Reproducing Kernel Functions: A general framework for Discrete Variable Representation

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Abstract

Since its introduction, the Discrete Variable Representation (DVR) basis set has become an invaluable representation of state vectors and Hermitian operators in non-relativistic quantum dynamics and spectroscopy calculations. On the other hand reproducing kernel (positive definite) functions have been widely employed for a long time to a wide variety of disciplines: detection and estimation problems in signal processing; data analysis in statistics; generating observational models in machine learning; solving inverse problems in geophysics and tomography in general; and in quantum mechanics.

In this article it was demonstrated that, starting with the axiomatic definition of DVR provided by Littlejohn et al. [1], it is possible to show that the space upon which the projection operator defined in ref [1] projects is a Reproducing Kernel Hilbert Space (RKHS) whose associated reproducing kernel function can be used to generate DVR points and their corresponding DVR functions on any domain manifold (curved or not). It is illustrated how, with this idea, one may be able to ‘neatly’ address the long-standing challenge of building multidimensional DVR basis functions defined on curved manifolds.

Keywords: Discrete Variable Representation, reproducing kernel functions, curved manifolds.

1. Introduction

Studies in basic and ordinary (non-relativistic) quantum dynamics and spectroscopy have made great progress in the past few decades. Arguably, expressing the relevant higher dimensional dynamic operators and state vectors in the so-called direct product DVR basis sets [2, 3] has been a major contributor to this progress. However, the configuration manifolds on which those states and Hermitian operators are described are in general not Euclidean [4, 5, 6]. In those scenarios, it was pointed out that proper multidimensional DVR basis set functions defined over curved manifolds cannot, in general, be written in a direct product form [3] (and references therein). Constructing the correct DVR basis set on curved configuration spaces has been a challenging problem since the mid 1980’s, when Light and co-workers demonstrated the enormous potential in using DVR techniques for solving the appropriate nuclear motion Schrodinger equations for polyatomic molecules [2].

To our knowledge, there has not been much progress on the issue until recently when a few promising papers appeared [1, 7, 8, 9]. The first of those was presented by Littlejohn et al. [1]. Here in this article one of the main objectives is to revisit the excellent work presented in that paper. We ‘restate’ the core idea in ref [1] as a definition and then demonstrate that the DVR concept can be connected with the theory of reproducing kernel functions. It is then illustrated how this observation may lead to a ‘neat’ solution to the aforementioned outstanding problem of building Multidimensional Non-direct Product (MNPDVR) basis sets on metric and differentiable manifolds. In the following section, we give a brief overview
of the DVR concept. In Section 3 the central idea of the paper is presented. The final section gives some concluding remarks. Note that all spaces, variables, matrices and manifolds considered here are real unless stated otherwise. Also note that the two statements ‘flat manifold’ and ‘Euclidean manifold’ are loosely used interchangeably.

2. Brief overview of Direct Product DVR

Although in this paper a familiarity with the DVR scheme \[2, 3, 11, 12, 13, 14, 15, 16, 17, 18\] and its employment in practice is assumed, a brief outline of the basics of the DVR concept is provided — albeit, an introduction tailored mainly to set the scene for us to introduce the reproducing kernel theory into the DVR techniques.

In nuclear, atomic (and, of course, molecular) levels it is acceptable to ignore the effects of gravity (and quantum gravity for that matter). In other words, the physical space is considered a homogeneous, isotropic, and continuum entity that is subject to the laws of Euclidean geometry. One important implication of these assumptions is that the spectrum of a position operator defined on the Euclidean ‘manifold’ is continuous. It also means if the molecular system consists of \(L\) atoms, it is unavoidable to consider the configuration space of the system as a Euclidean 3\(L\)-dimensional differentiable metric manifold, \(M\). In this setting, in global coordinate system descriptions, each point \((\alpha, \cdots, \alpha)\) in \(M\) is represented by a set of 3\(L\) (= \(d\)) coordinates, which are denoted here by \(x^{(\alpha)}_{\cdots, \cdots}\). A consequence of the physical system’s ‘arena’ being a flat \(d\)-dimensional manifold is that all the \(d\) components of the position operator \(\hat{x}^{(\alpha)}\) are mutually commutative, i.e., they are simultaneously diagonalisable on \(M\).

