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Finite Difference Approximation for Diffusion Equation

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Abstract- In this paper, the approximate solutions of differential equation are studied. Then, one-dimensional diffusion equation is solved by using Explicit and Crank- Nicolson methods to obtain local truncation errors. These schemes are presented using Taylor series expansion.

Indexed Terms- Diffusion equation, explicit method, Crank- Nicolson method, local truncation error.

I. INTRODUCTION

We shall find the approximate solutions of differential equations, that is, to find a function (or some discrete approximation to this function) which satisfies a given relationship between several of its derivatives on some given region of space and / or time, along with some boundary conditions along the edges of this domain. In general this is a difficult problem and only rarely can be found an analytic formula for the solution. A finite difference method proceeds by replacing the derivatives in the differential equations by finite difference approximations. This gives a large algebraic system of equations to be solved in place of the differential equation, something that is easily solved on a computer.

Before tackling this problem, we first consider the more basic question of how we can approximate the derivatives of a known function by finite difference formulas based only on values of the function itself at discrete points. Besides providing a basis for the later development of finite difference methods for solving differential equations, this allows us to investigate several key concepts such as the order of accuracy of an approximation in the simplest possible setting.

Let $u(x)$ represent a function of one variable that, unless otherwise stated, will always be assumed to be smooth, meaning that we can differentiate the function several times and each derivative is a well-defined bounded function over an interval containing a particular point of interest $\bar{x}$.

Suppose we want to approximate $u'(\bar{x})$ by a finite difference approximation based only on values of *u* at a finite number of points near $\bar{x}$. One obvious choice would be to use $D_+ u(\bar{x}) \equiv \dfrac{u(\bar{x}+h)-u(\bar{x})}{h}$ (1)
For some small value of *h*.

This is motivated by the standard definition of the derivative as the limiting value of this expression as $h \to 0$. Note that $D_+ u(\bar{x})$ is the slope of the line interpolating *u* at the points $\bar{x}$ and $\bar{x}+h$.

The Equation (1) is a one-sided approximation to u' since *u* is evaluated only at values of $x \geq \bar{x}$.
Another one-sided approximation would be

$$D_- u(\bar{x}) \equiv \frac{u(\bar{x})-u(\bar{x}-h)}{h}. \qquad (2)$$

Each of these formulas gives a first order accurate approximation to $u'(\bar{x})$, meaning that the size of the error is roughly proportional to *h* itself.
Another possibility is to use the centered approximation, $D_0 u(\bar{x}) \equiv \dfrac{u(\bar{x}+h)-u(\bar{x}-h)}{2h}$

$$= \frac{1}{2}(D_+ u(\bar{x}) + D_- u(\bar{x})) \cdot \qquad (3)$$

This is the slope of the line interpolating u at $\bar{x}-h$ and $\bar{x}+h$, and is simply the average of the two one-sided approximations defined above. From Figure 1.1 it should be clear that we would expect $D_0 u(\bar{x})$ to give a better approximation than either of the one-sided approximations. In fact this gives a second order accurate approximation which the error is proportional to h^2 and hence is much smaller than the error in a first order approximation when h is small.

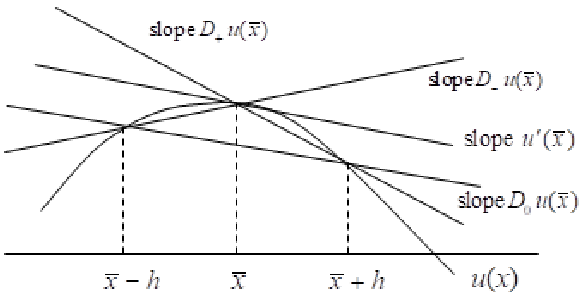

Figure 1: Various approximations to $u'(\bar{x})$ interpreted as the slope of secant lines.

Other approximations are also possible, for example $D_3 u(\bar{x}) \equiv \frac{1}{6h}\left[2u(\bar{x}+h)+3u(\bar{x})-6u(\bar{x}-h)+u(\bar{x}-2h)\right]$(4) .This is a third order accurate approximation which the error is proportional to h^3 when h is small.

