Exploring Gaussian quadrature with students: Part 1 – A forgotten idea

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Introduction

In this age of easy access to the internet and to spreadsheets, easy-to-apply numerical methods exist that are vastly superior to Simpson's rule and the (corrected) trapezoidal rule. Gaussian quadrature (GQ) is such a method. What follows tells how enthusiastic Year 9 students with a physics problem provoked a science teacher into re-discovering a mathematical idea, then together we played with the idea.

Numerical integration is taught for the HSC using Simpson's rule and the trapezoidal rule. The examples used are always analytical functions on the domain of interest; they can be well approximated by a polynomial using a Taylor series around the midpoint of the interval. These are 'nice' curves. Often these examples can be integrated exactly, so convergence is easily examined. Many problems in chemistry and physics cannot be solved using the integration rules taught in the HSC course. In such cases the *CRC Handbook of Chemistry and Physics* (Lide, 2004) is a good starting point, followed by Abramowitz and Stegun's (1965) *Handbook of Mathematical Functions*, the *NIST Handbook of Mathematical Functions* (Olver, Lozier, Boisvert & Clark, 2010), then *Table of Integrals, Series, and Products* (Gradshteyn & Ryzhik, 2007). After that, and often much earlier, we fall back on numerical methods.

Part 1 compares the convergence of Simpson's rule, the trapezoidal rule, the corrected trapezoidal rule and Gaussian quadrature for three simple problems of increasing challenge. If you just need a better tool for numerical integration, read only Part 1. Using GQ is like using logarithms, the hard work of calculating the values need only be done once then the results can be used for a multitude of problems. The values needed for GQ can be downloaded from a website, inserted into a spreadsheet, then applied to a multitude of problems. This part ends with a description of how the method can be extended to less 'nice' problems, where the height or the slope of the curve becomes infinite at the edges of the domain.

Part 2 shows how we (re)developed GQ for the simplest case, where the function can be well approximated by a polynomial. This part explains the logic of the method and shows how the abscissae and weights were found.

Part 3 shows the physics problem, which led to this work. We responded by (re)developing the work in Part 2 and developing the delta-weighted GQ in Part 3, which appears to be completely original. Its development is strongly parallel to Part 2.

Weighted sum

The *weighted sum* or *weighted average* is a useful idea in many areas of mathematics, science and education. For example, the average mark in a class test has equal weights, usually given as 1. If a student is away, their weight becomes 0.

$$\bar{x} = \frac{\sum_{i=1}^{n} w_i \cdot x_i}{\sum_{i=1}^{n} w_i}$$

The variance of the test, the square of its standard deviation, is also a weighted sum:

$$\text{var} = \frac{\sum_{i=1}^{n} w_i \left(x_i - \bar{x}\right)^2}{\sum_{i=1}^{n} w_i}$$

Simpson's rule is a weighted sum, with weights 1, 4, 1 on each subinterval. The trapezoidal rule is a weighted sum, with weights 1 at the ends of each subinterval.

In statistics and probability, the weights are often *normalised* so that their sum is one.

Gaussian quadrature is a weighted sum that optimises the points and weights used. The meaning and derivation of these values will be explored in part 2 in more depth, but once these values are known, evaluating the numerical integral is exactly as hard as adding up a shopping list. Compare Table 1 with Table 5 to see the structural similarities.

Table 1. Adding up a shopping list as an everyday example of a weighted sum.

Items	Mass (kg) = w	Price ($/kg) = f(x)	w·f(x)
2 bananas	0.567	3.30	1.87
3 oranges	0.789	2.80	2.21
5 pears	1.234	2.50	3.09
		TOTAL	7.17

A more detailed look at the methods

Simpson's rule exactly fits a parabola to three points, so its answer is correct for any polynomial of order 2 or lower. We start by considering a single strip on the domain $[-h, h]$ and fitting a parabola $y = ax^2 + bx + c$ through three points at $(-h, y_m)$, $(0, y_o)$ and (h, y_p).

$$y_m = ah^2 - bh + c;\ y_o = c;\ y_p = ah^2 + bh + c$$

$$a = \frac{y_p + y_m - 2y_o}{2h^2}$$

$$b = \frac{y_p - y_m}{2h};\ c = y_o$$

The area A under the curve on $[-h, h]$ is:

$$A = \frac{2}{3}ah^3 + 2ch$$

$$= \frac{1}{6}\left(y_p + 4y_o + y_m\right)(2h)$$

When considering the errors in Simpson's rule, the third order term about the midpoint does not contribute to the integral so Simpson's rule converges as the fourth power of the interval h between the points used. This is demonstrated in the examples that follow

The trapezoidal rule fits the heights at the two endpoints of each strip. When considering the errors, the trapezoidal rule converges as the square of the interval h between the points used.

