$$u''(x) = \frac{-2a^2}{(1+a^2x^2)^2} + \frac{2(2a^2x)^2}{(1+a^2x^2)^3} = \frac{-2a^2(1+a^2x^2)+8a^4x^2}{(1+a^2x^2)^3} = \frac{6a^4x^2-2a^2}{(1+a^2x^2)^3}$$ (5)

Whereas the derivatives of the exponential function remain bounded with the order, it is not so clear what happens in this second example. It turns out that the derivatives actually grow factorially with the order, making the convergence of the approximation problematic.

Roughly speaking, the reason for the growth of the derivative is to be found by extending the domain of definition of $u(x)$ to the complex plane. We then see that u has simple poles at $x = \pm 1/a$. By contrast, the exponential function is entire, i.e. it has no singularity in the complex plane.

[Show a numerical example on the interval $[-1,1]$ with $a=1$ and $a=5$]

If the approximation is sought in an interval that is "too close" to a singularity, interpolation will diverge as $r \to \infty$. This is called the Runge phenomenon. This phenomenon may be mitigated to some extent by choosing the interpolation points carefully. For instance, we see that the oscillations in the previous example occur near the endpoints. By choosing the distribution of the interpolation points so that they are more dense there, the approximation may be improved.

Example The Chebyshev polynomials are defined by

$$T_n(x) = \cos[n \arccos x]$$

We have

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2-1 \quad \text{etc.}$$

These polynomials are orthogonal with respect to a certain inner product. Indeed

$$\int_{-1}^{1} T_n(x)\, T_m(x) \frac{dx}{\sqrt{1-x^2}} \underset{x=\cos\theta}{=} \int_0^{\pi} \cos(n\theta)\cos(m\theta)$$

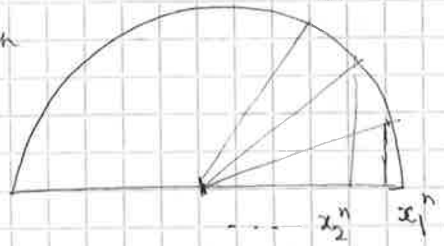
$$= \int_0^{\pi} \left\{ \frac{\cos[(m+n)x] + \cos[(m-n)x]}{2} \right\} dx = 0 \text{ unless } m=n.$$

By a well-known theorem in numerical analysis, it follows in particular that the n roots of T_n must be contained in the interval $[-1,1]$. In fact, from the definition, we see that

$$T_n(x) = 0 \text{ if } \arccos x = \frac{\pi}{2n}, \frac{3\pi}{2n}, \ldots \frac{(2n-1)\pi}{2n}$$

That is $x_j^n = \cos\left[\frac{(2j-1)\pi}{2n}\right]$

It is readily seen that the spacing between successive roots is not uniform. Rather, the roots are closer near the ends of the interval $[-1,1]$.



If we use these roots as interpolation points in the construction of the interpolant p_n, then we find that the error decreases nicely as $n \to \infty$, even for the case $a=5$.

<u>Parabolic problems</u> The simplest such problem is the heat equation

$$u_t = \frac{\sigma^2}{2} u_{xx}, \quad t>0, \; x \in \mathbb{R}.$$

s.t. $$u(x,0) = u_0(x), \quad x \in \mathbb{R}.$$

This problem is historically important for its connection with Brownian motion.

The problem may be solved explicitly as follows: we look for solutions of the form
$$u(x,t) = g(t)\, e^{i\xi x}$$

Then
$$g_t\, e^{i\xi x} = -\frac{\sigma^2}{2}\xi^2 g\, e^{i\xi x}$$

and so
$$g_t = -\frac{\sigma^2}{2}\xi^2 g$$

This yields the particular solution
$$e^{-\frac{\sigma^2}{2}\xi^2 t + i\xi x} \qquad (*)$$

The general solution is a "linear combination" of these particular solutions
$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(\xi)\, e^{-\frac{\sigma^2}{2}\xi^2 t + i\xi x}\, d\xi$$

The unknown function f may be determined by making use of the initial condition
$$u_0(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(\xi)\, e^{i\xi x}\, d\xi$$

One important feature of the heat eqn is the decay of the Fourier mode $(*)$ as $t \to \infty$.

