Initial value problems for ordinary differential equations

Xiaojing Ye, Math & Stat, Georgia State University

Spring 2019

IVP of ODE

We study numerical solution for initial value problem (IVP) of ordinary differential equations (ODE).

- A basic IVP:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t, y), \quad \text{for } a \le t \le b$$

  with initial value $y(a) = \alpha$.

Remark

- *f is given and called the defining function of IVP.*
- *α is given and called the initial value.*
- *$y(t)$ is called the solution of the IVP if*
  - $y(a) = \alpha$;
  - $y'(t) = f(t, y(t))$ *for all* $t \in [a, b]$.

IVP of ODE

Example

The following is a basic IVP:

$$y' = y - t^2 + 1, \quad t \in [0,2], \ \textit{and} \ y(0) = 0.5$$

- The defining function is $f(t, y) = y - t^2 + 1$.
- Initial value is $y(0) = 0.5$.
- The solution is $y(t) = (t+1)^2 - \frac{e^t}{2}$ because:
  - $y(0) = (0+1)^2 - \frac{e^0}{2} = 1 - \frac{1}{2} = \frac{1}{2}$;
  - We can check that $y'(t) = f(t, y(t))$:

$$y'(t) = 2(t+1) - \frac{e^t}{2}$$

$$f(t, y(t)) = y(t) - t^2 + 1 = (t+1)^2 - \frac{e^t}{2} - t^2 + 1 = 2(t+1) - \frac{e^t}{2}$$

IVP of ODE (cont.)

More general or complex cases:

- IVP of ODE system:

$$\begin{cases} \frac{\mathrm{d}y_1}{\mathrm{d}t} = f_1(t, y_1, y_2, \dots, y_n) \\ \frac{\mathrm{d}y_2}{\mathrm{d}t} = f_2(t, y_1, y_2, \dots, y_n) \\ \qquad \vdots \\ \frac{\mathrm{d}y_n}{\mathrm{d}t} = f_n(t, y_1, y_2, \dots, y_n) \end{cases} \quad \text{for } a \le t \le b$$

  with initial value $y_1(a) = \alpha_1, \dots, y_n(a) = \alpha_n$.

- High-order ODE:

$$y^{(n)} = f(t, y, y', \dots, y^{(n-1)}) \quad \text{for } a \le t \le b$$

  with initial value $y(a) = \alpha_1, y'(a) = \alpha_2, \dots, y^{(n-1)}(a) = \alpha_n$.

Why numerical solutions for IVP?

- ODEs have extensive applications in real-world: science, engineering, economics, finance, public health, etc.
- Analytic solution? Not with almost all ODEs.
- Fast improvement of computers.

Some basics about IVP

Definition (Lipschitz functions)

*A function $f(t, y)$ defined on $D = \{(t, y) : t \in \mathbb{R}_+, y \in \mathbb{R}\}$ is called **Lipschitz with respect to** y if there exists a constant $L > 0$*

$$|f(t, y_1) - f(t, y_2)| \le L|y_1 - y_2|$$

for all $t \in \mathbb{R}_+$, and $y_1, y_2 \in \mathbb{R}$.

Remark

We also call f is Lipschitz with respect to y with constant L, or simply f is L-Lipschitz with respect to y.

Some basics about IVP

Example

Function $f(t, y) = t|y|$ is Lipschitz with respect to y on the set $D := \{(t, y)|t \in [1, 2], y \in [-3, 4]\}$.

Solution: *For any $t \in [1, 2]$ and $y_1, y_2 \in [-3, 4]$, we have*

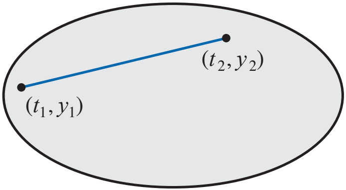
$$|f(t, y_1) - f(t, y_2)| = \big|t|y_1| - t|y_2|\big| \le t|y_1 - y_2| \le 2|y_1 - y_2|.$$

So $f(t, y) = t|y|$ is Lipschitz with respect to y with constant $L = 2$.

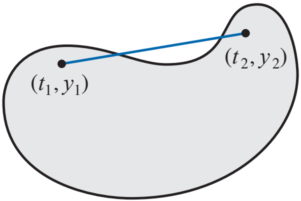
Some basics about IVP

Definition (Convex sets)

A set $D \in \mathbb{R}^2$ is ***convex*** *if whenever $(t_1, y_1), (t_2, y_2) \in D$ there is $(1-\lambda)(t_1, y_1) + \lambda(t_2, y_2) \in D$ for all $\lambda \in [0, 1]$.*



Convex



Not convex

Some basics about IVP

Theorem

If $D \in \mathbb{R}^2$ is convex, and $|\frac{\partial f}{\partial y}(t, y)| \leq L$ for all $(t, y) \in D$, then f is Lipschitz with respect to y with constant L.

Remark

This is a sufficient (but not necessary) condition for f to be Lipschitz with respect to y.

Some basics about IVP

Proof.

For any $(t, y_1), (t, y_2) \in D$, define function g by

$$g(\lambda) = f(t, (1-\lambda)y_1 + \lambda y_2)$$

for $\lambda \in [0, 1]$ (need convexity of D!). Then we have

$$g'(\lambda) = \partial_y f(t, (1-\lambda)y_1 + \lambda y_2) \cdot (y_2 - y_1)$$

So $|g'(\lambda)| \le L|y_2 - y_1|$. Then we have

$$|g(1) - g(0)| = \left| \int_0^1 g'(\lambda)\, \mathrm{d}\lambda \right| \le L|y_2 - y_1| \left| \int_0^1 \mathrm{d}\lambda \right| = L|y_2 - y_1|$$

Note that $g(0) = f(t, y_1)$ and $g(1) = f(t, y_2)$. This completes the proof. $\square$

Some basics about IVP

Theorem

Suppose $D = [a, b] \times \mathbb{R}$, a function f is continuous on D and Lipschitz with respect to y, then the initial value problem $y' = f(t, y)$ for $t \in [a, b]$ with initial value $y(a) = \alpha$ has a unique solution $y(t)$ for $t \in [a, b]$.

Remark

This theorem says that there must be one and only one solution of the IVP, provided that the defining f of the IVP is continuous and Lipschitz with respect to y on D.

Some basics about IVP

Example

Show that $y' = 1 + t\sin(ty)$ *for* $t \in [0, 2]$ *with* $y(0) = 0$ *has a unique solution.*

Solution: First, we know $f(t, y) = 1 + t\sin(ty)$ is continuous on $[0, 2] \times \mathbb{R}$. Second, we can see

$$\left|\frac{\partial f}{\partial y}\right| = \left|t^2\cos(ty)\right| \le |t^2| \le 4$$

So $f(t, y)$ is Lipschitz with respect to y (with constant 4). From theorem above, we know the IVP has a unique solution $y(t)$ on $[0, 2]$.

Some basics about IVP

Theorem (Well-posedness)

An IVP $y' = f(t, y)$ for $t \in [a, b]$ with $y(a) = \alpha$ is called ***well-posed*** *if*

- *It has a unique solution $y(t)$;*
- *There exist $\epsilon_0 > 0$ and $k > 0$, such that $\forall \epsilon \in (0, \epsilon_0)$ and function $\delta(t)$, which is continuous and satisfies $|\delta(t)| < \epsilon$ for all $t \in [a, b]$, the perturbed problem $z' = f(t, z) + \delta(t)$ with initial value $z(a) = \alpha + \delta_0$ (where $|\delta_0| \le \epsilon$) satisfies*

$$|z(t) - y(t)| < k\epsilon, \quad \forall t \in [a, b].$$

Remark

This theorem says that a small perturbation on defining function f by $\delta(t)$ and initial value $y(a)$ by δ_0 will only cause small change to original solution $y(t)$.

Some basics about IVP

Theorem

Let $D = [a, b] \times \mathbb{R}$. If f is continuous on D and Lipschitz with respect to y, then the IVP is well-posed.

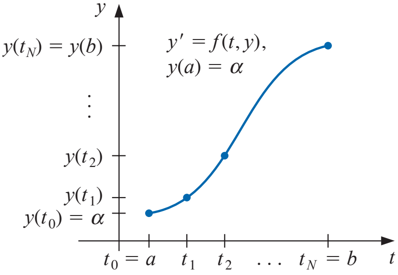
Remark

Again, a sufficient but not necessary condition for well-posedness of IVP.

