12. Lecture 12

Numerical Integration

We use polynomial interpolation techniques to derive numerical integration schemes to approximate

$$I(f) = \int_\alpha^\beta f(x)\ dx,$$

for $\alpha < \beta$. Let $\{x_0, ..., x_n\} \subset [a, b]$ be distinct, where $a < b$ are such that $[\alpha, \beta] \subseteq [a, b]$. Let $p \in \mathbb{P}^n$ interpolates f at $\{x_0, ..., x_n\}$. We propose to approximate $I(f)$ by

$$Q(f) = \int_\alpha^\beta p(x)\ dx.$$

Using the Lagrange polynomials $\{l_i(x)\}_{i=0}^n$ associated with the interpolations points $\{x_i\}_{i=0}^n$, we write

$$p(x) = \sum_{i=0}^n f(x_i) l_i(x)$$

so that

$$\begin{aligned} Q(f) &= \int_\alpha^\beta \left(\sum_{i=0}^n f(x_i) l_i(x) \right)\ dx = \sum_{i=0}^n f(x_i) \int_\alpha^\beta l_i(x)\ dx \\ &= \sum_{i=0}^n w_i f(x_i), \end{aligned}$$

where we defined

$$w_i := \int_\alpha^\beta l_i(x)\ dx.$$

This leads to the following definition of quadrature.

Definition 12.1 (Quadrature). *An integral approximation of the form*

$$I(f) \approx Q(f) = \sum_{i=0}^n w_i f(x_i)$$

is called a quadrature. *The real numbers $\{w_i\}$ are the weights and $\{x_i\}$ are the nodes.*

Example 12.1 (Rectangle quadrature). *Let $x_0 \in [a, b]$. Find the quadrature approximating*

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

based on polynomial interpolation using x_0 and $\mathbb{P}^0$. In this case, $p(x) = f(x_0) l_0(x) = f(x_0)$ and

$$Q(f) = \int_a^b f(x_0)\ dx = (b - a) f(x_0),$$

which is the area of the shaded region in Figure 4.

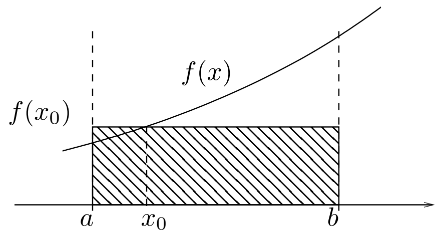

FIGURE 4. Rectangle quadrature. The approximation $Q(f)$ corresponds to the area of the shaded region.

Example 12.2 (Trapezoidal quadrature)**.** *Consider $p \in \mathbb{P}^1$ interpolating f at $x_0 = a$ and $x_1 = b$ to approximate*

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

In that case,

$$p(x) = l_0(x)f(a) + l_1(x)f(b) = \frac{b-x}{b-a}f(a) + \frac{x-a}{b-a}f(b)$$

so that

$$Q(f) = \int_a^b p(x)\ dx = \frac{f(a)}{b-a}\int_a^b (b-x)\ dx + \frac{f(b)}{b-a}\int_a^b (x-a)\ dx.$$

Both integrals equal $\frac{1}{2}(b-a)^2$ so

$$Q(f) = \frac{b-a}{2}\left(f(a) + f(b)\right).$$

See Figure 5 for an illustration.

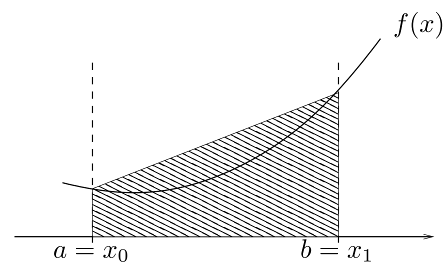

FIGURE 5. Trapezoidal quadrature. The approximation $Q(f)$ corresponds to the area of the shaded region.

Example 12.3 (3 Points Quadrature)**.** *Consider the interpolation nodes $\{x, x-h, x-2h\}$ for some $h > 0$ and $x \in \mathbb{R}$ and use a quadratic polynomial interpolant to derive a quadrature scheme to approximate*

$$I(f) = \int_{x-h}^{x} f(t)\ dt.$$

Note that this will use interpolation points outside the integration region. In Example 11.1, we have already computed the corresponding lagrange polynomials l_0,

l_1 and l_2. To derive such quadrature scheme, we need to compute

$$w_i = \int_{x-h}^{x} l_i(t)\ dt,$$

which seems like a lot of work... perhaps there is a better way (later).

We now discuss how well $Q(f)$ approximate $I(f)$.

Theorem 12.1 (Interpolation error)**.** *Let $f \in C^{(n+1)}[a,b]$, $\{x_0, ..., x_n\}$ distinct in $[a,b]$ and $a \le \alpha < \beta \le b$. If $p \in \mathbb{P}^n$ inteprolates f at x_i, $i = 0, ..., n$, and $Q(f) = \sum_{i=0}^{n} w_i f(x_i)$, with $w_i = \int_\alpha^\beta l_i(x)\ dx$, then we have*

$$I(f) - Q(f) = \frac{1}{(n+1)!} \int_\alpha^\beta f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)\ dx,$$

where for every $x \in [\alpha, \beta]$, $\xi_x \in [a,b]$. Moreover, if $\prod_{i=0}^{n}(x - x_i)$ does not change sign on $[a,b]$, then there exists $\xi \in [a,b]$ with

$$I(f) - Q(f) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_\alpha^\beta \prod_{i=0}^{n} (x - x_i)\ dx.$$

Proof. In view of the interpolation error provided by Theorem 4.1, for $x \in (\alpha, \beta)$ there exists $\xi_x \in (a,b)$ such that

$$I(f) - Q(f) = \int_\alpha^\beta (f(x) - p(x))\ dx = \frac{1}{(n+1)!} \int_\alpha^\beta f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)\ dx.$$

