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SOLVING 1-DIMENSIONAL DIFFUSION PROCESS BY PADE APPROXIMATION

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ABSTRACT
This paper explores the method of Pade approximation to solve a system of heat equation; The Pade method of solving PDEs is a well-established method because of its added advantage of naturally increasing the domain of convergence of truncated power series. The solution of the heat equation has been directly expressed as a rational power series of the independent variable known as the Pade approximant. Attempt is made to solve the heat equation and obtain solutions in terms of their exponential matrix. A test on the stability of the solutions via conventional numerical procedures through some form of John Neumann stability method confirmed the scheme to be $L_0 - stable$ and therefore produced solutions that are well behaved.

Keywords: Pade Approximation, stability, diffusion process, convergence, Taylor series

INTRODUCTION

Partial differential equations (PDEs) form the basis of very many mathematical models of physical, chemical and biological phenomena, and more recently their use has spread into economics, financial forecasting, image processing and other fields. To investigate the predictions of PDE models of such phenomena it is often necessary to approximate their solution numerically, commonly in combination with the analysis of simple special cases; while in some of the recent instances the numerical models play an almost independent role.

This paper is concerned with the solutions of Heat Equation using finite difference method and pade approximation. The Pade approximation deals with the construction of rational fraction with a numerator of degree N and denominator of degree M so that the Taylor series expansion agrees with the original function up to the term of order N+M. The obtained rational fraction is known as the Pade approximant of the original function. The coefficients of the rational fraction representing the function under consideration are obtained by comparison with known coefficients of the Taylor expansion of the original function itself. This was done explicitly for the first time by Johann Heinrich Lambert; see Mulhouse (1777) and Lambert (1758) or by means of continued fractions as presented by Joseph & Louis (1813), Lagrange (1776).

The one dimensional Heat equation is the model for consideration in this paper, it is given by:

$$\partial_t u(x,t) = \alpha \partial_{xx} u(x,t), \quad 0 \le x \le L, \quad t \ge 0 \qquad (1)$$

where $u = u(x,t)$ is the dependent variable, and α is a constant coefficient. Equation (1) is a model of transient heat conduction in a slab of material with thickness L. The domain of the solution is a semi-infinite strip of width L that continues indefinitely in time. The material property α is the thermal diffusivity. In a practical computation, the solution is obtained only for a finite time, say t_{max}. Solution to Equation (1) requires specification of boundary conditions at x = 0 and x = L, and initial conditions at t = 0. Subject to boundary and initial conditions:

$$u(0,t) = u_{0;}\, u(L,t) = u_L; u(x,0) = f_0(x) \qquad (2)$$

Other boundary conditions, e.g. gradient (Neumann) or mixed conditions, can be specified. To keep the presentation as simple as possible, only the conditions in (2) are considered. See [Cooper, 1998; Fletcher, 1988; Golub & James, 1993; Hoffman, 1992; Morton & Mayer, 1994; Williams, 1992] for more exposition on general description of heat equations.

PRELIMINARIES

Finite Difference Method and Pade Approximation. The finite difference method is one of several techniques for obtaining numerical solutions to Equation (1). In all numerical solutions the continuous partial differential equation (PDE) is replaced with a discrete approximation. In this context the word "discrete" means that the numerical solution is known only at a finite number of points in the physical domain. The number of those points can be selected by the user of the numerical method. In general, increasing the number of points not only increases the resolution (i.e., detail), but also the accuracy of the numerical solution. The discrete approximation results in a set of algebraic equations that are evaluated (or solved) for the values of the discrete unknowns.
The mesh is the set of locations where the discrete solution is computed. These points are called nodes, and if one were to draw lines between adjacent nodes in the domain the resulting image would resemble a net or mesh. Two key parameters of the mesh are Δx, the local distance between adjacent points in space, and Δt, the local distance between adjacent time steps. For the simple examples considered in this project Δx and Δt are uniform throughout the mesh. The core idea of the finite-difference method is to replace continuous derivatives with so-called difference formulas that involve only the discrete values associated with positions on the mesh. In this project, we develop a handful of difference formulae to solve heat equation. Applying the finite-difference method to a differential equation involves replacing all derivatives with difference formulas. In the heat equation there are derivatives with respect to time, and derivatives with respect to space. Using different combinations of mesh points in the difference formulas results in difference schemes. In the limit as the mesh spacing (Δx and Δt) go to zero, the numerical solution obtained with any useful scheme will approach the true solution to the original differential equation. However, the rate at which the numerical solution approaches the true solution varies with the scheme. In addition, there are some

practically useful schemes that can fail to yield a solution for bad combinations of Δx and Δt.

