Editors: Francis Sullivan, fran@super.org
William J. Thompson, wmjthompson@msn.com

GAUSS-LEGENDRE PRINCIPAL VALUE INTEGRATION

By Julian V. Noble

AS WE ATTEMPT MORE SOPHISTICATED PROJECTS IN SCIENCE AND ENGINEERING, THE MATHEMATICAL TOOLS WE APPLY TO THEM ALSO BECOME MORE SOPHISTICATED. BECAUSE SO few problems lend themselves to closed-form solution, we often need to convert formal definitions into practical numerical methods. One such problem deals with the Principal Value integral, which many students encounter in a course on functions of a complex variable. However, the prospect of evaluating one numerically might seem rather daunting. To the best of my knowledge, the subject remains outside the treatments of numerical quadrature found in treatises on numerical analysis.

The Principal Value integral

Early in the 19th century, Augustin Cauchy defined the PV integral as

$$I(x) = \mathrm{P}\int_a^b dt\,\frac{\rho(t)}{t-x} \equiv \lim_{\varepsilon\to 0^+}\left[\int_a^{x-\varepsilon} dt\,\frac{\rho(t)}{t-x} + \int_{x+\varepsilon}^b dt\,\frac{\rho(t)}{t-x}\right].$$

It arises in applications of Cauchy's residue theorem[1,2] when the pole lies on the real axis within the interval of integration, $a < x < b$. The function $\rho(t)$ in the preceding equation is assumed continuous on the interval of integration.

Familiar instances where PV integrals arise include integral transforms, Green's functions for scattering, and dispersion relations such as

$$\mathrm{Re}\, f(\omega) = -\frac{q^2}{4\pi mc^2} + \frac{\omega^2}{2\pi^2 c}\,\mathrm{P}\int_0^\infty d\omega'\,\frac{\sigma(\omega')}{\omega'^2-\omega^2}$$

which relates the real part of the forward scattering amplitude for photons of angular frequency ω to the total scattering cross section $\sigma(\omega)$. (Such relationships, because of the general nature of the assumptions underlying their derivation and because they relate quantities that can be measured, lead to important sum rules and consistency checks in atomic, nuclear, and particle physics.)

Contour deformation

When the function $\rho(t)$ or the interval (a, b) does not lend itself to closed-form evaluation of a PV integral, we must resort to numerical quadrature. Researchers have proposed various ways to perform this. For example, when $\rho(t)$ has an explicit analytic continuation to a portion of the complex plane including the line segment of integration and a region with $\mathrm{Im}(t) \neq 0$, we can deform the contour into the complex plane (see Figure 1).
Thus

$$\mathrm{P}\int_a^b dt\,\frac{\rho(t)}{t-x} = \mathrm{Re}\left(\int_\Gamma dz\,\frac{\rho(z)}{z-x}\right).$$

The above integral requires complex arithmetic, to be sure, but we can evaluate it using ordinary quadrature techniques. A simple example is

$$\mathrm{P}\int_0^\infty dt\,\frac{1}{1-t^3} = \mathrm{Re}\left(e^{-i\pi/3}\int_0^\infty dr\,\frac{1}{1+r^3}\right) = \frac{\pi}{3\sqrt{3}}$$

where we deform to the line $t = re^{-i\pi/3}$ and integrate numerically to get 0.604599788078..., in excellent agreement with the exact result, $\pi/(3\sqrt{3})$. Here I used an adaptive integration routine based on a three-point Gauss-Legendre rule for the subintervals, with the absolute precision set to 10^{-10}.

Not surprisingly, the PV integral can be numerically intractable. Figure 2 exhibits the integrand of a typical example. Clearly, significant cancellations come from contributions on either side of the singularity. This means that straightforward numerical quadrature will express the desired result as a small difference between large numbers, a situation notoriously prone to round-off error.

Computing the PV integral directly

The contour-deformation approach has two disadvantages: the explicit analytic continuation of $\rho(t)$ must be known; moreover, complex arithmetic is not available in all computer languages and entails a two- to fourfold increase in computational effort (that is, running time). So, William Thompson has proposed to compute the PV

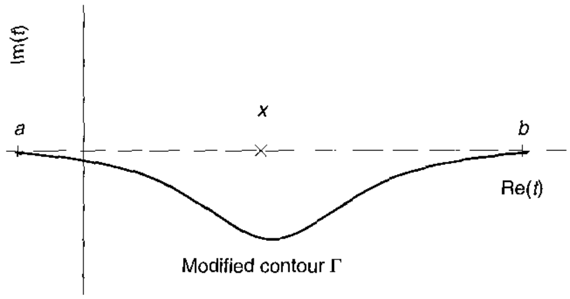

Figure 1. A contour deformed away from a singularity at the point x in the complex t-plane.