This is the first claim. To continue further, it suffices to note that $f^{(n+1)}(\xi_x)$ is continuous (see Remark 11.1) and invoke the mean value theorem for integrals to write

$$\frac{1}{(n+1)!} \int_\alpha^\beta f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)\ dx = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_\alpha^\beta \prod_{i=0}^{n} (x - x_i)\ dx,$$

for some $\xi \in (a,b)$. This implies the second claim. $\square$

Example 12.4 (Error for the Trapezoidal quadrature)**.** *For some $\xi \in (a,b)$ the above theorem guarantees that*

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

using the fact that $(x-a)(x-b)$ does not change sign. Hence, computing the integral leads to

$$\int_a^b f(x)\ dx - \frac{b-a}{2}\,(f(a) + f(b)) \overset{y=x-a}{=} \frac{f''(\xi)}{2} \int_0^{b-a} y(y-(b-a)\ dy = -\frac{f''(\xi)}{12}(b-a)^3.$$

Example 12.5 (Simpson quadrature)**.** *We want to approximate*

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

using a polynomial of degree 2 interpolating f at $x_0 = -1$, $x_1 = 0$ and $x_2 = 1$. We first compute the lagrange polynomials

$$l_0(x) = \frac{(x-0)(x-1)}{(-1-0)(-1-1)} = \frac{x^2 - x}{2}$$
$$l_1(x) = \frac{(x+1)(x-1)}{(0+1)(0-1)} = 1 - x^2$$
$$l_2(x) = \frac{(x-0)(x+1)}{(1-0)(1+1)} = \frac{x^2 + x}{2}$$

Therefore,

$$w_0 = \int_{-1}^{1} l_0(x)\ dx = \int_{-1}^{1} \frac{1}{2}x^2\ dx = \frac{1}{3}$$
$$w_1 = \int_{-1}^{1} l_1(x)\ dx = \int_{-1}^{1} (1 - x^2)\ dx = \frac{4}{3}$$
$$w_2 = \int_{-1}^{1} l_3(x)\ dx = \int_{-1}^{1} \frac{1}{2}x^2\ dx = \frac{1}{3}.$$

and the quadrature rule reads

$$I(f) \approx Q(f) = \frac{1}{3}f(-1) + \frac{4}{3}f(0) + \frac{1}{3}f(1).$$

However,

$$\prod_{i=0}^{2}(x - x_i) = (x+1)x(x-1) = (x^2 - 1)x$$

changes sign on $[-1, 1]$ so we cannot get a formula involving $f'''(\xi)$ for some (fixed) $\xi \in (-1, 1)$.

We now discuss a possibly simpler way to compute the weights w_i. This relies on the observation that when $f \in \mathbb{P}^n$ is a polynomial of degree n, then its interpolant $p \in \mathbb{P}^n$ is f itself (since interpolant are unique). This means

$$I(f) = \int_a^b f(x)\ dx = \int_a^b p(x)\ dx = Q(f)$$

for all $f \in \mathbb{P}^n$. In other words, the quadrature is *exact* for $p \in \mathbb{P}^n$. In particular, this means that

$$J_0 := \int_a^b 1\ dx = \sum_{i=0}^{n} w_i 1 = Q(1)$$
$$J_1 := \int_a^b x\ dx = \sum_{i=0}^{n} w_i x_i = Q(x)$$
$$\vdots$$
$$J_n := \int_a^b x^n\ dx = \sum_{i=0}^{n} w_i x_i^n = Q(x^n).$$

Hence, the weights $\{w_i\}_{i=0}^n$ satisfy the linear system

$$A^t w := \begin{pmatrix} 1 & 1 & 1 & ... & 1 \\ x_0 & x_1 & x_2 & ... & x_n \\ x_0^2 & x_1^2 & x_2^2 & ... & x_n^2 \\ & & \vdots & & \\ x_0^n & x_1^n & x_2^n & ... & x_n^n \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} J_0 \\ J_1 \\ \vdots \\ J_n \end{pmatrix}.$$

Recall that you get the linear system

$$Aw := \begin{pmatrix} 1 & x_0 & x_0^2 & ... & x_0^n \\ 1 & x_1 & x_1^2 & ... & x_1^n \\ 1 & x_2 & x_2^2 & ... & x_2^n \\ & & \vdots & & \\ 1 & x_n & x_n^2 & ... & x_n^n \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix},$$

when solving the interpolation problem $p(x_i) = y_i$, where

$$p(x) = c_0 + c_1 x + ... c_n x^n.$$

We already know that A is non-singular and it follows that A^t is also non-singular. As a consequence, we realize that

Remark 12.1 (Uniqueness of Weights). The weights w_i making the quadrature Q exact on $\mathbb{P}^n$ are uniquely determined from the exactness conditions

$$Q(x^j) = \sum_{i=0}^n w_i x_i^j = \int_a^b x^j \; dx, \qquad j = 0, ..., n.$$

Example 12.6 (Simpson's quadrature)**.**

$$Q(f) = w_0 f(-1) + w_1 f(0) + w_2 f(1) \approx \int_{-1}^1 f(x) \; dx.$$

The exactness conditions (for $\mathbb{P}^2$) are

$$\begin{aligned} 2 &= \int_{-1}^1 1 \; dx = w_0(1) + w_1(1) + w_2(1) \\ 0 &= \int_{-1}^1 x \; dx = w_0(-1) + w_1(0) + w_2(1) \\ \frac{2}{3} &= \int_{-1}^1 x^2 \; dx = w_0(-1)^2 + w_1(0)^2 + w_2(1)^2, \end{aligned}$$

i.e.

$$w_0 = w_2 = \frac{1}{3} \qquad \textit{and } w_1 = \frac{4}{3}$$

as previously obtained.

