Chapter 3

Numerical Integration

3.1 Introduction

Problem: *Given a real-valued function* f *that is continuous on* $[a, b]$, *can we find an estimate for*

$$I(f) := \int_a^b f(x)dx?$$

And if we can, can we say how accurate it is?

Why bother?

- many problems in applicable mathematics require definite integrals to be evaluated.[1]
- evaluating them by finding the anti-derivative can be hard, and very hard to automate.
- some times, although the function is integrable, its anti-derivative doesn't exist in a closed form.

The process of numerically estimating a definite integral is called *Numerical Integration* or *Quadrature*.

The formulae we'll derive all look like

$$Q_n(f) := q_0 f(x_0) + q_1 f(x_1) + q_2 f(x_2) + \dots q_n f(x_n).$$

Here the points x_i are called *quadrature points* and the q_i are *quadrature weights*. So we need a way of choosing these. The simplest approach is to take the points to be equally spaced, i.e., $x_i = a + hi$ where $h = (b - a)/n$.

How to choose the weights? We've spent quite a while talking and thinking about approximating functions with polynomials. So why not find a polynomial interpolant to f and take the integral of that to be the answer? The appeal of this approach is due to the fact that

- Finding polynomial interpolants is easy.
- Integrating polynomials is easy.
- We can estimate the error easily (yet again, we'll make use of Theorem 1.3.3)

[1]These methods were originally motivated by problems in astronomy. They're credited to the English mathematician/astronomer Roger Cotes (1682–1716), working with Isaac Newton.

This leads to the Newton-Cotes methods, which are the subject of this section, and Section 3.2 Later again, we'll look at more sophisticated methods, called *Gaussian Methods* which use non-uniformly spaced points.

3.1.1 Newton-Cotes methods

Definition 3.1.1. The *Newton-Cotes* quadrature rule for $\int_a^b f(x)dx$ with $n+1$ points is derived by integrating exactly the polynomial of degree n that interpolates f at the n equally spaced points $a = x_0 < x_1 < \dots < x_n = b$. The method is written as

$$Q_n(f) := q_0 f_0 + q_1 f_1 + q_2 f_2 + \dots q_n f_n.$$

That is, the quadrature weights are chosen so that

$$Q_n(f) = \int_a^b p_n(x)dx,$$

where p_n is the polynomial of degree n that interpolates f at the $n+1$ quadrature points. However, it turns out that we can compute the weights $q_0, \dots, q_n$, *without* knowing p_n. We'll do this for $n = 1$ in the next section, and $n = 2$ (the most interesting case) in Section 3.2.

3.1.2 The Trapezium rule

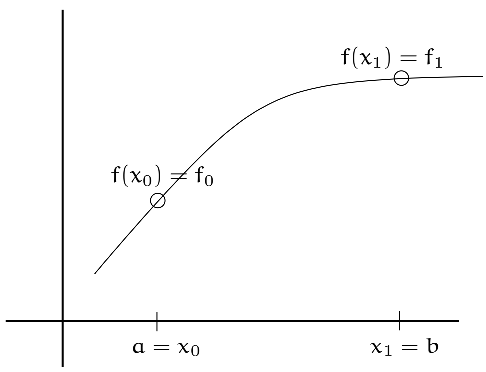

Fig. 3.1: Want to estimate $\int_a^b f(x)dx$

We want to estimate the integral of a function, f, on $[a,b]$, shown in Figure 3.1. Here are three approaches we could take.

Method 1: We could try to estimate the area of the trapezium the fits under the graph, as show in Figure 3.2. Clearly this comes to

$$Q_1(f) = (b-a)f_0 + (b-a)\frac{f_1 - f_2}{2} = (b-a)\frac{f_1+f_0}{2}. \quad (3.1)$$

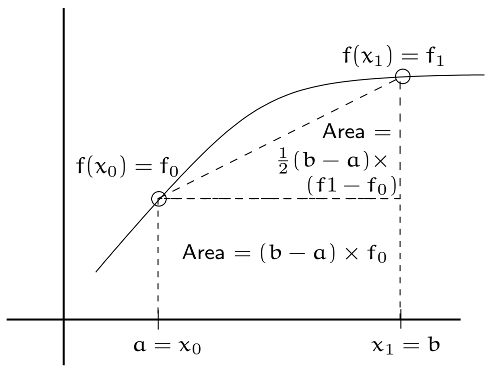

Fig. 3.2: Whats the area under the graph?

Method 2: As shown in Figure 3.3 we could find p_1, the polynomial of degree 1 that interpolates f at $x = a$ and $x = b$.

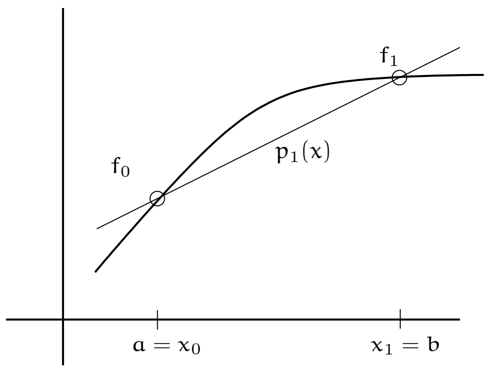

Fig. 3.3: Integrate $p_1(x)$ from x_0 to x_1

Take notes:

Note that this shows that $q_i = \int_a^b L_i(x)dx$, where, as usual, the L_i are the Lagrange Polynomials. (See §1.2.4).

