Supplementary Notes 7

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Abstract

We discuss numerical integration.

Contents

1 General overview of numerical integration

Given an integrable function f over the interval $[a, b]$, we want to compute $I(f) := \int_a^b f(x)\,dx$ but this may prove to be difficult or even impossible. The alternative is then to approximate its value:

$$\int_a^b f(x)\,dx \approx I_h(f) := \sum_{i=0}^{n} c_i f(x_i).$$

We call $I_h(f)$ numerical quadrature.

1.1 Lagrange interpolation approach

One method to find a numerical quadrature is to use Lagrange interpolation where the points $x_0, \ldots, x_n$ are taken to be equally spaced in the interval $[a, b]$ with $a = x_0$ and $b = x_n$. (Therefore $x_k = a + kh$ where $h = \frac{b-a}{n}$.) Let's take a look at an example:

Example 1.1 (Trapezoid Rule)**.** *Consider the Lagrange interpolation at two equally spaced nodes and let L_1 denote the corresponding first order Lagrange polynomial. We then have by the Newton's divided difference formula*

$$L_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a).$$

Hence

$$\begin{aligned}
\int_a^b f(x)\,dx &\approx \int_a^b L_1(x)\,dx \\
&= \int_a^b f(a) + \frac{f(b)-f(a)}{b-a}(x-a)\,dx \\
&= f(a)(b-a) + \frac{f(b)-f(a)}{b-a}\left.\frac{(x-a)^2}{2}\right|_{x=a}^{x=b} \\
&= f(a)(b-a) + \frac{f(b)-f(a)}{b-a}\frac{(b-a)^2}{2} \\
&= \frac{h}{2}\left(f(a)+f(b)\right)
\end{aligned}$$

where $h = b - a$. As for the error, one can show that

$$E(f) := \int_a^b f(x)\,dx - \frac{h}{2}(f(a)+f(b)) = -\frac{h^3}{12}f''(\xi)$$

where $\xi \in [a, b]$.

In general, we know that

$$\begin{aligned}
f(x) &= L_n(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n) \\
&= \sum_{i=0}^{n} f(x_i)l_i(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n)
\end{aligned}$$

where $\xi(x) \in [a, b]$ for each x and the l_i are the Lagrange basis polynomials which are given by

$$l_i(x) = \prod_{\substack{k=0\\k\neq i}} \frac{(x-x_k)}{(x_i-x_k)}.$$

We then get

$$\begin{aligned}
\int_a^b f(x)dx &= \int_a^b \sum_{i=0}^{n} f(x_i)l_i(x)\,dx + \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n)\,dx \\
&= \sum_{i=0}^{n} a_i f(x_i) + \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n)\,dx
\end{aligned}$$

with

$$c_i = \int_a^b l_i(x)dx \quad i = 0, \dots, n.$$

Therefore, the quadrature formula is given by

$$I_h(f) = \sum_{i=0}^{n} c_i f(x_i)$$

with error

$$E_n(f) = \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)\dots(x-x_n)\,dx.$$

Remark 1.1. *It's possible to obtain simpler formulas for the error. See Section 4.3 in [1] for that.*

Example 1.2 (Simpson's Rule)**.** *If we use the second order Lagrange polynomial with equally spaced nodes, we get*

$$\int_a^b f(x)\,dx = \frac{h}{3}\left(f(a)+4f(m)+f(b)\right) - \frac{h^5}{90}f^{(4)}(\xi)$$

where $h = \frac{b-a}{2}$, $m = \frac{a+b}{2}$ (midpoint of the interval) and $\xi \in [a, b]$.

1.2 Degree of accuracy approach

Another method to find a numerical quadrature is based on making it exact for a class of polynomials. We introduce the notion of degree of accuracy or precision to make the discussion easier.

Definition 1.2. *We say that $I_h(f)$ has degree of accuracy of p is p is the largest positive integer with $I(x^i) = I_h(x^i)$ for $i = 0, \ldots, p$.*

Remark 1.3. *For a quadrature to be exact for a function we need*

$$\int_a^b f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i)$$

and not just $\approx$. The bigger the degree of accuracy the better.

In practice one proceeds as follows. Check for $f(x) = x^0 = 1$ if the quadrature is exact, i.e., does the quadrature formula give the exact answer. If it does, then check for $f(x) = x^1 = x$. If it is not exact for this f, then the degree is zero. If it is exact, check for $f(x) = x^2$. If it is not exact for this f, the degree is one. We then check for $f(x) = x^3$ and so on.

