Online Lecture Notes

Prof. Boris Houska

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1 Numerical Integration

The goal of this lecture is to develop numerical integration schemes. The main idea is to start with an interpolation formala in order to approximate the given function f with a polynomial p, such that

$$f \approx p \qquad \Longrightarrow \qquad \int_a^b f(x)\,\mathrm{d}x \;\approx\; \int_a^b p(x)\,\mathrm{d}x \; .$$

Since the polynomial can be integrated explicitly (see the formula on the slides), this should yield an explicit numerical integration formula.

1.1 Derivation via Lagrange interpolation

Let $x_0, x_1, \ldots, x_n \in [a,b]$ be given interpolation points. Recall that the corresponding Lagrange polynomials are given by

$$\forall i \in \{0,1,\ldots,n\}, \qquad L_i(x) \;=\; \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \; .$$

The main reason why these Lagrange polynomials are useful is that they satisfy

$$L_i(x_j) = \delta_{i,j} = \left\{ \begin{array}{ll} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{array} \right. \; . \tag{1}$$

This means that the corresponding interpolation polynomial of a given function f has the form

$$p(x) = \sum_{i=0}^{n} f(x_i) L_i(x) \qquad \text{such that} \qquad p(x_j) = \sum_{i=0}^{n} f(x_i) L_i(x_j) \overset{(1)}{=} f(x_j) \; .$$

The next question is: What does this mean in terms of approximating the integral of f? Let us substitute the above polynomial directly in the integral approximation. This yields

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \int_a^b p(x)\,\mathrm{d}x \;=\; \int_a^b \sum_{i=0}^{n} f(x_i) L_i(x)\,\mathrm{d}x \;=\; \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\,\mathrm{d}x$$

Now, this means that we can precompute the terms

$$\int_a^b L_i(x)\,\mathrm{d}x$$

without know the function f in advance. BUT: these coefficients still depend on the choice of the interpolation points as well as on the integration inteval parameters a and b. Thus, in order two write this integration into an even more general / more practical form, it is helful to introduce a change of variables. One way to do is to start with the so-called closed Newton-Cotes interpolation points:

$$x_0 = a, \quad x_1 = a + H, \quad x_2 = a + 2H, \quad \ldots, \quad x_n = b$$

with equidistant grid constant $H = \frac{b-a}{n}$. Here, we have

$$x_i = a + iH \; . \tag{2}$$

This motivates to introduce a change of variables of the form

$$x = a + tH \qquad \text{with} \qquad t \in [0, n] \; .$$

Let us substitute this change of variables in our coefficient integral:

$$\int_a^b L_i(x)\,\mathrm{d}x = \int_0^n L_i(a+tH)\,H\,\mathrm{d}t \qquad \text{since} \qquad \frac{\mathrm{d}x}{\mathrm{d}t} = H \; .$$

We can make this even more explicit by substituting the epxlicit expression for the Lagrange basis polynomials:

$$\int_a^b L_i(x)\,\mathrm{d}x \quad = \quad \int_0^n L_i(a+tH)\,H\,\mathrm{d}t \tag{3}$$

$$= \quad \int_0^n \left(\prod_{j\neq i} \frac{a + tH - x_j}{x_i - x_j} \right) H\,\mathrm{d}t \tag{4}$$

$$\stackrel{(2)}{=} \quad \int_0^n \left(\prod_{j\neq i} \frac{a + tH - (a+jH)}{(a+iH) - (a+jH)} \right) H\,\mathrm{d}t \tag{5}$$

$$\stackrel{(2)}{=} \quad \int_0^n \left(\prod_{j\neq i} \frac{tH - jH}{iH - jH} \right) H\,\mathrm{d}t \tag{6}$$

$$\stackrel{(2)}{=} \quad H \underbrace{\int_0^n \left(\prod_{j\neq i} \frac{t - j}{i - j} \right) \mathrm{d}t}_{=\alpha_i} \tag{7}$$