Method 3: The third approach for generating the Trapezium Rule is called the *Method of Undetermined Coefficients*. Because the method is based on integrating a linear function we expect it to yield an exact solution for any constant or linear function (i.e., there should be no error). To keep the algebra simple, we'll take $a = 0$ and $b = 1$. So,

$$Q_1(f) = q_0 f(0) + q_1 f(1),$$

and, setting $f(x) \equiv 1$, and then $f(x) = x$ we get

Take notes:

Now we need to extend this to estimating $\int_a^b g(x)dx$ as follows:

Take notes:

Example 3.1.2. Use the Trapezium Rule to estimate

$$\int_0^{\pi/4} \cos(x)dx.$$

Calculate the (exact) error $|\int_a^b f(x)dx - Q_1(f)|$.

Take notes:

3.1.3 Exercises

Exercise 3.1. Let $q_0, q_1, \dots, q_n$ be the quadrature weights for the Newton-Cotes rule $Q_n(f)$. Show that $q_i = q_{n-i}$ for $i = 0, \dots n$.

Exercise 3.2. $\star$ Show that $\sum_{i=0}^n q_i = b - a$.

3.2 Simpson's Rule

Next we'll consider the *3-point Newton-Cotes scheme* which is based on integrating the quadratic interpolant to $f(x)$.

Simpson's Rule

$$Q_2(f) = \frac{b-a}{6}\big(f(a) + 4f(\frac{a+b}{2}) + f(b)\big). \tag{3.2}$$

This is called *Simpson's Rule*[2]. To show how to derive it, we'll use the Method of Undetermined Coefficients again. First restrict our attention to approximating $\int_0^1 g(x)dx$. This method should be exact for all constant, linear and quadratic polynomials. Taking $g(x) \equiv 1$, $g(x) = x$ and $g(x) = x^2$ we get the set of equations

Take notes:

This is easily solved giving

$$\int_0^1 g(x)dx \approx \frac{1}{6}g(0) + \frac{2}{3}g(1/2) + \frac{1}{6}g(1). \tag{3.3}$$

To extend this to the interval $[a, b]$, we again use a change of variables to get the general Simpson's Rule (3.2) .

Example 3.2.1. Use Simpson's rule to estimate $\int_0^{\pi/4} \cos(x)dx$, and calculate the (exact) error $|\int_a^b f(x)dx - Q_2(f)|$.

Take notes:

[2]Thomas Simpson, 1710–1761. One of the most distinguished of a group of itinerant lecturers who taught in the London coffee-houses, Hutton (famous text-book writer) said of him

> *It has been said that Mr Simpson frequented low company, with whom he used to guzzle porter and gin: but it must be observed that the misconduct of his family put it out of his power to keep the company of gentlemen, as well as to procure better liquor.*

The method was known well before Simpson's time: it had been used by Cavalieri (a student of Galileo) in 1639, James Gregory, Johannes Kepler, and others.

3.2.1 Newton-Cotes error estimates

We'll now derive error estimates for general Newton-Cotes methods, and look at the specific cases of the Trapezium and Simpson's rules.

Theorem 3.2.2. *Let*

$$M_{n+1} := \max_{a \leqslant x \leqslant b} |f^{(n+1)}(x)|,$$

and $\pi_{n+1}(x)$ be the usual nodal polynomial. Define

$$\mathcal{E}_n := \big|\int_a^b f(x)dx - Q_n(f)\big|.$$

Then

$$\mathcal{E}_n \leqslant \frac{M_{n+1}}{(n+1)!}\int_a^b |\pi_{n+1}(x)|dx,$$

The proof just comes directly Cauchy's Theorem (Theorem 1.3.3).

Take notes:

Error estimates for the Trapezium Rule

Theorem 3.2.3. *For the Trapezium Rule (3.1)*

$$\mathcal{E}_1 \leqslant \frac{(b-a)^3}{12}M_2. \tag{3.4}$$

The proof is an exercise.

Example 3.2.4. Use (3.4) to get an upper bound on the error for the estimate of $\int_0^{\pi/4} \cos(x)dx$ using the Trapezium rule. How does this compare with the actual error that we found in Example 3.1.2?

Take notes:

Example 3.2.5. If use the Trapezium Rule to estimate the integral of x^2 on the interval $[0, 1]$ we get

$$\int_0^1 x^2 dx = \frac{1}{3} \qquad \text{and} \qquad Q_1(x^2) = \frac{1}{2}(0+1) = \frac{1}{2}.$$

So the error is $1/6$, exactly as the theory predicts.

Error estimates for Simpson's rule

One could also use Theorem 3.2.2 to show that, for Simpson's Rule,

$$\mathcal{E}_2 \leqslant \frac{(b-a)^4}{196}M_3, \tag{3.5}$$

but don't bother because, although correct, it is not *sharp* (that is, it is pessimistic).

