

# **Applied Complex Analysis**

## **MATH60006/70006/97028, Chapter Two**

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## 2. Numerical approximation of contour integrals

When evaluating closed contour integrals

$$\oint_{\gamma} f(z) dz$$

there are often times when a residue calculation cannot be used. For example:

- We may not know the locations and/or the orders of the poles of  $f$ .
- We may only have an accurate expression for  $f$  in a neighbourhood of  $\gamma$ .
- Residue calculations can be tedious and prone to errors - we may want to verify such a calculation by evaluating the integral directly.

As is the case with much of applied mathematics and many real-world applications, a numerical approximation is required! The general term for approximating integrals is *quadrature*, which refers to an approximation taking the sum of weighted samples of the integrand:

$$\int_a^b f(x) dx \approx \sum_{n=1}^N f(x_j) w_j \quad (2.1)$$

for weights  $w_j$  and nodes  $x_j$ , for  $j = 1, \dots, N$ . Some rules will have  $N + 1$  nodes, instead of  $N$ .

### 2.1 The trapezium rule

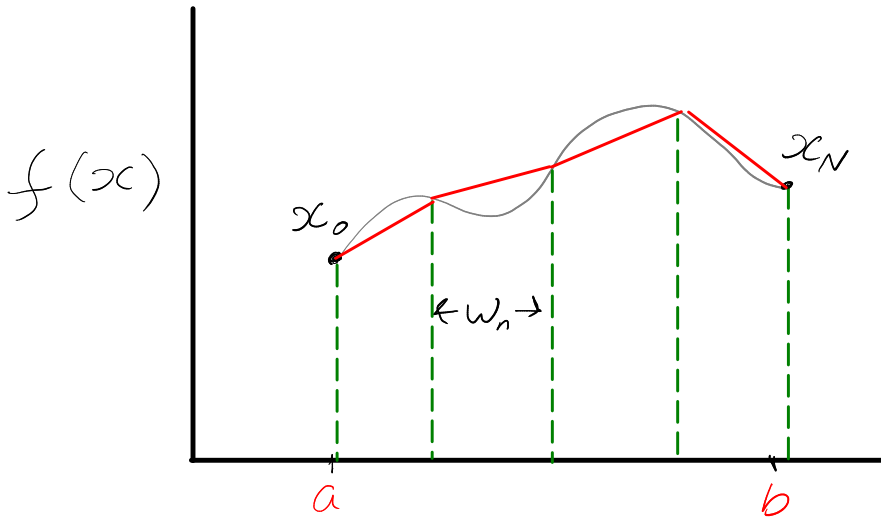


Figure 1: Visualisation of the trapezium rule.

We begin this chapter by recalling one of the simplest quadrature rules:

**Definition 2.1** (Trapezium rule). The  $(N + 1)$ -point trapezium rule is a quadrature rule of the form (2.1) with nodes  $x_j = a + (b - a)j/N$  for  $j = 0, \dots, N$  and weights  $w_0 = w_N = (b - a)/(2N)$  and  $w_j = (b - a)/N$

for  $j = 1, \dots, N - 1$ . Physically, it can be interpreted as approximating the area under the curve by  $N$  trapeziums, as in Figure 1.

In the case where  $f$  is periodic, the 0th and  $N$ th points coincide, and since  $w_0 + w_N = (b - a)/N$ , the trapezium rule can be simplified to an  $N$ -point rule with nodes  $x_j = a + j/N$  and weights  $w_j = (b - a)/N$  for  $j = 1, \dots, N$ .

It is likely that you first came across the trapezium rule back in school, and in many senses, this is as simple as a quadrature rule can get. If you learnt math(s) using American-English, it would have been called the *trapezoidal rule*.

Its simplicity is matched by a relatively slow convergence rate, as shown by the following theorem.

**Theorem 2.2** (Quadratic convergence of trapezium rule). *For an integral*

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

*if  $f$  has a bounded second derivative, then*

$$|I - I_N| = O(N^{-2}), \quad N \rightarrow \infty,$$

*where  $I_N$  is the  $N + 1$  point trapezium rule of Definition 2.1,*

*Proof.* Define the parameter  $h := (b - a)/N$ , which is the width of each trapezium base. Partition the integration range into the sum of smaller integrals over mesh elements defined as follows  $\mathcal{M}_0(x) = [x_0, x_0 + \frac{h}{2}]$ ;  $\mathcal{M}_j(x) = [x_j - \frac{h}{2}, x_j + \frac{h}{2}]$  for  $j = 1, \dots, N - 1$ ;  $\mathcal{M}_N(x) = [x_N - \frac{h}{2}, x_N]$ . Note that  $|\mathcal{M}_j| = w_j = O(h) = O(N^{-1})$  for  $j = 0, \dots, N$ .

$$I = \sum_{j=0}^N \int_{\mathcal{M}_j} f(x) dx$$

Now Taylor expand the integrands on the right-hand side about the midpoint of each integral:

$$I = \sum_{j=0}^N \int_{\mathcal{M}_j} \left( f(x_j) + (x - x_j)f'(x_j) + \frac{(x - x_j)^2}{2} f''(\xi_j(x)) \right) dx$$

where the third term on each line is the Taylor remainder;  $\xi_j \in \mathcal{M}_j$ . Now, moving some terms to the left-hand side, and moving constant terms outside of the integrals,

$$I - \sum_{j=0}^N f(x_j) \int_{\mathcal{M}_j} dx = \sum_{j=0}^N \left( \int_{\mathcal{M}_j} (x - x_j) f'(x_j) dx + \int_{\mathcal{M}_j} \frac{(x - x_j)^2}{2} f''(\xi_j(x)) dx \right)$$

We find the integrals on the left-hand side evaluates to  $|\mathcal{M}_j| = w_j$ , and the first sum of integrals on the right-hand side (linear integrands) are zero for  $j = 1, \dots, N - 1$ . This gives an exact formula for the error in the trapezium rule:

$$I - I_N = \sum_{j \in \{0, N\}} \int_{\mathcal{M}_j} (x - x_j) f'(x_j) dx + \sum_{j=0}^N \int_{\mathcal{M}_j} \frac{(x - x_j)^2}{2} f''(\xi_j(x)) dx.$$

Taking absolute value and moving it inside of the sum and integrand, then bounding,

$$\begin{aligned}
|I - I_N| &\leq \sum_{j \in \{0, N\}} \int_{\mathcal{M}_j} \frac{h}{2} \max_{x \in [a, b]} \{|f'(x)|\} + \sum_{j=1}^N \int_{\mathcal{M}_j} \frac{h^2}{8} \max_{x \in [a, b]} \{|f''(x)|\} dx \\
&= \frac{h^2}{2} \max_{x \in [a, b]} \{|f'(x)|\} + N \frac{h^3}{8} \max_{x \in [a, b]} \{|f''(x)|\} dx \\
&= O(N^{-2}) + N \times O(N^{-3}) \\
&= O(N^{-2}).
\end{aligned}$$

□

The above Theorem tells us that the trapezium rule converges quadratically for  $C^2(a, b)$  functions. As a rule of thumb, in most practical applications where most integrands are piecewise smooth, the midpoint rule should be considered a poor choice. Even if we only have access to equispaced data, Newton-Coates quadrature will converge at a faster rate, and can be made numerically stable by oversampling [3].

There are, however, a few significant (and closely-related) exceptions, which, fortunately, align precisely with our current goal: approximating closed contour integrals of analytic functions. Many applications are covered in the excellent review paper [4], and many of the results in this chapter were taken from, or inspired by this paper.

## 2.2 The trapezium rule on the unit circle

Suppose we want to approximate  $f(0)$  via the Cauchy integral around the unit circle, and that  $f$  is analytic in an annulus containing the circle:

$$I = f(0) = \frac{1}{2\pi i} \oint_{|z|=1} \frac{f(z)}{z} dz. \quad (2.2)$$

We will investigate the trapezium approximation to  $I$ .

Changing variables  $z = e^{i\theta}$ , for  $\theta \in [0, 2\pi]$ , noting that  $dz = ie^{i\theta}d\theta$ , we obtain

$$I = \frac{1}{2\pi} \int_0^{2\pi} f(e^{i\theta}) d\theta. \quad (2.3)$$

Since the integrand is periodic, we may apply the  $N$ -point trapezium rule with where  $\theta_j = 2\pi j/N$ ,  $w_j = 2\pi/N$  for  $j = 1, \dots, N$ . This yields the approximation

$$I \approx I_N = \frac{1}{N} \sum_{j=1}^N f(z_j) \quad (2.4)$$

where  $z_j = e^{2\pi i j/N}$  for  $j = 1, \dots, N$  are the  $N$  roots of unity.

Now for the big reveal. Despite only converging quadratically for analytic functions in general, the trapezium rule converges exponentially fast in the situation we are considering here.

**Theorem 2.3** (Exponential convergence of the trapezium rule for functions analytic inside the circle.). *Suppose  $f$  in (2.3) is analytic and satisfies  $|f(z)| < M$  inside the complex disk  $|z| < r$  for some  $r > 1$ . Then the approximation (2.4) enjoys the following exponential convergence rate:*

$$|I - I_N| \leq \frac{M}{r^N - 1} = O(r^{-N}) \quad \text{as } N \rightarrow \infty.$$

*Proof.* Define the function

$$m(z) = \frac{z^{-1}}{1 - z^{-N}}.$$

Multiplying by  $f$  and rearranging gives,

$$f(z)m(z) = \frac{f(z)}{z - z^{1-N}},$$

from which we can use the usual formula ( $A(x)/B'(x)$ ) to compute the residue

$$\text{Res}(fm, z_j) = \frac{f(z_j)}{1 - (1 - N)z_j^{-N}} = \frac{f(z_j)}{N},$$

hence by the residue theorem

$$\frac{1}{2\pi i} \oint_{|z|=r'} f(z)m(z)dz = I_N, \quad \text{for } r' \in (1, r).$$

We have used  $m(z)$  to convert a sum, specifically the trapezium rule on a circle, to an integral. This is useful; originally we were interested in the difference between a quadrature rule (sum) and the exact integral, but now we are interested in the difference between two integrals. If we deform the contour of  $I$  to the circle  $|z| = r'$ , by Cauchy's theorem this does not change the value of  $I$ , and we can compare like-for-like, hence:

$$I - I_N = \frac{1}{2\pi i} \oint_{|z|=r'} f(z) \left( \frac{1}{z} - m(z) \right) dz$$

is an exact integral representation for the error in the trapezium rule. We now manipulate part of the integrand with elementary adjustments:

$$\frac{1}{z} - m(z) = \frac{1 - z^{-N}}{z(1 - z^{-N})} - \frac{-1}{z(1 - z^{-N})} = \frac{-z^{-N-1}}{1 - z^{-N}} = \frac{-z^{-1}}{z^N - 1}.$$

Our aim is to apply the ML principle, but to bound a fraction above, we need to bound the denominator below. We can apply the negative triangle inequality on the denominator to obtain the desired result.

If you'd like a more physical interpretation - by considering the possible values of  $z^N$  for  $|z| = r'$ , it is clear (draw a circle of radius  $r'$  about the origin and mark  $\{1, r'\}$  on it!) that  $|z^N - 1|$  is minimised when  $z = r'$ , thus  $|z^N - 1| \geq r'^N - 1$ . The result follows by applying the ML principle and letting  $r' \rightarrow r$ .  $\square$

## 2.3 The trapezium rule for periodic analytic functions

Exponential convergence of the trapezium rule was originally observed by Alan Turing in [5], where he used it to calculate zeros of the Riemann-Zeta function. We have proved (in Theorem 2.3) that the trapezium rule converges exponentially fast for a Cauchy integral on the unit circle. This is much better than the quadratic rate predicted by Theorem 2.2, but it is for a very specific class of integral. Can we generalise this to a broader class of closed contour integrals? (Yes.)

In this course, we have frequently used the change of variables  $z = z_0 + Re^{i\theta}$  to transform a closed contour integral

$$I = \oint_{\gamma} \tilde{f}(z) dz$$

for  $f$  analytic in some neighbourhood of  $\gamma$ , into an integral of the form

$$I = \int_0^{2\pi} f(\theta) d\theta \quad (2.5)$$

where  $f(z) = \tilde{f}(z_0 + Re^{i\theta})Re^{i\theta}$  is periodic analytic in some neighbourhood of  $[0, 2\pi]$ . Note that while we have only considered circular parametrisations of  $\gamma$ , any contour  $\gamma$  with an analytic parametrisation (e.g. an ellipse) can be expressed in the form (2.5) with an analytic  $f$ . Similarly to (2.3), we can apply the  $N$ -point trapezium rule with  $\theta_j = 2\pi/N$  to obtain the approximation

$$I \approx I_N = \frac{2\pi}{N} \sum_{j=1}^N f(\theta_j), \quad (2.6)$$

where  $I$  refers to (2.5). The following theorem shows that the trapezium rule converges exponentially for this more general class of integral.

**Theorem 2.4** (Exponential convergence of the trapezium rule for periodic analytic functions). *If  $f$  of (2.5) is  $2\pi$ -periodic and analytic in the strip  $S_a := \{\theta : -a < \text{Im}\theta < a\}$  for  $a > 0$ , then*

$$|I_N - I| \leq \frac{4\pi \sup_{\theta \in S_a} |f(\theta)|}{e^{aN} - 1},$$

where  $I_N$  is the approximation (2.6).

