4 Numerical Integration

The foregoing formal content is now supplemented by an exploration of numerical aspects. The focus will be two-fold: first Newton-Cotes type approaches that are more elemental in character, and then more sophisticated techniques, specifically Gaussian quadrature, followed by a brief mention of Romberg's method.

4.1 Newton-Cotes Formulae

These derived from the elemental approach of Newton's theory of integration. The agenda is to compute areas under curves with increasing accuracy and complexity of algorithm. The first method is to approximate functional behavior on a sequence of intervals $[x_i,\, x_{i+1}]$ by a piecewise linear construct, thereby formulating the **trapezoidal rule**.

Plot: Trapezoidal Rule Construct

Then,

$$f(x) \;\approx\; f_i + \Bigl(f_{i+1} - f_i \Bigr) \, \frac{x - x_i}{x_{i+1} - x_i} \quad . \tag{48}$$

This then gives an integral approximation on this interval of

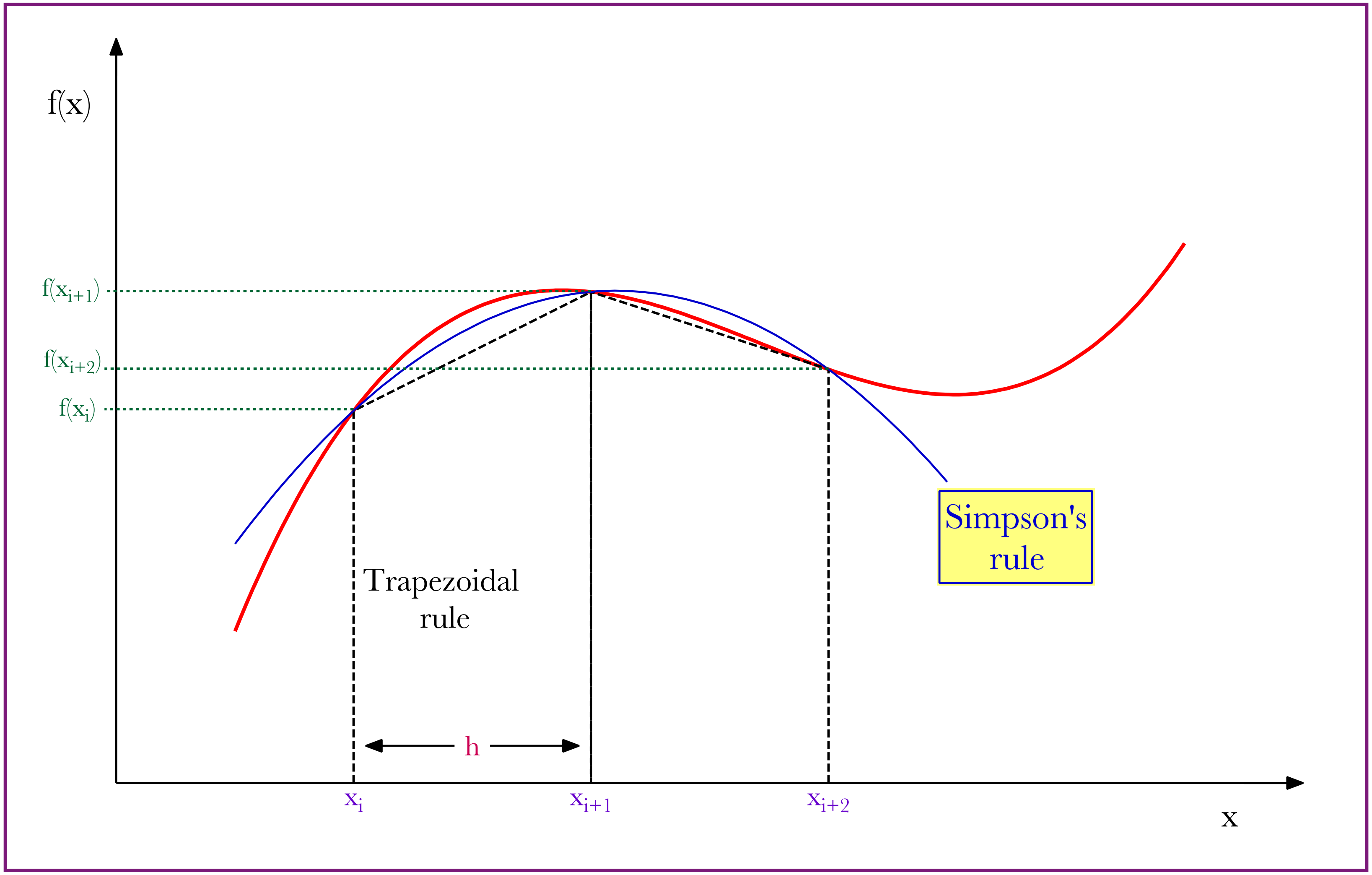
$$\int_{x_i}^{x_{i+1}} f(x)\, dx \;\approx\; \frac{h_i}{2} \Bigl(f_{i+1} + f_i \Bigr) \quad , \quad h_i \;=\; x_{i+1} - x_i \quad , \tag{49}$$