Euler's method

Given an IVP $y' = f(t, y)$ for $t \in [a, b]$ and $y(a) = \alpha$, we want to compute $y(t)$ on **mesh points** $\{t_0, t_1, \ldots, t_N\}$ on $[a, b]$.

To this end, we partition $[a, b]$ into N equal segments: set $h = \frac{b-a}{N}$, and define $t_i = a + ih$ for $i = 0, 1, \ldots, N$. Here h is called the **step size**.



Euler's method

From Taylor's theorem, we have

$$y(t_{i+1}) = y(t_i) + y'(t_i)(t_{i+1} - t_i) + \frac{1}{2}y''(\xi_i)(t_{i+1} - t_i)^2$$

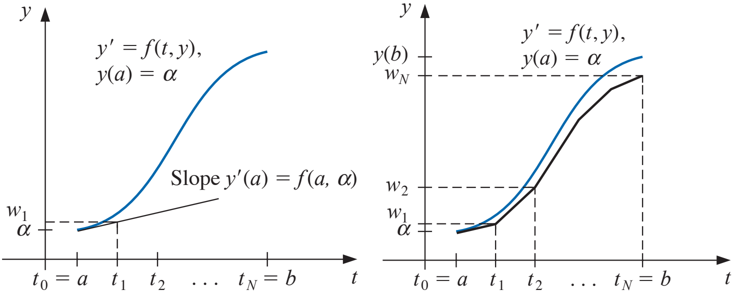
for some $\xi_i \in (t_i, t_{i+1})$. Note that $t_{i+1} - t_i = h$ and $y'(t_i) = f(t_i, y(t_i))$, we get

$$y(t_{i+1}) \approx y(t_i) + hf(t, y(t_i))$$

Denote $w_i = y(t_i)$ for all $i = 0, 1, \dots, N$, we get the **Euler's method**:

$$\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + hf(t_i, w_i), \quad i = 0, 1, \dots, N-1 \end{cases}$$

Euler's method



Euler's method

Example

Use Euler's method with $h = 0.5$ for IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ with initial value $y(0) = 0.5$.

Solution: We follow Euler's method step-by-step:

$$
\begin{aligned}
t_0 = 0: &\quad w_0 = y(0) = 0.5 \\
t_1 = 0.5: &\quad w_1 = w_0 + hf(t_0, w_0) = 0.5 + 0.5 \times (0.5 - 0^2 + 1) = 1.25 \\
t_2 = 1.0: &\quad w_2 = w_1 + hf(t_1, w_1) = 1.25 + 0.5 \times (1.25 - 0.5^2 + 1) = 2.25 \\
t_3 = 1.5: &\quad w_3 = w_2 + hf(t_2, w_2) = 2.25 + 0.5 \times (2.25 - 1^2 + 1) = 3.375 \\
t_4 = 2.0: &\quad w_4 = w_3 + hf(t_3, w_3) = 3.375 + 0.5 \times (3.375 - 1.5^2 + 1) = 4.437
\end{aligned}
$$

Error bound of Euler's method

Theorem

Suppose $f(t, y)$ in an IVP is continuous on $D = [a, b] \times \mathbb{R}$ and Lipschitz with respect to y with constant L. If $\exists M > 0$ such that $|y''(t)| \le M$ ($y(t)$ is the unique solution of the IVP), then for all $i = 0, 1, \dots, N$ there is

$$\left| y(t_i) - w_i \right| \le \frac{hM}{2L} \left(e^{L(t_i - a)} - 1 \right)$$

Remark

- *Numerical error depends on h (also called $O(h)$ error).*
- *Also depends on M, L of f.*
- *Error increases for larger t_i.*

Error bound of Euler's method

Proof. Taking the difference of

$$
\begin{aligned}
y(t_{i+1}) &= y(t_i) + hf(t_i, y_i) + \frac{1}{2}y''(\xi_i)(t_{i+1} - t_i)^2 \\
w_{i+1} &= w_i + hf(t_i, w_i)
\end{aligned}
$$

we get

$$
\begin{aligned}
|y(t_{i+1}) - w_{i+1}| &\le |y(t_i) - w_i| + h|f(t_i, y_i) - f(t_i, w_i)| + \frac{Mh^2}{2} \\
&\le |y(t_i) - w_i| + hL|y_i - w_i| + \frac{Mh^2}{2} \\
&= (1 + hL)|y_i - w_i| + \frac{Mh^2}{2}
\end{aligned}
$$

Error bound of Euler's method

Proof (cont).
Denote $d_i = |y(t_i) - w_i|$, then we have

$$d_{i+1} \le (1 + hL)d_i + \frac{Mh^2}{2} = (1 + hL)\left(d_i + \frac{hM}{2L}\right) - \frac{hM}{2L}$$

for all $i = 0, 1, \ldots, N - 1$. So we obtain

$$\begin{aligned} d_{i+1} + \frac{hM}{2L} &\le (1 + hL)\left(d_i + \frac{hM}{2L}\right) \\ &\le (1 + hL)^2\left(d_{i-1} + \frac{hM}{2L}\right) \\ &\le \cdots \\ &\le (1 + hL)^{i+1}\left(d_0 + \frac{hM}{2L}\right) \end{aligned}$$

and hence $d_i \le (1 + hL)^i \cdot \frac{hM}{2L} - \frac{hM}{2L}$ (since $d_0 = 0$).

Error bound of Euler's method

Proof (cont).
Note that $1 + x \le e^x$ for all $x > -1$, and hence $(1 + x)^a \le e^{ax}$ if $a > 0$.
Based on this, we know $(1 + hL)^i \le e^{ihL} = e^{L(t_i - a)}$ since $ih = t_i - a$. Therefore we get

$$d_i \le e^{L(t_i - a)} \cdot \frac{hM}{2L} - \frac{hM}{2L} = \frac{hM}{2L}(e^{L(t_i - a)} - 1)$$

This completes the proof.

Error bound of Euler's method

Example

Estimate the error of Euler's method with $h = 0.2$ for IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ with initial value $y(0) = 0.5$.

Solution: We first note that $\frac{\partial f}{\partial y} = 1$, so f is Lipschitz with respect to y with constant $L = 1$. The IVP has solution $y(t) = (t-1)^2 - \frac{e^t}{2}$ so $|y''(t)| = |\frac{e^t}{2} - 2| \le \frac{e^2}{2} - 2 =: M$. By theorem above, the error of Euler's method is

$$\left|y(t_i) - w_i\right| \le \frac{hM}{2L}\left(e^{L(t_i - a)} - 1\right) = \frac{0.2(0.5e^2 - 2)}{2}\left(e^{t_i} - 1\right)$$

Error bound of Euler's method

Example

Estimate the error of Euler's method with $h = 0.2$ for IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ with initial value $y(0) = 0.5$.

Solution: (cont)

t_i	w_i	$y_i = y(t_i)$	$\lvert y_i - w_i \rvert$
0.0	0.5000000	0.5000000	0.0000000
0.2	0.8000000	0.8292986	0.0292986
0.4	1.1520000	1.2140877	0.0620877
0.6	1.5504000	1.6489406	0.0985406
0.8	1.9884800	2.1272295	0.1387495
1.0	2.4581760	2.6408591	0.1826831
1.2	2.9498112	3.1799415	0.2301303
1.4	3.4517734	3.7324000	0.2806266
1.6	3.9501281	4.2834838	0.3333557
1.8	4.4281538	4.8151763	0.3870225
2.0	4.8657845	5.3054720	0.4396874

Round-off error of Euler's method

Due to round-off errors in computer, we instead obtain

$$\begin{cases} u_0 = \alpha + \delta_0 \\ u_{i+1} = u_i + hf(t_i, u_i) + \delta_i, \quad i = 0, 1, \dots, N-1 \end{cases}$$

Suppose $\exists \delta > 0$ such that $|\delta_i| \le \delta$ for all i, then we can show

$$\left|y(t_i) - u_i\right| \le \frac{1}{L}\left(\frac{hM}{2} + \frac{\delta}{h}\right)\left(e^{L(t_i - a)} - 1\right) + \delta e^{L(t_i - a)}.$$

Note that $\frac{hM}{2} + \frac{\delta}{h}$ does not approach 0 as $h \to 0$. $\frac{hM}{2} + \frac{\delta}{h}$ reaches minimum at $h = \sqrt{\frac{2\delta}{M}}$ (often much smaller than what we choose in practice).

Higher-order Taylor's method

Definition (Local truncation error)

We call the difference method

$$\begin{cases} w_0 = \alpha + \delta_0 \\ w_{i+1} = w_i + h\phi(t_i, w_i), \quad i = 0, 1, \dots, N-1 \end{cases}$$

to have ***local truncation error***

$$\tau_{i+1}(h) = \frac{y_{i+1} - (y_i + h\phi(t_i, y_i))}{h}$$

where $y_i := y(t_i)$.