Remark 12.2 (Higher order exactness for Simpson). Note that in addition of being exact for any polynomial of degree 2, the Simpson's quadrature rule also satisfy

$$0 = \int_{-1}^1 x^3 \; dx = \frac{1}{3}(-1)^3 + 0 + \frac{1}{3}(1)^3$$

but

$$\frac{2}{5} = \int_{-1}^{1} x^4 \; dx \neq \frac{1}{3}(-1)^4 + 0 + \frac{1}{3}(1)^4 = \frac{2}{3}.$$

Hence, the Simpson's quadrature rule is exact for $\mathbb{P}^3$ but not $\mathbb{P}^4$.

13. Lecture 13

Last lecture introduced the Simpson's rule

$$I(f) := \int_{-1}^{1} f(x)\ dx \approx \frac{1}{3}f(-1) + \frac{4}{3}f(0) + \frac{1}{3}f(1) =: Q(f).$$

We found that Q was exact for cubics.

Consider instead the quadrature scheme based on the nodes $\{x_0, x_1, x_2, x_3\} := \{-1, 0, 1/2, 1\}$, i.e.

$$I(f) \approx Q(f) = \sum_{i=0}^{3} w_i f(x_i).$$

We also saw during the last lecture that there exists a unique set of weights w_i, $i = 0, 1, 2, 3$ making Q exact for cubics (see Remark 12.1). Note that the Simpson's scheme can be interpreted as

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

and hence is the unique scheme. Applying the error formula provided by Theorem 12.1 gives

$$I(f) - Q(f) = \frac{1}{4!}\int_{-1}^{1} f^{(4)}(\xi_x)\prod_{i=0}^{3}(x - x_i)\ dx.$$

The quantity on the right side of the above relation is usually quite large. To get quadrature to approximate integrals, we need *composite schemes*.

Composite Schemes. Suppose you have a scheme

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

exact on $\mathbb{P}^n$, where $\{x_0, ..., x_n\}$ are distinct in $[a, b]$.

We want to deduce from a scheme on $[\alpha, \beta]$. Let λ be the linear mapping taking $[a, b]$ onto $[\alpha, \beta]$, i.e.

$$\lambda(x) = \alpha + \frac{x - a}{b - a}(\beta - \alpha)$$

($\lambda(a) = \alpha$ and $\lambda(b) = \beta$). As we saw in an early homework, if $p \in \mathbb{P}^n$, then so is $q(x) = p(\lambda(x))$. Also,

$$\lambda^{-1}(x) = a_{\frac{t-\alpha}{\beta-\alpha}}(b - a)$$

is a linear mapping from $[\alpha, \beta]$ to $[a, b]$. Now, for $q \in \mathbb{P}^n$

$$\tilde{I}(q) := \int_\alpha^\beta q(t)\ dt = \frac{\beta - \alpha}{b - a}\int_a^b q(\lambda(x))\ dx,$$

where we have used the change of variable $x = \lambda^{-1}(t)$ or $t = \lambda(x)$ so that $\frac{dx}{dt} = \frac{b-a}{\beta-\alpha}$ and $dt = \frac{\beta-\alpha}{b-a}dx$. Since the composition $q \circ \lambda$ is in $\mathbb{P}^n$ and the quadrature scheme is exact on $\mathbb{P}^n$

$$\tilde{I}(q) := \frac{\beta - \alpha}{b - a}\sum_{i=0}^{n} w_i q(\lambda(x_i)).$$

We set

$$\tilde{w}_i = \frac{\beta - \alpha}{b - a}w_i \qquad \text{and} \qquad \tilde{x}_i = \lambda(x_i) \tag{8}$$

to deduce that

$$\int_\alpha^\beta q(t)dt = \sum_{i=0}^n \tilde{w}_i q(\tilde{x}_i) =: \tilde{Q}(q).$$

In conclusion, given a scheme

$$I(f) = \int_a^b f(x)\ dx \approx Q(f) = \sum_{i=0}^n w_i f(x_i)$$

which is exact on $\mathbb{P}^n$, we get a *translated* scheme

$$\tilde{I}(f) = \int_\alpha^\beta f(t)\ dt \approx \tilde{Q}(f) = \sum_{i=0}^n \tilde{w}_i f(\tilde{x}_i)$$

which is also exact on $\mathbb{P}^n$ using the notation (8).

Remark 13.1 (Property of the translated scheme). The map λ is a linear map of $[a,b]$ onto $[\alpha,\beta]$ so it maps points in a proportional way: $a \to \alpha$ and $b \to \beta$ implies $(a+b)/2 \to (\alpha+\beta)/2$. More generally, for any $t \in [0,1]$

$$[a,b] \ni ta + (1-t)b \to t\alpha + (1-t)\beta \in [\alpha,\beta].$$

Composite Quadrature. We want to approximate

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

and introduce $N+1$ distinct points

$$a = x_0 < x_1 < ... < x_N = b$$

and set $h = \max_{i=1,\dots,N}(x_i - x_{i-1})$. Hence, we split the integral over $[a,b]$ onto N pieces

$$I(f) = \sum_{i=1}^N \int_{x_{i-1}}^{x_i} f(x)\ dx$$

and use a base (translated) quadrature scheme over each sub-interval.