Let us give a simple example of how to derive a finite-difference scheme for the heat eqn. We introduce spatial and temporal grids

$$x_j = jh, \quad j \in \mathbb{Z}, \quad t_n = nk, \quad n \in \mathbb{N}$$

where h and k are the step sizes. Then we may look for a scheme of the form

$$u_j^{n+1} = \alpha u_{j-1}^n + \beta u_j^n + \gamma u_{j+1}^n$$

and choose α, β and γ so that

$$L_j^n := u(x_j, t_{n+1}) - \alpha u(x_{j-1}, t_n) - \beta u(x_j, t_n) - \gamma u(x_{j+1}, t_n)$$

We expand at (x_j, t_n):

$$\begin{aligned} L_j^n = {} & u(x_j,t_n) + k\, u_t(x_j,t_n) + \frac{k^2}{2} u_{tt}(x_j,t_n) + O(k^3) \\ & - \alpha\Big[u(x_j,t_n) - h\, u_x(x_j,t_n) + \frac{h^2}{2} u_{xx}(x_j,t_n) - \frac{h^3}{3!} u_{xxx}(x_j,t_n) \\ & \qquad + O(h^4) \Big] \\ & - \beta u(x_j,t_n) \\ & - \gamma\Big[u(x_j,t_n) + h u_x(x_j,t_n) + \frac{h^2}{2} u_{xx}(x_j,t_n) + \frac{h^3}{3!} u_{xxx}(x_j,t_n) + O(h^4)\Big] \end{aligned}$$

We use the fact that $u_t(x,t) = \frac{\sigma^2}{2} u_{xx}(x,t)$. Then

$$\begin{aligned} L_j^n = {} & [1-\alpha-\beta-\gamma]\, u(x_j,t_n) + h u_x(x_j,t_n)\,[\alpha-\gamma] + u_{xx}(x_j,t_n)\left[\frac{\sigma^2 k}{2} - \frac{\alpha}{2}h^2 - \frac{\gamma}{2}h^2\right] \\ & \frac{h^3}{3!} u_{xxx}(x_j,t)\,[\alpha-\gamma] + O(h^4+k^2) \end{aligned}$$

We choose α, β, γ so that

$$1 = \alpha+\beta+\gamma, \quad \alpha = \gamma, \quad \alpha+\gamma = \frac{k\sigma^2}{h^2}$$

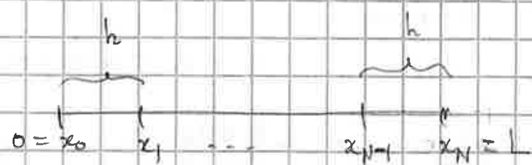
This yields the scheme

$$u_j^{n+1} = u_j^n + \mu\left[u_{j-1}^n - 2u_j^n + u_{j+1}^n\right], \quad \mu = \frac{k\sigma^2}{2h^2}$$

In practice, the scheme can only be implemented if the number of gridpoints is finite. This is possible if a boundary condition is imposed.

Example Assume a periodic boundary condition, i.e.

$$u(0,t) = u(L,t) \quad \forall\, t \in [0,T]$$



After discretisation this condition may be implemented as

$$u_0^n = u_N^n$$

For this simple problem, an explicit formula for u_j^n may be found as follows: we look for solutions of the form

$$u_j^n = g^n e^{i\xi x_j} \qquad (+)$$

The boundary condition dictates that $e^{i\xi L} = 1$. We use $Nh = L$ so that

$$\xi h = \xi_\ell h := \frac{\ell}{N} 2\pi, \quad \ell = 0, 1, \dots, N-1$$

For any one of these values, we then require (+) to solve the difference eqn:

$$g^{n+1} e^{i\xi x_j} = g^n e^{i\xi x_j} \left[1 + \mu \left(e^{-i\xi h} - 2 + e^{i\xi h} \right) \right]$$

After simplification, we find

$$g = 1 + \mu \left(e^{-i\xi h} - 2 + e^{i\xi h} \right) = 1 + 2\mu(\cos \xi h - 1) = 1 - 4\mu \sin^2 \frac{\xi h}{2}$$

