MATH50003 Numerical Analysis

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Contents

Chapter I

Calculus on a Computer

In this first chapter we explore the basics of mathematical computing and numerical analysis. In particular we investigate the following mathematical problems which can not in general be solved exactly:

1. Integration. General integrals have no closed form expressions. Can we instead use a computer to approximate the values of definite integrals? Numerical integration underpins much of modern scientific computing and simulations of physical systems modelled by partial differential equations.
2. Differentiation. Differentiating a formula as in calculus is usually algorithmic, however, it is often needed to compute derivatives without access to an underlying formula, eg, a function defined only in code. Can we use a computer to approximate derivatives? A very important application is in Machine Learning, where there is a need to compute gradients in training neural networks.
3. Root finding. There is no general formula for finding roots (zeros) of arbitrary functions, or even polynomials that are of degree 5 (quintics) or higher. Can we compute roots of general functions using a computer?

Each chapter is divided into sections that roughly correspond to individual lectures. In this chapter we investigate solving the above computational problems:

1. I.1 Rectangular rule: we review the rectangular rule for integration and deduce the *convergence rate* of the approximation. In the lab/problem sheet we investigate its implementation as well as extensions to the Trapezium rule.
2. I.2 Divided differences: we investigate approximating derivatives by a divided difference and again deduce the convergence rates. In the lab/problem sheet we extend the approach to the central differences formula and computing second derivatives. We also observe a mystery: the approximations may have significant errors in practice, and there is a limit to the accuracy.
3. I.3 Dual numbers: we introduce the algebraic notion of a *dual number* which allows the implementation of *forward-mode automatic differentiation*, a high accuracy alternative to divided differences for computing derivatives.

4. I.4 Newton's method: Newton's method is a basic approach for computing roots/zeros of a function. We use dual numbers to implement this algorithm.

Each week there are labs and problem sheets that further explore the mathematical material introduced in each section. The labs generally explore practical implementation and the impact of implementing methods in computer arithmetic. The problem sheets dig deeper into analysis of other methods and phenomena observed in the labs. The material introduced in the labs and problem sheets is also examinable so its important to study these as well.

I.1 Rectangular rule

One possible definition for an integral is the limit of a Riemann sum, for example:

$$\int_a^b f(x)\mathrm{d}x = \lim_{n\to\infty} h \sum_{j=1}^n f(x_j)$$

where $x_j = a + jh$ are evenly spaced points dividing up the interval $[a, b]$, that is with the *step size* $h = (b - a)/n$. This suggests an algorithm known as the *(right-sided) rectangular rule* for approximating an integral: choose n large so that

$$\int_a^b f(x)\mathrm{d}x \approx h \sum_{j=1}^n f(x_j).$$

In the lab we explore practical implementation of this approximation, and observe that the error in approximation is bounded by C/n for some constant C. This can be expressed using "Big-O" notation:

$$\int_a^b f(x)\mathrm{d}x = h \sum_{j=1}^n f(x_j) + O(1/n).$$

In these notes we consider the "Analysis" part of "Numerical Analysis": we want to *prove* the convergence rate of the approximation, including finding an explicit expression for the constant C.

To tackle this question we consider the error incurred on a single panel (x_{j-1}, x_j), then sum up the errors on rectangles.

Now for a secret. There are only so many tools available in analysis (especially at this stage of your career), and one can make a safe bet that the right tool in any analysis proof is either (1) integration-by-parts, (2) geometric series or (3) Taylor series. In this case we use (1):

Lemma 1 ((Right-sided) Rectangular Rule error on one panel)**.** *Assuming f is differentiable on $[a, b]$ and its derivative is integrable we have*

$$\int_a^b f(x)\mathrm{d}x = (b - a)f(b) + \delta$$

where $|\delta| \le M(b - a)^2$ *for* $M = \sup_{a\le x\le b} |f'(x)|$.

Proof We write

$$\begin{aligned}\int_a^b f(x)\mathrm{d}x &= \int_a^b (x-a)' f(x)\mathrm{d}x = [(x-a)f(x)]_a^b - \int_a^b (x-a)f'(x)\mathrm{d}x \\ &= (b-a)f(b) + \underbrace{\left(-\int_a^b (x-a)f'(x)\mathrm{d}x\right)}_{\delta}.\end{aligned}$$

Recall that we can bound the absolute value of an integral by the supremum of the integrand times the width of the integration interval:

$$\left|\int_a^b g(x)\mathrm{d}x\right| \leq (b-a) \sup_{a\leq x\leq b} |g(x)|.$$

The lemma thus follows since

$$\begin{aligned}\left|\int_a^b (x-a)f'(x)\mathrm{d}x\right| &\leq (b-a) \sup_{a\leq x\leq b} |(x-a)f'(x)| \\ &\leq (b-a) \sup_{a\leq x\leq b} |x-a| \sup_{a\leq x\leq b} |f'(x)| \\ &\leq M(b-a)^2.\end{aligned}$$

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Now summing up the errors in each panel gives us the error of using the Rectangular rule:

Theorem 1 (Rectangular Rule error)**.** *Assuming f is differentiable on $[a,b]$ and its derivative is integrable we have*

$$\int_a^b f(x)\mathrm{d}x = h\sum_{j=1}^n f(x_j) + \delta$$

where $|\delta| \leq M(b-a)h$ for $M = \sup_{a\leq x\leq b}|f'(x)|$, $h = (b-a)/n$ and $x_j = a + jh$.