13.1. **Simpson's Composite Quadrature Rule.** If we use the Simpson's rule

$$\int_{-1}^1 g(t)\ dt \approx \frac{1}{3}g(-1) + \frac{4}{3}g(0) + \frac{1}{3}g(1)$$

to approximate

$$\int_{x_{i-1}}^{x_i} f(x)\ dx,$$

we have

$$\int_{x_{i-1}}^{x_i} f(x)\ dx \approx \sum_{i=0}^2 \tilde{w}_i f(\tilde{x}_i),$$

where

$$\tilde{w}_2 = \tilde{w}_0 = \frac{x_i - x_{i-1}}{2}\frac{1}{3} \qquad \text{and} \qquad \tilde{w}_1 = \frac{x_i - x_{i-1}}{2}\frac{4}{3}$$

and the nodes are moved proportionally

$$-1 \to x_{i-1}, \qquad 1 \to x_i \qquad \text{and} \qquad 0 \to \frac{x_{i-1}+x_i}{2}.$$

This implies

$$\int_{x_{i-1}}^{x_i} f(x)\ dx \approx \frac{x_i - x_{i-1}}{6}\left(f(x_{i-1}) + 4f(x_{i-1/2}) + f(x_i)\right),$$

where

$$x_{i-1/2} := \frac{x_{i-1} + x_i}{2}.$$

Gathering all the approximations in all subinterval, we arrive at the *composite Simpson's rule* approximation

$$\int_a^b f(x)\ dx \approx \sum_{i=1}^{N} \frac{x_i - x_{i-1}}{6}\left(f(x_{i-1}) + 4f(x_{i-1/2}) + f(x_i)\right) =: \sum_{i=1}^{N} \tilde{Q}_i(f).$$

Regarding the integration error, the Simpson's rule is the rule based on $\{-1, 0, 1/2, 1\}$, which is exact for cubics. Since $\frac{1}{2} = \frac{3}{4}(1) + \frac{1}{4}(-1)$, the translated rule is the rule on

$$\{x_{i-1}, \frac{1}{2}(x_{i-1} + x_i), \frac{3}{4}x_i + \frac{1}{4}x_{i-1}, x_i\} := \{\tilde{x}_0, \tilde{x}_1, \tilde{x}_2, \tilde{x}_3\},$$

which is exact on cubics. The error formula (Theorem 12.1) gives

$$\int_{x_{i-1}}^{x_i} f(x)\ dx - \tilde{Q}_i(f) = \frac{1}{24}\int_{x_{i-1}}^{x_i} f^{(4)}(\xi_x)\prod_{j=0}^{3}(x - \tilde{x}_j)\ dx,$$

provided that $f \in C^4[a, b]$. Let $\|f^{(4)}\|_\infty = \max_{t\in[a,b]} |f^{(4)}(t)|$, then

$$\left|\int_{x_{i-1}}^{x_i} f(x)\ dx - \tilde{Q}(f)\right| \leq \frac{1}{24}\|f^{(4)}\|_\infty h^4 \int_{x_{i-1}}^{x_i} dx$$

(since $|x - \tilde{x}_i| \leq h$ as $x, \tilde{x}_j \in [x_{i-1}, x_i]$). Therefore, we obtain that

$$\left|\int_{x_{i-1}}^{x_i} f(x)\ dx - \tilde{Q}(f)\right| \leq \frac{1}{24}\|f^{(4)}\|_\infty h^4 (x_i - x_{i-1}).$$

Summing over all subintervals gives an estimate for the error

$$\left|\int_a^b f(x)\ dx - \sum_{i=1}^{N}\tilde{Q}_i(f)\right| \leq \sum_{i=1}^{N}\left|\int_{x_{i-1}}^{x_i} f(x)\ dx - \tilde{Q}_i(f)\right| \leq \frac{b-a}{24}\|f^{(4)}\|_\infty h^4.$$

In general, a quadrature rule which is exact on $\mathbb{P}^n$ translated to an interval of size h has a local accuracy of h^{n+2} and usually results in a global accuracy of h^{n+1} when used in a composite quadrature.

14. Lecture 14

Gaussian Quadrature. We noted last lecture that the order of a quadrature is determined by exactness on $\mathbb{P}^n$. It is natural to optimize the order by allowing the nodes to move.

We start with examples.

Example 14.1 (One point).

$$I(f) = \int_a^b f(x)\ dx \approx (b-a)f(x_i).$$

Note that the weight $(b-a)$ makes the quadrature exact on constants. For the quadrature to be exact on linears, we need that

$$\frac{b^2-a^2}{2} = \int_a^b x\ dx = (b-x)x_i,$$

or

$$x_i = \frac{b+a}{2},$$

which implies that

$$Q(f) = (b-a)f\left(\frac{b+a}{2}\right).$$

This is called the mid-point rule. *It is exact for linears but not quadratics since*

$$\frac{b^3-a^3}{3} = \int_a^b x^2 \neq (b-a)\left(\frac{a+b}{2}\right)^2.$$

Example 14.2 (Two points formula). *The two-points formula has 4 unknowns (2 weights and 2 interpolation points). We show that we can determine these unknowns for the quadrature to be exact on cubics. For this, the following* 4 *exactness conditions (see Remark 12.1)*

$$\begin{aligned}
2 &= \int_{-1}^{1} dx = w_1 + w_2 \\
0 &= \int_{-1}^{1} x\ dx = w_1x_1 + w_2x_2 \\
\frac{2}{3} &= \int_{-1}^{1} x^2\ dx = w_1x_1^2 + w_2x_2^2 \\
0 &= \int_{-1}^{1} x^3\ dx = w_1x_1^3 + w_2x_2^3.
\end{aligned}$$

From the second condition, we deduce that $w_1x_1 = -w_2x_2$. This into the 4*th condition yield*

$$0 = w_2x_2(x_1^2 - x_2^2).$$

Note that $w_1 \neq 0$, for otherwise it would be a one-point rule which cannot be exact for cubics, and $x_2 \neq 0$ for otherwise the second condition would imply that $x_1 = x_2 = 0$ and the interpolation points would not be distinct. Therefore, we must have $x_1^2 = x_2^2$, i.e.

