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The computation of radial integrals with nonclassical quadratures for quantum chemistry and other applications

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Abstract The computation of radial integrals on the semi-infinite axis is an important computationally intensive feature of quantum chemistry computer codes with additional applications to physics and engineering. There have been numerous algorithms proposed to evaluate these integrals efficiently. Many of these approaches involve the transformation of the semi-infinite axis , $r \in [0, \infty)$, to the finite interval, $x \in [-1, 1]$, and the use of the Gauss-Legendre or Gauss-Chebyshev quadratures to evaluate the integrals. These mappings redistribute the quadrature points in many different ways. The approach in this paper is to compute the radial integrals with the Gauss-Maxwell nonclassical quadrature defined by the weight function $w(r) = r^2 e^{-r^2}$ appropriate for the semi-infinite interval and to also use scaling of the quadrature points. We carry out numerical experiments with simple model radial integrands and compare with the results of previous workers.

1 Introduction

Quantum chemistry computer codes whether based on density functional theory [11, 32, 39] or otherwise require the efficient numerical evaluation of three dimensional integrals in spherical polar coordinates [4]. The angular portion of the integrals are often evaluated with Lebedev

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