Notes on Cauchy integration

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September 16th, 2017

Cauchy integration became a popular way to compute exponential integrators. This document describes briefly the background information on Cauchy integrals, how they are related to REXI and how to apply them for exponential integrators. For related work on which this work is based on, see [1, 2]

1 Cauchy's integration

Loosely stated, for a given function $f(x)$, the value of this function can be computed by the contour integral around the point x_0 where it should be integrated

$$f(x) = \frac{1}{2\pi i} \oint_\Gamma \frac{f(z)}{z-x} dz$$

Here, $f : \mathbb{C} \to \mathbb{C}$ is a holomorphic function (complex-valued function which is infinitely differentiable) and the inner area of the contour can be reconstructed by the values on the contour. (This can be imagined similar to a Taylor expansion).

2 Relation to exponential integrators

For exponential integrators, we have to deal with the ψ_n functions and approximate them with the function above:

$$\psi(x) = \frac{1}{2\pi i} \oint_\Gamma \frac{\psi(z)}{z-x} dz$$

Note, that the ψ_n function with $n > 0$ have a singularity at $x = 0$, however we can cope with this with the Cauchy integration easily

3 Cauchy's quadrature and Exponential integrators

First, we choose a contour which should enclose all x points which should be correctly approximated.

We can use a parametrization of this with (see e.g. [1])

$$\Gamma = \{R\exp(i\theta) + \mu | \theta \in [0; 2\pi]\}$$

with $\theta \in [0; 2\pi]$ and μ some shift. We use a change of variables

$$\begin{aligned} z &= R\exp(i\theta) + \mu \\ \frac{d}{d\theta} z &= \frac{d}{d\theta}\left(R\exp(i\theta) + \mu\right) \\ dz &= \left(iR\exp(i\theta)\right) d\theta \end{aligned}$$

which leads to

$$\psi(x) = \frac{1}{2\pi i} \oint_0^{2\pi} \frac{\psi(R\exp(i\theta) + \mu)}{R\exp(i\theta) + \mu - x} \left(iR\exp(i\theta)\right) d\theta$$

$$\psi(x) = \frac{1}{2\pi i} \oint_0^{2\pi} \frac{\psi(R\exp(i\theta) + \mu)\left(iR\exp(i\theta)\right)}{R\exp(i\theta) + \mu - x} d\theta$$

$$\psi(x) = \frac{1}{2\pi i} \oint_0^{2\pi} \frac{\psi(R\exp(i\theta) + \mu)\left(iR\exp(i\theta)\right)}{(R\exp(i\theta) + \mu) - x} d\theta$$

Using

$$\alpha(\theta) = (R\exp(i\theta) + \mu)$$

and

$$\beta(\theta) = -\psi(R\exp(i\theta) + \mu)\left(iR\exp(i\theta)\right)$$

we can write

$$\frac{1}{2\pi i} \oint_0^{2\pi} \frac{\beta(\theta)}{x - \alpha(\theta)} d\theta.$$

A discretization of the contour integral leads to

$$\frac{1}{N} \sum_{n=1}^{N} \frac{\beta_n}{x - \alpha_n},$$

hence leading to a REXI-like discretization.

In a similar way, a generic formulation for a parametrized contour integral around $z = g(s)$ with s the parameter can be obtained by

$$\begin{aligned} f(x) &= \frac{1}{2\pi i} \oint_\Gamma \frac{f(z)}{z - x} dz \\ &= \frac{1}{2\pi i} \oint_0^{2\pi} \frac{-f(g(s))}{-g(s) + x} \frac{\partial g(s)}{\partial s} ds \end{aligned}$$

3.1 Circle contour

4 Test cases

All test cases are conducted with $N = 64$, $\mu = 1$, $R = 10$ using the circle contour integral and initial conditions