with an error of the order of h_i^3. Often, the implementation is for a sequence of evenly-spaced intervals. With $h_i = h$ for all i, the total integration over two consecutive intervals becomes

$$\boxed{\int_{x_i}^{x_{i+2}} f(x)\, dx \;\approx\; \frac{h}{2} \Bigl(f_i + 2 f_{i+1} + f_{i+2} \Bigr) \quad .} \tag{50}$$

The accuracy of this trapezoidal rule can clearly be improved by choosing smaller intervals, unless their is a pathological problem with the integrand, for example a singularity or sharp peak within the overall integration range.

Simpson's Rule for Numerical Integration



However, integration accuracy is more efficiently improved by approximating the function more precisely, namely with a piecewise parabolic function. This now requires 3 points instead of two, to uniquely constrain the parabola. Without loss of generality, it is sufficient, and prudent, to space the two sub-intervals equally.

Plot: Simpson's Rule Construct

This method is known as **Simpson's rule**, and we derive the approximating function as follows. The parabolic form can be written

$$f(x) \;\approx\; f_i + a\,(x - x_i) + b\,(x - x_i)^2 \quad , \tag{51}$$

from which the specific evaluations at $x = x_{i+1}$ and $x = x_{i+2}$ yield the following simultaneous equations for a and b:

$$\begin{aligned} f_{i+1} &= f_i + a\,h + b\,h^2 \quad , \\ f_{i+2} &= f_i + a\,(2h) + b\,(2h)^2 \quad , \end{aligned} \tag{52}$$

where we have used the substitutions $h = x_{i+1} - x_i$ and $2h = x_{i+2} - x_i$. These can be solved to yield

$$\begin{aligned} 2ah &= -3f_i + 4f_{i+1} - f_{i+2} \quad , \\ 2bh^2 &= f_i - 2f_{i+1} + f_{i+2} \quad . \end{aligned} \tag{53}$$

From this, the final result for the integral on $[x_i,\, x_{i+2}]$ of Eq. (51) is

$$\boxed{\int_{x_i}^{x_{i+2}} f(x)\,dx \;\approx\; \frac{h}{3}\Big(f_i + 4f_{i+1} + f_{i+2}\Big) \quad .} \tag{54}$$

This is Simpson's rule, and is accurate to $O(h^5)$, and therefore *more precise than the trapezoidal rule, which possesses comparable computational needs.* Accordingly, it is of common usage, as is the alternative Simpson's $3/8$ rule:

$$\int_{x_i}^{x_{i+3}} f(x)\,dx \;\approx\; \frac{3h}{8}\Big(f_i + 3f_{i+1} + 3f_{i+2} + f_{i+3}\Big) \quad , \tag{55}$$

which uses a cubic fit, but is no more accurate, i.e. of $O(h^5)$.

