Numerical exponential integrators for dynamical systems

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- Title:

Numerical exponential integrators for dynamical systems

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- *2. Summary of the activities*
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- *Description and evaluation of institutional support received in the period*
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CHAPTER

ONE

1. SUMMARY OF THE PROPOSED PROJECT

This is a scientific initiation project that proposes the deep study of some of the main methods of exponential integration for problems in dynamic systems, with emphasis on the paper []. Here, the undergraduate will study the construction, analysis, implementation and application of them and at the end, it is expected that she is familiar with modern techniques of numerical methods.

Keywords: exponential integrator, numerical methods, dynamical systems.

CHAPTER

TWO

2. SUMMARY OF THE ACTIVITIES

To be done.

CHAPTER

THREE

3. PROJECT EXECUTION

3.1 Motivation - Stiffness

The reason for studying exponential methods is that those are good with **stiff differential equations** in terms of precision and how small the time step is required to be to achieve good accuracy.

3.1.1 Cauchy problem

A **Cauchy problem** is a ordinary differential equation (ODE) with initial conditions. Being its standard scalar form:

$$\begin{cases} y'(t) = f(y(t), t), t \in (t_0, T) \\ y(t_0) = y_0 \in \mathbb{K}, \end{cases}$$

with $\mathbb{K}$ a field, f function with image in $\mathbb{K}$ and $t_0, T \in \mathbb{R}$.

Sometimes, it is convenient to separate the linear part of f as indicated below:

$$f(y(t), t) = g(y(t), t) - \lambda y(t),$$

with $\lambda \in \mathbb{K}$ or $\mathcal{M}_{N\times N}(\mathbb{K})$.

So the system is:

$$\begin{cases} y'(t) + \lambda y(t) = g(y(t), t), t \in (t_0, T) \\ y(0) = y_0. \end{cases}$$

In this project, the stiff ones were those addressed.

Notation as in [1].

3.1.2 Stiffness

The error of the approximation given by a method trying to estimate the solution of a Cauchy problem is always given by a term multiplied by a higher derivative of the exact solution, because of the Taylor expansion with Lagrange form of the remainder. In that way, if that is enough information about this derivative, the error can be estimated.

If the norm of the derivative increases with the time, but the exact solution doesn't, that is possible that the error dominates the approximation and the precision is lost. Those problems are called **stiff equations**.

Between them, there are the **stiff differential equations**, that have exact solution given by the sum of a *transient solution* with a *steady state solution*.

The **transient solution** is of the form:

$$e^{-ct}\text{, with c >>1,}$$

which is known to go to zero really fast as t increases. But its nth derivative

$$\mp c^n e^{-ct}$$

doesn't go as quickly and may increase in magnitude.

The **steady state solution**, however, as its name implies, have small changes as time passes, with higher derivative being almost constant zero.

In a system of ODE's, these characteristics are most common in problems in which the solution of the initial value problem is of the form

$$e^A$$

being A a matrix such that λ_{min} and λ_{max} are the eigenvalue with minimum and maximum value in modulus and $\lambda_{min} << \lambda_{max}$. On the bigger magnitude eigenvalue direction, the behaviour is very similar to the transient solution, having drastic changes over time and on the smaller one, comparing to that, changes almost nothing as times passes, like the steady state solution.

Work around these problems and being able to accurately approximate these so contrasting parts of the solutions requires more robust methods than the more classic and common one-step methods addressed at the beginning of the study of numerical methods for Cauchy problems. For the systems, it is also required that that is a precise way to calculate the exponential of a matrix.

In this project, we studied the **exponential methods**, their capabilities to deal with these problems and the comparision with other simpler methods.

Definition from [2].

3.2 3.2 Chapter 2: Classical methods

In order to show that the exponential methods improve in dealing with Stiff problems, that is necessary to know how the previows methods deal with them, so a review on the theory of the classical methods is made in this chapter. In particular there will be focus on the one step methods. All the information is from [3].

