Applied Complex Analysis (2021)

1 Lecture 6: Trapezium rule, Fourier series and Laurent series

This lecture we cover

- 1. Periodic and complex Trapezium rule
- 2. Convergence via Laurent series
- 3. Numerical differentiation via numerical computation of Cauchy integrals

1.1 Periodic Trapezium rule

Quadrature rules are pairs of nodes x_0, \ldots, x_{N-1} and weights w_0, \ldots, w_{N-1} to approximate integrals

$$\int_{a}^{b} f(x)dx \approx \sum_{j=0}^{N-1} w_{j} f(x_{j})$$

In this lecture we construct quadrature rules on complex contours γ to approximate contour integrals.

The trapezium rule gives an easy approximation to integrals. On $[0,2\pi)$ for periodic $f(\theta)$, we have a simplified form:

Definition (Periodic trapezium rule) The *periodic trapezium rule* is the approximation

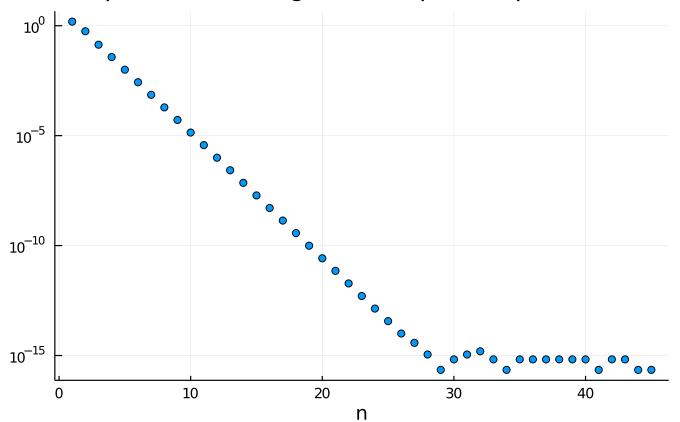
$$\int_0^{2\pi} f(\theta)d\theta \approx Q_N f := \frac{2\pi}{N} \sum_{j=0}^{N-1} f(\theta_k)$$

for
$$\theta_j = \frac{2\pi j}{N}$$
.

The periodic trapezium rule is amazingly accurate for smooth, periodic functions:

```
using Plots, ApproxFun f = \theta \rightarrow 1/(2 + \cos(\theta)) periodic_rule(N) = 2\pi/N*(0:(N-1)), 2\pi/N*ones(N) errs = [((x, w) = periodic_rule(N); abs(sum(w.*f.(x)) - sum(Fun(f, 0...2\pi)))) for N = 1:45]; scatter(errs.+eps(); yscale=:log10, title="exponential convergence of N-point trapezium rule", legend=false, xlabel="n")
```

exponential convergence of N-point trapezium rule



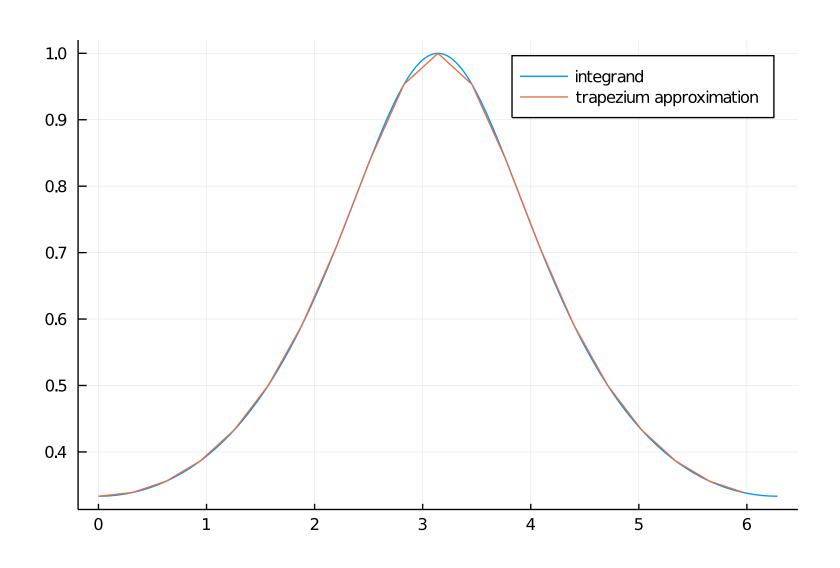
The accuracy in integration is remarkable as the trapezoidal interpolant does not accurately approximate f: we can see clear differences between the functions here:

```
N=20

(x, w) = periodic_rule(N)

plot(Fun(f, 0 .. 2\pi); label = "integrand")

plot!(x, f.(x); label = "trapezium approximation")
```