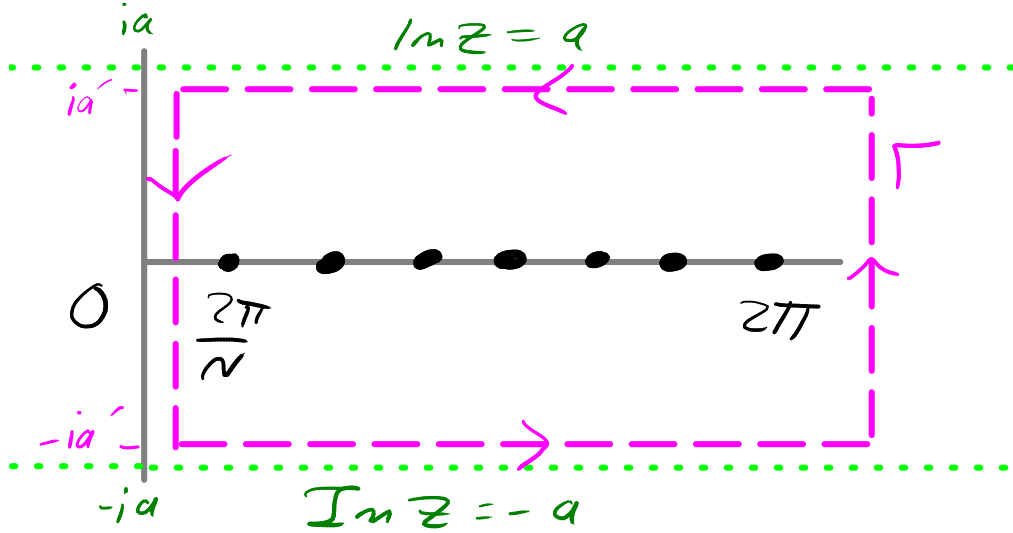


Figure 2: The contour  $\Gamma$  and poles for the proof of Theorem 2.4.

*Proof.* We follow a similar strategy to Theorem 2.3, in that we define a *characteristic function*

$$m(\theta) := \frac{1}{2} \cdot \frac{1 + e^{-iN\theta}}{1 - e^{-iN\theta}}$$

which, due to its simple poles at  $\theta_j = 2\pi j/N$ , enables us to write the periodic trapezium rule (2.6) as an integral:

$$I_N = \oint_{\Gamma} f(\theta) m(\theta) d\theta,$$

where  $\Gamma$  is any closed contour containing  $\{\theta_j\}_{j=1}^N$ . We will choose a rectangular contour, as in Figure 2, with the top and bottom at  $\text{Im} z = \pm a' \leq \pm a$ , and the vertical sides at  $\pi/N$  and  $2\pi + \pi/N$ . Our original integral is *not* expressed over a contour, so before we can compare like-for-like, we need to adjust this a little. The idea is to deform  $[0, 2\pi)$  onto a rectangular contour above the real line  $\gamma_+$ , specifically onto three sides of a rectangle, and add this to analogous deformation below the real line  $\gamma_-$ , hence

$$I = - \int_{\gamma_+} f(\theta) d\theta = \int_{\gamma_-} f(\theta) d\theta.$$

These contours can be combined to form a closed rectangular contour (with four sides)  $\Gamma = \gamma_+ \cup \gamma_-$ , which (as before) is chosen to contain  $\{\theta_j\}_{j=1}^N$  in its interior:

$$I = \int_{0+2\pi/N}^{2\pi+2\pi/N} f(\theta) d\theta = \frac{1}{2} \oint_{\Gamma} f(\theta) \mu(\theta) d\theta,$$

where the first step follows by the  $2\pi$ -periodicity of  $f$ , and

$$\mu(\theta) = \begin{cases} -1 & \text{if } \text{Im}\theta \geq 0, \\ +1 & \text{if } \text{Im}\theta < 0 \end{cases}$$

takes care of the different orientation / sign in each integral. Now we can write

$$I_N - I = \oint_{\gamma} f(\theta) (m(\theta) - \mu(\theta)) d\theta$$

On each smaller (three-sided) rectangle  $\gamma_{\pm}$ , because the vertical components of the rectangles are exactly  $2\pi$  apart, the contributions from the vertical components will cancel due to periodicity of  $f$ . Hence we only need to estimate the contribution from top and bottom horizontal components of  $\Gamma$ , which can be expressed as

$$\begin{aligned} I_N - I &= -\frac{1}{2} \int_{\frac{\pi}{N}+ia'}^{2\pi+\frac{\pi}{N}+ia'} (m(\theta) + 1) f(\theta) d\theta + \frac{1}{2} \int_{\frac{\pi}{N}-ia'}^{2\pi+\frac{\pi}{N}-ia'} (m(\theta) - 1) f(\theta) d\theta \\ &= \int_{\frac{\pi}{N}+ia'}^{2\pi+\frac{\pi}{N}+ia'} \left( \frac{1}{e^{iN\theta} - 1} \right) f(\theta) d\theta - \int_{\frac{\pi}{N}-ia'}^{2\pi+\frac{\pi}{N}-ia'} \left( \frac{1}{e^{-iN\theta} - 1} \right) f(\theta) d\theta \end{aligned}$$

The result follows by the ML principle. □

The above result generalises<sup>1</sup> Theorem 2.3 to a larger class of problems. If a closed contour  $\gamma$  has a parametrisation  $s(\theta)$  for  $[0, 2\pi)$  which is analytic, then the trapezium rule converges exponentially as  $N \rightarrow \infty$ . It is worth noting that the integral  $I$  may be defined entirely in terms of real numbers, but complex analysis still serves a practical purpose providing this proof. It is also possible to prove this result using Fourier series, alternative methods of proof are given in [4]. I have chosen this approach because (1) you

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<sup>1</sup>This is not a strict generalisation; if one applied a change of variables to Theorem 2.3 and then applied Theorem 2.4, the constant is twice as large, due to the theorem being to a function analytic in an annulus, rather than a circle.



are now all experts in residue calculus, and (2) we will return to the idea of a characteristic function later in the course - these can be used to *improve* convergence of a quadrature rules, rather than just analyse them. Now we consider a couple of examples of how we can apply the above theorem.

**Example 2.5.** *Estimate the error when the trapezium rule is applied to the integral*

$$I = \oint_{\gamma} \frac{e^{iz}}{z^2 + 2} dz$$

and  $\gamma$  is the unit circle.

Parametrising as usual  $z = e^{i\theta}$  we obtain

$$I = i \int_0^{2\pi} \frac{e^{ie^{i\theta}}}{e^{2i\theta} + 2} e^{i\theta} d\theta.$$

First, we must determine the domain of analyticity. Clearly the integral is singular for  $\theta$  such that

$$e^{2i\theta} + 2 = 0 \implies e^{2i\theta} = -2$$

now taking complex logarithms of both sides,

$$2i\theta = \log |2| + i\pi + 2\pi ki, \quad \text{for } k \in \mathbb{Z},$$

hence the singularities are at  $\theta = -\log |2|/2 + \pi/2 + k\pi$  for  $k \in \mathbb{Z}$ .

Now we can deduce the analytic strip around  $\mathbb{R}$ , this is  $|\text{Im}z| < a$  for  $a = \log(2)/2 \approx 0.34657$ . Hence, by Theorem 2.4, convergence is

$$|I - I_N| = O(e^{-a'N}), \quad N \rightarrow \infty$$

for any  $a' < a$ , noting that  $M$  (the maximum value) is unbounded at  $a' \rightarrow a$ , so we have to choose  $a'$  to be a little smaller.

**Example 2.6.** *Estimate the error, when using the trapezium rule on a circle of radius one, to approximate derivatives of*

$$f(z) = \frac{e^z - 1 - z}{z^2}.$$

Cauchy's integral theorem tells us

$$f^{(m)}(z_0) = \frac{m!}{2\pi i} \int_{\gamma} \frac{f(z)}{(z - z_0)^{m+1}} dz,$$

parametrising with  $z = z_0 + e^{i\theta}$ ,

$$f^{(m)}(z_0) = \frac{m!}{2\pi} \int_{\gamma} f(z_0 + e^{i\theta}) e^{-mi\theta} dz.$$

We first show that  $f(z)$  has a removable singularity at  $z = 0$ , expanding  $e^z$  shows

$$f(z) = \sum_{n=2}^{\infty} \frac{z^{n-2}}{n!} \implies f(z) \rightarrow 1/2 \text{ as } z \rightarrow 0,$$

confirming the removable singularity at zero. Our integrand is therefore entire (analytic in all of  $\mathbb{C}$ ), and thus when applying Theorem 2.4 we can choose  $a$  to be any value we like. We seek an optimal value. Re-indexing the sum, and bounding term-by-term via the triangle inequality:

$$|f(z)| \leq \sum_{n=0}^{\infty} \frac{|z|^n}{(n+2)!} \leq \sum_{n=0}^{\infty} \frac{|z|^n}{n!} = e^{|z|}.$$

Thus, our integrand is:

$$M = O\left(\exp\left(|e^{i\theta}| + m|\operatorname{Im}\{\theta\}|\right)\right).$$

Noting that Theorem 2.4 predicts convergence like  $O(e^{-aN})$ , we seek an  $a$  which is in some sense optimal. Bounding  $M$  further, and multiplying by the convergence rate,

$$Me^{-aN} = O(\exp(e^a + a(m - N))).$$

Let  $\varphi(a)$  be the argument of the exponent, and let's use calculus to find the optimal  $a$ .

$$\varphi'(a) = e^a + (m - N)$$

setting  $\varphi'(\tilde{a}) = 0$  and rearranging gives

$$\tilde{a} = \log(N - m)$$

differentiating again

$$\varphi''(a) = e^a > 0,$$

for all  $a \in \mathbb{R}$ , thus  $\tilde{a}$  is the minimum value of  $\varphi$ . Hence, choosing  $a = \tilde{a}$ , we have

$$Me^{-\tilde{a}N} = O(\exp(N - m + \log(N - m)(m - N))).$$

Absorbing the constants and focusing on large  $N$ , things become a little clearer:

$$Me^{-\tilde{a}N} = O(e^N N^{-N}) = O((N/e)^{-N}), \quad N \rightarrow \infty$$

which, despite the exponentially growing term, will result in is super-exponential decay/convergence. In practice however, we may have already reached machine precision accuracy before this rate becomes visible.

### Exactness of Trapezium rule for band-limited functions

You may have previously studied *Gaussian quadrature* in a numerical methods class, which enjoys the celebrated *polynomial exactness* property: An  $N$ -point Gauss rule can *exactly* evaluate the integral of a degree  $2N - 1$  polynomial. An analogous result holds for the trapezium rule for band-limited functions, equivalently, functions with a finite number of terms in the Laurent expansion.

**Theorem 2.7** (Exactness of the Trapezium Rule). *If a function  $f$  has a Laurent expansion of the form*

$$f(z) = \sum_{j=-N}^{N-2} a_j (z - z_0)^j,$$

*for  $z$  in some annulus  $D$ , then an  $N$ -point trapezium rule  $I_N$  can exactly approximate*

$$I = \oint_{\gamma} f(z) dz,$$

*where  $\gamma$  is a closed anti-clockwise-oriented contour in  $D$ .*

*Proof.* Deforming  $\gamma$  onto some circle in  $D$  of radius  $r$ , setting  $z = z_0 + re^{i\theta}$ , we have

$$I = \int_0^{2\pi} f(z_0 + re^{i\theta}) ire^{i\theta} d\theta = i \int_0^{2\pi} \sum_{j=-N}^N a_j r^{j+1} e^{(j+1)i\theta} d\theta$$

after substituting the Laurent expansion and simplifying. Now applying the trapezium rule to this integral, with  $\theta_n = 2\pi n/N$ , and weights  $2\pi/N$  we find

$$I_N = \frac{2\pi i}{N} \sum_{j=-N}^{N-2} \sum_{n=1}^N a_j r^{j+1} e^{2\pi(j+1)n/N} = \frac{2\pi i}{N} \sum_{j=-N}^{N-2} a_j r^{j+1} \sum_{n=1}^N e^{2\pi(j+1)n/N}. \quad (2.7)$$

Now the inner sum on the right-hand side can be considered as two cases. The first case, when  $(j+1)/N \in \mathbb{Z}$ , leads to

$$\sum_{n=1}^N e^{2\pi(j+1)n/N} = \sum_{n=1}^N e^{2\pi i} = N.$$

The second case,  $(j+1)/N \notin \mathbb{Z}$ , results in a sum of points equispaced around the unit circle. The average of these points will be zero,

$$\frac{1}{N} \sum_{n=1}^N e^{2\pi(j+1)n/N} = 0,$$

thus multiplying both sides by  $N$ ,

$$\sum_{n=1}^N e^{2\pi(j+1)n/N} = 0,$$

for the second case. Due to the range of the outer sum of (2.7),  $j = -N, \dots, N-2$ , the only time  $(j+1)/N \in \mathbb{Z}$  is when  $j = -1$ , and thus, this is the only non-zero summand in the outer sum of (2.7). Therefore,

$$I_N = \frac{2\pi i}{N} r^0 a_{-1} N = 2\pi i a_{-1}$$

We know from residue theory earlier in the course that this is the exact value of the integral;

$$I = 2\pi i a_{-1}.$$

□

Much like the polynomial exactness result for Gaussian quadrature, this is rarely useful practically (to the best of my knowledge). For integrals of polynomials, we can simply integrate by hand. Similarly, for closed contour integrals of Laurent polynomials, we can use residue calculus. There are exceptions. The simplest may be that you have been asked to write a trapezium rule for closed contour integrals (as you will be soon!) and you want to test it. This is the subject in the following (brief) example.

