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A Zoo of Numerical Schemes for the Diffusion Equation

2.1 Differentiation on a Grid

Our initial goal is to derive a family of difference schemes for investigation. We assume that one way or the other, our option-pricing problem has been reduced to the diffusion equation:

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2} \tag{1}$$

We introduce a discrete grid with steps $\Delta\tau$, Δx, where Δx is the grid step for the (log) stock price, and $\Delta\tau$ is the grid step for the time, and set

$$u_n^m = u(m\,\Delta\tau,\ n\,\Delta x) \tag{2}$$

All the difference schemes involve a parameter α that is given by

$$\alpha = \frac{\Delta\tau}{\Delta x^2} \tag{3}$$

What we need to establish first are some relations for approximating derivatives on a grid. We allow ourselves to consider a refined grid, so that e.g. $u_{n+\frac{1}{2}}^m$ makes sense.

The Difference Operators

Let's go back to one dimension and consider Taylor's Theorem in the form

$$f(h+x) = f(x) + h\,\frac{\partial f}{\partial x} + \frac{1}{2}\,h^2\,\frac{\partial^2 f}{\partial x^2} + \frac{h^3}{3!}\,\frac{\partial^3 f}{\partial x^3} + \ldots \tag{4}$$

Introduce the operator:

$$D\,f = \frac{\partial f}{\partial x} \tag{5}$$

Then Taylor's theorem can be written in the compact form:

$$f(h+x) = e^{h\,D}\,f(x) \tag{6}$$

The exponential function is used as a convenient encoding of the infinite sum of terms.

One-sided differences

First consider

$$\Delta\, f\ = f(h+x) - f(x) \tag{7}$$

Using the operator form of Taylor's theorem we can write

$$\Delta\, f = e^{h\,D}\, f(x) - f(x) = (e^{h\,D} - 1)\, f(x) \tag{8}$$

So as operators

$$\Delta\ = e^{h\,D} - 1 \tag{9}$$

We can invert this as (note that log is just used to encode an infinite sum):

$$D = \frac{\log(\Delta + 1)}{h} = \frac{1}{h}\left(\Delta - \frac{\Delta^2}{2} + \ldots\right) \tag{10}$$

Unpacking this expression, we obtain, first keeping just one term, the Euler approximation to the derivatives

$$D\, f \approx \frac{1}{h}\,\Delta\, f\ = \frac{1}{h}\,(f(x+h) - f(x)) \tag{11}$$

Keeping two terms we obtain instead

$$D\, f \approx \frac{\Delta\, f - \frac{\Delta^2\, f}{2}}{h} = \frac{f(h+x) - f(x) - \frac{1}{2}\,(f(x+2\,h) - 2\, f(x+h) + f(x))}{h} \tag{12}$$

which simplifies to the approximation:

$$D\, f \approx = \frac{4\, f(h+x) - 3\, f(x) - f(x+2\,h)}{2\,h} \tag{13}$$

This last formula is particularly useful for estimating derivatives at the edge of a grid. E.g. Theta, the option time derivative.

Central Differences

Now we consider a finite difference centred on a point of interest:

$$\delta\, f\ = f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right) \tag{14}$$

In terms of the D operator, proceeding as before, we can write

$$\delta = e^{\frac{h\,D}{2}} - e^{-\frac{1}{2}\,h\,D} = 2\sinh\left(\frac{h\,D}{2}\right) \tag{15}$$

Inverting this, we see that there is an *exact* relationship:

$$D = \frac{2\sinh^{-1}\left(\frac{\delta}{2}\right)}{\Delta x} \tag{16}$$

We can obtained various orders of approximation by taking various numbers of terms in the series. This series is interesting as it contains only odd powers, in particular no quadratic term arises:

$$D \;=\; \frac{1}{\Delta x}\,2\sinh^{-1}\left(\frac{\delta}{2}\right) \approx \frac{1}{\Delta x}\left(\delta - \frac{\delta^3}{24} + \frac{3\,\delta^5}{640} + O(\delta^7)\right) \tag{17}$$

We are going to need the square of this in the form:

$$D^2 \;\approx\; \frac{1}{(\Delta x)^2}\left(\delta^2 - \frac{\delta^4}{12} + \frac{\delta^6}{90} + O(\delta^8)\right) \tag{18}$$

