Numerical Methods

So far, we have seen several analytical technique for finding solutions to the PDEs. Another alternative approach is to use numerical techniques. This is also applicable to find solution of the nonlinear problem. Here we shall focus on the use of finite difference methods.

Polynomial approximations

From Taylor's theorem, we can find the polynomial approximation to f near a point $x = x_0$ by

$$f(x) = f(x_0) + (\Delta x) f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0) + \ldots + \frac{(\Delta x)^n}{n!} f^{(n)}(x_0) + R_n$$

Where $\underset{\substack{\text{(remainder term)} \\ \text{(usually called truncation error)}}}{R_n} = \frac{(\Delta x)^{n+1}}{(n+1)!} f^{(n+1)}(\xi) \quad , \; x_0 < \xi < x$

Here $x = x_0 + \Delta x$, Δx small

Ex For linear approximation $f(x) = f(x_0) + (\Delta x) f'(x_0)$

For quadratic approximation $f(x) = f(x_0) + (\Delta x) f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0)$

Truncation error usually denotes by the order notation i.e., $f = O(g)$ as $x \to x_0$ means $\lim_{x \to x_0} \frac{f}{g} = C$ or $|f| \le C|g|$.

Thus the truncation error for linear approximation is

$$f(x) = f(x_0) + (\Delta x) f'(x_0) + \underbrace{O(\Delta x^2)}_{\text{truncation error}} \qquad ✪$$

First derivative approximations

There are several ways to approximate the first derivative by using Taylor's theorem. For example, from ✪, we can write

$$\boxed{f'(x_0) = \frac{f(x) - f(x_0)}{\Delta x} = \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}} \qquad (1)$$

This is known as forward difference.

If we replace Δx by $-\Delta x$, another kind of approximation to $\frac{df}{dx}$ can be achieved ,i.e.,

$$\boxed{f'(x_0) = \frac{f(x_0 - \Delta x) - f(x_0)}{(-\Delta x)} = \frac{f(x_0) - f(x_0 - \Delta x)}{\Delta x}} \qquad (2)$$

This is known as backward difference. Both forward and backward difference approximations of $\frac{df}{dx}$ have truncation error of order $O(\Delta x)$.

To get a better approximation, we use Taylor series of $f(x_0+\Delta x)$ and $f(x_0-\Delta x)$.

$$f(x_0+\Delta x) = f(x_0) + (\Delta x) f'(x_0) + \frac{(\Delta x)^2}{2!} f''(x_0) + \frac{(\Delta x)^3}{3!} f'''(x_0) + \dots$$

$$f(x_0-\Delta x) = f(x_0) - (\Delta x) f'(x_0) + \frac{(-\Delta x)^2}{2!} f''(x_0) + \frac{(-\Delta x)^3}{3!} f'''(x_0) + \dots$$

Subtracting these series, we have

$$f(x_0+\Delta x) - f(x_0-\Delta x) = 2(\Delta x) f'(x_0) + \frac{2}{3!}(\Delta x)^3 f'''(x_0) + \frac{2}{5!}(\Delta x)^5 f^{(5)}(x_0)$$

Rewriting for $f'(x_0)$, we obtain

$$\boxed{f'(x_0) \;=\; \frac{f(x_0+\Delta x) - f(x_0-\Delta x)}{2\Delta x} + O(\Delta x^2)} \qquad (3)$$

This is known as the centered (or central) difference approximation to $\frac{df}{dx}$ at $x = x_0$ with error $O(\Delta x^2)$. Obviously (3) is more accurate than (1) and (2), and it is more preferable. These approximations are usually called finite difference formula for the first derivative $\frac{df}{dx}$ at $x = x_0$.

In summary, we can find the error of these finite difference approximation by using the estimate of the remainder term. Let E denotes the error.

For forward and backward differences, $E = \left|\frac{\Delta x}{2} f''(\xi)\right|$, $x_0 < \xi < x_0 + \Delta x$

For centered difference, $E = \left|\frac{(\Delta x)^2}{3!} f'''(\xi)\right|$, $x_0 < \xi < x_0 + \Delta x$

<u>Ex</u> Given $f(x) = \log x$. First derivative of $f(x)$ is $f'(x) = \frac{1}{x}$.

Thus at $x = 1$, we have $f'(1) = 1$.

Suppose we want to approximate $f'(x)$ at $x = 1.0$ by using forward difference formula, what is the error from this approximation of $f'(1)$ if $\Delta x = 0.1$?