The basic idea of the numerical approach to solving differential equations is to replace the derivatives in the heat equation by difference quotients and consider the relationships between u at (x, t) and its neighbours a distance Δx apart and at a time Δt later.

1. Forward Difference in Time

$$\frac{u(x,t+\Delta t)-u(x,t)}{\Delta t} = \frac{\partial u(x,t)}{\partial t} + O(\Delta t) \qquad (3)$$

Where $O(\Delta t)$ is the truncation of higher order derivatives upon performing a Taylor series expansion with $u(x, t + \Delta t)\ about\ \Delta t$

2. Central Difference Space:

$$\frac{u(x+\Delta x,t)-2u(x,t)+u(x-\Delta x,t)}{\Delta x^2} = \frac{\partial^2 u(x,t)}{\partial x^2} + O(\Delta x) \qquad (4)$$

By rewriting the heat equation in its discretized form using the expressions above and rearranging terms, one obtains:

$$u(x, t + \Delta t) = u(x,t) + \alpha^2 \frac{\Delta t}{\Delta x^2}(u(x + \Delta x, t) - 2u(x,t) + u(x - \Delta x, t)) \qquad (5)$$

Hence, given the values of u at three adjacent points $x + \delta x, x, and\ x - \delta x$ at a time t one can calculate an approximated value of u at x at a later time $t + \Delta t$, this is a standard numerical exercise.

We introduce next the pade approximation which helps to give the best approximation of a function by its rational presentation in a given order. In this technique, the approximant power series is in concord with the power series of the function being approximated. Since pade approximation provides a more accurate approximation of a function beyond the capacity of a truncated Taylor series, this method works fine where Taylor series fails to converge. Therefore, pade approximation is a preferred choice in this paper to strengthen the use of finite difference method for our numerical approximation of the diffusion equation.

PADE SCHEME FOR DIFFUSION EQUATION

We write the rational function:

$$R(x) = \frac{\sum_{j=0}^{M} a_j x^j}{1+\sum_{k=1}^{N} b_k x^k} = \frac{P_M}{Q_N} \qquad (6)$$

$where\ R(x)\ represents\ the\ pade\ approximant\ of\ order\ (M + N)\ to\ e^x$. By comparing coefficients with Taylor series of e^x, we give (2,1) pade approximant as follows:

$$R(x) = \frac{1+\frac{1}{3}x}{1-\frac{2}{3}x+\frac{1}{6}x^2}. \qquad (7)$$

This agrees with the function of interest to the highest possible order prescribed.

Now, for convenience, we could write equation (5) as:

$$\frac{du}{dt} = \frac{1}{(\Delta x)^2}\lfloor u(x + \Delta x, t) - 2u(x,t) + u(x - \Delta x, t)\rfloor. \qquad (8)$$

We subdivide the interval $0 \le x \le L$ in N equal subintervals by the grid lines $x_i = i\Delta x\ for\ i = 1, \dots, N\ where\ N.\Delta x = L.$ We compute (8) for every mesh point to obtain approximate solutions V_i(t) for the solutions u_i(t) from a system of (N-1) ordinary differential equations:

$$\frac{dV_i(t)}{dt} = \frac{1}{(\Delta x)^2}\{V_{i-1}(t) - 2V_i(t) + V_{i+1}(t)\}; \quad \text{where} \quad i = 1, \dots, N-1. \qquad (9)$$

The system (9) is reduced to the following ODE thus:

$$\frac{dV(t)}{dt} - AV(t) = b; \qquad (10)$$

$where$

$$A = \frac{1}{(\Delta x)^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ \ddots & \vdots & \ddots & & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}$$

and $b = \begin{pmatrix} V(0) \\ \vdots \\ V_N \end{pmatrix}$ are given boundary conditions.

From (10)

$$V(t) = -bA^{-1} + ce^{At} \qquad (11)$$

$V(0) = f_0$(x)= $= -bA^{-1} + c \implies c = f_0(0) + bA^{-1}$ which yields

$$V(t) = -bA^{-1} + (f_0(0) + bA^{-1})e^{At}. \qquad (12)$$

Since the solution is computed at every mesh point we have:

$V(t + k) = -bA^{-1} + (f_0(0) + bA^{-1})e^{A(t+p)}$; which simplifies to

$$V(t + k) = -bA^{-1} + \left(bA^{-1} + V(t)\right)e^{Ap}. \qquad (13)$$

Now, we consider, for simplicity, a situation where b=0 so that (13) gives:

$$V(t + k) = V(t)e^{Ap}; \qquad (14)$$

Next, we recall (7) and substitute into (14) to get:

$$V(t + k) = \frac{1+\frac{1}{3}Ap}{1-\frac{2}{3}Ap+\frac{1}{6}(Ak)^2}V(t) \qquad (15)$$

where $e^{Ap} = \frac{1+\frac{1}{3}Ap}{1-\frac{2}{3}Ap+\frac{1}{6}(Ap)^2}$.