Going back to our grid with both a space and time dimension, we need this operator form for the x-direction, that is: we define the central difference operator δ_x by

$$\delta_x\, u_n^m = u_{n+\frac{1}{2}}^m - u_{n-\frac{1}{2}}^m \tag{19}$$

Its square is

$$\delta_x^2\, u_n^m = \; u_{n+1}^m + u_{n-1}^m - 2\,u_n^m \tag{20}$$

2.2 Overview of Difference Schemes

The Operator Approach

We introduce the operators L, D, given by

$$L\,f = \frac{\partial f}{\partial t} \qquad D\,f = \frac{\partial f}{\partial x} \tag{21}$$

So the diffusion equation is just $L\,f \;=\; D^2\,f$. Assuming that the Taylor series expansion holds, we can write

$$u(\tau + \Delta\,\tau,\, x) = e^{\Delta\tau\,L}\,u(\tau,\, x) \tag{22}$$

In other words

$$u_n^{m+1} = e^{\Delta\tau\,L}\,u_n^m = \; e^{\Delta\tau\,D^2}\,u_n^m \tag{23}$$

More generally, if we consider the value, u_θ of u at $x = n\,\Delta\,x$, and $\tau \;=\; \theta\,n\,\Delta\tau + \;(1-\theta)\,(n+1)\,\Delta\tau$, we can write it in two ways. First, by using a forwards Taylor expansion, we have

$$u_\theta = e^{\Delta\tau\,(1-\theta)\,L}\,u_n^m = e^{\Delta\tau\,(1-\theta)\,D^2}\,u_n^m \tag{24}$$

By considering a Taylor series backwards from the next time-level, we can also say that

$$u_\theta = e^{-\Delta\tau\,\theta\,L}\,u_n^{m+1} = e^{-\Delta\tau\,\theta\,D^2}\,u_n^{m+1} \tag{25}$$

So on the assumption that we have such Taylor series, we can equate the two to obtain

$$e^{-\Delta\tau\,\theta\,D^2}\,u_n^{m+1} = e^{\Delta\tau\,(1-\theta)\,D^2}\,u_n^m \tag{26}$$

Note that no approximations have been made.

General High Order Difference Versions of the Diffusion Equation

Now our diffusion equation involves $\Delta\tau\,D^2$, which, after some algebra, we can expand out as

$$\alpha\left(\delta_x^2 - \frac{\delta_x^4}{12} + \frac{\delta_x^6}{90} + \ldots\right) \tag{27}$$

We can combine our exact diffusion equation with the series expansion of the operators contained within it to obtain a description of the problem to any desired order. Keeping all terms up to order δ_x^6, and performing some tedious simplifications, the combination of the last two equations becomes, neglecting eighth and higher order differences

$$\begin{aligned}&-\alpha\,\theta\left(\frac{\alpha^2\,\theta^2}{6} + \frac{\alpha\,\theta}{12} + \frac{1}{90}\right)\delta_x^6\,u_n^{m+1} + \frac{1}{2}\left(\alpha\,\theta + \frac{1}{6}\right)\alpha\,\theta\,\delta_x^4\,u_n^{m+1} - \alpha\,\theta\,\delta_x^2\,u_n^{m+1} + u_n^{m+1} = \\ &\quad\left(\frac{1}{2}\,(1-\theta)^2\,\alpha^2 - \frac{1}{12}\,(1-\theta)\,\alpha\right)\delta_x^4\,u_n^m + \alpha\,(1-\theta)\,\delta_x^2\,u_n^m + u_n^m \\ &+\left(\frac{1}{6}\,(\alpha^2\,(1-\theta))^2 - \frac{1}{12}\,\alpha\,(1-\theta) + \frac{1}{90}\right)\alpha\,(1-\theta)\,\delta_x^6\,u_n^m\end{aligned} \tag{28}$$

This in general is a matrix equation, and can be represented in terms of "difference matrices", A, B that govern the mapping from one time level to the next. All such schemes can be written in the form $B\,u^{m+1} = A\,u^m$ for suitable difference matrices.