For forward difference, $f'(x_0) = \frac{f(x_0+\Delta x) - f(x_0)}{\Delta x}$

Here $x_0 = 1.0$, $\Delta x = 0.1$

$$f'(1.0) \;=\; \frac{f(1.1) - f(1)}{0.1} \;=\; \frac{0.09531 - 0}{0.1} \;=\; 0.9531$$

Centered difference $\quad f'(1.0) \;=\; \frac{f(1.1) - f(0.9)}{0.1} \;=\; \frac{0.09531 + 0.10536}{0.1} \;=\; 1.00335$

Error (centered) $E \;=\; \left|\frac{\Delta x^2}{3!} f'''(\xi)\right| \;=\; \left|\frac{(0.1)^2}{6}\frac{2}{1^3}\right| \;=\; 3.3\times 10^{-3}$

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Second derivatives

We look at

$$f(x_0+\Delta x)= f(x_0)+(\Delta x)f'(x_0)+\frac{(\Delta x)^2}{2!}f''(x_0)+\frac{(\Delta x)^3}{3!}f'''(x_0)+\frac{(\Delta x)^4}{4!}f^{(iv)}(x_0)+\ldots$$

and

$$f(x_0-\Delta x)= f(x_0)-(\Delta x)f'(x_0)+\frac{(\Delta x)^2}{2!}f''(x_0)-\frac{(\Delta x)^3}{3!}f'''(x_0)+\frac{(\Delta x)^4}{4!}f^{(iv)}(x_0)-\ldots$$

Adding these two series, we have

$$f''(x_0)=\frac{f(x_0+\Delta x)-2f(x_0)+f(x_0-\Delta x)}{(\Delta x)^2}-\frac{(\Delta x)^2}{12}f^{(iv)}(\xi)$$

where $x_0<\xi<x_0+\Delta x$. This gives a finite difference formula for $f''(x_0)$ with $O(\Delta x^2)$ truncation error:

$$\boxed{f''(x_0)=\frac{f(x_0+\Delta x)-2f(x_0)+f(x_0-\Delta x)}{(\Delta x)^2}} \qquad (4)$$

This is called the centered (or central) difference approximation for $f''(x_0)$.

Note: The coefficient $\frac{1}{(\Delta x)^2}$, $-\frac{2}{(\Delta x)^2}$ and $\frac{1}{(\Delta x)^2}$ of $f(x_0+\Delta x)$, $f(x_0)$ and $f(x_0-\Delta x)$ represent the weight average and they must sum to zero for any finite difference approximations.

General technique for finding finite difference approximation to derivatives can be derived based on Taylor's approximation. As an example, suppose that we want to find the approximation to $f''(x_0)$ using $f(x_0+\Delta x)$, $f(x_0)$ and $f(x_0-\Delta x)$, we consider

$$f''(x_0)=af(x_0+\Delta x)+bf(x_0)+cf(x_0-\Delta x)+O(\Delta x^m)$$

The coefficients a,b,c and m are to be found. Let's begin with

$$af(x_0+\Delta x) = af(x_0)+a(\Delta x)f'(x_0)+a\frac{(\Delta x)^2}{2!}f''(x_0)+a\frac{(\Delta x)^3}{3!}f'''(x_0)+a\frac{(\Delta x)^4}{4!}f^{(iv)}(x_0)+\ldots$$

$$bf(x_0) = bf(x_0)$$

$$cf(x_0-\Delta x) = cf(x_0)-c(\Delta x)f'(x_0)+c\frac{(\Delta x)^2}{2!}f''(x_0)-c\frac{(\Delta x)^3}{3!}f'''(x_0)+c\frac{(\Delta x)^4}{4!}f^{(iv)}(x_0)+\ldots$$

$$\Rightarrow \quad af(x_0+\Delta x)+bf(x_0)+cf(x_0-\Delta x) = (a+b+c)f(x_0)+(a-c)\Delta x f'(x_0)$$
$$+(a+c)\frac{\Delta x^2}{2}f''(x_0)+(a-c)\frac{(\Delta x)^3}{3!}f'''(x_0)$$
$$+(a+c)\frac{(\Delta x)^4}{4!}f^{(iv)}(x_0)+\ldots$$

Setting $a+b+c=0$ (1)

$a-c=0$ (2)

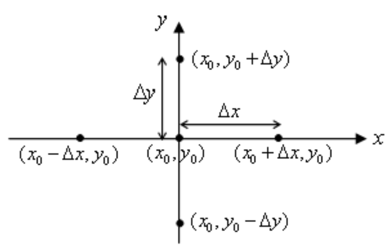
and $a+c=\frac{1}{\Delta x}$ (3)

It is clear from (2)&(3) that $a = c = \dfrac{1}{\Delta x}$. From (1), we have $b = -\dfrac{2}{\Delta x}$. The question now is how to find m. If we look at the coefficient of $f'''(x_0)$, it is $a - c$ which is zero. The next non zero term would be $(a+c)\dfrac{\Delta x^4}{4!} f^{(iv)}(x_0)$. Hence $m = 2$. This is the centered difference formula for $f''(x_0)$ obtained earlier.