The corrected trapezoidal rule fits the heights at all of the points but needs the slopes only at the two endpoints. It converges as the fourth power of the interval width h.

We start by considering a single strip on the domain $\left[-\frac{h}{2}, \frac{h}{2}\right]$. This problem has four variables so a cubic polynomial is needed.

$$y = ax^3 + bx^2 + cx + d$$

$$y_m = -\frac{1}{8}ah^3 + \frac{1}{4}bh^2 - \frac{1}{2}ch + d$$

$$y_p = \frac{1}{8}ah^3 + \frac{1}{4}bh^2 + \frac{1}{2}ch + d$$

The slope is then given as $s = 3ax^2 + 2bx + c$.

$$s_m = \frac{3}{4}ah^2 - bh + c$$

$$s_p = \frac{3}{4}ah^2 + bh + c$$

$$b = \frac{s_p - s_m}{2h}$$

$$d = \frac{1}{2}\left(y_p + y_m\right) + \frac{1}{8}\left(s_p - s_m\right)h$$

The area A under the curve on $\left[-\frac{h}{2}, \frac{h}{2}\right]$ is:

$$
\begin{aligned}
A &= dh + \frac{1}{12} bh^3 \\
&= \frac{1}{2}\left(y_p + y_m\right)h - \frac{1}{12}\left(s_p - s_m\right)h^2
\end{aligned}
$$

For a set of evenly spaced points, the slope terms for all interior points cancel. For the same number of points, the corrected trapezoidal rule has a smaller error and is easier to program than Simpson's rule, but the HSC mathematics course neglects it.

Gaussian quadrature is a weighted sum where the points and the weights given to those points have been chosen to fit the highest order polynomial possible. The variable is changed to a standard domain of integration [–1, 1] so the odd order polynomial terms drop out. For n points the method is exact for a polynomial of order $(2n - 1)$. This is explained in detail in Part 2.

$$
\begin{aligned}
\int_a^b f(x)\,dx &= \frac{(b-a)}{2}\int_{-1}^{1} f(\xi)\,d\xi \\
&= \frac{(b-a)}{2} S_n \\
&= \frac{(b-a)}{2}\sum_{i=1}^{n} w_i f(\xi_i)
\end{aligned}
$$

Using the same number of points, Gaussian quadrature is superior to the numerical integration rules taught in the HSC mathematics courses. We compare it with Simpson's rule, the trapezoidal rule, and the corrected trapezoidal rule for small numbers of points. The errors appear in the last two digits. The highlighted entries for GQ have basically reached Excel's limit of precision. Using a spreadsheet makes numerical integration easy, but few students are familiar with the simple task of programming a spreadsheet. (This should be an assessed skill in Science and Mathematics, so more students will take it seriously.)

Example 1

The integral

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos(x)\,dx = 2$$

was chosen because it is 'nice', varying smoothly over the chosen range, not rising to large values and easily approximated by a polynomial, but not exactly expressed by a polynomial of finite order. The results below compare the four numerical integration methods evaluating this integral for small numbers of points. The errors in the calculations appear in the last two digits shown.

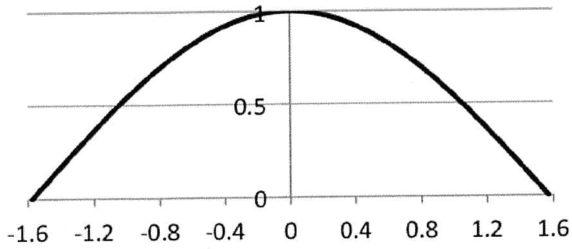

Figure 1. The cosine function on $\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$.

Table 2. Comparing methods of numerical integration for the cosine function, using only n points. The integral is exactly 2.

n	Simpson	Trap	Corr. trap	Gaussian
3	2.094	1.57	1.982	2.0014
5	2.0046	1.90	1.9989	2.00000011
7	2.00086	1.954	1.99979	2.0000000000019
9	2.00027	1.974	1.999934	2.0000000000000
11	2.00011	1.984	1.999973	
17	2.000017	1.9936	1.9999959	
33	2.0000010	1.9984	1.99999974	
65	2.000000065	1.99960	1.999999984	

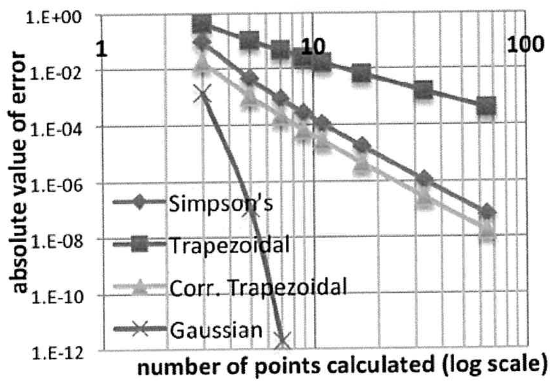

Figure 2. Log-log plot of the error against the number of points used, to show convergence.

