Online Lecture Notes

Prof. Boris Houska

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1 Numerical Integration: Extensions & Examples

Recall from the last two lectures: we dicussed two ways of deriving integration formulas of the form

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

where the weights α_i are independent of f and the points $x_0, x_1, \ldots, x_n$ are chosen inside the interval $[a, b]$. The appoximation error is typically of order

$$\left| \int_a^b f(x)\,\mathrm{d}x \;-\; \sum_{i=0}^{n} \alpha_i f(x_i) \right| \leq \mathbf{O}(|b-a|^m) \;,$$

where m depends on which integration formula is used. The maximum possible order is given $m = 2n+2$, which is obtained by choosing the Gauss-points (Gauss-Quadrature).

1.1 Integration on large intervals

If $|b-a|$ is large, then a single integration formula may have a large approximation error. In this case, we can, of course, break the whole interval into smaller intervals and use the integration formula on each of the interval pieces, and sum-up. For instance, we could choose an equidistant grid

$$y_0 = a, \quad y_1 = a+h \quad y_2 = a+2h, \quad \ldots, \quad y_N = b = a+Nh$$

This means that here we choose $h = \frac{b-a}{N}$. Use that

$$\int_a^b f(x)\,\mathrm{d}x \;=\; \int_{y_0}^{y_1} f(x)\,\mathrm{d}x + \int_{y_1}^{y_2} f(x)\,\mathrm{d}x + \ldots + \int_{y_{N-1}}^{y_N} f(x)\,\mathrm{d}x \;.$$

Next, we can apply the integration formula for each of the smaller intervals separately. Eventually, if the last interpolation point of the current interval equals the first evaluation point of the next interval, we can simply the sum-up formula. For example, we could sum-up Simpson's formula, which gives

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{b-a}{6N}\left[f(a) + 4f\left(a+\frac{h}{2}\right) + \mathbf{2}f(a+h) + 4f\left(a+3\frac{h}{2}\right) + \ldots + f(b) \right]$$

The factors 2 in the sum expression correspond to the simplification at the boundaries of the smaller integration intervals. In this example, the numerical integration would be bounded by

$$\mathbf{O}\left(\left(\frac{b-a}{N}\right)^5\right)$$

Thus, the integration error can be made arbitrarily small by choosing N sufficiently large. Similar sum-up formulas can be found for other Newton-Cotes methods as well.

1.2 Integration on infinite intervals

If we have an interval of the form, say

$$\int_a^\infty f(x)\,\mathrm{d}x$$

we cannot directly use the above integration formula. The sum-up trick also doesn't work, since we would need infinitely many smaller intervals. In such cases it is sometimes possible to introdoce a variable transformation. For instance, if $a = 1$, we could try to substitute

$$x = \frac{1}{y} \qquad \text{such that} \qquad \frac{\mathrm{d}x}{\mathrm{d}y} = -\frac{1}{y^2}.$$

This yields

$$\int_1^\infty f(x)\,\mathrm{d}x \;=\; \int_1^0 f\left(\frac{1}{y}\right)\left(-\frac{1}{y^2}\right)\mathrm{d}y \;=\; \int_0^1 f\left(\frac{1}{y}\right)\frac{1}{y^2}\,\mathrm{d}y\,.$$

The latter integral can be evaluated by a standard integration for the interval $[0,1]$, but we need to ensure that the limit

$$\lim_{y\to 0^+} f\left(\frac{1}{y}\right)\frac{1}{y^2}$$

exists and can be evaluated. An example would be

$$\int_1^\infty e^{-x}\,\mathrm{d}x \;=\; \int_0^1 e^{-\frac{1}{y}}\frac{1}{y^2}\,\mathrm{d}y \;\approx\; \frac{1}{6}\left[0 + 16e^{-2} + e^{-1}\right]$$

where the latter approximation is based on Simpon's formula. In principle, we could also try to derive an error bound (Exercise!). Notice that other variable substitution might also work—there is in general no unique way of doing this substitution.

1.3 Integration of function of more than one variable

In general, we could also consider functions of the form $f : \mathbb{R}^n \to \mathbb{R}$ and integrate over a multivariate interval. In the easiest vector-valued, we could consider the 2D integration problem ($n = 2$). In this case, we wish to evaluate the integral

$$\int_X f(x)\,\mathrm{d}x \;=\; \int_a^b \int_c^d f(x_1, x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2$$

on the interval domain $X = [a, b] \times [c, d]$. If we want to use an integration formula to approximate such 2D integral, we can first use a parametric integration formula to evaluate the inner integral and then integrate the parametrix expression once more with respect to the other variable.