Example 3.2.6. Use (3.5) to get an upper bound on the error for the estimate of $\int_0^{\pi/4} \cos(x)dx$ using **Simpson's** rule. How does this compare with the actual error that we found in Theorem 3.2.1?

Take notes:

Example 3.2.7. We expect Simpson's Rule to give *exactly* the right answer for integrals of constant, linear and quadratic functions. If we take $f(x) = x^3$, $a = 0$ and $b = 1$, then formula above suggests that (approx) $\mathcal{E}_2 \leqslant 0.03$. But

Take notes:

3.2.2 Exercises

Exercise 3.3. Deduce the 4-point Newton-Cotes Rule for estimating the integral $\int_0^1 f(x)dx$:

$$Q_3(f) = q_0 f(x_0) + q_1 f(x_1) + q_2 f(x_2) + q_3 f(x_3).$$

Extend the rule to estimate the integral of functions over $[a, b]$.

Exercise 3.4. Prove the error bound given for the Trapezium rule. That is, show that

$$|\int_a^b f(x)dx - Q_1(f)| := \mathcal{E}_1 \leqslant \frac{(b-a)^3}{12} M_2.$$

3.3 Precision and Composition

3.3.1 Precision

We know from Example 3.2.7 that Simpson's Rule applied to approximating $\int_0^1 x^3 dx$ yields exactly the right answer (i.e., the error is zero).

We now claim that Simpson's Rule is exact for *any* polynomial of degree 3 or less.

In class to simplified by taking $a = -1$ and $b = 1$. Here are the **details** for the general case. Denote by $Q_2(f)$ the approximation of $\int_a^b f(x)dx$ with Simpson's Rule:

$$Q_2(f) = \frac{b-a}{6}\Big(f(a) + 4f(\frac{a+b}{2}) + f(b)\Big).$$

Since the method can be derived by integrating the quadratic that interpolates $f(x)$ at the three points a, $(a+b)/2$, and b, it is clearly exact for all quadratics. (We also know this from Theorem 3.2.3).

Let $f(x) = c_0 + c_1x + c_2x^2 + c_3x^3$. Then

$$\int_a^b f(x)dx = \int_a^b (c_0 + c_1x + c_2x^2)dx + c_3\int_a^b x^3dx = \int_a^b (c_0 + c_1x + c_2x^2)dx + c_3\frac{b^4-a^4}{4}.$$

Also,

$$Q_2(f) = Q_2(c_0 + c_1x + c_2x^2) + Q_2(c_3x^3) = \int_a^b (c_0 + c_1x + c_2x^2)dx + c_3(\frac{b-a}{6})\Big(a^3 + 4(\frac{a+b}{2})^3 + b^3\Big). \quad (3.6)$$

With a bit of symbolic manipulation we get that

$$\frac{b^4-a^4}{4} = (\frac{b-a}{6})\Big(a^3 + 4(\frac{a+b}{2})^3 + b^3\Big),$$

as required.

In (3.5) we gave the result of a nïeve attempt to derive an upper bound for the error in Simpson's rule:

$$\mathcal{E}_2 \leqslant \frac{(b-a)^4}{196}M_3.$$

This is not wrong – just not sharp. For example it does not give that Simpson's Rule is exact for all cubics. The sharp result is

Theorem 3.3.1.

$$|E_2(x)| = |\int_a^b f(x)dx - Q_2\big(f(x)\big)| \leqslant \frac{(b-a)^5}{2880}M_4.$$

For the proof see the text book (Theorem 7.2 of [SM03]). Instead of working through it in class we'll prove a more general version of a consequence of Theorem 3.3.1.

Definition 3.3.2 (Precision of a Quadrature Rule)**.** A quadrature rule has *precision* n if it is exact for all polynomials of degree n or less. That is, the rule $Q(f)$ has precision n if

$$Q(p_n) = \int_a^b p_n(x)dx \quad \text{for all } p_n \in \mathcal{P}_n.$$

Example 3.3.3. By construction, the $(n{+}1)$-point Newton-Cotes rule has precision n.

Theorem 3.3.4. *If $Q_{2k}(\cdot)$ is a Newton-Cotes quadrature rule on $2k+1$ points, then $Q_{2k}(\cdot)$ has in fact precision $2k+1$.*

Proof: Let p_{n+1} be a polynomial of degree $n+1$. We wish to show that $Q_n(p_{n+1}) = \int_a^b p_{n+1}(x)dx$. We can take $a = -1$, $b = 1$ because a simple linear transformation can be used to map to an arbitrary interval.

Also, since the quadrature points are equally spaced on $[-1, 1]$ we have that $x_i = -x_{n-i}$.

Furthermore (see Exercise 3.1), the quadrature weights are symmetric: $q_i = q_{n-i}$.