We write $1 + \frac{1}{3}Ap$ explicitly as:

$$1 + \frac{1}{3}Ap = \begin{bmatrix} 1 & \cdots & & \vdots \\ & 1 & \ddots & 0 \\ 0 & \cdots & & 1 \end{bmatrix} + \frac{1}{3}p\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ \vdots & \ddots & & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}$$

and

$$1 - \frac{2}{3}Ak + \frac{1}{6}(Ak)^2 = \begin{bmatrix} 1 & \cdots & & \vdots \\ & 1 & \ddots & 0 \\ 0 & \cdots & & 1 \end{bmatrix} - \frac{2}{3}p\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ \vdots & \ddots & & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} + + \frac{1}{6}p^2\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ \vdots & \ddots & & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}^2 \qquad (16)$$

Using that

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$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ \vdots & \ddots & & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}^2 = \begin{bmatrix} 5 & -4 & 1 & & & & & & \\ -4 & 6 & -4 & 1 & & & & & \\ 1 & -4 & 6 & -4 & 1 & & & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & & & & & & \\ 0 & 0 & 0 & 0 & 1 & -4 & 6 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -4 & 6 & -4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -4 & 5 \end{bmatrix}$$

so that (15) becomes:

$$V(t+p) = \frac{\begin{bmatrix} 1-\frac{2}{3}p & \frac{1}{3}p & & \\ \frac{1}{3}p & 1-\frac{2}{3}p & \frac{1}{3}p & \\ & & & \ddots \\ \vdots & \ddots & \frac{1}{3}p & 1-\frac{2}{3}p \end{bmatrix}}{\begin{bmatrix} 1+\frac{4}{3}p+\frac{5}{6}p^2 & -\frac{2}{3}(p+p^2) & \frac{1}{6}p^2 & & & & \\ -\frac{2}{3}(p+p^2) & 1+\frac{4}{3}p+p^2 & -\frac{2}{3}(p+p^2) & \frac{1}{6}p^2 & & & \\ \frac{1}{6}p^2 & -\frac{2}{3}(p+p^2) & 1+\frac{4}{3}p+p^2 & -\frac{2}{3}(p+p^2) & \frac{1}{6}p^2 & & \\ \vdots\ \ddots\ \ddots & & & \ddots\ \ddots\ \ddots & & \ddots\ \ddots\ \ddots & \\ & & & & \frac{1}{6}p^2 & -\frac{2}{3}(p+p^2) & 1+\frac{4}{3}p+\frac{5}{6}p^2 \end{bmatrix}} V(t)$$

We write,

$$\begin{bmatrix} 1+\frac{4}{3}p+\frac{5}{6}p^2 & -\frac{2}{3}(p+p^2) & \frac{1}{6}p^2 & & & & \\ -\frac{2}{3}(p+p^2) & 1+\frac{4}{3}p+p^2 & -\frac{2}{3}(p+p^2) & \frac{1}{6}p^2 & & & \\ \frac{1}{6}p^2 & -\frac{2}{3}(p+p^2) & 1+\frac{4}{3}p+p^2 & -\frac{2}{3}(p+p^2) & \frac{1}{6}p^2 & & \\ \vdots\ \ddots\ \ddots & & & \ddots\ \ddots\ \ddots & & \ddots\ \ddots\ \ddots & \\ & & & & \frac{1}{6}p^2 & -\frac{2}{3}(p+p^2) & 1+\frac{4}{3}p+\frac{5}{6}p^2 \end{bmatrix} \begin{bmatrix} V_{1,j+1} \\ V_{2,j+1} \\ V_{3,j+1} \\ V_{3,j+1} \\ \vdots \\ V_{N-4,j+1} \\ V_{N-3,j+1} \\ V_{N-2,j+1} \\ V_{N-1,j+1} \end{bmatrix} =$$

$$= \begin{bmatrix} 1-\frac{2}{3}p & \frac{1}{3}p & & \\ \frac{1}{3}p & 1-\frac{2}{3}p & \frac{1}{3}p & \\ & & & \ddots \\ \vdots & \ddots & \frac{1}{3}p & 1-\frac{2}{3}p \end{bmatrix} \begin{bmatrix} V_{1,j} \\ V_{2,j} \\ \vdots \\ V_{N-2,j} \\ V_{N-1,j} \end{bmatrix}.;$$