Partial derivatives

Some of the partial derivatives can be approximated by the earlier results for $f'(x_0)$. For examples, if we use the centered difference formulas,

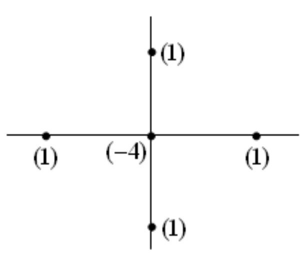
$$
\begin{aligned}
\frac{\partial u}{\partial x}(x_0, y_0) &= \frac{u(x_0+\Delta x, y_0) - u(x_0 - \Delta x, y_0)}{2\Delta x} \\
\frac{\partial u}{\partial y}(x_0, y_0) &= \frac{u(x_0, y_0+\Delta y) - u(x_0, y_0 - \Delta y)}{2\Delta y} \\
\frac{\partial^2 u}{\partial x^2}(x_0, y_0) &= \frac{u(x_0+\Delta x, y_0) - 2u(x_0, y_0) + u(x_0 - \Delta x, y_0)}{(\Delta x)^2} \\
\frac{\partial u^2}{\partial^2 y}(x_0, y_0) &= \frac{u(x_0, y_0+\Delta y) - 2u(x_0, y_0) + u(x_0, y_0 - \Delta y)}{(\Delta y)^2}
\end{aligned}
$$



For Laplacian ∇^2, we have (based on centered formula with $\Delta x = \Delta y = \Delta$)

$$\nabla^2 u(x_0, y_0) = \frac{u(x_0+\Delta x, y_0) + u(x_0 - \Delta x, y_0) + u(x_0, y_0+\Delta y) + u(x_0, y_0 - \Delta y) - 4u(x_0, y_0)}{\Delta^2} + O(\Delta^2)$$

This is known as 5-point finite difference approximation for the Laplacian.



Homework 11 (b) Derive an approximation for $\dfrac{\partial^2 u}{\partial x \partial y}$ whose truncation error is $O(\Delta x^2)$ for $\Delta x = \Delta y = \Delta$. (Hint: use centered difference approximations for first order derivative.)

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Heat equation

Let's replace the heat equation $\frac{\partial u}{\partial t}-\alpha^2\frac{\partial^2 u}{\partial x^2}=0$ at the point $x=x_0$ and $t=t_0$ by a forward difference time and a centered difference in space.

$$\frac{u(x_0,t_0+\Delta t)-u(x_0,t_0)}{\Delta t}=\alpha^2\frac{u(x_0+\Delta x,t_0)-2u(x_0,t_0)+u(x_0-\Delta x,t_0)}{(\Delta x)^2}+E \qquad (1)$$

Where the (discretization) truncation error $E=\frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_0,\tau)-\alpha^2\frac{(\Delta x)^2}{12}\frac{\partial^4 u}{\partial x^4}(\xi,t_0)$ for $t_0<\tau<t_0+\Delta t$, $x_0<\xi<x_0+\Delta x$. Here we look for the approximation $\tilde{u}(x_0,t_0)$ of the exact solution $u(x_0,t_0)$ satisfying.

$$\frac{\tilde{u}(x_0,t_0+\Delta t)-\tilde{u}(x_0,t_0)}{\Delta t}=\alpha^2\frac{\tilde{u}(x_0+\Delta x,t_0)-2\tilde{u}(x_0,t_0)+\tilde{u}(x_0-\Delta x,t_0)}{(\Delta x)^2} \qquad (2)$$

This approximation is said to be <u>consistent</u> with the heat equation $\frac{\partial u}{\partial t}=\alpha^2\frac{\partial^2 u}{\partial x^2}$ when $E\to 0$ as $\Delta x\to 0$ and $\Delta t\to 0$.