3.2.1 One step methods for ODE

In order to find a approximation for the solution of the problem $\begin{cases} y'(t) = f(t, y(t)), t \in [t_0, T] \\ y(t_0) = y_0, \end{cases}$

they are of the form: \$$y_{k+1} = y_k + h\phi(t_k, y_k, t_{k+1}, y_{k+1}, h)$,\$

with \$$k = 0, 1, ..., n-1$;$N \in \mathbb{N}$; $h = \frac{T-t_0}{N}$;
$\{t_i = t_0 + ih : i = 0, 1, ..., N\}$;
$y_n \approx y(t_n)$.\$

To analyse the method, there is a model problem $\begin{cases} y'(t) = -\lambda y(t) \ ; t \in [t_0, T] \\ y(t_0) = y_0, \end{cases}$

whose solution is $y(t) = y_0 e^{-\lambda(t-t_0)}$ with $\lambda > 0$.

If that is possible to manipulate the method so that, for this problem, can be written as $y_{k+1} = \zeta(\lambda, h) y_k$, then $\zeta(\lambda, h)$ is called **amplification factor** of the method.

By induction, it gives $y_{k+1} = \zeta(\lambda, h)^{k+1} y_0$.

It is well known that this expression only converges as k goes to infinity if $|\zeta(\lambda, h)| < 1$ and then converges to zero.

When it occurs, i.e., $k \to \infty \Rightarrow y_k \to 0$ such as the exact solution $y(t) = y_0 e^{-\lambda(t-t_0)}$, it is said that there is **stability**.

The inequation gives a interval for which values of λh, $|\zeta(\lambda, h)| < 1$, called **interval of stability**.

And if the interval of stability contains all the points z such that $Re(z) < 0$, the method is said **A-stable**.

The reason for taking this specific problem is that it models the behaviour of the difference between the approximation and the solution on a small neighbourhood of any Cauchy problem:

Taking $\begin{cases} y'(t) = f(y(t), t), t \in (t_0, T) \\ y(t_0) = y_0 \in \mathbb{K} \end{cases}$

and a approximation z of the solution y, doing $\sigma(t) = z(t) - y(t) \Rightarrow$

$$\dot{\sigma}(t) = \dot{z}(t) - \dot{y}(t) = f(z(t), t) - f(y(t), t) \Rightarrow$$

$$\dot{\sigma}(t) + \dot{y}(t) = \dot{z}(t) = f(z(t), t) = f(y(t) + \sigma(t), t)$$
$$= f(y(t), t) + \sigma(t)\frac{\partial f}{\partial y} + O(\sigma^2(t)),$$

so $\begin{cases} \dot{\sigma}(t) \approx \sigma(t) \frac{\partial f}{\partial y} (y(t), t) \\ \sigma(t_k) = \sigma_k. \end{cases}$

Other important definitions are:

Local truncation error: Is the difference between the exact expression and its numerical approximation in a certain point and with a certain domain discretization. If the domain is equally spaced by h is often denoted by $\tau(h, t_0)$ being t_0 the point.

Order of the local truncation error: the local truncation error (which depends on the h spacing of the discretized domain) $\tau(h)$ has order $n \in \mathbb{N}$ if $\tau(h) = O(h^n)$, i.e., if there is constant $M \in \mathbb{R}$ and $h_0 \in \mathbb{R}$ such that $\tau(h) \leq Mh^n$, $\forall h \leq h_0$.

Global error: Is the difference between the approximation given by the method for the solution of the problem on a certain point and the exact one (unlike the local truncation error, here we take the solution we got, not the expression used to find the approximation).

Consistency: The method is said consistent if $\lim_{h \to 0} \frac{1}{h} \tau(h, x_0) = 0$.

Obs.: For consistency, we usually only analyse for the linear part of the Cauchy problem, since this is the part that most influences in the consistency.

Order of consistency: is the smallest order (varying the points at which the local error is calculated) of the local truncation error.

Convergence: A numerical method is convergent if, and only if, for any well-posed Cauchy problem and for every $t \in (t_0, T)$, $\lim_{h \to 0} e_k = 0$ with $t - t_0 = kh$ fixed and e_k denoting the global error on t_k (following the past notation).

Theorem: A one-step explicit method given by $y_0 = y(t_0)$
$y_{k+1} = y_k + h\phi(t_k, y_k, h)$ such that ϕ is Lipschitzian in y, continuous in their arguments, and consistent for any well-posed Cauchy problem is convergent. Besides that, the convergence order is greater or equal to the consistency order.