Now, the really useful observation is that the coefficients α_i depend only on i (and on n). But this means that these coefficients neither depend on f nor on a nor on b. Since we can work out the numbers α_i explicitly, we are "hiding" the Lagrange polynomials including all the products over the divided differences. This means that all of numerical troubles that we had with numerical interpolation formulas regarding the conditioning of divided difference schemes automatically goes away if we derive numerical integration formulas. The final integration formula is then taking the simple form

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \sum_{i=0}^n f(x_i) \int_a^b L_i(x)\,\mathrm{d}x \;\stackrel{(7)}{=}\; \sum_{i=0}^n f(x_i) H \alpha_i$$

This can be written in the very practical form

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \frac{b-a}{n}\sum_{i=0}^{n}\alpha_i f(x_i)\ .$$

This is extremely easy to implement!!!

1.2 Example: Simpson's integration formula

The idea of Simpson's is to work out the Newton Cotes coefficients for $n = 2$. This means that our interpolation points will be located at

$$x_0 = a, \qquad x_1 = \frac{a+b}{2}, \quad \text{and} \quad x_2 = b\ .$$

The corresponding coefficients are given by

$$\alpha_0 \;=\; \int_0^2 \left(\prod_{j\neq 0}\frac{t-j}{-j}\right)\mathrm{d}t = \int_0^2 \frac{t-1}{-1}\frac{t-2}{-2}\,\mathrm{d}t \;=\; \frac{1}{3} \tag{8}$$

$$\alpha_1 \;=\; \int_0^2 \left(\prod_{j\neq 1}\frac{t-j}{1-j}\right)\mathrm{d}t = \frac{4}{3} \tag{9}$$

$$\alpha_2 \;=\; \int_0^2 \left(\prod_{j\neq 2}\frac{t-j}{2-j}\right)\mathrm{d}t = \frac{1}{3} \tag{10}$$

This means we obtain an explicit integration formula (Simpson's rule), which is given by

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; H\sum_{i=0}^{2}\alpha_i f(x_i) \;=\; \frac{b-a}{2}\left[\frac{1}{3}f(a) + \frac{4}{3}f\left(\frac{a+b}{2}\right) + \frac{1}{3}f(b)\right]$$

The Simpson formula can also be further simplified as

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]\ .$$

1.3 Approximation Accuracy of Simpson's Formula

First recall from Lecture 2 that the accuracy of the Lagrange interpolation is given by

$$\forall x\in[a,b], \qquad |f(x)-p(x)| \;\leq\; \max_{\xi\in[a,b]}\frac{f^{(3)}(\xi)}{3!}|b-a|^3 \tag{11}$$

Now, a "naive" bound on the approximation error is thus given by

$$\begin{aligned}\left|\int_a^b f(x)\,\mathrm{d}x - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]\right| \;&\leq\; \int_a^b |f(x)-p(x)|\,\mathrm{d}x \\ &\overset{(11)}{\leq}\; \max_{\xi\in[a,b]}\frac{f^{(3)}(\xi)}{3!}|b-a|^3|b-a| \\ &=\; \max_{\xi\in[a,b]}\frac{f^{(3)}(\xi)}{3!}|b-a|^4\ . \quad (12)\end{aligned}$$

Notice that this formula gives us a valid upper bound on the approximation error of Simpson's formula. But actually a big surprise is that this error bound can be improved orders of magnitude (at least for the case that the interval length $|b-a|$ is sufficiently small). The basic intuition of why Simpson's formula is much more accurate than one would expect by looking at the worst-case interpolation error is the following: the interpolant p is in some intervals over-approximating f but in other intervals under approximating f, since p interpolates f at all points. An interesting effect here is that the integral approximation error contributions from the parts where we overestimate f and the parts where we underestimate f partially cancel out with each other. In a way, this is some kind "symmetry effect" that we can exploit here. This intuition is exploited systematically in the following section:

1.4 Tighter error bounds for Simpon's formula

If we want to get a more accurate error estimate for Simpson's formula, we need to work a bit harder. Our goal is to work out a bound on the integration error

$$\begin{aligned} E_{\text{Simpson}} &= \left| \int_a^b f(x)\,\mathrm{d}x - \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]\right| \\ &= \left| \int_a^b f[x_0, x_1, \ldots, x_n, x](x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,\mathrm{d}x\right| \end{aligned} \tag{13}$$

In the last equation we have substituted the standard divided difference error bound (see Lecture 2; the proof of this error bound is using generalized Rolle's theorem). The main idea is to add and substract a term in order to exploit symmetry around the point $\frac{a+b}{2}$:

$$\begin{aligned} E_{\text{Simpson}} &= \left| \int_a^b f[x_0, x_1, \ldots, x_n, x](x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,\mathrm{d}x\right| \\ &= \left| \int_a^b f[x_0, x_1, \ldots, x_n, x](x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,\mathrm{d}x \right. \\ &\quad - \int_a^b f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right](x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,\mathrm{d}x \\ &\quad \left. + \int_a^b f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right](x-a)\left(x - \frac{a+b}{2}\right)(x-b)\,\mathrm{d}x \right| \end{aligned} \tag{14}$$

In the next we use the triangle inequality to write this in the form

$$
\begin{aligned}
E_{\text{Simpson}} \quad &\leq \quad \left| \int_a^b \frac{f[x_0, x_1, \ldots, x_n, x] - f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right]}{x - \frac{a+b}{2}} (x-a) \left(x - \frac{a+b}{2}\right)^2 (x-b)\, \mathrm{d}x \right| \\
&\quad + \left| \int_a^b f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right] (x-a) \left(x - \frac{a+b}{2}\right) (x-b)\, \mathrm{d}x \right| \\
&= \quad \left| \int_a^b \frac{f[x_0, x_1, \ldots, x_n, x] - f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right]}{x - \frac{a+b}{2}} (x-a) \left(x - \frac{a+b}{2}\right)^2 (x-b)\, \mathrm{d}x \right| \\
&\quad + \left| f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right] \int_a^b (x-a) \left(x - \frac{a+b}{2}\right) (x-b)\, \mathrm{d}x \right|
\end{aligned}
\tag{15}
$$

Due to symmetry around the point $\frac{a+b}{2}$ we have that

$$
\int_a^b (x-a) \left(x - \frac{a+b}{2}\right) (x-b)\, \mathrm{d}x = 0 \; .
$$

Moreover, we can bound the divided difference by

$$
\left| \frac{f[x_0, x_1, \ldots, x_n, x] - f\left[x_0, x_1, \ldots, x_n, \frac{a+b}{2}\right]}{x - \frac{a+b}{2}} \right| \leq \max_{\xi \in [a,b]} \frac{|f^{(4)}(\xi)|}{4!} \; .
$$

Additionally, we find that

$$
\int_a^b (x-a) \left(x - \frac{a+b}{2}\right)^2 (x-b)\, \mathrm{d}x \;=\; \frac{(b-a)^5}{120} \; .
$$

By substituting all of these relations we find the error bound of Simpson's formula:

$$
E_{\text{Simpson}} \leq \max_{\xi \in [a,b]} \frac{f^{(4)}(\xi)}{4!} \frac{(b-a)^5}{120} \;=\; \frac{(b-a)^5}{2880} \max_{\xi \in [a,b]} |f^{(4)}(\xi)| \; .
$$

1.5 Example

Let us apply Simpson's formula to the integral

$$
\int_0^1 e^x \, \mathrm{d}x = e - 1 \;\approx\; \frac{1}{2}\left[1 + 4\sqrt{e} + e\right] \approx 1.7188611518765928
$$

and the approximation error is bounded by

$$
\begin{aligned}
|e - 1 - 1.7188611518765928| \;&=\; 0.0005793234175477391 \\
&\leq\; \frac{e^1}{2880} = 0.0009438478571038351
\end{aligned}
$$

This verifies numerically that the error bound is correct for this example.