Numerical integration of singular functions by finite-difference methods

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In various fields of physical and quantum chemistry, e. g. in solid state theory and in the Dirac theory of a hydrogen-like atom with a point-like nucleus, singular functions are encountered. The functions themselves or their derivatives beyond a certain order behave singularly for some value(s) of the argument. Closed expressions of these functions are known only in simple cases (as in the examples just mentioned). In general, such functions are known only numerically for a set of argument values.

Definite integration of such functions is frequently required, and must be performed numerically (except for simple cases, which can be treated in closed form). Special numerical methods are usually needed to cope with the singular behaviour in low-order derivatives (including the function itself as zeroth derivative).

A suitable integration method, to be used in connection with finite-difference methods, was given by Biegler-König. We have further developed this method, and coded it into a computer program for ease of application. The method promulgated, which avoids any singularity in the integration step, is of wide applicability and, in principle, allows for extremely high accuracy. Preliminiary results will be presented.