*The following Jupyter notebook example can be run interactively in a browser by clicking on **this link**.*

## 1 Testing the trapezium rule on a circle

```
[3]: function closed_circle_contour_int(f, N, z_0, r)
      z(θ) = z_0 + r*exp(im*θ)
      dz(θ) = im*r*exp(im*θ)
      θ_nodes = 2*π*[n for n=1:N]/N
      weight = 2π / N
      weight * sum(f.(z.(θ_nodes)) .* dz.(θ_nodes))
end
```

[3]: closed\_circle\_contour\_int (generic function with 1 method)

**First test:** a polynomial of degree greater than  $N - 2$ . We know from Cauchy's integral theorem that

$$\oint f(z)dz = 0$$

But due to our choice of degree, the approximation should not be accurate.

```
[8]: f(z) = 2z^3 - 5z^4
      N = 5
      closed_circle_contour_int(f, N, 0, 1)
```

[8]: -2.1974153077364703e-14 - 31.415926535897928im

**Second tests:** We fix the above inaccuracy by (first) increasing  $N$  and (second) reducing the polynomial degree. We now expect to see zero, up to machine precision ( $10^{-16}$ ).

```
[10]: f(z) = 2z^3 - 5z^4
       N = 6
       closed_circle_contour_int(f, N, 0, 1)
```

[10]: 9.591153752931802e-15 - 6.045638729881628e-15im

```
[12]: f(z) = 2z^3
       N = 5
       closed_circle_contour_int(f, N, 0, 1)
```

[12]: 1.6252100484418195e-15 + 1.6741768790441432e-15im

**Third tests:** Let's add a simple pole to our polynomial. For any polynomial  $p$ , from residue theory we expect

$$\oint_{\gamma} p(z) + \frac{1}{z} dz = 2\pi i,$$

again, to machine precision accuracy.

```
[14]: f(z) = 2z^3 + z^(-1)
      N = 5
      closed_circle_contour_int(f, N, 0, 1)
```

```
[14]: 1.3461805686011284e-15 + 6.283185307179589im
```

```
[109]: display(2π*im)
```

```
0.0 + 6.283185307179586im
```

**A slightly more interesting example**

```
[5]: f(z) = (z^2 + z^(-2) - 2)/(-4*im*z)
      N = 2
      closed_circle_contour_int(f, N, 0, 1)-π
```

```
[5]: -3.141592653589793 + 0.0im
```

```
[ ]:
```

## 2.4 Applications of closed contour integrals

### 2.4.1 Stable evaluation near removable singularities

Functions with removable singularities are analytic and well-behaved *in theory*; in practice however, such functions typically require cancellation of very large numbers, which can lead to numerical instabilities close to the removable singularity.

To understand this in a bit more detail, we briefly consider how 64-bit double precision floating point numbers are stored:

$$(-1)^S \times 2^{E-1023} \times (1 + M)$$

where one bit is allocated for the sign  $S$ , 11 bits are allocated for the exponent  $E$ , and 52 bits are allocated for the Manissa  $M$ , this gives us 16 digits of precision. This could just be interpreted as a binary form of standard scientific representation. If the difference of two numbers is significantly smaller than the magnitude of those two numbers, we are combining two numbers with a similar (or equal) value of  $E$ , to produce one with a significantly smaller value of  $E$ . For example, on a computer:

$$1.000000012345678 - 1.0000000000000000 = 0.000000012345678$$

We are moving from 16 significant digits to 8 significant digits - the only way to get 16 significant digits on the right-hand side would be to start with 24 digits in both numbers on the left-hand side.

As an analogy, imagine you take a photograph, and then you decide you just want to keep a small part of that picture. If you did not take the original picture at a high enough resolution, then your zoomed-in image will be grainy, and there is no way to reconstruct the resolution. Rounding errors occur because we require more numerical detail than was originally stored.

This is highlighted in the following example:

**Example 2.8.** *The function*

$$f(z) = \frac{e^z - 1 - z}{z^2},$$

*has a removable singularity at  $z = 0$  (as shown in an earlier example). Let's consider what happens in a numerical evaluation of  $f(\varepsilon)$ , for small  $\varepsilon$ . Theoretically, a simple Taylor expansion can show that  $\exp(\varepsilon) - 1 - \varepsilon = O(\varepsilon^2)$ , but  $\exp(\varepsilon) = O(1)$  and  $-1 = O(1)$ , so the top of the fraction will be subject to rounding errors. Indeed, choosing  $\varepsilon = 10^{-8}$  means that  $\varepsilon^2 = 10^{-16}$ , thus we are losing significant 16 digits of information on the top of the fraction, which in standard machine precision, is all of our digits! So we expect the answer to be complete nonsense.*

The following Jupyter notebook example can be run interactively in a browser by clicking on ***this link***.

```
[1]: include("trapezium.jl")
      using Plots, LaTeXStrings
```

Define our function  $f$ , and instead of  $\epsilon$  I am writing `small_val`, (due to technical formatting reasons about converting this notebook into a form which can be imported into your lecture notes :/)

```
[2]: f(z) = (exp(z) - 1 - z) / z^2
      small_val = 10^(-8)
```

1.0e-8

To machine precision (16 digits), the correct value is  $f(x) = 0.500000001666667$

```
[3]: f_at_small_val = 0.500000001666667
```

0.500000001666667

Represent via Cauchy integral around unit circle

$$f(x) = \frac{1}{2\pi i} \int_{|z|=1} \frac{f(z)}{z-x} dz = \frac{1}{2\pi i} \int_0^{2\pi} \frac{f(z(\theta))}{z(\theta)-x} \frac{dz}{d\theta}(\theta) d\theta$$

where we have made the usual change of variable  $z(\theta) = e^{i\theta}$ .

```
[7]: z(θ) = exp(im*θ)
      dz_dθ(θ) = im*exp(im*θ)
```

`dz_dθ` (generic function with 1 method)

Now define the integrand as  $U(\theta)$  for simplicity, and define the  $N$ -point trapezium rule approximation:

$$f(x) = \frac{1}{2\pi i} \int_0^{2\pi} U(\theta) d\theta \approx f_N(x) = \frac{1}{N} \frac{1}{2\pi i} \sum_{j=1}^N U(\theta_j)$$

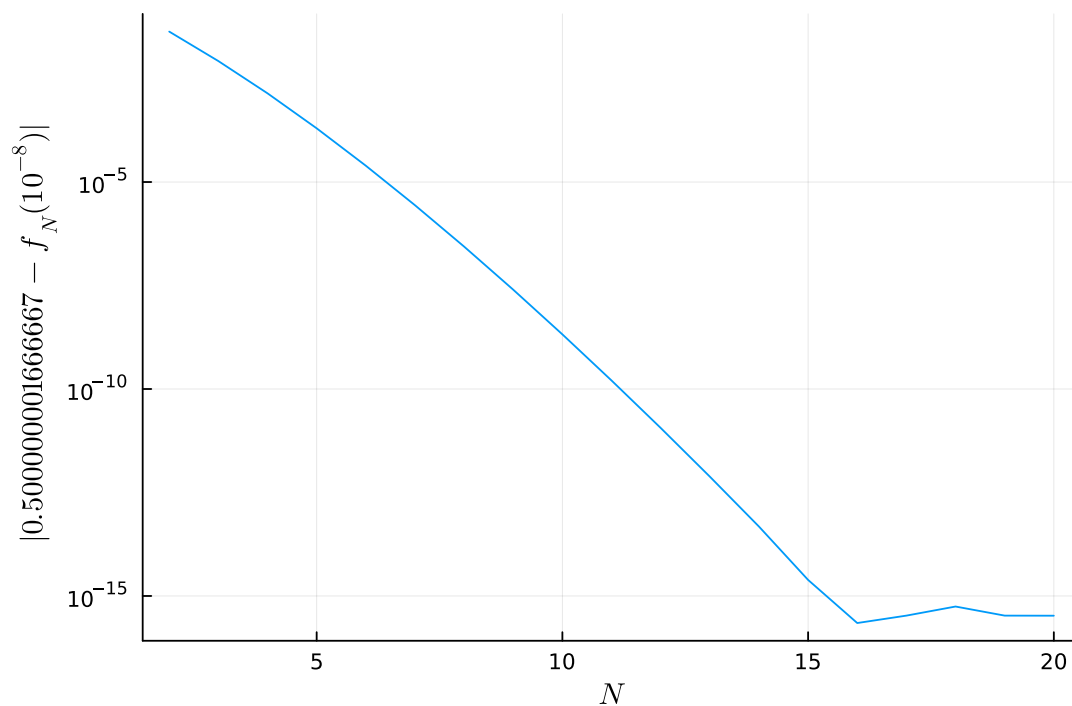
where  $\theta_j := 2\pi j/N$  for  $j = 1, \dots, N$ .

Note that `trap` used below is defined in a neighbouring `trapezium.jl` file, which is imported as the top of this one.

```
[ ]: U(θ, x) = f(z(θ)) * dz_dθ(θ) / (z(θ) - x) #integrand for Cauchy integral
      f_N(x, N=10) = (1/(2π*im)) * trap(θ->U(θ, x), N, periodic=true) # trapezium rule
      ↪ approximation
      # defaults to N=10 points
```

f\_N (generic function with 2 methods)

```
[6]: #plot the difference between the estimates and f(small_val)
N_range = 2:20
plot(N_range, abs.(f_at_small_val .- f_N.(small_val, N_range)),
      xlabel=L"N",
      ylabel=L"|0.500000001666667-f_N(10^{-8})|",
      yaxis=:log, labels="")
```





### 2.4.2 The argument principle

We now consider the following result:

**Theorem 2.9** (Argument principle). *For  $f$  meromorphic (all non-analytic points are poles), and  $g$  analytic in  $\Omega$ ,*

$$\frac{1}{2\pi i} \oint_{\gamma} \frac{f'(z)}{f(z)} g(z) dz = \sum_{a \in \{\text{zeros of } f\}} g(a) m_a - \sum_{b \in \{\text{poles of } f\}} g(b) m_b.$$

where  $m_a$  and  $m_b$  represent the order of the zeros and poles respectively,  $\gamma$  is a closed contour in  $\Omega$  with no loops, such that  $f(z) \neq 0$  for  $z \in \gamma$ .

*Proof.* Suppose  $z_0$  is a zero of  $f$ , order  $m$ . We know from a theorem in the previous chapter that we can write  $f(z) = (z - z_0)^m \phi(z)$ , for analytic  $\phi$  with  $\phi(z_0) \neq 0$ . By the product rule,

$$f'(z) = m(z - z_0)^{m-1} \phi(z) + (z - z_0)^m \phi'(z),$$

thus

$$\frac{f'(z)}{f(z)} g(z) = \frac{m(z - z_0)^{m-1} \phi(z) + (z - z_0)^m \phi'(z)}{(z - z_0)^m \phi(z)} g(z) = \frac{mg(z)}{z - z_0} + \frac{\phi'(z)g(z)}{\phi(z)}.$$

Likewise, if  $z_0$  is a pole of order  $m$ , we have  $f(z) = (z - z_0)^{-m} \varphi(z)$  for analytic  $h$  with  $\varphi(z_0) \neq 0$ , and

$$\frac{f'(z)}{f(z)} g(z) = \frac{-mg(z)}{z - z_0} + \frac{\varphi'(z)g(z)}{\varphi(z)}.$$

Clearly the function  $gf'/f$  is analytic except for zeros and poles of  $f$ . By summing residues at these points, we obtain the result.  $\square$

This can be useful in a variety of situations. It is often applied to analytic  $f$  with  $g = 1$ , in which case the integral counts the number of roots inside  $\omega$ . We now demonstrate with a couple of examples.

**Example 2.10.** *Find (numerically) all roots of  $f(x) = \sin(x) - \cos(2x) + e^{3x}$  inside the unit circle.*

*We can compute by hand  $f'(x) = \cos(x) + 2\sin(2x) + 3e^{3x}$ . Thus, assuming that  $f(z) \neq 0$  on the unit circle  $\gamma = \{|z| = 1\}$ , we can write*

$$I = \frac{1}{2\pi i} \oint_{|z|=1} \frac{\cos(z) + 2\sin(2z) + 3e^{3z}}{\sin(z) - \cos(2z) + e^{3z}} dz$$

*to count the number of roots. Let's pause to appreciate this surprising fact for just a moment:*

$$I \in \mathbb{N}_0.$$

*To approximate, we change variables  $z = e^{i\theta}$ , and write*

$$I = \frac{1}{2\pi} \int_0^{2\pi} e^{i\theta} \frac{\cos(e^{i\theta}) + 2\sin(2e^{i\theta}) + 3e^{3e^{i\theta}}}{\sin(e^{i\theta}) - \cos(2e^{i\theta}) + e^{3e^{i\theta}}} d\theta.$$

*We now approximate this integral with the  $N$ -point periodic trapezium rule. As we don't know the location of the zeros, we cannot determine the strip in which the integrand is analytic, thus we cannot estimate a in Theorem 2.4, nor can we bound  $f$  in the corresponding analytic strip. Therefore, we cannot predict the accuracy of the trapezium rule, but we can be sure that it will converge exponentially to some integer.*

The following Jupyter notebook example can be run interactively in a browser by clicking on **this link**.

```
[40]: include("trapezium.jl")
      using Plots, LaTeXStrings
```

This notebook example uses the argument principle to count and find zeros of the analytic function

$$f(z) = \sin(z - 1) + \cos(4z) + e^{3z}.$$

Initially, we will define our function  $f$  and perform a suitable change of variables to integrate around the circle.

```
[42]: # function with unknown zeros:
      f(z) = sin(z-1) + cos(4z) + exp(3z)

      # its derivative
      df_dz(z) = cos(z-1) - 4sin(4z) + 3exp(3z)
```

```
[42]: df_dz (generic function with 1 method)
```

```
[44]: # change integration variable
      z(r,θ,z) = z + r*exp(im*θ)
      dz_dθ(r,θ) = im*r*exp(im*θ)

      # default to unit circle to simplify syntax
      z(θ) = z(1,θ,0)
      dz_dθ(θ) = dz_dθ(1,θ)

      # resulting integrand of argument principle
      F(θ) = (1/(2π*im)) * df_dz(z(θ))/f(z(θ)) * dz_dθ(θ)
```

```
[44]: F (generic function with 1 method)
```

Let's assume that there are no zeros on the unit circle, and apply the argument principle, which says that

$$I = \frac{1}{2\pi i} \int_{|z|=1} \frac{f'(z)}{f(z)} dz = \int_0^{2\pi} F(\theta) d\theta$$

is equal to the number of zeros inside the unit circle. We will use the trapezium rule, as this will converge exponentially fast.

```
[46]: # test for a smallish number of points
      println("15-point trapezium rule estimates the number of zeros as: ",
```

```
trap(F, 15, periodic=true))
```

15-point trapezium rule estimates the number of zeros as: 3.009675822582812 - 3.4097361544549064e-16im

We know the answer is an integer, and it's looking likely to be 3. Note that the exact integral may be three, but there may be just two, or one zeros - there will only be three zeros if each zero is simple. Let's perform a numerical test to check if the midpoint approximation converges to 3.

