Discrete Variable Representation

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Introduction

Discrete Variable Representation (DVR) methods were introduced long ago [3, 2, 6, 5, 7, 1, 4], but only recently have been put on a firm theoretical basis [12, 10, 9, 8, 11]. Here, we give a brief (and simplified) account of the recent work by Littlejohn and Cargo.

1 Definition and properties

Let $\mathcal{H}$ be the Hilbert space of a quantum mechanical system and P the projector onto a subspace $\mathcal{S} = P\mathcal{H}$ in which we are interested. Let M be the configuration space of the system upon which the coordinate representation of $\mathcal{H}$ is based; for example, for a single particle $\mathrm{M} = \mathbb{R}^3$ and $\mathcal{H}_{\mathrm{x}} = L^2(\mathbb{R}^3)$. Finally, let $\{x_\alpha\}$ be a set of grid points in M. Then, we say that the combination of the projector P and the grid $\{x_\alpha\}$ forms a DVR set if the set of vectors

$$|\Delta_\alpha\rangle = P\,|x_\alpha\rangle$$

is *orthogonal*

$$\langle\Delta_\alpha|\Delta_\beta\rangle = N_\alpha\delta_{\alpha\beta}\ N_\alpha > 0$$

and *complete* in S. In this case, the complete, orthonormalized set of vectors

$$|F_\alpha\rangle = \frac{1}{\sqrt{N_\alpha}}\,|\Delta_\alpha\rangle$$

is the DVR set of the space $\mathcal{S}$ on the grid $\{x_\alpha\}$.

The above definition makes clear that each DVR state $|F_\alpha\rangle$ is, in some sense, localized around the grid point x_α, thereby establishing a natural correspondence between points in configuration space and state vectors. The following, schematic interpretation may be useful. Close to $\mathcal{H}$ there are two simple spaces, the *Schwartz space* of 'rapid decreasing functions' and the *temperated distribution space* of continuous linear functionals on the Schwartz space. The first space is *dense* in $\mathcal{H}$; the latter is somewhat larger than $\mathcal{H}$ and contains 'exotic' elements such as *improper* vectors. A simple map between M and the distribution space is given by the (improper) eigenvectors of the coordinate operator

$$\mathrm{M} \ni x \rightsquigarrow |x\rangle$$

Then, the DVR maps a set of point of M directly on $\mathcal{H}$ and almost preserves the metric properties, in the sense

$$\langle x_\alpha | x'_\beta \rangle = \delta(x_\alpha - x'_\beta) \rightsquigarrow \langle F_\alpha | F_\beta \rangle = \delta_{\alpha\beta}$$

By definition, using $P^\dagger = P^2 = P$, it follows

$$\langle \Delta_\alpha | \Delta_\beta \rangle = \langle x_\alpha | P x_\beta \rangle = \Delta_\beta(x_\alpha) = \Delta^*_\alpha(x_\beta) = N_\alpha \delta_{\alpha\beta}$$

or equivalently

$$F_\beta(x_\alpha) = \delta_{\alpha\beta}\sqrt{N_\alpha}$$

that is, the coordinate representation of a DVR set is made up of functions which vanish at each other grid points, but at their own. In other words, DVR functions satisfy simultaneously two properties: *orthogonality* and *interpolation* property. These properties can be used to get two different representations of vectors.

Let us first consider the case $|\psi\rangle \in \mathcal{S}$. Then, $|\psi\rangle$ can exactly be represented by the DVR set

$$|\psi\rangle = \sum_\alpha |F_\alpha\rangle \langle F_\alpha|\psi\rangle = \sum_\alpha \frac{1}{N_\alpha} \psi(x_\alpha) |F_\alpha\rangle$$

where the property $\langle F_\alpha|\psi\rangle = \frac{1}{\sqrt{N_\alpha}} \langle P x_\alpha|\psi\rangle = \frac{1}{\sqrt{N_\alpha}} \langle x_\alpha|\psi\rangle$ has been used. The DVR representation of the state vector $|\psi\rangle$, $\psi^{DVR}_\alpha = \langle F_\alpha|\psi\rangle$, is therefore simply related to the values of the wavefunction at grid points; in this case, one may indifferently use the 'scalar product definition'