`Take notes`:

3.3.2 Composite Rules

Suppose that we want to estimate $\int_a^b f(x)dx$ and the Trapezium rule is not sufficiently accurate. We could try Simpson's Rule, which should be better. Failing that, we could try a Newton-Cotes rule that uses more points. However, quite apart from the fact that it might be tedious to derive these rules, such schemes are based on poynomial interpolation, and we know (Runge's example again!) that high-order polynomial interpolation can be very inaccurate. See Exercise 3.5

It is better to use a *Composite Rule*. This is analogous to the piecewise polynomial interpolation introduced in Section 2.1. For the Composite Trapezium Rule, as shown in Figure 3.4, we divide $[a, b]$ into N intervals of size $h = (b - a)/N$. Applying the Trapezium Rule on each interval $[x_{i-1}, x_i]$ we get

$$\int_{x_{i-1}}^{x_i} f(x)dx \approx h\frac{f_{i-1} + f_i}{2}.$$

Summing for the n intervals we get

$$\int_a^b f(x)dx \approx \frac{b-a}{N}\Big(\frac{f_0}{2} + f_1 + f_2 + \cdots + f_{N-1} + \frac{f_N}{2}\Big). \quad (3.7)$$

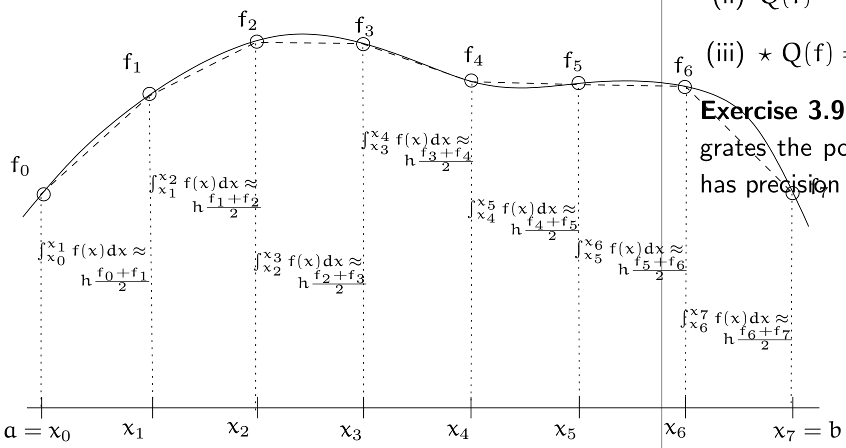

Fig. 3.4: Estimating $\int_a^b f(x)dx$ using the Composite Trapezium Method

3.3.3 Exercises

Exercise 3.5. Explain clearly, with an example, why in general it is not true that $Q_n(f) \to \int_a^b f(x)dx$ as $n \to \infty$.

Exercise 3.6.

(i) Use Theorem 3.2.2 to deduce an error estimate for the Composite Trapezium Rule (3.7).

(ii) Taking $N = 10$, give an upper bound for the error in the Composite Trapezium Rule when approximating $\int_1^2 \ln(x)dx$.

(iii) What value of n would you have to take to ensure that the error was less that 10^{-5}?

Exercise 3.7.

(i) Deduce the formula for the *composite Simpson's Rule*, and use Theorem 3.3.1 to derive an error estimate.

(ii) What value of N would you have to take to ensure that the error in the estimate of $\int_1^2 \ln(x)dx$ is less that 10^{-6}?

(iii) Denote the $(N+1)$-point Composite Simpson's Rule by $S_N(f) \approx \int_a^b f(x)dx$. Show that, for sufficiently smooth $f(x)$,

$$\lim_{n\to\infty} S_N(f) = \int_a^b f(x)dx.$$

Exercise 3.8. Determine the precision of the following schemes for estimating $\int_0^1 f(x)dx$.

(i) $Q(f) = f(\frac{1}{2})$.

(ii) $Q(f) = \frac{1}{4}f(0) + \frac{3}{4}f(\frac{2}{3})$.

(iii) $\star$ $Q(f) = \frac{3}{2}f(\frac{1}{3}) - 2f(\frac{1}{2}) + \frac{3}{2}f(\frac{2}{3})$.

Exercise 3.9. Suppose that a quature rule exactly integrates the polynomials 1, x, x^2, $\ldots$, x^n. Show that it has precision n.

3.4 Gaussian Quadrature

3.4.1 Introduction

To date we have found some numerical schemes that approximate $\int_a^b f(x)dx$ as the weighted average of values of f at $n+1$ equally spaced points. These methods have precision n (or $n+1$ in special cases).

With Gaussian Quadrature [3] **we choose both the quadrature weights and points in such as way as to maximize the precision of the method**. There are three equivalent approaches to doing this.

(i) *Undetermined Coefficients*: The obvious way for, say, $n = 2$. But, unlike Newton-Cotes, we have to solve a system of *nonlinear* equations. Even for $n = 3$ this can become difficult.

(ii) *Base the method on integrating the Hermite Interpolant of the integrand,* f *(see §1.5)*, and choose the points so that the coefficients of $f'(x_i)$ are zero. This approach is the easiest to analyse, but less useful for construction.

(iii) *Finding the zeros of the members of a sequence of orthogonal monic polynomials*. This is the approach we will emphasise most, as it gives us an easy way of proving the precision of the methods.