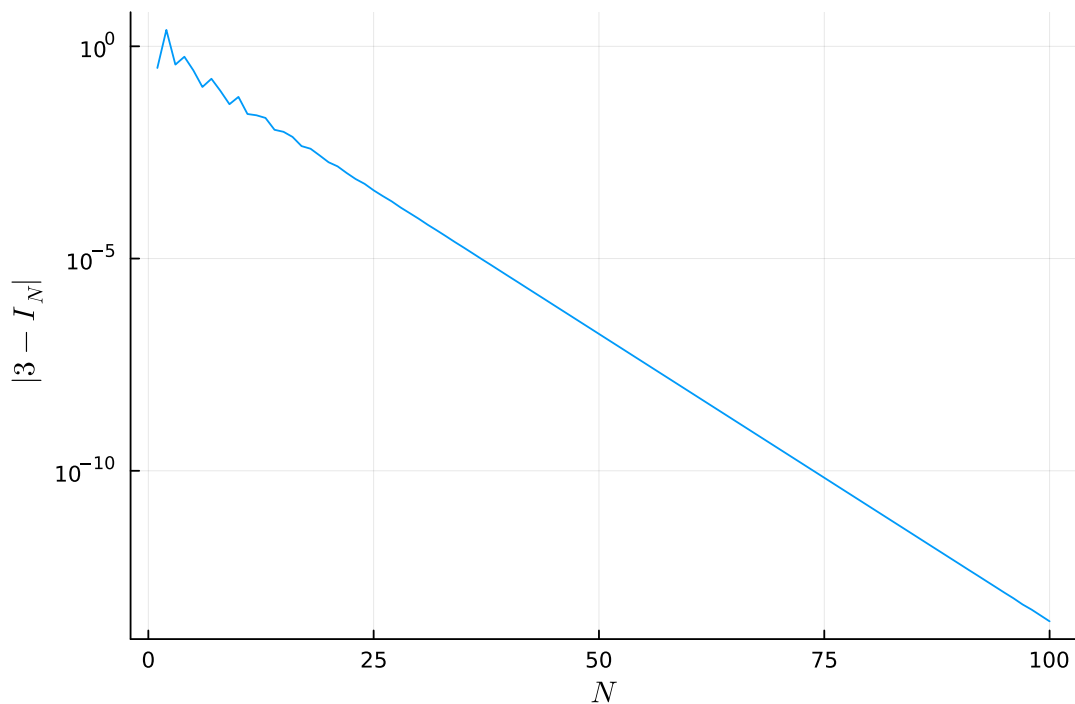
```
[54]: N_range = 1:100 # range of points to apply trapezium rule
```

```
#initialise blank vector of approximations
count_ests = zeros(ComplexF64, length(N_range))

# record estimate for each N
for N in N_range
    count_ests[N] = trap(F, N, periodic=true)
end

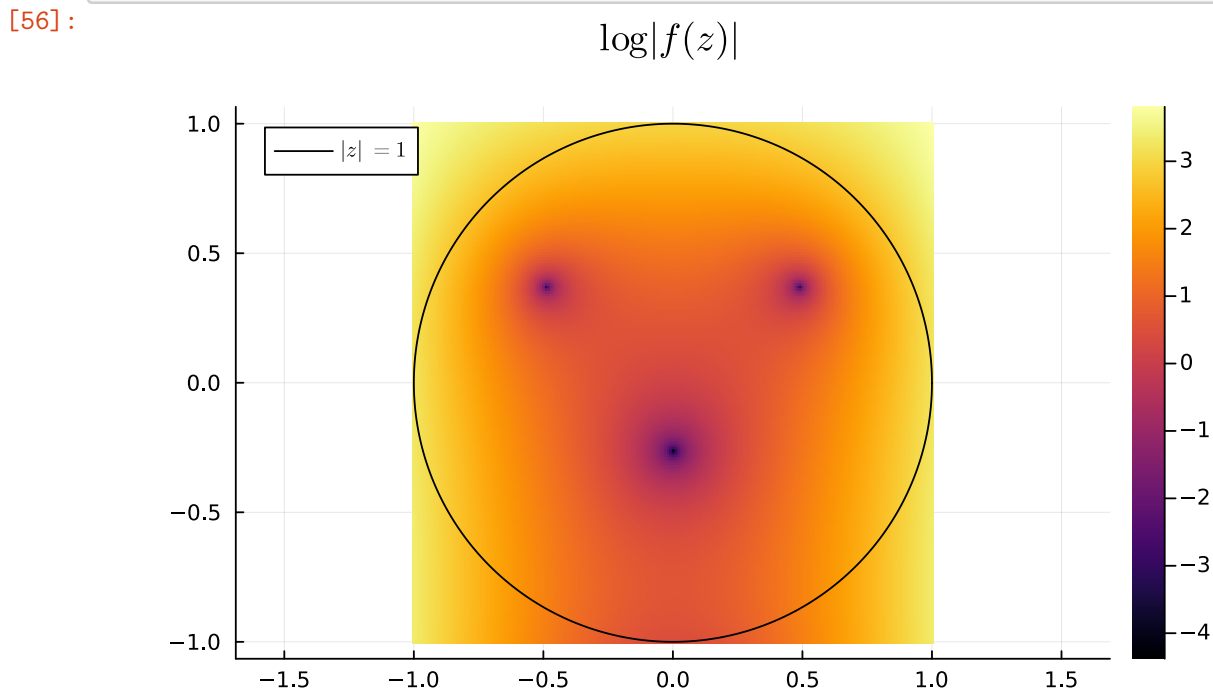
#plot the difference between the estimates and 3
plot(N_range, abs.(3 .- real.(count_ests)),
      xlabel=L"N",
      ylabel=L"|3-I_N|",
      axis=:log, labels="")
```

```
[54]:
```



Now let's plot the  $\log|f|$  in the unit circle and look for large negative values, as a (more computationally expensive) rough way of looking for zeros.

```
[56]: r = 1.0 #radius of square
      δ = 0.01 #pixel size for plot
      t = -r:δ:r
      z_vals = t .+ (im*t')
      heatmap(t, t, log.(abs.(f.(z_vals))))
      plot!(real(z.(0:δ:2π)),
             imag(z.(0:δ:2π)),
             color=:black,
             label=L"$|z|=1$",title=L"$\log|f(z)|$",
             aspect_ratio=1)
```

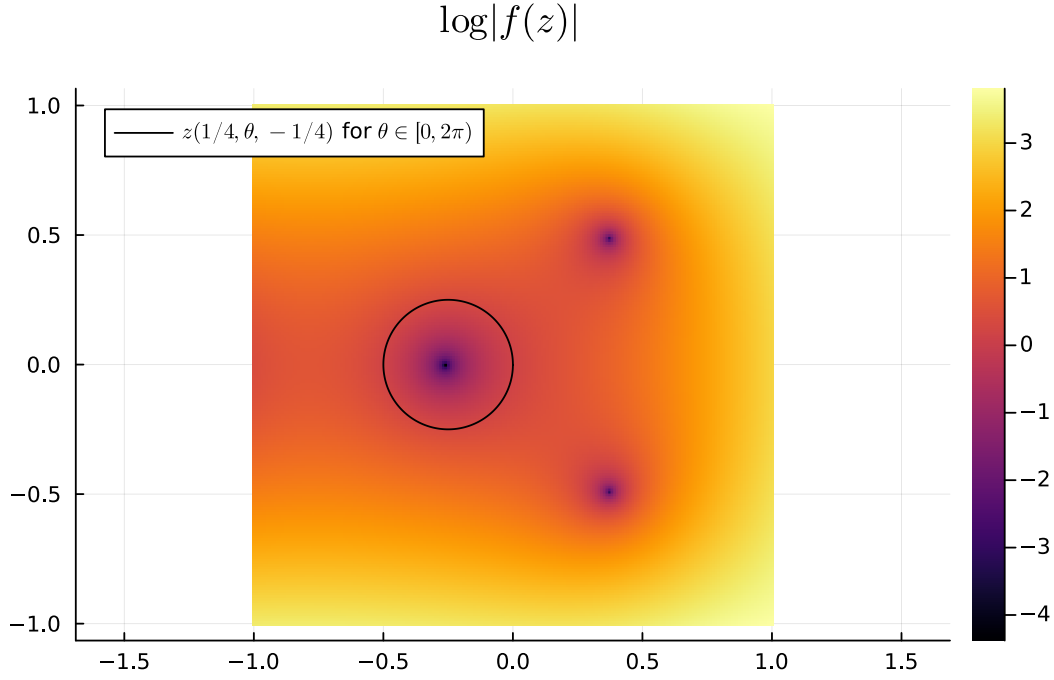


We see that there are definitely three zeros! Now let's use the argument principle again, to get the value of the zero in the left half-plane. Start by putting a smaller ball around that one:

```
[58]: heatmap(t, t, log.(abs.(f.(z_vals))))'
      r = 1/4
      z = -1/4
      plot!(real(z.(r,0:δ:2π,z)),
             imag(z.(r,0:δ:2π,z)),
             color=:black,
             label=L"$z(1/4,\theta,-1/4)$ for $\theta\in[0,2\pi)$",
```

```
title=L"$\log|f(z)|$",
aspect_ratio=1)
```

[58]:



Now use these values of  $r, z_0$  to construct the circle that we search inside. As we expect there is just one zero in here, we can modify the argument principle slightly, to find this zero  $z_0$  such that  $f(z_0) = 0$ :

$$z_0 = \frac{1}{2\pi} \oint_{\gamma} \frac{f'(z)}{f(z)} z \, dz = \int_0^{2\pi} G(\theta) \, d\theta,$$

where

$$G(\theta) = \frac{1}{2\pi i} \frac{f'(z(1/4, \theta, -1/4))}{f(z(1/4, \theta, -1/4))} z(1/4, \theta, -1/4) \frac{dz}{d\theta}(z(1/4, \theta, -1/4)),$$

noting the new circle  $z(1/4, \theta, -1/4) = -\frac{1}{4} + e^{i\theta}/4$ .

