CHAPTER 3

Initial Value Problems for Ordinary Differential Equations

1. Motivation

ODE numerical methods are directly applicable to solving PDE's. A simple example is the class of semi-discrete methods. Consider for instance the problem of finding $q(x,t)$ defined on $[0,1]\times[0,T]$ that satisfies

$$\left\{\begin{array}{c} q_t = q_{xx} \\ q(x,t=0)=f(x) \\ q(x=0,t)=g_0(t),\ q(x=1,t)=g_1(t) \end{array}\right. . \tag{1.1}$$

One approach to this PDE problem is to transform into a system of ODE's by introducing a discretization in space

$$x_i = ih,\ h=1/M \tag{1.2}$$

and the functions $Q_i(t)$ that approximate $q(x_i,t)$

$$Q_i(t)\cong q(x_i,t),\ i=0,\ldots,M \tag{1.3}$$

at the nodes x_i. A finite difference approximation of the spatial derivative in (1.1) leads to

$$\frac{dQ_i(t)}{dt}=\frac{Q_{i+1}(t)-2Q_i(t)+Q_{i-1}(t)}{h^2},\ i=1,\ldots,M-1 \tag{1.4}$$

a system of $M-1$ ODE's. Initial conditions are given by $Q_i(0)=f(x_i)$ and we can apply the boundary conditions through $Q_0(t)=g_0(t)$, $Q_M(t)=g_1(t)$. Thus the IVBP for the heat equation given by Eq. (1.1) has been approximated by the ODE system (1.4).

Not only are the methods that we devise for ODE's applicable to PDE's but also much of the theoretical tools used in analyzing ODE's can be applied to the more difficult case of PDE's.

2. Existence of solutions

One of the basic ODE problems is the Cauchy or initial value problem given in general by (3.1). Let us consider the scalar form

$$\left\{\begin{array}{l} q'=f(t,q) \\ q(t=0)=q_0 \end{array}\right. , \tag{2.1}$$

with $f:\mathbb{R}^2\to\mathbb{R}$ and establish the conditions under which solutions exist. The natural language translation of the above ODE is: *given the instantaneous rate of change for* q *and a starting value* q_0 *at* $t=0$ *find* $q(t)$ *for later times* $t>0$. We suspect that f should be smooth in order for a solution to exist. If f were discontinuous at some q^* we would be hard put to choose the proper rate of change.

It could conceivably be anywhere from the left limit $f(t,q^*-0)$ to the right limit $f(t,q^*+0)$. In fact mere continuity of the function f is not sufficient to establish a unique solution as shown by the following counter-example.

Example 1. *Consider the IVP* $q'=f(q)=3q^{2/3}$, $q(t=0)=0$. *Both* $q(t)=0$ *and* $q(t)=t^3$ *are solutions of the problem, so the IVP does not specify a unique solution even though* $f(q)$ *is continuous.*

Looking at the counter-example we might presume that the non-uniqueness is somehow associated with f not being differentiable at $q=0$. Indeed, if we impose that f is differentiable everywhere then a unique solution to the IVP (2.1) does exist. From ODE theory it is known that the necessary and sufficient condition is stronger that continuity but weaker than differentiability. Continuity in q at q^*would require $|f(t,q)-f(t,q^*)|\to 0$ as $q\to q^*$ while differentiability would require that there exist a limit value of the ratio

$$\frac{f(t,q)-f(t,q^*)}{q-q^*} \tag{2.2}$$

as $q\to q^*$ which we denote by

$$f_q(t,q^*)=\frac{\partial f}{\partial q}(t,q^*)\ . \tag{2.3}$$

An intermediate condition would be that the ratio (2.2) be bounded over some neighborhood of q^*, $|q-q^*|<\varepsilon$ for all t. This is known as Lipschitz continuity.

Definition 1. *The function* $f(t,q)$ *is* ***Lipschitz continuous*** *in* q *over* $S=\{(t,q)\ \mid 0\le t\le T,\ q\in\mathbb{R}\}$*if there exists* $L>0$ *such that*

$$|f(t,q_1)-f(t,q_2)|\le L\,|q_1-q_2|\ . \tag{2.4}$$

This equivalent with stating that the function difference is of the same order as the difference in the q arguments: $|f(t,q_1)-f(t,q_2)|=O(|q_1-q_2|)$ at any given time t. It is easy to see that if f is differentiable and $f_q=\partial f/\partial q$ is bounded, we can take L as the maximum value of the differential over the neighborhood of q