Example

Euler's method has local truncation error

$$\tau_{i+1}(h) = \frac{y_{i+1} - (y_i + hf(t_i, y_i))}{h} = \frac{y_{i+1} - y_i}{h} - f(t_i, y_i)$$

Higher-order Taylor's method

Note that Euler's method has local truncation error $\tau_{i+1}(h) = \frac{y_{i+1}-y_i}{h} - f(t_i, y_i) = \frac{hy''(\xi_i)}{2}$ for some $\xi_i \in (t_i, t_{i+1})$. If $|y''| \le M$ we know $|\tau_{i+1}(h)| \le \frac{hM}{2} = O(h)$.

Question: What if we use higher-order Taylor's approximation?

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \cdots + \frac{h^n}{n!}y^{(n)}(t_i) + R$$

where $R = \frac{h^{n+1}}{(n+1)!}y^{(n+1)}(\xi_i)$ for some $\xi_i \in (t_i, t_{i+1})$.

Higher-order Taylor's method

First note that we can always write $y^{(n)}$ using f:

$$
\begin{aligned}
y'(t) &= f \\
y''(t) &= f' = \partial_t f + (\partial_y f) f \\
y'''(t) &= f'' = \partial_t^2 f + (\partial_t \partial_y f + (\partial_y^2 f) f) f + \partial_y f (\partial_t f + (\partial_y f) f) \\
&\cdots \\
y^{(n)}(t) &= f^{(n-1)} = \cdots
\end{aligned}
$$

albeit it's quickly getting very complicated.

Higher-order Taylor's method

Now substitute them back to high-order Taylor's approximation (ignore residual R)

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \cdots + \frac{h^n}{n!}y^{(n)}(t_i) \\ &= y(t_i) + hf + \frac{h^2}{2}f' + \cdots + \frac{h^n}{n!}f^{(n-1)} \end{aligned}$$

We can get the n**-th order Taylor's method**:

$$\begin{cases} w_0 = \alpha + \delta_0 \\ w_{i+1} = w_i + hT^{(n)}(t_i, w_i), \quad i = 0, 1, \dots, N-1 \end{cases}$$

where

$$T^{(n)}(t_i, w_i) = f(t_i, w_i) + \frac{h}{2}f'(t_i, w_i) + \cdots + \frac{h^{n-1}}{n!}f^{(n-1)}(t_i, w_i)$$

Higher-order Taylor's method

- Euler's method is the first order Taylor's method.
- High-order Taylor's method is more accurate than Euler's method, but at much higher computational cost.
- Together with Hermite interpolating polynomials, it can be used to interpolate values not on mesh points more accurately.

Higher-order Taylor's method

Theorem

If $y(t) \in C^{n+1}[a, b]$, then the n-th order Taylor method has local truncation error $O(h^n)$.

Runge-Kutta (RK) method

Runge-Kutta (RK) method attains high-order local truncation error **without** expensive evaluations of derivatives of f.

Runge-Kutta (RK) method

To derive RK method, first recall Taylor's formula for two variables (t, y):

$$f(t, y) = P_n(t, y) + R_n(t, y)$$

where $\partial_t^{n-k}\partial_y^k f = \frac{\partial^n f(t_0, y_0)}{\partial t^{n-k}\partial y^k}$ and

$$\begin{aligned} P_n(t, y) = {} & f(t_0, y_0) + (\partial_t f \cdot (t - t_0) + \partial_y f \cdot (y - y_0)) \\ & + \frac{1}{2}\left(\partial_t^2 f \cdot (t - t_0)^2 + 2\partial_y \partial_t f \cdot (t - t_0)(y - y_0) + \partial_y^2 f \cdot (y - y_0)^2\right) \\ & + \cdots + \frac{1}{n!}\sum_{k=0}^{n}\binom{n}{k}\partial_t^{n-k}\partial_y^k f \cdot (t - t_0)^{n-k}(y - y_0)^k \end{aligned}$$

$$R_n(t, y) = \frac{1}{(n+1)!}\sum_{k=0}^{n+1}\binom{n+1}{k}\partial_t^{n+1-k}\partial_y^k f(\xi, \mu) \cdot (t - t_0)^{n+1-k}(y - y_0)^k$$

Runge-Kutta (RK) method

The second order Taylor's method uses

$$T^{(2)}(t, y) = f(t, y) + \frac{h}{2} f'(t, y) = f(t, y) + \frac{h}{2}(\partial_t f + \partial_y f \cdot f)$$

to get $O(h^2)$ error.

Suppose we use $af(t + \alpha, y + \beta)$ (with some a, α, β to be determined) to reach the same order of error. To that end, we first have

$$af(t + \alpha, y + \beta) = a\left(f + \partial_t f \cdot \alpha + \partial_y f \cdot \beta + R\right)$$

where $R = \frac{1}{2}(\partial_t^2 f(\xi, \mu) \cdot \alpha^2 + 2\partial_y \partial_t f(\xi, \mu) \cdot \alpha\beta + \partial_y^2 f(\xi, \mu) \cdot \beta^2)$.

Runge-Kutta (RK) method

Suppose we try to match the terms of these two formulas (ignore R):

$$T^{(2)}(t,y) = f + \frac{h}{2}\partial_t f + \frac{hf}{2}\partial_y f$$
$$af(t+\alpha, y+\beta) = af + a\alpha\partial_t f + a\beta\partial_y f$$

then we have

$$a = 1, \quad \alpha = \frac{h}{2}, \quad \beta = \frac{h}{2}f(t,y)$$

So instead of $T^{(2)}(t,y)$, we use

$$af(t+\alpha, y+\beta) = f\left(t + \frac{h}{2}, y + \frac{h}{2}f(t,y)\right)$$

Runge-Kutta (RK) method

Note that R we ignored is

$$R = \frac{1}{2}\left(\partial_t^2 f(\xi,\mu)\cdot\left(\frac{h}{2}\right)^2 + 2\partial_y\partial_t f(\xi,\mu)\cdot\left(\frac{h}{2}\right)^2 f + \partial_y^2 f(\xi,\mu)\cdot\left(\frac{h}{2}\right)^2 f^2\right)$$

which means $R = O(h^2)$.

Also note that

$$R = T^{(2)}(t,y) - f\left(t + \frac{h}{2}, y + \frac{h}{2}f(t,y)\right) = O(h^2)$$

and $T^{(2)}(t,y) = O(h^2)$, we know

$$f\left(t + \frac{h}{2}, y + \frac{h}{2}f(t,y)\right) = O(h^2)$$

Runge-Kutta (RK) method

This is the **RK2 method (Midpoint method)**:

$$\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + h\, f\left(t_i + \dfrac{h}{2}, w_i + \dfrac{h}{2} f(t_i, w_i)\right), \quad i = 0, 1, \dots, N-1. \end{cases}$$

Remark

If we have (t_i, w_i), we only need to evaluate f twice (i.e., compute $k_1 = f(t_i, w_i)$ and $k_2 = f(t_i + \frac{h}{2}, w_i + \frac{h}{2} k_1)$) to get w_{i+1}.

Runge-Kutta (RK) method

We can also consider higher-order RK method by fitting

$$T^{(3)}(t,y) = f(t,y) + \frac{h}{2}f'(t,y) + \frac{h}{6}f''(t,y)$$

with $af(t,y) + bf(t+\alpha, y+\beta)$ (has 4 parameters a, b, α, β).

Unfortunately we can make match to the $\frac{hf''}{6}$ term of $T^{(3)}$, which contains $\frac{h^2}{6}f \cdot (\partial_y f)^2$, by this way But it leaves us open choices if we're OK with $O(h^2)$ error: let $a = b = 1$, $\alpha = h$, $\beta = hf(t,y)$, then we get the **modified Euler's method**:

$$\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + \dfrac{h}{2}\Big(f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))\Big), \; i = 0, 1, \dots, N-1. \end{cases}$$

Also need evaluation of f twice in each step.

Runge-Kutta (RK) method

Example

Use Midpoint method (RK2) and Modified Euler's method with $h = 0.2$ to solve IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ and $y(0) = 0.5$.

