'(x)$$

and $n = n'$.

Now if the algorithm is applied in $(\mathcal{K}, (\cdot, \cdot))$ with the initialization $k(x_0, \cdot)$, where $x_0$ is the element in $\mathcal{X}$ that maps to the initialization $\phi(x_0)$ that we use in Proposition[4] then sequences of elements $x_i$ and of weights $w_i$ are generated. The weights $w_i$ are of the form $k(x_0, \cdot) + \sum_{t=1}^{i} k(x_t, \cdot) - tn$. The sequence $x_1, x_2, \ldots$ also maximizes the objective in $(\mathcal{H}, \langle \cdot, \cdot \rangle)$. This can be seen by an induction over the weights $w_i \in \mathcal{H}$ that are generated by
the algorithm. The induction step is the following.

\[
\max_{x \in [0,1]} \langle \tilde{w}_t, \phi(x) \rangle = \max_{x \in [0,1]} \left( \langle \phi(x_0), \phi(x) \rangle + \sum_{i=1}^{t} \langle \phi(x_i), \phi(x) \rangle - t \langle m, \phi(x) \rangle \right)
\]

\[
= \max_{x \in [0,1]} \left( k(x_0, \cdot), k(x, \cdot) \right) + \sum_{i=1}^{t} \left( k(x_i, \cdot), k(x, \cdot) \right) - t \left( n, k(x, \cdot) \right) = (w_t, k(x_{t+1}, \cdot))
\]

\[
= (k(x_0, \cdot), k(x_{t+1}, \cdot)) + \sum_{i=1}^{t} (k(x_i, \cdot), k(x_{t+1}, \cdot)) - t (n, k(x_{t+1}, \cdot))
\]

\[
= \left( \langle \phi(x_0) + \sum_{i=1}^{t} \phi(x_i) - tm, \phi(x_{t+1}) \rangle \right) = \langle \tilde{w}_t, \phi(x_{t+1}) \rangle.
\]

From Proposition 4, we can now infer that the sequence \{\|\tilde{w}_t\|_H\}_{t \in \mathbb{N}} = \{\|w_t\|_K\}_{t \in \mathbb{N}} is unbounded and the algorithm does not converge with the fast rate in \(K\).

\[\square\]

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