In terms of the theorem statement, this returns the value of  $g(z) = z$  at  $z_0$ , i.e. the zero  $z_0$ .

```
[60]: # resulting integrand of argument principle
G(theta) = (1/(2*pi*im)) * df_dz(z(r,theta,z))/f(z(r,theta,z)) * dz_dtheta(r,theta) * z(r,theta,z)
```

[60]: G (generic function with 1 method)

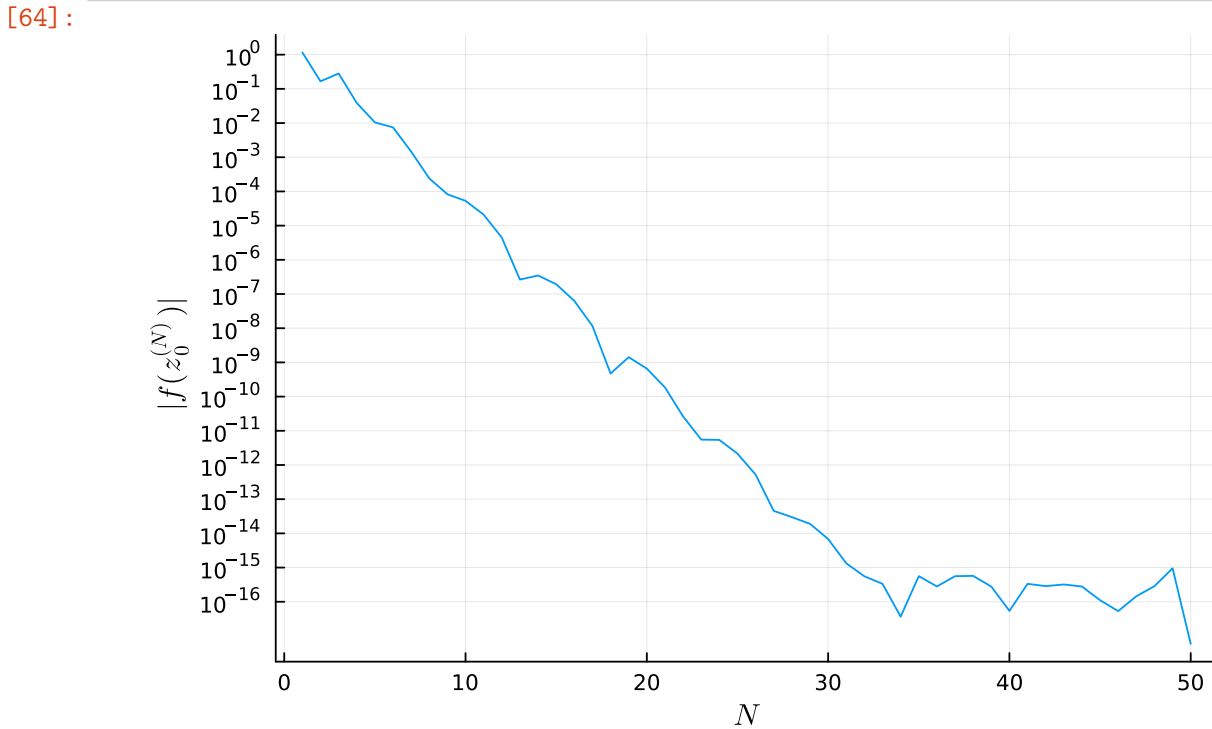
```
[62]: # now we know there is just one zero, we can estimate it using the argument_
      ↪principle:
println("100-point trapezium rule estimates the zero as: ", trap(G, 100))
```

100-point trapezium rule estimates the zero as:  $-0.2624416049064458 - 6.906480170210255e-17im$

Finally, we compute the  $N$ -point trapezium rule approximation to  $z_0^{(N)}$ , and measure the convergence of residual error  $|f(z_0^{(N)})|$  (as we do not know the exact value of  $z_0$ )

```
[64]: # resulting integrand of argument principle
G(θ) = (1/(2π*im)) * df_dz(z(r,θ,z))/f(z(r,θ,z)) * dz_dθ(r,θ) * z(r,θ,z)

# evaluate using trapezium rule
N_range = 1:50
zero_ests = zeros(ComplexF64, length(N_range))
for N in N_range
    zero_ests[N] = trap(G, N, periodic=true)
end
plot(N_range, abs.(f.(zero_ests)),
     xlabel=L"N",
     ylabel=L"|f(z^{(N)})_0|",
     yaxis=:log,
     yticks=:10.0.^(-16:1:0),
     labels="")
```



Reading off the above chart, we observe close to machine (residual) error ( $10^{-16}$ ) with  $N = 33$

```
[66]: println("33-point trapezium rule estimates the zero as: ", trap(G, 33), "; with_↵  
↵residual error: ", f(trap(G, 33)))
```

```
33-point trapezium rule estimates the zero as: -0.2624416049064456 -  
4.011683991942889e-18im; with residual error: 3.3306690738754696e-16 -  
2.0611634816863823e-17im
```

```
[ ]:
```

## 2.5 The trapezium rule for unbounded contours

In Chapter One, a common technique for evaluating integrals  $\int_{-\infty}^{\infty} f(x)dx$  for absolutely integrable  $f$  was to close the integral in a semi-circle of radius  $r$ , and compute the residue contribution from inside this closed integral. We then let  $r \rightarrow \infty$  and show contribution from the semi-circular arc was zero in this limit.

This isn't always possible, for example, if  $f(x) = e^{ix^2}/(1+x^2)$ . Here  $f(x)$  grows exponentially for  $\arg x \in (\pi/2, \pi)$  or  $\arg x \in (-\pi/2, 0)$ , because then  $ix^2 > 0$ , and the contribution from the semicircular arc does not vanish as  $|x| \rightarrow \infty$ . In such a case, numerical approximation of the integral may be necessary.

Our process here will follow similarly to the case for closed contours; we will define a version of the trapezium rule for integrals on  $\mathbb{R}$ , use complex analysis to show that it converges exponentially, and then apply it to some practical applications in complex variables.

**Definition 2.11** (Trapezium rule on  $\mathbb{R}$ ). For an integral  $I = \int_{\mathbb{R}} f$ , for some  $h > 0$  we define the *unbounded* Trapezium rule  $I_h \approx I$  as

$$I_h := h \sum_{j=-\infty}^{\infty} f(x_j),$$

where  $x_j = jh$ . We define the *truncated* Trapezium rule  $I_h^{(N)} \approx I$  as

$$I_h^{(N)} := h \sum_{j=-N}^N f(x_j),$$

for  $N \in \mathbb{N}_0$ .

The unbounded trapezium rule cannot be applied in practice, as it requires the evaluation of infinitely many points. It is, however, useful for analysis purposes, serving as an intermediary between the exact integral and the truncated Trapezium rule.

For the truncated version, we now have two parameters:  $N$  and  $h$ . These must be balanced carefully, an equivalent interpretation is that we are approximating  $\int_{\mathbb{R}} f \approx \int_{-Nh}^{Nh} f$  and applying the trapezium rule of Definition 2.1 (with  $2N$  instead of  $N$  points). We want to truncate our integration range in a way which does not significantly increase the error.

**Theorem 2.12.** Suppose  $f(z)$  is analytic in the complex strip  $|\operatorname{Im}(z)| < a$  for some  $a > 0$ . Suppose further that  $f(z) \rightarrow 0$  uniformly as  $|z| \rightarrow \infty$  in the strip and

$$\int_{-\infty}^{\infty} |f(t + ia')| dt \leq M, \quad (2.8)$$

for all  $a' \in (-a, a)$ . Then  $I_h$  of Definition 2.11 satisfies

$$|I - I_h| \leq \frac{2M}{e^{2\pi a/h} - 1}.$$

*Proof.* Now, our characteristic function is

$$m(z) = -\frac{i}{2} \cot\left(\frac{\pi z}{h}\right),$$

chosen for its simple poles at  $x_j = jh$  each with  $\operatorname{Res}(m, jh) = h/(2\pi i)$  for  $j \in \mathbb{N}_0$ , thus if  $\gamma$  is a closed contour containing  $x_j$  for  $j = -N, \dots, N$ , we have an integral representation of the truncated Trapezium rule:

$$I_h^{(N)} = \int_{\gamma} m(z) f(z) dz \quad (2.9)$$



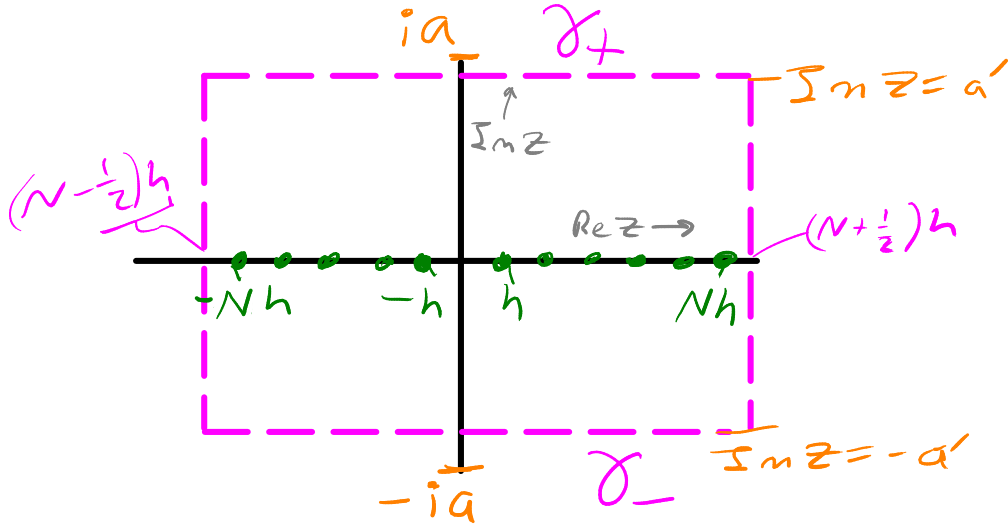


Figure 3: The contour  $\Gamma$  and poles for the proof of Theorem 2.12.

Now consider the complex rectangle  $\gamma$  with vertices at  $\pm(N + \frac{1}{2})h + ia'$  and  $\pm(N + \frac{1}{2})h - ia'$ , and define  $\gamma_+$  and  $\gamma_-$  to be the intersections of these contours with the upper- and lower-half planes respectively. It follows by Cauchy's theorem that we can represent the truncated integral as

$$\int_{-(N+\frac{1}{2})h}^{(N+\frac{1}{2})h} f(x)dx = \mp \int_{\gamma_{\pm}} f(z)dz = \frac{1}{2} \sum_{\pm} \int_{\gamma_{\pm}} \mp f(z)dz. \quad (2.10)$$

See Figure 3 for a visualisation.

Now combining (2.9) and (2.10),

$$I_h^{(N)} - \int_{-(N+\frac{1}{2})h}^{(N+\frac{1}{2})h} f(x)dx = \frac{1}{2} \sum_{\pm} \int_{\gamma_{\pm}} f(z) (2m(z) \pm 1) dz. \quad (2.11)$$

Now we focus on simplifying the integrand. From standard identities:

$$\cot(x) = \frac{1}{\tan(x)} = \frac{\cos(x)}{\sin(x)} = \frac{\frac{1}{2}(e^{ix} + e^{-ix})}{\frac{1}{2i}(e^{ix} - e^{-ix})} = i \frac{e^{ix} + e^{-ix}}{e^{ix} - e^{-ix}},$$

we can then take, for  $x = \pi z/h$  (to keep the algebra simple)

$$2m(z) \pm 1 = -i \cot(x) \pm 1 = \frac{e^{ix} + e^{-ix}}{e^{ix} - e^{-ix}} \pm \frac{e^{ix} - e^{-ix}}{e^{ix} - e^{-ix}} = \frac{e^{ix}(1 \pm 1) + (1 \mp 1)e^{-ix}}{e^{ix} - e^{-ix}} = 2 \frac{e^{\pm ix}}{e^{ix} - e^{-ix}} = \pm \frac{2}{1 - e^{\mp 2ix}}.$$

Subbing this back into (2.11),

$$I_h^{(N)} - \int_{-(N+\frac{1}{2})h}^{(N+\frac{1}{2})h} f(x)dx = \sum_{\pm} \pm \int_{\gamma_{\pm}} \frac{f(z)}{1 - e^{\mp 2\pi iz/h}} dz$$

We are getting there! The next step is to show that the vertical sides of  $\gamma_{\pm}$  tend to zero as  $n \rightarrow \infty$ . We show this on just the upper-right side, the argument is identical on the other three sides:

$$\int_0^{a'} \frac{f((N + \frac{1}{2})h + it)}{1 - e^{-2\pi i[(N+\frac{1}{2})h+it]/h}} idt$$

We can bound the denominator below:

$$1 - \exp\left(-2\pi i \left[\left(N + \frac{1}{2}\right)h + it\right]/h\right) = 1 + \exp(2\pi t/h) \geq 2, \quad \text{for } t \geq 0,$$

where we have used  $\exp(-2\pi i N) = 1$  and  $\exp(-\pi i) = -1$ . Thus by the ML principle and condition (2.8),

$$\left| \int_0^{a'} \frac{f((N + \frac{1}{2})h + it)}{1 - e^{-2\pi i [(N + \frac{1}{2})h + it]/h}} dt \right| \leq \frac{a' \max_{t \in [0, a']} |f((N + \frac{1}{2})h + it)|}{2} \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Returning to (2.11) and taking the limit as  $N \rightarrow \infty$  gives (noting the extra negation over  $\gamma_+$  due to the reverse orientation)

$$I_h - I = - \sum_{\pm} \int_{-\infty \pm ia'}^{\infty \pm ia'} \frac{f(z)}{1 - e^{\mp 2\pi i x/h}} dz, \quad (2.12)$$

the result follows by the triangle inequality (over  $\pm$ ) and the ML principle.  $\square$

We have a bound on the accuracy of  $I_h$ , which as stated earlier, cannot be used in practice, due to infinitely many nodes. We would instead like an estimate about the accuracy of  $I_h^{[N]}$ , which has finitely many nodes, and thus *can be used in practice*. By the triangle inequality, we can write

$$|I - I_h^{[N]}| \leq |I - I_h| + |I_h - I_h^{[N]}|. \quad (2.13)$$

The first term on the right-hand side can be estimated by Theorem 2.12. We can express the second term, which is often referred to the *truncation error*, using Definition 2.11:

$$I_h - I_h^{[N]} = h \left( \sum_{j=-\infty}^{-N-1} + \sum_{j=N+1}^{\infty} \right) f(x_j)$$

Exponential decay of  $f$  is sufficient to bound  $|I_h - I_h^{[N]}|$ , we will show this now for a fairly general case.