Thus, ideally, the so-called ‘generalised eigenfunction’ of (say) \(\hat{x}^{(\alpha)}\) at \(x^{(\alpha)}\) can be seen as a Dirac’s tempered distribution, \(\delta(x^{(\alpha)} - x^{(\alpha)}_{\cdots, \cdots})\), and the eigenfunction of \(\hat{x}^{(\alpha)}\) can then be expressed as \(\delta(x^{(\alpha)} - x^{(\alpha)}_{\cdots, \cdots}) = \prod_{i=1}^{d} \delta(x_{\cdots, \cdots}^{(\alpha)} - x^{(\alpha)}_{\cdots, \cdots})\) in Cartesian coordinates. Obviously, these ‘functions’ do not belong to \(\mathcal{L}(M)\) — an infinite-dimensional space whose elements are square-integrable functions on \(M\), which in the rest of the paper we denote \(\mathcal{H}\). However, given a set of \(N\) (finite number) orthonormal functions \(\{\psi_{j}(x^{(\alpha)})\}_{j=1}^{\alpha} \in \mathcal{H}\), one can (in principle) for \(\hat{x}^{(\alpha)}\) yield \(N\) eigenvalues \(\{x_{\alpha}^{(\alpha)}\}_{\alpha=1}^{N}\) in \(M\) and their corresponding eigenfunctions \(\{u_{\alpha}(x^{(\alpha)})\}_{\alpha=1}^{N}\) in \(\mathcal{H}\), such that \(u_{\alpha}(x^{(\alpha)}) = \prod_{i=1}^{d} \rho_{\alpha}^{(\alpha)}(x^{(\alpha)})\); with \(\rho_{\alpha}(x^{(\alpha)})\) being the eigenfunction associated with \(x^{(\alpha)}_{\cdots, \cdots}\) and an element of \(\mathcal{H}\) \[10\], that in the \(\lim\) becomes a Dirac delta function which, as pointed out, earlier does not belong to \(\mathcal{H}\). \(\mathcal{H}\) is represented by \(\mathcal{H}\) with its \(\times\) being the eigenfunction

\[
\left\{x_{\alpha}^{(\alpha)}\right\}_{\alpha=1}^{N} \text{ and } \left\{u_{\alpha}(x^{(\alpha)})\right\}_{\alpha=1}^{N}
\]

The DVR basis functions expressed in the above composite form is an example of what is commonly termed the direct product DVR basis set \[2, 3\]. Computing \(\{x_{\alpha}^{(\alpha)}\}, u_{\alpha}(x^{(\alpha)})\} \) on \(M\) is a straightforward matter. One simple way of achieving this is to express (say) \(\hat{x}^{(\alpha)}\) in \(\{\psi_{j}(x^{(\alpha)})\}_{j=1}^{\alpha} \) which yields a \(N \times N\) matrix for this particular position operator component. The eigen-pairs of the matrix are the DVR points and DVR eigenvectors of \(\hat{x}^{(\alpha)}\), respectively \[11, 19\]. For later reference, we provide below a formal form of the eigenfunction for (as an
example) \( \hat{x}^{(i)} \) represented in \( \{\psi_j(x^i)\}_{j=1}^N \):

\[
\rho^i_{\alpha}(x^i) = \sum_j R_{\alpha j} \psi_j(x^i)
\]

where

\[
R_{\alpha j} = \int_{-\infty}^{\infty} dx^{(i)} \psi_j(x^{(i)}) \rho^i_{\alpha}(x^{(i)}) \tag{2}
\]
denotes the matrix elements of the unitary transformation matrix \( [11, 19] \). If the quadrature

\[
\int_{-\infty}^{\infty} dx^{(i)} \psi_j(x^{(i)}) \rho^i_{\alpha}(x^{(i)}) = \sum_\beta \psi_j(x^{(i)}) \rho^i_{\alpha}(x^{(i)})
\]
exists, then

\[
R_{\alpha j} = \int_{-\infty}^{\infty} dx^{(i)} \psi_j(x^{(i)}) \rho^i_{\alpha}(x^{(i)}) = c_{\alpha} \psi_j(x^{(i)}) \tag{3}
\]
because by definition \( \rho^i_{\alpha}(x^{(i)}) \propto \delta_{\alpha \beta} \) \([11]\); and \( c_{\alpha} \in \mathcal{R} \). (Note that the superscripts in \( \rho^i, x^{(1:d)}, \) etc., are merely for labelling.)

In summary, superficially, one may view DVR basis functions as the representation of physically realizable position states. In that case, finding a DVR basis function is mathematically equivalent to obtaining bounded functional of \( \mathcal{D} \subseteq \mathcal{L}^2(\mathbb{M}) \) that approximates (in the \( N \to \infty \) ) a Dirac delta functional of \( \mathcal{L}^2(\mathbb{M}) \). A potent tool for this is the rich theory of operators and functionals on Hilbert spaces \([20, 21, 22]\). However, this approach would be too abstract for the purpose of this paper.

