Department of Mathematics and Statistics
620–295
Real analysis with applications

Before starting, copy the folder `Lab3` from the lab server `M&S Lab Materials\620-295` to `D:MATLAB` and set the path to `D:MATLAB` including subfolders.

Laboratory Class 4: Numerical integration

Since many functions that are (Riemann) integrable do not have a closed form indefinite integral in terms of simple functions, it is useful to evaluate definite integrals

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

using approximations with well-understood error behaviour.

All numerical approximations for I involve sampling the integrand f at a set of points $\{x_j\} \in [a, b]$ and approximating I as a weighted sum of the sampled values of f. Any such process is called *numerical integration* or *quadrature*.

$$Q_N = \sum_{j=0}^{N} w_j f(x_j) \approx \int_a^b f(x)\ dx.$$

1 Trapezoid rule

Adding up areas of trapezoids gives an approximation to $\int_a^b f(x)\ dx$ given by

$$T_N = \frac{\Delta x}{2}\left(f(a) + 2f(a+\Delta x) + 2f(a+2\Delta x) + \cdots + 2f(b-\Delta x) + f(b)\right), \qquad \text{where } \Delta x = (b-a)/N.$$

The M-file `trapez.m` computes the approximation T_N for $\displaystyle\int_a^b f(x)\ dx$ with N intervals.

The M-file `trapDriver.m` specifies the integrand f and interval $[a, b]$ and produces trapezoid rule estimates for a range of N values. It is set up to use the trapezoid rule to approximate

$$\int_0^1 x^4 - x^2\ dx = 1/5 - 1/3 = -2/15 \approx -0.1333333333333333.$$

1.0.1 Exercise

Run `trapDriver`. By editing `trapDriver`, find out (experimentally) how large N has to be for the trapezoid estimate to be accurate to 5 significant figures.

Numerical integration is most useful when you don't know the exact answer. The function $f = \exp(-x^2)$ is integrable but the indefinite integral $\int e^{-x^2} dx$ does not have an expansion in terms of simple functions.

1.0.2 Exercise

Edit and run `trapDriver` to estimate the integral $\int_0^1 \exp(-x^2)\ dx$ to 6 significant figures.

Using the Taylor expansion of e^{-x^2}, express $\int_0^1 \exp(-x^2)\ dx$ as a (convergent) infinite series.

1.1 Testing the error bound

The trapezoid rule has an error estimate if $f''\colon [a,b] \to \mathbb{R}$ is continuous,

$$\left| \int_a^b f(x)dx - T_N \right| \leq (\Delta x)^2 \frac{(b-a)M}{12}, \qquad \text{where } \Delta x = \tfrac{b-a}{N}, \tag{1}$$

and M is an upper bound for $\{|f''(x)| \mid x \in [a,b]\}$.

We can see how well this error bound describes the performance of the trapezoid rule by computing successive estimates with finer and finer meshes (smaller and smaller values of Δx).

1.1.1 Exercise

If you compute successive trapezoid rule estimates with $N = 10, 20, 40, 80 \cdots$, how would you expect the errors to behave, according to the error bound? Explain why a log-log plot is a sensible way to plot the errors versus N.

The M-file `trapErrors.m` extends `trapDriver` by computing, displaying and plotting the errors, if the exact value of the integral is known. It is set up to use the trapezoid rule to approximate

$$\int_0^1 x^4 - x^2\ dx = 1/5 - 1/3 = -2/15 \approx -0.1333333333333333.$$

1.1.2 Exercise

Run `trapErrors`. Do the errors behave the way you expect? How can you tell? By editing `trapErrors`, find out (experimentally) how large n has to be for the trapezoid estimate to be accurate to 5 decimal places.

1.2 Non-smooth integrand

Apart from $(\Delta x)^2$ behaviour, the other important information from the error bound is that it relies on the continuity of the second derivative $f''\colon [a,b] \to \mathbb{R}$. What happens if that is not the case?

1.2.1 Exercise

Edit and run `trapErrors` to estimate the integral $\int_0^1 \sqrt{x}\ dx = 2/3$.

Do the errors behave the way you expect? How can you tell? How large does N have to be for the trapezoid estimate to be accurate to 5 significant figures? *Don't try to explain what you see — it's enough to see it!*

1.3 Unusually accurate cases

1.3.1 Exercise

Edit and run `trapDriver` to estimate the integral $\int_0^1 x\ dx = 1/2$.

How big are the errors? Is this what you expect? Are the results consistent with Eq. 1?
Errors $\approx 10^{-16}$ can be taken to be numerical approximations to zero in this context.

1.3.2 Exercise

Edit and run `trapErrors` to estimate the integral $\int_0^{2\pi} \frac{1}{2+\cos(x)}\ dx = 2\pi/\sqrt{3}$.

How big are the errors? Is this what you expect? Are the results consistent with Eq. 1?

2 Simpson's rule

Simpson's approximation rule to $\int_a^b f(x)dx$ is obtained by adding up parabola topped slices,

$$S_N = \frac{\Delta x}{3}\left(f(a) + 4f(a+\Delta x) + 2f(a+2\Delta x) + \cdots + 4f(b-\Delta x) + f(b)\right), \qquad \text{where } \Delta x = \tfrac{b-a}{N}$$

and N must be even. The M-file `simpson.m` computes the Simpson's rule estimate for $\int_a^b f(x)dx$ with N intervals.

2.0.3 Exercise

Modify `trapDriver.m` to create an M-file `simpDriver.m` and test it on the integral

$$\int_0^1 x^4 - x^2 \, dx = 1/5 - 1/3 = -2/15 \approx -0.1333333333333333.$$

2.0.4 Exercise

Edit and run `simpDriver` to estimate the integral $\displaystyle\int_0^1 \exp(-x^2)\, dx$ to 6 significant figures.

2.1 Testing the error bound

Simpson's rule has an error estimate if the fourth derivative $f^{(4)}\colon [a,b] \to \mathbb{R}$ is continuous,

$$\left| \int_a^b f(x)dx - S_N \right| \le (\Delta x)^4 \frac{(b-a)M}{180}, \qquad \text{where } \Delta x = \tfrac{b-a}{N} \tag{2}$$

and M is an upper bound for $\{|f^{(4)}(x)| \mid x \in [a,b]\}$.

2.1.1 Exercise

Modify `trapErrors.m` to create an M-file `simpErrors.m` and test it on the integral

$$\int_0^1 (x^4 - x^2)\, dx = 1/5 - 1/3 = -2/15 \approx -0.1333333333333333.$$

2.2 Non-smooth integrand

2.2.1 Exercise

Edit and run `simpErrors` to estimate the integral $\displaystyle\int_0^1 \sqrt{x}\, dx = 2/3.$
Do the errors behave the way you expect? How can you tell?

2.3 An unusually accurate case

2.3.1 Exercise

Edit and run `simpDriver` to estimate the integral $\displaystyle\int_0^1 x^2\, dx = 1/3.$
How big are the errors? Is this what you expect?

2.3.2 Exercise

Edit and run `simpDriver` to estimate the integral $\displaystyle\int_0^1 x^3\, dx = 1/4.$
How big are the errors? Is this what you expect? Are the results consistent with Eq. 2?