Principle of Heun's method: the ODE case

Let us consider an ODE $y' = f$, whose fundamental variable is time, denoted by t. f changes with time but is not necessarily an explicit function of time. Let y^k and f^k be the values of y and f at $t = t^k$ respectively. Heun's method is

$$\begin{cases} \tilde{y}^{k+1} = y^k + \Delta t f^k \\ y^{k+1}_{Heun} = y^k + \frac{\Delta t}{2}(f^k + \tilde{f}^{k+1}) \end{cases} \tag{1}$$

where $\tilde{y}^{k+1}$ is a forward Euler approximation of y^{k+1} and $\tilde{f}^{k+1}$ is the corresponding value of f^{k+1}.

Let us consider the example where $y' = y$. Here f is an explicit function of y, but it is important to realize that in general it is not necessarily so. In such a case we can write

$$\tilde{f}^{k+1} = f(y^k + \Delta t f^k) = y^k + \Delta t y^k \tag{2}$$

Thus, using the second equation of (1)

$$y^{k+1}_{Heun} = y^k + \Delta t y^k + \frac{\Delta t^2}{2} y^k$$

Alternatively, since f is an explicit function only of y, we can take its Taylor expansion with respect to y with an increment $\Delta t y^k$:

$$\tilde{f}^{k+1} = f(y^k + \Delta t f^k) = f(y^k + \Delta t y^k) = f^k + (\Delta t y^k) f^k_y + (\Delta t y^k)^2 f^k_{yy} + O((\Delta t y^k)^3) \tag{3}$$

We know that $f^k = y^k$, $f^k_y = 1$ and $f^k_{yy} = f^k_{yyy} = ... = 0$, so we recover (2)

Let us define the error of the numerical scheme as $\boldsymbol{e} = \boldsymbol{y}_{numerical} - \boldsymbol{y}_{exact}$

The Taylor expansion of y^{k+1}_{exact} is $y^k + \Delta t y'^k + \frac{\Delta t^2}{2} y''^k + \frac{\Delta t^3}{6} y'''^k + O(\Delta t^4)$

For this example, $y'^k = y''^k = y'''^k = y^k$, which means that in this case the Heun scheme is simply the first three terms of the Taylor expansion of the exact value. The said Taylor expansion can be rewritten as

$$y^{k+1}_{exact} = y^k + \Delta t y^k + \frac{\Delta t^2}{2} y^k + \frac{\Delta t^3}{6} y^k + O(\Delta t^4) \tag{4}$$

Ignoring higher order terms, the error is

$$e = -\frac{\Delta t^3}{6} y^k \tag{5}$$

Wrong approach

Since f is a function of time, and Heun's method is used as a time integration scheme in this case, when formulated in the following way

$$\begin{cases} \tilde{y}^{k+1} = y^k + \Delta t f^k \\ y^{k+1}_{Heun} = y^k + \frac{\Delta t}{2}(f^k + f^{k+1}) \end{cases} \tag{6}$$

it is tempting to decide to take the Taylor expansion of f^{k+1} with respect to time:

$$f^{k+1} = f^k + \Delta t {f'}^k + \frac{\Delta t^2}{2} {f''}^k \tag{7}$$

Since we also know $y' = f$, we can then rewrite

$$f^{k+1} = {y'}^k + \Delta t {y''}^k + \frac{\Delta t^2}{2} {y'''}^k \tag{8}$$

and thus

$$y^{k+1}_{Heun} = y^k + \Delta t {y'}^k + \frac{\Delta t^2}{2} {y''}^k + \frac{\Delta t^3}{4} {y'''}^k \tag{9}$$

Using this approach instead of the one outlined earlier, one finds the following deceivingly wrong expression for the error of the scheme applied to simple equation of the previous case:

$$e_{wrong} = \frac{\Delta t^3}{12} y^k \tag{10}$$

This approach is wrong because while f is a function of time, it is not explicitly so, contrary to y. It is only an explicit function of y. Therefore, the Taylor expansion of f should be taken with respect to y and not t.

When dealing with such problems, it is perhaps a good idea to define f^k as the value of f corresponding to the value of y at t^k to avoid the ambiguity, even though there is nothing intrinsically wrong in calling f^k the value of f at t^k.