$$L=\max_q\ |f_q(t,q)|\ . \tag{2.5}$$

Whenever we can establish a single L value that holds over the entire strip S we say that f is *uniformly Lipschitz continuous* over S. There is a natural extension to vector valued functions $\mathbf{f}:\mathbb{R}^{n+1}\to\mathbb{R}^n$ in which instead of the absolute value we use some norm $\|\|$, saying that $\mathbf{f}$ is Lipschitz continuous if there exists $L>0$ such that

$$\|\mathbf{f}(t,\mathbf{q}_1)-\mathbf{f}(t,\mathbf{q}_2)\|\le L\,\|\mathbf{q}_1-\mathbf{q}_2\| \tag{2.6}$$

over a strip $\mathbf{S}=\{(t,\mathbf{q})\ \mid 0\le t\le T,\ \mathbf{q}\in\mathbb{R}^n\}$

With this preparation we can state the basic theorem for existence of solutions to the IVP.

Theorem 2. *If* f *in (2.1) is Lipschitz continuous in* q *over* S *then there exists a unique solution* $q(t)$ *to (2.1) for some interval* $t\in[0,\tau]$. *The solution* $q(t)$ *is continuous and continuously differentiable. If* f *is uniformly Lipschitz continuous over* S *then the solution* $q(t)$ *exists over the entire interval* $t\in[0,T]$.

Furthermore, the solution to (2.1) depends continuously on the initial data. Suppose we have two IVP's which have the same f but different initial conditions q_0^1, q_0^2 leading to two different solutions $q\left(t; q_0^1\right)$, $q\left(t; q_0^2\right)$. Under the same conditions as the above theorem we can show that

$$\left|q\left(t; q_0^1\right) - q\left(t; q_0^2\right)\right| \leq e^{Lt}\left|q_0^1 - q_0^2\right| \; . \tag{2.7}$$

This states that later differences in the function values remain bounded by e^{Lt} times the difference in the initial conditions. We see the role played by the Lipschitz constant L. It describes how quickly the two different solutions could diverge from one another.

3. Finite difference approximations

We shall first concentrate on solving the IVP (3.1) using a finite difference approach. A discretization of the interval $[0, T]$ over which the solution is sought is introduced by

$$t^{(n)} = nk,\ n = 0, 1, \ldots, N,\ k = T/N, \tag{3.1}$$

with k the step size. This is known as an *uniform discretization* of the interval $[0, T]$. Non-uniform discretizations are also widely used but we shall restrict our attention to uniform discretizations for now. The notation $Q^{(n)}$ shall be used to denote approximations of the exact value of the unknown function at $t^{(n)}$

$$Q^{(n)} \cong q(t^{(n)}) \; . \tag{3.2}$$

Superscripts shall be used to denote discretization in time with a view to using subscripts for spatial discretization later on. To simplify the notation the parantheses around superscripts shall be omitted as in t^n, Q^n, when there is no risk of confusing superscripts with exponentiation.

Simple finite difference approximations of the derivative can be deduced by geometric reasoning. Thus

$$\frac{Q^{n+1} - Q^n}{k},\ \frac{Q^n - Q^{n-1}}{k},\ \frac{Q^{n+1} - Q^{n-1}}{2k}$$

can be interpreted as approximations of the true slope of the function $q(t)$ at t^n, $q'(t^n)$ obtained by various secants passing through points on the graph of $q(t)$. Such geometric constructions are difficult to extend to arbitrary accuracy though. One analytical procedure for achieving arbitrary accuracy is the *method of undetermined coefficients* which makes use of Taylor series expansions of $q(t^n + mk)$.

Example 2. *A fourth-order accurate finite difference approximation of $q'(t)$ can be obtained by*

$$\left\{\begin{array}{r} a\ q(t-2k) = a\left[q - 2kq' + \frac{(2k)^2}{2!}q'' - \frac{(2k)^3}{3!}q''' + \frac{(2k)^4}{4!}q^{(iv)} + O(k^5)\right] \\ b\ q(t-k) = b\left[q - kq' + \frac{k^2}{2!}q'' - \frac{k^3}{3!}q''' + \frac{k^4}{4!}q^{(iv)} + O(k^5)\right] \\ c\ q(t) = c\ q(t) \\ d\ q(t+k) = d\left[q + kq' + \frac{k^2}{2!}q'' + \frac{k^3}{3!}q''' + \frac{k^4}{4!}q^{(iv)} + O(k^5)\right] \\ e\ q(t+2k) = e\left[q + 2kq' + \frac{(2k)^2}{2!}q'' + \frac{(2k)^3}{3!}q''' + \frac{(2k)^4}{4!}q^{(iv)} + O(k^5)\right] \end{array}\right. . \tag{3.3}$$