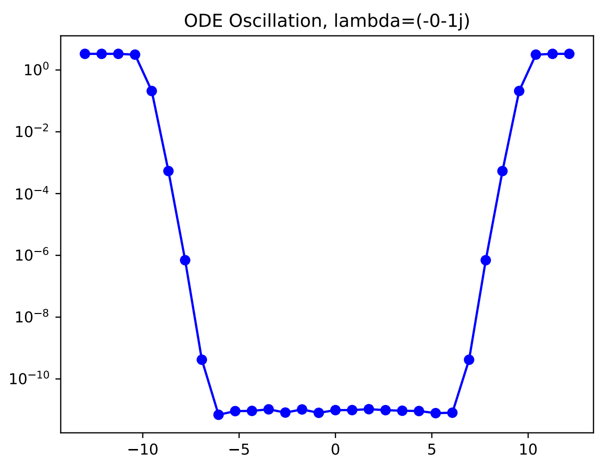
$$U_i = \begin{cases} 1.66 & \text{if } i = 0 \\ 0 & \text{else} \end{cases}$$

4.1 Contour integration

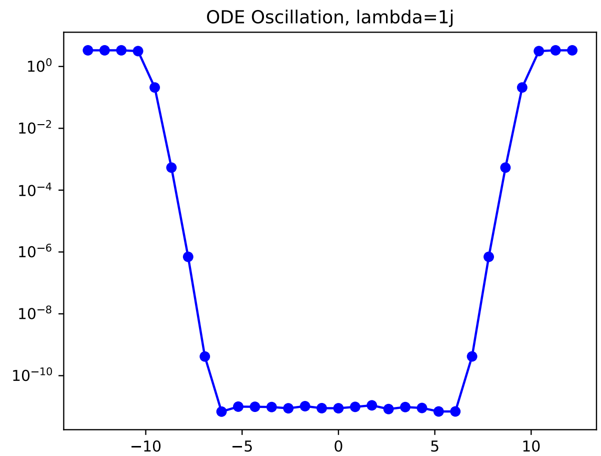
4.1.1 Oscillatory ODE I

$$u(t) = \exp(\lambda t) u(0)$$

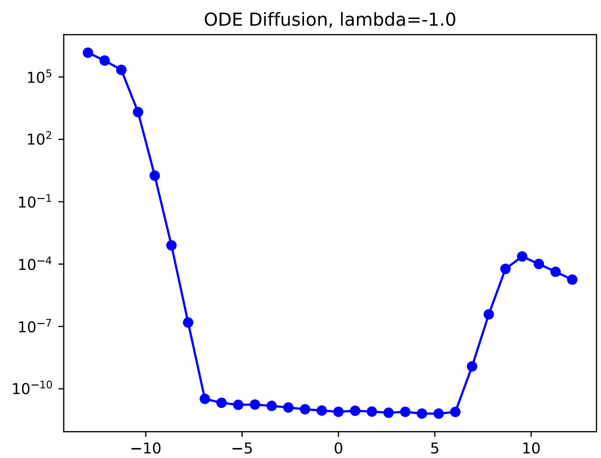
$$\lambda = 1i$$



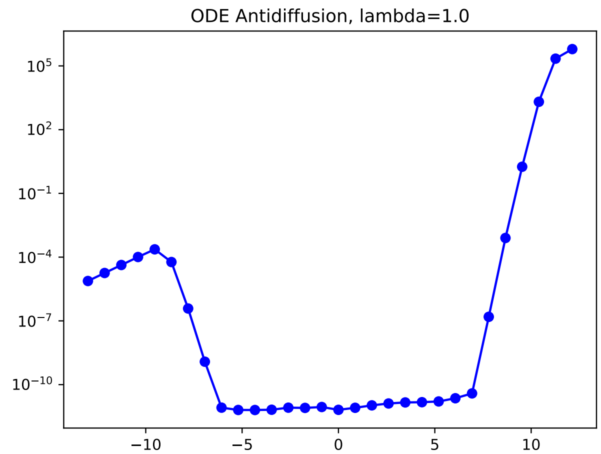
4.1.2 Oscillatory ODE II



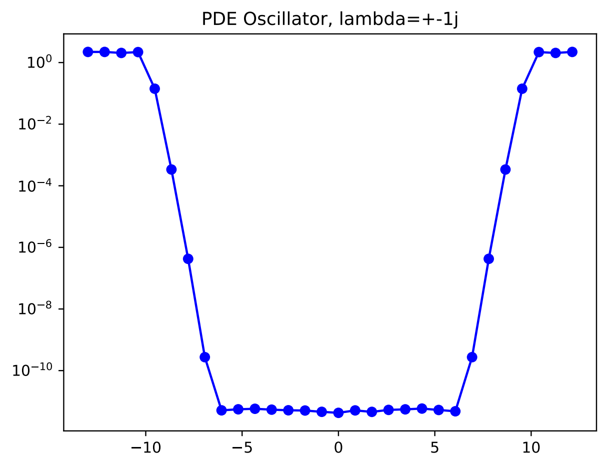
4.1.3 Diffusive ODE



4.1.4 Anti-Diffusive ODE



4.1.5 Oscillatory PDE (2x2 matrix)



5 Relation of REXI to Cauchy contour

Next, we can try to relate coefficients which are given in the "REXI" format to the contour of the Cauchy quadrature. For the α terms, this is trivial since the contour is given by

$$\Gamma = R\exp(i\theta) + \mu$$

and the alphas by

$$\alpha(\theta) = (R \exp(i\theta) + \mu)$$

Hence, the quadrature points are given by $-\alpha_n$. Note, that here these coefficients are independent of the function to be approximated (This is also what Terry stated at the very end of his paper with his method).

The β coefficients correspond simply to the quadrature weights and depend on the function.

$$\beta(\theta) = -\psi(R \exp(i\theta) + \mu) \, (R \exp(i\theta))$$

6 Numerical cancellation problems

For a radius > 10, the Cauchy contour integration suffers increasingly from numerical cancellation effects because of very large and small coefficients with alternating signs:

```
beta_re[0] = (-2585.75,-2120.81)
beta_re[1] = (1344.27,-2563.9)
beta_re[2] = (2100.59,553.566)
beta_re[3] = (3.77547,1416.9)
beta_re[4] = (-767.79,247.343)
beta_re[5] = (-254.154,-312.771)
beta_re[6] = (76.3302,-160.693)
beta_re[7] = (69.6664,-6.12502)
beta_re[8] = (16.2192,18.6306)
beta_re[9] = (-0.930128,7.85576)
beta_re[10] = (-1.71593,1.55317)
beta_re[11] = (-0.613435,0.0849086)
beta_re[12] = (-0.138315,-0.0537611)
beta_re[13] = (-0.0156466,-0.0254132)
beta_re[14] = (0.00955142,-0.00808595)
...
```

6.1 Origins of numerically ill-conditioned betas

Using the CI, we get $\max_\theta |\alpha(\theta)| = R$, hence α behaves linear regarding R.

The real problem arises with $\beta(\theta)$. Using the previous derivation, we can see that $\beta(\theta) = -\psi(R \exp(i\theta) + \mu) \, (R \exp(i\theta))$ where

$$\max_\theta |R \exp(i\theta)| = R$$

for the 2nd term and

$$\max_\theta |Im(\exp(R \exp(i\theta) + \mu))| = R$$

for the imaginary (oscillatory) components for the 1st term. However, for positive real parts (anyhow related to unphysical "anti-diffusion"), we get **exponential growth for approximating positive real Eigenvalues** and we account this for the instabilities. Therefore we could try to get around this by using a rectangle which is mainly extended along the oscillatory components by simply putting a rectangle around it.