An interested reader should check that the Trapezoid Rule has a degree of accuracy 1 and that the degree of accuracy of Simpson's Rule is 3 using the procedure described above.

There is however a shortcut to compute degrees of accuracy provided that we know the error of the quadrature. A quadrature formula is exact for some f if and only if error is zero for that f. Consequently it is sufficient to simply check the derivative of f in the error term and do that minus one to get the degree of accuracy. Let's look at the Trapezoid Rule as an example. The error is proportional to $f''(\xi)$ hence the degree of accuracy is $2 - 1 = 1$. The reasoning is the following: if $f(x) = 1$, $f''(x) = 0$, so $f''(\xi) = 0$ and thus the error is zero. If $f(x) = x$, $f''(x) = 0$, so $f''(\xi) = 0$ and thus the error is again zero. If $f(x) = x^2$, we don't have $f''(x) = 0$ and therefore the error will (most likely) be nonzero. We can then conclude the degree of accuracy is indeed 1, without having to do many computations.

Exercise 1.1. *Find the degree of accuracy of the quadrature formula*

$$\int_{-1}^{1} f(x)\,dx = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

Solution: According to the definition we need to check if the quadrature is exact for polynomials.

- $f(x) = 1$

We have

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} 1\,dx = 2$$

and

$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = 1 + 1 = 2.$$

Thus the formula is exact for this f.

- $f(x) = x$

We have

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} x\,dx = \left[\frac{x^2}{2}\right]_{-1}^{1} = \frac{1}{2} - \frac{(-1)^2}{2} = 0$$

and

$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = -\frac{\sqrt{3}}{3} + \frac{\sqrt{3}}{3} = 0.$$

Hence the formula is again exact and the degree of accuracy is at least 1.

- $f(x) = x^2$

We have
$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} x^2\,dx = \left[\frac{x^3}{3}\right]_{-1}^{1} = \frac{1}{3} - \frac{(-1)^3}{3} = \frac{2}{3}$$
and
$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \left(-\frac{\sqrt{3}}{3}\right)^2 + \left(\frac{\sqrt{3}}{3}\right)^2 = 2\frac{3}{9} = \frac{2}{3}.$$
Therefore the degree of accuracy is at least 2.

- $f(x) = x^3$

We have
$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} x^3\,dx = \left[\frac{x^4}{4}\right]_{-1}^{1} = \frac{1}{4} - \frac{(-1)^4}{4} = 0$$
and
$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \left(-\frac{\sqrt{3}}{3}\right)^3 + \left(\frac{\sqrt{3}}{3}\right)^3 = 0.$$
Therefore the degree of accuracy is at least 3.

- $f(x) = x^4$

We have
$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} x^4\,dx = \left[\frac{x^5}{5}\right]_{-1}^{1} = \frac{1}{5} - \frac{(-1)^5}{5} = \frac{2}{5}$$
and
$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \left(-\frac{\sqrt{3}}{3}\right)^4 + \left(\frac{\sqrt{3}}{3}\right)^4 = 2\frac{9}{81} = \frac{2}{9}.$$
Therefore the degree of accuracy is 3.

The degree of accuracy provides us with another method to find a numerical quadrature. We can fix the nodes a priori (e.g., setting them to be equally spaced) and look at the weights as unknowns. Then the weights should be such that the quadrature formula has the highest degree possible.

Exercise 1.2. *The quadrature formula*
$$\int_0^2 f(x)\,dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$$
has degree of accuracy at least 2*. Determine* c_0*,* c_1 *and* c_2 *and the degree of accuracy.*

Solution: Let $f(x) = 1$. We know that the quadrature is exact for this f. Then
$$2 = \int_0^2 1\,dx = \int_0^2 f(x)\,dx = c_0 f(0) + c_1 f(1) + c_2 f(2) = c_0 + c_1 + c_2$$
which leads to the equation $c_0 + c_1 + c_2 = 2$.

Now take $f(x) = x$. Hence

$$2 = \int_0^2 x\, dx = \int_0^2 f(x)\, dx = c_0 f(0) + c_1 f(1) + c_2 f(2) = c_1 + 2c_2$$

leading to the equation $c_1 + 2c_2 = 2$. Finally we take $f(x) = x^2$. We have

$$\frac{8}{3} = \int_0^2 x^2\, dx = \int_0^2 f(x)\, dx = c_0 f(0) + c_1 f(1) + c_2 f(2) = c_1 + 4c_2$$

and so we get the equation $c_1 + 4c_2 = \frac{8}{3}$.