**Lemma 2.13.** *Suppose that, for some  $\alpha > 0$  independent of  $y_0 > 0$ , the function  $g$  satisfies the mild growth condition*

$$g(y + \delta) - g(y) \geq \alpha \delta, \quad (2.14)$$

*for all  $\delta > 0$  and  $y > y_0$ . Furthermore, suppose either that (i) the meshwidth  $h$  is independent of  $N$ , or (ii) the meshwidth  $h \rightarrow 0$  as  $N \rightarrow \infty$ , but with a rate  $1/N \ll h$ . Then the positive terms in the truncation error satisfies:*

$$h \sum_{n=N+1}^{\infty} e^{-g(hn)} = O(e^{-g(h(N+1))}), \quad N \rightarrow \infty.$$

*Proof.* Rearranging the sum,

$$\begin{aligned} h \sum_{n=N+1}^{\infty} e^{-g(hn)} &= h e^{-g(h(N+1))} \sum_{n=N+1}^{\infty} e^{g(h(N+1)) - g(hn)} \\ &= h e^{-g(h(N+1))} \sum_{n=0}^{\infty} e^{g(h(N+1)) - g(h(N+1+n))} \end{aligned}$$

From the condition on  $h$ , we have that  $(N+1)h \rightarrow \infty$  as  $N \rightarrow \infty$ , so we can consider  $N$  sufficiently large that  $(N+1)h > y_0$ . Now applying (2.14) to each term with  $\delta = hn$  and  $y = h(N+1)$ , we find

$$\sum_{n=N+1}^{\infty} e^{-g(hn)} \leq e^{-g(h(N+1))} h \sum_{n=0}^{\infty} e^{-\alpha hn}$$

In the case (i) where  $h$  is independent of  $N$ , we are done. In the case where  $h \rightarrow 0$  as  $N \rightarrow \infty$ , we can write as a geometric series:

$$h \sum_{n=0}^{\infty} e^{-\alpha hn} = h \sum_{n=0}^{\infty} \left( \frac{1}{e^{\alpha h}} \right)^n = \frac{h}{1 - e^{\alpha h}} = \frac{h}{-\alpha h + O(h^2)} = -\frac{1}{\alpha} + O(h),$$

thus the sum is bounded as  $h \rightarrow 0$  and thus in a small neighbourhood of  $h = 0$ . This completes the proof.  $\square$

The key message from Lemma 2.13 is the following: *if the integrand  $f$  is exponentially decaying, then  $I_h - I_h^{[N]} = O(f(h(N+1)))$ .* We turn our attention to  $f$  analytic and exponentially decaying along the real line<sup>2</sup>, for which we now have a process to estimate both contributors to the error (2.13).

Note that we have two approximation parameters to adjust:  $h$  and  $N$ . For the version of the trapezium rule in Definition 2.1, these parameters were linearly dependent - it was not necessary to consider the optimal interplay between them. For the unbounded trapezium rule,  $h$  and  $N$  can be chosen independently. From a practical point of view  $N$  is limited by computational resources, so we now ask the question: *Given  $N$ , what is the optimal choice of  $h$ ?* By *optimal* we mean that the contribution from both parts of (2.13) have the same asymptotic rate as  $N \rightarrow \infty$ , if one contribution is larger than the other then we are, in some sense, not allocating our computational resources evenly. We will see that the optimal choice of  $h$  depends on  $f$ , and now consider a few examples.

**Example 2.14.** *Using the Trapezium rule, we will approximate*

$$I = \int_{-\infty}^{\infty} e^{-x^2} (1+x^2)^{1/2} dx,$$

*and choose meshwidth  $h(N)$  which gives the optimal rate as the number of nodes  $N \rightarrow \infty$ .*

*The integrand clearly has singularities at  $\pm i$ , so is analytic in the strip  $|\operatorname{Im} z| \leq 1$ , applying Theorem 2.12 gives*

$$|I - I_h| \leq \frac{2M}{e^{2\pi/h} - 1} = O(e^{-2\pi/h}), \quad \text{as } h \rightarrow 0$$

*Clearly  $M$  and therefore the constant term hidden in the  $O$  could be made smaller by choosing a narrower strip, but this is just a constant, and we would like the rate to be as rapid as possible, which was achieved by choosing a (of Theorem 2.12) to be one.*

*Now we analyse the discretisation error. By Lemma 2.13, this can be bounded by the final terms in  $I_h^{[N]}$ ,*

$$|I_h - I_h^{[N]}| = O(e^{-(Nh)^2}).$$

---

<sup>2</sup>Recall that any analytic  $f$  exponentially decaying along the real line must grow in other sectors in the complex plane, if it were decaying in all directions then this would imply a local maximum, which violates the maximum modulus principle.

Now we want to balance the contributions from both terms to estimate the error in (2.13), so that both contributions decay at the same rate. This boils down to elementary algebraic manipulation of the exponents, setting

$$-(Nh)^2 = -2\pi/h \implies h = (2\pi/N^2)^{1/3}.$$

Substituting this into (either of) the previous rates, we obtain the optimal rate:

$$\text{For } h(N) = (2\pi/N^2)^{1/3} : \quad |I - I_h^{[N]}| = O(\exp(-2\pi N)^{2/3}), \quad \text{as } N \rightarrow \infty.$$

The next example has obvious real-world applications, but the analysis needed is only a minor extension of the previous example.

**Example 2.15.** *The complementary error function arises in a wide range of statistical applications, describing the cumulative normal distribution. At some point in your studies, you may have seen this in a statistical table in a formula book (especially if you are a millennial). It has the representation (from [1, 7.7.1])*

$$\operatorname{erfc}(z) = \frac{2e^{-z^2}}{\pi} \int_0^\infty \frac{e^{-z^2 t^2}}{t^2 + 1} dt, \quad z \in \mathbb{R}.$$

As written, this integral is on the half-line, and we cannot expect the trapezium rule to converge exponentially. Noting the symmetry of the integral, we can instead write

$$\operatorname{erfc}(z) = \frac{e^{-z^2}}{\pi} I, \quad \text{where } I = \int_{-\infty}^\infty \frac{e^{-z^2 t^2}}{t^2 + 1} dt, \quad z \in \mathbb{R},$$

to which the truncated trapezium rule, and Theorem 2.12 can be applied.<sup>3</sup>

Following similar arguments to the previous example, and assuming  $z \neq 0$ , we find for any  $a < 1$

$$|I - I_h| = O(e^{-2a\pi/h}), \quad \text{as } h \rightarrow 0$$

and

$$|I_h - I_h^{[N]}| = O(e^{-(zNh)^2}).$$

To balance the errors, we can take  $a$  arbitrarily close to one, and the same reasoning applies as in the previous example, with  $N$  replaced by  $zN$ . The optimal rate is given by:

$$\text{For } h(N) = (2\pi/(zN)^2)^{1/3} : \quad |I - I_h^{[N]}| = O(\exp(-2\pi|z|N)^{2/3}), \quad \text{as } N \rightarrow \infty.$$

A couple of points are worth noting at this stage.

In the two examples above, the optimal meshwidth  $h$  and the convergence rate are optimal for sufficiently large  $N$ . In practice, a different choice may be optimal for fixed  $N$ . A separate consideration is that beyond some  $N$  there will be summands in  $I_h^{[N]}$  which are below machine precision in magnitude; some of these samples may be redundant before we hit the optimal rate.

Finally, in the second example, it may be necessary to compute  $\operatorname{erfc}(z)$  for a range of values of  $z$ . In this instance, it may be more efficient to use the same weights and nodes for each value of  $z$ , potentially reducing the number of computations overall.

Now we consider an example which looks easier, but is actually slightly more involved.

---

<sup>3</sup>Note that this trick only worked because we were able to extend the integral to  $\mathbb{R}$  any maintain analyticity of the integrand! In practice, to apply the truncated trapezium rule of Definition 2.11, one could simply sum from  $j = 0$  to  $j = N$ , and double the value of each weight for  $j \geq 1$ , to simplify computations.

**Example 2.16.** Compute the optimal meshwidth and rate for trapezium rule evaluation of

$$I = \int_{-\infty}^{\infty} e^{-x^2} dx.$$

This integrand is entire, so we can choose  $a$  in Theorem 2.12 to be any value we please. We will not fix it, and later seek to choose the value of  $a$  which maximises convergence rate. The integrand is  $O(e^{a^2})$  in the strip  $|\operatorname{Im}(z)| < a$ , thus Theorem 2.12 tells us

$$|I - I_h| \leq \frac{2M}{e^{2\pi a/h} - 1} = O(\exp(a^2 - 2\pi a/h)), \quad h \rightarrow 0.$$

The approach here is (i) first choose the  $a$  which **maximises** the discretisation error and then (ii) choose  $h$  which balances this error with the truncation error.

We want to choose  $a$  which maximises this rate, solving

$$\frac{d}{da}[a^2 - 2\pi a/h] = 0 \implies a = \pi/h,$$

and thus

$$|I - I_h| = O(\exp(-\pi^2/h^2))$$

The truncation error follows similar arguments to the previous two examples, simply

$$|I_h - I_h^{(N)}| = O(\exp(-(hN)^2)), \quad N \rightarrow \infty.$$

As in the previous examples, we aim to match the two rates,

$$-\pi/h = -hN \implies h(N) = (\pi/N)^{1/2},$$

leading to the following convergence rate:

$$\text{For } h(N), \quad |I - I_h^{(N)}| = O(\exp(-\pi N)), \quad \text{as } N \rightarrow \infty.$$

## 2.6 Adding a residue correction to the trapezium rule

We have seen that the trapezium rule converges exponentially fast,  $O(e^{-aN})$  for some  $a > 0$  for periodic analytic integrals, and unbounded analytic integrals. In this chapter, we will explore a beautiful trick which makes the trapezium rule converge exponentially *more* fast, i.e.  $O(e^{-\tilde{a}N})$  for some  $\tilde{a} > a$ . This is a valuable trick, and was used recently for the rapid calculation of Fresnel integrals in [2]. Fresnel integrals are a type of special function (see [1, §7]) which occur frequently in diffraction and scattering theory. They also occur, considerably less frequently, in rollercoaster design.

We consider integrals of the form:

$$\int_{-\infty}^{\infty} \frac{g(z)}{z - z_0} dz,$$

where  $\operatorname{Im}\{z_0\} = a > 0$ , and  $g$  is analytic and bounded in a strip  $|\operatorname{Im}\{z\}| < \tilde{a}$ , for  $0 < a < \tilde{a}$ . To simplify the calculations that follow, we choose  $\operatorname{Im}\{z_0\} > 0$ . If we apply Theorem 2.12, the integrand is analytic in  $\operatorname{Im}\{z\} < a$  due to the presence of the pole at  $z_0$ , thus we expect convergence at a rate of  $O(e^{-a'N})$  as  $N \rightarrow \infty$ , for any  $a' < a$ . Given that we are only non-analytic at a single point in  $|\operatorname{Im}\{z\}| < \tilde{a}$ , can we do better than this? Recalling (2.11), we have

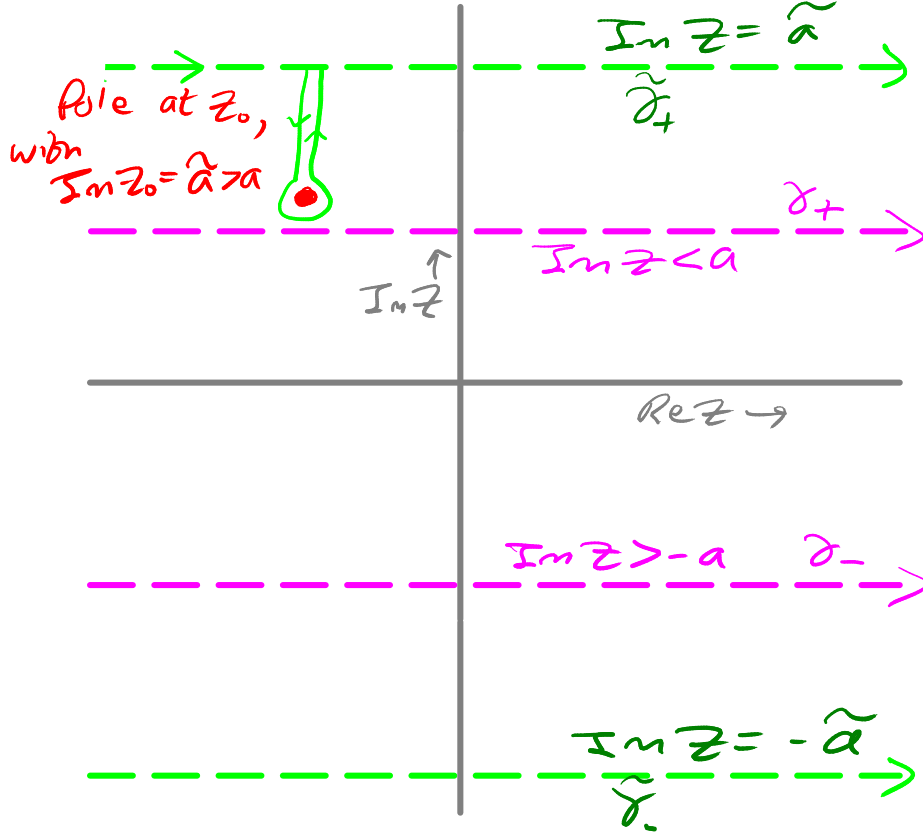


Figure 4: Visualisation of the trapezium rule correction process.

$$I_h^{(N)} - \int_{-(N+\frac{1}{2})h}^{(N+\frac{1}{2})h} f(x)dx = \sum_{\pm} \pm \int_{\gamma_{\pm}} \frac{f(z)}{1 - e^{\mp 2\pi iz/h}} dz,$$

where  $f(z) = g(z)/(z - z_0)$ .