Solution:

Apply the main steps in the two methods:

$$\textbf{Midpoint}: \quad w_{i+1} = w_i + h\, f\left(t_i + \frac{h}{2}, w_i + \frac{h}{2} f(t_i, w_i)\right)$$

$$\textbf{Modified Euler's}: \quad w_{i+1} = w_i + \frac{h}{2}\Big(f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))\Big)$$

Runge-Kutta (RK) method

Example

Use Midpoint method (RK2) and Modified Euler's method with $h = 0.2$ to solve IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ and $y(0) = 0.5$.

Solution: (cont)

t_i	$y(t_i)$	Midpoint Method	Error	Modified Euler Method	Error
0.0	0.5000000	0.5000000	0	0.5000000	0
0.2	0.8292986	0.8280000	0.0012986	0.8260000	0.0032986
0.4	1.2140877	1.2113600	0.0027277	1.2069200	0.0071677
0.6	1.6489406	1.6446592	0.0042814	1.6372424	0.0116982
0.8	2.1272295	2.1212842	0.0059453	2.1102357	0.0169938
1.0	2.6408591	2.6331668	0.0076923	2.6176876	0.0231715
1.2	3.1799415	3.1704634	0.0094781	3.1495789	0.0303627
1.4	3.7324000	3.7211654	0.0112346	3.6936862	0.0387138
1.6	4.2834838	4.2706218	0.0128620	4.2350972	0.0483866
1.8	4.8151763	4.8009586	0.0142177	4.7556185	0.0595577
2.0	5.3054720	5.2903695	0.0151025	5.2330546	0.0724173

Midpoint (RK2) method is better than modified Euler's method.

Runge-Kutta (RK) method

We can also consider higher-order RK method by fitting

$$T^{(3)}(t,y) = f(t,y) + \frac{h}{2}f'(t,y) + \frac{h}{6}f''(t,y)$$

with $af(t,y) + bf(t+\alpha_1, y+\delta_1(f(t+\alpha_2, y+\delta_2 f(t,y)))\ )$ (has 6 parameters $a, b, \alpha_1, \alpha_2, \delta_1, \delta_2$) to reach $O(h^3)$ error.

For example, Heun's choice is $a = \frac{1}{4}$, $b = \frac{3}{4}$, $\alpha_1 = \frac{2h}{3}$, $\alpha_2 = \frac{h}{3}$, $\delta_1 = \frac{2h}{3}f$, $\delta_2 = \frac{h}{3}f$.

Nevertheless, methods of order $O(h^3)$ are rarely used in practice.

4-th Order Runge-Kutta (RK4) method

Most commonly used is the **4-th order Runge-Kutta method (RK4)**: start with $w_0 = \alpha$, and iteratively do

$$\begin{cases} k_1 = f(t_i, w_i) \\ k_2 = f(t_i + \frac{h}{2}, w_i + \frac{h}{2}k_1) \\ k_3 = f(t_i + \frac{h}{2}, w_i + \frac{h}{2}k_2) \\ k_4 = f(t_{i+1}, w_i + hk_3) \\ w_{i+1} = w_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \end{cases}$$

Need to evaluate f for 4 times in each step. Reach error $O(h^4)$.

4-th Order Runge-Kutta (RK4) method

Example

Use RK4 (with $h = 0.2$) to solve IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ and $y(0) = 0.5$.

Solution: With $h = 0.2$, we have $N = 10$ and $t_i = 0.2i$ for $i = 0, 1, \dots, 10$. First set $w_0 = 0.5$, then the first iteration is

$$
\begin{aligned}
k_1 &= f(t_0, w_0) = f(0, 0.5) = 0.5 - 0^2 + 1 = 1.5 \\
k_2 &= f(t_0 + \frac{h}{2}, w_0 + \frac{h}{2}k_1) = f(0.1, 0.5 + 0.1 \times 1.5) = 1.64 \\
k_3 &= f(t_0 + \frac{h}{2}, w_0 + \frac{h}{2}k_2) = f(0.1, 0.5 + 0.1 \times 1.64) = 1.654 \\
k_4 &= f(t_1, w_0 + hk_3) = f(0.2, 0.5 + 0.2 \times 1.654) = 1.7908 \\
w_1 &= w_0 + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.8292933
\end{aligned}
$$

So w_1 is our RK4 approximation of $y(t_1) = y(0.2)$.

4-th Order Runge-Kutta (RK4) method

Example

Use RK4 (with $h = 0.2$) to solve IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ and $y(0) = 0.5$.

Solution: (cont) Continue with $i = 1, 2, \cdots, 9$:

t_i	Exact $y_i = y(t_i)$	Runge-Kutta Order Four w_i	Error $\|y_i - w_i\|$
0.0	0.5000000	0.5000000	0
0.2	0.8292986	0.8292933	0.0000053
0.4	1.2140877	1.2140762	0.0000114
0.6	1.6489406	1.6489220	0.0000186
0.8	2.1272295	2.1272027	0.0000269
1.0	2.6408591	2.6408227	0.0000364
1.2	3.1799415	3.1798942	0.0000474
1.4	3.7324000	3.7323401	0.0000599
1.6	4.2834838	4.2834095	0.0000743
1.8	4.8151763	4.8150857	0.0000906
2.0	5.3054720	5.3053630	0.0001089

High-order Runge-Kutta method

Can we use even higher-order method to improve accuracy?

$\#f$ eval	2	3	4	$5 \le n \le 7$	$8 \le n \le 9$	$n \ge 10$
Best error	$O(h^2)$	$O(h^3)$	$O(h^4)$	$O(h^{n-1})$	$O(h^{n-2})$	$O(h^{n-3})$

So RK4 is the sweet spot.

Remark

Note that RK4 requires 4 evaluations of f each step. So it would make sense only if it's accuracy with step size $4h$ is higher than Midpoint with $2h$ or Euler's with h!

High-order Runge-Kutta method

Example

Use RK4 (with $h = 0.1$), Midpoint (with $h = 0.05$), and Euler's method (with $h = 0.025$) to solve IVP $y' = y - t^2 + 1$ for $t \in [0, 0.5]$ and $y(0) = 0.5$.

Solution:

t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order Four $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

RK4 is better with same computation cost!

Error control

Can we control the error of Runge-Kutta method by using variable step sizes?

Let's compare two difference methods with errors $O(h^n)$ and $O(h^{n+1})$ (say, RK4 and RK5) for fixed step size h, which have schemes below:

$$
\begin{aligned}
w_{i+1} &= w_i + h\phi(t_i, w_i, h) && O(h^n) \\
\tilde{w}_{i+1} &= \tilde{w}_i + h\tilde{\phi}(t_i, \tilde{w}_i, h) && O(h^{n+1})
\end{aligned}
$$

Suppose $w_i \approx \tilde{w}_i \approx y(t_i) =: y_i$. Then for any given $\epsilon > 0$, we want to see how small h should be for the $O(h^n)$ method so that its error $|\tau_{i+1}(h)| \le \epsilon$?

Error control

We recall that the local truncation errors of these two methods are:

$$\tau_{i+1}(h) = \frac{y_{i+1} - y_i}{h} - \phi(t_i, y_i, h) \approx O(h^n)$$
$$\tilde{\tau}_{i+1}(h) = \frac{y_{i+1} - y_i}{h} - \tilde{\phi}(t_i, y_i, h) \approx O(h^{n+1})$$

Given that $w_i \approx \tilde{w}_i \approx y_i$ and $O(h^{n+1}) \ll O(h^n)$ for small h, we see

$$\begin{aligned}\tau_{i+1}(h) &\approx \tau_{i+1}(h) - \tilde{\tau}_{i+1}(h) = \tilde{\phi}(t_i, y_i, h) - \phi(t_i, y_i, h) \\ &\approx \tilde{\phi}(t_i, \tilde{w}_i, h) - \phi(t_i, w_i, h) = \frac{\tilde{w}_{i+1} - \tilde{w}_i}{h} - \frac{w_{i+1} - w_i}{h} \\ &\approx \frac{\tilde{w}_{i+1} - w_{i+1}}{h} \approx K h^n\end{aligned}$$

for some $K > 0$ independent of h, since $\tau_{i+1}(h) \approx O(h^n)$.

Error control

Suppose that we can scale h by $q > 0$, such that

$$|\tau_{i+1}(qh)| \approx K(qh)^n = q^n K h^n \approx q^n \frac{|\tilde{w}_{i+1} - w_{i+1}|}{h} \leq \epsilon$$

So we need q to satisfy

$$q \leq \left(\frac{\epsilon h}{|\tilde{w}_{i+1} - w_{i+1}|} \right)^{1/n}$$

- $q < 1$: reject the initial h and recalculate using qh.
- $q \geq 1$: accept computed value and use qh for next step.

