Numerical Methods
Differential Equations

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Introduction to Differential Equations

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Examples

- Exponential growth $\dot{y} = ky$ or decay $\dot{y} = -ky$.

- Logistic growth $\dot{y} = ky(y_{\max} - y)$.

- Linear (first order): $\dot{y} + p(t)y = q(t)$

- Predator-prey $\dot{x} = ax - bxy; \quad \dot{y} = -cy + dxy$.

- Forced damped oscillations $\ddot{x} + \delta\dot{x} + kx = A\cos(\omega t)$.
  Equivalently: $\dot{x} = v, \dot{v} = \ddot{x} = -\delta v - kx + A\cos(\omega t)$.

Scientific applications

Differential equations are one of the most common modeling frameworks in the natural sciences and engineering.

Physics   All major theories: dynamics (Newton), elastics (Euler), electromagnetism (Maxwell), fluids (Navier-Stokes), relativity (Einstein), quantum (Schrödinger).

e.g. Newton's law $F(x) = ma = m\ddot{x}$.

e.g. Maxwell's equations

$$\nabla \cdot \mathbf{E} = \rho/\varepsilon_0; \quad \nabla \cdot \mathbf{B} = 0;$$

$$\mu_0(\varepsilon_0\dot{\mathbf{E}} + \mathbf{J}) = \nabla \times \mathbf{B}; \quad \dot{\mathbf{B}} = -\nabla \times \mathbf{E}.$$

Chemistry   Systems of reactions.

e.g. $\dot{a} = -k_1 a; \quad \dot{x} = k_1 a - k_2 x^2$.

Biology   Cellular processes, population/disease dynamics.

e.g. SIR model $\dot{S} = -\beta SI; \quad \dot{I} = \beta SI \gamma I; \quad \dot{R} = \gamma I$.

Engineering   Power systems, engines, robotics.

Computational, data science and artificial intelligence

Computer science   Since differential equations are ubiquitous in scientific modelling, their solution is one of the most important parts of scientific computing.

Many data sources are systems modelled by differential equations, so require fitting of differential equation models (system identification).

The physical behaviour of autonomous agents is described by differential equations, so agents need to understand their properties in order to operate successfully.

Checking solutions

We can check a candidate solution of a differential equation by substitution:
- A solution of the differential equation $\dot{y} = 2y$ is $y(t) = e^{2t}$, since

$$\frac{dy}{dt} = \frac{d}{dt}e^{2t} = 2e^{2t} = 2y.$$

- A solution of $\dot{y} = y(1-y)$ is $y(t) = 1/(1+2e^{-t})$, since

$$\frac{dy}{dt} = \frac{d}{dt}\left(1/(1+2e^{-t})\right) = 2e^{-t}/(1+2e^{-t})^2$$

$$y(1-y) = \frac{1}{1+2e^{-t}}\left(1 - \frac{1}{1+2e^{-t}}\right) = \frac{1}{1+2e^{-t}}\frac{(1+2e^{-t})-1}{1+2e^{-t}} = \frac{2e^{-t}}{(1+2e^{-t})^2}.$$

- A solution of $\dot{y} + y/t = \cos(t)$ is $y(t) = (\cos(t)-1)/t + \sin(t)$, since

$$\frac{dy}{dt} + y/t = \frac{d}{dt}\left((\cos(t)-1)/t + \sin(t)\right) + \left((\cos(t)-1)/t + \sin(t)\right)/t$$

$$= -\sin(t)/t - (\cos(t)-1)/t^2 + \cos(t) + (\cos(t)-1)/t^2 + \sin(t)/t = \cos(t).$$

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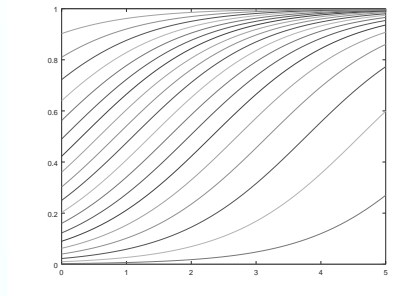 Check by substitution: $\frac{\mathrm{d}y}{\mathrm{d}t} = Cke^{kt} = kCe^{kt} = ky$.