6.2 Rectangle contour

Using a rectangle as the contour, we can decompose this into the "bottom", "right", "top" and "left" edges as follows

$$\oint_{\Gamma} = \oint_{\Gamma_B} + \oint_{\Gamma_R} + \oint_{\Gamma_T} + \oint_{\Gamma_L}.$$

Furthermore we assume the rectangle being centered at the origin and being of extension S_{Re} along the real axis and S_{Im} along the imaginary axis. This yields

$$\begin{aligned}
\Gamma_B &= \left\{-i\frac{1}{2}S_{Im} + p | p \in \left[-\frac{1}{2}S_{Re}; \frac{1}{2}S_{Re}\right]\right\} \\
\Gamma_R &= \left\{+\frac{1}{2}S_{Re} + ip | p \in \left[-\frac{1}{2}S_{Im}; \frac{1}{2}S_{Im}\right]\right\} \\
\Gamma_T &= \left\{+i\frac{1}{2}S_{Im} - p | p \in \left[-\frac{1}{2}S_{Re}; \frac{1}{2}S_{Re}\right]\right\} \\
\Gamma_L &= \left\{-\frac{1}{2}S_{Re} - ip | p \in -\left[-\frac{1}{2}S_{Im}; \frac{1}{2}S_{Im}\right]\right\}
\end{aligned}$$

We continue with an example for the bottom partial contour integral where we can set

$$z = -i\frac{1}{2}S_{Im} + p$$

and perform a change of integration variable

$$\begin{aligned}
\frac{dz}{dp} &= \frac{d}{dp}\left(-i\frac{1}{2}S_{Im} + p\right) = 1 \\
dz &= dp.
\end{aligned}$$

for the "bottom" contour integral. For all boundaries, we can get in a similar way

$$\begin{aligned}
dz_B &= dp \\
dz_R &= idp \\
dz_T &= -dp \\
dz_L &= -idp.
\end{aligned}$$

Finally, we can write for the bottom contour integral

$$\oint_{\Gamma_B} \frac{\psi(z)}{z-x} dz = \oint_{\Gamma_B} \frac{\psi(-i\frac{1}{2}S_{Im} + p)}{(-i\frac{1}{2}S_{Im} + p) - x} dp$$

using N quadrature points, we get

$$\oint_{\Gamma_B} \frac{\psi(-i\frac{1}{2}S_{Im}+p)}{(-i\frac{1}{2}S_{Im}+p)-x}dz \approx \frac{S_{Re}}{N_{Re}} \sum_{n=1}^{N} \frac{\psi(-i\frac{1}{2}S_{Im}+p_{Re}^n)}{(-i\frac{1}{2}S_{Im}+p_{Re}^n)-x}.$$

Specifying the sampling distances with

$$D_{Re} = \frac{S_{Re}}{N_{Re}}$$

$$D_{Im} = \frac{S_{Im}}{N_{Im}}$$

we can write

$$p_{Re}^n = \frac{1}{2}\left(D_{Re} - S_{Re}\right) + nD_{Re}$$

$$p_{Im}^n = \frac{1}{2}\left(D_{Im} - S_{Im}\right) + nD_{Im}.$$

This leads to the approximation of the CI in the order of "bottom", "right", "top", "left"

$$\begin{aligned}
\frac{1}{2\pi i}\oint_{\Gamma} \frac{\psi(z)}{z-x}dz \quad \approx \quad & \frac{1}{2\pi i}(\\
& + \frac{S_{Re}}{N_{Re}} \sum_{n=1}^{N_{Re}} \frac{\psi(-i\frac{1}{2}S_{Im}+p_{Re}^n)}{(-i\frac{1}{2}S_{Im}+p_{Re}^n)-x} \\
& + \frac{S_{Im}}{N_{Im}} \sum_{n=1}^{N_{Im}} \frac{\psi(\frac{1}{2}S_{Re}+ip_{Im}^n)}{(\frac{1}{2}S_{Re}+ip_{Im}^n)-x} \\
& - \frac{S_{Re}}{N_{Re}} \sum_{n=1}^{N_{Re}} \frac{\psi(i\frac{1}{2}S_{Im}-p_{Re}^n)}{(i\frac{1}{2}S_{Im}-p_{Re}^n)-x} \\
& - \frac{S_{Im}}{N_{Im}} \sum_{n=1}^{N_{Im}} \frac{\psi(-\frac{1}{2}S_{Re}-ip_{Im}^n)}{(-\frac{1}{2}S_{Re}-ip_{Im}^n)-x} \\
&)
\end{aligned}$$