Suppressed arguments denote function evaluation at t. Adding the above equations gives

$$\begin{aligned}
& aq(t-2k)+bq(t-k)+cq(t)+dq(t+k)+eq(t+2k) = (a+b+c+d+e)\,q+ \tag{3.4}\\
& \qquad k(-2a-b+d+2e)q'+ \tag{3.5}\\
& \qquad k^2\left(2a+\frac{b}{2}+\frac{d}{2}+2e\right)q''+ \tag{3.6}\\
& \qquad k^3\left(-\frac{4a}{3}-\frac{b}{6}+\frac{d}{6}+\frac{4e}{3}\right)q'''+ \tag{3.7}\\
& \qquad k^4\left(\frac{2a}{3}+\frac{b}{24}+\frac{d}{24}+\frac{2e}{3}\right)q^{(iv)}+ \tag{3.8}\\
& \qquad O(k^5) \tag{3.9}
\end{aligned}$$

Setting the coefficient of kq' to 1 and those of $q, q'', q''', q^{(iv)}$ to zero leads to the formula

$$q'(t)=\frac{-q(t+2k)+8q(t+k)-8q(t-k)+q(t-2k)}{12k}+O(k^4) \tag{3.10}$$

3.1. Finite difference operators. Finite difference approximations of arbitrarily high order of accuracy can be obtained using operator methods. Let E be the translation operator defined by

$$Eq(t)=q(t+k)\ . \tag{3.11}$$

Repeated applications of E lead to

$$E^n q(t)=q(t+nk) \tag{3.12}$$

with n any integer. E^0 is the identity operator

$$E^0 q(t)=Iq(t)=q(t) \tag{3.13}$$

Define the forward and backward difference operators by

$$\Delta_+ = E-E^0 \tag{3.14}$$

$$\Delta_- = E^0-E^{-1}\ . \tag{3.15}$$

We can also define a central difference operator by

$$\delta = E^{1/2}-E^{-1/2} \tag{3.16}$$

whose action is given by

$$\delta q(t)=q(t+k/2)-q(t-k/2)\ . \tag{3.17}$$

Say we're given a set of values of the function q at nodes $t^n = nk$, $n=0,\dots,N$ that we denote by Q^n. One way we can determine values of the derivative q' would be to construct the interpolating polynomial passing through the points (t^n, Q^n) and then differentiate the polynomial. The Newton form of the interpolating polynomial $p_N(t)$ is given by

$$\begin{aligned}
p_N(t) &= Q^0+\left[Q^1,Q^0\right](t-t^0)+\left[Q^2,Q^1,Q^0\right](t-t^1)(t-t^0)+\dots+ \tag{3.18}\\
&\quad \left[Q^N,Q^{N-1},\dots,Q^0\right](t-t^{N-1})(t-t^{N-2})\dots(t-t^0) \tag{3.19}
\end{aligned}$$

with the divided differences $\left[Q^n, Q^{n-1}, \ldots, Q^0\right]$ defined recursively by

$$\left[Q^1, Q^0\right] = \frac{Q^1 - Q^0}{t^1 - t^0} \tag{3.20}$$

$$\left[Q^n, Q^{n-1}, \ldots, Q^0\right] = \frac{\left[Q^n, Q^{n-1}, \ldots, Q^1\right] - \left[Q^{n-1}, Q^{n-2}, \ldots, Q^0\right]}{t^n - t^0} \tag{3.21}$$

One could just differentiate (3.18), replace t by the point of interest and thus obtain a finite difference approximation to the derivative. The resulting formula is unwieldy though since it involves divided differences evaluated recursively. We can however express the divided differences in terms of the finite difference operators Δ_+, Δ_-. The first divided difference is

$$\left[Q^1, Q^0\right] = \frac{\Delta_+ q(t_0)}{k} = \frac{\Delta_+ Q^0}{k} \tag{3.22}$$

and one can verify by induction that

$$\left[Q^n, Q^{n-1}, \ldots, Q^0\right] = \frac{\Delta_+^n Q^0}{n!\, k^n} = \frac{\Delta_-^n Q^n}{n!\, k^n} \,. \tag{3.23}$$