This section is perhaps the most mathematically rich in the course. I'd encourage you to read further: Chapter 10 of Süli and Mayers [SM03] is devoted to this. However, much of the basic theory is developed in Section 9.4 on Orthogonal Polynomials. See also [S96, Lectures 22 and 23] and [SB92, §3.6].

3.4.2 Undetermined Coefficients

Example 3.4.1. *Find a two point rule*

$$\int_{-1}^{1} f(x)dx \approx G_1(f) := w_0 f(x_0) + w_1 f(x_1),$$

that is exact for all polynomials of degree 3 or less.

This leads a the non-linear system which we must solve

<u>Take notes</u>:

3 

Johann Carl Friedrich Gauß, born 1777 in Braunschweig, died 1855 in Göttingen.

Image source: `http://jeff560.tripod.com/stamps.html`

That is

$$\int_{-1}^{1} f(x)dx \approx G_1(f) := f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right). \qquad (3.8)$$

Example 3.4.2. Let $f(x) = \exp(-x)$. If we estimate $\int_{-1}^{1} f(x)dx$ using each of the Trapezium Rule, Simpson's Rule and the Gaussian Rule above we find the errors are, respectively, 0.735, 0.01165 and 0.00771. Using the composite trapezium rule, we find we would have to take $N = 11$ to obtain an estimate that is more accurate than the two-point Gaussian Rule.

Example 3.4.3. If you use the $G_1(\cdot)$ rule to estimate $\int_0^{\pi/4} \cos(x)dx$ you'll find that

$$\left|\int_0^{\pi/4} \cos(x)dx - G_1(\cos)\right| = \left|\frac{1}{\sqrt{2}} - 0.07070432596\right| \approx 6.35 \times 10^{-5}.$$

Compare with results for the same problem when

- The trapezium rule is used (Theorem 3.1.2).
- Simpson's rule is used (Theorem 3.2.1).

Example 3.4.4. A variation of Gaussian quadrature is *constrained Gaussian quadrature*, also known is the *Gauss-Lobatto method*. Rather than allowing all of the quadrature points to vary in order to maximize the precision of the method, we fix some of them — usually the end points. Use undetermined coefficients to derive the 3-point *Gauss-Lobatto rule*:

$$\int_{-1}^{1} f(x)dx \approx w_0 f(-1) + w_1 f(x_1) + w_2 f(1),$$

where we fixed $x_0 = 0$ and $x_2 = 1$.

<u>Take notes</u>:

3.4.3 Exercises

Exercise 3.10. Use a change of variables, as we did with the Trapezium rule, to show that the rule for approximating $\int_0^1 f(x)dx$ is

$$G_1(f) = \frac{1}{2}\Big(f(\frac{1}{2} - \frac{1}{2\sqrt{3}}) + f(\frac{1}{+}\frac{1}{2\sqrt{3}})\Big).$$

More generally, extend the $G_1(f)$ rule in (3.8) to an arbitrary interval $[a, b]$.

Exercise 3.11. Use $G_1(x)$ to estimate $\int_1^2 \ln(x)dx$. How does this compare with the Trapezium and Simpson's Rule?

Exercise 3.12. Derive a 3-point Gaussian Quadrature Rule to estimate $\int_{-1}^1 f(x)dx$. *Hint:* $x_1 = 0$.

3.5 Orthogonal Polynomials

High order Newton-Cotes methods are of little use because of the problems associated with interpolation be high degree polynomials at equally spaced points. However, high-order Gaussian methods are very useful.

Driving such methods by undetermined coefficients is not practical, however. There is a simpler way, but some mathematical preliminaries are required.

3.5.1 Inner products

Definition 3.5.1 (Vector Space)**.** V is a *vector space* (a.k.a., a *linear space*) over a field F (e.g, the real or complex numbers) if for all $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$ and $a, b \in F$:

(i) $\mathbf{u}+\mathbf{v} \in V$ (closed under addition)

(ii) $\mathbf{u}+\mathbf{v} = \mathbf{v}+\mathbf{u}$ (Commutativity)

(iii) $(\mathbf{u}+\mathbf{v})+\mathbf{w} = \mathbf{u}+(\mathbf{v}+\mathbf{w})$ (Associativity)

(iv) V has a zero vector $\mathbf{0}$ such that $\mathbf{u}+\mathbf{0} = \mathbf{u}$.

(v) $-\mathbf{u} \in V$

(vi) $a\mathbf{u} \in V$

(vii) $a(b\mathbf{u}) = (ab)\mathbf{u}$

(viii) F contains 0 and 1 such that $1\mathbf{u} = \mathbf{u}$, $0\mathbf{u} = \mathbf{0}$.

(ix) $a(\mathbf{u}+\mathbf{v}) = a\mathbf{u}+a\mathbf{v}$, and $(a+b)\mathbf{u} = a\mathbf{u}+b\mathbf{u}$.

Examples:

Definition 3.5.2 (Inner Product)**.** Let V is a real vector space. An **Inner Product** (IP) is a real-valued function $(\cdot,\cdot)$ on $V \times V$ such that, for all $f, g, h \in V$,

(i) $(f+g, h) = (f, h) + (g, h)$,

(ii) $(\lambda f, g) = \lambda(f, g)$, for $\lambda \in \mathbb{R}$.