II. DERIVING FINITE DIFFERENCE APPROXIMATION

Suppose we want to derive a finite difference approximation to $u'(\bar{x})$ base on some given set of points. We can use Taylor series to derive an appropriate formula, using the method of undetermined coefficients. As an example, we suppose a one-sided approximation to $u'(\bar{x})$ base on $u(\bar{x})$, $u(\bar{x}-h)$ and $u(\bar{x}-2h)$ of the form, $D_2u(\bar{x}) = au(\bar{x})+bu(\bar{x}-h)+cu(\bar{x}-2h)$. (5)

We can determine the coefficients a, b, and c to give the best possible accuracy by expanding in Taylor series and collecting terms. Equation (5) gives

$$D_2u(\bar{x}) = au(\bar{x})+bu(\bar{x}-h)+cu(\bar{x}-2h).$$

$$= au(\bar{x})+b\left[u(\bar{x})-hu'(\bar{x})+\frac{1}{2}h^2u''(\bar{x})-\frac{1}{6}h^3u'''(\bar{x})+\cdots\right]$$

$$+c\left[u(\bar{x})-2hu'(\bar{x})+\frac{1}{2}(2h)^2u''(\bar{x})-\frac{1}{6}(2h)^3u'''(\bar{x})+\cdots\right]$$

$$\cdot -\frac{1}{6}(b+8c)h^3u'''(\bar{x})+\cdots.$$

If this is going to agree with $u'(\bar{x})$ to high order then we need, $a+b+c=0$, $b+2c=-\frac{1}{h}$ (6)

$$b+4c=0.$$

We might like to require that higher order coefficients be zero as well, but since there are only three unknowns a, b and c we cannot in general hope to satisfy more than three such conditions. Solving the linear system (6) gives $a=\frac{3}{2h}$, $b=-\frac{2}{h}$, $c=\frac{1}{2h}$.

So that the formula is

$$D_2u(\bar{x}) = \frac{3}{2h}u(\bar{x})-\frac{2}{h}u(\bar{x}-h)+\frac{1}{2h}u(\bar{x}-2h)$$

$$= \frac{1}{2h}\left[3u(\bar{x})-4u(\bar{x}-h)+u(\bar{x}-2h)\right].$$

(7) The error in this approximation is clearly

$$D_2u(\bar{x}) = u'(\bar{x})-\frac{1}{6}(b+8c)h^3u'''(\bar{x})+\cdots$$

$$D_2u(\bar{x})-u'(\bar{x}) = \frac{1}{6}\left(-\frac{2}{h}+\frac{4}{h}\right)h^3u'''(\bar{x})+\cdots$$

$$= -\frac{1}{3}h^2u'''(\bar{x})+O(h^3).$$

Next, suppose we want to a one-sided approximation to $u'(\bar{x})$ base on $u(\bar{x})$, $u(\bar{x}+h)$ and $u(\bar{x}+2h)$.

$$D_2u(\bar{x}) = au(\bar{x})+bu(\bar{x}+h)+cu(\bar{x}+2h)$$

$$= au(\bar{x})+b\left[u(\bar{x})+hu'(\bar{x})+\frac{1}{2!}h^2u''(\bar{x})+\frac{1}{3!}h^3u'''(\bar{x})+\cdots\right]$$

$$+c\left[u(\bar{x})+2hu'(\bar{x})+\frac{1}{2!}(2h)^2u''(\bar{x})+\frac{1}{3!}(2h)^3u'''(\bar{x})+\cdots\right]$$

$$= (a+b+c)u(\bar{x})+(b+2c)hu'(\bar{x})+\frac{1}{2}(b+4c)h^2u''(\bar{x})$$

$$+\frac{1}{6}(b+8c)h^3u'''(\bar{x})+\cdots.$$

If this is going to agree with $u'(\bar{x})$ to high order then we need, $a+b+c=0$

$b+2c=\frac{1}{h}$, $b+4c=0$.

Solving this linear system, we get

$a=-\frac{3}{2h}$, $b=\frac{2}{h}$, $c=-\frac{1}{2h}$

$$D_2u(\bar{x}) = -\frac{1}{2h}\left[3u(\bar{x})-4u(\bar{x}+h)+u(\bar{x}+2h)\right].$$

The error in this approximation is

$$D_2 u(\bar{x}) - u'(\bar{x}) = \frac{1}{6}(b+8c)h^3 u'''(\bar{x}) + \cdots$$

$$= -\frac{1}{3}h^2 u'''(\bar{x}) + O(h^3)\cdot$$

III. BOUNDARY VALUE PROBLEM FOR DIFFUSION EQUATIONS

We shall study finite difference methods for time-dependent partial differential equations, where variations in space are related to variations in time. The heat equation (or diffusion equation)

$$u_t = k\,u_{xx}\,. \qquad (8)$$

This is the classical example of a parabolic equation, and many of the general properties seen here carry over to the design of numerical methods for other parabolic equations. We will assume $k=1$ for simplicity but some comments will be made about how the results scale to other values of $k>0$.

