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New Formulae for Differentiation and Techniques in Numerical Integration

We present new formulae, called the Slevinsky-Safouhi's formulae (SSF) I and II [1] for the analytical development of derivatives. The SSF, which are analytic and exact, represent the derivative as a discrete finite sum involving coefficients that can be computed recursively and they are not subject to any computational instability.

There are numerous applications in science and engineering for special functions and higher order derivatives. As an example, the nonlinear G transformation has proven to be a very powerful tool in numerical integration [3]. However, this transformation requires higher order derivatives of the integrands for the calculation, which can be a severe computational impediment.

As examples of applications of the SSF, we present higher order derivatives of Bessel functions which are prevalent in oscillatory integrals and provide tables illustrating our results. We also present an efficient recursive algorithm for the implementation of the G transformation. The incomplete Bessel function is presented as an example of application. Lastly, we present a generalized and formalized integration by parts to create equivalent representations to some challenging integrals. As an example of application, we present the Twisted tail.

[1] R. M. Slevinsky and H. Safouhi. New formulae for higher order derivatives and applications. J. Comput. App. Math., 233:405–419, 2009.

[2] H. L. Gray and S. Wang. A new method for approximating improper integrals. SIAM J. Numer. Anal., 29:271–283, 1992.

[3] R. M. Slevinsky and H. Safouhi. The S and G transformations for computing three-center nuclear attraction integrals. Int. J. Quantum Chem., 109:1741–1747, 2009.