This gives the following scheme:

$$\frac{1}{6}p^2V_{i-2,j+1} - \frac{2}{3}(p^2+p)V_{i-1,j+1} +$$
$$+(p^2+\frac{4}{3}p+1)V_{i,j+1} - \frac{2}{3}(p^2+p)V_{i+1,j+1} + \frac{1}{6}p^2V_{i+2,j+1} = \frac{1}{3}pV_{i-1,j} + \left(1-\frac{2}{3}p\right)V_{i,j} + \frac{1}{3}pV_{i+1,j}.$$

Now, it is left to be seen whether the scheme above displays any form of stability i.e. whether or not a small perturbation of the initial data leads to only small changes on the solution or changes on initial data would result to significant changes on the solution. The next theorem answers this important question.

STABILITY TEST OF THE SCHEME

It is important to check that the scheme is stable before any attempt to search for solution; an unstable scheme cannot produce reasonable solution that converges to the exact solution. It is imperative to check that a small perturbation of the initial data would lead to only a small change in the solution; it need be also emphasized here that testing stability of the scheme is of greater importance to obtaining a reasonable solution in an explicit numerical computation. The following results are obtained for our scheme:

Theorem 1:

The following Pade approximant $R(x)=\frac{1+\frac{1}{3}x}{1-\frac{2}{3}x+\frac{1}{6}x^2}$ is such that |R(x)|<1 and that $\lim_{x\to\infty} R(x)=0.$

Obviously, the L_0 stability holds true.

Theorem 2

If $\sin^2\frac{p\pi}{2L}=K\ then\ for \begin{cases} r<\frac{1-\sqrt{13}K}{4K} \\ or \\ r>\frac{1+\sqrt{13}K}{4K}\end{cases}$ then the scheme is stable.

Proof:

Suppose that $\alpha_{t,} t=1,2,\ldots N-1\ are\ the\ eigenvalues\ of\ the\ matrix\ A, so$

$\alpha_t=-\frac{4}{h^2}\sin^2\frac{p\pi}{2L}$ and $\gamma_{t,} t=1,2,\ldots N-1$ are the eigenvalues of the matrix $e^{(pA)}$=$\frac{1+\frac{1}{3}Ap}{1-\frac{2}{3}Ap+\frac{1}{6}(Ap)^2}$. Hence,

$\gamma_t\ =\frac{1+\frac{1}{3}A\alpha_t}{1-\frac{2}{3}A\alpha_t+\frac{1}{6}(A\alpha_{t,})^2}$; plugging $\alpha_t=-\frac{4}{h^2}\sin^2\frac{p\pi}{2L}$ yields:

$\gamma_t\ =\frac{1+\frac{1}{3}A(-\frac{4}{h^2}\sin^2\frac{p\pi}{2L})}{1-\frac{2}{3}A(-\frac{4}{h^2}\sin^2\frac{p\pi}{2L})+\frac{1}{6}(A(-\frac{4}{h^2}\sin^2\frac{p\pi}{2L}))^2}$, where r=$\frac{A}{h^2}$. Should we claim that $\gamma_t\ \ is\ stable, we\ necessarily\ should\ obtain$

$-1<\frac{1+\frac{1}{3}A\left(-\frac{4}{h^2}\sin^2\frac{p\pi}{2L}\right)}{1-\frac{2}{3}A\left(-\frac{4}{h^2}\sin^2\frac{p\pi}{2L}\right)+\frac{1}{6}\left(A\left(-\frac{4}{h^2}\sin^2\frac{p\pi}{2L}\right)\right)^2}<1$. This is possible if we put

$$\sin^2\frac{p\pi}{2L}=K\ where$$
$$\begin{cases} r<\dfrac{1-\sqrt{13}K}{4K} \\ or \\ r>\dfrac{1+\sqrt{13}K}{4K}\end{cases}$$

Conclusion

The diffusion equation is solved by the Pade approximation of the exponential matrix; we presented a robust scheme that is tested to be $L_0\ stable$ so should have a solution that is well behaved (Converges to the exact solution) should the scheme proceed to execution using any numerical method. The deployment of Pade approximation for solving the diffusion equation is a preferred choice because rational approximants increases the domain of convergence than the traditional Taylor series.

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