Proof. Formula (3.23) is true for $n = 1$ by Eq. (3.22). Assuming the above statement to be true for n, we must show that

$$\left[Q^{n+1}, Q^n, \ldots, Q^0\right] = \frac{\Delta_+^{n+1} Q^0}{(n+1)!\, k^{n+1}} = \frac{\Delta_-^{n+1} Q^{n+1}}{(n+1)!\, k^{n+1}} \,. \tag{3.24}$$

By the recursive definition of divided differences we have

$$\left[Q^{n+1}, Q^n, \ldots, Q^0\right] = \frac{\left[Q^{n+1}, Q^n, \ldots, Q^1\right] - \left[Q^n, Q^{n-1}, \ldots, Q^0\right]}{t^{n+1} - t^0} \,. \tag{3.25}$$

Using (3.23) we have

$$\left[Q^{n+1}, Q^n, \ldots, Q^0\right] = \frac{\dfrac{\Delta_+^n Q^1}{n!\, k^n} - \dfrac{\Delta_+^n Q^0}{n!\, k^n}}{(n+1)k} = \frac{\dfrac{\Delta_-^n Q^{n+1}}{n!\, k^n} - \dfrac{\Delta_-^n Q^n}{n!\, k^n}}{(n+1)k} \tag{3.26}$$

or

$$\left[Q^{n+1}, Q^n, \ldots, Q^0\right] = \frac{\Delta_+^n}{(n+1)! k^{n+1}} \left(Q^1 - Q^0\right) = \frac{\Delta_+^{n+1} Q^0}{(n+1)! k^{n+1}} \tag{3.27}$$

$$= \frac{\Delta_-^n}{(n+1)! k^{n+1}} \left(Q^{n+1} - Q^0\right) = \frac{\Delta_-^n Q^{n+1}}{(n+1)! k^{n+1}} \,. \; \square \tag{3.28}$$

□

Using these and replacing t by $t = t_0 + \alpha k$ the Newton interpolating polynomial becomes

$$p_N(t) = Q^0 + \alpha \Delta_+ Q^0 + \frac{\alpha(\alpha - 1)}{2} \Delta_+^2 Q^0 + \ldots + C_\alpha^n \Delta_+^n Q^0 \tag{3.29}$$

with $\alpha \in [0, n]$. There is a corresponding formula using backward differences

$$p_N(t) = Q^N + \beta \Delta_- Q^N + \frac{\beta(\beta + 1)}{2} \Delta_-^2 Q^N + \ldots + (-1)^n C_{-\beta}^n \Delta_-^n Q^N \tag{3.30}$$

with $t = t_n + \beta k$ and $\beta \in [-n, 0]$. The above formulas may be succintly written as

$$p_N(t) = \left(E^0 + \Delta_+\right)^\alpha Q^0 = \left(E^0 - \Delta_-\right)^{-\beta} Q^N \tag{3.31}$$

using the binomial expansion. Differentiation of the interpolating polynomial with respect to t may be rewritten as

$$\frac{dp_N(t)}{dt} = \frac{dp_N(t^0+\alpha h)}{d\alpha}\frac{d\alpha}{dt} = \frac{1}{h}\left[\left\{\ln(E^0+\Delta_+)\right\}(E^0+\Delta_+)^{\alpha}\right]Q^0 \tag{3.32}$$

where the quantity between the brackets is an operator. But the first operator to act on u_0 gives just the evaluation of the Newton interpolant

$$\left[(E^0+\Delta_+)^{\alpha}\right]Q^0 = p_N(t) \tag{3.33}$$

so

$$\frac{dp_N(t)}{dt} = \frac{1}{k}\left[\ln(E^0+\Delta_+)\right]p_N(t) \tag{3.34}$$

Identifying the operators on the two sides leads to the identity

$$\frac{d}{dt} = \frac{1}{k}\left[\ln(E^0+\Delta_+)\right] \tag{3.35}$$

Analogously, if we use backward differences we have

$$\frac{d}{dt} = -\frac{1}{k}\left[\ln(E^0-\Delta_-)\right] \tag{3.36}$$

The logarithm of an operator is defined by its series representation so we obtain

$$\frac{d}{dt} = \frac{1}{k}\left(\Delta_+ - \frac{1}{2}\Delta_+^2 + \frac{1}{3}\Delta_+^3 - \frac{1}{4}\Delta_+^4 + \ldots\right) \tag{3.37}$$

$$= \frac{1}{k}\left(\Delta_- + \frac{1}{2}\Delta_-^2 + \frac{1}{3}\Delta_-^3 + \frac{1}{4}\Delta_-^4 + \ldots\right) \tag{3.38}$$