At any rate, for both physical insight and calculation expedience, in molecular physics the internal motions \( \text{(i.e., shape defining motions)} \) of polyatomic molecules is described in a \( \tilde{d} \)-dimensional surface embedded in \( \mathbb{M} \), where \( \tilde{d} < d \) \([4, 5, 6, 23]\). This is achieved by introducing some appropriate constraints. The imposition of these constraints turns the physical system’s configuration space from Euclidean to Riemannian \([5, 6]\), denoted here by \( \mathbb{M}_c \). In simple terms, the \( \tilde{d} \)-dimensional subspace embedded in the original and larger \( d \)-dimensional Euclidean configuration space does not have any internal/inherent Euclidean metric (hence it is curved), but this subspace looks like a Euclidean space locally. Unfortunately, on the Riemannian manifold the molecular system can only intrinsically be described in curvilinear co-ordinate systems, and besides there is no single internal curvilinear co-ordinate system which can cover \( \mathbb{M}_c \) globally. This means there are some of the embedded molecular configurations, such that their curvilinear coordinates are not defined. In other words, there is no co-ordinate system on this curved manifold that can provide a unique label for each constrained molecular configuration. In the following discussion, in lieu of explicitly reciting each time the full rigmarole about the mapping relationship between co-ordinate systems and manifolds, the statement ‘a function is defined over \( \mathbb{M}_c \)’ means that the function is defined over a patch in the manifold where the co-ordinates are valid, see Refs.\([24, 25, 26]\). This is also discussed in the chemical physics literature, see Refs.\([4, 5]\) for more accessible details.

Owing to the aforementioned constraints, it can no longer guaranteed that all \( \tilde{d} \) components of the co-ordinate operators defined in these curvilinear co-ordinates are mutually commutative. In other words, the components may not be diagonalisable simultaneously on \( \mathbb{M}_c \).
Thus, employing a direct product DVR approach to represent higher dimensional Hermitian operators defined in the curvilinear co-ordinates in $\mathbb{M}_c$ might lead to erroneous estimates of the observables.

As briefly noted in the introduction, for the last two decades there has been active research on finding a way to build MNPDVR basis set on curved manifolds. Recently Littlejohn et al [1]; Dawes and Carrington [7]; Yu [8]; and Degani and Tennor [9] reported some promising results. Dawes and Carrington’s work is based on an approximate simultaneous diagonalization of the multidimensional co-ordinate operators described in $\mathbb{M}_c$. Yu presented a scheme somewhat apparently related to that reported in ref [7]. The basis of the work presented in ref [9] is that introduced in ref [1] by Littlejohn et al, which is the work we intend to look into (albeit briefly) here.

3. Reproducing Kernel functions and MNPDVR basis sets

Littlejohn et al took a novel approach to solving the ongoing problem of building MNPDVR basis sets. The authors ‘axiomize’ the known properties of a one-dimensional DVR basis set in the hope of deducing some underlying mathematical structures of the DVR concept with which one can formulate a general framework for constructing higher dimensional DVR basis sets. The essence of their work is given in the following definition. (Note that in the following discussion — for the sake of clarity — $x$ denotes $x^{(1:d)}$, unless stated otherwise.)

**Definition 1 (adapted from ref [1, 27, 28]):** Let $\mathbb{M}_c$ and $\mathcal{H}$ be as defined before; $\mathcal{P}$ a projection operator on $\mathcal{H}$; $\mathcal{I} = \mathcal{P}\mathcal{H}$, the space upon which $\mathcal{P}$ projects, with a dimension of $N$. Then $\{\Delta_\alpha(x) = \mathcal{P}\delta(x - x_\alpha)\}$ and $\{x_\alpha\}$, where $\alpha = 1, .., N$, is a DVR set.

To our knowledge, apart from two special cases [27, 28], the authors have not managed to achieve their ultimate goal of generating a general framework upon which MNPDVR basis sets can be built. Before we come to the central idea presented in this article, it is perhaps useful to recall that the so-called Dirac’s $\delta$ function (or more precisely tempered distribution) is not an element of $\mathcal{H}$ [21, 22, 29] – it is a functional that acts on $\mathcal{H}$ and resides in a dual space that is defined with reference to $\mathcal{H}$. We think the beauty of **Def.1** becomes clear if one replaces $\mathcal{H}$ in the definition with a ‘Rigged Hilbert Space’. With this minor amendment, it is then possible to use loosely $\Delta_\alpha(x) = \mathcal{P}\delta(x - x_\alpha)$ and $\Delta_\alpha(x) = <x|\mathcal{P}|x_\alpha>$ interchangeably. In the following discussion, for both pedantry and convenience, we elect to use the former which can obviously be expressed as

$$\Delta_\alpha(x) = \int_{\mathbb{M}}^{N} \mathcal{P}(x,x'')\delta(x'' - x_\alpha)dx''$$

$$= \sum_{j=1}^{N} \psi_j(x)\psi_j(x_\alpha)$$

where $\mathcal{P}(x,x'') = \sum_{j=1}^{N} \psi_j(x)\psi_j(x'')$ [30]