Example 2

The function e^x on [−4, 4] is less 'nice', varying smoothly over the domain, but rising to large values as x approaches 4, and needing a higher order polynomial.

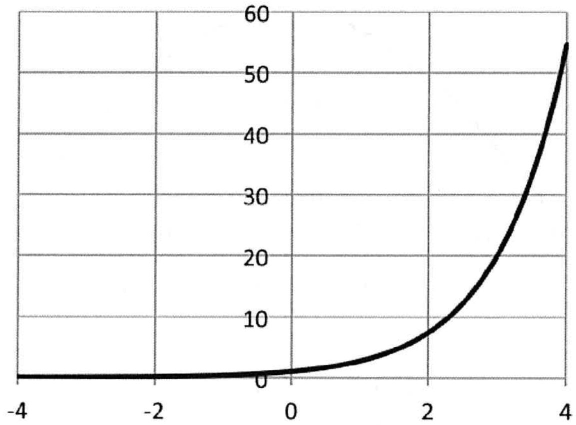

Figure 3. *The exponential function on* [−4 ,4].

Table 3. *Comparing methods of numerical integration of* e^x, *using small numbers of points.* *The integral of exp(x) on* [−4,4] *is* 54.5798343942555.

n	Simpson	Trap.	Corr. trap.	Gaussian
3	78	113	40	52.91
5	58	72	53.5	54.575
7	55.4	62	54.3	54.579831
9	54.85	59	54.51	54.5798343936
11	54.70	57.5	54.549	54.5798343942553
17	54.598	55.7	54.5751	
33	54.5810	54.86	54.57954	
65	54.57991	54.65	54.579816	

Figure 4 shows the log-log plot of the error versus the number of points, to show the different convergence. The slope of lines for Simpson's rule and the corrected trapezoidal rule are roughly equal. GQ converges much more rapidly as more points are used. Again, the last GQ value shown is limited by the finite precision arithmetic.

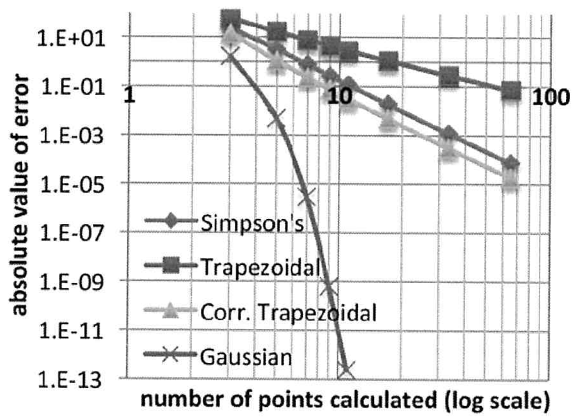

Figure 4. *Log-log plot of the error versus the number of points.*

Example 3

The function $f(x)=\sqrt{r^2-x^2}$ on $[-r,r]$ is not 'nice'. The function varies smoothly over the chosen range, but the slope becomes infinite as $|x|$ approaches r, so it cannot be approximated by a polynomial of finite order. Away from these problem areas, a finite polynomial is a much better approximation. Using a smaller angle improves the convergence. The internal angle of this sector is 60°; when the radius of the circle is $\sqrt{6}$, the pale grey area, which lies on the domain $\left[-\frac{\sqrt{6}}{2},\frac{\sqrt{6}}{2}\right]$ has area π.

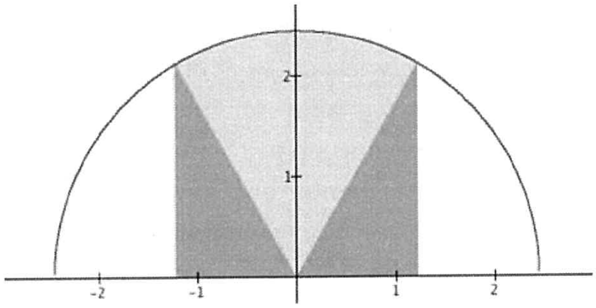

Figure 5. The sextant integral. The pale sector or sextant has area π, approximated by integrating under the curve then subtracting the darker triangles.

