

Discrete Variable Representations Using Incomplete Quadrature Formulas

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Abstract

A new type of multidimensional discrete variable representation (DVR) is developed. The construction involves finding an exact quadrature formula over a set of polynomials. The set is generally too small to admit a DVR set over the grid points. A linear algebra technique selects the requisite remaining functions. A modification of the kinetic energy matrix is presented which should not modify the correct spectrum of the hamiltonian while eliminating spurious eigenvalues. The modification also greatly simplifies the computation of the DVR kinetic energy matrix.