$\boxed{7.1}$

$$\begin{cases} \dot{u} = u - u^3 \\ u(0) = u^0 \end{cases}$$

- exact solution : $u(t) = \dfrac{u^0}{u^0 + (1-u^0)e^{-t}}$ (*)

check by substitution

or derive by separation of variables

$$\frac{u^{n+1} - u^n}{1 - e^{-\Delta t}} = u^{n+1}(1 - u^n)$$

↓ re-write

$$u^{n+1} = u^n + (1 - e^{-\Delta t})u^{n+1}(1-u^n)$$

↓ solve for $u^{n+1}$

$$u^{n+1} = \frac{u^n}{1 - (1 - e^{-\Delta t})(1-u^n)}$$

$$= \frac{u^n}{u^n + (1-u^n)e^{-\Delta t}}$$

compare with (*)

## 7.2

first order nonlinear PDE

$$\begin{cases} u_t + u_x = u(1-u) \\ u(x,0) = f(x) \end{cases}$$

$$\Rightarrow \text{exact sol} \quad u(x,t) = \frac{f(x-t)}{e^{-t} + (1-e^{-t}) f(x-t)}$$

exact FD's:

$$\underbrace{\frac{u_i^{n+1} - u_i^n}{\phi(\Delta t)}}_{\approx u_t|_i^n} + \underbrace{\frac{u_i^n - u_{i-1}^n}{\phi(\Delta x)}}_{\approx u_x|_i^n} = u_{i-1}^n \left(1 - u_i^{n+1}\right)$$

!

$$\phi(z) = e^z - 1 \quad \leftrightarrow \quad \phi(z) = 1 + z + \frac{z^2}{2} + \dots - 1 = z + O(z^2)$$

solve for $u_i^{n+1}$, $h \stackrel{d}{=} \Delta t = \Delta x$

$$u_i^{n+1} = \frac{u_{i-1}^n}{1 + (e^h - 1) u_{i-1}^n}$$

explicit scheme!

$\boxed{7.3}$

$$\begin{cases} \dfrac{du}{dt} = u^2(1-u) = u^2 - u^3 \\ u(0) = u^0 > 0 \end{cases}$$

$\exists$ three fixed points $\bar{u}^{(1)} = \bar{u}^{(2)} = 0$ and $\bar{u}^{(3)} = 1$

all solutions go monotonically to $\bar{u}^{(3)} = 1$

we have $R_1 = R_2 = 0, R_3 = 1 \Rightarrow R^* = 1$ $(T^* = 1)$

and $\phi(\Delta t) = 1 - e^{-\Delta t}$ (note: $0 < \phi(\Delta t) < 1$)

(instead of $\dfrac{u^{n+1} - u^n}{\Delta t}$ standard 2)

$$\Rightarrow \frac{du}{dt} \to \frac{u^{n+1} - u^n}{1 - e^{-\Delta t}} \quad \text{nonstandard}$$

note that $u(t) > 0$ for example a concentration or a population density

therefore must hold (discrete): $\boxed{\text{if } u^n \geq 0 \Rightarrow u^{n+1} \geq 0}$

This can be enforced by (not taking the "local" approx's)

$$\begin{cases} u^2 \mapsto 2(u^n)^2 - u^{n+1} u^n \\ u^3 \mapsto u^{n+1} (u^n)^2 \end{cases}$$

substitute & solve

$$u^{n+1} = \frac{(1 + 2\phi u^n) u^n}{1 + \phi (u^n + (u^n)^2)} \quad \text{explicit scheme !}$$

It can be shown for the discrete scheme $\forall \Delta t > 0$ !!

1) it has also 3 fixed points (!) $\bar{u}^{(1)} = \bar{u}^{(2)} = 0$, $\bar{u}^{(3)} = 1$

2) first two are unstable, 3rd is stable (as in ODE itself!)

3) $u^0 > 0$: $u^n \to \bar{u}^{(3)} = 1$ monotonically ! important property

7.4

# Fisher PDE

$$u_t = u_{xx} + u(1-u)$$

$u(x,t)$ satisfies: $0 \le u(x,0) \le 1$
$\Rightarrow 0 \le u(x,t) \le 1 \quad \forall t \ge 0$

property: "boundedness"

nonstandard FD:

$$\underbrace{\frac{u_i^{n+1} - u_i^n}{\Delta t}}_{FT} = \underbrace{\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}}_{CS} + 2\bar{u}_i^n - u_i^{n+1} - \bar{u}_i^n u_i^{n+1}$$

standard — standard — non-standard part

where $\bar{u}_i^n \stackrel{def}{=} \dfrac{u_{i+1}^n + u_i^n + u_{i-1}^n}{3}$

"nonlocal": $\begin{cases} u = 2u - u \longrightarrow 2\bar{u}_i^n - u_i^{n+1} \\ u^2 \longrightarrow \bar{u}_i^n \, u_i^{n+1} \end{cases}$ instead of $u_i^n$, $(u_i^n)^2$

can be solved explicitly

substitute and solve with $R = \dfrac{\Delta t}{(\Delta x)^2} = \dfrac{1}{2}$

$$u_i^{n+1} = \frac{\frac{1}{2}(u_{i+1}^n + u_{i-1}^n) + 2\Delta t\, \bar{u}_i^n}{1 + \Delta t + \Delta t\, \bar{u}_i^n}$$

explicit expression

for positivity: need $R = \frac{\Delta t}{(\Delta x)^2} \le \frac{1}{2}$ (OK) ($= \frac{1}{2}$, in fact)

also boundedness with this FD-scheme!