Prove: [3] pág 29-31.

3.2.2 Examples

Euler method:

$$\phi(t_k, y_k, h) = f(t_k, y_k)$$

Modified Euler method:

$$\phi(t_k, y_k, h) = \frac{1}{2}\left[f(t_k, y_k) + f(t_{k+1}, y_k + hf(t_k, y_k))\right]$$

Midpoint method:

$$\phi(t_k, y_k, h) = f(t_k + \frac{h}{2}, y_k + \frac{h}{2}f(t_k, y_k))$$

Classic Runge-Kutta (RK 4-4):

$$\begin{aligned}\phi(t_k, y_k, h) = \frac{1}{6}\left(\kappa_1 + 2\kappa_2 + 2\kappa_3 + \kappa_4\right), \text{with}\\ \kappa_1 = f(t_k, y_k)\\ \kappa_2 = f(t_k + \frac{h}{2}, y_k + \frac{h}{2}\kappa_1)\\ \kappa_3 = f(t_k + \frac{h}{2}, y_k + \frac{h}{2}\kappa_2)\\ \kappa_4 = f(t_k + h, y_k + h\kappa_3)\end{aligned}$$

3.2.3 Euler method

Further detailing this explicit one-step method of

$$\phi(t_k, y_k, h) = f(t_k, y_k),$$

an analysis on stability, convergence and order of convergence is done.

Stability

For the problem $\begin{cases} y'(t) = -\lambda y(t)\ ; t \in [t_0, T] \\ y(t_0) = y_0, \end{cases}$

with known solution

$$y(t) = y_0 e^{-\lambda(t-t_0)},$$

the method turn into:

$$\begin{aligned} y_0 = y(t_0)\\ \textbf{for } k = 0, 1, 2, ..., N-1:\\ y_{k+1} = y_k + h\lambda y_k\\ t_{k+1} = t_k + h.\end{aligned}$$

Then the amplification factor is: $(1 - h\lambda).$

If

$$|1 - h\lambda| > 1, \text{for fixed } N,$$

it will be a divergent series

$$(k \to \infty \Rightarrow y_k \to \infty),$$

so, since the computer has a limitant number that can represent, even if the number of steps is such that h is not small enought, it might have sufficient steps to reach the maximum number represented by the machine.

However, if $|1 - h\lambda| < 1$ and N is fixed,

it converges to zero $(k \to \infty \Rightarrow y_k \to 0)$.

Besides that,

$$|1 - h\lambda| < 1$$

is the same as $0 < h\lambda < 2$.

So the interval of stability is $(0, 2)$.

That's why the method suddenly converged, it was when h got small enought to $h\lambda$ be in the interval of stability, i.e.,

$$h < 2/\lambda.$$

It is worth mentioning here that if

$$-1 < 1 - h\lambda < 0,$$

the error will converge oscillating since it takes positive values with even exponents and negative with odd ones.

Convergence

Since $\lim_{m\to+\infty} \left(1 + \frac{p}{m}\right)^m = e^p$, and $h = \frac{T-t_0}{N}$, for y_N we have $\lim_{N\to+\infty} y_N = \lim_{N\to+\infty} (1 - h\lambda)^N y_0 = \lim_{N\to+\infty} \left(1 - \frac{(T-t_0)\lambda}{N}\right)^N y_0$. It is reasonable to take $p = -(T-t_0)\lambda$ and conclude that the last point estimated by the method will converge to $y_0 e^{-\lambda(T-t_0)}$. Which is precisely $y(T)$ and proves the convergence.

Order of convergence

Being $\tau(h, t_k)$ the local truncation error.

From $y(t_{k+1}) = y(t_k) + hf(y(t_k), t_k) + O(h^2)$,

we have $h\tau(h, t_k) \doteq \frac{y(t_{k+1}) - y(t_k)}{h} - f(t_k, y(t_k)) = O(h^2)$,

so $\tau(h, t_k) = O(h)$.

Since for one step methods the order of convergence is the order of the local truncation error, the order is of $O(h)$, order 1.