A PDE case

In a general form, a PDE of time and 1D-space can be written as $\dfrac{\partial y}{\partial t} = f(t, y, y', ..., y_x, y_{xx}, ...)$

For now, let us assume that we are working with a **linear** PDE of the form $y' = f(y_x)$, such as the advection equation. In this case, f is an explicit function of y_x only. As with the ODE case

$$\begin{cases} \tilde{y}^{k+1} = y^k + \Delta t f^k \\ y^{k+1}_{Heun} = y^k + \frac{\Delta t}{2}(f^k + \tilde{f}^{k+1}) \end{cases} \tag{11}$$

where $\tilde{y}^{k+1}$ is a forward Euler approximation of y^{k+1} and $\tilde{f}^{k+1}$ is the corresponding value of f^{k+1}.
Since y^k is continuous in x, the first equation of (11) implies that

$$\tilde{y}_x^{k+1} = \frac{\partial \tilde{y}^{k+1}}{\partial x} = \frac{\partial (y^k + \Delta t f^k)}{\partial x} = y_x^k + \Delta t f_x^k = y_x^k + \Delta t {y'}_x^k \tag{12}$$

Thus

$$\tilde{f}^{k+1} = f(\tilde{y}_x^{k+1}) = f(y_x^k + \Delta t {y'}_x^k) \tag{13}$$

Let us define $Y = y_x$ and $K = \Delta t {y'}_x^k$. Taking a Taylor expansion of $\tilde{f}^{k+1}$

$$\tilde{f}^{k+1} = f^k + K f_Y^k + \frac{K^2}{2} f_{YY}^k + O(K^3) \tag{14}$$

For equations of the form $y' = f(y_{xx})$, such as the diffusion equation, the reasoning is the same, except this time $Y = y_{xx}$ and $K = \Delta t {y'}_{xx}^k$.

Combination with Space discretization

Let e_S^k be the spatial truncation error of a numerical scheme used to approximate a function f by a a function g at time t^k. Let us define e_S as

$$e_S = g - f \tag{15}$$

so as to be **consistent with the convention used for the time error** in previous sections.

When a PDE is solved numerically it is the time derivative of g that is taken, so (15) is rearranged as:

$$g = f + e_S \tag{16}$$

The Heun's method is thus:

$$\begin{cases} \tilde{\tilde{y}}^{k+1} = y^k + \Delta t g^k \\ y_{Heun}^{k+1} = y^k + \frac{\Delta t}{2}(g^k + \tilde{g}^{k+1}) \end{cases} \tag{17}$$

and

$$\tilde{g}^{k+1} = g(\tilde{\tilde{y}}^{k+1}) = g(y^k + \Delta t g^k) = g(y^k + \Delta t f^k + \Delta t e_S) \tag{18}$$

Since e_S is at least of order $O(\Delta x)$, $\Delta t e_S$ is asymptotically small compared to the other terms.

Thus

$$\tilde{g}^{k+1} = g(y^k + \Delta t f^k) = g(\tilde{y}^{k+1}) = \tilde{f}^{k+1} + \tilde{e_S}^{k+1} \tag{19}$$

where $\tilde{y}^{k+1}$ is defined in (11) and $\tilde{e_S}^{k+1} = e_S(\tilde{y}^{k+1})$. Note that since g is a discrete spatial approximation of f and e_S is the associated error, it is correct to write those values as explicit functions of y. However, remember that f is not necessarily an explicit function of y. It is then better to refer to $\tilde{f}^{k+1}$ as **the value of f that corresponds to $\tilde{y}^{k+1}$**.

$$y^{k+1}_{Heun} = y^k + \frac{\Delta t}{2}(f^k + \tilde{f}^{k+1}) + \frac{\Delta t}{2}(e^k_S + \tilde{e}^{k+1}_S) \tag{20}$$

Taking the Taylor expansion $\tilde{e}^{k+1}_S = e^k_S + \Delta t e'^k_S + ...\ e_S$, we can see that since $\tilde{e}^{k+1}_S$ is of order at least $O(\Delta x)$, again the terms that are multiplied by Δt are negligible compared to e^k_S

So in the end

$$y^{k+1}_{Heun} = y^k + \frac{\Delta t}{2}(f^k + \tilde{f}^{k+1}) + \Delta t e^k_S \tag{21}$$

Error due to spatial discretization

The Talyor expansion of y in space at a fixed time t^k in the general case is

$$y^k(x+\Delta x) = y^k + y^k_x \Delta x + \frac{1}{2} y^k_{xx} \Delta x^2 + \frac{1}{6} y^k_{xxx} \Delta x^3 + \frac{1}{24} y^k_{xxxx} \Delta x^4 + O(\Delta x^5) \tag{22}$$