$$x_1 = -x_2$$

(again, we want distinct interpolation points). Using the second constraint again, this implies that $w_2 x_1 - w_2 x_1 = 0$ *or*

$$w_1 = w_2.$$

Now the second and fourth constraints hold. The first condition requires

$$w_1 + w_2 = 2 \qquad \Longrightarrow \qquad w_1 = w_2 = 1.$$

Finally, the third condition implies

$$\frac{2}{3} = 2w_1 x_1^2 \qquad or \qquad x_1 = \pm\sqrt{\frac{1}{3}}.$$

Finally, the scheme is

$$\int_{-1}^{1} f(x)\ dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) := Q(f)$$

and is exact on cubics. It is not exact on quartics since

$$\frac{2}{5} = \int_{-1}^{1} x^4\ dx \neq Q(x^4) = \frac{1}{9} + \frac{1}{9}.$$

Example 14.3 (Three points)**.** *Can we make a three points quadrature rule exact on* $\mathbb{P}^5$*? Here the unknowns are* $\{w_i, x_i\}_{i=0}^2$*. Assume the scheme is* symmetric *about the origin, i.e.*

$$Q(f) = w_1 f(-x_1) + w_0 f(0) + w_1 f(x_1).$$

Notice that the symmetry implies that for all odd degree conditions:

$$0 = \int_{-1}^{1} x^{2j+1}\ dx = -w_1 x_1^{2j+1} + w_0 0 + w_1 x_1^{2j+1} = Q(x^{2j+1}), \qquad j \geq 0.$$

We now check the even degree conditions:

$$\begin{aligned} 2 &= \int_{-1}^{1} 1\ dx \stackrel{?}{=} 2w_1 + w_0 \\ \frac{2}{3} &= \int_{-1}^{1} x^2\ dx \stackrel{?}{=} 2w_1 x_1^2 \\ \frac{2}{5} &= \int_{-1}^{1} x^4\ dx \stackrel{?}{=} 2w_1 x_1^4. \end{aligned}$$

Divide the third relation by the second to get

$$\frac{3}{5} = x_1^2 \qquad \Longrightarrow \qquad x_1 = \sqrt{\frac{3}{5}}.$$

From the second relation we compute w_1*:*

$$\frac{1}{3} = w_1 \frac{3}{5} \qquad \Longrightarrow \qquad w_1 = \frac{5}{9}.$$

This in the first constraint implies that

$$\frac{10}{9} + w_0 = 2 \qquad \Longrightarrow \qquad w_0 = \frac{8}{9}$$

and the scheme reads

$$Q(f) = \frac{5}{9} f(-\sqrt{3/5}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{3/5}).$$

This scheme is exact on $\mathbb{P}^5$ *but not on* $\mathbb{P}^6$*.*

Definition 14.1 (Gaussian Quadrature). *A quadrature involving n points, which is exact on* $\mathbb{P}^{2n+1}$ *is called a* Gaussian quadrature.

Generalization: Weighted Gaussian Quadrature. Given a non-negative weight functions $w(x)$ only vanishing at a discrete set of points, we want to derive Gaussian quadrature schemes such that

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

Notice that the assumption on the weight function implies that when $[\alpha, \beta] \subseteq [a, b]$ with $\alpha < \beta$ then

$$\int_\alpha^\beta w(x)\ dx > 0.$$

We define

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

The mapping $\langle ., .\rangle_w$ provides an inner product on $C[a, b]$, i.e.

(1) $\langle ., .\rangle_w$ is bilinear, i.e.

$$\langle \alpha f + \beta g, h\rangle_w = \alpha\langle f, h\rangle_w + \beta\langle f, h\rangle_w,$$

and

$$\langle h, \alpha f + \beta g\rangle_w = \alpha\langle h, f\rangle_w + \beta\langle h, g\rangle_w,$$

for $f, g, h \in C[a, b]$ and $\alpha, \beta \in \mathbb{R}$.

(2) $\langle ., .\rangle_w$ is symmetric, i.e.

$$\langle f, g\rangle_w = \langle f, g\rangle_w, \qquad f, gC^[a, b].$$

(3) $\langle ., .\rangle_w$ is positive definite, i.e.

$$\langle f, f\rangle_w \geq 0, \qquad f \in C[a, b]$$

and equals 0 only if f is the zero function, i.e. $f(x) = 0$.

The above three properties implies that

$$\|f\|_w := (\langle f, f\rangle_w)^{1/2}$$

is a norm on $C[a, b]$ and

$$|\langle f, g\rangle_w| \leq \|f\|_w\|g\|_w$$

(Cauchy-Schwartz inequality).

Definition 14.2 (w-orthogonality). *We say that* f *is* $w-$orthogonal *to* $\mathbb{P}^k$ *is*

$$\langle f, p\rangle_w = 0 \qquad \textit{for all} \quad p \in \mathbb{P}^k.$$

Theorem 14.1 (Gaussian Quadrature). *Suppose there is a nonzero* $q_{k+1} \in \mathbb{P}^{k+1}$ *which is* $w-$*orthogonal to* $\mathbb{P}^k$*. If* q_{k+1} *has* $k+1$ *distinct roots* $\{x_0, ..., x_k\}$*, then quadrature based on the nodes* $\{x_0, ..., x_k\}$ *approximating*

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

which is exact on $\mathbb{P}^k$ *is in fact exact on* $\mathbb{P}^{2k+1}$*, i.e. a Gaussian quadrature.*

Note that the quadrature Q is exact on $\mathbb{P}^k$ (or $\mathbb{P}^{2k+1}$) means that

$$I(p) = \int_a^b w(x)p(x)\ dx = Q(p)$$

for every $p \in \mathbb{P}^k$ (or $\mathbb{P}^k$). As in the case $w(x) = 1$, the exactness conditions uniquely determine the quadrature weights.

We postpone the proof of this theorem for later. For now, we make the following remark.