We must then solve the linear system

$$\begin{cases} c_0 + c_1 + c_2 = 2 \\ c_1 + 2c_2 = 2 \\ c_1 + 4c_2 = \frac{8}{3} \end{cases}$$

We get

$$\begin{cases} c_0 = 2 - c_1 - c_2 = 2 - \frac{4}{3} - \frac{1}{3} = \frac{1}{3}, \\ c_1 = 2 - 2c_2 = 2 - \frac{2}{3} = \frac{4}{3}, \\ c_2 = \frac{1}{2}\left(\frac{8}{3} - 2\right) = \frac{1}{3}. \end{cases}$$

To determine the degree of accuracy of the quadrature we have to, according to its definition, find the largest positive integer n such that the formula is exact for x^i for each $i = 0, \ldots n$. Hence we have to keep trying with x^3, x^4 and so on, until the formula is no longer exact. Only then, we will know the degree of accuracy.

If let $f(x) = x^3$, we get

$$\int_0^2 x^3\, dx = 4$$

and

$$c_0 f(0) + c_1 f(1) + c_2 f(2) = \frac{0 + 4 + 8}{3} = 4.$$

If we now let $f(x) = x^4$ then

$$\int_0^2 x^4\, dx = \frac{32}{5}$$

and

$$c_0 f(0) + c_1 f(1) + c_2 f(2) = \frac{0 + 4 + 16}{3} = \frac{20}{3} \neq \frac{32}{5}.$$

We can then conclude the degree of accuracy of the numerical quadrature is 3.

Exercise 1.3. *Find the constants x_0, x_1 and c_1 so that the quadrature formula*

$$\int_0^1 f(x)\, dx = \frac{1}{2} f(x_0) + c_1 f(x_1)$$

has the highest possible degree of accuracy. Find the degree of accuracy.

Solution: The procedure is the same as in the previous exercise. Taking $f(x) = 1$ leads to

$$\frac{1}{2} + c_1 = 1 \iff c_1 = \frac{1}{2}.$$

Taking now $f(x) = x$, we get
$$\frac{1}{2}x_0 + \frac{1}{2}x_1 = \frac{1}{2}.$$
Letting now $f(x) = x^2$ gives us
$$\frac{1}{2}x_0^2 + \frac{1}{2}x_1^2 = \frac{1}{3}.$$
We have two equations which should be enough to find x_0 and x_1:
$$\begin{cases} x_0 + x_1 = 1 \\ x_0^2 + x_1^2 = \frac{2}{3} \end{cases} \iff \begin{cases} x_0 = 1 - x_1 \\ 2x_1^2 - 2x_1 + \frac{1}{3} = 0 \end{cases} \iff \begin{cases} x_0 = \frac{1}{2} \mp \frac{\sqrt{3}}{6} \\ x_1 = \frac{1}{2} \pm \frac{\sqrt{3}}{6} \end{cases}$$
Since the weights of the quadrature are equal, we have indeed
$$\begin{cases} x_0 = \frac{1}{2} - \frac{\sqrt{3}}{6} \\ x_1 = \frac{1}{2} + \frac{\sqrt{3}}{6} \end{cases}$$

By construction we know that the degree of accuracy is at least 2. Taking $f(x) = x^3$ we easily verify that
$$\frac{1}{4} = \int_0^1 f(x)\,dx = \frac{1}{2}f\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right) + \frac{1}{2}f\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right).$$
Taking now $f(x) = x^4$, we get
$$\frac{1}{5} = \int_0^1 f(x)\,dx \neq \frac{1}{2}f\left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right) + \frac{1}{2}f\left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right) = \frac{7}{36}.$$
The order of accuracy is therefore 3.

1.3 Gaussian quadrature

The idea behind Gaussian quadrature is that we not only choose the weights in an optimal way, but also the nodes. Assuming that the best choice to minimize the expected error is the one with the highest degree of accuracy, we want to choose nodes $x_0, \dots, x_n$ in the interval $[a, b]$ and weights $c_0, \dots, c_n$ that make the quadrature exact
$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i)$$
for the largest class of polynomials.

The weights $c_0, \dots, c_n$ are arbitrary and the nodes $x_0, \dots, x_n$ are restricted only by the fact that they must lie in $[a, b]$, the interval of integration. We then have $2n + 2$ parameters to choose. A polynomial of degree $2n + 1$ has $2n + 2$ parameters and, therefore, is the largest class of polynomials for which it is reasonable to expect a formula to be exact.

One way to find the Gaussian quadrature is to use the method used in Exercises 1.2 and 1.3: we consider both the weights $c_0, \dots, c_n$ and the nodes $x_0, \dots, x_n$ as unknowns and choose them in order for the numerical quadrature to have the highest degree of accuracy possible.