Explicit Schemes

These are obtained by setting $\theta = 0$, thereby obtaining, to sixth order,

$$u_n^{m+1} = u_n^m + \alpha\;\delta_x^2\,u_n^m + \;\frac{\alpha}{2}\left(\alpha - \frac{1}{6}\right)\delta_x^4\,u_n^m + \frac{\alpha}{6}\left(\alpha^2 - \frac{1}{2}\,\alpha + \frac{1}{15}\right)\;\delta_x^6\,u_n^m \tag{29}$$

Second Order Explicit and Binomial Schemes

If we keep terms to second order we obtain

$$u_n^{m+1} = u_n^m + \alpha\ \delta_x^2\, u_n^m \tag{30}$$

The choice $\alpha = 1/2$ in fact gives the scheme embodied by the binomial model (if a tree-shaped grid is used instead of a rectangular grid).

Fourth Order Explicit and Pentanomial/Trinomial Schemes

If we keep terms to fourth order we obtain the family of pentanomial schemes

$$u_n^{m+1} = u_n^m + \alpha\ \delta_x^2\, u_n^m + \frac{\alpha}{2}\left(\alpha - \frac{1}{6}\right)\delta_x^4\, u_n^m \tag{31}$$

The choice $\alpha = 1/6$ gives the scheme embodied by the trinomial model (if a tree-shaped grid is used instead of a rectangular grid) - the fourth order terms then vanish identically, and we have a simple scheme but with high order accuracy.

Implicit Crank-Nicolson and Douglas Schemes

Working to second order, the choice $\theta = 1/2$ gives the scheme known as the Crank-Nicolson scheme. If we write it out it becomes

$$u_n^{m+1} - \frac{1}{2}\,\alpha\,(u_{n-1}^{m+1} + u_{n+1}^{m+1} - 2\,u_n^{m+1}) = u_n^m + \frac{1}{2}\,\alpha\,(u_{n-1}^m + u_{n+1}^m - 2\,u_n^m) \tag{32}$$

Another interesting set of schemes can be derived by taking the general high order scheme with $\theta = 1/2$, and multiplying both sides by

$$1 + \mu\,\delta_x^2 - \lambda\,\delta_x^4 \tag{33}$$

The choice $\mu = 1/12,\ \lambda = \alpha^2/8$ leads to a very interesting equation where the fourth order terms disappear:

$$u_n^{m+1} - (1/12 - \alpha/2)\ \delta_x^2\, u_n^{m+1} + O(\,\delta_x^6\, u_n^{m+1}) = u_n^m + (1/12 + \alpha/2)\,\delta_x^2\, u_n^m + O(\,\delta_x^6\, u_n^m) \tag{34}$$

The second order truncated form, i.e.

$$u_n^{m+1} - (1/12 - \alpha/2)\ \delta_x^2\, u_n^{m+1} = u_n^m + (1/12 + \alpha/2)\,\delta_x^2\, u_n^m \tag{35}$$

is called the *Douglas* scheme. It is very important due to the fact that it is exact to order δ_x^4, even though it contains terms only of order δ_x^2.

2.3 Binomial and Trinomial Schemes

The following links may be helpful in appreciating the importance of the Douglas scheme, and its relationship to the explicit schemes that are common to FD models and binomial/trinomial tree models.

(1) When θ = 0 and α = 1/2, our schemes, as noted already, become the same difference rule as in a binomial tree, but on a rectangular grid in standard coordinates.

(2) When we use a Douglas scheme with α = 1/6, we obtain a highly accurate explicit scheme. This is none other than the trinomial tree model, but on a rectangular grid. So the Douglas scheme is the natural implicit form of the trinomial model. We have already seen that this case also corresponds to a special case of a high order explicit scheme based on five points (the pentanomial scheme).

The relationship to standard tree models may be made clearer if we state up front the simplest form of the change of variables used to reduce an option-pricing problem to the diffusion equation. For a problem with a flat term-structure parametrized by a variable K (e.g. strike or barrier) the change of coordinates being used here is, for an underlying S, time variable T, volatility σ,

$$x = \log\left(\frac{S}{K}\right) \tag{36}$$

$$\tau = \frac{\sigma^2 T}{2} \tag{37}$$

so that

$$\Delta S = S\,\sigma\sqrt{\frac{\Delta T}{2\,\alpha}} \tag{38}$$

In these coordinates the relationship between FD schemes with α = 1/2, 1/6 and binomial, trinomial trees becomes clear. To practitioners, we emphasize the following:

***The two-time-level Douglas scheme is the natural implicit generalization of the trinomial tree*.**