1.2 Trapezium rule and Fourier coefficients

Write

$$f(\theta) = \sum_{k=-\infty}^{\infty} \hat{f}_k e^{ik\theta}$$

and assume that the Fourier coefficients are absolutely summable (true if f is smooth enough):

$$\sum_{k=-\infty}^{\infty} |\hat{f}_k| < \infty.$$

Note that geometric series tells us that

$$\begin{split} \frac{1}{2\pi}Q_N\mathrm{e}^{\mathrm{i}k\theta} &= \frac{1}{N}\sum_{j=0}^{N-1}(\mathrm{e}^{2\pi\mathrm{i}k/N})^j\\ &= \begin{cases} 1 & \text{if } k=mN \text{ for some integer } m\\ 0 & \text{otherwise} \end{cases} \end{split}$$

It follows that we can express the Trapezium rule exactly in terms of a sum of Fourier coefficients:

$$\frac{1}{2\pi}Q_Nf = \sum_{k=-\infty}^{\infty} \hat{f}_k \frac{1}{2\pi}Q_N \mathrm{e}^{\mathrm{i}k\theta} = \sum_{k=-\infty}^{\infty} \hat{f}_k \begin{cases} 1 & \text{if } k=mN \text{ for some integer } m \\ 0 & \text{otherwise} \end{cases}$$
$$= \cdots + \hat{f}_{-2N} + \hat{f}_{-N} + \hat{f}_0 + \hat{f}_N + \hat{f}_{2N} + \cdots$$

In other words, the error in the Trapezium rule is bounded by

$$\left| \int_{0}^{2\pi} f(\theta) d\theta - Q_N f \right| \le 2\pi \sum_{m=1}^{\infty} \left[|\hat{f}_{mN}| + |\hat{f}_{-mN}| \right]$$

if we can show fast decay in the coefficients we can prove the observation that trapezium rule converges fast.

1.3 Decay in Fourier/Laurent coefficients

Now we consider g(z) such that $g(e^{i\theta}) = f(\theta)$, that is, g has the Laurent series

$$g(z) = \sum_{k=-\infty}^{\infty} g_k z^k$$

where $g_k = \hat{f}_k$. Interestingly, analytic properties of g can be used to show decaying properties in Fourier coefficients of f:

Theorem (Decay in Fourier/Laurent coefficients) Suppose g(z) is analytic in a closed annulus $A_{r,R}$ around 0: $A_r(z_0) = \{z : r \le |z| \le R, 0 < r < 1, R > 1\}$. Then for all $k = |g_k| \le M \min\left\{\frac{1}{R^k}, \frac{1}{r^k}\right\}$ where $M = \sup_{z \in A_{r,R}} |g(z)|$.

Proof This is a simple application of the ML lemma: let $k \geq 0$, then

$$|g_k| = \frac{1}{2\pi} \left| \oint_{C_1} \frac{g(\zeta)}{\zeta^{k+1}} d\zeta \right| = \frac{1}{2\pi} \left| \oint_{C_R} \frac{g(\zeta)}{\zeta^{k+1}} d\zeta \right| \le \sup_{\zeta \in C_R} |f(\zeta)| R^{-k} \le M R^{-k}.$$

For k < 0, we deform the contour to C_r .

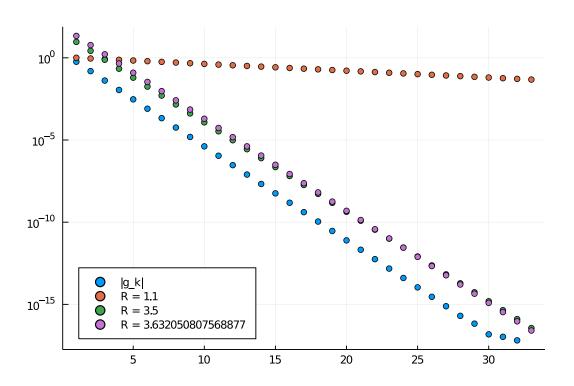
We thus can show fast convergence of Trapezium rule again using geometric series:

$$\sum_{m=1}^{\infty} \left[|f_{mN}| + |f_{-mN}| \right] \le M \sum_{m=1}^{\infty} \left[R^{-mN} + r^{mN} \right] \le M \left[\frac{R^{-N}}{1 - R^{-N}} + \frac{r^{N}}{1 - r^{N}} \right].$$

Demonstration The Laurent coefficients of $g(\theta) = \frac{1}{2-\cos\theta}$ satisfies for $k \geq 0$

$$|g_k| \le \frac{2}{4 - R - R^{-1}} R^{-k}$$

for all $R \le 2 + \sqrt{3}$. The following shows this bound is quite accurate:



This fast decay in coefficients explains the fast convergence of the trapezium rule.

