Numerical analysis: Week 8: ODEs, one-step methods

Dr. Dmitry Batenkov

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Task: solve the initial value problem

$$\begin{aligned} y' &= f(x,y) \\ y(x_0) &= y_0 \end{aligned} \tag{1}$$

1. Vast majority of interesting cases has no closed-form solution, so need to resort to numerical methods.
2. Will compute approximation to the solution on the grid of step size $h \ll 1$:

$$\begin{aligned} x_n &= x_0 + nh, \quad n = 0, 1, \dots, \\ y_n &\approx y(x_n) \end{aligned}$$

3. Euler's scheme:

$$\begin{aligned} y'(x_n) &\approx \frac{y(x_n+h) - y(x_n)}{h} \\ \frac{y(x_n+h) - y(x_n)}{h} &\approx f(x_n, y(x_n)) \\ y_{n+1} &= y_n + hf(x_n, y_n) \end{aligned}$$

4. Vector field picture intuition: see figure.
5. Example: $f(x,y) = Ry$ with $x_0 = 0$, $y_0 = 2$
   (a) Exact solution: $y = 2e^{Rx}$
   (b) Compute: $y_n = 2(1+Rh)^n$
   (c) Check: take any x, put $nh = x = x_n$, compare as $h \to 0$.
6. Error analysis.

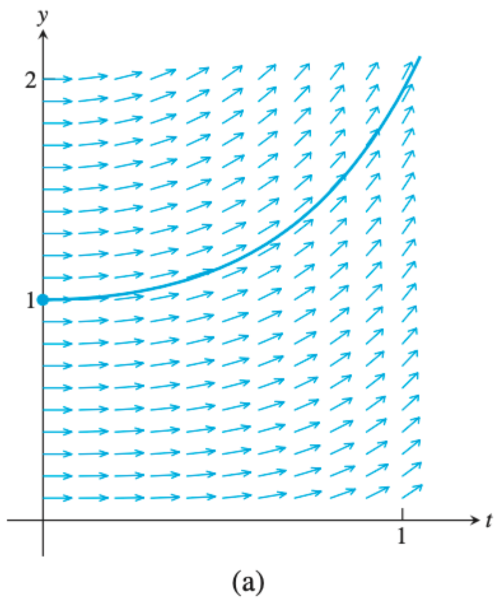

Figure 1: IVP solution, approximation and the slope field

(a) Taylor series for $h > 0$

$$
\begin{aligned}
y(x_{n+1}) &= y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(\xi_n) \\
&= y(x_n) + hf(x_n, y(x_n)) \\
&\quad + \underbrace{\frac{h^2}{2}y''(\xi_n)}_{\text{truncation error=local discretization error after one step of Euler}} \\
e_{n+1} &= y(x_{n+1}) - y_{n+1} \\
&= e_n + hf(x_n, y(x_n)) - hf(x_n, y_n) + \frac{h^2}{2}y''(\xi_n) \\
|e_{n+1}| &\leq |e_n| + h\,|f(x_n, y(x_n)) - f(x_n, y_n)| + \frac{h^2}{2}\,|y''(\xi_n)| \\
\text{mean value thm.} &\leq |e_n| + h\,|f_y(x_n, \eta_n)|\,|y(x_n) - y_n| + \frac{h^2}{2}\,|y''(\xi_n)| \\
&= |e_n|\,(1 + h\,|f_y(x_n, \eta_n)|) + \frac{h^2}{2}\,|y''(\xi_n)|\,, \quad \eta_n \text{between } y_n, y(x_n)
\end{aligned}
$$

(b) suppose the exact solution is C^2 in $[a, b]$ with $|y''| \leq Y$, f is C^1 (in both variables) in a sufficiently large rectangle R around (x_0, y_0), with $|f_y| \le M$ in R. Then

$$|e_{n+1}| \le |e_n| \underbrace{(1+hM)}_{S} + \underbrace{\frac{h^2 Y}{2}}_{Q}, \; e_0 = 0$$

$$\begin{aligned} |e_1| &\le Q \\ |e_2| &\le Q(1+S) \\ |e_3| &\le Q(1+S)S + Q = Q\left(1+S+S^2\right) \\ &\dots \\ |e_n| &\le Q\left(1+S+S^2+\dots+S^{n-1}\right) = Q\frac{S^n-1}{S-1} = \frac{hY}{2M}\left\{(1+hM)^n - 1\right\} \end{aligned}$$

(c) Taylor series for exp:

$$\begin{aligned} e^{hM} &= 1 + hM + \frac{(hM)^2}{2} e^{\zeta} \\ 1 + hM &\le e^{hM} \end{aligned}$$

(d) Substitute:

$$|e_n| \le \frac{hY}{2M}\left\{e^{hMn} - 1\right\} = \frac{hY}{2M}\left(e^{M(x-x_0)} - 1\right).$$

