Numerical Matrix Exponentiation for Large Matrices

Bruno Beltran, Avery St. Dizier, Morgan Matchett, Tyler Wales

Department of Mathematics
Louisiana State University
bbeltr1@lsu.edu, astdiz1@lsu.edu, mmatch1@lsu.edu, twales2@lsu.edu

Introduction

- Systems of linear ordinary differential equations are pervasive throughout the engineering disciplines and the sciences. The solution to these systems, e^{tA}, or the matrix exponential, can be solved for and approximated using a variety of methods. Our research investigated the use of
- A nice little section on the results of the calculations will go here, however, Bruno needs more time to get the best results so in the meantime he put a long section of text here which really doesn't say much as far as Mathematics goes in order to take up the appropriate amount of space.

1. Background

An Easy Problem

- Consider the following variation on the canonical heat dissipation problem often presented in an introductory Differential Equations class.
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The temperature of the system can be modelled using Newton's law of heating and cooling as

$$\frac{dT_1}{dt} = a(T_2 - T_1) + b(T_{e_1} - T_1)$$
$$\frac{dT_2}{dt} = c(T_1 - T_2) + d(T_{e_2} - T_2)$$

where a, b, c, d are constants, and T_1, T_2, T_{e_i} are the temperatures of their respective regions. If $T_e = 0$ (the homogenous case,) then the classical way to solve these equations involves rearranging them to get

$$\frac{dT_1}{dt} = -(a+b)T_1 + aT_2$$
$$\frac{dT_2}{dt} = cT_1 - (c+d)T_2$$

which can simply be written as a matrix product

$$A\begin{pmatrix} T_1 \\ T_2 \end{pmatrix} = \begin{pmatrix} T_1' \\ T_2' \end{pmatrix}$$

In order to see the way in which the classical method lacks generalizability for larger matrices, let us solve a particular system, $A = \begin{pmatrix} -3 & 4 \\ -1 & 1 \end{pmatrix}$.

2. Retarded and Neutral Equations

- To approximate the solutions of (DDE) we use new numerical methods for the inversion of the Laplace transform as described in [1]. The solution $u(t)$ of (DDE) can be approximated by a function $u_a(t)$ given by the Laplace Transform inversion formula

$$u_a(t) = \frac{B_0}{t}\hat{u}\left(\frac{\lambda_0}{t}\right) + \frac{B_1}{t}\hat{u}\left(\frac{\lambda_1}{t}\right) + \cdots + \frac{B_q}{t}\hat{u}\left(\frac{\lambda_q}{t}\right), \qquad (*)$$

where the constants $B_0, \ldots, B_q$ and $\lambda_0, \ldots, \lambda_q$ are uniquely determined by the partial fraction decomposition of the subdiagonal rational Padé-approximation $r(z) = \frac{P(z)}{Q(z)}$ of the exponential; i.e., $r(z)$ is a rational function of the form

$$r(z) = \frac{P(z)}{Q(z)} = \frac{B_0}{\lambda_0 - z} + \cdots + \frac{B_q}{\lambda_q - z}, \text{ where}$$

$$P(z) = \sum_{j=0}^{q-1} \frac{(m-j)!(q-1)!}{m!j!(q-1-j)!} z^j \text{ and } Q(z) = \sum_{j=0}^{q} \frac{(m-j)!q!}{m!j!(q-j)!}(-z)^j.$$

- To check the numerical accuracy of the approximation method, we study a DDE that can be solved explicitly and compare the true solution with its approximation. One of the few first-order DDEs that can be solved explicitly is the "greedy bank" problem

$$u'(t) - ru(t-1) = 0 \text{ with } u(t) = 1 \text{ for } t \in [-1, 0]. \qquad \text{(GB)}$$

(see below for an explanation of the problem). For $r = 1$, the solution is $u(t) = t + 1$ on the interval $[0, 1]$, $u(t) = (\frac{t^2}{2} + \frac{3}{2})$ on $[1, 2]$, and, more generally,

$$u(t) = \sum_{n=0}^{N}\left[1 + \sum_{j=0}^{n} \frac{(t-j)^{j+1}}{(j+1)!} X_{[n,n+1]}(t)\right],$$

where $X_{[n,n+1]}$ is the characteristic function of the interval $[n, n+1]$.