Because of the closure property of $\{\psi_j(x)\}_{j=1}^{\infty}$,
\[ \sum_{j=1}^{\infty} \psi_j(x) \psi_j(x_\alpha) = \delta(x - x_\alpha). \] In other words,

\[ \lim_{N \to \infty} \Delta_\alpha(x) = \lim_{N \to \infty} \sum_{j=1}^{N} \psi_j(x) \psi_j(x_\alpha) = \delta(x - x_\alpha) \]  

(5)

(cf. Eqs. 16 and 17 in ref. [17]).

This means that \( \lim_{N \to \infty} \Delta_\alpha(x_\alpha) = \lim_{N \to \infty} \sum_{j=1}^{N} |\psi_j(x_\alpha)|^2 = \infty \)

Then by deduction, it can be argued that

\[ \Delta_\alpha(x_\alpha) = \sum_{j=1}^{N} |\psi_j(x_\alpha)|^2 < \infty \]  

which implies that \( \Delta_\alpha(x) \in \mathcal{D} (\subset \mathcal{H}) = \text{span} \{ \psi_j(x) \}_{j=1}^{N} \) even though \( \lim_{N \to \infty} \Delta_\alpha(x) \notin \mathcal{H} \), Eq. 5. By definition \[1, 31\] \( x_\alpha \) is a DVR point whose corresponding DVR function is given by \( \Delta_\alpha(x) = \sum_{j=1}^{N} \psi_j(x) \psi_j(x_\alpha) \) where \( R_\alpha j = \psi_j(x_\alpha) \) (cf. Eq. 3), i.e. \( R_\alpha R = R_\alpha R^{-1} R = I_N \);

this means \( \Delta_\alpha(x_\beta) = \delta_{\alpha \beta} = \sum_{j=1}^{N} \psi_j(x_\beta) \psi_j(x_\alpha) \) when \( x_\alpha \) and \( x_\beta \) are DVR points. Since \( R \) is unitary, then \( \mathcal{D} \) is in the span of the set \( \{ \Delta_\alpha(x) \}_{\alpha=1}^{N} \) as well. (Note that we used \( R_{\alpha j} = \psi_j(x_\alpha) \) instead of \( R_{\alpha j} = c_\alpha \psi_j(x_\alpha) \) as \( c_\alpha \) can be absorbed into \( \psi_j(x_\alpha) \); this is also an implicit assumption made in the rest of the paper.)

Now we come to the nub of this paper. Using the facts given in the preceding paragraphs, Eq. 4 can obviously be rewritten as

\[ \Delta_\alpha(x) = \sum_{\beta=1}^{N} (R^{-1})_{\alpha \beta} \sum_{j=1}^{N} \psi_j(x) \psi_j(x_\beta) \]  

where

\[ k(x, x_\alpha) = \sum_{j=1}^{N} \psi_j(x) \psi_j(x_\alpha) \]  

From Eqs. 7 and 8, it is clear that \( k(x, x_\alpha) \) is symmetric and strictly positive definite \[32\]. According to Eq. 6, \( \sup_{x_\alpha \in M} k(x_\alpha, x_\alpha) < \infty \) which implies \( k \) is a valid representation of the inner-product in the span \( \{ \psi_j(x) \}_{j=1}^{N} \). In other words, \( k(x, x_\alpha) \) is a reproducing kernel (positive definite) function \[32, 33, 34, 35\]. All these points indicate that generating a DVR
function, $\Delta_\alpha(x)$, via $P_\delta(x - x_\alpha)$ can be viewed as finding a reproducing kernel function $k(x, x_\alpha)$ defined over $\mathcal{M}$, such that equations 7 holds.

First a brief description of the reproducing kernel theory is given in the following paragraph in the form of a definition. For more detailed discussions on the subject, the reader is referred to the seminal papers of N. Aronszajn [32] and E. H. Moore [33]. More descriptions on the subject, both on its application and theory, may be found in Refs. [34, 35, 36, 37, 38].

