

# Coursework

In this coursework, you will use the *argument principle* to implement and analyse a root-finding algorithm. For  $f$  analytic in a simply connected domain  $D \subset \mathbb{C}$ , we define

$$I[f; \beta, \gamma] := \frac{1}{2\pi i} \oint_{\gamma} \frac{f'(z)}{f(z)} z^{\beta} dz, \quad \text{for } \beta \in \mathbb{N} \cup \{0\}, \quad (1)$$

where  $\gamma$  is a closed anti-clockwise-oriented contour in  $D$ , without any loops. Below, Algorithm 1 uses equation (1) to search for a root of  $f$  inside of a circular subset of  $D$ .

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**Algorithm 1** Basic root-finder

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1: function BASICROOTFINDER( $f, \tilde{z}, \mathcal{R}$ )
2:
3:    $\gamma_{\mathcal{R}} \leftarrow \{\tilde{z} + \mathcal{R}e^{i\theta} : \theta \in [0, 2\pi]\}$ 
4:   if  $m_0 \geq 1$  then
5:      $m_0 \leftarrow I[f; 0, \gamma_{\mathcal{R}}]$ 
6:   return  $z_0, m_0$ 
7:   end if
8: end function
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Throughout this project, you should assume the following:

**Assumption 1** For all contour integrals over  $\gamma_{\mathcal{R}}$  (as defined in Algorithm 1),  $\mathcal{R}$  is chosen such that  $\gamma_{\mathcal{R}} \subset D$  and  $f(z) \neq 0$  for  $z \in \gamma_{\mathcal{R}}$ .

1. This question is about understanding when Algorithm 1 works, and when it fails. For this question, you should assume that all integrals in lines 3 and 5 are calculated in exact arithmetic.

- (a) State further assumptions about the roots of  $f$  and the contour  $\gamma_{\mathcal{R}}$ , such that Algorithm 1 returns an output.

[1 mark]

- (b) State further assumptions about the roots of  $f$  and the contour  $\gamma_{\mathcal{R}}$ , such that the output

$$z_0, m_0 = \text{BasicRootFinder}(f, \tilde{z}, \mathcal{R}),$$

satisfies  $f(z_0) = 0$ .

[2 marks]

- (c) Given  $\tilde{z}$  and  $\mathcal{R}$ , construct an  $f$  such that Algorithm 1 returns

$$z_0, m_0 = \text{BasicRootFinder}(f, \tilde{z}, \mathcal{R}),$$

where

$$f(z_0) \neq 0.$$

[2 marks]

2. Typically in practice, we are unable to compute the integrals on lines 3 and 5 of Algorithm 1 in exact arithmetic. This question is about the design and analysis of an approximation to the general case, as defined in (1).

- (a) For  $\gamma_{\mathcal{R}}$  defined as in line 2 of Algorithm 1, show that an  $N$ -point trapezium rule approximation to (1) is given by

$$\begin{aligned} I[f; \beta, \gamma_{\mathcal{R}}] &\approx I_N[f; \beta, \gamma_{\mathcal{R}}] \\ &:= \frac{\mathcal{R}}{N} \sum_{n=1}^N \frac{f'(\tilde{z} + \mathcal{R}e^{i\theta_n})}{f(\tilde{z} + \mathcal{R}e^{i\theta_n})} (\tilde{z} + \mathcal{R}e^{i\theta_n})^{\beta} e^{i\theta_n}, \end{aligned} \quad (2)$$

where  $\theta_n := 2\pi n/N$  for  $n = 1, \dots, N$ .

[2 marks]

- (b) Assuming convergence

$$I_N[f; 0, \gamma_{\mathcal{R}}] \rightarrow I[f; 0, \gamma_{\mathcal{R}}], \quad \text{as } N \rightarrow \infty,$$

explain why

$$I[f; 0, \gamma_{\mathcal{R}}] = \text{round}(\text{Re}\{I_N[f; 0, \gamma_{\mathcal{R}}]\}),$$

for sufficiently large  $N$ , where

$$\text{round}(x) : \mathbb{R} \rightarrow \mathbb{Z}$$

rounds to the nearest integer.