1.4 Complex Trapezium rule

We can use the map γ that defines a closed contour to construct an approximation to integrals over γ :

Definition (Complex trapezium rule) The *complex trapezium rule* on a contour γ (mapped from $[0,2\pi)$) is the approximation

$$\oint_{\gamma} f(z)dz \approx \sum_{j=0}^{N-1} w_j f(z_j)$$

for

$$z_j = \gamma(heta_j)$$
 and $w_j = rac{2\pi}{N} \gamma'(heta_j)$

Example (Circle trapezium rule) On a circle $C_r = \{re^{i\theta} : 0 \le \theta < 2\pi\}$, we have

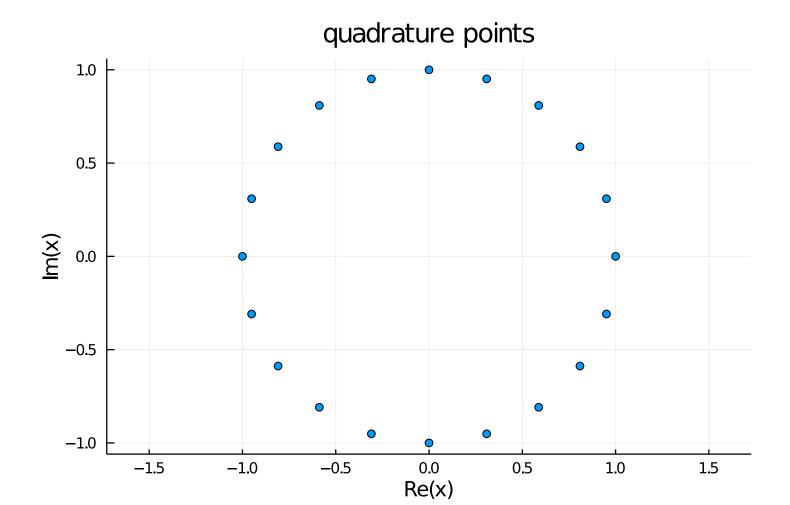
$$\oint_{C_r} f(z)dz \approx \sum_{j=0}^{N-1} w_j f(z_j)$$

for $z_j = r \mathrm{e}^{\mathrm{i} heta_j}$ and $w_j = \frac{2\pi \mathrm{i} r}{N} \mathrm{e}^{\mathrm{i} heta_j}$.

Here we plot the quadrature points:

```
function circle_rule(N, r)
      θ = periodic_rule(N)[1]
      r*exp.(im*θ), 2π*im*r/N*exp.(im*θ)
end

ζ, w = circle_rule(20, 1.0)
scatter(ζ; title="quadrature points", legend=false, ratio=1.0)
```



The Circle trapezium rule is surprisingly accurate for analytic functions, following from the explanation above:

```
\zeta, w = circle_rule(20, 1.0)

f = z -> cos(z)

z = 0.1+0.2im

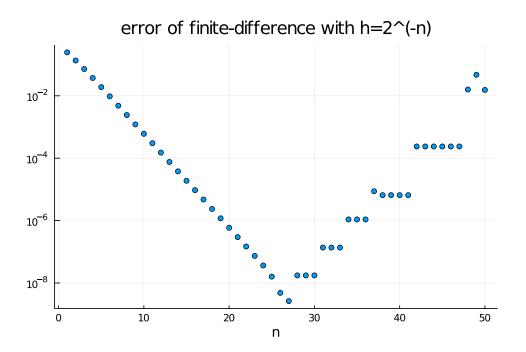
sum(f.(\zeta)./(\zeta .- z).*w)/(2\pi*im) - f(z)

-9.814371537686384e-14 - 1.3076345561913172e-14im
```

1.5 Application: Numerical differentiation

Calculating high-order derivatives using limits is numerically unstable. Here is a demonstration using finite-differences: making h small does not increase the accuracy after a certain point:

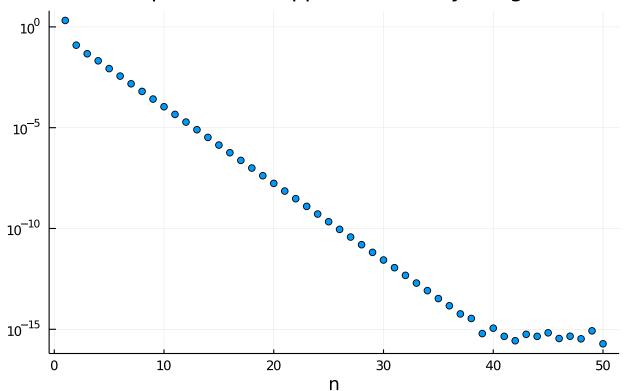
```
using SpecialFunctions f = z \rightarrow gamma(z) fp = z \rightarrow gamma(z)polygamma(0,z) \# exact derivative x = 1.2 fp_fd = [(h=2.0^(-n); (f(x+h)-f(x))/h) for n = 1:50] scatter(abs.(fp_fd - fp(x)); yscale=:log10, legend=false, title = "error of finite-difference with h=2^(-n)", xlabel="n")
```



But the Cauchy integral formula for derivatives tells us that we can reduce a derivative to a contour integral, which can be computed stably:

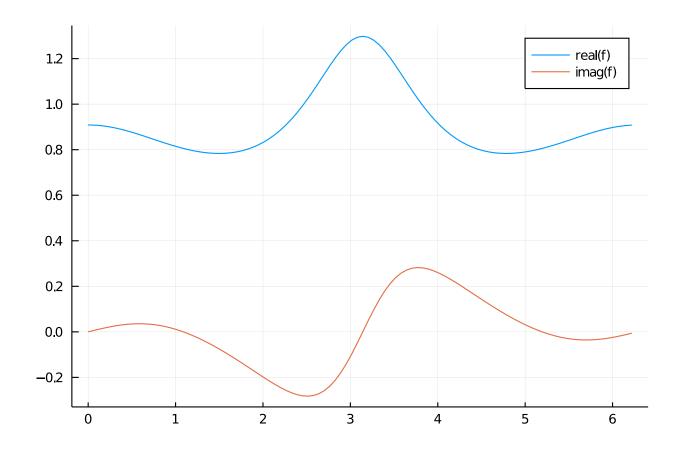
```
 \begin{aligned} \text{trap\_fp} &= \left[ ((\zeta, \, \mathbf{w}) \, = \, \text{circle\_rule}(\mathbf{n}, \, 0.5); \\ &\quad \zeta \, . + = \, \mathbf{x}; \, \# \, \, \text{circle around } \, \mathbf{x} \\ &\quad \text{sum}(\mathbf{f}.(\zeta)./(\zeta \, . - \, \mathbf{x}).^2 \, . * \mathbf{w})/(2\pi*\mathrm{im})) \, \, \text{for n=1:50} \right] \\ \text{scatter(abs.(trap\_fp \, . - \, fp.(\mathbf{x})); yscale=:log10,} \\ &\quad \text{title="Error of trapezium rule applied to Cauchy integral formula", xlabel="n", legend=false)} \end{aligned}
```

Error of trapezium rule applied to Cauchy integral formula



The exponential convergence of the complex trapezium rule is a consequence of $f(\gamma(t))$ being 2π -periodic:

```
\theta = \operatorname{periodic\_rule}(100)[1]
\zeta = x .+ 0.5*\exp.(\operatorname{im}*\theta)
\operatorname{plot}(\theta, \operatorname{real.}(f.(\zeta)); \operatorname{label="real}(f)")
\operatorname{plot!}(\theta, \operatorname{imag.}(f.(\zeta)); \operatorname{label="imag}(f)")
```



Therefore, the integrand of Cauchy's integral formula is periodic and analytic (if f is analytic) on the circular contour.

We can take things further and use this to calculate higher order derivatives, with some care taken for choosing the radius:

```
k=100

r = 1.0k

g = Fun(\zeta \rightarrow exp(\zeta)/(\zeta - 0.1)^{(k+1)}, Circle(0.1,r))

factorial(1.0k)/(2\pi*im) * sum(g) - exp(0.1)

-7.993605777301127e-15 + 3.675487826103639e-16im
```

Bornemann 2011 investigates this further and optimizes the radius.

Example (Ellipse trapezium rule) On an ellipse $\{a\cos\theta + bi\sin\theta : 0 \le \theta < 2\pi\}$ we have

$$\oint_{\gamma} f(z)dz \approx \sum_{j=0}^{N-1} w_j f(z_j)$$

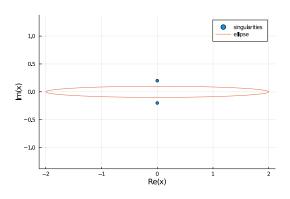
for $z_j = a \cos \theta_j + b i \sin \theta_j$ and $w_j = \frac{2\pi}{N} (-a \sin \theta_j + i b \cos \theta_j)$.