Remark 14.1 (Leading Coefficient of $w-$orthogonal polynomial). If $q_{k+1} \in \mathbb{P}^{k+1}$ is $w-$orthogonal to $\mathbb{P}^k$ and nonzero then

$$q_{k+1}(x) = a_{k+1}x^{k+1} + a_k x^k + ... + a_0$$

and $a_{k+1} \neq 0$. Indeed, if $a_{k+1} = 0$ then $q_{k+1} \in \mathbb{P}^k$ and

$$0 = \langle q_{k+1}, q_{k+1} \rangle_w = \int_a^b w(x) q_{k+1}^2(x)\ dx,$$

which implies that $q_{k+1} = 0$ and contradicts our assumption. Moreover, since we are only interested in the roots of q_{k+1}, we may assume that q_{k+1} is monic, i.e. $a_{k+1} = 1$ and

$$q_{k+1}(x) = x^{k+1} + a_k x^k + ... + a_0.$$

Example 14.4 ($k = 1$ and $w(x) = 1$). *Find a monic $q \in \mathbb{P}^2$ with*

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

We are looking for α and β such that

$$0 = \langle q, 1 \rangle_w = \int_{-1}^1 (x^2 + \alpha x + \beta)\ dx = \frac{2}{3} + \alpha 0 + 2\beta,$$

i.e. $2\beta = -\frac{2}{3}$ or $\beta = -\frac{1}{3}$. In addition, we want

$$0 = \langle q, x \rangle_w = \int_{-1}^1 (x^3 + \alpha x^2 + \beta x)\ dx = \frac{2}{3}\alpha,$$

and so $\alpha = 0$. This implies that the desired polynomial is

$$q(x) = x^3 - \frac{1}{3},$$

which has two roots, namely

$$\pm\frac{1}{\sqrt{3}}.$$

There are the quadrature nodes derived in Example 14.2.

Example 14.5 ($k = 2$ and $w(x) = 1$). *Find $q \in \mathbb{P}^3$,*

$$q(x) = x^3 + \alpha x^2 + \beta x + \gamma,$$

which is $w-$*orthogonal to* $\mathbb{P}^2$ *with* $w(x) = 1$. *The desired polynomial must satisfy the following 3 constraints*

$$\begin{aligned} \alpha\frac{2}{3} + 2\gamma &= \langle q, 1\rangle_w = 0 \\ \frac{2}{5} + \frac{2}{3}\beta &= \langle q, x\rangle_w = 0 \\ \alpha\frac{2}{5} + \frac{2}{3}\gamma &= \langle q, x^2\rangle_w = 0. \end{aligned}$$

The first and last constraints hold only if

$$A := \begin{pmatrix} \frac{2}{3} & 2 \\ \frac{2}{5} & \frac{2}{3} \end{pmatrix} \begin{pmatrix} \alpha \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Note that $\det(A) = \frac{4}{9} - \frac{4}{5} \neq 0$, *so the only solution is* $\alpha = \gamma = 0$. *From the second constraint, we find that*

$$\frac{1}{5} + \frac{\beta}{3} = 0 \qquad \Longrightarrow \qquad \beta = -\frac{3}{5}.$$

The desired polynomial reads

$$q(x) = x^3 - \frac{3}{5}x = (x^2 - \frac{3}{5})x$$

and has roots $-\sqrt{3/5}$, 0, $\sqrt{3/5}$.

15. Lecture 15

We start with the proof of the quadrature theorem (Theorem 14.1).

Proof of Theorem 14.1. Let $\{x_0, .., x_k\}$ be distinct roots of q_{k+1} and let Q be the associated exact quadrature scheme exact on $\mathbb{P}^k$. The latter is assumed to be non zero, belongs to $\mathbb{P}^{k+1}$ and is $w-$orthogonal to $\mathbb{P}^k$. Let $p \in \mathbb{P}^{2k+1}$ and factor (using polynomial division with reminder)

$$p = qs + r,$$

with $r, s \in \mathbb{P}^k$. Then,

$$I(p) = \int_a^b w(x)p(x)\ dx = \underbrace{\int_a^b w(x)q(x)s(x)\ dx}_{=0} + \int_a^b w(x)r(x)\ dx$$

using the fact that q is $w-$orthogonal to $\mathbb{P}^k$ and $s \in \mathbb{P}^k$. Now, since Q is exact on $\mathbb{P}^k$, then

$$I(p) = \sum_{j=0}^{k} w_j r(x_j).$$

Moreover, the nodes $\{x_0, ..., x_k\}$ are the roots of p, so that computing further

$$I(p) = \sum_{j=0}^{k} w_j r(x_j) = \sum_{j=0}^{k} w_j \left(\underbrace{q(x_j)}_{=0} s(x_j) + r(x_j) \right) = Q(p),$$

which proves the quadrature is exact on $\mathbb{P}^{2k+1}$. □

Lemma 15.1 (Roots of $w-$orthogonal polynomial)**.** *If $q \in \mathbb{P}^{k+1}$ is non zero and is $w-$orthogonal to $\mathbb{P}^k$, then all of the roots of q are distinct and in (a, b).*

Proof. We will see in the next lemma (Lemma 15.2) that q as real coefficients. If q does not have any root in (a, b) then $q > 0$ or $q < 0$ in (a, b) and so

$$\int_a^b w(x)q(x)\ dx > 0 \qquad \text{and} \qquad \int_a^b w(x)q(x)\ dx < 0,$$

either contradicting the $w-$orthogonality of q in $\mathbb{P}^0 \subset \mathbb{P}^k$.