(e) We have proved

Theorem 1. *Suppose the exact solution to (1) is C^2 in $[a,b]$ with $|y''| \le Y$, f is C^1 (in both variables) in a sufficiently large rectangle R around (x_0, y_0), with $|f_y| \le M$ in R. Then for each $x = x_n \in [a,b]$*

$$|e_n| = |y(x_n) - y_n| \le \frac{hY}{2M}\left(e^{M(x_n - x_0)} - 1\right).$$

7. Order of convergence: the scheme is of order p if $\exists K > 0$ s.t. $|e_n| \le Kh^p$. **Euler's scheme is of 1st order.** Compare with local discretization error which is of second order. This is a general feature (as in integration rules), as we are accumulating errors in $n = \frac{x - x_0}{h}$ steps.

8. Example: $y' = -2y, y(0) = 3$. $|e_n| \le \dots \le 20h$.

9. Taylor series method:

$$\begin{aligned} y(x_{n+1}) =& y(x_n) + hy'(x_n) + \frac{h^2}{2}y''(x_n) + \frac{h^3}{3!}y'''(x_n) + \dots + \\ &+ \frac{h^m}{m!}y^{(m)}(x_n) + \frac{h^{m+1}}{(m+1)!}y^{(m+1)}(\xi_n) \end{aligned}$$

(a) $m = 1$ and putting $y'(x_n) = f(x_n, y_n)$ gives Euler's method

(b) $m=2$: need to approximate $y''(x_n)$:

$$y''(x) = f_x(x,y) + f_y(x,y)\underbrace{y'(x)}_{=f(x,y)} = f_x + f_y f$$

$$y_{n+1} = y_n + hf(x_n,y_n) + \frac{h^2}{2}\{f_x(x_n,y_n) + f_y(x_n,y_n)f(x_n,y_n)\}$$

(c) $m=3$: working in the same way, we get

$$\begin{aligned} y_{n+1} =& y_n + hf(x_n,y_n) + \frac{h^2}{2}[f_x(x_n,y_n) + f(x_n,y_n)f_y(x_n,y_n)] + \\ &+ \frac{h^3}{3!}\left[f_{xx} + 2ff_{xy} + f^2 f_{yy} + f_x f_y + f(f_y)^2\right]\Big|_{(x_n,y_n)} \end{aligned} \tag{2}$$

10. Euler's scheme is of low accuracy, and Taylor method is not convenient. We will see methods of degree 2 and 4 which are also easy to implement.

11. <u>Runge-Kutta of order 2</u>

(a) Main idea: find constants α, β, a, b in the scheme

$$\begin{cases} y_{n+1} = y_n + ak_1 + bk_2 \\ k_1 = hf(x_n,y_n) \\ k_2 = hf(x_n + \alpha h, y_n + \beta k_1) \end{cases} \tag{3}$$

to achieve maximal order of convergence.

(b) Taylor expanding $f(x_n + \alpha h, y_n + \beta k_1)$ around (x_n,y_n) (in 2D) gives (all evaluations are at (x_n,y_n))

$$\begin{aligned} f(x_n + \alpha h, y_n + \beta h f(x_n,y_n)) &= f + \alpha h f_x + \beta h f f_y \\ &+ \frac{1}{2}\left[\alpha^2 h^2 f_{xx} + 2\alpha\beta h^2 f f_{xy} + \beta^2 h^2 f^2 f_{yy}\right] + O\left(h^3\right) \end{aligned} \tag{4}$$

(c) Taylor expansion up to order 3 gives (2) with a remainder $\frac{h^4}{4!}y^{(4)}(\xi_n)$. Substituting (3) and (4) gives

$$\begin{aligned} y_{n+1} &= y_n + ahf + bh\{f + \alpha h f_x + \beta h f f_y \\ &+ \frac{1}{2}\left[\alpha^2 h^2 f_{xx} + 2\alpha\beta h^2 f f_{xy} + \beta^2 h^2 f^2 f_{yy}\right]\} \\ &+ O\left(h^4\right) \\ &= y_n + hf + \frac{h^2}{2}[f_x + ff_y] + \frac{h^3}{3!}\left[f_{xx} + 2ff_{xy} + f^2 f_{yy} + f_x f_y + f(f_y)^2\right] \end{aligned}$$

(d) Comparing coefficients of $h^0, \ldots, h^3$ gives

- $1: \quad y_n = y_n$
- $h: \quad (a+b)f = f$
- $h^2: \quad b\alpha f_x + b\beta f f_y = \frac{1}{2}\left[f_x + f f_y\right]$
- $h^3: \quad b\frac{1}{2}\left[\alpha^2 f_{xx} + 2\alpha\beta f f_{xy} + \beta^2 f^2 f_{yy}\right] = \frac{1}{3!}\left[f_{xx} + 2f f_{xy} + f^2 f_{yy} + f_x f_y + f\left(f_y\right)^2\right]$

(e) 2nd and 3rd equations can be satisfied for all f if $a+b=1, \quad b\alpha = b\beta = \frac{1}{2}$, but the last equation cannot be in general true for arbitrary f.