(iii) $(f, g) = (g, f)$,

(iv) $(f, f) \geqslant 0. \quad (f, f) = 0 \iff f \equiv 0.$

Example 3.5.3. Let $\mathbb{R}^n$ be our vector space, with $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ and $\mathbf{y} = (y_1, y_2, \dots, y_n)^T$. Then

$$(\mathbf{x}, \mathbf{y}) := \sum_{i=1}^{n} x_i y_i,$$

is an inner product.

Example 3.5.4. The set of real-valued functions that are continuous and defined on the ionterval $[a, b]$, denoted $C[a, b]$, is a vector space. And

$$(f, g) := \int_a^b f(x)g(x)dx, \tag{3.9}$$

is an inner product on this space.

We could consider the more general family "weighted" inner products:

$$(f, g) := \int_a^b w(x)f(x)g(x)dx,$$

where $w(x)$ is some positive "weight function." However the IP we will use for the remainder of this chapter is always the one defined in (3.9). That is, we are just concerned with the case $w(x) \equiv 1$.

3.5.2 A Sequence of Orthogonal Monic Polynomials

(Please see [S96, Lecture 23] for more details).

Definition 3.5.5 (Monic Polynomial)**.** A polynomial is *monic* if the coefficient of its leading term is 1.

Example 3.5.6.

<u>`Take notes`</u>:

Definition 3.5.7. Two elements a, b, of a vector space are *orthogonal* with respect to a given inner product $(\cdot,\cdot)$ if $(a, b) = 0$.

Example 3.5.8. <u>`Take notes`</u>:

Example 3.5.9. Take the space of polynomials of degree 2 or less and the IP

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

Let $p(x) \equiv 1$, $q(x) \equiv x$, $r(x) \equiv x^2 - 1/3$, and $f(x) = 3x - 4$, then:
Take notes:

3.5.3 A sequence of orthogonal polynomials

As given in Definition 3.5.5, a polynomial is *monic* if the coefficient of the leading term is 1:

$$p_n = x^n + c_{n-1}x^{n-1} + c_{n-2}x^{n-1} + \cdots + c_1 x + c_0.$$

We'll now look at a sequence of such polynomials $\{\widetilde{p}_0, \widetilde{p}_1, \widetilde{p}_2, \ldots, \widetilde{p}_n, \ldots\}$ that have the property they are orthogonal to each other:

$$(\widetilde{p}_i, \widetilde{p}_j) := \int_a^b \widetilde{p}_i(x)\widetilde{p}_j(x)dx = 0 \quad \text{if } i \neq j.$$

We want to establish some important facts about monic polynomials:

- A set of monic polynomials of degrees 1, 2, ..., n, forms a basis for $\mathcal{P}_n$.
- If the members of that set are orthogonal to each other, then they are orthogonal to *all* polynomials of lower degree.
- We can construct such as set.

Lemma 3.5.10. *Let $\{p_i\}_{i=0}^n$ be a sequence of polynomials where each p_i is monic an* exactly *of degree i. This sequence forms as basis for $\mathcal{P}_n$.*

Proof:
Take notes:

This lemma means that if q is a polynomial of degree n then it can be written uniquely as a linear combination of the p_i:

$$q(x) = \sum_{i=0}^{n} a_i p_i(x),$$

for some unique choice of the real coefficients a_i.

Definition 3.5.11. The sequence $\{\widetilde{p}_i\}_{i=0}^n$ is a sequence of *monic*, *orthogonal* polynomials if each $\widetilde{p}_i$ is monic and *exactly* of degree i and

$$(\widetilde{p}_i, \widetilde{p}_j) = 0 \quad \text{if } i \neq j.$$

Lemma 3.5.12. *If $\widetilde{p}_j \in \{\tilde{p}_i\}_{i=0}^{\infty}$ then $\widetilde{p}_j$ is orthogonal to all polynomials of degree less than j.*

Proof:
Take notes:

3.5.4 Constructing the Sequence

Theorem 3.5.13. *The sequence $\{\tilde{p}_i\}_{i=0}^{\infty}$ exists and can be constructed as follows: Let α and β be defined as*

$$\alpha_{n+1} = \frac{(x\widetilde{p}_n, \widetilde{p}_n)}{(\widetilde{p}_n, \widetilde{p}_n)}, \quad \textit{and} \quad \beta_{n+1} = \frac{(x\widetilde{p}_n, \widetilde{p}_{n-1})}{(\widetilde{p}_{n-1}, \widetilde{p}_{n-1})},$$

then the sequence is given by

$$\widetilde{p}_0(x) \equiv 1, \qquad \widetilde{p}_1(x) = x - \alpha_1$$

and

$$\widetilde{p}_{n+1}(x) = (x - \alpha_{n+1})\widetilde{p}_n(x) - \beta_{n+1}\widetilde{p}_{n-1}(x),$$

for $n \geqslant 1$.

The proof uses *Gram-Schmidt Orthogonalization*.