To find the Gaussian quadrature for an arbitrary interval $[a, b]$ the idea is to rewrite the integral as an integral on the interval $[-1, 1]$ for which we know what the Gaussian quadrature is. Consider then the change of variables
$$t = \frac{2x - a - b}{b - a} \iff x = \frac{1}{2}\left((b - a)t + a + b\right)$$

n	weights w_i	nodes t_i	degree of accuracy
0	2	0	1
1	$1, 1$	$-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}$	3
2	$\frac{5}{9}, \frac{8}{9}, \frac{5}{9}$	$-\sqrt{\frac{3}{5}}, 0, \sqrt{\frac{3}{5}}$	5

Table 1: Nodes and weights of the Gaussian quadrature in the interval $[-1, 1]$.

that takes the interval $[a, b]$ into the interval $[-1, 1]$. Thus, it's now enough to observe that

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_{-1}^{1} f\left(\frac{(b-a)t + (b+a)}{2}\right)\frac{(b-a)}{2}\,dt \\ &\approx \sum_{i=0}^{n} w_i f\left(\frac{(b-a)t_i + (b+a)}{2}\right)\frac{(b-a)}{2}\end{aligned}$$

We can then write the Gaussian quadrature for an arbitrary interval as

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i)$$

where the weights are given by

$$c_i = \frac{b-a}{2} w_i$$

and the nodes given by

$$x_i = \frac{(b-a)t_i + (b+a)}{2}$$

for $i = 0, \ldots, n$.

2 Review numerical integration

Numerical integration is a method to used to approximate the value of a definite integral. Here, given a function f and an interval $[a, b]$ we look for

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} c_i f(x_i).$$

We call the above formula a numerical quadrature with the constants a_i begin denominated weights and the x_i nodes.

If the nodes are picked to be equally spaced with $x_0 = a$ and $x_n = b$, then by using Lagrange interpolation, we obtained a numerical quadrature which we call Newton-Cotes. If instead we look at both the weights and the nodes as unknown and choose them to make the numerical quadrature have the highest degree possible, we obtain what we call the Gaussian quadrature. In Table 2, we can see the degree of accuracy of each numerical quadrature.

3 Composite quadratures

To reduce the quadrature error, one can divide the interval into smaller subintervals and apply known quadrature rules to each one of the subintervals. The error is reduced by taking smaller and smaller

Numerical Quadrature	Number of points ($N = n+1$)	Degree of accuracy
Newton-Cotes	N (odd)	N
	N (even)	N-1
Gaussian quadrature	N	$2N-1$

Table 2: Degree of accuracy of the Newton-Cotes and Gaussian quadratures.

subintervals of length h.

$$I(f) = \int_a^b f(x)\,dx = \sum_{k=0}^{n} \int_{x_k}^{x_{k+1}} f(x)\,dx = \sum_{k=0}^{n} I_{h,k}(f) + E_k(f)$$

where $I_{h,k}(f)$ is the quadrature on $[x_k, x_{k+1}]$ and $E_k(f)$ is the local error on $[x_k, x_{k+1}]$. This is the idea of composite quadrature.

Example 3.1 (Composite Midpoint Rule)**.** *On each* $[x_k, x_{k+1}]$*, there is some* $\xi_k \in (x_k, x_{k+1})$*,*

$$\int_{x_k}^{x_{k+1}} f(x)\,dx = hf\left(x_{k+\frac{1}{2}}\right) + f''(\xi_k)\frac{h^3}{24}$$

where $x_{k+\frac{1}{2}} = \frac{x_k + x_{k+1}}{2}$*. Hence*

$$I(f) = h\sum_{k=0}^{n-1} f\left(x_{k+\frac{1}{2}}\right) + \frac{h^3}{24}\sum_{k=0}^{n-1} f''(\xi_k) = h\sum_{k=0}^{n-1} f\left(\frac{x_k + x_{k+1}}{2}\right) + \frac{b-a}{24} f''(\xi)h^2$$

since

$$\frac{1}{n}\sum_{k=0}^{n-1} f''(\xi_k) = f''(\xi)$$

for some $\xi \in (a,b)$ *by the intermediate value theorem.*

References

[1] R. L. Burden and J. D. Faires. *Numerical Analysis.* 9^{th} edition. Brookes/Cole, 2004.

[2] A. Quarteroni, R. Sacco and F. Saleri. *Numerical Mathematics.* 2^{nd} edition. Springer, 2006.

[3] Tutorial notes written by Jan Feys