The contours  $\gamma_{\pm}$  were chosen to remain inside of the domain of analyticity  $|\text{Im}\{z\}| < a$ . The only thing preventing this domain of analyticity being larger, i.e.  $|\text{Im}\{z\}| < \tilde{a}$  is the presence of the pole at  $z_0$ . By deforming the contour vertically into this larger domain, so that  $\tilde{\gamma}_{\pm}$  now have horizontal edges at  $\tilde{a}' < \tilde{a}$ , we pick up a residue contribution from the pole:

$$I_h^{(N)} - \int_{-(N+\frac{1}{2})h}^{(N+\frac{1}{2})h} f(x)dx = 2\pi i \text{Res} \left( \frac{-\tilde{g}(z)}{1 - e^{-2\pi iz/h}}, z_0 \right) + \sum_{\pm} \pm \int_{\tilde{\gamma}_{\pm}} \frac{f(z)}{1 - e^{\mp 2\pi iz/h}} dz.$$

Following the same arguments as in the original proof, we obtain

$$I_h - I = 2\pi i \text{Res} \left( \frac{-\tilde{g}(z)}{1 - e^{-2\pi iz/h}}, z_0 \right) - \sum_{\pm} \int_{-\infty \pm \tilde{a}i}^{\infty \pm \tilde{a}i} \frac{f(z)}{1 - e^{\mp 2\pi iz/h}} dz.$$

The pole at  $z_0$  is simple, so we can calculate the residue easily, and subtract it from both sides

$$\left(I_h - \frac{-2\pi ig(z_0)}{1 - e^{-2\pi iz_0/h}}\right) - I = - \sum_{\pm} \int_{-\infty \pm \tilde{a}'i}^{\infty \pm \tilde{a}'i} \frac{f(z)}{1 - e^{\mp 2\pi iz/h}} dz.$$

Now we can apply the ML principle as before, to obtain

$$\left|\left(I_h - \frac{-2\pi ig(z_0)}{1 - e^{-2\pi iz_0/h}}\right) - I\right| \leq \frac{2\tilde{M}}{e^{2\pi\tilde{a}/h} - 1}, \quad (2.15)$$

where  $\tilde{M}$  is the analogue of  $M$  over the new horizontal contours.

To summarise, by adding a small correction to our trapezium rule, it will converge at a faster rate! I feel that this is a particularly beautiful result, for the following reasons. Usually, we derive a numerical method, and then prove that it works. Here, we have derived a method, proved it worked, then taken a particular component of the proof, namely the *characteristic function*  $m(z)$ , and used this to represent the bulk of the error, which we can subtract off explicitly in a more accurate method.

As you might expect, the idea could be generalised to the periodic trapezium rule, poles in the lower half plane, and multiple poles, but we do not consider this in these notes (see problem sheet 2 for a more general example). We apply this method to the following example, which demonstrates its power.

**Example 2.17.**

$$I = \int_{-\infty}^{\infty} \frac{e^{-z^2} \sqrt{z - 2i}}{z - i} dz.$$

Applying the standard techniques initially, this is analytic in the strip  $|\operatorname{Im} z| < a$  for any  $a < 1$ , which gives us the discretisation error

$$|I - I_h| = O(e^{-2\pi a/h}), \quad \text{for any } a < 1.$$

The truncation error is bounded by Theorem 2.13:

$$|I_h - I_h^{(N)}| \leq O(e^{-(Nh)^2}), \quad (2.16)$$

balancing the discretisation and truncation error:

$$-2\pi a/h = -(Nh)^2$$

implies, as in earlier examples, that  $h = (2\pi a/N^2)^{1/3} \approx (2\pi/N^2)^{1/3}$

However, we notice that there is a simple pole at  $z = i$ , and by correcting for this, we can extend the domain of analyticity to  $|\operatorname{Im} z| < \tilde{a} = 2$ . Using the formula (2.15),

$$\left|\left(I_{\tilde{h}} - \frac{-2\pi ie\sqrt{-i}}{1 - e^{2\pi/\tilde{h}}}\right) - I\right| \leq \frac{2\tilde{M}}{e^{2\pi\tilde{a}/\tilde{h}} - 1} = O(e^{-4\pi/h}).$$

Now, balancing this discretisation error with the truncation error (2.16):

$$-4\pi a/\tilde{h} = -(N\tilde{h})^2 \implies \tilde{h} = (4\pi/N^2)^{1/3},$$

thus we have a different mesh size for the corrected trapezium rule.

The following Jupyter notebook example can be run interactively in a browser by clicking on **this link**.

In this example, we improve the convergence rate of the trapezium rule by adding a **residue correction**. As we have shown in the notes, the error can be represented as a residue plus a contour integral. The residue is the largest component, but fortunately, we can evaluate this component of the error exactly, so we can effectively subtract it from the error!

```
[2]: using Plots, LaTeXStrings
```

Now define the a function which returns the nodes of the truncated trapezium rule  $I_h^{(N)}$ :

```
[4]: trap_rule_trunc(N, h) = [j*h for j in -N:N] #, repeat([h], 2N+1)
```

```
[4]: trap_rule_trunc (generic function with 1 method)
```

The integral for this experiment is

$$\int_{-\infty}^{\infty} f(z) dz = \int_{-\infty}^{\infty} \frac{e^{-z^2} \sqrt{z-2i}}{z-i} dz,$$

where the branch cut of the square root function is chosen not to cross the real axis, thus the integrand  $f$  is analytic. Note that there is a pole at  $z = i$ , and a branch point at  $z = 2i$ . The convergence of the standard trapezium rule will be limited by the pole at  $z = i$ .

```
[8]: f(z) = exp(-z^2) * sqrt(z-2im) / (z-im)
```

```
[8]: f (generic function with 1 method)
```

### Convergence of standard trapezium rule

In the notes, we have derived the optimal meshwidth as:

$$h = \left( \frac{2\pi}{N^2} \right)^{1/3}$$

We now test the standard trapezium rule, and observe exponential convergence.

```
[10]: N_max = 40
approx_val = zeros(ComplexF64, N_max)
for N=1:N_max
    h = (2*pi/N^2)^(1/3) # optimal h
    x = trap_rule_trunc(N, h)
    approx_val[N] = h*sum(f.(x)) # apply trap rule
end
```



```

# Need a high order reference solution, as we don't have an exact value for this
→ integral
N_ref = 100
h_ref = (2*pi/N_ref^2)^(1/3)
x = trap_rule_trunc(N_ref, h_ref)
I_ref = h_ref*sum(f.(x))

# compute absolute errors
errs = abs.(approx_val .- I_ref);

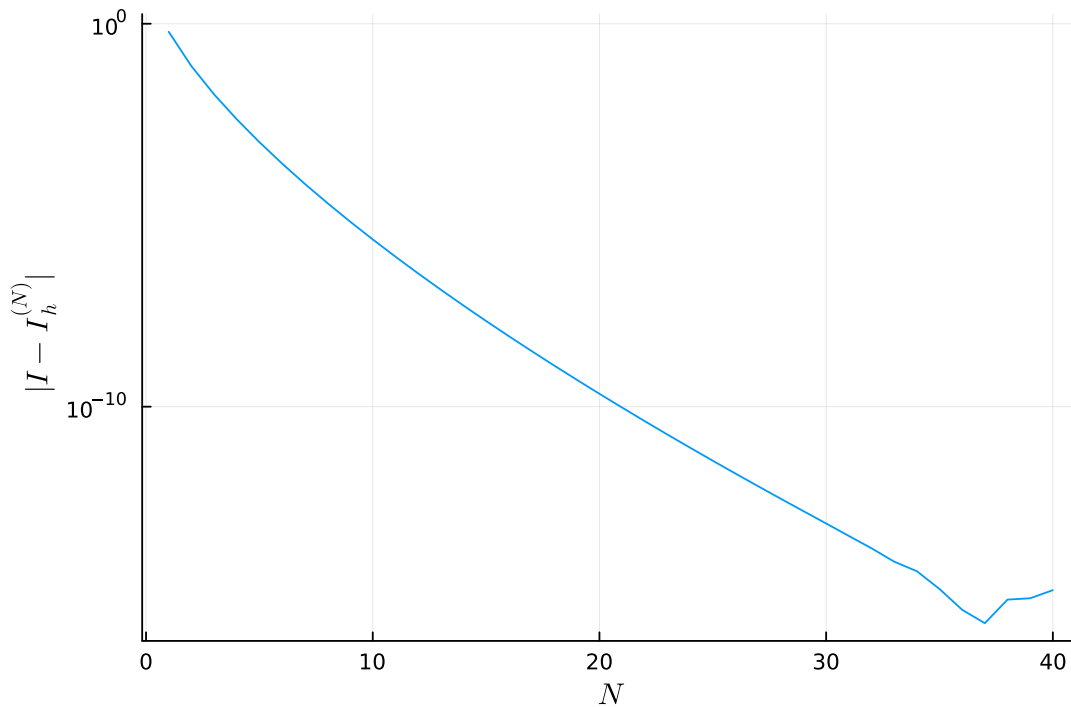
```

```

[12]: plot(1:N_max, errs,yscale=:log10, xlabel=L"$N$", ylabel=L"$|I-I_h^{(N)}|$",
→ labels=false)

```

[12]:



### Convergence of the trapezium rule with a residue correction

We have an exponentially convergent method... but can we converge at a *faster* exponential rate? Using the formula in the nodes, we subtract the residue:

$$2\pi i \operatorname{Res} \left( \frac{-g(z)}{1 - e^{-2\pi i z/h}}, i \right) = \frac{-2\pi i g(z_0)}{1 - e^{\mp 2\pi i z_0/h}} = \frac{-2\pi i e \sqrt{-i}}{1 - e^{2\pi/h}},$$

recalling that:

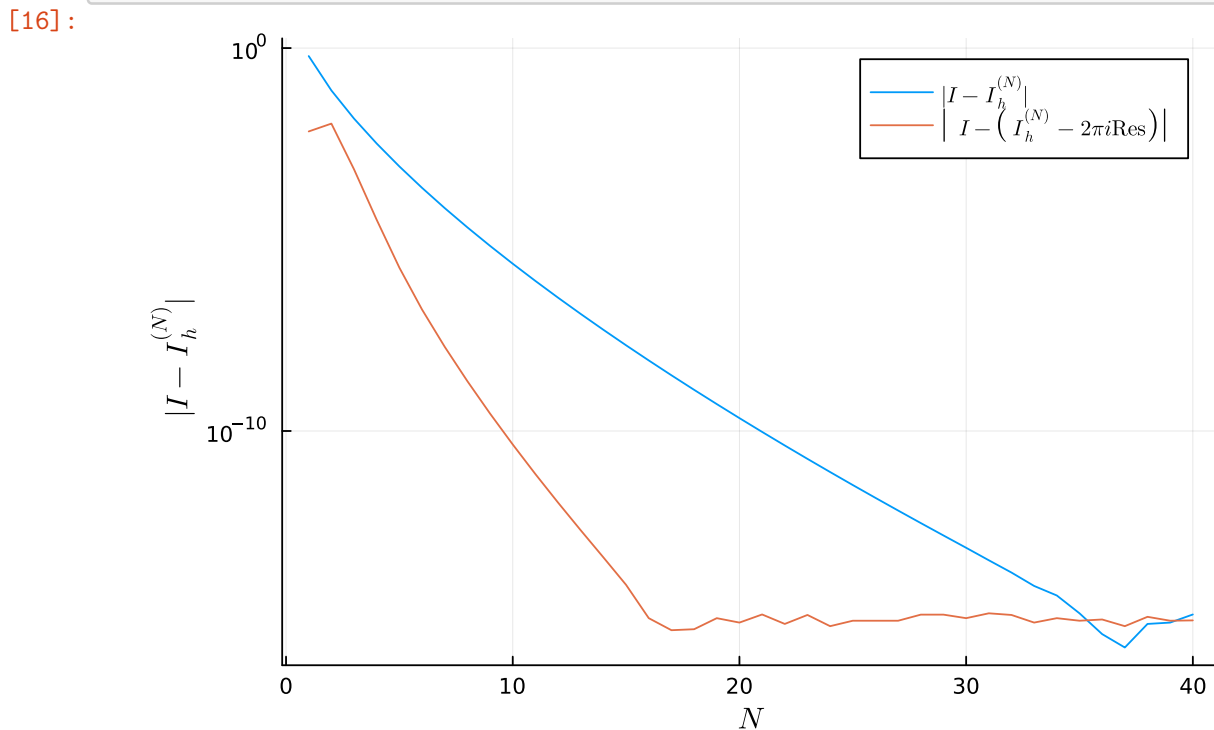
$$g(z) = e^{-z^2} \sqrt{z - 2i}$$

This allows us to take  $a = 2$ , and thus gives us a new meshwidth parameter  $h$ . We now observe a faster convergence rate!

```
[14]: N_max = 40
approx_val_corrected = zeros(ComplexF64, N_max)
for N=1:N_max
    h = (4*pi/N^2)^(1/3) # optimal meshwidth
    x = trap_rule_trunc(N, h)
    res = -2*pi*im*exp(1)sqrt(-im) / (1-exp(2*pi/h)) # residue
    approx_val_corrected[N] = h*sum(f.(x)) - res # trapezium rule + residue
end

# compute absolute errors
errs_after_correction = abs.(approx_val_corrected .- I_ref);
```

```
[16]: plot(1:N_max, [errs, errs_after_correction],yscale=:log10, xlabel=L"$N$",
    →ylabel=L"$|I-I_h^{(N)}|$",
    label=[L"$|I-I_h^{(N)}| $" L"$\left|I-\left(I_h^{(N)}-2\pi i\right.\right.$
    →i\mathrm{Res}\right)\right|$"])
```



[ ]:

## 2.7 An introduction to numerical steepest descent

For the final example of this chapter, we will investigate the idea of *steepest descent*. Not to be confused with *gradient descent* in optimisation methods, steepest descent originally dates back to Riemann and Cauchy. The main idea is to deform the path of integration onto one where the integrand is exponentially decaying, or negligibly small. Broadly speaking, exponentially decaying integrals are much easier to approximate, both numerically and asymptotically. For centuries, steepest descent has been presented as an asymptotic method (indeed, it is sometimes featured in Imperial's Asymptotic Methods course), and the deformed integrals were approximated asymptotically. In recent decades, numerical methods have been used to evaluate the deformed contours, in so-called *numerical steepest descent methods*.