Take notes:

Example 3.5.14. If we use the inner product $(f, g) := \int_0^1 f(x)g(x)$ then the first 4 polynomials in the sequence are:

Take notes:

Example 3.5.15. The zeros of $\widetilde{p}_2$ are ...

Take notes:

3.5.5 Properties of the sequence

One of the ways of constructing Gaussian Quadrature rule $G_n(\cdot)$ on $n+1$ is to take the quadrature points as the roots of $\widetilde{p}_{n+1}$. We know (from the fundamental theorem of algebra) a polynomial of degree $n+1$ has exactly $n+1$ roots in $\mathbb{C}$ up to multiplicity.

However, the polynomials $\widetilde{p}$ have the special properties, established by the following result.

Lemma 3.5.16. *Let* $\widetilde{p}_i \in \{\tilde{p}_i\}_{i=0}^{\infty} = \{\widetilde{p}_0, \widetilde{p}_1, \dots,\}$ *be the set of monic polynomials that are orthogonal with respect to the (usual) inner product.*

(i) The zeros of each $\widetilde{p}_i \in \{\tilde{p}_i\}_{i=0}^{\infty}$ *are simple (not repeated).*

(ii) All the zeros of $\widetilde{p}_i$ *are real numbers in the interval* $[a, b]$.

(*A slightly different proof of these facts are given in [SM03, Thm 9.4].*

Take notes:

3.5.6 Exercises

Exercise 3.13. Suppose that $(\cdot, \cdot)$ is an inner product. Show that $\|u\| := \sqrt{(u, u)}$ is a norm.

Exercise 3.14. $\mathcal{P}_n$, the space of polynomials of degree (at most) n forms a vector space. Is it true that the space of *monic* polynomials of degree n forms a vector space?

Exercise 3.15. (i) Using the Inner Product

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

find $\widetilde{p}_0(x)$, $\widetilde{p}_1(x)$, $\widetilde{p}_2(x)$ and $\widetilde{p}_3(x)$.

(ii) Find the zeros of $\widetilde{p}_2(x)$ and call them x_0 and x_1. Construct a quadrature rule for $\int_{-1}^{1} f(x)dx$ taking these as the quadrature points, and the weights as the integrals to the corresponding Lagrange polynomials. Verify that this is the same rule as given in (3.8).

(iii) Repeat this exercise using the zeros of $\widetilde{p}_3(x)$ as the quadrature points. Verify that the rule you get is the same as Exercise 3.12.

3.6 Gaussian Quadrature via Orthogonal Polynomials

At the start of this section, we introduced the using Gaussian Quadrature technique for estimating integrals

$$\int_a^b f(x)dx \approx G_n(f) := \sum_{k=0}^{n} w_k f(x_k),$$

where the points x_k and weights w_k are chosen to maximise the precision of the method.

We now have an equivalent way of defining the method, $G_n(\cdot)$, and deriving the coefficients:

(a) Write down the set of monic polynomials $\{\widetilde{p}_0, \widetilde{p}_1, \dots, \widetilde{p}_{n+1}\}$ that is orthogonal with respect to the inner product

$$(u, v) := \int_a^b u(x)v(x)dx.$$

Note that a and b, the limits of integration for the IP, are the same as for the integral we are trying to estimate.

(b) From Theorem 3.5.16, we know that $\widetilde{p}_{n+1}$ has $n+1$ zeros in the interval $[a, b]$. Let these be the quadrature points of the method.[4]

For example, the polynomial $\widetilde{p}_5 = x^5 - (10/9)x^3 + (5/21)x$ is shown in Figure 3.5, with its zeros highlighted.

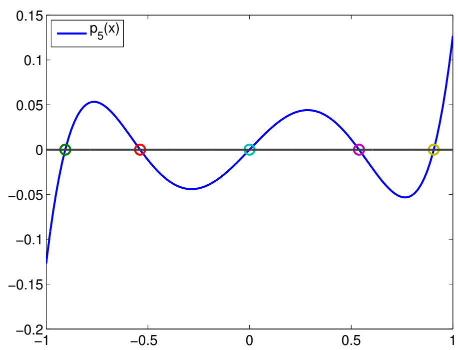

Fig. 3.5: The polynomial $\widetilde{p}_5 = x^5 - (10/9)x^3 + (5/21)x$

(c) Take the quadrature weights to be $w_k = \int_a^b L_k(x)dx$, where the L_k are the usual Lagrange polynomials for this set of points.

The key property of this method in stated in the following theorem.[5]

[4]In practice one would take a simpler IP such as

$$(u, v) = \int_{-1}^{1} u(x)v(x)dx,$$

and then transform the zeros from $[-1, 1]$ to $[a, b]$ using a linear transformation.

[5]In an earlier version of these notes, this was number Theorem 3.6.16

Theorem 3.6.1. *Let $x_0, \dots, x_n$ to be the zeros of $\widetilde{p}_{n+1}$, the $(n+1)$th polynomial in the sequence of orthogonal monic polynomials $\{\tilde{p}_i\}_{i=0}^{\infty}$. Set*

$$G_n(f) = w_0 f(x_0) + \cdots + w_n f(x_n)$$

$$\text{where } w_i = \int_a^b L_i(x)dx. \qquad (3.10)$$

Then $G_n(f)$ has precision $2n+1$.