$$\psi^{DVR}_\alpha = \langle F_\alpha|\psi\rangle$$

or the 'grid definition'

$$\psi^{DVR}_\alpha = \frac{1}{\sqrt{N_\alpha}} \psi(x_\alpha)$$

When $|\psi\rangle \notin \mathcal{S}$ the two expressions above are different and only the projection of $|\psi\rangle$ onto $\mathcal{S}$ can exactly be represented by the DVR. That is, two different approximation to the state vector are possible, one based on its projection on $\mathcal{S}$

$$|\psi\rangle \simeq |\psi^S\rangle = P|\psi\rangle = \sum_\alpha |F_\alpha\rangle \langle F_\alpha|\psi\rangle$$

and one based on the DVR formula

$$|\psi\rangle \simeq |\psi^{DVR}\rangle = \sum_\alpha \frac{1}{\sqrt{N_\alpha}} \psi(x_\alpha) |F_\alpha\rangle \tag{1}$$

The two vectors $|\psi^S\rangle$ and $|\psi^{DVR}\rangle$ lie in the same space $\mathcal{S}$ but they are only approximately equal, since in this case $\langle x_\alpha|P\psi\rangle = \psi^S(x_\alpha) \simeq \psi(x_\alpha)$. *Both* vectors are approximate representation of $|\psi\rangle$ and, in some sense, they are exponentially close to $|\psi\rangle$ in the measure that $|\psi\rangle$ is close to $\mathcal{S}$ [12]. Equation 1 defines the (approximate) Discrete Variable representation of the state vector, $\psi_\alpha^{DVR} = \langle F_\alpha|\psi^{DVR}\rangle = \psi(x_\alpha)N_\alpha^{-1/2}$.

Now, let $|\psi\rangle\,, |\phi\rangle \in \mathcal{S}$ and let us consider the scalar product

$$\langle\psi|\phi\rangle = \sum_\alpha \langle\phi|F_\alpha\rangle\,\langle F_\alpha|\psi\rangle = \sum_\alpha \frac{1}{N_\alpha}\phi^*(x_\alpha)\psi(x_\alpha)$$

In other words, the DVR introduces an exact *quadrature rule* for the scalar product,

$$\langle\psi|\phi\rangle = \sum_\alpha \omega_\alpha\phi^*(x_\alpha)\psi(x_\alpha) \text{ with } \omega_\alpha = N_\alpha^{-1} \tag{2}$$

When $|\psi\rangle\,, |\phi\rangle \notin \mathcal{S}$ this formula is the DVR approximation to the scalar product, according to

$$\langle\psi|\phi\rangle \simeq \langle\psi^{DVR}|\phi^{DVR}\rangle$$

where vectors on r.h.s. are defined by equation 1.

Note that once a DVR set has been defined in a space $\mathcal{S} = P\mathcal{H}$ with the grid points $\{x_\alpha\}$ one can obtain further DVR sets by simply throwing out grid points. This is useful if the wavefunction we are interested in is known to be vanishing small at some grid points. The proof follows directly from the definition using the projector $P' = \sum'_\alpha |F_\alpha\rangle\,\langle F_\alpha|$ in which the sum is restricted to a subset of the original grid.

2 Finite Basis Representations

Let $\{|\phi_n\rangle\}$ be a complete, orthonormal set in $\mathcal{S}$. This set can be used to obtain an alternative representation of any vector in $\mathcal{S}$ which we call the Finite Basis Representation,

$$|\psi\rangle = \sum_n |\phi_n\rangle\,\langle\phi_n|\psi\rangle \quad \psi_n^{FBR} = \langle\phi_n|\psi\rangle$$

A unitary transformation exists such that

$$|F_\alpha\rangle = \sum_n |\phi_n\rangle\, U_{n\alpha}$$

and this can be used to transform FB representations to DV representations,

$$\psi^{DVR} = \sum_n (U^\dagger)_{\alpha n}\psi_n^{FBR} \tag{3}$$

where

$$U_{n\alpha} = \langle\phi_\alpha|F_\alpha\rangle = \sqrt{\omega_\alpha}\phi_n^*(x_\alpha) \tag{4}$$

It is clear, however, from the discussion of the previous section, that eq. 3 is exact only for vectors of $\mathcal{S}$; for a generic vector $|\psi\rangle$, eq. 3 relates different representations of its projection on $\mathcal{S}$, $|\psi^S\rangle$. The assumption is always made that $|\psi^S\rangle \simeq |\psi^{DVR}\rangle$.

