

Generalized techniques in numerical integration

Richard M. Slevinsky¹, Hassan Safouhi²

¹Mathematical section, Campus Saint-Jean, University of Alberta, Canada
email: rms8@ualberta.ca

²Mathematical section, Campus Saint-Jean, University of Alberta, Canada
email: hassan.safouhi@ualberta.ca

Abstract

Integration by parts is one of the most popular techniques in the analysis of integrals. The product of the technique is usually a divergent series formed from evaluating boundary terms [1]; however, sometimes the remaining integral is also evaluated [2].

Due to the successive differentiation and antidifferentiation required to form the series or the remaining integral, the technique in its raw form is difficult to apply to problems more complicated than the simplest. In this talk, we explore a generalized and formalized integration by parts to create equivalent representations to some challenging integrals. Coupled with sequence transformations and/or extrapolation methods, we assess each of the different methods that can be formed from our formalized integration by parts.

As a demonstrative archetype, we examine the infinite-range Fresnel integrals. We also examine some peculiarities with the methods applied to the Twisted Tail. And lastly, we examine the most challenging molecular integrals that arise in molecular structure calculation using exponential type functions as a basis set of atomic orbitals.

References

- [1] E. J. Weniger, Nonlinear sequence transformations for the acceleration of convergence and the summation of divergent series, *Comp. Phys. Rep.*, 10, 189–371, 1989.
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