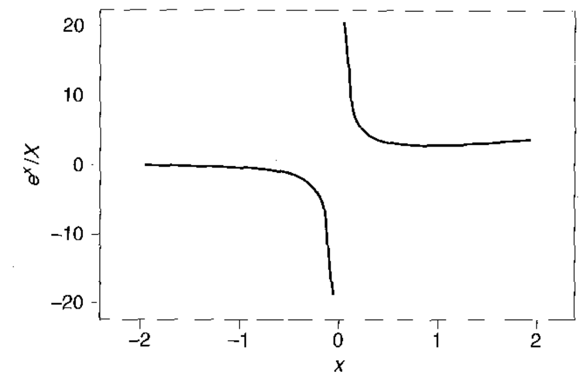

Figure 2. The integrand e^x/x illustrating the large cancellations near $x = 0$ and the consequent possibilities of round-off error.

integral directly, in real arithmetic.[3] Thompson isolates the singularity within a symmetric interval of finite size:

$$\mathrm{P}\int_a^b dt\,\frac{\rho(t)}{t-x}=\int_a^{x-\Delta} dt\,\frac{\rho(t)}{t-x}+\int_{x+\Delta}^{b} dt\,\frac{\rho(t)}{t-x}+\mathrm{P}\int_{x-\Delta}^{x+\Delta} dt\,\frac{\rho(t)}{t-x}.$$

The crucial portion,

$$I_\Delta(x)=\mathrm{P}\int_{-\Delta}^{\Delta} dt\,\frac{\rho(t+x)}{t}$$

can be integrated term-by-term using the Taylor series expansion of $\rho(t+x)$ about $t = 0$:

$$\hat{I}_\Delta(x)\approx 2\sum_{n=0}^{N_{\max}}\rho^{(2n+1)}(x)\frac{\Delta^{2n+1}}{(2n+1)(2n+1)!}.$$

The order of the first neglected term is $2N_{\max} + 3$.

In the absence of explicit expressions for the high-order derivatives, Thompson advocates computing them by differentiating interpolation formulas. In either case, the procedure might become somewhat clumsy because, to achieve an absolute error ε, the order of the highest retained derivative must be

$$2N_{\max}+3\sim\frac{\log(\varepsilon)}{\log(\Delta/R)}$$

where R is the distance from the point $x + i0$ to the nearest singularity of $\rho(t + x)$. This estimate is based on Cauchy's bound on derivatives of an analytic function.

A better way

Let's look at a simpler, more efficient procedure for evaluating numerically the Cauchy PV integral. We approximate I_Δ by a Gauss-Legendre[4] quadrature formula:

$$I_\Delta=\int_{-\Delta}^{\Delta} dt\,\frac{\rho(t+x)-\rho(x)}{t}\equiv\int_{-1}^{1} dt\,\frac{\rho(t\Delta+x)-\rho(x)}{t}$$
$$\approx\sum_{k=-K}^{K}\frac{w_k}{\xi_k}\left[\rho(\xi_k\Delta+x)-\rho(x)\right]$$

where ξ_k are the zeros of the Legendre polynomial P_{2K} or P_{2K+1} and w_k are the corresponding weights. Although the Gauss-Legendre family of quadrature rules has no special virtue (Gauss-Hermite, Gauss-Laguerre, or Gauss-Chebyshev could work equally well—any natural interval and scaling rule would do), the problem's symmetry makes scaling $(-\Delta, \Delta)$ to $(-1, 1)$ the simplest alternative. Because the points and weights that the Gauss-Legendre formula uses are respectively antisymmetric and symmetric about $\xi = 0$, we can drop the constant term $\rho(x)$. However, if we choose an odd-order formula, we must account for the point $\xi = 0$ by including the term $w_0\rho'(x)$.

The usual wisdom prefers odd-order Gauss-Legendre formulas to even-order ones. In this case, however, because we want to avoid evaluating any derivatives of $\rho(t)$, we should employ an even-order (that is, $n_{points} = 2K$) formula because it avoids the derivative term at $\xi = 0$. Table 1 lists the points and weights for Gauss-Legendre rules of two, four, and six points, to 15 decimal places. As an illustration, Table 2 lists the results of applying Gauss-Legendre integration to

Table 1. Gauss-Legendre weights and points.