(f) One choice is $a = b = \frac{1}{2}$ and $\alpha = \beta = 1$. We get **Modified Euler Method/Heun method/Explicit Trapezoid Method**

$$\begin{cases} y_{n+1} = y_n + \frac{1}{2}\left[k_1 + k_2\right] \\ k_1 = hf\left(x_n, y_n\right) \\ k_2 = hf\left(x_n + h, y_n + k_1\right) \end{cases} \tag{5}$$

(g) Equivalence of Explicit Trapezoidal Method and the composite Trapezoidal rule for integration of $y' = f(x), y(x_0) = 0$ (so f is independent of y)

(h) Example: one step of (5) for $y' = -\frac{y}{x}, y'(1) = 1$ with $(x_0, y_0) = (1, 1)$

$$\begin{aligned} y_1 &= y_0 + \tfrac{1}{2}\left[k_1 + k_2\right] = y_0 + \tfrac{1}{2}\left[hf\left(x_0, y_0\right) + hf\left(x_0 + h, y_0 + hf\left(x_0, y_0\right)\right)\right] \\ &= y_0 + \tfrac{h}{2}\left[\frac{-y_0}{x_0} + \frac{-\left(y_0 + h\left(\frac{-y_0}{x_0}\right)\right)}{x_0 + h}\right] = y_0 + \tfrac{h}{2}\left[\frac{-y_0(x_0+h)}{x_0(x_0+h)} + \frac{-(x_0 y_0 - h y_0)}{x_0(x_0+h)}\right] = \\ &= y_0 + \tfrac{h}{2}\left[\frac{-2x_0 y_0}{x_0(x_0+h)}\right] = y_0\left\{1 + \tfrac{h}{2}\left[\frac{-2}{1+h}\right]\right\} = y_0\left(1 - \frac{h}{1+h}\right) = \frac{y_0}{1+h} = \frac{1}{1+h} \end{aligned}$$

The exact solution is $y = \frac{1}{x}$, so at $x_1 = 1+h$ the approximation is exact. However, this is not true for the next steps $x_2 = 1 + 2h, x_3 = 1 + 3h$ etc.

(i) Another popular choice is $a = 0, b = 1$ and $\alpha = \beta = \frac{1}{2}$, giving the **Midpoint method**

$$\begin{cases} y_{n+1} = y_n + k_2 \\ k_1 = hf\left(x_n, y_n\right) \\ k_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right) \end{cases}$$

(j) Interpretation of flows and vector fields: see figure.

12. Runge-Kutta of order 4. Same type of computation (although more lengthy) gives the 4th order scheme

$$\begin{cases} y_{n+1} = y_n + \frac{1}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right] \\ k_1 = hf\left(x_n, y_n\right) \\ k_2 = hf\left(x_n + h/2, y_n + k_1/2\right) \\ k_3 = hf\left(x_n + h/2, y_n + k_2/2\right) \\ k_4 = hf\left(x_n + h, y_n + k_3\right) \end{cases}$$

which has truncation error $O\left(h^5\right)$ and the global error $O\left(h^4\right)$. k_1/h is the initial slope, k_2/h is the midpoint slope, k_3/h is the improved midpoint slope, and k_4/h is the approximate slope at the right endpoint.

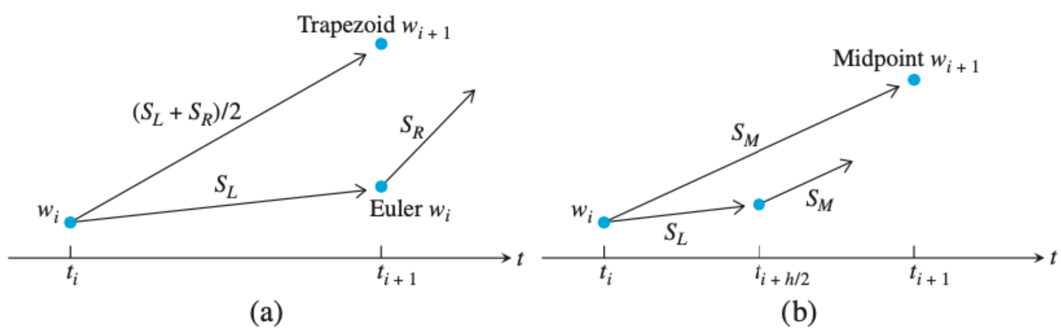

Figure 6.14 Schematic view of two members of the RK2 family. (a) The Trapezoid Method uses an average from the left and right endpoints to traverse the interval. (b) The Midpoint Method uses a slope from the interval midpoint.

Figure 2: RK family of order 2