[2 marks]

- (c) Suppose now that  $f$  has no zeros in the closed annulus

$$\Omega_{\mathcal{R}_-, \mathcal{R}_+} := \{z \in \mathbb{C} : \mathcal{R}_- \leq |\tilde{z} - z| \leq \mathcal{R}_+\},$$

for  $0 < R_- < \mathcal{R} < R_+$ . By referring to an appropriate theorem in the course notes, show that

$$|I_N[f; \beta, \gamma_{\mathcal{R}}] - I[f; \beta, \gamma_{\mathcal{R}}]| = O(e^{-aN}), \quad \text{as } N \rightarrow \infty,$$

where

$$a = \max \left\{ \log \frac{R_+}{\mathcal{R}}, \log \frac{\mathcal{R}}{R_-} \right\}.$$

[6 marks]

3. In this question, you will implement and test a modified version of Algorithm 1.

(a) Some guidance:

- Use a programming language of your choice. You should choose a language which supports complex arithmetic. My advice would be to use Matlab/Octave, Python, or Julia. You will need to be able to compute complex values of the Riemann-Zeta function, further information is given in (3(b)iii).
- The integrals in lines 3 and 6 of Algorithm 1 should be approximated using the trapezoidal approximation (defined in equation (2) above); therefore your algorithm should contain an additional input  $N$ . You should also pass  $f'$  as a separate input. With this in mind, your function inputs should look similar to that in Algorithm 2 below.
- You should manually code the trapezium rule yourself.
- You should improve the accuracy for large  $N$  by incorporating knowledge from question (2b), adding a further modification to line 3.
- Comment your code clearly.
- Label your axes in your plots.
- In each problem below, you should achieve machine precision accuracy, typically stagnating between  $10^{-14}$  and  $10^{-16}$  error, for larger values of  $N$ .
- Noting the result of question (2c), you should observe exponential convergence for your method. Using a logarithmic scale for the absolute error on the vertical axis, this will look (roughly) like a straight line.

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**Algorithm 2** Your root-finder

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1: function YOURROOTFINDER( $f, f', \tilde{z}, \mathcal{R}, N$ )
2:   :
3: end function
```

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(b) Plot the absolute error (on a logarithmic scale, on the vertical axis) of your algorithm, against  $N$  (standard scale, on the horizontal axis), for the following experiments:

- i. Approximate the *golden ratio*  $z_0 = (1 + \sqrt{5})/2$ , which is the positive root of the equation  $f(z) = z^2 - z - 1$ . Use  $\mathcal{R} = 1$  with an initial guess of  $\tilde{z} = 1$ , for  $N = 1, 2, \dots, 80$
- ii. Approximate  $z_0 = \pi$  using  $f(z) = (1 + e^{iz})/e^{iz}$ , for which  $\pi$  is a simple root (you do not need to prove this). Use  $\mathcal{R} = 1$ , with an initial guess of  $\tilde{z} = 3$ , for  $N = 1, 2, \dots, 25$ .
- iii. Approximate the first non-trivial zero

$$z_0 = \frac{1}{2} + i14.13472514173469\dots$$

of the *Riemann-Zeta function*  $f(z) = \zeta(z)$ . Use initial guess  $\tilde{z} = 1/2 + 15i$ ,  $\mathcal{R} = 1$ , for  $N = 10, 20, \dots, 400$ .

You should use pre-existing software to compute  $\zeta$ , **do not attempt to code this yourself**. In Matlab/Octave this is simply `zeta`, in Python this can be done using recent versions of the SciPy library, and in Julia this can be done using the SpecialFunctions package. However, to compute  $\zeta'(z)$ , **you must use Cauchy's integral formula** over a circular contour of radius  $1/10$  centred at  $z$ , approximated with an  $N$ -point trapezium rule (the same  $N$  as for your argument principle approximation, in the ‘outer’ integral).

[15 marks for full question]