We consider the integral

$$I = \int_{-\infty}^{\infty} f(z) e^{i\omega z^p} dz, \quad \text{for } \omega > 0, \quad 2 \leq p \in \mathbb{N} \text{ and even,}$$

where for now, we assume that  $|f(z)|$  is bounded by some  $M$  as  $z \rightarrow \infty$ , and  $f$  decays sufficiently to ensure that  $I$  converges.

The idea behind steepest descent methods is to deform onto a new contour  $\gamma$ , where the integrand exponentially decays. As we have earlier in this chapter, we can often expect the trapezium rule to converge exponentially fast in such a case. We introduce three contours for  $R > 0$ :

- $\gamma_R$  parametrised by  $z = te^{i\pi/(2p)}$ , for  $t \in [-R, R]$
- $\gamma_1$  parametrised by  $z = Re^{i\theta}$ , for  $\theta \in [\pi, (2p+1)\pi/(2p)]$
- $\gamma_2$  parametrised by  $z = Re^{i\theta}$ , for  $\theta \in [0, \pi/(2p)]$

We define  $\gamma = \cup \gamma_1 \cup \gamma_R \cup \gamma_2$ . By the corollary of Cauchy's integral theorem, under suitable analyticity assumptions about  $f$ , we have

$$\int_{-R}^R f(z) e^{i\omega z^p} dz = \int_{\gamma} f(z) e^{i\omega z^p} dz.$$

First we examine the integral along  $\gamma_R$ . Applying our parametrisation:

$$\int_{\gamma_R} f(z) e^{i\omega z^p} dz = e^{i\pi/(2p)} \int_{-R}^R f(te^{i\pi/(2p)}) \exp\left(i\omega (te^{i\pi/(2p)})^p\right) dt.$$

Inside the exponent we see  $i\omega (te^{i\pi/(2p)})^p = i\omega t^p e^{i\pi/2} = i\omega t^p i = -\omega t^p$ ; we have converted our oscillating exponential into pure exponential decay! We now have

$$\int_{\gamma_R} f(z) e^{i\omega z^p} dz = e^{i\pi/(2p)} \int_{-R}^R f(te^{i\pi/(2p)}) e^{-\omega t^p} dt.$$

Now we aim to show that the contribution from the two circular arcs  $\gamma_1$  and  $\gamma_2$  vanishes as  $R \rightarrow \infty$ . First we write the integral in parametrised form and rearrange:

$$\begin{aligned} \int_{\gamma_2} f(z) e^{i\omega z^p} dz &= \int_0^{\pi/(2p)} f(Re^{i\theta}) \exp\left(i\omega (Re^{i\theta})^p\right) Rie^{i\theta} d\theta \\ &= \int_0^{\pi/(2p)} f(Re^{i\theta}) \exp\left(i\omega R^p e^{pi\theta}\right) Rie^{i\theta} d\theta \\ &= \int_0^{\pi/(2p)} f(Re^{i\theta}) \exp\left(i\omega R^p [\cos(p\theta) + i \sin(p\theta)]\right) Rie^{i\theta} d\theta. \end{aligned}$$

Bounding, taking the absolute value sign inside of the integral, we obtain

$$\left| \int_{\gamma_2} f(z) e^{i\omega z^p} dz \right| \leq \int_0^{\pi/(2p)} M \exp(-\omega R^p \sin(p\theta)) R d\theta.$$

Now, noting the convexity of  $\sin$  and hence  $-\sin x \leq -2x/\pi$  for  $x \in [0, \pi/2]$ , subbing  $x = p\theta$  we can write

$$\begin{aligned} \left| \int_{\gamma_2} f(z) e^{i\omega z^p} dz \right| &\leq MR \int_0^{\pi/(2p)} \exp(-2p\omega R^p \theta/\pi) d\theta \\ &= M\pi \frac{1 - e^{-\omega R^p}}{2p\omega R^{p-1}} \rightarrow 0 \quad \text{as } R \rightarrow \infty. \end{aligned}$$

Putting everything together, we have

$$\begin{aligned} I &= \int_{-\infty}^{\infty} f(z) e^{i\omega z^p} dz \\ &= \lim_{R \rightarrow \infty} \int_{-R}^R f(z) e^{i\omega z^p} dz \\ &= \lim_{R \rightarrow \infty} \int_{\gamma} f(z) e^{i\omega z^p} dz \\ &= \lim_{R \rightarrow \infty} \left( \int_{\gamma_1} f(z) e^{i\omega z^p} dz + \int_{\gamma_R} f(z) e^{i\omega z^p} dz + \int_{\gamma_2} f(z) e^{i\omega z^p} dz \right) \\ &= 0 + \lim_{R \rightarrow \infty} \left( \int_{\gamma_R} f(z) e^{i\omega z^p} dz \right) + 0 \\ &= e^{i\pi/(2p)} \int_{-\infty}^{\infty} f(te^{i\pi/(2p)}) e^{-\omega t^p} dt. \end{aligned} \tag{2.17}$$

As we will see, this new representation for our integral is particularly advantageous. We now consider an example.

**Example 2.18.** *Numerically evaluate the integral*

$$I = \int_{-\infty}^{\infty} \frac{e^{10ix^2}}{\sqrt{x-i}} dx,$$

where  $\sqrt{z}$  is the principle / positive branch of the square root function.

We begin by applying (2.17), to obtain

$$I = e^{i\pi/4} \int_{-\infty}^{\infty} \frac{e^{-10t^2}}{\sqrt{te^{i\pi/4} - i}} dt.$$

We choose the branch cut of the square root to be along the negative real axis, i.e.  $\arg z \in [-\pi, \pi)$ . Then, the deformation used to obtain (2.17) is justified, as it does not cross the branch cut. The original representation for  $I$  is not exponentially decaying, so using our current techniques, we have no means to estimate its truncation error. After deforming on to the steepest descent path, we immediately see an advantage of the exponential decay; we are able to estimate the truncation error of a truncated trapezium rule approximation:

$$|I_h - I_h^{(N)}| \leq O(e^{-10(Nh)^2}).$$

Before choosing  $h$ , we must determine the imaginary strip of  $t$ . Considering that the branch cut is chosen to be horizontal line parallel to the real axis, the imaginary strip is clearly determined by the point  $t^*$  such that the denominator is zero, hence we must solve

$$t^* e^{i\pi/4} - i = 0,$$

which can be rearranged to obtain

$$t^* = e^{i\pi/2} e^{-i\pi/4} = e^{i\pi/4},$$

thus the integrand is analytic inside of the strip  $|\operatorname{Im}\{z\}| < a$ , where

$$a = \operatorname{Im}\{t^*\} = \sin(\pi/4) = \sqrt{2}/2.$$

Thus, from Theorem 2.12, we can expect discretisation error

$$O(e^{-(\sqrt{2}\pi/h)});$$

balancing the errors to determine  $h$ , we solve

$$\sqrt{2}\pi/h = 10(Nh)^2$$

to find

$$h = \left( \frac{\sqrt{2}\pi}{10N^2} \right)^{1/3}$$

as the optimal mesh width.

The following Jupyter notebook example can be run interactively in a browser by clicking on ***this link***.

# NSD0

February 14, 2025

```
[82]: using Plots, LaTeXStrings
```

```
[84]: function trunc_trap(f, h, N)
      # get (truncated) trapezium rule points
      x = [n*h for n= -N:N]
      # sum up function at each point
      return h*sum(f.(x))
end
```

```
[84]: trunc_trap (generic function with 1 method)
```

Example:

$$I = \int_{-\infty}^{\infty} f(x)e^{\omega ix^2} dx, \quad \text{where } f(x) = \frac{1}{x^2 + 1}$$

```
[119]: f(x) = 1/(x^2+1)
      ω = 100
      F(x) = exp(ω*im*x^2) * f(x)
```

```
[119]: F (generic function with 1 method)
```

Deforming onto the steepest descent (SD) path gives us:

$$I = e^{i\pi/4} \int_{-\infty}^{\infty} f(re^{i\pi/4})e^{-\omega r^2} dr$$

```
[150]: # integrand of deformed contour
      F_sd(r) = exp(im*π/4) * exp(-ω*r^2) * f(r*exp(im*π/4))
```

```
[150]: F_sd (generic function with 1 method)
```

Optimal mesh width, which balances truncation and discretisation error, is:

$$h(N) = \left( \frac{\sqrt{2}\pi}{\omega N^2} \right)^{1/3}$$

```
[153]: max_N = 50

      # define optimal h for SD case
```

```

h_sd(N) = (sqrt(2)* $\pi$ /( $\omega$ *N2))^(1/3)

# cannot define optimal h for non-SD case, so let's try a few!
h_1 = 10/ $\omega$ 
h_2 = 1/ $\omega$ 
h_3 = 0.1/ $\omega$ 

# get reference solution:
N_ref = 1000
I = trunc_trap(F_sd, h_sd(N_ref), N_ref)

# initialise vectors to store errors
errs_h1 = zeros(max_N)
errs_h2 = zeros(max_N)
errs_h3 = zeros(max_N)
errs_sd = zeros(max_N)
for N=1:max_N
    errs_h1[N] = abs(I - trunc_trap(F, h_1, N)) + eps()
    errs_h2[N] = abs(I - trunc_trap(F, h_2, N)) + eps()
    errs_h3[N] = abs(I - trunc_trap(F, h_3, N)) + eps()
    errs_sd[N] = abs(I - trunc_trap(F_sd, h_sd(N), N)) + eps()
end

```

```

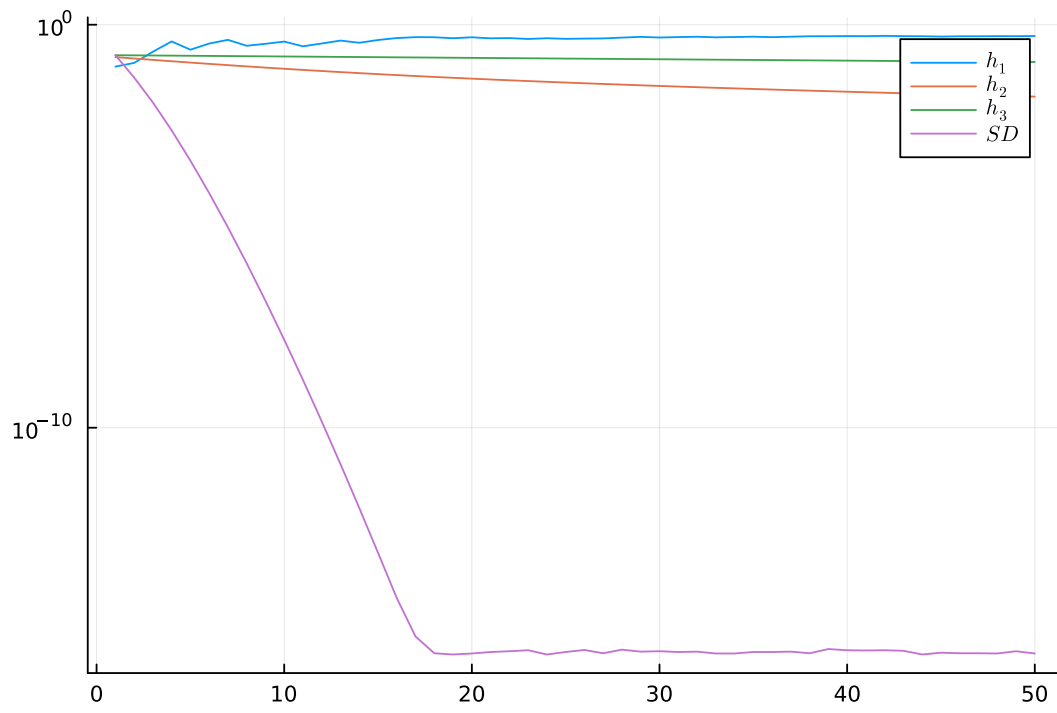
[155]: plot(1:max_N,
    [errs_h1, errs_h2, errs_h3, errs_sd],
    yscale=:log10,
    labels=[L"h_1" L"h_2" L"h_3" L"SD"])

```

```

[155]:

```



We see exponential convergence along our deformed contour, with our optimal mesh width. The other approaches converge at a much slower rate, if at all!



## References

- [1] Digital Library of Mathematical Functions. National Institute of Standards and Technology, from <http://dlmf.nist.gov/>, release date: 2010-05-07.
- [2] Mohammad Alazah, Simon N Chandler-Wilde, and Scott La Porte. Computing fresnel integrals via modified trapezium rules. *Numerische Mathematik*, 128(4):635–661, 2014.
- [3] Daan Huybrechs. Stable high-order quadrature rules with equidistant points. *Journal of computational and applied mathematics*, 231(2):933–947, 2009.
- [4] Lloyd N Trefethen and JAC Weideman. The exponentially convergent trapezoidal rule. *SIAM review*, 56(3):385–458, 2014.
- [5] Alan M Turing. A method for the calculation of the zeta-function. *Proceedings of the London Mathematical Society*, 2(1):180–197, 1945.