Suppose now that q has $1 \leq l < k+1$ roots in (a, b), denoted y_1, y_2, ..., y_l (repeated according to their multiplicity), and set

$$r(x) = \prod_{y_j \text{ root of odd multiplicity}} (x - y_j).$$

As the polynomial q changes sign across a root of odd multiplicity (as does $r(x)$), the product $q(x)r(x)$ has the same sign except for $x = y_j$, where y_j is a root of odd multiplicity. This implies that

$$\int_a^b w(x)q(x)r(x)\ dx \neq 0.$$

As $r \in \mathbb{P}^k$, this is a contradiction with the $w-$orthogonality in $\mathbb{P}^k$. As a consequence, there must be $k+1$ roots of q in (a, b) and so they must be distinct for the resulting r to belongs to $\mathbb{P}^{k+1}$. □

Lemma 15.2 (Real coefficients)**.** *There is a unique monic real polynomial $q \in \mathbb{P}^{k+1}$, which is $w-$orthogonal to $\mathbb{P}^k$.*

Proof. Let $q = x^{k+1} + \alpha_k x^k + ... + \alpha_0$. Then q is a $w-$orthogonal to $\mathbb{P}^k$ if and only if

$$\langle q, x^j \rangle_w = 0, \qquad j = 0, ..., k,$$

i.e.

$$\langle x^{k+1}, x^j \rangle_w + \sum_{l=0}^{k} \alpha_l \langle x^l, x^j \rangle_w = 0, \qquad j = 0, ..., k.$$

This is equivalent to

$$A \begin{pmatrix} \alpha_0 \\ ... \\ \alpha_k \end{pmatrix} = F,$$

where the coefficients of the matrix A are given by

$$A_{j,l} = \langle x^l, x^j \rangle_w \qquad j, l = 0, ..., k$$

and

$$F_j = -\langle x^{k+1}, x^j \rangle_w, \qquad j = 0, ..., k.$$

Suppose that $A\beta = 0$ for some $\beta \in \mathbb{R}^{k+1}$. Set

$$r(x) = \beta_k x^k + \beta_{k-1} x^{k-1} + ... + \beta_0.$$

The jth equation of $A\beta = 0$ is

$$0 = \sum_{l=0}^{k} A_{j,l}\beta_l = \sum_{l=0}^{k} \langle x^l, x^j \rangle_w \beta_l = \sum_{l=0}^{k} \langle \beta_l x^l, x^j \rangle_w = \langle r(x), x^j \rangle_w, \quad j = 0, 1, ..., k,$$

i.e. $r(x)$ is $w-$orthogonal to $\mathbb{P}^k$. As $r \in \mathbb{P}^k$

$$0 = \langle r(x), r(x) \rangle_w \qquad \Longrightarrow \qquad r(x) = 0, \quad \text{i.e.} \quad \beta = 0.$$

This proves that A is nonsingular. As A is real valued, so is A^{-1}. (For instance, the inverse can be computed by row reducing $(A : I) \to (I : A^{-1})$.) $\square$

Every weighted quadrature problem gives rise to a sequence of orthogonal polynomial. The sequence follows a 3 term recurrence.

Start with $\tilde{p}_0 = 1 \in \mathbb{P}^0$ (nothing to be orthogonal to). Then $\tilde{p}_1 \in \mathbb{P}^1$ must be orthogonal to 1. If $\tilde{p}_1(x) = x + \alpha$ then α must satisfy

$$0 = \langle x + \alpha, 1 \rangle_w, \qquad \text{or} \qquad \alpha = -\langle x, 1 \rangle_w.$$

Suppose we have computed $\tilde{p}_{j-1}$ and $\tilde{p}_j$. Write

$$\tilde{p}_{j+1} = (x + \alpha)\tilde{p}_j + \beta \tilde{p}_{j-1}.$$

Then for $\theta \in \mathbb{P}^{j-2}$

$$\langle \tilde{p}_{j+1}, \theta \rangle_w = \langle (x + \alpha)\tilde{p}_j, \theta \rangle_w + \beta \underbrace{\langle \tilde{p}_{j-1}, \theta \rangle_w}_{=0} = \underbrace{\langle \tilde{p}_j, (x + \alpha)\theta \rangle_w}_{=0} = 0.$$

We also need

$$0 = \langle \tilde{p}_{j+1}, \tilde{p}_{j-1} \rangle_w = \langle (x + \alpha)\tilde{p}_j, \tilde{p}_{j-1} \rangle_w + \beta \langle \tilde{p}_{j-1}, \tilde{p}_{j-1} \rangle_w.$$

The α term goes away so

$$\beta = -\frac{\langle x\tilde{p}_j, \tilde{p}_{j-1} \rangle_w}{\langle \tilde{p}_{j-1}, \tilde{p}_{j-1} \rangle_w}.$$

Also

$$0 = \langle \tilde{p}_{j+1}, \tilde{p}_j \rangle_w = \langle (x+\alpha)\tilde{p}_j, \tilde{p}_j \rangle_w + \beta \underbrace{\langle \tilde{p}_{j-1}, \tilde{p}_j \rangle_w}_{=0},$$

and so we find

$$\alpha = -\frac{\langle x\tilde{p}_j, \tilde{p}_j \rangle_w}{\langle \tilde{p}_j, \tilde{p}_j \rangle_w}.$$

The values of α and β determines $\tilde{p}_{j+1}$. Note that the orthogonal polynomials always satisfy 3 term recurrence relations!

Rodrigues Formula for Legendre Polynomials.

Example 15.1. *$w(x) = 1$, $a = -1$, $b = 1$] Consider the approximation $I(f) = \int_{-1}^{1} f(x)\, dx$.. Then*

$$\tilde{p}_n(x) = \frac{1}{(2n)(2n-1)\cdot \ldots \cdot (n+1)} \frac{d^n}{dx^n}[(x^2-1)^n].$$

To see this, we check that it is a monic polynomial of degree n and $w-$orthogonal to $\mathbb{P}^{n-1}$. We leave the first part as an exercise (Exercise 15.1). Now, if $p \in \mathbb{P}^{n-1}$

$$\int_{-1}^{1} \frac{d^n}{dx^n}[(x^2-1)^n] p(x)\, dx = \underbrace{\frac{d^n}{dx^n}[(x^2-1)^n]\Big|_{-1}^{1}}_{=0} - \int_{-1}^{1} \frac{d^{n-1}}{dx^{n-1}}[(x^2-1)^n] p'(x)\, dx.$$

Repeating this by moving all derivatives over to p, we arrive at

$$\int_{-1}^{1} \frac{d^n}{dx^n}[(x^2-1)^n] p(x)\, dx = (-1)^n \int_{-1}^{1} (x^2-1)^n \underbrace{p^{(n)}(x)}_{=0}\, dx = 0$$

because $p \in \mathbb{P}^{n-1}$.

