7   Mathematical Methods

7.4   Airy Functions and Stokes' Phenomenon   (9 units)

This project uses ideas from the Further Complex Methods course. It also covers some material which is lectured as part of the Asymptotic Methods course, but students not taking this course are at no disadvantage.

1   Introduction

The Airy functions $\mathrm{Ai}(z)$ and $\mathrm{Bi}(z)$, where z is a complex variable, are two linearly independent solutions of the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}z^2}\,y(z) = zy(z) \tag{1}$$

satisfying

$$\mathrm{Ai}(0) = \alpha, \qquad \mathrm{Ai}'(0) = -\beta, \qquad \mathrm{Bi}(0) = \sqrt{3}\,\alpha, \qquad \mathrm{Bi}'(0) = \sqrt{3}\,\beta$$

where

$$\alpha = \frac{1}{3^{2/3}\,\Gamma(\frac{2}{3})} \approx 0.355028053887817, \qquad \beta = \frac{1}{3^{1/3}\,\Gamma(\frac{1}{3})} \approx 0.258819403792807.$$

Here Γ is the Gamma function, defined by

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1}\mathrm{d}t, \tag{2}$$

but you do not need to know anything about its properties for this project. The Airy functions are useful in many problems involving transition regions of all kinds, for example in optical diffraction (the transition between relatively light and dark regions), wave theory, electron tunnelling, and asymptotic analysis. Ai and Bi have Maclaurin series given by

$$\mathrm{Ai}(z) = \alpha f(z) - \beta g(z), \qquad \mathrm{Bi}(z) = \sqrt{3}\big(\alpha f(z) + \beta g(z)\big)$$

where

$$f(z) = 1 + \frac{1}{3!}z^3 + \frac{1\cdot 4}{6!}z^6 + \frac{1\cdot 4\cdot 7}{9!}z^9 + \cdots$$

and

$$g(z) = z + \frac{2}{4!}z^4 + \frac{2\cdot 5}{7!}z^7 + \frac{2\cdot 5\cdot 8}{10!}z^{10} + \cdots.$$

For large $|z|$, any solution $y(z)$ of (1) is given asymptotically by the relation

$$y(z) \sim AF(z) + BG(z)$$

where A and B are complex constants, and where

$$F(z) = \frac{1}{\sqrt{\pi}}\,z^{-1/4}\exp(-\frac{2}{3}z^{3/2})(1 - \frac{5}{48}z^{-3/2} + \cdots)$$

and

$$G(z) = \frac{1}{\sqrt{\pi}}\,z^{-1/4}\exp(\frac{2}{3}z^{3/2})(1 + \frac{5}{48}z^{-3/2} + \cdots),$$

where the principal value is taken for any multi-valued function. The values of the constants A and B depend, of course, on precisely which solution y is being considered (Ai and Bi have different asymptotic behaviour, for instance). More surprisingly, perhaps, the values of A and B may also depend on which region of the complex plane is under consideration. This is known as Stokes' phenomenon, and the rays from the origin that divide the complex plane into different regions are known as Stokes lines. In the current case, there are three Stokes lines, two of which are given by the rays $\arg z = \pm \pi/3$.

In this project, we shall concentrate to start with on the region R given by $|\arg z| < \pi/3$. In that region, the appropriate values of A and B are $\frac{1}{2}$ and 0 respectively for Ai(z); for Bi(z), $B = 1$ but A is not important and can take any value (because $F(z)$ is negligible compared to $G(z)$ for large $|z|$ in R; that is, F is *subdominant*). Hence Ai$(z) \to 0$ and $|\text{Bi}(z)| \to \infty$ as $|z| \to \infty$ in R.

Programming note: You should write your own programs to compute the Airy functions: it is not sufficient simply to use the inbuilt MATLAB functions, or equivalent inbuilt functions for other software packages or programming languages, to calculate Airy functions although they are, of course, a convenient way to check your results. All calculations and evaluations are to be performed for *complex* numbers, not just real ones. You should use MATLAB's 64-bit (8-byte) double-precision floating-point and complex number values or the equivalent in other programming languages. Although MATLAB handles complex numbers quite well, most programming languages handle only real numbers, so you may have to write your own code to perform simple complex number operations such as multiplication.

Question 1 Show that

$$y(z) = \frac{1}{2\pi i} \int_C \exp(zt - \frac{1}{3}t^3)\,\mathrm{d}t$$

is a solution of 1. Here C is any contour that starts at $\infty e^{-2\pi i/3}$ and ends at $\infty e^{2\pi i/3}$. Show furthermore that this solution satisfies $y(0) = \alpha$, $y'(0) = -\beta$ and that it is therefore equal to Ai(z). [*Hint: deform C into two (straight) rays that meet at the origin. You may assume without proof the reflection formula for the Gamma function, viz. $\Gamma(z)\,\Gamma(1-z) = \pi/\sin(\pi z)$.*]

This integral representation of Ai(z) can be used to check the asymptotic expansion given above for large $|z|$, but you are not required to do this.