The general soln is then

$$u_j^n = \sum_{\ell=0}^{N-1} c_\ell \left[1 - 4\mu \sin^2 \frac{\xi_\ell h}{2} \right]^n e^{i\xi_\ell x_j}$$

and the c_ℓ may be determined by using the initial condition. We note that the ℓth mode remains bounded iff

$$-1 \le 1 - 4\mu \sin^2 \frac{\xi_\ell h}{2} \le 1$$

<u>Consistency, stability and convergence</u> Having discussed this particular example at some length, we can now introduce some important concepts that are relevant more generally. To introduce them, we consider an abstract initial-value problem of the form

$$u_t = \mathcal{L} u, \quad 0 \le t \le T, \quad u(\cdot, 0) = u_0$$

where $\mathcal{L}$ is some linear operator on a space of functions, say X, with a norm $\|\cdot\|$. The solution may be expressed formally as

$$u(\cdot, t) = \underbrace{S(t)}_{e^{t\mathcal{L}}} u_0, \qquad 0 \le t \le T$$

<u>Definition</u> The problem is said to be <u>well posed</u> if $\exists\, M > 0$ s.t.

$$\forall\, t \in [0,T] \quad \|S(t)\| \le M.$$

<u>Notation</u> $$\|S(t)\| = \sup_{\|u_0\| = 1} \|S(t) u_0\|$$

We consider a finite difference method for computing an approximation u^n of $u(t_n)$. It will be convenient to express the finite difference scheme in the form

$$u^{n+1} = S_k u^n$$

where S_k can be thought of as an operator on X that approximates $S(k)$. Generally, S_k may also depend on the spatial mesh size h but, to simplify the situation, we shall suppose that h is a function of k.

Definitions (1) We say that the finite-difference scheme has order of accuracy p if

$$\| u(t+k) - S_k u(t) \| = O(k^{p+1}) \quad \text{as } k \to 0$$

for every $t \in [0,1)$.

(2) We say that the scheme is consistent if $p > 0$.

(3) We say that the scheme is stable if $\exists\, C > 0$ s.t.

$$\| S_k^n \| \leq C$$

for every $n \in \mathbb{N}$, $k > 0$ s.t. $0 \leq nk \leq T$.

(4) We say that the scheme is convergent if

$$\lim_{\substack{k \to 0 \\ nk = t}} \| S_k^n u(0) - u(t) \| = 0$$

The Lax Equivalence Theorem says that, if the problem is well-posed, then the scheme is convergent iff it is consistent and stable.

Proof of $[\Leftarrow]$ We prove the necessity of convergence:

We have

$$S_k^n u(0) - u(t_n) = S_k^n u(0) - S_k^{n-1} u(t_1) + S_k^{n-1} u(t_1) - S_k^{n-2} u(t_2) + S_k^{n-2} u(t_2)$$
$$- S_k^{n-3} u(t_2) + \cdots + S_k u(t_{n-1}) - u(t_n)$$

Hence

$$\| S_h^k u(0) - u(t_n) \| \leq \| S_k^{n-1} \| \, \| S_k u(0) - u(t_1) \| + \| S_k^{n-2} \| \, \| S_k u(t_2) - u(t_2) \|$$
$$+ \cdots + \| S_k u(t_{n-1}) - u(t_n) \|$$
$$\leq C\, n\, O(k^{p+1}) = O(k^p) \quad \text{as } k \to 0. \quad \blacksquare$$

The proof of necessity has made no use of the well-posedness; that hypothesis only enters in the proof of sufficiency.

Example Let us return to our earlier example in order to illustrate these new concepts:

$$u_j^{n+1} = u_j^n + \mu \left[u_{j-1}^n - 2u_j^n + u_{j+1}^n \right] \qquad (+)$$

where, for the sake of concreteness, we shall again assume periodic boundary conditions:

$$u_0^n = u_N^n$$

We may then take as our space

$$X = l_2(\mathbb{C}^N) = \left\{ v,\ v \in \mathbb{C}^N : \sum_{j=0}^{N-1} h|v_j|^2 < \infty \right\}$$

equipped with the norm

$$\|v\| = \left(\sum_{j=0}^{N-1} h\,|v_j|^2 \right)^{\frac{1}{2}}$$

Clearly, the soln $u(x,t)$ of the pde problem does not itself belong to X, but we can replace u by the vector, say $u(t)$, whose entries are the values $u(x_j,t)$.

