Difference schemes as Markov chains

Recall that the explicit Euler scheme was first derived as describing the transition density of a discrete-time random walk on a grid $\Delta x\mathbb{Z}$. It is a natural question to ask whether the implicit scheme has a similar interpretation, ie is there a random walk X_t on the state space $\Delta x\mathbb{Z}$, such that the associated transition density $U_n^m = \mathbb{P}(X_{m\Delta t} = n\Delta x)$ satisfies the implicit Euler scheme?

We have already shown in (2.3.2) that the solution to the implicit Euler scheme has the making of a probability density – non-negativity and "preserves probability",

$$\sum_{n=-\infty}^{\infty} u_n^m = \sum_{n=-\infty}^{\infty} u_n^{m-1}. \tag{2.33}$$

A prime candidate for a random walk is therefore defined by the one-step transition densities,

$$X_{t_m+\Delta t} = X_{t_m} + \xi_m \Delta x,$$

where

$$\mathbb{P}(\xi_m = n) := U_n^1 := u_n^1 \Delta x$$

with $u_n^1 = c\Delta x z^{|n|}$ as defined in (2.24), and all ξ_m independent.

The process X is a *Markov chain* because it satisfies the *Markov property*

$$\mathbb{P}(X_{t_m} = y_m | X_{t_0} = y_0, \ldots, X_{t_{m-1}} = y_{m-1}) = \mathbb{P}(X_{t_m} = y_m | X_{t_{m-1}} = y_{m-1}).$$

See e.g. [Grimmet and Stirzaker, 2001], pp214, for more details. We can think of the process having an infinite transition matrix

$$P_{nk} = \mathbb{P}(X_{t_m} = x_k | X_{t_{m-1}} = x_n) = \mathbb{P}(X_{t_m} = x_{k-n} | X_{t_{m-1}} = 0) = P_{0,k-n} = U_{k-n}^1.$$

For the implicit scheme on a finite grid, where we approximate $U_N^m = U_{-N}^m = 0$ for sufficiently large N, (2.33) is no longer exactly given, but instead

$$\sum_{n=-N}^{N} U_n^m = \sum_{n=-N}^{N} U_n^{m-1} - p\,(U_{-N+1}^m + U_{N-1}^m) < \sum_{n=-N}^{N} U_n^{m-1}.$$

The boundaries are absorbing and the probability of staying in the interval $(-N\Delta x, N\Delta x)$ goes down by the probability $pU_{\pm(N-1)}^m$ of moving out to $\pm N\Delta x$ from $\pm(N-1)\Delta x$. We could account for this by introducing "absorbed" states into the Markov chain.

We try a different tack and see if we can modify the boundary conditions at $\pm N\Delta x$ in order to preserve probability. For reasons that will become apparent shortly it is useful to define the vector $(1) = (1, \ldots, 1) \in \mathbb{R}^{2N+1}$. With this notation, we want

$$1 = \sum_{n\in\mathbb{Z}} U_n^m = (1)'U^m = (1)'(K^{-1}U^{m-1}) = ((1)'K^{-1})U^{m-1},$$

but because $(1)'U^{m-1} = 1$, it is sufficient that

$$(1)'K^{-1} = (1)' \quad \Leftrightarrow \quad (1)' = (1)'K,$$

that is to say all columns sum up to one,

$$\sum_{k=-N}^{N} K_{kn} = 1 \quad \forall n. \tag{2.34}$$

Taken the coefficients for interior points as given, this is only possible if

$$\begin{aligned} K_{N,N} &= 1 + p \\ K_{N,N-1} &= -p \end{aligned}$$

and zero elsewhere in the last line, and similarly for $-N$. The corresponding equation is

$$U_N^m = U_N^{m-1} - p(U_N^m - U_{N-1}^m) \quad \Leftrightarrow \quad \frac{U_N^m - U_N^{m-1}}{\Delta t} = \frac{1}{2}\frac{U_N^m - U_{N-1}^m}{\Delta x^2},$$

which is consistent with

$$\frac{U_N^m - U_N^{m-1}}{\Delta t} = \frac{1}{2}\frac{U_{N+1}^m - 2U_N^m + U_{N-1}^m}{\Delta x^2}$$

only if

$$\frac{U_{N+1}^m - U_N^m}{\Delta x} = 0.$$

This is the discrete counterpart of a *Neumann boundary condition*

$$\frac{\partial u}{\partial x}(x_{max}, t) = 0$$

for the heat equation. It is left as an exercise to check that the heat equation with Neumann boundary conditions at the upper and lower boundary preserves the integral of the solution.

Back to the discretised equations, we already know that for any $u \geq 0$ the solution to $Kv = u$ has $v = K^{-1}u \geq 0$, and since this is true for all u,

$$P_{nk} = (K^{-1})_{nk} \geq 0. \tag{2.35}$$

It follows that

$$P = K^{-1}$$

is a so-called *stochastic matrix* defined through properties (2.34) and (2.35). The *transition matrix* P therefore defines a *Markov chain.*

In an appropriate limit $\Delta t, \Delta x \to 0$, the Markov chain approaches Brownian motion. It is an interesting question to ask what happens if we consider continuous time ($\Delta t \to 0$) but keep the states x_n fixed. (We leave the Δx limit for fixed Δt to Exercise 6, Section 4.4.)