The approximations at $x = x_{i+1}$, $x = x_{i-1}$, and $x = x_{i-2}$ respectively are

$$\begin{aligned}
y^k_{i+1} &= y^k(x+\Delta x) = y^k_i + y^k_{i_x} \Delta x + \frac{1}{2} y^k_{i_{xx}} \Delta x^2 + \frac{1}{6} y^k_{i_{xxx}} \Delta x^3 + \frac{1}{24} y^k_{xxxx} \Delta x^4 + O(\Delta x^5) \\
y^k_{i-1} &= y^k(x-\Delta x) = y^k_i - y^k_{i_x} \Delta x + \frac{1}{2} y^k_{i_{xx}} \Delta x^2 - \frac{1}{6} y^k_{i_{xxx}} \Delta x^3 + \frac{1}{24} y^k_{xxxx} \Delta x^4 + O(\Delta x^5) \\
y^k_{i-2} &= y^k(x-2\Delta x) = y^k_i - 2 y^k_{i_x} \Delta x + 2 y^k_{i_{xx}} \Delta x^2 - \frac{4}{3} y^k_{i_{xxx}} \Delta x^3 + \frac{2}{3} y^k_{xxxx} \Delta x^4 + O(\Delta x^5)
\end{aligned} \tag{23}$$

A second order upwind scheme approximates a first derivative such that:

$$\frac{\partial y}{\partial x}|_{t=t^k} = ay_i^k + by_{i-1}^k + cy_{i-2}^k \tag{24}$$

The solution to the system of equation is $a = \frac{3}{2\Delta x}$, $b = -\frac{2}{\Delta x}$ and $c = \frac{1}{2\Delta x}$

The 3rd order term of $\frac{\partial y}{\partial x}|_{t=t^k}$ using this approximation is thus

$$(-2 \times \frac{-1}{6} + \frac{1}{2} \times \frac{-4}{3})y_{i_{xxx}}^k \frac{\Delta x^3}{\Delta x} = \boldsymbol{-\frac{1}{3} y_{i_{xxx}}^k \Delta x^2} \tag{25}$$

A second order central scheme approximation of a second derivative is

$$\frac{\partial^2 y}{\partial x^2}|_{t=t^k} = ay_{i-1}^k + by_i^k + cy_{i+1}^k \tag{26}$$

The solution to the system of equation is $a = \frac{1}{\Delta x^2}$, $b = -\frac{2}{\Delta x^2}$ and $c = \frac{1}{\Delta x^2}$

The 3rd order term of $\frac{\partial^2 y}{\partial x^2}|_{t=t^k}$ using this approximation is thus

$$(\frac{1}{\Delta x^2}\frac{1}{24} + \frac{1}{\Delta x^2}\frac{1}{24})y_{i_{xxxx}}^k \Delta x^4 = \boldsymbol{\frac{1}{12} y_{i_{xxxx}}^k \Delta x^2} \tag{27}$$

Application to the advection-diffusion equation

We now apply the above results to the advection-diffusion equation, solving with Heun's method in time, a second order upwind scheme for advection and a second order central scheme for diffusion. The equation is of the form $y' = f(y_x) + g(y_{xx})$.

Applying the results from the previous sections, one find that the corresponding Heun's scheme approximation of y^{k+1} can be expressed as:

$$y^{k+1}_{numerical} = y^k + \frac{\Delta t}{2}\Big(f^k + K f^k_Y + \frac{K^2}{2} f^k_{YY} + O(K^3) + h^k + L h^k_Z + \frac{K^2}{2} h^k_{ZZ} + O(L^3)\Big) + \Delta t(e^k_{f_S} + e^k_{h_S}) \tag{28}$$

where $Y = y_x$, $K = \Delta t {y'}^k_x$ and $Z = y_{xx}$, $L = \Delta t {y'}^k_{xx}$, and $e^k_{f_S}$ and $e^k_{h_S}$ are the spatial errors due to f and h respectively.

In our case, $f = -Uy_x$ and $h = \nu y_{xx}$ where U and ν are constants. Thus, $f_Y = -U$ and $h_Z = \nu$, and higher order derivatives are all 0, and

$$y^{k+1}_{numerical} = y^k + \frac{\Delta t}{2}\Big(f^k - U\Delta t {y'}^k_x + h^k + \nu \Delta t {y'}^k_{xx}\Big) + \Delta t(e^k_{f_S} + e^k_{h_S}) \tag{29}$$

and remembering that

$$\begin{cases} {y'}^k = f^k + h^k \\ {y''}^k = -U{y'}^k_x + \nu {y'}^k_{xx} \\ e^k_{f_S} = \frac{U}{3} y^k_{i_{xxx}} \Delta x^2 \\ e^k_{h_S} = \frac{\nu}{12} y^k_{i_{xxxx}} \Delta x^2 \end{cases} \tag{30}$$

we obtain

$$y^{k+1}_{numerical} = y^k + \frac{\Delta t}{2}(2{y'}^k + \Delta t {y''}^k) + \Delta t(\frac{U}{3} y^k_{i_{xxx}} \Delta x^2 + \frac{\nu}{12} y^k_{i_{xxxx}} \Delta x^2) \tag{31}$$