Proof We split the integral into a sum of smaller integrals:

$$\int_a^b f(x)\mathrm{d}x = \sum_{j=1}^n \int_{x_{j-1}}^{x_j} f(x)\mathrm{d}x = \sum_{j=1}^n \left[(x_j - x_{j-1})f(x_j) + \delta_j\right] = h\sum_{j=1}^n f(x_j) + \underbrace{\sum_{j=1}^n \delta_j}_{\delta}$$

where δ_j, the error on each panel as in the preceding lemma, satisfies

$$|\delta_j| \leq (x_j - x_{j-1})^2 \sup_{x_{j-1}\leq x\leq x_j} |f'(x)| \leq Mh^2.$$

Thus using the triangular inequality we have

$$|\delta| = \left|\sum_{j=1}^n \delta_j\right| \leq \sum_{j=1}^n |\delta_j| \leq Mnh^2 = M(b-a)h.$$

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Note a consequence of this lemma is that the approximation converges as $n \to \infty$ (i.e. $h \to 0$). In the labs and problem sheets we will consider the left-sided rule:

$$\int_a^b f(x)\mathrm{d}x \approx h\sum_{j=0}^{n-1} f(x_j).$$

We also consider the *Trapezium rule*. Here we approximate an integral by an affine function:

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

Subdividing an interval $a = x_0 < x_1 < \ldots < x_n = b$ and applying this approximation separately on each subinterval $[x_{j-1}, x_j]$, where $h = (b-a)/n$ and $x_j = a + jh$, leads to the approximation

$$\int_a^b f(x)\mathrm{d}x \approx \frac{h}{2}f(a) + h\sum_{j=1}^{n-1} f(x_j) + \frac{h}{2}f(b)$$

We shall see both experimentally and provably that this approximation converges faster than the rectangular rule.

I.1.1 Lab and problem sheet

In the lab, we explore the practical implementation of the right-sided rectangular rule and extensions to other rules like the left-sided rectangular rule and trapezium rule. We also see how the error rate can be deduced *experimentally*: by applying a rule to specific integrals with known formula we can see the error rate visually by plotting it. We also observe that in practice there are some subtleties: the error can bounce around at an extremely small, but not zero, level on the order of 10^{-15}. In the problem sheet we explore the *analysis* of these other rules, proving that the Trapezium rule converges to the true integral at a faster quadratic ($O(h^2)$) error rate. This is a guarantee that the integral can be computed much more accurately for the same amount of work by taking into account the analysis of the method.

I.2 Divided Differences

Given a function, how can we approximate its derivative at a point? We consider an intuitive approach to this problem using *(Right-sided) Divided Differences*:

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Note by the definition of the derivative we know that this approximation will converge to the true derivative as $h \to 0$. But in numerical approimxations we also need to consider the rate of convergence.

Now in the previous section I mentioned there are three basic tools in analysis: (1) integration-by-parts, (2) geometric series or (3) Taylor series. In this case we use (3):

Proposition 1 (divided differences error)**.** *Suppose that f is twice-differentiable on the interval $[x, x+h]$. The error in approximating the derivative using divided differences is*

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \delta$$

where $|\delta| \leq Mh/2$ for $M = \sup_{x \leq t \leq x+h} |f''(t)|$.

Proof Follows immediately from Taylor's theorem: recall that

$$f(x+h) = f(x) + f'(x)h + \frac{f''(t)}{2}h^2$$

for some $t \in [x, x+h]$. Rearranging we get

$$f'(x) = \frac{f(x+h) - f(x)}{2} + \underbrace{\left(-\frac{f''(t)}{2h^2}\right)}_{\delta}.$$

We then bound:

$$|\delta| \leq \left|\frac{f''(t)}{2}h\right| \leq \frac{Mh}{2}.$$

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Unlike the rectangular rule, the computational cost of computing the divided difference is independent of h! We only need to evaluate a function f twice and do a single division. Here we are assuming that the computational cost of evaluating f is independent of the point of evaluation. Later we will investigate the details of how computers work with numbers via floating point, and confirm that this is a sensible assumption.

So why not just set h ridiculously small? In the lab we explore this question and observe that there are significant errors introduced in the numerical realisation of this algorithm. We will return to the question of understanding these errors after learning floating point numbers.

There are alternative versions of divided differences. Left-side divided differences evaluates to the left of the point where we wish to know the derivative:

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

and central differences:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

We can further arrive at an approximation to the second derivative by composing a left- and right-sided finite difference:

$$f''(x) \approx \frac{f'(x+h) - f'(x)}{h} \approx \frac{\frac{f(x+h)-f(x)}{h} - \frac{f(x)-f(x-h)}{h}}{h} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

In the lab we investigate the convergence rate of these approximations (in particular, that central differences is more accurate than standard divided differences) and observe that they too suffer from unexplained (for now) loss of accuracy as $h \to 0$. In the problem sheet we prove the theoretical convergence rate, which is never realised because of these errors.

I.2.1 Lab and problem sheet

In the lab, we explore the practical implementation of the right-sided divided differences and extensions to central differences and second-order divided differences. We see *experimentally* that the central differences converges much faster to the true value of the derivative as h becomes moderately small. However, we observe a serious issue: if h becomes too small, the eror mysteriously starts growing extremely large, and hence these rules do not actually converge at all to the true value of the derivatives!

The problem sheet explores the *analysis* of these different rules, proving the precise theoretical convergence rates observed for moderately small h. This presents a bit of a contradiction: why does the theory say the method converges but in practice it diverges, and spectacularly so! This is a mystery that we will return to later.