The proof of this is an exercise.

3.6.1 Error estimates

Our final task associated with numerical integration is to prove that, as $n \to \infty$, so $G_n(f) \to \int_a^b f(x)dx$.

We are not going to do this in full detail, but the key ideas will be presented.

We would like to prove the following error estimate, which is closely related to Theorem 1.5.2 (error in Hermitian interpolation):

Theorem 3.6.2.

$$\int_a^b f(x)dx - G_n(f) = \frac{f^{(2n+2)}(\tau)}{(2n+2)!} \int_a^b \pi_{n+1}(x)^2 dx.$$

The trick here is that we are claiming that Gaussian Quadrature is the same as integrating the Hermite interpolant to f, even though the latter depends on $f'(x_k)$ although the former does not.

Moreover, we would like to show that

$$G_n(f) \to \int_a^b f(x)dx \text{ as } n \to \infty.$$

To do this we need to establish several facts. In each case we make use of Theorem 3.6.1, a consequence of which is that, if f is a polynomial of degree at most $2n-1$, then

$$\int_a^b f(x)dx = \sum_{k=0}^{n} w_k f(x_k).$$

First, recall the basis functions that we use for Hermite Interpolation Section 1.5:

$$H_i(x) = [L_i(x)]^2(1 - 2L_i'(x_i)(x - x_i)),$$

$$K_i(x) = [L_i(x)]^2(x - x_i).$$

<u>`Take notes`</u>:

Now we can deduce Theorem 3.6.2.

Take notes:

Next we want to show that each of the w_k are positive. From (3.10) we have that the Gaussian Quadrature weights are $w_k = \int_a^b L_k(x)dx$ where the L_k are the usual Lagrange Polynomials:

$$L_k(x_j) = \begin{cases} 1 & k = j \\ 0 & k \neq j, \end{cases}$$

associated with the Gaussian interpolation points. Then in fact
Take notes:

and so that the w_k are all positive. It follows directly that $0 < w_k < (b-a)$, for $k = 0, 1, 2, \ldots, n$:
Take notes:

3.6.2 Convergence

Section 10.4 of [SM03] also covers this, though from a different angle. One of the most interesting aspects of this theory is given in Theorem 10.2:

Theorem 3.6.3.

$$\lim_{n\to\infty} G_n(f) = \int_a^b f(x)dx.$$

(*Here we'll just given an out line of the proof. You are not required to know this for the exam*).

The Weierstrass approximation theorem, which we mentioned back in Section 1.6.1, tells us that, for any $\epsilon > 0$, there exists a polynomial p such that $|f(x)-p(x)| \leqslant \epsilon$. Let n be the degree of this polynomial. Let $G_n(\cdot)$ be the $n+1$ point Gaussian Quadrature rule. Then

$$\int_a^b f(x)dx - G_n(f) = \int_a^b f(x) - p(x)dx + \int_a^b p(x)dx - G_n(p) + G_n(p) - G_n(f).$$

But because $G_n(\cdot)$ is exact for polynomials of degree n, $\int_a^b p(x)dx - G_n(p) = 0$. Using this, and the triangle inequality,

$$\left|\int_a^b f(x)dx - G_n(p)\right| \leqslant \left|\int_a^b f(x) - p(x)dx\right| + \left|G_n(p) - G_n(f)\right|.$$

But

$$\left|\int_a^b f(x) - p(x)dx\right| \leqslant \int_a^b \varepsilon dx = \varepsilon(b-a).$$

Also,

$$|G_n(f) - G_n(p)| = |G_n(p-f)| = \Big|\sum_{k=0}^{n} w_k\big(f(x_k) - p(x_k)\big)\Big| = \sum_{k=0}^{n} w_k\big|f(x_k) - p(x_k)\big|,$$

because all the w_i are positive. Then, using that $\sum_k w_k = b-a$ and $|f(x) - p(x)| \leqslant \varepsilon$, we get

$$\big|G_n(f) - G_n(p)\big| \leqslant \varepsilon(b-a).$$

Combining these we have shown that for any ε, one can always find n such that

$$\left|\int_a^b f(x)dx - G_n(p)\right| \leqslant 2\varepsilon(b-a).$$

. . . .

One of the key ingredients to this proof was that the w_i are all positive. That is not the case for Newton-Cotes methods—for large enough n their quadrature weights can be negative—so no similar result is possible.

3.6.3 Exercise

Exercise 3.16. Prove Theorem 3.6.1.

Exercise 3.17. ⋆ Show that it is impossible to choose $n+1$ quadrature points and weights so that the $n+1$-point quadrature rule

$$\int_a^b f(x)dx \approx \sum_{k=0}^{n} w_k f(x_k)$$

has precision $2n+2$.

Hint: To show the method does not have precision $2n+2$*, you just need to give a an example of a single polynomial* p *of degree exactly* $2n+2$ *for which* $\int_a^b p(x)dx \neq \sum_{k=0}^{n} w_k f(x_k)$.