CLASS NOTES

Models, Algorithms and Data: Introduction to computing

2019

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IMPORTANT DISCLAIMERS

Much of the material (ideas, definitions, concepts, examples, etc) in these notes is taken for teaching purposes, from several references:

- Numerical Analysis by R. L. Burden and J. D. Faires
- The Nature of Mathematical Modeling by N. Gershenfeld
- A First Course in Numerical methods by U. M. Ascher and C. Greif

These notes are only informally distributed and intended ONLY as study aid for the final exam of ETHZ students that were registered for the course Models, Algorithms and Data (MAD): Introduction to computing 2019. The notes have been checked, however they may still contain errors so use with care.

LECTURE 9 Numerical integration II: Richardson and Romberg

What are requirements for a good numerical integrator?

1. Ease of use: User specifies the function to be integrated, integration bounds and desired accuracy. The code should produce the required result.

2. Cost: minimal time to solution (or alternatively: minimal energy, etc.)

In principle, any of the Newton–Cotes formulas can produce the desired result by halving the subintervals repeatedly until convergence. Such a procedure may be problematic for complex functions with large peaks and valleys.

A better approach is the **Romberg integration** that is based on the concept of **Richardson extrapolation** (also called “deferred approach to the limit”). The concept of Richardson extrapolation is a simple and elegant way to extend the accuracy by which we compute numerically *any quantity* (not necessarily an integral).

9.1 Richardson Extrapolation

If we work on a computer we have to discretize our quantity of interest G. This approximations depend on the chosen discretization, which is normally characterized by some grid-spacing h so that we write

$$G \approx G(h) \tag{9.1.1}$$

In other word, if we calculate any quantity on the computer, the result depends on our choice of the grid via the spacing h. As this grid spacing is usually small $h \ll 1$ and we want to have a consistent discretization (i.e. one for which $G(h) \xrightarrow{h\to 0} G$) we can expand our approximation in terms of a Taylor series for h:

$$G(h) = G(0) + c_1 h + c_2 h^2 + \cdots, \tag{9.1.2}$$

where $c_1, c_2, \ldots$ are the typical constants we obtain from this expansion $G'(0), G''(0)/2, \ldots$ (some constants may be 0). As already remarked above, the term $G(0)$ is the exact value ($G = G(0)$), while the rest of the terms are the errors we wish to eliminate. As said at the beginning one way to go about that is to splitt h into $h/2$ so that

$$G(h/2) = G + \frac{1}{2} c_1 h + \frac{1}{4} c_2 h^2 + \cdots. \tag{9.1.3}$$

We have now doubled the operations (assuming that we compute $G(h)$ in $O(1/h)$) and halved the error. Richardson's ingenious idea is to combine Eq. (9.1.2) and Eq. (9.1.3) to reduce the error:

$$G_1(h) = 2\,G(h/2) - G(h) = G + c_2' h^2 + c_3' h^3 + \cdots, \tag{9.1.4}$$

where c_2', c_3' are fractions of c_2, c_3. Now for $G_1(h)$ the leading error term is h^2. So as $h \to 0$, $G_1(h)$ is much more accurate than $G(h)$ and $G(h/2)$ at very little extra cost (one subtraction). We can repeat this process to obtain

$$G_2(h) = \frac{1}{3}\big(4\,G_1(h/2) - G_1(h)\big) = G + O(h^3), \tag{9.1.5}$$

which is even more accurate. Finally, we define $G_0(h) = G(h)$ and obtain

$$\boxed{G_n(h) = \frac{1}{2^n - 1}\big(2^n\, G_{n-1}(h/2) - G_{n-1}(h)\big) = G + O(h^{n+1})} \tag{9.1.6}$$

Example 9.1

Compute 2π by measuring the perimeter of a regular polygon inscribed in the unit circle. A polygon with E edges in the unit circle will have an edge length of $2\sin(\pi/E)$. We can use a Taylor expansion of $\sin(\pi/E)$ around $\sin(0)$ and obtain:

$$P_0(E) = 2E\sin(\pi/n) = 2E\Big((\pi/E) - (\pi/E)^3/6 + O(1/E^5)\Big) = 2\pi + O(1/E^2).$$

Since the error contains only even terms $(O(1/E^2), O(1/E^4), \ldots)$, we can adapt Eq. (9.1.6) and write

$$P_n(E) = \frac{1}{4^n - 1}\big(4^n\, P_{n-1}(2E) - P_{n-1}(E)\big) = 2\pi + O(1/E^{2n+2}).$$

9.2 Error Estimation

The same idea can be used to estimate the error of an approximation. We have

$$G(h/2) - G(h) = -\frac{1}{2}c_1 h - \frac{3}{4}c_2 h^2 + O(h^3). \tag{9.2.1}$$

On the other hand, we can rearrange Eq. (9.1.3) to get

$$\epsilon(h/2) = G - G(h/2) = -\frac{1}{2}c_1 h - \frac{1}{4}c_2 h^2 + O(h^3). \tag{9.2.2}$$

So to first order (i.e. dropping $O(h^2)$ terms), the error of the approximation with $h/2$ can be estimated as

$$\boxed{\epsilon(h/2) \approx G(h/2) - G(h)} \tag{9.2.3}$$

If h is small, this will be a good estimate of the error. If the error is not small enough, then this tells the user to keep subdividing.