We can use the ellipse trapezium rule in place of the circle trapezium rule and still achieve accurate results. This gives us flexibility in avoiding singularities. Consider

$$f(z) = 1/(25z^2 + 1)$$

which has poles at $\pm i/5$. Using an ellipse allows us to design a contour that avoids these singularities:

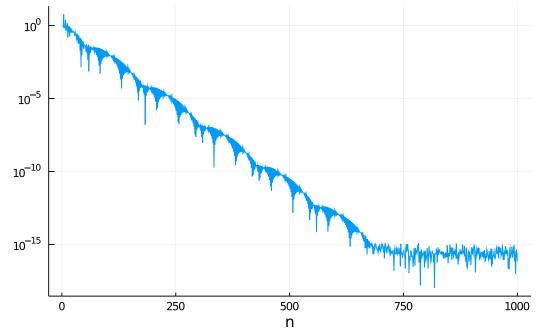
```
scatter([1/5im,-1/5im]; label="singularities") \theta = \text{range}(0; \text{stop}=2\pi, \text{length}=2000) a = 2; b = 0.1 \text{plot!}(a * \cos.(\theta) + im*b * \sin.(\theta); \text{label}="ellipse", ratio = 1.0)
```



Thus we can still use Cauchy's integral formula:

```
 \begin{array}{l} x = 0.1 \\ f = z \rightarrow 1/(25z^2 + 1) \\ \\ function \ ellipse\_rule(n, a, b) \\ \theta = periodic\_rule(n)[1] \\ a*cos.(\theta) + b*im*sin.(\theta), 2\pi/n*(-a*sin.(\theta) + im*b*cos.(\theta)) \\ \\ end \\ f\_ellipse = [((z, w) = ellipse\_rule(n, a, b); \\ sum(f.(z)./(z.-x).*w)/(2\pi*im)) \ for \ n=1:1000] \\ plot(abs.(f\_ellipse .- f(x)); \ yscale=:log10, \ title="convergence of n-point ellipse approximation", legend= false, xlabel="n") \\ \end{array}
```

convergence of n-point ellipse approximation



1.6 Taylor series versus Cauchy integral formula

The Taylor series gives a polynomial approximation to f. The Cauchy's integral formula discretisation gives a rational approximation, which is more adaptable and does not require knowing the derivatives of f:

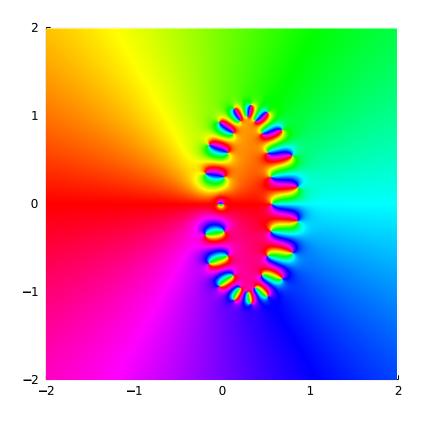
```
using ComplexPhasePortrait
f = z \rightarrow sqrt(z)
function sqrt_n(n,z,z_0)
    ret = sqrt(z_0)
    c = 0.5/ret*(z-z_0)
    for k=1:n
        ret += c
        c *= -(2k-1)/(2*(k+1)*z) *(z-z)
    end
    ret
end
z = 0.3
n = 40
phaseplot(-2..2, -2..2, z -> sqrt_n.(n,z,z_0))
```

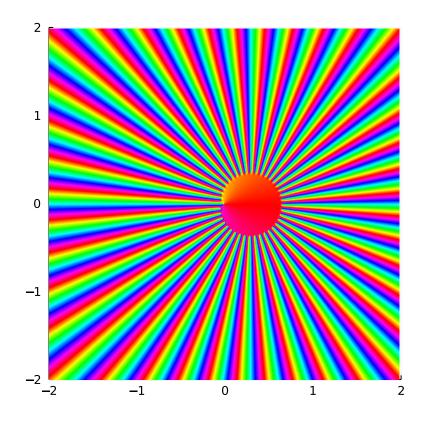
```
(\zeta, w) = ellipse\_rule(20, 0.28, 1.0);

\zeta = \zeta + 0.3;

f_c = z -> sum(f.(\zeta)./(\zeta.-z).*w)/(2\pi*im)

phaseplot(-2..2, -2 ... 2, f_c)
```





$$(\zeta, w) = ellipse_rule(1000, 0.28, 1.0);$$

 $\zeta = \zeta + 0.3;$
 $f_c = z -> sum(f.(\zeta)./(\zeta.-z).*w)/(2\pi*im)$
 $f_c(0.5) - sqrt(0.5)$

-3.907985046680551e-14 - 2.9403565414571575e-17im