$2K$	w_k	ξ_k
2	1.0	0.577350269189626
	1.0	−0.577350269189626
4	0.347854845137454	0.861136311594053
	0.652145154862546	0.339981043584856
	0.652145154862546	−0.339981043584856
	0.347854845137454	−0.861136311594053
6	0.171324492379170	0.932469514203152
	0.360761573048139	0.661209386466265
	0.467913934572691	0.238619186083197
	0.467913934572691	−0.238619186083197
	0.360761573048139	−0.661209386466265
	0.171324492379170	−0.932469514203152

Table 2. PV integral by Gauss-Legendre integration.

$2K$	$Ei(1) + E_1(1)$
2	2.11297772844928
4	2.11450171810538
6	2.11450175075134

Table 3. PV integral by the derivatives method.

N_{max}	$Ei(1) + E_1(1)$
0	2.00000000000000
1	2.11111111111111
2	2.11444444444444
3	2.11450113378685
4	2.11450174617172
5	2.11450175072665
6	2.11450175075135

Table 4: Six-point Gauss-Legendre evaluation of J(Δ).

Δ	Exact	Six-point Gaussian
1.00	0.7363873204869	0.736386792355803
0.50	0.3425632583545	0.342563258302464
0.25	0.1678238552951	0.167823855295059

$$Ei(1) + E_1(1) = \mathrm{P}\int_{-1}^{1} dt\,\frac{e^t}{t} = 2.11450175075\ldots\ .$$

We can compare Table 2's results with Thompson's method requiring derivatives. Table 3 evaluates $Ei(1) + E_1(1)$ by summing the terms of Thompson's formula. Obtaining the precision given by the sixth-order Gauss-Legendre formula (which would seldom be necessary in practice) requires keeping terms 0 to 6 in the sum. That is, we must evaluate the 13th derivative of the function $\rho(t + x)$ for absolute precision of 10^{-15}.

Given that we must evaluate a 13th derivative, how many function evaluations do we need? This depends on whether we know the derivatives in closed form at the point of singularity. For the simple case e^t at $t = 0$, we do know them—all the derivatives are unity. With more complicated functions, however, computing the derivatives—even if known in closed form through the application of a computer algebra program—will be somewhat more time-consuming. If we must evaluate 13th derivatives by interpolation, we will need a uniformly spaced interpolation polynomial of at least order 15 to yield the desired precision. That is, we must evaluate the function at least 16 times.

As a second example, Table 4 lists results for the integral

$$\mathcal{J}(\Delta) = \mathrm{P}\int_{1-\Delta}^{1+\Delta} dt\,\frac{1}{1-t^3} = \frac{1}{6}\ln\left(\frac{\left(\Delta+\frac{3}{2}\right)^2+\frac{3}{4}}{\left(-\Delta+\frac{3}{2}\right)^2+\frac{3}{4}}\right) + \frac{1}{\sqrt{3}}\left[\tan^{-1}\left(\frac{\sqrt{\frac{3}{4}}}{\Delta+\frac{3}{2}}\right) - \tan^{-1}\left(\frac{\sqrt{\frac{3}{4}}}{-\Delta+\frac{3}{2}}\right)\right].$$

The agreement is already very good for a reasonably wide interval. Again comparing with Thompson's formula, we see that for the function $(1 + t^2)^{-1}$, whose singularities lie a distance $\sqrt{2}$ from the point $t = 1$, $N_{max} \approx 10$ for the interval width $\Delta = 0.25$. That is, we must evaluate terms through the 21st derivative, requiring either at least 24 function evaluations (for interpolation) or the storage of 10 derivative formulas (direct algebraic computation). The sixth-order Gauss-Legendre method requires only six evaluations of the function itself.

The Gauss-Legendre rule is more efficient than the Taylor series approach-cum-interpolation for one simple reason. In deriving the above estimates, I assumed interpolation in a table of uniform spacing. Gauss-Legendre quadrature of nth order approximates the integrand $[\rho(t + x) - \rho(x)]/t$ by a polynomial of order $2n - 1$ (the points and weights comprise $2n$ free parameters[4]). For $n = 6$, we fit an 11th-order polynomial, with the error proportional to the 12th derivative of the integrand but with an exceedingly small coefficient, of order 1.5×10^{-12}. No wonder the precision is good.