Operator representations and transformations follow easily from

$$\langle F_\alpha | A | F_\beta \rangle = \sum_{nm} \langle F_\alpha | \phi_n \rangle \langle \phi_n | A | \phi_m \rangle \langle \phi_m | F_\beta \rangle$$

i.e.

$$A^{DVR} = U^\dagger A^{FBR} U \tag{5}$$

which is exact only for operators projected onto $\mathcal{S}$, $A_P = PA$ and, as before, the assumption is always made that $|\alpha^S\rangle = PA|F_\alpha\rangle \simeq |\alpha^{DVR}\rangle$. Local operators may be approximated as follows

$$\langle F_\alpha | A | F_\beta \rangle = A(x_\alpha)\delta_{\alpha\beta} \tag{6}$$

if one takes into account the localized properties of the DVR vectors. As before, this formula is exact only if $A = PA$.

In practice, one uses the DVR approximation of eq. 6 for operators which are local in system coordinates and, starting from an appropriate FBR for non-local operators, (s)he gets (approximate) DV representations for the latter using eq. 5. Usually, the FB set diagonalizes the operator A and thus

$$(A^{DVR})_{\alpha\beta} = \sum_n \sqrt{\omega_\alpha \omega_\beta}\phi_n(x_\alpha)\phi_n^*(x_\beta)a_n$$

where a_n are the eigenvalues of A. A more general result is

$$(f(A)^{DVR})_{\alpha\beta} = \sum_n \sqrt{\omega_\alpha \omega_\beta}\phi_n(x_\alpha)\phi_n^*(x_\beta)f(a_n)$$

3 Simple examples

Defining a DVR set is generally difficult and not even always possible. Usually, one starts with a set of orthogonal vectors $\{|\phi_n\rangle\}$, defines the projector

$$P = \sum_n |\phi_n\rangle \langle \phi_n|$$

and looks for grid points x_α such that the vectors

$$P|x_\alpha\rangle = |\Delta_\alpha\rangle = \sum_n |\phi_n\rangle \phi_n^*(x_\alpha)$$

are orthogonal,

$$\langle \Delta_\alpha | \Delta_\beta \rangle = \sum_n \phi_n(x_\alpha)\phi_n^*(x_\beta) = N_\alpha \delta_{\alpha\beta} \tag{7}$$

This task may be very difficult or even impossible. However, for several one-dimensional problems a convenient choice for $\{|\phi_n\rangle\}$ is a *real orthogonal polynomial set* times the square root of some weighting function $W(x)$,

$$\phi_n(x) = W^{1/2}(x)P_n(x)$$

$$\langle \phi_n | \phi_m \rangle = \int W(x)P_n(x)P_m(x)dx = \delta_{nm}$$

In such case, given that $P_n(x)\,(n=0,..N-1)$ are polynomials of degree n one chooses as grid points the *zero* of $P_N(x)$, the first neglected polynomial

$$P_N(x_\alpha)=0\,\alpha=1,..N$$

They are known as Gauss-quadrature points. The above DVR condition of eq. 7 may be rewritten as follows

$$\Delta_\alpha(x_\beta)=\sum_{n=0}^{N-1}\sqrt{W(x_\alpha)W(x_\beta)}P_n(x_\alpha)P_m(x_\beta)\propto\delta_{\alpha\beta}$$