2 Numerical Integration of the Differential Equation

Question 2 Write a program to find Bi(z) for any $z \in R$, accurate to at least 4 significant figures, by performing a numerical integration of the defining differential equation (1) using any standard method. You should perform your integration along a ray joining the origin to z, using a real variable t to denote distance along the ray: this will require you to find a system of differential equations satisfied by Re y and Im y along the ray. Include the derivation of this system of equations in your write-up as well as the initial conditions (over which you are advised to take care). Also explain what checks you carried out to ensure the accuracy of your solutions. As a very simple first check, you may find it useful to know that Bi$(1) \approx 1.20742$.

Use your program to evaluate Bi(z) at $z = 2, 4, 8, 16, e^{\pm i\pi/6}$ and one other non-real point of your choosing. Draw a graph of the behaviour of the (modulus of the) solution along

one particular non-real ray of your choosing and give a plausible demonstration that the leading order asymptotic behaviour, $G(z)$, is indeed as stated in the Introduction.

Question 3 Modify your program to instead calculate $\text{Ai}(z)$, and try to evaluate $\text{Ai}(z)$ at the same points as in Question 2. You may find it useful to know that $\text{Ai}(1) \approx 0.13529$. Draw a graph of $\text{Ai}(z)$ for real positive z. Which of your evaluations are you confident are accurate? What goes wrong with the method? Why is this unavoidable?

One way to avoid this problem is, instead of integrating from $z = 0$ towards infinity, to start from a value of z with *large* modulus, and step towards the origin. The asymptotic expansion for $\text{Ai}(z)$ (and the derivative of this expansion) can be used to approximate the initial conditions.

Question 4 Explain why this alternative approach should work. Write a program to implement it; start from $|z| = a$, for some large fixed constant a, and integrate towards the origin. Use only the zeroth order term of the asymptotic expansion (i.e., ignore $\frac{5}{48}z^{-3/2}$ and higher order terms in $F(z)$); a more advanced implementation might take more terms into account.

To start with you might like to use $a = 20$; but you should experiment with other values and explain what difference they might make. State the value you finally settle on and why.

Use your program to evaluate $\text{Ai}(z)$ at the same points as in Question 2.

3 Matched expansions

Question 5 By finding series expansions about the origin, or otherwise, prove that the given expressions for the Maclaurin series of $\text{Ai}(z)$ and $\text{Bi}(z)$ are correct.

A much quicker, and more accurate, approach to evaluating the Airy functions is to avoid numerical integration altogether and instead use the analytic series expansions. In theory, the Maclaurin series for Ai and Bi are valid for all z, but in practice they are not very helpful for larger values of $|z|$ because of rounding errors caused by adding together large numbers of terms. Here we will try an approach based on using the Maclaurin series when $|z| < b$, for some fixed constant b, and using the asymptotic expansion when $|z| \geqslant b$; we hope to achieve accuracy at least as high as 4 significant figures, and preferably more.

Question 6 Investigate the feasibility and potential accuracy of this approach for evaluating $\text{Ai}(z)$ on the positive real axis. You should use only the first two terms in the asymptotic expansion (i.e., do not attempt to find more terms in $F(z)$ than are given above), though you may use as many terms of the Maclaurin series as you wish. You should try various different values of b, and experiment with the number of terms to use from the Maclaurin series for best results. What level of accuracy is attainable?

Include a plot of your composite approximation and some sample values close to $|z| = b$.

How did you sum the Maclaurin series in order to minimize rounding errors?

How do you expect the time taken by this algorithm to compare with that for Question 4?

A professional implementation of this method (at least for real z) would use a selection of Chebyshev polynomial approximations in different overlapping regions and choose the best one automatically.

4   Stokes lines

Question 7   Use the programs you have developed in previous questions to describe how the behaviour of Ai and Bi with $|z|$ changes as the rays approach the Stokes line at $\arg z = \pi/3$ from within R.

Question 8   By experimenting with rays *outside* R, determine the location of the third Stokes line. How do Ai and Bi behave on this line?

Question 9   What can you say about the values of A and B in each of the three regions which lie between each pair of Stokes lines? Can you estimate these values from your numerical results?

What, if anything, can you say *on* the Stokes lines?

5   A particle in a constant force field

[Note that no knowledge of Quantum Mechanics is required for this section of the project: all required equations are given below.]

A one-dimensional quantum-mechanical particle is confined to the region $x > 0$ and is subjected to a force of constant magnitude k directed towards the origin. The governing equation for the wavefunction $\psi(x)$ is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + kx\psi = \lambda\psi$$

with boundary conditions $\psi(0) = 0$, $\psi(x) \to 0$ as $x \to \infty$, where λ is the energy of the particle. This is a Sturm–Liouville problem with eigenvalue λ.

Question 10   Show, using your computed results from earlier questions, that there is a discrete set of energy eigenvalues λ_n. Find an approximate value for the first two of these eigenvalues in units where $\hbar^2 k^2/2m = 1$.