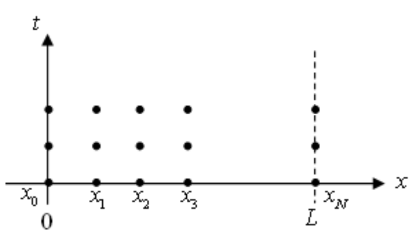
Let's now discretize the domain $0<x<L$ into N equal intervals with a mesh size of $\Delta x=\frac{L}{N}$ (That is, $x_0=0$, $x_1=\Delta x$, $x_2=2\Delta x$, … , $x_N=N\Delta x=L$). In particular, we use the notation

$$x_j=j\Delta x \qquad (3)$$

Similarly, we define the time step Δt such that

$$t_m=m\Delta t \qquad (4)$$

Here, m and j are integers. The exact solution of (2) is denoted by



$$\tilde{u}(x_j,t_m)=u_j^m \qquad (5)$$

<u>Note</u> : $x_0+\Delta x\to x_j+\Delta x=x_{j+1}$

and $t_0+\Delta t \;\to\; t_m+\Delta t=t_{m+1}$

Equation (2) can be written as

$$\frac{u_j^{m+1}-u_j^m}{\Delta t}=\alpha^2\frac{u_{j+1}^m-2u_j^m+u_{j-1}^m}{(\Delta x)^2} \qquad (6)$$

For $i=1,2,\ldots,N-1$ and $m=1,2,\ldots$ Note that $u_0^m=u(0,t)$ and $u_N^m=u(L,t)$ are values of u at boundaries which are generally given (for Dirichlet problem).
To perform the calculations, we rewrite (6) as

$$\boxed{u_j^{m+1}=u_j^m+\alpha^2\frac{\Delta t}{(\Delta x)^2}\left(u_{j+1}^m-2u_j^m+u_{j-1}^m\right)} \qquad (7)$$

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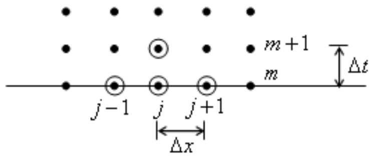


To find $u(x_j, t_{m+1})$, we use the values of u at previous time step t_m at $x = x_{j-1}$, $x = x_j$ and $x = x_{j+1}$.

This is known as the forward time and central space finite difference scheme. The scheme is explicit as it can compute u_j^{m+1} directly from the values of u at previous time t_m. Define $s = \alpha^2 \dfrac{\Delta t}{(\Delta x)^2}$ a dimensionless parameter of this finite difference equation. This discrete problem can be solved numerically. To obtain numerical stability, it is required that $\boxed{s \le \frac{1}{2}.}$

For non-homogeneous problem $u_t = \alpha^2 u_{xx} + Q(x,t)$, the source term $Q(x,t)$ is usually discretized based on the numerical scheme. If explicit scheme is used then $Q(x,t)$ will be replaced by $Q(j\Delta x, m\Delta t)$ or (in our notation) Q_j^m.

Other numerical schemes

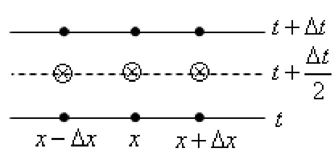
(a) More accurate scheme can be derived by using centered difference in both space and time

$$\frac{u_j^{m+1} - u_j^{m-1}}{\Delta t} = \frac{\alpha^2}{(\Delta x)^2}\left(u_{j+1}^m - 2u_j^m + u_{j-1}^m\right)$$

or $$u_j^{m+1} = u_j^{m-1} + s(u_{j+1}^m - 2u_j^m + u_{j-1}^m) \qquad (8)$$

The scheme is known as Richardson's scheme. It is an explicit scheme with second order accuracy in space and time $O(\Delta t^2)$ and $O(\Delta x^2)$. Although, this scheme is more accurate than the forward-time, centered-space but should never be used (since the scheme is always unstable).

(b) Crank-Nicholson scheme



Centered difference approximation can be achieved with higher accuracy by expanding the Taylor's series around

$$t + \frac{\Delta t}{2} \;\Rightarrow\; \left.\frac{\partial u}{\partial t}\right|_{t+\frac{\Delta t}{2}} = \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

For $\dfrac{\partial^2 u}{\partial x^2}$, the original approximation is done at t ,i.e.,

$$u_{xx}\big|_t = u_{j+1}^m - 2u_j^m + u_{j-1}^m$$

To find $u_{xx}\big|_{t+\frac{\Delta t}{2}}$ we average u_{j+1}, u_j and u_{j-1} at t and $t+\Delta t$. Hence, the finite difference equation for $u_t = \alpha^2 u_{xx}$ is

$$\frac{u_j^{m+1}-u_j^m}{\Delta t}=\frac{\alpha^2}{2}\left[\frac{u_{j+1}^{m+1}-2u_j^{m+1}+u_{j-1}^{m+1}}{\Delta x^2}+\frac{u_{j+1}^m-2u_j^m+u_{j-1}^m}{\Delta x^2}\right]$$

or $$\frac{s}{2}u_{j+1}^{m+1}-(1+s)u_j^{m+1}+\frac{s}{2}u_{j-1}^{m+1}=-\frac{s}{2}u_{j+1}^m-(1-s)u_j^m-\frac{s}{2}u_{j-1}^m \qquad (9)$$

This is called an implicit scheme with $O(\Delta t^2)$ and $O(\Delta x^2)$. The advantage of this scheme is that it is always stable for all values of s.