Proof (by induction): suppose $0 \le u_i^n \le 1 \quad \forall i$ for certain index $n$

$\Rightarrow \frac{1}{2}(u_{i+1}^n + u_{i-1}^n) \le 1$

$\bar{u}_i^n \le \frac{u_{i+1}^n + u_i^n + u_{i-1}^n}{3} \le \frac{1+1+1}{3} = 1$

and $2\Delta t \bar{u}_i^n \overset{\text{now}}{=} \Delta t \bar{u}_i^n + \Delta t \bar{u}_i^n$

$\le \Delta t + \Delta t \bar{u}_i^n$

adding these two: $\frac{1}{2}(u_{i+1}^n + u_{i-1}^n) + 2\Delta t \bar{u}_i^n$

$\le 1 + \Delta t + \Delta t \bar{u}_i^n$

divide by: $1 + \Delta t + \Delta t \bar{u}_i^n$:

$$\underbrace{\frac{\frac{1}{2}(u_{i+1}^n + u_{i-1}^n) + 2\Delta t \bar{u}_i^n}{1 + \Delta t + \Delta t \bar{u}_i^n}}_{= u_i^{n+1} \text{ (is what we want for } n+1)} \le 1 \qquad \left(\le \frac{1 + \Delta t + \Delta t \bar{u}_i^n}{1 + \Delta t + \Delta t \bar{u}_i^n} = 1\right)$$

By induction: $0 \le u_i^0 \le 1 \Rightarrow 0 \le u_i^n \le 1$ $\forall n \ge 1$ and all $i$.

! Collocation examples in extra files on web page !

7.5

a) $\begin{cases} \dot{u} = \sqrt{u} \\ u(0) = 1 \end{cases} \Rightarrow \int \frac{du}{\sqrt{u}} = \int dt$

$2\sqrt{u} = t + c$

$2\sqrt{1} = 0 + c$

$\underline{c = 2}$

$2\sqrt{u} = t + 2$

$\Downarrow$

$u = \left(\frac{1}{2}t + 1\right)^2$ exact sol.

call $u^+ = u^{n+1} = \left(\frac{1}{2}(t + h) + 1\right)^2$ ($h = \Delta t$)

call $u^- = u^{n-1} = \left(\frac{1}{2}(t - h) + 1\right)^2$ ($h = \Delta t$)

$$\Rightarrow \frac{u^+ - u^-}{\Delta t} = \frac{\left(\frac{1}{2}(t + \Delta t) + 1\right)^2 - \left(\frac{1}{2}(t - \Delta t) + 1\right)^2}{\Delta t}$$

$$= \frac{\left(\frac{1}{4}\left(t^2 + 2\Delta t\, t + (\Delta t)^2\right) + 1 + t + \Delta t\right) - \left(\frac{1}{4}\left(t^2 - 2\Delta t \cdot t + (\Delta t)^2\right) + 1 + (t - \Delta t)\right)}{\Delta t}$$

$$= \frac{\Delta t \cdot t + 2 \cdot \Delta t}{2 \cdot \Delta t} = \frac{1}{2}t + 1 = \sqrt{u^n}$$

b) nonstandard FD's:

1) denominator function $\phi(\Delta t)$ instead of $\Delta t$
$\phi(\Delta t) = \Delta t + O((\Delta t)^2)$

2) nonlocal approximation of RHS
example: $u_j^2 \to u_{j+1} u_j$

3) -- ---

Assume for $A$ a two-term splitting

7.7

$$A = A_1 + A_2 .$$

System (1.1) may for example be seen as a semi-discretization of a linear PDE problem with homogeneous or periodic boundary conditions. The solution of (1.1) is given by

$$w(t_{n+1}) = e^{\tau A} w(t_n) , \tag{1.2}$$

where $\tau = t_{n+1} - t_n$. If we wish to use only $A_1$ and $A_2$ separately, instead of the full $A$, then (1.2) can be approximated by

$$w_{n+1} = e^{\tau A_2} e^{\tau A_1} w_n \tag{1.3}$$

with $w_n$ approximating $w(t_n)$. This is the simplest splitting, in which we solve the two subproblems

$$\begin{aligned} &\tfrac{d}{dt} w^*(t) = A_1 w^*(t) \quad \text{for } t_n < t \leq t_{n+1} \text{ with } w^*(t_n) = w_n , \\ &\tfrac{d}{dt} w^{**}(t) = A_2 w^{**}(t) \quad \text{for } t_n < t \leq t_{n+1} \text{ with } w^{**}(t_n) = w^*(t_{n+1}) , \end{aligned}$$

one after another, starting from $w_n$, and take $w_{n+1} = w^{**}(t_{n+1})$ to complete the splitting integration step.