**Definition 2 (adapted from ref. [39]):** Let $\mathbb{X}$ be any domain and let $q(s, r) - s$ and $r \in \mathbb{X}$ — be symmetric and positive definite function if for any $M \in \mathbb{N}$, and any $r_1, r_2, \ldots, r_M \in \mathbb{X}$, the $H_{M \times M}$ matrix is positive definite; with the $(l,m)$th element given by $q(s_l, r_m)$. Then $q(s, r)$ is a reproducing kernel function, with which a unique RKHS $\mathcal{H}_k$ is associated, and can be described as having the representation

$$q(s, r) = \sum_{j=1}^{N} \zeta_j(s)\zeta_j(r)$$

where $\zeta_j(.)$ is defined on $\mathbb{X}$. A function is a reproducing kernel in the sense of $\langle f(\cdot), q(\cdot, r) \rangle = f(r), \forall f(\cdot) \in \mathcal{H}_k$.

The last statement means $q(s, r)$ is a representer of a bounded linear functional which acts on RKHS (here onwards denoted by $\mathcal{H}_q$) [32, 34]. It also means that the set $q(s, r_i), i = 1, 2, \ldots, M$ can span $\mathcal{H}_q$ [32]. It should also be noted that just $q(s, r)$ being a positive definite function on $\mathbb{X}$ is a sufficient condition for that function to be a reproducing kernel [32, 34], an observation the importance of which becomes clear later in the article. (Without lost of generality in the following discussions, $M$ is set to $N$ — and it is worth noting that $M$ can not be $> N$ [42].)

As stated in the definition, a function is positive definite over the given domain if $a^T H_{N \times N} a = \sum_{l,m} a_l a_m q(s_l, r_m) \geq 0, \forall a_l$ and $a_m \in \mathbb{R}\setminus 0$.

For the purpose of generating MNPDVR basis sets, another equally crucial property of $q$ is that if (say) $t_1, t_2$, and so on, are reproducing kernel functions defined over a manifold, then using these kernel functions we may be able to design other reproducing kernels defined over the same domain [35, 39].

Clearly, based on the above definition, $k(x, x_\alpha)$ (see Eq. 8) is a reproducing kernel function [32, 40] whose associated $\mathcal{H}_k$ can be viewed as $\mathcal{S}$ (cf. $\mathcal{S}$ noted in Def.1) provided that $N < \infty$. In the following discussion we demonstrate how a DVR function can be generated from a positive definite function.

If $Q$ is strictly positive definite [1], i.e., $\sum_{l,m} a_l a_m q(s_l, r_m) > 0$, then $Q^{-1}Q = I_N$. In other words,

$$(Q^{-1}Q)_{\alpha\beta} = \delta_{\alpha\beta} = \sum_{\beta=1}^{N} (Q^{-1})_{\alpha\beta} q(x_\beta, x_\alpha), \quad s_l = x_\beta; \quad r_m = x_\alpha$$

\[1\] Recall that if $q(x, x_\alpha)$ is not strictly positive definite, it can be turned into one, see Refs. [32, 39].
\[ v_\alpha(x) = \sum_{\beta=1}^{N} (Q)_{\alpha\beta}^{-1} q(x_\beta, x) \]  

is a function that \( v_\alpha(x_\beta) = \delta_{\alpha\beta} \), with \( \alpha = 1, \ldots, N \).

Of course, as \( v_\alpha(x) \) is a linear combination of a set of reproducing kernels, \( v_\alpha(x) \) itself is a reproducing kernel function \([35, 39]\) whose relation to \( \Delta_\alpha(x) \) can be readily shown as follows

\[ v_\alpha(x) = \sum_{\beta=1}^{N} (Q)_{\alpha\beta}^{-1} q(x_\beta, x) = \sum_{\beta=1}^{N} (Q)_{\alpha\beta}^{-1} \sum_{j=1}^{N} \zeta_j(x_\beta) \zeta_j(x) \]

\[ = \sum_{j=1}^{N} \left[ \sum_{\beta=1}^{N} (Q)_{\alpha\beta}^{-1} \zeta_j(x_\beta) \right] \zeta_j(x) = \sum_{j=1}^{N} c_\alpha \zeta_j(x_\alpha) \zeta_j(x) \]

\[ = \sum_{j=1}^{N} \psi_j(x_\alpha) \psi_j(x) \]

\[ = P[\delta(x-x_\alpha)] = \Delta_\alpha(x) \]

which is what we set out to show. (Note that \( \psi_j(.) = \sqrt{(c_\alpha)} \zeta_j(.) \).

Now we briefly analyze the implications of Eqs. 12–14. The equivalence of Eqs. 12–14 implies that the knowledge of a positive definite function defined on the specified domain is sufficient to construct a DVR basis set. In other words, it is not necessary to know that set \( \{ \zeta_j(x) \}_{j=1}^{N} \) that yields \( q(x, x_\alpha) \). A function that represents a valid inner-product in the span \( \{ \zeta_j(x) \}_{j=1}^{N} \), i.e., the appropriate \( q(x, x_\alpha) \), is all that is required \([41]\).

