INTEGRATION OF PARAMETRIZED INTEGRANDS

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Abstract. Computer simulations involving numerical integration typically rely upon subroutines from sources such as the GNU Scientific Library, Netlib, or the Numerical Algorithms Group. Routines are often quadrature based and employ acceleration heuristics based on linear or nonlinear sequence transformations. Most accept user specified limits on absolute and relative error. The underlying assumptions are violated in practice, however. Subroutines may return an incorrect result accompanied by a small error estimate, telling the caller that the incorrect result should be trusted. This talk presents a case study where such behavior resulted in the loss of a large block of computation time due to the consequent meaningless simulation. The alternative methods which were employed to obtain reliable integration results are described.

1. Introduction

Integration routines provided by computation packages and scientific libraries are widely used in support of computer simulations. Their numerical inaccuracy can make consequent computations meaningless, however. Subroutines may return an incorrect answer accompanied by a small error estimate, misleading the caller.

We have encountered this situation when evaluating the integral $I(\alpha, \beta, \gamma, \delta, \xi)$ defined by

$$\int_0^1 \int_0^\infty \frac{\exp(-((u-\alpha)/\beta)^2 - ((v-\gamma)/\delta)^2 - v/(c_0 - uc_1) - \xi)}{c_0 - uc_1} \, dv \, du \tag{1}$$

For example, with $c_0 = 1$ and $c_1 = 0.9$, we naively believed Maple would give a reasonable answer using 16 digits of decimal precision (default precision is 10).

```
> Digits := 16; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
     0.00097...
```

Thinking that result too small, we tried repeatedly but doubled each time the number of digits:

```
> Digits := 32; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
     0.00687...
> Digits := 64; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
     0.02194...
> Digits := 128; I_(0.9138181, 0.09564921, 0.5759114, 4.1584, 1.47815);
     0.03221...
```

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The relative error of the last answer is over 6%, and Maple is excruciatingly slow.[1] The Gnu Scientific Library is comparatively fast, taking 0.0365 seconds to do the outer integral when provided with an explicit solution for the inner integral. But it returned 0.00013... with estimated relative error below $2.0e{-}08$. That was useless; our application needed the *correct* answer 0.03436... and it needed it produced *thousands* of times faster. We found no package or library which returned reasonable answers within reasonable amounts of time for a sampling of parameter values generated by our application.

We interchanged the order of integration and hand-coded 128-point Gauss-Laguerre quadrature of the form

$$(2)\quad \int_0^\infty e^{-x} \exp\Big(-\big(\frac{(c_0 - \alpha c_1)x - \gamma}{\varphi_x}\big)^2\Big) \Big\{ \mathrm{erf}\Big(\frac{\psi_x}{\varphi_x \beta\delta}\Big) - \mathrm{erf}\Big(\frac{\psi_x - \varphi_x^2}{\varphi_x\beta\delta}\Big)\Big\} \frac{dx}{\varphi_x}$$

where

$$\psi_x \;=\; x\beta^2 c_1(xc_0 - \gamma) + \delta^2\alpha \qquad \text{and} \qquad \varphi_x \;=\; \sqrt{\delta^2 + x^2\beta^2 {c_1}^2}$$

This was suitably fast and accurate for the specific parameter values above (integrals (1) and (2) are not equal, but the value of one is easily obtained from the value of the other). After further testing, 128-point Gauss-Laguerre quadrature was incorporated into our application.

The story does not end here. Our application was later observed to generate integrals which double precision 256-point Gauss-Laguerre could not evaluate with less than 160% relative error. To make matters worse, it had become apparent that significant additional speedup was desired. The following sections describe our initial steps towards solving these problems. We hope our case study will serve as a useful tutorial to others facing similar situations (which may vary in the technical details).

2. Complex Variables

Cauchy's integral theorem is a well-known tool for integration. A lesser known method described by Boas and Schoenfeld [1] dispenses with having to choose suitable contours by focusing instead on residues of the integrand over the Riemann sphere. They discuss integrals of three types, the second of which is covered by the following theorem.