Truncation of the operator series at term n leads to a finite difference formula of $O(k^n)$. The procedure may be extended to higher order derivatives. The result for the second order derivative is

$$\frac{d^2}{dt^2} = \frac{1}{k^2}\left(\Delta_+^2 - \Delta_+^3 + \frac{11}{12}\Delta_+^4 - \ldots\right) \tag{3.39}$$

$$= \frac{1}{k^2}\left(\Delta_-^2 + \Delta_-^3 + \frac{11}{12}\Delta_-^4 + \ldots\right) \tag{3.40}$$

Example 3. *A second order forward difference formula is obtained by truncating the series (3.37) to the first two terms*

$$\frac{dq(t)}{dt} \cong \frac{1}{k}\left(\Delta_+ - \frac{1}{2}\Delta_+^2\right)q(t) \tag{3.41}$$

$$= \frac{1}{k}\left\{q(t+k) - q(t) - \frac{q(t+2k) - 2q(t+k) + q(t)}{2}\right\} \tag{3.42}$$

$$= \frac{-q(t+2k) + 4q(t+k) - 3q(t)}{2k} \tag{3.43}$$

$$= q'(t) + O(k^2) \tag{3.44}$$

From the above left and right formulas we can also construct a centered finite difference representation of the derivative operator. Let D denote the time differentiation operator, i.e. $D = d/dt$. From (3.35) and (3.36) we can write

$$\Delta_+ = e^{kD} - 1,\ \Delta_- = 1 - e^{-kD}\ . \tag{3.45}$$

The average of the forward and backward difference operators is

$$\frac{1}{2}\left(\Delta_+ + \Delta_-\right) = 2\sinh kD \; . \tag{3.46}$$

Note that the centered difference operator δ can be expressed as the average of the forward and backward operators for a half step size, so we obtain

$$\delta = 2\sinh\frac{kD}{2} \; , \tag{3.47}$$

from where

$$D = \frac{2}{k}\,\mathrm{arcsinh}\,\frac{\delta}{2} \; . \tag{3.48}$$

The Taylor series expansion of $\mathrm{arcsinh}\,x$ around $x = 0$ is

$$\mathrm{arcsinh}\,x = x - \frac{x^3}{6} + \frac{3x^5}{40} - \frac{5x^7}{112} + \frac{35x^9}{1152} - \tag{3.49}$$

so the first few terms from (3.48) are

$$D = \frac{1}{k}\left(\delta - \frac{1}{24}\delta^3 - \frac{3}{640}\delta^5 - \frac{5}{7168}\delta^7 + \frac{35}{294912}\delta^9 - \dots\right) . \tag{3.50}$$

Notice that the series only contains odd powers of δ. We can show by induction that truncation of the series at δ^{2n-1} gives a formula of $O(k^{2n})$ accuracy.

4. Common finite difference methods

Let us now consider how numerical algorithms may be built to solve the IVP (2.1) using finite differences.

4.1. Taylor series. The basic task of a finite difference method that solves (2.1) numerically is to furnish a value at the next time step $q(t+k)$ in terms of known values at previous time steps. An immediate way of doing this is by use of a Taylor series expansion

$$q(t+k) = q + kq' + \frac{k^2}{2!}q'' + \frac{k^3}{3!}q''' + \dots \tag{4.1}$$

To ease notation, function arguments not explicitly written out are considered to be t, i.e. q' means $q'(t)$. The ODE specifies that $q' = f(t,q)$. From this we can compute higher derivatives

$$q'' = \frac{d}{dt}f(t,q(t)) = f_t + f_q q' = \tag{4.2}$$

$$q''' = \frac{d}{dt}q'' = \frac{d}{dt}\left(f_t + f_q f\right) = f_{tt} + f_{tq}f + \left(f_{qt} + f_{qq}f\right)f + f_q\left(f_t + f_q f\right) \tag{4.3}$$

Truncation of the Taylor series to various orders leads to the algorithms:

(1) $O(k)$, Euler's method

$$Q^{n+1} = Q^n + kf(Q^n) \tag{4.4}$$

(2) $O(k^2)$

$$Q^{n+1} = Q^n + kf(Q^n) + \frac{k^2}{2}\left[f_t(Q^n) + f_q(Q^n)f(Q^n)\right] \tag{4.5}$$