The finite-difference scheme (+) corresponds to the operator $S_k : X \to X$ defined by

$$(S_k v)_j = v_j + \mu\left[v_{j-1} - 2v_j + v_{j+1} \right]$$

Our earlier calculation (based on Taylor expansions at (x_j,t_n)) then showed that

$$\| u(t+k) - S_k u(t) \| = O(k^2)$$

where we consider that $\mu = k/h^2$ is fixed as $k \to 0$. It follows that the scheme has order of accuracy 1.

Let us now investigate stability. Let $v \in X$ and write

$$v_j = \sum_{l=0}^{N-1} \hat{v}_l\, e^{i\xi_l x_j} \qquad (\text{cf Sheet 2, Q1})$$

Then

$$(S_k v)_j = \sum_{l=0}^{N-1} \left[1 - 4\mu \sin^2 \frac{\xi_l h}{2} \right] \hat{v}_l\, e^{i\xi_l x_j}$$

Iterating, we find

$$(S_k^n v)_j = \sum_{l=0}^{N-1} \left[1 - 4\mu \sin^2 \frac{\xi_l h}{2} \right]^n \hat{v}_l\, e^{i\xi_l x_j}$$

Parseval's identity then says that

$$\| S_k^n v \|^2 = L \sum_{l=0}^{N-1} \left[1 - 4\mu \sin^2 \frac{\xi_l h}{2} \right]^{2n} |\hat{v}_l|^2$$

We distinguish three cases

(1) $$\max_{0 \le \xi h \le 2\pi} \left| 1 - 4\mu \sin^2 \frac{\xi h}{2} \right| \le 1$$

In that case

$$\| S_k^h v \|^2 \le L \sum_{l=0}^{N-1} |\hat{v}_l|^2 \overset{\text{Parseval}}{=} \|v\|^2$$

This shows that

$$\| S_k^h \| \le 1$$

and so the scheme is stable; the condition on μ is

$$\mu \le 1/2$$

(2) $\exists\ \alpha > 0$ independent of k and h s.t.

$$\max_{0 \le \xi h \le 2\pi} \left| 1 - 4\mu \sin^2 \frac{\xi h}{2} \right| \le 1 + \alpha k$$

Using $k = t/n$, we may then write

$$\| S_k^h v \|^2 \le L \sum_{l=0}^{N-1} \underbrace{\left(1 + \frac{\alpha t}{n}\right)^n}_{\le e^{\alpha t}} |\hat{v}_l|^2 \le e^{\alpha t} \|v\|^2$$

and again the scheme is stable

(3) $\exists\ \beta > 0$ s.t.

$$\max_{0 \le \xi h \le 2\pi} \left| 1 - 4\mu \sin^2 \frac{\xi h}{2} \right| \ge 1 + \beta$$

Then, for every h (i.e. k) small enough we can always find $0 \le l < N$ with

$$\left| 1 - 4\mu \sin^2 \frac{\xi_l h}{2} \right| > 1 + \beta/2 .$$

Choose

$$v_j = e^{-i \xi_l x_j}, \quad 0 \le j < N$$

Then

$$\| S_k^h v \|^2 > L \left(1 + \beta/2\right)^n \|v\|^2$$

and the scheme is unstable.

Summary The Lax equivalence theorem enables us to reduce the study of convergence to that of stability and consistency. Consistency can be investigated by using Taylor expansions. Stability may be investigated by looking for particular solutions of the form $u_j^n = g^n e^{i \xi x_j}$, $\xi h \in [0, 2\pi]$

The scheme is stable if every such solution satisfies

$$\max_{0 \leq \xi h \leq 2\pi} |g(\xi h)| \leq 1 + \alpha k$$

for some $\alpha \geqslant 0$ independent of k and unstable otherwise. This approach to the study of stability is called <u>von Neumann</u> analysis. Its validity has been demonstrated for the particular case of <u>periodic</u> boundary conditions but it is more generally a useful guide in more general situations, such as

(1) Other boundary conditions

(2) No boundary condition, i.e. pure initial-value problems.

(3) variable coefficients

(4) nonlinear problems

(5) Equation's of other types.