Simpson's Rule: Mathematica Example

```
Functional definition:

f[x_] := Sin[Pi x/2]  (* on [0,1] *)

Simpson's rule integration algorithm on [xmin, xmax]:

Simpson[xmin_, xmax_, n_]:= h/3 ( f[xmin] +
              2 Sum[ f[xmin+ k h], {k,2,2n-2,2}] +
              4 Sum[ f[xmin+ k h], {k,1,2n-1,2}] +
                f[xmax] ) /. h-> N[(xmax-xmin)/(2 n)];

Performing a sequence of improved precision, with
n pairs of intervals, equally spaced:

Simpson[0,1,2] -> 0.636705
Simpson[0,1,4] -> 0.636625
Simpson[0,1,6] -> 0.636621

the last of which is almost exact (2/Pi).

This demonstrates how around 25 terms each involving a
functional evaluation leads to precision at the 0.001% level.
```

4.2 Gaussian Quadrature

The essence of the **Gaussian quadrature** technique is to approximate the integral by a weighted sum over values of the function at selected abscissa points. The finite number of abscissa points are chosen based on the integration limits, and the nature of the integrand. They form zeros for a select class of polynomials (or functions) for which the *integral evaluation is exact* on the particular integral. As no formal derivation is offered here (see Stroud & Secrest 1966, "Gaussian Quadrature Formulas"), the method is expounded by illustration.

• This example will define **two-point Gauss-Legendre quadrature** for integrals of the form

$$\int_{-1}^{1} f(x)\, dx \;\approx\; w_1\, f(x_1) + w_2 f(x_2) \quad . \tag{56}$$

The key elements are the integration range, $[-1, 1]$, upon which the Legendre polynomials form an orthogonal set of **basis states**, and the weighting factor of unity in the integrand. The approach embellished here is viable provided that $f(x)$ is not extraordinarily rapidly varying on $[-1, 1]$, i.e. is not exponential in character, nor possesses singularities or cusp points.

• Eq. (56) has four unknowns, so we require the quadrature to be exact for functions $f(x) = 1, x, x^2, x^3$, and, consequently, for all cubic polynomials. This establishes the system of simultaneous equations:

$$\begin{aligned} f(x) &= 1 &:&\quad w_1 + w_2 = 2 \quad , \\ f(x) &= x &:&\quad w_1 x_1 + w_2 x_2 = 0 \quad , \\ f(x) &= x^2 &:&\quad w_1 x_1^2 + w_2 x_2^2 = \frac{2}{3} \quad , \\ f(x) &= x^3 &:&\quad w_1 x_1^3 + w_2 x_2^3 = 0 \quad , \end{aligned} \tag{57}$$

for which the solution is elementary:

$$x_1 = -\frac{1}{\sqrt{3}} = -x_2 \quad , \quad w_1 = w_2 = 1 \quad , \tag{58}$$

so that $x_{1,2}$ are the roots of the Legendre polynomial $P_2(x) = (3x^2 - 1)/2$, and the two-point Gauss-Legendre rule is

$$\int_{-1}^{1} f(x)\, dx \;\approx\; f\Bigl(-\frac{1}{\sqrt{3}}\Bigr) + f\Bigl(\frac{1}{\sqrt{3}}\Bigr) \quad . \tag{59}$$

• If one extends this to three-point quadrature on $[-1,\, 1]$, then by a similar construct, one finds that

$$\int_{-1}^{1} f(x)\, dx \;\approx\; \frac{5}{9}\, f\biggl(-\sqrt{\frac{3}{5}}\biggr) + \frac{8}{9}\, f(0) + \frac{5}{9}\, f\biggl(\sqrt{\frac{3}{5}}\biggr) \quad , \tag{60}$$

which is exact for polynomials up to and including 5th order. Here the roots of the Legendre polynomial $P_3(x) = x(5x^2 - 3)/2$ are sampled.