9.3 Romberg integration

The key idea is to take inaccurate integration methods and improve them by using Richardson's extrapolation. We start with the trapezoidal rule with a single interval. Then recalculate with two intervals, four, eight, and so on with the results:

$$I_0^1, I_0^2, I_0^4, \cdots \tag{9.3.1}$$

In the calculation of I_0^n for n intervals, half of the needed functions have been computed earlier.

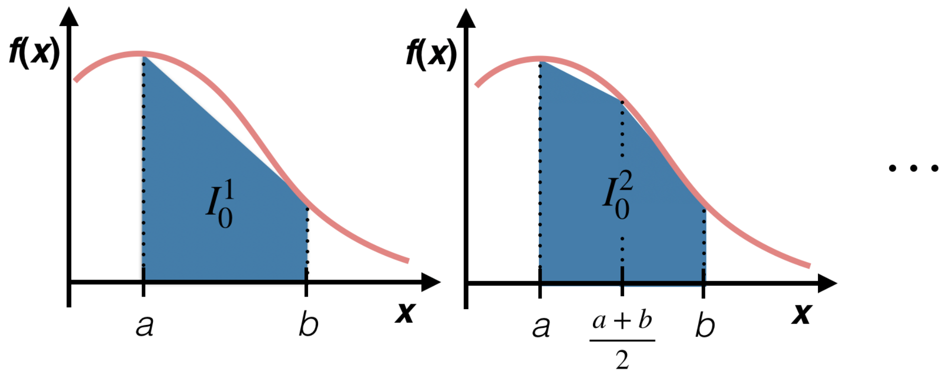

Figure 9.1: Graphical representation of the refinement step on the example of the trapezoidal rule.

From our numerical analysis of the error of the trapezoidal rule we have

$$I = \int_a^b f(x)dx = \underbrace{\frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f_j\right]}_{I_0^n} + c_1 h^2 + c_2 h^4 + c_3 h^6 + \cdots, \tag{9.3.2}$$

where we have equidistant intervals of length $h = (b-a)/n$ with $f_j = f(a + jh)$. Then the exact I and I_0^n are related as

$$I_0^n = I - c_1 h^2 - c_2 h^4 - c_3 h^6 \tag{9.3.3}$$

Now we evaluate with half the grid size $h_1 = h/2$:

$$I_0^{2n} = I - c_1 \frac{h^2}{4} - c_2 \frac{h^4}{16} - c_3 \frac{h^6}{64} \cdots \tag{9.3.4}$$

We eliminate the $O(h^2)$ term by using Richardson extrapolation:

$$(\star)\ I_1^n = \frac{4 I_0^{2n} - I_0^n}{3} = I + \frac{1}{4} c_2 h^4 + \frac{5}{16} c_3 h^6 \tag{9.3.5}$$

This is a fourth order approximation for I. In fact we rediscovered Simpson's rule. For $h_2 = h_1/2 = h/4$ we get

$$I_0^{4n} = I - c_1 \frac{h^2}{16} - c_2 \frac{h^4}{256} - c_3 \frac{h^6}{4096} - \cdots \tag{9.3.6}$$

To get another fourth order estimate we combine I_0^{2n} and I_0^{4n}

$$(\star\star)\ I_1^{2n} = \frac{4I_0^{4n} - I_0^{2n}}{3} = I + \frac{1}{64}c_2 h^4 + \frac{5}{1024}c_3 h^6 \tag{9.3.7}$$

So now we can combine I_1^n and I_1^{2n} and eliminate the $O(h^4)$ terms and get a 6th order accurate

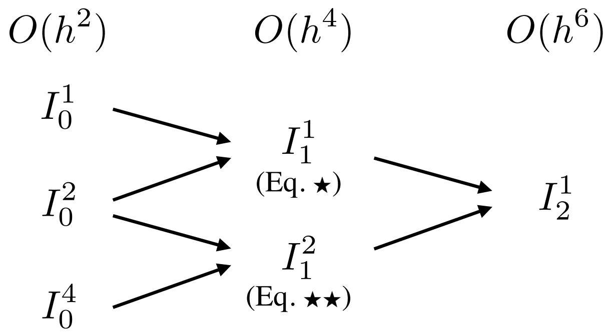

Figure 9.2: Graphical representation of Romberg integration.

formula. The process may be continued to get

$$\boxed{I_k^n = \frac{4^k I_{k-1}^{2n} - I_{k-1}^n}{4^k - 1}} \tag{9.3.8}$$

In principle, arbitrary accuracy can be achieved.

Exam checklist

After this class, you should understand the following points regarding numerical integration:

- How to use Richardson extrapolation to improve the accuracy of a numerically estimated quantity and to estimate errors
- How to use Romberg integration to improve the accuracy of trapezoidal rule