Theorem 1. *Let F be holomorphic in the extended plane except for a finite number of singularities, let F be holomorphic on (a, b) except for simple poles, and let F be holomorphic at a and at b. Then*

$$P.V. \int_a^b F(t)\, dt \;=\; -(R + r)$$

where R is the sum of the residues of $F(z)\log\{(z - a)/(z - b)\}$ for z in the extended plane but not on $[a, b]$, and r is the sum of the residues of $F(z)\log\{(z - a)/(b - z)\}$ for z on (a, b).

[1]For the example parameter values above, we discovered later that Maple returns an acceptable answer using default precision provided specialized syntax is used for the query. That syntax shifts problems elsewhere, however; unacceptable results are returned when using it with other parameter values.

After performing the inner integration, changing variables and rearranging, our original integration problem (1) reduces to the form

$$\int_u^v \exp(-(\frac{t-a}{b})^2 + (t^{-1}-d)^2)\,\{1-\mathrm{erf}(t^{-1}-d)\}\,\frac{dt}{t} \tag{3}$$

Difficulty using Theorem 1 arises from the integrand's singularity at ∞ (see appendix) which contributes the residue at $z = 0$ of

$$-z^{-1}\exp(-(\frac{z^{-1}-a}{b})^2 + (z-d)^2)\,\{1-\mathrm{erf}(z-d)\}\log\{(1-uz)/(1-vz)\}$$

The singularity at 0 likewise involves an essential singularity and contributes the residue at $z = 0$ of

$$z^{-1}\exp(-(\frac{z-a}{b})^2 + (z^{-1}-d)^2)\,\{1-\mathrm{erf}(z^{-1}-d)\}\log\{(z-u)/(z-v)\}$$

Because determining these residues for different values of parameters a, b, d, u, v is problematic (except for infinite series, we are unaware of any method producing parametrized results), we first approximate the integrand by functions meromorphic on the Riemann sphere so as to remove all essential singularities.

This approach introduces other difficulties, since functions meromorphic on the Riemann sphere are rational [3]. Suitably approximating the integrand involves a trade-off between the number of poles or complexity of residues and the number of sub intervals involved; a rational approximation suitable over all of (u, v) – one sub interval – would have high degree – either many poles or computationally expensive residue(s). Moreover, u and v are parameters; neither computing infinitely many rational approximations at compile-time nor computing rational approximations at run-time is feasible.

Fortunately, exp satisfies a functional equation enabling approximation with a single rational function (at the potential price of many sub intervals of (u, v)):

$$\begin{aligned} \exp(-f(t)) &= \exp(s)\exp(-s-f(t)) \\ &\approx \exp(s)\,\mathrm{rational}_0(f(t)+s) \end{aligned} \tag{4}$$

If $\mathrm{rational}_0(t)$ suitably approximates $\exp(-t)$ over $[x, y]$, the approximation above is valid for $t \in [u', v']$ provided f maps $[u', v']$ into $[x-s, y-s]$. By first subdividing (u, v) into sub intervals over which f is monotonic, we may assume without loss of generality that f is invertible. Hence

$$\{u', v'\} = f^{-1}(\{x-s, y-s\}) \tag{5}$$

and s parametrizes a sub range $t \in [u', v'] \subset [u, v]$ of integration. In our case, both subdividing (u, v) into sub intervals over which f is monotonic and determining $[u', v']$ via (5) involve solving quartic polynomials at run-time.

We chose among four approximations for $g(x) = \exp(x^2)(1-\mathrm{erf}(x))$, based upon the value of $w = t^{-1} - d$:

$$\begin{array}{rll} 2\exp(w^2) & \text{if} & w \le -3 \\ \mathrm{rational}_1(w) & \text{if} & -3 \le w \le 0 \\ \mathrm{rational}_2(w) & \text{if} & 0 \le w \le 10 \\ \mathrm{rational}_3(w) & \text{if} & 10 \le w \end{array}$$