Definition 15.1 (Legendre Polynomials)**.** *The polynomial*

$$\frac{1}{2^n n!} \frac{d^n}{dx^n}[(x^2-1)^n].$$

is called the Legendre polynomial (different normalization) and satisfies

$$(n+1)p_{n+1}(x) = (2n+1)xp_n(x) - np_n(x).$$

Exercise 15.1. *Show that*

$$\tilde{p}_n(x) = \frac{1}{(2n)(2n-1)\cdot \ldots \cdot (n+1)} \frac{d^n}{dx^n}[(x^2-1)^n]$$

is a polynomial of degree n and is monic (i.e. the leading coefficient is 1).

Rodrigues Formula for Chebyshev Polynomials.

Example 15.2 (Chebyshev polynomials)**.** *We recall that the Chebyshev are given by*

$$T_n(x) = \cos(n \cos^{-1}(x)).$$

Note that for $n \neq j$

$$\int_0^{\pi} \cos(n\theta)\cos(j\theta)\, d\theta = 0.$$

We leave the above claim as exercise.

Set $\theta = \cos^{-1}(x)$*, then* $x = \cos(\theta)$ *and*

$$dx = -\sin(\theta)d\theta = -\sqrt{1-\cos^2(\theta)}\ d\theta = -\sqrt{1-x^2}\ d\theta.$$

Using the orthogonality above

$$\begin{aligned} 0 = \int_0^{\pi} \cos(n\theta)\cos(j\theta)\ d\theta &= \int_{-1}^{1} \cos(n\cos^{-1}(x))\cos(j\cos^{-1}(x))\frac{dx}{\sqrt{1-x^2}} \\ &= \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} T_n(x)T_j(x)\ dx, \end{aligned}$$

i.e. the Chebyshev polynomial T_n *are orthogonal polynomials on* $-1, 1$ *with weights* $w(x) = \frac{1}{\sqrt{1-x^2}}$ *and satisfy the recurrence*

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

as we have seen already in Section 5.1.

16. Lecture 16

We saw last lecture that the Chebyshev polynomials are orthogonal with respect to the scalar product

$$\langle f, g\rangle_w = \int_{-1}^{1} \underbrace{\frac{1}{\sqrt{1-x^2}}}_{=:w(x)} f(x)g(x)\ dx,$$

i.e. T_{n+1} satisfies $T_{n+1} \in \mathbb{P}^{n+1}$ and

$$\langle T_{n+1}, T_j\rangle_w = 0, \qquad 0 \le j \le m.$$

As $\{T_j\}_{j=0}^{n}$ is a basis for $\mathbb{P}^n$, T_{n+1} is $w-$orthogonal to $\mathbb{P}^n$.

The Rodrigues formula for the Chebyshev polynomials reads

$$\tilde{T}_n = w(x)\frac{d^n}{dx^n}\left(w(x)(1-x^2)^n\right) = \frac{1}{(1-x^2)^{1/2}}\frac{d^n}{dx^n}\left((1-x^2)^{n-1/2}\right)$$

using the definition of the weight $w(x) = (1-x^2)^{-1/2}$. Note that

$$\frac{d^n}{dx^n}(fg) = \sum_{j=0}^{n}\binom{n}{j} f^{(j)}g^{(n-j)}$$

(you can prove this by induction). Therefore,

$$\begin{aligned}
\tilde{T}_n(x) &= \frac{1}{(1-x^2)^{1/2}}\frac{d^n}{dx^n}\left((1-x)^{n-1/2}(1+x)^{n-1/2}\right)\\
&= \frac{1}{(1-x^2)^{1/2}}\sum_{j=0}^{n}\binom{n}{j} c_{j,n}(1-x)^{n-j-1/2}(1+x)^{j-1/2}\\
&= \sum_{j=0}^{n}\binom{n}{j} c_{j,n}(1-x)^{n-j}(1+x)^{j}.
\end{aligned}$$

This proves that $\tilde{T}_n \in \mathbb{P}^n$. We now check that it is $w-$orthogonal. We use integration by parts again:

$$\begin{aligned}
I &:= \int_{-1}^{1}(1-x^2)^{-1/2}\tilde{T}_n(x)p(x)\ dx\\
&= \int_{-1}^{1}\frac{d^n}{dx^n}\left((1-x^2)^{-1/2}(1-x^2)^n\right)p(x)\ dx\\
&= p(x)\frac{d^{n-1}}{dx^{n-1}}\left((1-x)^{n-1/2}(1+x)^{n-1/2}\right)\Big|_{x=-1}^{x=1} - \int_{-1}^{1}\frac{d^{n-1}}{dx^{n-1}}\left((1-x^2)^{-1/2}(1-x^2)^n\right)p'(x)\ dx\\
&= -\sum_{j=0}^{n-1}\binom{n-1}{j} c_{n-1,j}(1-x)^{n-j-1/2}(1+x)^{j+1-1/2}.
\end{aligned}$$

Note that all terms evaluated at either $x=-1$ or $x=1$ are zero because the have positive powers of $(1-x)$ and $(1+x)$. Repeating the argument gives

$$I = (-1)^n\int_{-1}^{1}(1-x^2)^{-1/2}(1-x^2)^n p^{(n)}(x)\ dx = 0$$

for $p \in \mathbb{P}^{n-1}$. Since, T_n and $\tilde{T}_n$ differ at most by a normalization constant, T_n is also a polynomial of degree n, $w-$orthogonal to $\mathbb{P}^{n-1}$.