• The principal of Gaussian quadrature is based on identifying orthogonal functions, usually n^{th} order polynomials $P_n(x)$, on the chosen integration interval $[a,\, b]$. These satisfy

$$\int_a^b w(x)\, P_n(x)\, P_m(x)\, dx \;=\; 0 \quad , \quad m \;\neq\; n\, ; \;\; m,\, n \;=\; 0, 1, 2, \dots \tag{61}$$

The polynomials $P_n(x)$ form an **orthogonal** sequence on the interval $[a,\, b]$ with respect to the weight function $w(x)$, which is usually non-negative. Then, one can trivially identify the normalization

$$\kappa_n^2 \;\equiv\; \int_a^b w(x)\; \bigl[P_n(x)\bigr]^2\; dx \;>\; 0 \quad . \tag{62}$$

Observe that the orthogonality constraint generally forces the sequence to polynomials that *exhibit real roots only.*

∗ In the case of Legendre polynomials, $w(x) = 1$ and also $\kappa_n^2 = 2/(1{+}2n)$.

• For an n-point quadrature, the integration is represented by a finite sum:

$$\boxed{\int_a^b w(x)\, f(x)\, dx \;\approx\; \sum_{i=1}^{n} w_i\, f(x_i) \quad .} \tag{63}$$

Without loss of generality, the abscissa points *can be chosen to be the roots* x_i *of* $P_n(x)$. It then automatically follows from Eq. (61), by choosing $m = 0$ so that $P_m(x)$ is a constant, that the quadrature in Eq. (63) is exact (and zero) for $f(x) = P_n(x)$.

• It is straightforward to prove that the quadrature is also exact in polynomials of lower order $m < n$. This assertion is based on the basis vector decomposition

$$\begin{aligned} f(x) \; &= \; \mathcal{P}_m(x) \; &&= \; \sum_{j=0}^{m} \alpha_j \, P_j(x) \qquad (\text{for}\, m \; < \; n) \\ \Rightarrow \int_a^b w(x)\, f(x)\, dx \; &&&= \; \sum_{j=0}^{m} \alpha_j \int_a^b w(x)\, P_j(x)\, dx \quad . \end{aligned} \tag{64}$$

and proceed from there.

∗ Note that general ranges of integration $a \le t \le b$ can be transformed onto $-1 \le x \le 1$ using the substitution $x = (2t - b - a)/(b - a)$.

• The weights for the quadrature can be shown to be given by a variety of formulae:

$$w_i \; = \; \frac{\kappa_{n-1}^2}{P_n'(x_i)\, P_{n-1}(x_i)} \; = \; -\frac{\kappa_n^2}{P_n'(x_i)\, P_{n+1}(x_i)} \; = \; \int_a^b \frac{w(x)\, P_n(x)\, dx}{(x - x_i) P_n'(x_i)} \; . \tag{65}$$

• The categories of Gaussian quadrature depend on the integration limits and the weighting function; other common types are **Gauss-Jacobi**, **Gauss-Hermite** and **Gauss-Laguerre** quadrature.

$\boxed{\textbf{Plot:}}$ Types of Gaussian Quadrature

• The primary algorithmic task is to identify the type of quadrature that will best suit the integral, reworking the integral via changes of variable and then extracting the appropriate weight function before performing the quadrature.

Types of Gaussian Quadrature

$\int_{-1}^{1} f(x)\,dx$	$\approx \sum_{i=1}^{n} w_i\,f(x_i)$	Gauss-Legendre
$\int_{-1}^{1} \frac{f(x)\,dx}{\sqrt{1-x^2}}$	$\approx \sum_{i=1}^{n} w_i\,f(x_i)$	Gauss-Chebyshev
$\int_{-1}^{1} (1-x^2)^{\alpha}\,f(x)\,dx$	$\approx \sum_{i=1}^{n} w_i\,f(x_i)$	Gauss-Gegenbauer
$\int_{-1}^{1} (1+x)^{\beta}\,f(x)\,dx$	$\approx \sum_{i=1}^{n} w_i\,f(x_i)$	Gauss-Jacobi
$\int_{0}^{\infty} e^{-x}\,f(x)\,dx$	$\approx \sum_{i=1}^{n} w_i\,f(x_i)$	Gauss-Laguerre
$\int_{-\infty}^{\infty} e^{-x^2}\,f(x)\,dx$	$\approx \sum_{i=1}^{n} w_i\,f(x_i)$	Gauss-Hermite