Replacing (1.2) by (1.3) normally introduces an error, the so-called *splitting error*. Inserting the exact solution $w$ of the original problem into (1.3) gives

$$w(t_{n+1}) = e^{\tau A_2} e^{\tau A_1} w(t_n) + \tau \rho_n ,$$

with local truncation error $\rho_n$. Recall that $\tau \rho_n$ is the error introduced per step starting from the true solution, hence it is the *local* splitting error. We have

$$\begin{aligned} e^{\tau A} &= I + \tau(A_1 + A_2) + \tfrac{1}{2}\tau^2 (A_1 + A_2)^2 + \cdots , \\ e^{\tau A_2} e^{\tau A_1} &= I + \tau(A_1 + A_2) + \tfrac{1}{2}\tau^2 (A_1^2 + 2A_2A_1 + A_2^2) + \cdots . \end{aligned}$$

The truncation error thus satisfies

$$\rho_n = \frac{1}{\tau}\Big(e^{\tau A} - e^{\tau A_2} e^{\tau A_1}\Big) w(t_n) = \tfrac{1}{2}\tau \, [A_1, A_2] \, w(t_n) + O(\tau^2) , \tag{1.4}$$

with

$$[A_1, A_2] = A_1 A_2 - A_2 A_1 \tag{1.5}$$

being the *commutator* of $A_1$ and $A_2$. Obviously (1.3) is a first-order process unless $A_1$ and $A_2$ commute. In case $A_1$ and $A_2$ do commute we have

$$e^{\tau A_2} e^{\tau A_1} = e^{\tau A_2 + \tau A_1} = e^{\tau A} ,$$

which can be seen by using the power series expansion (I.2.19) for the exponential function. It follows that for commuting matrices the splitting (1.3) is exact, it leaves no splitting error.

$\boxed{7.8}$ & $\boxed{7.9}$

### The Baker-Campbell-Hausdorff Formula

The Baker-Campbell-Hausdorff (BCH) formula expresses the product of two exponentials as one new exponential:

$$e^{\tau A_2}\, e^{\tau A_1} = e^{\tau \tilde{A}} \tag{1.6}$$

with

$$\begin{aligned}\tilde{A} = A + \tfrac{1}{2}\tau[A_2, A_1] + \tfrac{1}{12}\tau^2\Big([A_2,[A_2,A_1]] + [A_1,[A_1,A_2]]\Big) \\ + \tfrac{1}{24}\tau^3[A_2,[A_1,[A_1,A_2]]] + \mathcal{O}(\tau^4)\,.\end{aligned} \tag{1.7}$$

Clearly, if $A_1, A_2$ commute all higher-order terms in the expansion vanish and $\tilde{A} = A$. This formula can be derived from the power series development for the three exponentials by comparing terms with the same power of $\tau$. The calculation of the terms in $\tilde{A}$ quickly becomes cumbersome if done in a straightforward fashion, but it can also be done in a recursive way, see Sanz-Serna & Calvo (1994) and the references given there. Using a Lie operator formalism, a similar formula can also be derived for nonlinear autonomous equations

### Second-Order Symmetrical Splitting

#### Linear ODE problems

The splitting (1.3) starts in all steps with application of $A_1$. Interchanging the order of $A_1$ and $A_2$ after each step will lead to symmetry and better accuracy. Carrying out two half steps with reversed sequence gives

$$w_{n+1} = \left(e^{\frac{1}{2}\tau A_1} e^{\frac{1}{2}\tau A_2}\right)\left(e^{\frac{1}{2}\tau A_2} e^{\frac{1}{2}\tau A_1}\right) w_n = e^{\frac{1}{2}\tau A_1} e^{\tau A_2} e^{\frac{1}{2}\tau A_1} w_n\,. \tag{1.10}$$

This idea of symmetry in splitting has been proposed by Strang (1968) and Marchuk (1971). It is commonly called *Strang splitting*.

By a series expansion, and after some tedious calculations, the local truncation error is found to satisfy

$$\rho_n = \tfrac{1}{24}\tau^2\Big([A_1,[A_1,A_2]] + 2[A_2,[A_1,A_2]]\Big) w(t_{n+\frac{1}{2}}) + \mathcal{O}(\tau^4)\,, \tag{1.11}$$

revealing a formal consistency order of two