1.3.1 Example: 2D Simpson formula

The first step would be to apply Simpson's formula for the inner integral,

$$F(x_1) = \int_c^d f(x_1, x_2)\,\mathrm{d}x_2 \;\approx\; \frac{d-c}{6}\left[f(x_1, c) + 4f\left(x_1, \frac{c+d}{2}\right) + f(x_1, d)\right] = G(x_1)\;.$$

Now, it only remains to work out the integral over $G(\cdot)$. This yields

$$\begin{aligned}\int_a^b \int_c^d f(x_1, x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \;&=\; \int_a^b F(x_1)\,\mathrm{d}x_1 \;\approx\; \int_a^b G(x_1)\,\mathrm{d}x_1 \\ &=\; \frac{b-a}{6}\left(G(a) + 4G\left(\frac{a+b}{2}\right) + G(b)\right) \qquad (1)\end{aligned}$$

In principle, we could substitute the above expression for G, which would give a lengthly explicit integration formula for a 2D interval. Essentially, we need to evaluate f at the 9 grid points in the rectangle $[a, b]$. The 4 vertices, the 4 midpoints of the edges, and the midpoint of the rectangle (9 evaluation points in total). Details: Exercise!

Remark: Similar tricks also work if the integration domain is not an interval, but given in parametric form. For instance the integral

$$\int_X f(x_1, x_2)\,\mathrm{d}x \quad \text{over the unit disk} \quad X = \{x \in \mathbb{R}^2 \mid x_1^2 + x_2^2 \le 1\}$$

we could write this integral in parametric form

$$\int_{-1}^{1} \underbrace{\left[\int_{x_1^2-1}^{1-x_1^2} f(x_1, x_2)\mathrm{d}x_2\right]}_{=F(x_1)} \mathrm{d}x_1\;.$$

A numerical approximation of this integral can be found by first applying the integration formula to F in dependence on x_1 and then using the same integration formula once more to integrate the corresponding integral approximation of F.

1.4 Short introduction to multivariate orthogonal polynomials

If we want to derive more advanced approximation or integration formulas based on orthononal polynomials, we can still use the standard L_2-scalar product, but for multivariate functions. For instance if we want to have multivariate Legendre polynomials on the two dimensional interval box $[-1,1]^2$. We could take the polynomials

$$
\begin{aligned}
Q_0(x) &= q_0(x_1)q_0(x_2) && (2)\\
Q_1(x) &= q_1(x_1)q_0(x_2) && (3)\\
Q_2(x) &= q_0(x_1)q_1(x_2) && (4)\\
Q_3(x) &= q_1(x_1)q_1(x_2) && (5)\\
Q_4(x) &= q_2(x_1)q_0(x_2) && (6)\\
&\vdots && (7)
\end{aligned}
$$

with $q_0, q_1, \ldots$ denoting the scalar Legendre polynomials. The multivariate polynomials $Q_0, Q_1, Q_2, \ldots$ are orthogonal on the 2D interval $[-1,1]^2$, since

$$
\begin{aligned}
\int_{-1}^{1}\int_{-1}^{1} q_i(x_1)q_j(x_2)q_k(x_1)q_l(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 &= \int_{-1}^{1} q_i(x_1)q_k(x_1)\,\mathrm{d}x_1 \int_{-1}^{1} q_j(x_2)q_l(x_2)\,\mathrm{d}x_2\\
&= \delta_{i,k}\delta_{j,l} \qquad (8)
\end{aligned}
$$

This means that the L_2-scalar product is one if $i = k$ and $j = l$ and zero otherwise. From here on everything that we discussed in the lecture is applicable (both Gauss approximation as well as Gauss Quadrature), since we have found an orthogonal basis for the Hilbert space of square integrable functions on the 2-dimensional domain $[-1,1]^2$.

Remark: In general, multivariate integration is very expensive. In two dimension, this usually no problem, but in higher dimensions, we might have to evaluate the integrand at a very large number of grid points. The optimal choice of grid point is, in general, an open research problem, but there is a lot of literature on so-called "smart grids", which are essentially evaluation points in higher dimensions, which lead to accurate intgration formulas—but this would be a research topic on its own.

2 Summary of lecture on numerical integration

In this lecture we have discussed:

1. Lagrange quadrature rules with a particular emphasis on Newton Cotes formulas. Example: Simpson's formula + error bound.

2. Gauss quadrature rules and their construction by using orthogonal polynomials.

3. Sum-up formulas for larger intervals (Rhomberg quadrature).

4. Variable transformations for the case that one or both integration bounds are equal $\pm\infty$.
5. Multivariate integration domains; parametric cascaded application of integration formulas for the derivation of 2D or higher dimensional integration formulas.
6. Finally, we briefly discussed the construction of multivariate orthogonal polynomials.