6. FOURIER SERIES AND TRANSFORMS

Matthew Baring — Lecture Notes for PHYS 516, Fall 2022

1 Fourier Series

In physics and engineering applications, periodic functions frequently appear, and efficient means of computing them with good approximation are needed. This becomes the domain of **Fourier series**. A function that is defined, and well-behaved on the interval $[0, 2\pi]$ (or periodic with period 2π) can be represented by the infinite series **A&W Sec. 14.1**

$$f(\theta) \; = \; \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos n\theta + b_n \sin n\theta \right) \quad . \tag{1}$$

There is no unique definition of *well-behaved* functions, but a sufficient (but not necessary) condition is that $f(\theta)$ be *piecewise very smooth*, meaning that f, f' and f'' are piecewise continuous. Then the series converges to $f(\theta)$, or to the limit

$$\lim_{\epsilon\to 0} \frac{1}{2} \Bigl[f(\theta_0+\epsilon) + f(\theta_0-\epsilon) \Bigr] \quad , \tag{2}$$

if $f(\theta)$ is discontinuous at $\theta = \theta_0$.

$*$ For even functions, $f(-\theta) = f(\theta)$ and $b_n = 0$ for all n. For odd functions, $f(-\theta) = -f(\theta)$ and $a_n = 0$ for all n.

• To uniquely determine the Fourier coefficients a_n and b_n, we employ the orthogonality relations for trigonometric functions:

$$\int_0^{2\pi} \sin n\theta \, \cos m\theta \, d\theta \; = \; 0 \tag{3}$$

for all m and n, and

$$\int_0^{2\pi} \cos n\theta \, \cos m\theta \, d\theta \;=\; \pi \, \delta_{nm} \;=\; \int_0^{2\pi} \sin n\theta \, \sin m\theta \, d\theta \tag{4}$$

for $n \neq 0 \neq m$. Here δ_{nm} is the **Kronecker delta** and is non-zero only for integers $n = m$. The orthogonality relations then permit evaluation of integral moments of $f(\theta)$ with appropriate trigonometric weights:

$$\int_0^{2\pi} f(\theta) \, d\theta \;=\; \int_0^{2\pi} \left[\frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta) \right] d\theta \;=\; \pi a_0 \tag{5}$$

for the $m = 1$ cosine integral moment. Hence,

$$a_0 \;=\; \frac{1}{\pi} \int_0^{2\pi} f(\theta) \, d\theta \;=\; 2\langle f(\theta) \rangle \quad . \tag{6}$$

Similarly,

$$\begin{aligned} \int_0^{2\pi} f(\theta) \, \cos m\theta \, d\theta \;&=\; \frac{1}{2} \int_0^{2\pi} a_0 \cos m\theta \, d\theta \\ &+ \sum_{n=1}^{\infty} \left\{ a_n \int_0^{2\pi} \cos n\theta \, \cos m\theta \, d\theta + b_n \int_0^{2\pi} \sin n\theta \, \cos m\theta \, d\theta \right\} \\ &=\; 0 + \sum_{n=1}^{\infty} \pi a_n \delta_{nm} + 0 \;=\; \pi \, a_m \quad . \end{aligned} \tag{7}$$

The sine integral moment isolates the b_m coefficient in similar fashion. The results are

$$\begin{aligned} a_n \;&=\; \frac{1}{\pi} \int_0^{2\pi} f(\theta) \, \cos n\theta \, d\theta \\ b_n \;&=\; \frac{1}{\pi} \int_0^{2\pi} f(\theta) \, \sin n\theta \, d\theta \quad . \end{aligned} \tag{8}$$

These forms uniquely determine the Fourier series in Eq. (1), whose convergence to $f(\theta)$ is dictated by the number of terms evaluated in the series.

$*$ Often, a_n and b_n are declining functions of n, since the oscillatory character of the integrands in Eq. (8) is a destructive influence in controlling contributions to the integrals.