From Def.2, Eqs. 12–14 are true for both \( \mathcal{M} \) and \( \mathcal{M}_c \). One inference that can be made from Eqs. 12–14 is that the commonly employed DVR schemes, such as the Sinc-DVR of Colbert and Miller \([16]\) and the 'conventional' DVR of Light and co-workers \([2]\) are different instances of the proposed scheme. Furthermore when the domain over which \( q(x, x_\alpha) \) is defined is one-dimensional, the Lagrangian functions of Baye and co-workers (as defined in Ref. \([43]\)) are similar to \( h(x, x_\alpha) \).

The equations, Eqs. 12–14, also imply that one now has control over the choice of the DVR points unlike the currently used conventional DVR techniques where the global basis functions determine where on \( \mathcal{M}/\mathcal{M}_c \) the DVR points appear.

Possible simple reproducing kernel functions: The class of parameterisable functions \([4]\),

\[ \frac{a}{\pi} \lim_{a \to \infty} \frac{a \sin(x-x_\alpha)}{(x-x_\alpha)}, \quad \frac{1}{\sqrt{\pi}} \lim_{\epsilon \to 0} \frac{1}{\sqrt{\pi}} \exp(-\epsilon^2 x^2), \quad \frac{1}{\pi} \lim_{\epsilon \to 0} \frac{\epsilon}{(x-x_\alpha)^2 + \epsilon^2} \] 

(with \( a \) and \( \epsilon \) (\( \in \mathbb{R} \) > 0), that are widely used in physics to approximate/represent the Dirac's delta function \( \delta(x^{(i)}-x^{(i)}_\alpha) \) on \( \mathcal{M}/\mathcal{M}_c \) provides a good example of positive definite functions. In the cases of \( a < \infty \) and \( \epsilon > 0 \), these functions are valid reproducing kernels. In fact, the Lorentzian \( h(x, x_\alpha) = \frac{1}{\pi} \lim_{\epsilon \to 0} \frac{\epsilon}{(x-x_\alpha)^2 + \epsilon^2} \), with \( \epsilon > 0 \), can be modified to \( q(x, x_\alpha) = \frac{1}{\gamma(x-x_\alpha)^2 + 1} \). \[\text{8}^{2}\text{with parametric values that are different from their limiting values of the parameters}\].
where \( \gamma(\in R) > 0 \) — a function that is a fine positive definite function on any inner-product manifold, of which, of course, \( M \) and \( \overline{M} \) are examples. In the high dimensional case, \( x \) becomes \( x_{i=1, \ldots, d} \).

In the literature on DVR basis sets a 2-dimensional surface \( S^2 \) of a unit sphere is cited frequently as an example of a curved manifold. In the reproducing kernel function context, the issue of what kind of functions defined on \( S^\infty \) are positive definite was comprehensively addressed in the early 1940’s by I. J. Schoenberg. Recently it was demonstrated that, for example,

\[
\sum_{l=0}^{\infty} a_l P_l(p,p') \text{ is strictly positive definite on } S^2 \text{ if } a_l \geq 0,
\]

\[
\sum_{l=0}^{\infty} a_l P_l(1) < \infty \text{ and the set } \{ l : a_l > 0 \} \text{ contains infinitely many odd and infinitely many even integers.}
\]

\( P_l(p,p') = \cos \theta \cos \theta_a + \sin \theta \sin \theta_a \cos(\phi - \phi_a); \) \( P_l \) are Legendre polynomials; \( 0 \leq \theta \leq 2\pi; 0 \leq \phi \leq \pi; p = (\theta, \phi); p' = (\theta_a, \phi_a). \)

This means

\[
\lim_{N \to \infty} \frac{1}{4\pi} \sum_{l=0}^{N} (2l+1)P_l(p,p') \to \delta(p-p')
\]

is a strictly positive definite function on the 2-dimensional spherical surface if \( N < \infty \), while \( P_l(p,p') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^m(p)(Y_l^m(p'))^* \) (where \( Y_l^m \) are spherical harmonics) is a reproducing kernel function on the surface of the unit sphere. \( \frac{3}{2} - \cos(p,p') \), \( e^{(p,p')} \), to name but few, are other (strictly) positive definite functions on \( S^\infty \).

In passing, the practical issues such as the inversion of \( Q \) when \( d(\text{or } \overline{d}) \) is large, the calculation of the matrix elements of \( Q \) on multi-dimensional flat and curved manifolds, etc, will be discussed and elaborated upon in detail elsewhere. In the following subsection we illustrate (and demonstrate) the proposed scheme via solving the eigen-problem for a bound system that is described on ‘one-dimensional manifold’.