Runge-Kutta-Fehlberg method

The **Runge-Kutta-Fehlberg (RKF) method** uses specific 4th-order and 5th-order RK schemes, which share some computed values and together only need 6 evaluation of f, to estimate

$$q = \left(\frac{\epsilon h}{2|\tilde{w}_{i+1} - w_{i+1}|}\right)^{1/4} = 0.84 \left(\frac{\epsilon h}{|\tilde{w}_{i+1} - w_{i+1}|}\right)^{1/4}$$

This q is used to tune step size so that error is always bounded by the prescribed ϵ.

Multistep method

Definition

*Let $m > 1$ be an integer, then an m**-step multistep method** is given by the form of*

$$\begin{aligned} w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i-m+1} \\ &\quad + h\left[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) + \cdots + b_0 f(t_{i-m+1}, w_{i-m+1})\right] \end{aligned}$$

for $i = m-1, m, \dots, N-1$.

Here $a_0, \dots, a_{m-1}, b_0, \dots, b_m$ are constants. Also $w_0 = \alpha, w_1 = \alpha_1, \dots, w_{m-1} = \alpha_{m-1}$ need to be given.

- *$b_m = 0$: Explicit m-step method.*
- *$b_m \neq 0$: Implicit m-step method.*

Multistep method

Definition

*The **local truncation error** of the m-step multistep method above is defined by*

$$
\begin{aligned}
\tau_{i+1}(h) = {} & \frac{y_{i+1} - (a_{m-1} y_i + \cdots + a_0 y_{i-m+1})}{h} \\
& - \left[b_m f(t_{i+1}, y_{i+1}) + b_{m-1} f(t_i, y_i) + \cdots + b_0 f(t_{i-m+1}, y_{i-m+1}) \right]
\end{aligned}
$$

where $y_i := y(t_i)$.

Adams-Bashforth Explicit method

Adams-Bashforth Two-Step Explicit method:

$$\begin{cases} w_0 = \alpha, \quad w_1 = \alpha_1, \\ w_{i+1} = w_i + \dfrac{h}{2}\left[3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\right] \end{cases}$$

for $i = 1, \ldots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = \frac{5}{12} y'''(\mu_i) h^2$$

for some $\mu_i \in (t_{i-1}, t_{i+1})$.

Adams-Bashforth Explicit method

Adams-Bashforth Three-Step Explicit method:

$$\begin{cases} w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \\ w_{i+1} = w_i + \dfrac{h}{12}\Big[23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})\Big] \end{cases}$$

for $i = 2, \ldots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = \frac{3}{8} y^{(4)}(\mu_i) h^3$$

for some $\mu_i \in (t_{i-2}, t_{i+1})$.

Adams-Bashforth Explicit method

Adams-Bashforth Four-Step Explicit method:

$$\begin{cases} w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3 \\ w_{i+1} = w_i + \dfrac{h}{24}\Big[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})\Big] \end{cases}$$

for $i = 3, \dots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = \frac{251}{720} y^{(5)}(\mu_i) h^4$$

for some $\mu_i \in (t_{i-3}, t_{i+1})$.

Adams-Bashforth Explicit method

Adams-Bashforth Five-Step Explicit method:

$$\begin{cases} w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3, \quad w_4 = \alpha_4 \\ w_{i+1} = w_i + \dfrac{h}{720}[1901 f(t_i, w_i) - 2774 f(t_{i-1}, w_{i-1}) + 2616 f(t_{i-2}, w_{i-2}) \\ \qquad\qquad - 1274 f(t_{i-3}, w_{i-3}) + 251 f(t_{i-4}, w_{i-4})] \end{cases}$$

for $i = 4, \ldots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = \frac{95}{288} y^{(6)}(\mu_i) h^5$$

for some $\mu_i \in (t_{i-4}, t_{i+1})$.

Adams-Moulton Implicit method

Adams-Moulton Two-Step Implicit method:

$$\begin{cases} w_0 = \alpha, \quad w_1 = \alpha_1, \\ w_{i+1} = w_i + \frac{h}{12}[5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})] \end{cases}$$

for $i = 1, \ldots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = -\frac{1}{24} y^{(4)}(\mu_i) h^3$$

for some $\mu_i \in (t_{i-1}, t_{i+1})$.

Adams-Moulton Implicit method

Adams-Moulton Three-Step Implicit method:

$$\begin{cases} w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2 \\ w_{i+1} = w_i + \dfrac{h}{24}[9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})] \end{cases}$$

for $i = 2, \ldots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = -\frac{19}{720} y^{(5)}(\mu_i) h^4$$

for some $\mu_i \in (t_{i-2}, t_{i+1})$.

Adams-Moulton Implicit method

Adams-Moulton Four-Step Implicit method:

$$
\begin{cases}
w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3 \\
w_{i+1} = w_i + \dfrac{h}{720}[251f(t_{i+1}, w_{i+1}) + 646f(t_i, w_i) - 264f(t_{i-1}, w_{i-1}) \\
\qquad\qquad + 106f(t_{i-2}, w_{i-2}) - 19f(t_{i-3}, w_{i-3})]
\end{cases}
$$

for $i = 3, \ldots, N-1$.

The local truncation error is

$$\tau_{i+1}(h) = -\frac{3}{160} y^{(6)}(\mu_i) h^5$$

for some $\mu_i \in (t_{i-3}, t_{i+1})$.

Steps to develop multistep methods

- Construct interpolating polynomial $P(t)$ (e.g., Newton's backward difference method) using previously computed $(t_{i-m+1}, w_{i-m+1}), \dots, (t_i, w_i)$.
- Approximate $y(t_{i+1})$ based on

$$\begin{aligned} y(t_{i+1}) &= y(t_i) + \int_{t_i}^{t_{i+1}} y'(t)\,\mathrm{d}t = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t))\,\mathrm{d}t \\ &\approx y(t_i) + \int_{t_i}^{t_{i+1}} f(t, P(t))\,\mathrm{d}t \end{aligned}$$

and construct difference method:

$$w_{i+1} = w_i + h\phi(t_i, \dots, t_{i-m+1}, w_i, \dots, w_{i-m+1})$$

Explicit vs. Implicit

- Implicit methods are generally more accurate than the explicit ones (e.g., Adams-Moulton three-step implicit method is even more accurate than Adams-Bashforth four-step explicit method).
- Implicit methods require solving for w_{i+1} from

$$w_{i+1} = \cdots + \frac{h}{xxx} f(t_{i+1}, w_{i+1}) + \cdots$$

  which can be difficult or even impossible.
- There could be multiple solutions of w_{i+1} when solving the equation above in implicit methods.

Predictor-Corrector method

Due to the aforementioned issues, implicit methods are often cast in "predictor-corrector" form in practice.

In each step i:

- **Prediction:** Compute w_{i+1} using an explicit method ϕ to get $w_{i+1,p}$ using

$$w_{i+1,p} = w_i + h\phi(t_i, w_i, \dots, t_{i-m+1}, w_{i-m+1})$$

- **Correction:** Substitute w_{i+1} by $w_{i+1,p}$ in the implicit method $\tilde{\phi}$ and compute w_{i+1} using

$$w_{i+1} = w_i + h\tilde{\phi}(t_{i+1}, w_{i+1,p}, t_i, w_i, \dots, t_{i-m+1}, w_{i-m+1})$$

Predictor-Corrector method

Example

*Use the Adams-Bashforth 4-step explicit method and Adams-Moulton 3-step implicit method to form the **Adams 4th-order Predictor-Corrector** method.*

With initial value $w_0 = \alpha$, suppose we first generate w_1, w_2, w_3 using RK4 method. Then for $i = 3, 4, \ldots, N-1$:

- Use Adams-Bashforth 4-step explicit method to get a predictor $w_{i+1,p}$:

$$w_{i+1,p} = w_i + \frac{h}{24}\left[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})\right]$$

- Use Adams-Moulton 3-step implicit method to get a corrector w_{i+1}:

$$w_{i+1} = w_i + \frac{h}{24}[9f(t_{i+1}, w_{i+1,p}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})]$$

Predictor-Corrector method

Example

Use Adams Predictor-Corrector Method with $h = 0.2$ to solve IVP $y' = y - t^2 + 1$ for $t \in [0, 2]$ and $y(0) = 0.5$.

t_i	$y_i = y(t_i)$	w_i	Error $\lvert y_i - w_i \rvert$
0.0	0.5000000	0.5000000	0
0.2	0.8292986	0.8292933	0.0000053
0.4	1.2140877	1.2140762	0.0000114
0.6	1.6489406	1.6489220	0.0000186
0.8	2.1272295	2.1272056	0.0000239
1.0	2.6408591	2.6408286	0.0000305
1.2	3.1799415	3.1799026	0.0000389
1.4	3.7324000	3.7323505	0.0000495
1.6	4.2834838	4.2834208	0.0000630
1.8	4.8151763	4.8150964	0.0000799
2.0	5.3054720	5.3053707	0.0001013

Other Predictor-Corrector method

We can also use Milne's 3-step explicit method and Simpson's 2-step implicit method below:

$$w_{i+1,p} = w_{i-3} + \frac{4h}{3}\left[2f(t_i, w_i) - f(t_{i-1}, w_{i-1}) + 2f(t_{i-2}, w_{i-2})\right]$$

$$w_{i+1} = w_{i-1} + \frac{h}{3}[f(t_{i+1}, w_{i+1,p}) + 4f(t_i, w_i) + f(t_{i-1}, w_{i-1})]$$

This method is $O(h^4)$ and generally has better accuracy than Adams PC method. However it is more likely to be vulnurable to sound-off error.