Now, from *Gauss' quadrature theory* it is known that the following relation holds

$$\begin{aligned}\delta_{nm} &= \int W(x)P_n(x)P_m(x)dx \\ &\equiv \sum_\alpha w_\alpha W(x_\alpha)P_n(x_\alpha)P_m(x_\alpha) \end{aligned} \tag{8}$$

for $n,m=0,1,..N-1$. Here $\{x_\alpha\}$ are Gauss quadrature points and w_α are Gauss quadrature weights. This formula tells us that scalar products involving $P_n(x)\,n=0,..N-1$ polynomials (and their linear combinations) are *exactly* computed by quadrature with a careful choice of grid points. From eq. 8 it follows that the vectors $\mathbf{X}_\beta=\{X_m^\beta\}_{m=1}^{N-1}=\{\sqrt{W(x_\beta)}P_m(x_\beta)\}_{m=1}^{N-1}$ are linearly independent since they are orthogonal with respect to the weights w_β, and

$$\sum_\beta^N w_\beta\Delta_\alpha(x_\beta)X_m^\beta=\sqrt{W(x_\alpha)}P_m(x_\alpha)$$

holds. In other words

$$\sum_{\beta=1}^N w_\beta\Delta_\alpha(x_\beta)\mathbf{X}_\beta=\mathbf{X}_\alpha$$

or, equivalently, $w_\beta\Delta_\alpha(x_\beta)=\delta_{\alpha\beta}$. Thus, the set

$$F_\alpha(x)=\sqrt{w_\alpha}\sum_{n=0}^{N-1}\sqrt{W(x)W(x_\alpha)}P_n(x)P_m(x_\alpha)$$

is the DVR set.

Another very common, one-dimensional set is the *sync set.* To introduce it, let us consider $\mathrm{M}=\mathbb{R}$ and the following projection operator

$$P=\int_{-p_{max}}^{+p_{max}}dp\,|p\rangle\,\langle p|$$

where $|p\rangle$ are momentum eigenstates. This operator and the grid

$$\{x_\alpha=\frac{\pi}{p_{max}}\alpha\}_{\alpha\in\mathbb{Z}}$$

allow us to define a DVR set. Indeed,

$$|\Delta_\alpha\rangle=\int_{-p_{max}}^{+p_{max}}dp\,|p\rangle\,\frac{e^{-ipx_\alpha}}{\sqrt{2\pi}}$$

and

$$\langle\Delta_\alpha|\Delta_\beta\rangle = \int_{-p_{max}}^{+p_{max}} dp \frac{e^{ip(x_\alpha - x_\beta)}}{\sqrt{2\pi}} = \delta_{\alpha\beta}\frac{p_{max}}{\pi}$$

Therefore, a DVR set can be defined,

$$F_\alpha(x) = \sqrt{\frac{\pi}{p_{max}}}\Delta_\alpha(x) = \frac{1}{\sqrt{\pi p_{max}}}\frac{sin[p_{max}(x - x_\alpha)]}{(x - x_\alpha)}$$

which is known as sync DVR set. Note that in this case the space $\mathcal{S} = P\mathcal{H}$ is infinite dimensional and the DVR set is infinite. Its completeness follows from its momentum representation

$$\langle p|F_\alpha\rangle = \sqrt{\frac{\pi}{p_{max}}}\langle p|\Delta_\alpha\rangle = \frac{1}{\sqrt{2p_{max}}}e^{-i\frac{\pi}{p_{max}}p\alpha}$$

which is the known *complete* Fourier basis set for square-integrable functions in $\mathcal{M} = [-p_{max}, p_{max}]$. Note also that this DVR set allows one to exactly represent any *band-limited* function through an infinite but *discrete* set of function evaluations (or measurements)

$$\mathcal{S} \ni |\psi\rangle \quad |\psi\rangle = \sum_\alpha |F_\alpha\rangle \sqrt{\frac{\pi}{p_{max}}}\psi(x_\alpha)$$

Actual sync sets used in practice are obtained from that defined above by throwing out points, e.g. retaining points $|\alpha| \leq N$. The corresponding space $\mathcal{S}'$ comprises only discrete momentum values, $p_\alpha = \frac{p_{max}}{N}\alpha$, and is the space of band-limited, square-integrable functions in M $=[-L, L]$ with $L = \pi N/p_{max}$. This set underlies the use of Fast Fourier Transforms[1].

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