### 3.1. One Dimensional Test Case:

The one-dimensional Hamiltonian operator is in the form

\[
H(x) = -\frac{1}{2} \frac{d^2}{dx^2} + V(x)
\]

In the basis set \( \{v_n(x)\}_{n=1}^{N} \), the Hamiltonian and (possible) overlap matrix elements \( (H_{\alpha\alpha'}, B_{\alpha\alpha'}) \) can be written as

\[
H_{\alpha\alpha'} = T_{\alpha\alpha'} + V_{\alpha\alpha'}
\]

\[
B_{\alpha\alpha'} = \langle v_{\alpha'} | v_\alpha \rangle
\]
with

\[<v_\alpha'|v_\alpha> = \sum_{\beta',\beta}^N (Q^{-1})_{\alpha'\beta'}^{T} Q_{\alpha\beta}^{-1} C_{\beta'\beta}\; q(x_{\beta'},x) q(x_\beta,x) \] (20)

\[T_{\alpha'\alpha} = \sum_{\beta',\beta}^N (Q^{-1})_{\alpha'\beta'}^{T} Q_{\alpha\beta}^{-1} <q(x_{\beta'},x)|\frac{d^2}{dx^2}|q(x_\beta,x)> \] (21)

Since \(v_\alpha(x)\) are the DVR functions, which are not necessarily orthonormal, then

\[V_{\alpha'\alpha} = <v_{\alpha'}(x)|V(x)|v_\alpha(x)> \] (23)

\[= \sum_{\beta',\beta}^N (Q^{-1})_{\alpha'\beta'}^{T} Q_{\alpha\beta}^{-1} <q(x_{\beta'},x)|V(x)|q(x_\beta,x)> \] (24)

\[\approx V(x_\alpha) \sum_{\beta',\beta}^N (Q^{-1})_{\alpha'\beta'}^{T} Q_{\alpha\beta}^{-1} <q(x_{\beta'},x)|q(x_\beta,x)> \] (25)

\[= V(x_\alpha) \sum_{\beta',\beta}^N (Q^{-1})_{\alpha'\beta'}^{T} Q_{\alpha\beta}^{-1} C_{\beta'\beta} = V(x_\alpha) <v_{\alpha'}|v_\alpha> \] (26)

i.e., in matrix form the Hamiltonian operator is given as

\[H = (Q^{-1})^{T} T Q^{-1} + VB \] (27)

Thus yielding the solution of the eigen-problem amounts to determining the eigenpairs \((E_n, u_n)\) of a general eigenproblem

\[\left[(Q^{-1})^{T} T Q^{-1} + VB\right] u_n = E_n Bu_n \] (28)

As a concrete example we chose a Gaussian function \(q(x,x_\alpha) = (\frac{2A}{\pi})^{1/4} \exp\left[-A(x-x_\alpha)^2\right]\) as a reproducing kernel, which is defined over \(\mathbb{R}\). \(A\) is a parameter that is tuned to render the kernel strictly positive definite in the interval \([x_{\text{min}}, x_{\text{max}}]\) on which the potential function is defined. Recall that when \(q(x,x_\alpha)\) is strictly positive definite \(Q\) is invertible, which in turn implies the functions \(\{q(x_\alpha,x)\}\) are linearly independent over the chosen coordinate range. In other words, the small eigenvalues of \(B\) are not too small to create numerical problems (and references therein).

When \(q(x,x_\alpha)\) is Gaussian, the evaluation of \(<q(x_\beta',x)|\frac{d^2}{dx^2}|q(x_\beta,x)>\) and \(C_{\beta'\beta} = <q(x_\beta',x)|q(x_\beta,x)>\) is straightforward, see Eqs. 9–11 of Ref. [51].

In this test case, the potential function in the Hamiltonian operator was the Morse potential, \(v(x) = D(e^{-2\xi x} - 2e^{-\xi x})\), that was considered in Refs. [51, 52]. With \(D = 12\) and \(\xi = 0.2041241\), this potential function supports 24 bound eigenstates.
Finally the range \([x_{\text{max}}, x_{\text{min}}]\) was set to \([-4., 45.\]). In the example, \(x_\alpha = x_{\text{min}} + \frac{x_{\text{max}} - x_{\text{min}}}{L} (\alpha - 1), \ i=1,...,L\). The \(x_\alpha\) points (\(L\) of them) were used to generate a positive definite \(Q\) matrix of \(L \times L\). \(Q\) was then inverted employing a LU decomposition algorithm. The chosen points became the DVR points while their corresponding functions were obtained using Eq. 12.