Predictor-Corrector method

- PC methods have comparable accuracy as RK4, but often require only 2 evaluations of f in each step.
- Need to store values of f for several previous steps.
- Sometimes are more restrictive on step size h, e.g., in the stiff differential equation case later.

Variable step-size multistep method

Now let's take a closer look at the errors of the multistep methods. Denote $y_i := y(t_i)$.

The Adams-Bashforth 4-step explicit method has error

$$\tau_{i+1}(h) = \frac{251}{720} y^{(5)}(\mu_i) h^4$$

The Adams-Moulton 3-step implicit method has error

$$\tilde{\tau}_{i+1}(h) = -\frac{19}{720} y^{(5)}(\tilde{\mu}_i) h^4$$

where $\mu_i \in (t_{i-3}, t_{i+1})$ and $\tilde{\mu}_i \in (t_{i-2}, t_{i+1})$.

Question: Can we find a way to scale step size h so the error is under control?

Variable step-size multistep method

Consider the their local truncation errors:

$$y_{i+1} - w_{i+1,p} = \frac{251}{720} y^{(5)}(\mu_i) h^5$$
$$y_{i+1} - w_{i+1} = -\frac{19}{720} y^{(5)}(\tilde{\mu}_i) h^5$$

Assume $y^{(5)}(\mu_i) \approx y^{(5)}(\tilde{\mu}_i)$, we take their difference to get

$$w_{i+1} - w_{i+1,p} = \frac{1}{720}(19 + 251) y^{(5)}(\mu_i) h^5 \approx \frac{3}{8} y^{(5)}(\mu_i) h^5$$

So the error of Adams-Moulton (corrector step) is

$$\tilde{\tau}_{i+1}(h) = \frac{|y_{i+1} - w_{i+1}|}{h} \approx \frac{19|w_{i+1} - w_{i+1,p}|}{270h} = Kh^4$$

where K is independent of h since $\tilde{\tau}_{i+1}(h) = O(h^4)$.

Variable step-size multistep method

If we want to keep error under a prescribed ϵ, then we need to find $q > 0$ such that with step size qh, there is

$$\tilde{\tau}_{i+1}(qh) = \frac{|y(t_i + qh) - w_{i+1}|}{qh} \approx \frac{19q^4|w_{i+1} - w_{i+1,p}|}{270h} < \epsilon$$

This implies that

$$q < \left(\frac{270h\epsilon}{19|w_{i+1} - w_{i+1,p}|}\right)^{1/4} \approx 2\left(\frac{h\epsilon}{|w_{i+1} - w_{i+1,p}|}\right)^{1/4}$$

To be conservative, we may replace 2 by 1.5 above.

In practice, we tune q (as less as possible) such that the estimated error is between $(\epsilon/10, \epsilon)$

System of differential equations

The IVP for a system of ODE has form

$$\begin{cases} \dfrac{\mathrm{d}u_1}{\mathrm{d}t} = f_1(t, u_1, u_2, \ldots, u_m) \\ \dfrac{\mathrm{d}u_2}{\mathrm{d}t} = f_2(t, u_1, u_2, \ldots, u_m) \\ \qquad \vdots \\ \dfrac{\mathrm{d}u_m}{\mathrm{d}t} = f_m(t, u_1, u_2, \ldots, u_m) \end{cases} \quad \text{for } a \le t \le b$$

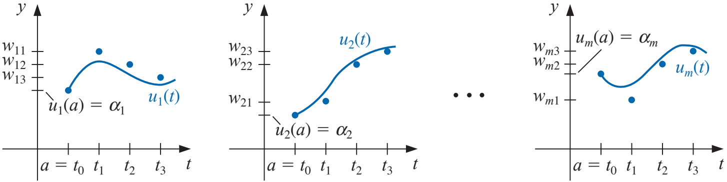
with initial value $u_1(a) = \alpha_1, \ldots, u_m(a) = \alpha_m$.

Definition

*A set of functions $u_1(t), \ldots, u_m(t)$ is a **solution** of the IVP above if they satisfy both the system of ODEs and the initial values.*

System of differential equations

In this case, we will solve for $u_1(t), \ldots, u_m(t)$ which are interdependent according to the ODE system.



System of differential equations

Definition

*A function f is called **Lipschitz** with respect to $u_1, \ldots, u_m$ on $D := [a, b] \times \mathbb{R}^m$ if there exists $L > 0$ s.t.*

$$|f(t, u_1, \ldots, u_m) - f(t, z_1, \ldots, z_m)| \le L \sum_{j=1}^{m} |u_j - z_j|$$

for all $(t, u_1, \ldots, u_m), (t, z_1, \ldots, z_m) \in D$.

System of differential equations

Theorem

If $f \in C^1(D)$ and $|\frac{\partial f}{\partial u_j}| \leq L$ for all j, then f is Lipschitz with respect to $u = (u_1, \dots, u_m)$ on D.

Proof.

Note that D is convex. For any $(t, u_1, \dots, u_m), (t, z_1, \dots, z_m) \in D$, define

$$g(\lambda) = f(t, (1-\lambda)u_1 + \lambda z_1, \dots, (1-\lambda)u_m + \lambda z_m)$$

for all $\lambda \in [0, 1]$. Then from $|g(1) - g(0)| \leq \int_0^1 |g'(\lambda)| \, \mathrm{d}\lambda$ and the definition of g, the conclusion follows. $\square$

System of differential equations

Theorem

If $f \in C^1(D)$ and is Lipschitz with respect to $u = (u_1, \ldots, u_m)$, then the IVP with f as defining function has a unique solution.

System of differential equations

Now let's use vector notations below

$$\begin{aligned} \mathbf{a} &= (\alpha_1, \ldots, \alpha_m) \\ \mathbf{y} &= (y_1, \ldots, y_m) \\ \mathbf{w} &= (w_1, \ldots, w_m) \\ \mathbf{f}(t, \mathbf{w}) &= (f_1(t, w_1), \ldots, f_m(t, w_m)) \end{aligned}$$

Then the IVP of ODE system can be written as

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \quad t \in [a, b]$$

with initial value $\mathbf{y}(a) = \mathbf{a}$.

So the difference methods developed above, such as RK4, still apply.

System of differential equations

Example

Use RK4 (with $h = 0.1$) to solve IVP for ODE system

$$\begin{cases} I_1'(t) = f_1(t, I_1, I_2) = -4I_1 + 3I_2 + 6 \\ I_2'(t) = f_2(t, I_1, I_2) = -2.4I_1 + 1.6I_2 + 3.6 \end{cases}$$

with initial value $I_1(0) = I_2(0) = 0$.

Solution: The exact solution is

$$\begin{cases} I_1(t) = -3.375e^{-2t} + 1.875e^{-0.4t} + 1.5 \\ I_2(t) = 2.25e^{-2t} + 2.25e^{-0.4t} \end{cases}$$

for all $t \geq 0$.

System of differential equations

Example

Use RK4 (with $h = 0.1$) to solve IVP for ODE system

$$\begin{cases} I_1'(t) = f_1(t, I_1, I_2) = -4I_1 + 3I_2 + 6 \\ I_2'(t) = f_2(t, I_1, I_2) = -2.4I_1 + 1.6I_2 + 3.6 \end{cases}$$

with initial value $I_1(0) = I_2(0) = 0$.