Subtracting the Taylor expansion of y^{k+1} with respect to time, one obtains that the total local truncation error is

$$\Delta t(\frac{U}{3} y^k_{i_{xxx}} + \frac{\nu}{12} y^k_{i_{xxxx}})\Delta x^2 - \frac{\Delta t^3}{6} {y'''}^k_i \tag{32}$$

Numerical results

Very good agreement is found between the analytical derived error in (32) and the numerically computed error. One notices that while it is possible to observe second order convergence in space, it is not possible to observe it in time. This behavior can in fact be explained mathematically.

Let us consider the case of pure advection, i.e. $\nu = 0$. Since $y' = -Uy_x$ one can express the third derivative in time as $y''' = -U^3 y_{xxx}$. (**??**) can thus be rewritten as:

$$\text{SPATIAL ERROR} + \text{TIME ERROR} = \frac{U\Delta t}{3} y^k_{i_{xxx}} \Delta x^2 + \frac{(U\Delta t)^3}{6} y^k_{i_{xxx}} \tag{33}$$

For a second order upwind scheme, the CFL condition is *at best* $\frac{U\Delta t}{\Delta x} \leq 2$. Thus, when CFL is satisfied exactly, i.e. $\Delta x = \frac{U\Delta t}{2}$, (33) becomes:

$$\text{SPATIAL ERROR} + \text{TIME ERROR} = \frac{2}{3} y^k_{i_{xxx}} \Delta x^3 + \frac{4}{3} y^k_{i_{xxx}} \Delta x^3 \tag{34}$$

This shows that the temporal error, which is the term on the right, can be at most twice as large as the spatial error. Now, (33) can be rewritten as

$$\text{SPATIAL ERROR} + \text{TIME ERROR} = \left(\frac{U}{3} y^k_{i_{xxx}} \Delta x^2\right)\Delta t + \left(\frac{U^3}{6} y^k_{i_{xxx}}\right)\Delta t^3 \tag{35}$$

$$\text{SPATIAL ERROR} + \text{TIME ERROR} = \alpha\Delta t + \beta\Delta t^3 \tag{36}$$

Let us call Δt_{CFL} the time step value that exactly satisfies CFL. We know that for this v value of Δt, the time error is twice as large as the space error, so we can express α in terms of β and Δt_{CFL}

$$\alpha = \frac{\beta}{2} \Delta t^2_{CFL} \tag{37}$$

Plugging (37) into (36), we obtain

$$\text{SPATIAL ERROR} + \text{TIME ERROR} = \beta\Delta t\left(\frac{\Delta t^2_{CFL}}{2} + \Delta t^2\right) \tag{38}$$

One can see that the temporal error decreases two orders faster than the spatial error. Since it can start at most twice as large and $\Delta t \leq \Delta t_0$, one cannot observe convergence in time close to second order without violating CFL. It is important to note that this result holds true regardless of the shape of the analytical solution.

Trapezoidal rule

If we wish to use an numerical scheme to solve a PDE of the form $\frac{\partial y}{\partial t} = f$, and we use a discrete approximation g of f, such that $g = f + e_S$ where e_S is the spatial trunctation error, we can derive the total local truncation error when integrating from t^k to t^{k+1} as follows:

$$\int_{t^k}^{t^{k+1}} \frac{\partial y}{\partial t} dt = \int_{t^k}^{t^{k+1}} g(t, x_i) dt \tag{39}$$

$$y^{k+1} - y^k = \int_{t^k}^{t^{k+1}} (f(t, x_i) + e_S(t, x_i)) dt \tag{40}$$

$$y^{k+1} = y^k + \int_{t^k}^{t^{k+1}} f(t, x_i) dt + \int_{t^k}^{t^{k+1}} e_S(t, x_i) dt \tag{41}$$

The Trapezoidal rule is defined as follows:

$$y^{k+1} = y^k + \Delta t \frac{f(t^k, x_i) + f(t^{k+1}, x_i)}{2} \tag{42}$$

If the Trapezoidal rule is used, we can express the first integral as

$$\int_{t^k}^{t^{k+1}} f(t, x_i) dt = \Delta t \frac{f(t^k, x_i) + f(t^{k+1}, x_i)}{2} - \int_{t^k}^{t^{k+1}} (t - \frac{\Delta t}{2}) f'(t, x_i) dt \tag{43}$$

See Cruz-Uribe and Neugebauer (2003) for details.