6.3 Shifted circle

Next, we focus on shifting the circle away from the large positive real values by shifting it to the negative values. It's very easy to catch all values for purely diffusive problems by shifting the circle along the real axis. The real "challenge" is to perform this shift optimally to also include oscillatory Eigenvalues. According to a previous Section, the numerical cancellation effects arise from large real Eigenvalues. Therefore we should limit them by enforcing the circle not to cross this point. Let this limiting point on the circle line be denoted by x_0 with $Im(x_0) = 0$.

Furthermore, we'd like an approximation including a particular imaginary spectrum. Let the two points maximum points on the circle including the maximum EValue be given by $x_{\pm 1}$.

Finally, we search for the radius r and the center point x_c of the circle which can be computed as follows:

$$|x_i - x_c| = r$$
$$(Re(x_i) - Re(x_c))^2 + (Im(x_i) - Im(x_c))^2 = r^2$$

We get the following system of equations:

$$\begin{aligned}
(Re(x_{-1}) - Re(x_c))^2 + (Im(x_{-1}) - Im(x_c))^2 &= r^2 \\
(Re(x_0) - Re(x_c))^2 + (Im(x_0) - Im(x_c))^2 &= r^2 \\
(Re(x_1) - Re(x_c))^2 + (Im(x_1) - Im(x_c))^2 &= r^2
\end{aligned}$$

Using $Im(x_{-1}) = Im(x_1)$, $Re(x_{\pm 1}) = 0$, $Im(x_0) = 0$ and $Im(x_c) = 0$ we get

$$\begin{aligned}
Re(x_c)^2 + Im(x_{-1})^2 &= r^2 \\
(Re(x_0) - Re(x_c))^2 &= r^2 \\
Re(x_c)^2 + Im(x_{-1})^2 &= r^2
\end{aligned}$$

where the 1st and 3rd line are identical.

The placement of the centroid on the real axis can be computed from the 2nd line by choosing the signs wisely

$$Re(x_c) = Re(x_0) - r$$

and the required radius by replacing $Re(x_c)$ in the 1st line:

$$\begin{aligned}
(Re(x_0) - r)^2 + (Im(x_{-1}))^2 &= r^2 \\
r^2 - 2rRe(x_0) + Re(x_0)^2 + (Im(x_{-1}))^2 &= r^2 \\
r &= \frac{Re(x_0)^2 + (Im(x_{-1}))^2}{2Re(x_0)}
\end{aligned}$$

7 Conclusions

1. Cauchy quadrature is easy and efficient. The circle quadrature seems to beat Terry's REXI method in it's elegance and efficiency. However it's limited by the numerical cancellation effects to $R < 30$ for simple test problems.

2. Using a circle for quadrature is not the most efficient way. An ellipsoid might be better and focused on oscillatory or diffuse approximation.

3. There could be a relation between every time stepping method which can be expressed to be REXI-like and a Cauchy contour integral.

References

[1] Tommaso Buvoli. A class of exponential integrators based on spectral deferred correction. *arXiv preprint arXiv:1504.05543*, 2015.

[2] Aly-Khan Kassam and Lloyd N Trefethen. Fourth-order time-stepping for stiff pdes. *SIAM Journal on Scientific Computing*, 26(4):1214–1233, 2005.