Solution: (cont) The result by RK4 is

t_j	$w_{1,j}$	$w_{2,j}$	$\lvert I_1(t_j) - w_{1,j}\rvert$	$\lvert I_2(t_j) - w_{2,j}\rvert$
0.0	0	0	0	0
0.1	0.5382550	0.3196263	0.8285×10^{-5}	0.5803×10^{-5}
0.2	0.9684983	0.5687817	0.1514×10^{-4}	0.9596×10^{-5}
0.3	1.310717	0.7607328	0.1907×10^{-4}	0.1216×10^{-4}
0.4	1.581263	0.9063208	0.2098×10^{-4}	0.1311×10^{-4}
0.5	1.793505	1.014402	0.2193×10^{-4}	0.1240×10^{-4}

High-order ordinary differential equations

A general **IVP for *m*th-order ODE** is

$$y^{(m)} = f(t, y, y', \dots, y^{(m-1)}), \quad t \in [a, b]$$

with initial value $y(a) = \alpha_1, y'(a) = \alpha_2, \dots, y^{(m-1)}(a) = \alpha_m$.

Definition

*A function $y(t)$ is a **solution of IVP for the mth-order ODE** above if $y(t)$ satisfies the differential equation for $t \in [a, b]$ and all initial value conditions at $t = a$.*

High-order ordinary differential equations

We can define a set of functions $u_1, \dots, u_m$ s.t.

$$u_1(t) = y(t), \quad u_2(t) = y'(t), \quad \dots, \quad u_m(t) = y^{(m-1)}(t)$$

Then we can convert the mth-order ODE to a system of first-order ODEs:

$$\begin{cases} u_1' = u_2 \\ u_2' = u_3 \\ \quad \vdots \\ u_m' = f(t, u_1, u_2, \dots, u_m) \end{cases} \qquad \text{for } a \le t \le b$$

with initial values $u_1(a) = \alpha_1, \dots, u_m(a) = \alpha_m$.

High-order ordinary differential equations

Example

Use RK4 (with $h = 0.1$) to solve IVP for ODE system

$$y'' - 2y' + 2y = e^{2t} \sin t, \quad t \in [0, 1]$$

with initial value $y(0) = -0.4, y'(0) = -0.6$.

Solution:

The exact solution is $y(t) = u_1(t) = 0.2e^{2t}(\sin t - 2\cos t)$. Also $u_2(t) = y'(t) = u_1'(t)$ but we don't need it.

High-order ordinary differential equations

Example

Use RK4 (with $h = 0.1$) to solve IVP for ODE system

$$y'' - 2y' + 2y = e^{2t}\sin t, \quad t \in [0, 1]$$

with initial value $y(0) = -0.4$, $y'(0) = -0.6$.

Solution: (cont) The result by RK4 is

t_j	$y(t_j) = u_1(t_j)$	$w_{1,j}$	$y'(t_j) = u_2(t_j)$	$w_{2,j}$	$\lvert y(t_j) - w_{1,j}\rvert$	$\lvert y'(t_j) - w_{2,j}\rvert$
0.0	−0.40000000	−0.40000000	−0.6000000	−0.60000000	0	0
0.1	−0.46173297	−0.46173334	−0.6316304	−0.63163124	3.7×10^{-7}	7.75×10^{-7}
0.2	−0.52555905	−0.52555988	−0.6401478	−0.64014895	8.3×10^{-7}	1.01×10^{-6}
0.3	−0.58860005	−0.58860144	−0.6136630	−0.61366381	1.39×10^{-6}	8.34×10^{-7}
0.4	−0.64661028	−0.64661231	−0.5365821	−0.53658203	2.03×10^{-6}	1.79×10^{-7}
0.5	−0.69356395	−0.69356666	−0.3887395	−0.38873810	2.71×10^{-6}	5.96×10^{-7}
0.6	−0.72114849	−0.72115190	−0.1443834	−0.14438087	3.41×10^{-6}	7.75×10^{-7}
0.7	−0.71814890	−0.71815295	0.2289917	0.22899702	4.05×10^{-6}	2.03×10^{-6}
0.8	−0.66970677	−0.66971133	0.7719815	0.77199180	4.56×10^{-6}	5.30×10^{-6}
0.9	−0.55643814	−0.55644290	1.534764	1.5347815	4.76×10^{-6}	9.54×10^{-6}
1.0	−0.35339436	−0.35339886	2.578741	2.5787663	4.50×10^{-6}	1.34×10^{-5}

A brief summary

The difference methods we developed above, e.g., Euler's, midpoints, RK4, multistep explicit/implicit, predictor-corrector methods, are

- based on step-by-step derivation and easy to understand;
- widely used in many practical problems;
- fundamental to more advanced and complex techniques.

Stability of difference methods

Definition (Consistency)

*A difference method is called **consistent** if*

$$\lim_{h\to 0}\left(\max_{1\le i\le N}\tau_i(h)\right)=0$$

where $\tau_i(h)$ is the local truncation error of the method.

Remark

Since local truncation error $\tau_i(h)$ is defined assuming previous $w_i = y_i$, it does not take error accumulation into account. So the consistency definition above only considers how good $\phi(t, w_i, h)$ in the difference method is.

Stability of difference methods

For any step size $h > 0$, the difference method $w_{i+1} = w_i + h\phi(t_i, w_i, h)$ can generate a sequence of w_i which depend on h. We call them $\{w_i(h)\}_i$. Note that w_i gradually accumulate errors as $i = 1, 2, \ldots, N$.

Definition (Convergent)

A difference method is called ***convergent*** *if*

$$\lim_{h \to 0} \left(\max_{1 \le i \le N} |y_i - w_i(h)| \right) = 0$$

Stability of difference methods

Example

Show that Euler's method is convergent.

Solution: We have showed before that for fixed $h > 0$ there is

$$\left|y(t_i) - w_i\right| \le \frac{hM}{2L}\left(e^{L(t_i - a)} - 1\right) \le \frac{hM}{2L}\left(e^{L(b-a)} - 1\right)$$

for all $i = 0, \dots, N$. Therefore we have

$$\max_{1 \le i \le N}\left|y(t_i) - w_i\right| \le \frac{hM}{2L}\left(e^{L(b-a)} - 1\right) \to 0$$

as $h \to 0$. Therefore $\lim_{h \to 0}(\max_{1 \le i \le N}\left|y(t_i) - w_i\right|) = 0$.

Stability of difference method

Definition
A numerical method is called ***stable*** *if its results depend on the initial data continuously.*

Stability of difference methods

Theorem

For a given IVP $y' = f(t, y)$, $t \in [a, b]$ with $y(a) = \alpha$, consider a difference method $w_{i+1} = w_i + h\phi(t_i, w_i, h)$ with $w_0 = \alpha$. If there exists $h_0 > 0$ such that ϕ is continuous on $[a, b] \times \mathbb{R} \times [0, h_0]$, and ϕ is L-Lipschitz with respect to w, then

- *The difference method is stable.*
- *The difference method is convergent if and only if it is consistent (i.e., $\phi(t, y, 0) = f(t, y)$).*
- *If there exists bound $\tau(h)$ such that $|\tau_i(h)| \le \tau(h)$ for all $i = 1, \dots, N$, then $|y(t_i) - w_i| \le \tau(h)e^{L(t_i - a)}/L$.*

Stability of difference methods

Proof.
Let h be fixed, then $w_i(\alpha)$ generated by the difference method are functions of α. For any two values $\alpha, \hat{\alpha}$, there is

$$\begin{aligned}
|w_{i+1}(\alpha) - w_{i+1}(\hat{\alpha})| &= |(w_i(\alpha) - h\phi(t_i, w_i(\alpha))) - (w_i(\hat{\alpha}) - h\phi(t_i, w_i(\hat{\alpha})))| \\
&\le |w_i(\alpha) - w_i(\hat{\alpha})| + h|\phi(t_i, w_i(\alpha)) - \phi(t_i, w_i(\hat{\alpha}))| \\
&\le |w_i(\alpha) - w_i(\hat{\alpha})| + hL|w_i(\alpha) - w_i(\hat{\alpha})| \\
&= (1 + hL)|w_i(\alpha) - w_i(\hat{\alpha})| \\
&\le \cdots \\
&\le (1 + hL)^{i+1}|w_0(\alpha) - w_0(\hat{\alpha})| \\
&= (1 + hL)^{i+1}|\alpha - \hat{\alpha}| \\
&\le (1 + hL)^{N}|\alpha - \hat{\alpha}|
\end{aligned}$$

Therefore $w_i(\alpha)$ is Lipschitz with respect to α (with constant at most $(1 + hL)^N$), and hence is continuous with respect to α. We omit the proofs for the other two assertions here. $\square$

Stability of difference method

Example

Use the result of Theorem above to show that the Modified Euler's method is stable.