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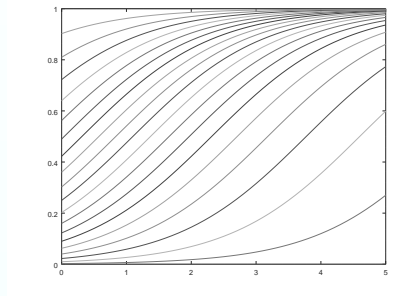 $y(t) = 1/(Ce^{-t}+1)$ is a solution.

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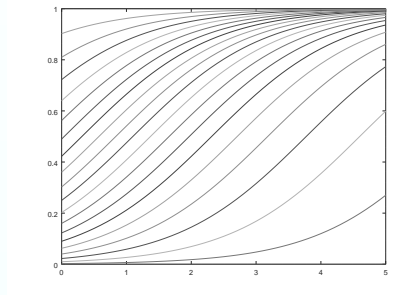
- Hence solution curves do not cross each other or merge.

- Given $y(t_0) = y_0$, there is a unique solution of the *initial-value problem*
  $\dot{y} = f(t,y)$; $y(t_0) = y_0$.

Degenerate solutions

Unbounded solutions   The solution of the initial-value problem

$$\dot{y} = y^2; \quad y(0) = y_0$$

is

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If $y_0 > 0$, then solutions are *unbounded*, with $y(t) \to \infty$ as $t \to 1/y_0$.

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Multiple solutions The initial-value problem

$$\dot{y} = \sqrt{|y|}; \quad y(0) = 0$$

has solutions

$$y(t) = \begin{cases} 0 \text{ for } t \leq t_c; \\ (t - t_c)^2/4 \text{ for } t \geq t_c. \end{cases}$$

This is possible since $f(t, y) = \sqrt{|y|}$ is not differentiable when $y = 0$.

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Linear equations   Linear first-order equations $\dot{y}(t) + p(t)y(t) = q(t)$.

Multiply through by $e^{\int p(t)\mathrm{d}t}$. Then by the product and chain rules

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\left(e^{\int p(t)\mathrm{d}t}y(t)\right) = e^{p(t)\mathrm{d}t}\left(\dot{y}(t) + p(t)y(t)\right) = e^{\int p(t)\mathrm{d}t}q(t)$$

Hence the general solution is

$$y(t) = e^{-\int p(t)\mathrm{d}t}\left(C + \int e^{\int p(t)\mathrm{d}t}\, q(t)\,\mathrm{d}t\right).$$

Separable equations   If $\dot{y} = f(y)g(t)$, then

$$\int 1/f(y)\,\mathrm{d}y = \int g(t)\,\mathrm{d}t.$$

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$$y(t) = 1 + t + \tfrac{3}{2}t^2 + \tfrac{4}{3}t^3 + \tfrac{17}{12}t^4 + \cdots .$$

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They also avoid the need for complicated algebraic analysis!!

Initial-Value Problems

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Initial-Value Problem   Find a function $y : [t_0, t_{\mathrm{f}}] \to \mathbb{R}$ satisfying

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Then $h = (t_{\mathrm{f}} - t_0)/N$ and $t_i = t_0 + ih$.

Chemical reactions

Example   Reactions $A \longrightarrow Y$ and $Y + Y \longrightarrow B$.

The concentrations $a = [A]$ and $y = [Y]$ satisfy the differential equations
$$\frac{\mathrm{d}a}{\mathrm{d}t} = -k_1 a; \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = k_1 a - k_2 y^2$$
where k_1, k_2 are rate constants.

Since a decays exponentially as $a = a_0 e^{-k_1 t}$ where $a_0 = [A(0)]$, we have
$$\frac{\mathrm{d}y}{\mathrm{d}t} = a_0 k_1 e^{-k_1 t} - k_2 y^2.$$

Use initial condition $t_0 = 0$ and $y_0 = [Y](0) = 0$.