The limit will have the form $U_n(t)$, where $n \in \mathbb{Z}$ and $t \geq 0$. Neither the explicit nor the implicit scheme have difficulties for small Δt, and letting $t \to 0$ in either one formally gets

$$\frac{\mathrm{d}}{\mathrm{d}t}U_n(t) = \frac{1}{2}\frac{U_{n-1}(t) - 2U_n(t) + U_{n+1}(t)}{\Delta x^2}, \tag{2.36}$$

with initial condition

$$U_n(0) = \delta_{n0}.$$

In matrix form,

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = AU(t) \tag{2.37}$$

with $A = 1/(2\Delta x^2)\mathrm{tridiag}(1,-2,1,2N+1)$. Writing the explicit Euler scheme as

$$\frac{U^{m+1}-U^m}{\Delta t} = AU^m \quad \Leftrightarrow \quad U^{m+1} = (I+\Delta t A)U^m$$

gives

$$U^m = (I+\Delta t A)^m U^0 = (I+\Delta t A)^{t/\Delta t}U^0 \quad \to \quad U(t) = \mathrm{e}^{At}U^0 \quad \text{for } \Delta t \to 0.$$

A similar derivation using the implicit scheme, of course, gives the same result. This defines a continuous-time Markov process X_t on the state space $\mathbb{Z}$ with transition probabilities

$$p_{kn}(t) = \mathbb{P}(X_t = n | X_0 = k) = U_{n-k}(t).$$

The matrix

$$P_t = \mathrm{e}^{At}$$

satisfies the forward equation

$$\frac{\mathrm{d}}{\mathrm{d}t}P_t = P_t A.$$

The process X_t jumps between states at exponentially distributed times, specifically the time of the first jump, $\tau = \inf\{t \geq 0 : \ X_t \neq 0\}$, is exponentially distributed with parameter $-A_{00} = 1/\Delta x^2$. The chain jumps to ± 1 with equal probability $1/2$. An analogous statement is true for the following inter-jump times.

2.5 Exercises

1. Given is the setup from Sections 2.1.1 and 2.1.2.

   (a) Show that for $m \geq 0$, $0 \leq n \leq m$,

   $$U_n^m = U_{-n}^m = \sum_{k=0}^{\lfloor \frac{m-n}{2} \rfloor} \frac{m! p^{n+2k}(1-2p)^{m-n-2k}}{(n+k)!k!(m-n-2k)!}. \tag{2.38}$$

   (b) By insertion, show that (2.38) solves the recursion (2.7) and initial condition (2.8).

   (c) Show directly that in the limit $\Delta x \to 0$, $\Delta t = 2p\Delta x^2$,

   $$\frac{1}{\Delta x}U_n^m \to \frac{1}{\sqrt{2\pi t}}\mathrm{e}^{-\frac{x^2}{2t}},$$

   where $t = m\Delta t$ and $x = n\Delta x$ fixed.

2. Given is the setup from Section 2.3.1.

(a) For $m = 1$, the scheme takes the special form

$$-pu_{-1}^1 + (1+2p)u_0^1 - pu_1^1 = \Delta x^{-1}, \tag{2.39}$$
$$-pu_{n-1}^1 + (1+2p)u_n^1 - pu_{n+1}^1 = 0, \quad n \neq 0. \tag{2.40}$$

Show that the general solution to (2.40) for $n > 0$ is of the form

$$u_n^1 = c_- z_-^n + c_+ z_+^n,$$

where you have to determine z_- and z_+. Use (2.39) to find the (unique) bounded symmetric solution. Verify that

$$\Delta x \sum_{n \in \mathbb{Z}} u_n^1 = 1.$$

(b) Show that

$$u_n^m = \sum_{k \in Z} u_k^{m-1} u_{n-k}^1 \Delta x$$

defines a solution to the implicit scheme. What is the counterpart for continuous x and discrete time?

(c) Explicitly find u_n^2 for all n. Does this lead to a computationally efficient method?

3. Consider the implicit Euler finite difference scheme for the heat equation with Dirac initial data, for $x \in [-5, 5]$, $t \in [0, 1]$, with zero boundary conditions at -5 and 5. Use a grid $(-N\Delta x, \ldots, -\Delta x, 0, \Delta x, \ldots, N\Delta x)$, where $N\Delta x = 5$, and M timesteps, $\Delta t = 1/M$.

(a) Show that for $\Delta t \to 0$, and Δx *fixed*, the finite difference scheme approaches a system of ODEs

$$\frac{\partial u}{\partial t} = Au \tag{2.41}$$
$$u(0) = u^0 \tag{2.42}$$

where $u(t) = (u_1(t), \ldots, u_{2N+1}(t)) \in \mathbb{R}^N$, $u^0 \in \mathbb{R}^N$, $A \in \mathbb{R}^{N \times N}$. State A and u^0. Explain why this is often called the *method of lines*.

(b) Show that a solution to (2.41), (2.42) is given by $u(t) = e^{At} u^0$. Hence compute the solution to this semi-discrete problem (x discrete, t continuous) in MATLAB for $t = 1$, $N = 10$ and plot over x together with the exact solution.

(c) Compute the error for $x = 0$, $t = 1$, for $N = 10, 20, 40, 80, 160, 320$. What do you observe?

4. (a) Implement the explicit as well as the implicit Euler finite difference scheme for the heat equation with Dirac initial data, for $x \in [-5, 5]$, $t \in [0, 1]$, with zero boundary conditions at -5 and 5. Use a grid $(-N\Delta x, \ldots, -\Delta x, 0, \Delta x, \ldots, N\Delta x)$, where $N\Delta x = 5$, and M timesteps, $\Delta t = 1/M$.

(b) Table the difference between

i. the discrete solutions and the analytical one,

ii. the discrete solutions and the semi-discrete solution from 3. (with the same number of grid points),

at $x = 0$, $t = 1$, for both schemes for $N = 10, 20, 40, 80, 160, 320$, M =10, 20, 40, 80, 160, 320, 640, 1280, 2560. Discuss the different patterns.