Table 4. Comparing numerical integrals to find pi, using small numbers of points. The radius is $\sqrt{6}$. The sextant area is π = 3.14159265358979

n	Simpson	Trap.	Corr. trap.	Gaussian
3	3.1340	3	3.1443	3.14177
5	3.14093	3.105	3.14178	3.14159307
7	3.14145	3.126	3.141631	3.1415926549
9	3.141545	3.1326	3.141605	3.1415926535942
11	3.141573	3.1358	3.1415977	3.14159265358980
17	3.1415896	3.1393	3.14159343	
33	3.141592459	3.14103	3.141592702	
65	3.141592641	3.14145	3.141592657	

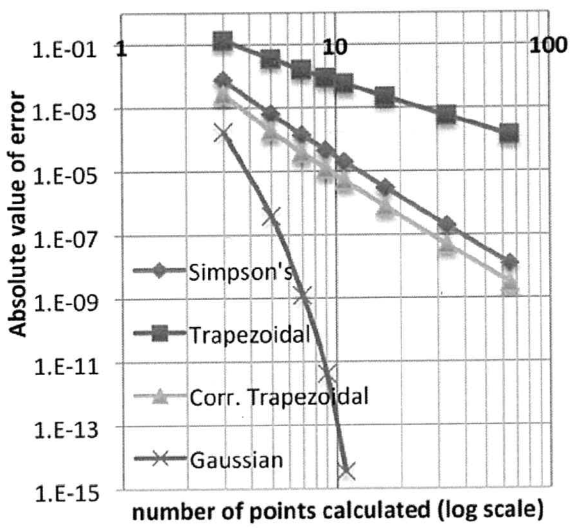

Figure 6. Log-log plot of the error versus the number of points to show the different convergence.

The examples above show that the trapezoidal rule converges more slowly (second order) than the corrected trapezoidal rule and Simpson's rule (fourth order) while Gaussian quadrature converges much more quickly and the convergence improves as more points are used. GQ owes its precision to optimising the placement of both the points at which the function is evaluated and the weigh given to those points. Using n points, the method exactly fits any polynomial of order $(2n - 1)$ or lower. Enormous effort was made throughout the 20th century to extend Gaussian quadrature to higher orders.

We found an excellent website (Casio Computer, 2018) that gives high (and variable) precision abscissae and weightings for a range of Gaussian methods, including methods that allow for integrable poles at the extrema. Part 2 derives and lists the solutions up to 13 points.

In practice, GQ is easily implemented on a spreadsheet. For the calculations above, our spreadsheet used only four columns, labelled a for the abscissae or points on the $[-1, 1]$ domain, w for their weightings, x for the points on the $[a, b]$ domain, and $w \cdot f(x)$ for weighted functional values. Doing a new problem added only two columns. The integral is found by summing the $w \cdot f(x)$ column and scaling for the width of the domain. GQ with only a small number of points converges to the limit of the spreadsheet's arithmetic, where using Simpson's rule to get comparable precision requires hundreds of points. Writing the program in Python is even easier.

Table 5 shows the evaluation of the numerical integral of $\cos(x)$, using small numbers of points. The first two columns contain values that can be downloaded from the Internet and re-used in many calculations. This GQ calculation is no harder than the shopping list shown in Table 1. Structurally they are almost identical.

Table 5. Evaluating the numerical integral of cos(x), using small numbers of points.

		GAUSSIAN QUADRATURE	
abscissae	weights	x	w*cos(x)
–0.906179845938664	0.236926885056189	–1.423423973	0.03479022
–0.538469310105683	0.478628670499366	–0.845825614	0.317385143
0.000000000000000	0.568888888888888	0	0.568888889
0.538469310105683	0.478628670499366	0.845825614	0.317385143
0.906179845938664	0.236926885056189	1.423423973	0.03479022
N = 5		integral=	2.00000011

Why is GQ not taught? Australia seems to have forgotten GQ. Australia needs to encourage STEM education of students and staff. Simple accurate methods attract greater student effort.

Building on a good idea

Gauss-Legendre quadrature (as used above and developed in more detail in Part 2) does not deal well with poles at the extrema nor with fractional powers such as square roots where the slope becomes infinite at one or both extrema. Gauss-Jacobi quadrature introduces weighting functions $(x + 1)^{\alpha}$ and $(x - 1)^{\beta}$ at these extrema. Such problems are common in physics and chemistry. GQ can be extended for appropriate functions on the semi-infinite and infinite domains $[0, \infty)$ and $(-\infty, \infty)$. Again, such problems are common in physics and chemistry.

References

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