You can find `pval.f`, a program that evaluates $I_\Delta(x)$ by the sixth-order Gauss-Legendre method, at landau1.phys.virginia.edu/classes/551/programs.htm. The program is written in ANS Forth (my current language of choice) but employs a Fortran-like style for ease of translation. A more general routine would take as input parameters the interval's endpoints, (a, b); the singularity's location; and the desired interval's width, Δ. It might even adjust Δ adaptively to obtain the best convergence. The program `adpt_g3.f` (and the auxiliary FORmula TRANSlator `ftran111.f`) is available at the same site and could easily be used to create an efficient generalized subroutine.

References

1. E.T. Copson, *An Introduction to the Theory of Functions of a Complex Variable*, Clarendon Press, Oxford, UK, 1955.
2. E.T. Whittaker and G.N. Watson, *A Course of Modern Analysis*, 4th ed., Cambridge Univ. Press, New York, 1963.
3. W.J. Thompson, "Principal-Value Integrals by a Simple and Accurate Finite-Interval Method," *Computers in Physics*, Vol. 12, No. 1, Jan. 1998, pp. 94–96.
4. A. Ralston and P. Rabinowitz, *A First Course in Numerical Analysis*, 2nd ed., McGraw-Hill, New York, 1978.

Julian Noble is a professor of physics at the University of Virginia's Commonwealth Center of Nuclear and Particle Physics. His interests include nuclear and particle phenomenology, the astrophysics of neutron stars and supernovas, quantum collision theory, and computational methods; he also consults in accident reconstruction. His interest in computing began at Grumman Aircraft Engineering Corp., where he used Fortran I (on an IBM 704) to compute neutron activation cross sections. He began to use Forth in 1985 from necessity, and has never looked back (although occasionally he writes in C, Fortran, or Basic). He received his BS in physics from Caltech and his MA and PhD from Princeton University. Contact him at the Commonwealth Center of Nuclear and Particle Physics, Univ. of Virginia, Charlottesville, VA 22901; jvn@virginia.edu; www.phys.Virginia.edu/People/personal.asp?UID=jvn.

WEB MECHANICS

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Generating problem formulas with symbolic programming languages

Here is a Mathematica script that solves Kirchhoff's rules for the currents in Problem 4 in terms of the randomly set resistor values.

```
Solve[{30 -i1 * (r1 + r2) -i3 * r4 == 0, 6 + i3 * r4 -i2 * r3
== 0, i1 == i2 + i3}, {i1, i2, i3}]
```

This will generate expressions for the three currents, which you can then reformat for use with VbScript. For example, examine the lines beginning with "correct = " in 4_1.asp to see the result for I_3. When you are through, you can check your new Web problem using specific answers generated by Mathematica. For example, suppose your browser contains the following data for this problem: R1 = 9 Ω, R2 = 8 Ω, R3 = 6 Ω, and R4 = 1Ω. Append the string " ./ {r1 -> 9, r2 -> 8, r3 -> 6, r4 -> 1}" (do not include the quotes) to the end of the line above. Mathematica will return 78/125 for I_3, which you should then enter into the form as a decimal number. If this answer is accepted, you have programmed the formula script correctly.

answer scripts must utilize symbolic expressions for the three currents in terms of arbitrary resistor values. In cases where the algebra is quite involved (such as Problem 4), symbolic programming environments such as Mathematica or Maple can help generate the required formulas (for more details, see the sidebar "Generating problem formulas with symbolic pro- gramming languages").

After more than three years of using this Web application for calculus-based introductory physics courses, I can give testimonial evidence that Web homework has made a remarkable difference in my students' ability to tackle standard physics problems, improving both their competency and their grades. My students also do better on tests now. I get beautiful vector diagrams on problems that involve vectors, and far more accurate numbers.

Although I have no formal assessment results to report, I have a few hypotheses about the success of the system. Maybe it's the instantaneous feedback, or the happy face—but students rarely give up on a Web homework problem. They can't hurt their grade by tinkering, so they tinker a lot. Sometimes they waste a lot of time spinning their wheels with silly mistakes, but mostly they spend a lot of time reading the book or working in groups to resolve their difficulties. I consistently get overall homework averages of around 90%. Overall, the entire learning experience is positive.

Reference

1. A.P. Titus, L.W. Martin, and R.J. Beichner, "Web-Based Testing in Physics Education: Methods and Opportunities," *Computers in Physics*, Vol. 12, 1998, pp. 117–123.

Chuck Bennett is professor of physics and director of the Center for Teaching and Learning at the University of North Carolina at Asheville. His research interests include quantum optics, high-temperature plasma diagnostics of fusion plasmas, and education. He received his PhD in physics from North Carolina State University. Contact him at bennett@unca.edu.