Sophisticated Techniques for Numerical Integration of Challenging Integrals: Extrapolation Methods and Asymptotics

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Abstract. Integration by parts is one of the most popular techniques in the analysis of integrals and it has frequently been used to create divergent series or asymptotic expansions of integral representations. The product of the technique is usually a divergent series formed from evaluating boundary terms; however, sometimes the remaining integral is also evaluated. As an example, we consider the Euler series arising from integrating the Euler integral by parts:

$$\int_x^\infty \frac{e^{-t}}{t}\mathrm{d}t \sim \frac{e^{-x}}{x}\sum_{l=0}^{\infty}(-1)^l\frac{l!}{x^l}, \quad x\to\infty, \tag{1}$$

where the remaining integral after n integrations by parts $(-1)^n n!\int_x^\infty \frac{e^{-t}}{t^{n+1}}\mathrm{d}t$ is often discarded and the divergent series has either been summed straightforwardly or through the use of sequence transformations.

Another example arises in molecular structure calculation. Through a reformalized integration by parts with respect to $x\,\mathrm{d}x$, the initial integral is transformed into the simple sine function integral:

$$\int_0^\infty x^{n_x}\frac{\hat{k}_\nu\left[R_2\gamma(s,x)\right]}{\left[\gamma(s,x)\right]^{n_\gamma}}j_\lambda(vx)\,\mathrm{d}x = \int_0^\infty\left[\left(\frac{\mathrm{d}}{x\,\mathrm{d}x}\right)^\lambda\left(x^{n_x+\lambda-1}\,\frac{\hat{k}_\nu\left[R_2\gamma(s,x)\right]}{\left[\gamma(s,x)\right]^{n_\gamma}}\right)\right]\sin(x)\,\mathrm{d}x. \tag{2}$$

Due to the successive differentiation and anti-differentiation required to form the series or the remaining integral, the technique is difficult to apply to problems more complicated than the simplest. In this contribution, we explore a generalized and formalized integration by parts to create equivalent representations to some challenging integrals and we introduce a recursive algorithm based on the theoretically powerful G transformation, which was handicapped by the lack of an algorithmic implementation. The recurrence relations reduce considerably the complexity of the algorithm, which is shown to be robust and leads to an unprecedented accuracy.

As a demonstrative archetype, we examine the infinite-range Fresnel integrals, the Twisted Tail, Airy functions, Bessel integrals, and the incomplete Bessel functions.

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