Along with this equation we need initial conditions at some time t_0, which we typically take to be $t_0 = 0$,

$$u(x,0) = \eta(x) \quad (9)$$

And also boundary conditions if we are working on a bounded domain,

For example, the Dirichlet conditions

$$u(0,t) = g_0(t) \text{ For } t>0$$

$$u(1,t) = g_1(t) \text{ For } t>0 \qquad (10)$$

if $0 \le x \le 1$.

We have already studied the steady state version of this equation and spatial discretizations of u_{xx}. We have also studied discretizations of the time derivatives.

In practice we generally apply a set of finite difference equations on a discrete grid with grid points (x_i, t_n) where

$$x_i = ih,\ t_n = nk\,.$$

Here $h = \Delta x$ is the mesh spacing on the x-axis and $k = \Delta t$ is the time step. Let $U_i^n \approx u(x_i, t_n)$ represent the numerical approximation at grid point (x_i, t_n).

Since the heat equation is an evolution equation that can be solved forward in time, we set up our difference equations in a form where we can march forward in time, determining the value U_i^{n+1} for all i from the values U_i^n at the previous time level, or perhaps using also values at earlier time levels with a multistep formula

As an example,

One natural discretization of Equation (8) would be

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{1}{h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n)\cdot \qquad (11)$$

This uses our standard centered difference in space and a forward difference in time. This is an explicit method since we can compute each U_i^{n+1} explicitly in terms of the previous data:

$$U_i^{n+1} = U_i^n + \frac{k}{h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n) \qquad (12)$$

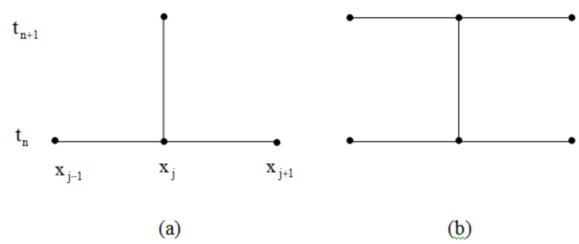

Figure 2 the stencil of this method

This is a one-step method in time, which is also called a two-level method in the context of partial differential equations since it involves the solution at two different time levels.

Another one step method, Crank-Nicolson method, Equation (8) can be written as

$$\frac{U_i^{n+1} - U_i^n}{k} = \frac{1}{2}(D^2 U_i^n + D^2 U_i^{n+1}) \qquad (13)$$

$$= \frac{1}{2h^2}(U_{i-1}^n - 2U_i^n + U_{i+1}^n + U_{i-1}^{n+1} - 2U_i^{n+1} + U_{i+1}^{n+1})$$

Which can be rewritten as, or

$$-rU_{i-1}^{n+1} + (1+2r)U_i^{n+1} - rU_{i+1}^{n+1} = rU_{i-1}^n + (1-2r)U_i^n + rU_{i+1}^n \quad (14)$$

where $r = \dfrac{k}{2h^2}$. This is an implicit method and gives a tridiagonal system of equations to solve for all the values U_i^{n+1} simultaneously.

In matrix form this is

$$\begin{bmatrix} (1+2r) & -r & & & & \\ -r & (1+2r) & -r & & & \\ & -r & (1+2r) & -r & & \\ & & \ddots & \ddots & \vdots & \\ & & & -r & (1+2r) & -r \\ & & & & -r & (1+2r) \end{bmatrix} \begin{bmatrix} U_1^{n+1} \\ U_2^{n+1} \\ U_3^{n+1} \\ \vdots \\ U_{m-1}^{n+1} \\ U_m^{n+1} \end{bmatrix}$$

$$= \begin{bmatrix} r\left(g_0(t_n)+g_0(t_{n+1})\right)+(1-2r)U_1^n+rU_2^n \\ rU_1^n+(1-2r)U_2^n+rU_3^n \\ rU_2^n+(1-2r)U_3^n+rU_4^n \\ \vdots \\ rU_{m-2}^n+(1-2r)U_{m-1}^n+rU_m^n \\ rU_{m-1}^n+(1-2r)rU_m^n+r\left(g_1(t_n)+g_1(t_{n+1})\right) \end{bmatrix}. \quad (15)$$

The boundary conditions $u(0,t)=g_0(t)$ and $u(1,t)=g_1(t)$ come into these equations.

Since a tridiagonal system of m equations can be solved with $O(m)$ work, this method is essentially as efficient per time step as an explicit method. The heat equation is “stiff”, and hence this implicit method, which allows much larger time steps to be taken than an explicit method, is a very efficient method for the heat equation.

Solving a parabolic equation with an implicit method requires solving a system of equations with the same structure as the 2-point boundary value problem. Similarly, a multidimensional parabolic equation requires solving a problem with the structure of a multidimensional elliptic equation.