Except for rational_3 which is the first two terms from the series expansion of g at ∞, we used Maple's implementation of the Remez algorithm (provided by the numapprox package) to obtain rational approximations (see [2] for a survey of widely used methods for generating rational or polynomial approximations to continuous functions). Our approximations are holomorphic in the sub intervals over which they are used, hence there is no contribution to the integral from r as described in Theorem 1. As functions of t, each of our rational approximations has a numerator with degree not exceeding that of its denominator. Therefore

$$-t^{-2}\,\text{rational}(t^{-1})/t^{-1}\log\frac{1-ta}{1-tb}$$

is holomorphic at $t=0$, hence there is no contribution from poles at ∞ to R as described in Theorem 1. Except for $\text{rational}_3(z)$ which has a single pole of order 3 at $z=0$, our approximations have simple poles located off the real line, and their partial fraction expansions are sums of terms of the form

$$\frac{\xi}{z-\zeta}$$

where all ξ and ζ are known at compile-time (numerators of approximations have degree less than that of denominators).

The most complicated residues arise from sub intervals involving both rational_0 and rational_3; residues are needed at $t=1/d$ for

$$\text{rational}_3(t^{-1}-d)/t\;\frac{\xi}{((t-a)/b)^2+s-\zeta}\;\log\frac{t-u'}{t-v'}$$

Maple computes symbolically the residue as a function of the parameters a, b, d, ξ, ζ, u', v', and the result of Maple's symbolic computation is evaluated as needed at run-time (see appendix).

Simpler residues arise from sub intervals involving rational_0 and rational_k for $k\in\{1,2\}$; residues are needed at $t=a\pm b\sqrt{\zeta-s}$ for

$$\text{rational}_k(t^{-1}-d)/t\;\frac{\xi}{((t-a)/b)^2+s-\zeta}\;\log\frac{t-u'}{t-v'}$$

and at $t=1/(d+\zeta)$ for

$$\text{rational}_0(((t-a)/b)^2+s)\;\frac{\xi}{t^{-1}-d-\zeta}\;\frac{1}{t}\;\log\frac{t-u'}{t-v'}$$

These residues are obtained easily via the following lemmas (Lemma 3 is from [1]). The first lemma allows one to focus on the factor containing the singularity, the second deals with forms having singularities – such as $\xi/(z+s-\zeta)$ – that have been complicated by function composition – such as $z=((t-a)/b)^2$.

Lemma 2. *Let ψ have a simple pole at ζ with residue ξ. If ϕ is holomorphic at ζ, then the residue of $\psi(z)\phi(z)$ at $z=\zeta$ is $\xi\phi(\zeta)$*

Lemma 3. *Let ζ be a point of the Riemann sphere where either $\phi'(\zeta)\neq 0$ or else ϕ has a simple pole. Let $\omega=\phi(\zeta)$ and let ψ either be holomorphic at ω or have an isolated singularity there. If φ is a local inverse of ϕ in a neighborhood of ω, then the residue of $\psi(\phi(z))$ at $z=\zeta$ is equal to the residue of $\psi(z)\varphi'(z)$ at $z=\omega$.*

The residues arising from sub intervals involving rational_0 alone are those of

$$\frac{\xi}{((t-a)/b)^2 - (t^{-1}-d)^2 + s - \zeta}\,\frac{1}{t}\,\log\frac{t-u'}{t-v'}$$

and are easily obtained using Lemmas 2 and 3. The expression above equals

$$\frac{b^2\xi}{t^4 - 2at^3 + (a^2 - b^2(\zeta + d^2 - s))t^2 + 2b^2dt - b^2}\,t\log\frac{t-u'}{t-v'}$$

Focusing on the first factor (via Lemma 2), we take ψ and ϕ of Lemma 3 to be

$$\begin{aligned}\psi(z) &= \frac{b^2\xi}{z-b^2}\\ \phi(z) &= z^4 - 2az^3 + (a^2 - b^2(\zeta + d^2 - s))z^2 + 2b^2dz\end{aligned}$$

The ζ of Lemma 3 are roots of $\phi(z) = b^2$, the $\varphi'(\omega)$ of Lemma 3 is $1/\phi'(\zeta)$ (which follows from the chain rule, since φ is a local inverse to ϕ), and ω is b^2.