In the end

$$y^{k+1} = y^k + \Delta t \frac{f(t^k, x_i) + f(t^{k+1}, x_i)}{2} - \int_{t^k}^{t^{k+1}} (t - \frac{\Delta t}{2}) f'(t, x_i) dt + \int_{t^k}^{t^{k+1}} e_S(t, x_i) dt \tag{44}$$

We obtain the total truncation error by subtracting (44) from (41):

$$\boldsymbol{\int_{t^k}^{t^k + \Delta t} (t - \frac{\Delta t}{2}) f'(t, x_i) dt - \int_{t^k}^{t^k + \Delta t} e_S(t, x_i) dt} \tag{45}$$

Note that while the spatial error is approximate, the temporal error is exact. Numerical results are in agreement with the analytically derived result.

Second order diagonally implicit Runge-Kutta scheme

Again, let us assume we are working with a linear PDE of the form $y' = f(Y)$, where Y is the nth derivative of y.

$$\begin{cases} y_\alpha = y^k + \alpha \Delta t f(y_\alpha) \\ y_D^{k+1} = y^k + \beta \Delta t f(y_\alpha) + \alpha \Delta t f(y_D^{k+1}) \end{cases} \tag{46}$$

For this scheme to be second order, it can be shown that α and β need to satisfy

$$\begin{cases} \alpha + \beta = 1 \\ \alpha\beta + \alpha = \frac{1}{2} \end{cases} \tag{47}$$

See original paper on DIRK

$$\begin{aligned} f(y_\alpha) &= f\Big(y^k + \alpha \Delta t f(y_\alpha)\Big) \\ &= f\Big(y^k + \alpha \Delta t y'_\alpha\Big) \\ &= f\Big(y^k + \alpha \Delta t (y'^k + \alpha \Delta t f(y'_\alpha))\Big) \\ &= f\Big(y^k + \alpha \Delta t y'^k + \alpha^2 \Delta t^2 y''^k\Big) + O(\Delta t^3) \\ &= y'^k + (\alpha \Delta t y'^k + \alpha^2 \Delta t^2 y''^k) f_Y(y^k) + O(\Delta t^3) \end{aligned} \tag{48}$$

Then

$$\begin{aligned} f(y_D) &= f\Big(y^k + \alpha \Delta t f(y_D) + \beta \Delta t f(y_\alpha)\Big) \\ &= f\Big(y^k + \alpha \Delta t y'_D + \beta \Delta t y'_\alpha\Big) \\ &= f\Big(y^k + \alpha \Delta t\big(y'^k + \alpha \Delta t f(y'_D) + \beta \Delta t f(y'_\alpha)\big) + \beta \Delta t\big(y'^k + \alpha \Delta t f(y'_\alpha)\big)\Big) \\ &= f\Big(y^k + \alpha \Delta t\big(y'^k + \alpha \Delta t y''^k + \beta \Delta t y''^k\big) + \beta \Delta t\big(y'^k + \alpha \Delta t y''^k\big)\Big) + O(\Delta t^3) \\ &= f\Big(y^k + \big(\alpha \Delta t y'^k + \alpha^2 \Delta t^2 y''^k + \alpha\beta \Delta t^2 y''^k\big) + \big(\beta \Delta t y'^k + \alpha\beta \Delta t^2 y''^k\big)\Big) + O(\Delta t^3) \\ &= f\Big(y^k + (\alpha + \beta) \Delta t y'^k + (\alpha^2 + 2\alpha\beta) \Delta t^2 y''^k\Big) + O(\Delta t^3) \\ &= y'^k + \Big((\alpha + \beta) \Delta t y'^k + (\alpha^2 + 2\alpha\beta) \Delta t^2 y''^k\Big) f_Y(y^k) + O(\Delta t^3) \end{aligned} \tag{49}$$

Plugging the two equations in and using the conditions on alpha and beta

$$y_{DIRK}^{k+1} = y^k + \Delta t {y'}^k + \frac{\Delta t^2}{2} {y'}^k f_y(y^k) + (3\alpha^2 - 2\alpha^3) \Delta t^3 {y''}^k f_y(y^k) + O(\Delta t^4) \tag{50}$$

Using a similar reasoning as for the Heun scheme, we can find that the error for the advection-diffusion equation is

$$\Delta t\Big(\frac{U}{3}y^k_{i_{xxx}} + \frac{\nu}{12}y^k_{i_{xxxx}}\Big)\Delta x^2 + \Big(3\alpha^2 - 2\alpha^3 - \frac{1}{6}\Big)\Delta t^3 y_i'''^k \tag{51}$$