Solution:

Recall the Modified Euler's method is given by

$$w_{i+1} = w_i + \frac{h}{2}\Big(f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))\Big)$$

So we have $\phi(t, w, h) = \frac{1}{2}(f(t, w) + f(t + h, w + hf(t, w)))$.
Now we want to show ϕ is continuous in (t, w, h), and Lipschitz with respect to w.

Stability of difference method

Solution: (cont) It is obvious that ϕ is continuous in (t, w, h) since $f(t, w)$ is continuous. Fix t and h. For any $w, \bar{w} \in \mathbb{R}$, there is

$$\begin{aligned}
|\phi(t, w, h) - \phi(t, \bar{w}, h)| &= \frac{1}{2}|f(t, w) - f(t, \bar{w})| \\
&\quad + \frac{1}{2}|f(t + h, w + hf(t, w)) - f(t + h, \bar{w} + hf(t, \bar{w}))| \\
&\leq \frac{L}{2}|w - \bar{w}| + \frac{L}{2}|(w + hf(t, w)) - (\bar{w} + hf(t, \bar{w}))| \\
&\leq L|w - \bar{w}| + \frac{Lh}{2}|f(t, w) - f(t, \bar{w})| \\
&\leq L|w - \bar{w}| + \frac{L^2 h}{2}|w - \bar{w}| \\
&= (L + \frac{L^2 h}{2})|w - \bar{w}|
\end{aligned}$$

So ϕ is Lipschitz with respect to w. By first part of Theorem above, the Modified Euler's method is stable.

Stability of multistep difference method

Definition

Suppose a multistep difference method given by

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i-m+1} + hF(t_i, h, w_{i+1}, \ldots, w_{i-m+1})$$

*Then we call the following the **characteristic polynomial** of the method:*

$$\lambda^m - (a_{m-1}\lambda^{m-1} + \cdots + a_1\lambda + a_0)$$

Definition

*A difference method is said to satisfy the **root condition** if all the m roots $\lambda_1, \ldots, \lambda_m$ of its characteristic polynomial have magnitudes ≤ 1, and all of those which have magnitude =1 are single roots.*

Stability of multistep difference method

Definition

- *A difference method that satisfies root condition is called* ***strongly stable*** *if the only root with magnitude* 1 *is* $\lambda = 1$*.*
- *A difference method that satisfies root condition is called* ***weakly stable*** *if there are multiple roots with magnitude 1.*
- *A difference method that does not satisfy root condition is called* ***unstable****.*

Stability of multistep difference method

Theorem

- *A difference method is stable if and only if it satisfies the root condition.*
- *If a difference method is consistent, then it is stable if and only if it is covergent.*

Stability of multistep difference method

Example

Show that the Adams-Bashforth 4-step explicit method is strongly stable.

Solution: Recall that the method is given by

$$w_{i+1} = w_i + \frac{h}{24}\left[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})\right]$$

So the characteristic polynomial is simply $\lambda^4 - \lambda^3 = \lambda^3(\lambda - 1)$, which only has one root $\lambda = 1$ with magnitude 1. So the method is strongly stable.

Stability of multistep difference method

Example

Show that the Milne's 3-step explicit method is weakly stable but not strongly stable.

Solution: Recall that the method is given by

$$w_{i+1} = w_{i-3} + \frac{4h}{3}\left[2f(t_i, w_i) - f(t_{i-1}, w_{i-1}) + 2f(t_{i-2}, w_{i-2})\right]$$

So the characteristic polynomial is simply $\lambda^4 - 1$, which have roots $\lambda = \pm 1, \pm \mathrm{i}$. So the method is weakly stable but not strongly stable.

Remark

This is the reason we chose Adams-Bashforth-Moulton PC rather than Milne-Simpsons PC since the former is strongly stable and likely to be more robust.

Stiff differential equations

Stiff differential equations have e^{-ct} terms ($c > 0$ large) in their solutions. These terms $\to 0$ quickly, but their derivatives (of form $c^n e^{-ct}$) do not, especially at small t.

Recall that difference methods have errors proportional to the derivatives, and hence they may be inaccurate for stiff ODEs.

Stiff differential equations

Example

Use RK4 to solve the IVP for a system of two ODEs:

$$\begin{cases} u_1' = 9u_1 + 24u_2 + 5\cos t - \dfrac{1}{3}\sin t \\ u_2' = -24u_1 - 51u_2 - 9\cos t + \dfrac{1}{3}\sin t \end{cases}$$

with initial values $u_1(0) = 4/3$ *and* $u_2(0) = 2/3$*.*

Solution: The exact solution is

$$\begin{cases} u_1(t) = 2e^{-3t} - e^{-39t} + \dfrac{1}{3}\cos t \\ u_2(t) = -e^{-3t} + 2e^{-39t} - \dfrac{1}{3}\cos t \end{cases}$$

for all $t \geq 0$.

Stiff differential equations

Solution: (cont) When we apply RK4 to this stiff ODE, we obtain

t	$u_1(t)$	$w_1(t)$ $h = 0.05$	$w_1(t)$ $h = 0.1$	$u_2(t)$	$w_2(t)$ $h = 0.05$	$w_2(t)$ $h = 0.1$
0.1	1.793061	1.712219	−2.645169	−1.032001	−0.8703152	7.844527
0.2	1.423901	1.414070	−18.45158	−0.8746809	−0.8550148	38.87631
0.3	1.131575	1.130523	−87.47221	−0.7249984	−0.7228910	176.4828
0.4	0.9094086	0.9092763	−934.0722	−0.6082141	−0.6079475	789.3540
0.5	0.7387877	9.7387506	−1760.016	−0.5156575	−0.5155810	3520.00
0.6	0.6057094	0.6056833	−7848.550	−0.4404108	−0.4403558	15697.84
0.7	0.4998603	0.4998361	−34989.63	−0.3774038	−0.3773540	69979.87
0.8	0.4136714	0.4136490	−155979.4	−0.3229535	−0.3229078	311959.5
0.9	0.3416143	0.3415939	−695332.0	−0.2744088	−0.2743673	1390664.
1.0	0.2796748	0.2796568	−3099671.	−0.2298877	−0.2298511	6199352.

which can blow up for larger step size h.

Stiff differential equations

Now let's use a simple example to see why this happens: consider an IVP $y' = \lambda y$, $t \geq 0$, and $y(0) = \alpha$. Here $\lambda < 0$. We know the problem has solution $y(t) = \alpha e^{\lambda t}$.

Suppose we apply Euler's method, which is

$$\begin{aligned} w_{i+1} &= w_i + hf(t_i, w_i) = w_i + h\lambda w_i = (1 + \lambda h) w_i \\ &= \cdots = (1 + \lambda h)^{i+1} w_0 = (1 + \lambda h)^{i+1} \alpha \end{aligned}$$

Therefore we simply have $w_i = (1 + \lambda h)^i \alpha$. So the error is

$$|y(t_i) - w_i| = |\alpha e^{\lambda i h} - (1 + \lambda h)^i \alpha| = |e^{\lambda i h} - (1 + \lambda h)^i||\alpha|$$

In order for the error not to blow up, we need at least $|1 + \lambda h| < 1$, which yields $h < \frac{2}{|\lambda|}$. So h needs to be sufficiently small for large λ.

Stiff differential equations

Similar issue occurs for other one-step methods, which for this IVP can be written as $w_{i+1} = Q(\lambda h)w_i = \cdots = (Q(\lambda h))^{i+1}\alpha$. For the solution not to blow up, we need $|Q(\lambda h)| < 1$.

For example, in nth-order Taylor's method, we need

$$|Q(\lambda h)| = \left|1 + \lambda h + \frac{\lambda^2 h^2}{2} + \cdots + \frac{\lambda^n h^n}{n!}\right| < 1$$

which requires h to be very small.

The same issue occurs for multistep methods too.

Stiff differential equations

A remedy of stiff ODE is using implicit method, e.g., the implicit Trapezoid method:

$$w_{i+1} = w_i + \frac{h}{2}(f(t_{i+1}, w_{i+1}) + f(t_i, w_i))$$

In each step, we need to solve for w_{i+1} from the equation above.
Namely, we need to solve for the root of $F(w)$:

$$F(w) := w - w_i - \frac{h}{2}(f(t_{i+1}, w) + f(t_i, w_i)) = 0$$

We can use Newton's method to solve $F(x) = 0$. For ODE system with **f** of high dimension, use secant method.