

1 Theory

1.1 Fourier transforms

- State the convolution theorem for two functions f and g .
- Define the rectangular pulse function:

$$\text{rect}(t) = \begin{cases} 1 & \text{if } |t| < \frac{1}{2} \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

Calculate the function $\text{tri}(t)$ obtained by the convolution of $\text{rect}(t)$ with itself. Sketch $\text{tri}(t)$.

- Show that the Fourier transform of $\text{rect}(t)$ is

$$\frac{\sin(\pi f)}{\pi f}.$$

- Hence show that the Fourier transform of $\text{tri}(t)$ is

$$\frac{\sin^2(\pi f)}{\pi^2 f^2}.$$

1.2 Finite difference formulae

- Derive a finite difference approximation for the first derivative of a function, $f(x)$, at the point x_i based on the (asymmetric) stencil $(x_i - \alpha h, x_i, x_i + h)$ with $\alpha \neq 1$. What is the error in this approximation?
- Adapt these calculations to obtain a finite difference formula for the second derivative of $f(x)$ at x_i . What is the error in this approximation?
- What are the possible choices of stencil for approximation of the first derivative of $f(x)$, at the point x_i using 4 *equally spaced* points?
- Pick one of these stencils and derive the finite difference approximation for the first derivative. What is the error?

1.3 Derivation of integration rules

- Write down:
 1. the interpolating polynomial of degree 1 passing through the points $(0, f_0)$ and (h, f_1) .
 2. the interpolating polynomial of degree 2 passing through the points $(0, f_0)$, (h, f_1) and $(2h, f_2)$.
- Use these results to derive the trapezoidal rule and Simpson's rule.
- Consider the integral

$$\int_0^1 \frac{1+x^2}{\sqrt{x}} dx \quad (2)$$

What is the exact value of this integral?

- Write down a change of variables which removes the singularity in the integrand at $x = 0$ and write the integral in the new variables.

1.4 Finding roots

- Derive the Newton-Raphson method for finding roots of the complex equation

$$f(z) = 0.$$

- Consider the equation

$$f(z) = z^3 - 2z + 2. \quad (3)$$

Write down the iterated map defined by applying the Newton-Raphson method to this equation. That is, find G such that the Newton-Raphson iteration can be written in the form

$$z_{n+1} = G(z_n). \quad (4)$$

- Write down the second iterate of the map (4). Use it to find a starting value for which the Newton-Raphson method applied to Eq. (3) enters an infinite loop (better to use trial and error here since the second iterate is complicated).
- Using the methods you learned in MA998 (or any introductory course on dynamical systems), try to determine if starting values near to the one which you have found above would also enter an infinite loop.

1.5 Bracketing of minima

Consider the problem of minimising a smooth function $f(x)$ which has a minimum at $x = x_*$.

- Show that if $x \approx x_*$ then

$$f(x) \approx f(x_*) \left[1 + \frac{f''(x_*)}{2f(x_*)} (x - x_*)^2 \right].$$

Quantify the error in this approximation.

- Use this result to show that it is not possible to bracket a minimum to an accuracy greater than

$$|x - x_*| \sim \sqrt{\varepsilon_m} \sqrt{\frac{2f(x_*)}{f''(x_*)}}$$

where ε_m is the machine precision.

- In Numerical Recipes this criterion is written

$$|x - x_*| \sim \sqrt{\varepsilon_m} |x_*| \sqrt{\frac{2f(x_*)}{x_*^2 f''(x_*)}}$$

on the basis that for "most" functions the latter factor is $O(1)$. Check whether this is true for three simple choices of $f(x)$ for which you already know the answer.

- Can you derive a comparable condition for the highest accuracy which can be achieved when bracketing a root?

2 Implementation

2.1 The Fast Fourier Transform*

Make sure you have installed the fftw3 implementation of the FFT algorithm. A skeleton code and makefile can be downloaded from the class website to help you get started.

- Look up the documentation of the fftw3 library and write down what the fftw algorithm actually computes.
- Consider the function $\text{tri}(t)$ defined

$$\text{tri}(t) = \begin{cases} 1 - |t| & \text{if } |t| < 1 \\ 0 & \text{otherwise.} \end{cases} \quad (5)$$

Write a code which samples this function using N points uniformly spaced on the interval $[-5, 5]$. Calculate the discrete Fourier transform of the resulting values using the fftw3 library. Plot the modulus squared of the elements of the output array as a function of the output array index.

- Rescale and re-order the output of the discrete Fourier transform to plot a numerical approximation to the power spectrum of $\text{tri}(t)$. Plot the numerical power spectrum against the analytic expression for the power spectrum for $N = 16$ and $N = 512$.
- Write down an estimate for the error in the numerical power spectrum. Use your code to compute this error for a range of values of N and use your results to determine empirically how the error scales with N .

2.2 Finding roots and minima*

- Considering $f(z)$ defined in Eq. (3), write a code which evaluates $f(z)$ and $f'(z)$ for complex arguments z and use these to write a function which performs the Newton-Raphson iteration for seeking roots of the equation $f(z) = 0$.
- Plot $f(x)$ to obtain a reasonable guess for the real root of this equation and use your code to compute it.
- Considered as a function of a complex variable, f , has three roots. Use your Newton-Raphson code to find them. Using a "grid" of initial guesses in an appropriately sized region of the complex plane containing all three roots, try to determine the basin of attraction of each root under Newton-Raphson iteration. (Beware: you already know from the theory section that there is at least one initial guess for which the method doesn't converge to any root and there may be more!)
- Considered as a function of a real variable, f , has a local minimum. Write a programme to find this root using the golden section search. Plot the size of the bracketing interval as a function of the number of refinements and compare the rate of convergence to the theoretical expectation. Estimate how many significant figures of accuracy you are able to obtain using this method.