Wave equation

$$u_{tt}=c^2u_{xx} \qquad , \ 0<x<1$$
$$u(x,0)=f(x),\ u_t(x,0)=g(x)$$

with Dirichlet boundary conditions

We can find numerical solution to this wave equation by using finite difference approximation.

$$\frac{u_j^{m+1}-2u_j^m+u_j^{m-1}}{\Delta t^2}=c^2\left(\frac{u_{j+1}^m-2u_j^m+u_{j-1}^m}{\Delta x^2}\right) \qquad (1)$$

With truncation error $O(\Delta x^2)$ and $O(\Delta t^2)$. Initial conditions are

$$u_j^0=f(x_j)=f(j\Delta x) \qquad (2)$$

and $$\frac{u_j^1-u_j^{-1}}{2\Delta t}=g(x_j)=g(j\Delta x) \qquad (3)$$

Question now is about how to deal with u_j^{-1}. From (1) we set $m=0$ which gives

$$u_j^1=2u_j^0-u_j^{-1}+\frac{c^2}{\left(\frac{\Delta x}{\Delta t}\right)^2}\left(u_{j+1}^0-2u_j^0+u_{j-1}^0\right) \qquad (4)$$

Eliminating u_j^1 from (3) and (4), we have

$$0 \ = \ 2f(j\Delta x)-2u_j^{-1}-2\Delta t g(j\Delta x)+\left(\frac{c\Delta t}{\Delta x}\right)^2\left(u_{j+1}^0-2u_j^0+u_{j-1}^0\right)$$

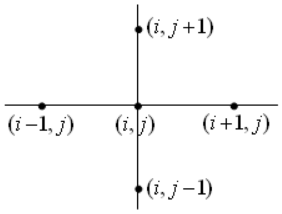
or $$u_j^{-1} \ = \ f(j\Delta x)-\Delta t g(j\Delta x)+\frac{1}{2}\left(\frac{c\Delta t}{\Delta x}\right)^2\left(u_{j+1}^0-2u_j^0+u_{j-1}^0\right)$$

Now that u_j^0 and u_j^{-1} are known, other u_j^m's can be found by using (1) and the boundary conditions can be imposed as usual.

Note: To have stable solution, the parameter $c\frac{\Delta t}{\Delta x}\le 1$. This is known as the Courant-Friedrichs-Lewy condition (CFL). Physical meaning of this is that the speed of the propagating wave (c) must be smaller than the speed of propagation of the numerical discretization of the wave equation.

Laplace's equation $\nabla^2 u=0$ (2-D)

Generally, the standard centered difference (5-point difference approximation) formula is used to find the partial difference equation with $\Delta x=\Delta y=\Delta$. That is



$$\frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}}{\Delta^2} = 0 \qquad (1)$$

Rearranging terms,

$$u_{i,j} = \frac{1}{4}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right) \qquad (2)$$

(value of u_j is the average of the four neighboring point)

We can solve (1) directly by writing as a linear system and using Gaussian elimination. But it costs too much and too expensive. It is more instructive to use approximation iterative scheme for (2). There are two basic scheme Jacobi and Gauss-Seidel iterations.

Jacobi method

$$u_{i,j}^{m+1} = \frac{1}{4}\left(u_{i+1,j}^{m} + u_{i-1,j}^{m} + u_{i,j+1}^{m} + u_{i,j-1}^{m}\right)$$

where the superscript m refers to number to iteration. Normally, we stop the iteration scheme when the convergence is achieved, i.e., $\left|u_{i,j}^{m+1} - u_{i,j}^{m}\right| < \varepsilon$.

Gauss-Seidel method

To accelerate the computation, we can update the values in (2)

$$u_{i,j}^{m+1} = \frac{1}{4}\left(u_{i+1,j}^{m} + u_{i-1,j}^{m+1} + u_{i,j+1}^{m} + u_{i,j-1}^{m+1}\right)$$