With \(L\) and \(A\) set to 90 and 0.9, respectively, the matrix elements \(V_{\alpha' \alpha}\) were calculated using Eq. 27. Then Eq. 29 was solved by employing \(DSYGV\), a \text{LAPACK} routine \([53]\). The yielded 24 bound eigenvalues are as shown in Column 3 of the table. Since strictly speaking the potential operator is not diagonal when expressed in DVR basis functions \([2, 10, 12]\), the above calculation was repeated. In this time round, the potential matrix elements were computed exactly using \text{Mathematica} \([54]\). Self-evidently, the two results are in excellent agreement, Column 4. seemingly this confirms the validity of the proposed scheme, \textit{albeit} in one-dimensional problems. Note that the above discussion is valid whether the coordinate domain is flat or curved. In the presented results, the coordinate domain was considered flat. Thus, \((x - x_\alpha)^2\) in \(q(x, x_\alpha) = \left(\frac{2A}{\pi}\right)^{1/4} \exp \left[-A(x - x_\alpha)^2\right]\) was a simple Euclidean distance.

The analytic solutions of the Hamiltonian problem are as given in Column 2. As Column 5 illustrates, the accuracy of the computed lower eigenvalues is good compared to that of the computed higher eigenvalues. As explained by Hamilton and Light \([51]\), this can be addressed by employing unequally distributed Gaussian functions – instead of the equally distributed Gaussian functions that we chose for clarity, to demonstrate the proposed algorithm.

4. Conclusion

In this article it was demonstrated that, starting off with the axiomatic definition of DVR provided in ref \([1]\), it is possible to show the space upon which the projection operator (noted in that reference) projects is a Reproducing Kernel Hilbert Space whose associated reproducing kernel function can be used to generate DVR points and their corresponding DVR functions on any manifold (curved or not).

The results of the simple example that was presented as a preliminary test of the new scheme seemingly confirms our mathematical prediction. Nonetheless, a more realistic test of the new method will be given in subsequent publications.

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Table 1: Comparison of errors of the calculated eigenvalues for Morse Potential. Exact: Analytic eigenvalues; RKSDVR= eigenvalues computed with $V_{\alpha',\alpha}$ computed via Eq. 26; RKS eigenvalues computed with $V_{\alpha',\alpha}$ computed exactly, Eq. 24.

| State Number | Exact     | RKSDVR   | RKSDVR-RKS | Exact-RKSDVR |
|--------------|-----------|----------|------------|--------------|
| 0            | -11.5052  | -11.5052 | 0.000000   | 3.5150666E-07|
| 1            | -10.5469  | -10.5469 | 0.000000   | 1.6017819E-06|
| 2            | -9.6302   | -9.6302  | 0.000000   | 2.1581170E-06|
| 3            | -8.7552   | -8.7552  | 0.000000   | 2.7113422E-06|
| 4            | -7.9219   | -7.9219  | 0.000000   | 3.3694112E-06|
| 5            | -7.1302   | -7.1302  | 0.000000   | 4.3132356E-06|
| 6            | -6.3802   | -6.3802  | 0.000000   | 5.8555934E-06|
| 7            | -5.6719   | -5.6719  | 0.000000   | 8.4396995E-06|
| 8            | -5.0052   | -5.0052  | 0.000000   | 1.2556453E-05|
| 9            | -4.3802   | -4.3802  | 0.000000   | 1.8664048E-05|
| 10           | -3.7969   | -3.7969  | 0.000000   | 2.7037027E-05|
| 11           | -3.2552   | -3.2552  | 0.000000   | 3.7583833E-05|
| 12           | -2.7552   | -2.7552  | 0.000000   | 4.9771613E-05|
| 13           | -2.2969   | -2.2969  | 0.000000   | 6.2608957E-05|
| 14           | -1.8802   | -1.8803  | 0.000000   | 7.4703949E-05|
| 15           | -1.5052   | -1.5053  | 0.000000   | 8.4475342E-05|
| 16           | -1.1719   | -1.1720  | 0.000000   | 9.0389726E-05|
| 17           | -0.8802   | -0.8803  | 0.000000   | 9.1175405E-05|
| 18           | -0.6302   | -0.6303  | 0.000000   | 9.6037056E-05|
| 19           | -0.4219   | -0.4220  | 0.000000   | 7.4869651E-05|
| 20           | -0.2552   | -0.2553  | 0.000000   | 5.8097745E-05|
| 21           | -0.1302   | -0.1303  | 0.000000   | 3.6435728E-05|
| 22           | -0.0469   | -0.0469  | 0.000000   | 6.946361E-05  |
| 23           | -0.0052   | -0.0043  | 0.000000   | -9.3466361E-04|

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