(a) $u_a(t)$ (b) $Error = u_a(t) - u(t)$

The Greedy Bank Problem(GB)

- The delay equation (GB) models an investment plan in which a bank continuously compounds interest at an annual interest rate r on the amount of what the account had in it a year ago (and works with the withhold interest for one year for its own greed). If r is compounded n-times per year on the amount of what the account had in it a year ago, then the discrete version of (GB) is

$$u_{t+\frac{1}{n}} = u_t + \frac{r}{n}u_{t-1}.$$

If one sets $t = \frac{j}{n}$ and defines $a_j := u_{\frac{j}{n}}$, then this becomes

$$a_{j+1} = a_j + \frac{r}{n}a_{j-n}, \qquad \text{(DE)}$$

where the initial values $a_0, \ldots, a_n$ are given. Thus, we expect that the solutions of (GE) can be approximated by solutions of (DE) for n sufficiently large.

Figure 2: *Discrete* → *Continuous*

- After having established that there are a variety of ways that we can approximate the solutions of retarded DDEs like (GB), we now turn to our main research issue, namely the investigation of advanced DDEs. First we show that advanced DDEs appear when one considers "backward-in-time" problems for retarded DDEs.

Retarded Backwards Equals Advanced Forward

- The problem we are considering is as follows. Let us assume that we know that a system is governed by a retarded DDE of the form

$$a_0u'(t) + b_0u(t) + b_1u(t - \omega) = f(t)$$

and that we can observe the solution $u(t)$ for $t \in [T, T + \omega]$. The question is then what we can say about the (unknown) initial function $u(t) = g(t)$ for $t \in [-\omega, 0]$. To solve this problem, we set $v(t) := u(T - t)$ and the problem becomes to compute $v(t)$ for $t \in [T, T + \omega]$. To do so, an easy computation shows that $v(t)$ satisfies the advanced DDE

$$-a_0v'(t - \omega) + b_1v(t) + b_0v(t - \omega) = \tilde{f}(t), \qquad (**)$$

where $\tilde{f}(t) := f(T - t + \omega)$ and $v(t) = u(T - \omega)$ is given for $t \in [-\omega, 0]$.

Uniqueness

- Using finite Laplace transform methods and a well known uniqueness theorem of Laplace transform theory, we can show that the solutions of advanced DDEs of the form (**) are unique. This seems to be a new result. As we will see next, the real problem with advanced DDEs of the form (**) lies within the existence and computability of the solutions.

The Backwards Greedy Bank Problem

- If one applies (**) to the greedy bank problem $u'(t) - ru(t-1) = 0$, then the corresponding backward-in-time problem is the advanced DDE

$$v'(t - 1) + rv(t) = 0, \qquad \text{(BGB)}$$

where $v(t) = u(T - t)$ is given for $t \in [-1, 0]$ by a solution $u(t)$ of the greedy bank problem for $t \in [T, T + 1]$.
- Since the greedy bank problem is a limit of the difference equations (DE), we are now investigating the "backward-in-time" versions of (DE) by setting $b_j := a_{N-j}$, where a_j solves (DE). It is easy to see that the sequence b_j satisfies the difference equation

$$b_{j+1} = \frac{n}{r}[-b_{j+1-n} - b_{j-n}], \qquad \text{(BDE)}$$

where the initial data is given by $b_j = a_{N-j}$ for $0 \le j \le n$. As we will see below, solving a (BDE) for a given solution a_j of a (DE) seems to be "as hard" as solving the advanced DDE corresponding to a solution of a retarded DDE.

(a) Given [0,1] (b) Given [2,3] (c) Given [4,5]

(d) Given [6,7]

Conclusion

In our research we made first steps towards understanding the fundamental problems that come with solving "backward-in-time" problems associated with linear first order differential-difference equations or higher order linear difference equations. Although the problems are perfectly well-posed if one goes forward in time (i.e., solutions can be computed and depend continuously on the initial values), just the opposite is true if one attempts to go backwards in time. Our research shows that the computed solutions $v(t)$ of (BGB) and b_j of (BDE) are entirely nontrustworthy. As a next step, we will try to regularize these inverse problems. That is, we will now search for functions $k(t)$ or sequences k_j such that the quantities $(k * v)(t) := \int_0^t k(t-s)v(s)\,ds$ and $(k * b)_j := \sum_{i=0}^{j} k_{j-i}b_i$ are more easily computable and depend continuously on the initial data.

Future Work

- In the future, we will investigate the use of this method in the inversion of the Laplace Transform; namely, that

$$e^{tA} = \sum_{i=1}^{q} \frac{B_i}{t} R\left(\frac{\lambda_i}{t}, A\right) = \sum_{k=0}^{n-1} \mathcal{L}^{-1}\left(\frac{\lambda^{n-k-1}}{c(\lambda)}\right) A_k,$$

where $c(\lambda)$ is the characteristic polynomial.

References & Acknowledgments

References

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