IV. LOCAL TRUNCATION ERRORS AND ORDER OF ACCURACY

We can define the local truncation error a usual, we insert the exact solution $u(x,t)$ of the partial differential equation into the finite difference equation and determine by how much it fails to satisfy the discrete equation.

4.1 Example

The local truncation error of the Equation (8) is based on Equation (4): $\tau_i^n=\tau(x_i,t_n)$. The diffusion equation is $u_t=u_{xx}$,

$$\frac{U_i^{n+1}-U_i^n}{k}-\frac{1}{h^2}(U_{i-1}^n-2U_i^n+U_{i+1}^n)=0$$

$$\frac{u(x_i,t_n+k)-u(x_i,t_n)}{k}-\frac{1}{h^2}(u(x_i-h,t_n)$$
$$-2u(x_i,t_n)+u(x_i+h,t_n))=0$$

$$\tau(x,t)=\frac{u(x,t+k)-u(x,t)}{k}$$
$$-\frac{1}{h^2}(u(x-h,t)-2u(x,t)+u(x+h,t))$$

$$u(x,t+k)=u(x,t)+ku_t+\frac{1}{2!}k^2u_{tt}+\frac{1}{3!}k^3u_{ttt}+\frac{1}{4!}k^4u_{tttt}+\cdots$$

$$u(x-h,t)=u(x,t)-hu_x+\frac{1}{2!}h^2u_{xx}-\frac{1}{3!}h^3u_{xxx}+\frac{1}{4!}h^4u_{xxxx}-\cdots$$

$$u(x+h,t)=u(x,t)+hu_x+\frac{1}{2!}h^2u_{xx}+\frac{1}{3!}h^3u_{xxx}+\frac{1}{4!}h^4u_{xxxx}+\cdots$$

we can find that,

$$\tau(x,t)=\left\{u_t+\frac{1}{2!}ku_{tt}+\frac{1}{3!}k^2u_{ttt}+\frac{1}{4!}k^3u_{tttt}+\cdots\right\}$$
$$-\left\{u_{xx}+\frac{1}{12}h^2u_{xxxx}+\frac{1}{180}h^4u_{xxxxxx}+\cdots\right\}$$

.

Since $u_t=u_{xx}$, the O(1) terms drop out. By differentiating $u_t=u_{xx}$, we find that $u_{tt}=u_{txx}=u_{xxxx}$ and so $\tau(x,t)=\left(\frac{1}{2}k-\frac{1}{12}h^2\right)u_{xxxx}+O(k^2+h^4)$.

This method is said to be second order accurate in space and first order accurate in time since the truncation error is $O(h^2+k)$.

The Crank-Nicolson method is centered in both space and time,

$$\frac{U_i^{n+1}-U_i^n}{k}=\frac{1}{2}(D^2U_i^n+D^2U_i^{n+1})$$
$$=\frac{1}{2h^2}(U_{i-1}^n-2U_i^n+U_{i+1}^n+U_{i-1}^{n+1}-2U_i^{n+1}+U_{i+1}^{n+1})$$

$$\tau(x,t)=\frac{1}{k}\left[u(x,t+k)-u(x,t)\right]$$
$$-\frac{1}{2h^2}\big[u(x-h,t)-2u(x,t)+u(x+h,t)$$
$$+u(x-h,t+k)-2u(x,t+k)+u(x+h,t+k)\big],$$

Where

$$u(x-h,t+k)=u(x,t)-\frac{h}{1!}u_x+\frac{k}{1!}u_t+\frac{h^2}{2!}u_{xx}+\frac{k^2}{2!}u_{tt}-\frac{hk}{1!1!}u_{xt}$$
$$-\frac{h^3}{3!}u_{xxx}+\frac{k^3}{3!}u_{ttt}+\frac{h^2k}{2!1!}u_{xxt}-\frac{hk^2}{1!2!}u_{xtt}+\cdots.$$

$$u(x+h,t+k)=u(x,t)+\frac{h}{1!}u_x+\frac{k}{1!}u_t+\frac{h^2}{2!}u_{xx}+\frac{k^2}{2!}u_{tt}+\frac{hk}{1!1!}u_{xt}$$
$$+\frac{h^3}{3!}u_{xxx}+\frac{k^3}{3!}u_{ttt}+\frac{h^2k}{2!1!}u_{xxt}+\frac{hk^2}{1!2!}u_{xtt}+\cdots.$$

The local truncation error shows that it is second order accurate in both space and time, $\tau(x,t)=\mathrm{O}(k^2+h^2)$ .A method is said to be consistent $\tau(x,t)\to 0$ ask, $h\to 0$.

V. CONCLUSION

In this paper, we study derivation of finite difference approximation of solution by method of undermined coefficients.Then,the diffusion equation has been solved by two finite difference techniques to obtain local truncation errors.

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