3. Accuracy and Speed

If A is any approximation to a positive integrand F, then

$$\left|1 - \frac{\int A}{\int F}\right| = \left|\frac{\int F\,\{1 - A/F\}}{\int F}\right| \le \frac{\int F\,|1 - A/F|}{\int F} \le \|1 - A/F\|_\infty$$

To achieve an integration tolerance of 1% relative error, we conservatively used rational approximations having less than 0.1% relative error. Underpinning assumptions of our calculation (like $\phi'(\zeta) \neq 0$ in Lemma 3 for instance) are checked at run-time. Although any serious consideration of accuracy must investigate the numerical stability of methods used, including an analysis of round-off, we have not yet done that.

To reduce execution time, our code implements a version of "lazy evaluation" by first evaluating sub intervals where the integrand is large, and terminating early when later sub intervals are estimated to contribute less than 0.1% of what has so far been accumulated. Typical time to evaluate our original integration problem (1) by way of residues is 0.000048 seconds (on a single 2.5 GHz AMD K10 core).

4. Acknowledgements

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References

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[2] W.J.Cody, A Survey of Practical Rational and Polynomial Approximation of Functions, *SIAM Review*, v 12, n 3 (1970), 400-423.

[3] R.Nevalinna, V.Paatero, *Introduction to Complex Analysis*, AMS Chelsea Publishing (2007).

Appendix

The *extended plane* (*Riemann sphere*) is the set of complex numbers together with ∞. The residue of $F(z)$ at $z = \infty$ is the residue of $-z^2 F(z^{-1})$ at $z = 0$. The *residue* of $F(z)$ at $z = \zeta$ is the coefficient of z^{-1} in the Laurent expansion of $F(z)$ about the point ζ. The *Laurent expansion* of $F(z)$ about the point ζ is the right-hand side of

$$F(z) = \sum_{k=-\infty}^{\infty} a_k (z - \zeta)^k \tag{6}$$

It exists and converges absolutely for $0 < |z-\zeta| < R$ provided F is differentiable (*holomorphic*) there. If F is also differentiable at ζ, then $a_k = 0$ for $k < 0$; otherwise ζ is called a *singularity*. Suppose (6) represents F for $0 < |z-\zeta| < R$ but ζ is a singularity. If there exists integer p maximal such that $a_k = 0$ for $k < -p$, then ζ is a *pole* of order p; otherwise ζ is an *essential singularity*. A *simple* pole is a pole of order 1.

If $F(z^{-1})$ is holomorphic at $z = 0$ then F is said to be holomorphic at ∞; otherwise F has a singularity at ∞. If $F(z^{-1})$ has a pole at $z = 0$, then F has a pole at $z = \infty$. If $F(z^{-1})$ has an essential singularity at $z = 0$, then F has an essential singularity at $z = \infty$. A *meromorphic* function is one which is everywhere differentiable except at a finite number of singularities which are poles. A *rational* function is the quotient of two polynomials.

The *principal* logarithm is the function $\log z = \log |z| + \sqrt{-1}\arg(z)$ where $-\pi < \arg(z) < \pi$ and $z = |z|\exp(\sqrt{-1}\arg(z))$. Formulae useful for computing residues include:

$$\begin{aligned}
\log \frac{z-a}{z-b} &= \log \frac{a}{b} + \sum_{k=1}^{\infty} \frac{b^{-k} - a^{-k}}{k} z^k \\
\log \frac{1/z-a}{1/z-b} &= \log \frac{1-az}{1-bz} = \sum_{k=1}^{\infty} \frac{b^k - a^k}{k} z^k \\
\left(\sum_{k=-\infty}^{\infty} a_k z^k\right)\left(\sum_{k=-\infty}^{\infty} b_k z^k\right) &= \sum_{k=-\infty}^{\infty}\left(\sum_{j=-\infty}^{\infty} a_j b_{k-j}\right) z^k
\end{aligned}$$

In particular, the residue of the left-hand side of the product above (at $z = 0$) is

$$\sum_{j=-\infty}^{\infty} a_j b_{-1-j}$$

which reduces to

$$\sum_{j=-p}^{-1} a_j b_{-1-j}$$

when the first factor has a pole of order p and the second factor is holomorphic.

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