Henceforth, take constants $a_0 = k_1 = k_2 = 1$ (in appropriate units) so
$$\frac{\mathrm{d}y}{\mathrm{d}t} = e^{-t} - y^2.$$

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Example Solve the following initial value problem in Matlab.
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Plot the solution:

```
plot(ts,ys)
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Taylor Methods

Euler's method

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Euler's method   Compute $w_i \approx y(t_i)$ by $w_0 = y(t_0)$ and
$$w_{i+1} = w_i + h_i f(t_i, w_i)$$
where $h_i = t_{i+1} - t_i$ is the step size.

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Evaluate $f(t_0, w_0) = (e^{-t_0} - w_0^2) = e^{-0} - 0^2 = 1$, so

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Evaluate $f(t_0, w_0) = (e^{-t_0} - w_0^2) = e^{-0} - 0^2 = 1$, so
$$y(1.0) \approx w_1$$

Euler's method

Example   Solve $\mathrm{d}y/\mathrm{d}t = f(t,y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Initialise $t_0 = 0$ and $w_0 = y_0 = y(0) = 0$.
Take $t_f = 1$, and aim to approximate $y(1)$ i.e. $y(t)$ when $t = 1$.

Try a single step, $h = 1.0$:
Formula $w_1 = w_0 + hf(t_0, w_0)$.
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$$y(1.0) \approx w_1 = w_0 + hf(t_0, w_0) = 0.0000 + 1.0 \times 1.0000$$

Euler's method

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Euler's method

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$$y(1.0) \approx w_1 = w_0 + hf(t_0, w_0) = 0.0000 + 1.0 \times 1.0000 = 1.0000.$$
The exact value is $y(1) = 0.503347\,(6\,\mathrm{sf})$.

Euler's method

Example   Solve $dy/dt = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Initialise $t_0 = 0$ and $w_0 = y_0 = y(0) = 0$.
Take $t_f = 1$, and aim to approximate $y(1)$ i.e. $y(t)$ when $t = 1$.

Try a single step, $h = 1.0$:
Formula $w_1 = w_0 + hf(t_0, w_0)$.
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Absolute error ≈ 0.50.

Euler's method

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The exact value is $y(1) = 0.503347 \, (6\,\mathrm{sf})$.
Absolute error ≈ 0.50.
Relative error
$$|w_1 - y(1)|/|y(1)| = 0.4967/0.503347 \approx 99\%!$$

Euler's method

Example   Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

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The exact value is $y(1) = 0.503347 \,(6\,\mathrm{sf})$.
Absolute error ≈ 0.50.
Relative error

$$|w_1 - y(1)|/|y(1)| = 0.4967/0.503347 \approx 99\%!$$

Very poor approximation...

Euler's method

Example Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Euler's method

Example Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Take $n = 2$ steps, each with step size $h = 0.5$.

Euler's method

Example   Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Take $n = 2$ steps, each with step size $h = 0.5$.

Times $t_0 = 0$, $t_1 = t_0 + h = 0.5$, $t_2 = t_1 + h = 1.0$.

Euler's method

Example   Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Take $n = 2$ steps, each with step size $h = 0.5$.

Times $t_0 = 0$, $t_1 = t_0 + h = 0.5$, $t_2 = t_1 + h = 1.0$.

Initialise $w_0 = y(t_0) = y(0) = 0.000$.

Euler's method

Example   Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Take $n = 2$ steps, each with step size $h = 0.5$.

Times $t_0 = 0$, $t_1 = t_0 + h = 0.5$, $t_2 = t_1 + h = 1.0$.

Initialise $w_0 = y(t_0) = y(0) = 0.000$. Solution is $y(1) = y(t_2) \approx w_2$

Euler's method

Example Solve $\mathrm{d}y/\mathrm{d}t = f(t, y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

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Initialise $w_0 = y(t_0) = y(0) = 0.000$. Solution is $y(1) = y(t_2) \approx w_2$

$$
\begin{aligned}
y(0.5) \approx w_1 &= w_0 + hf(t_0, w_0) \\
&= 0.000 + 0.5 \times f(0.0, 0.000) \\
&= 0.0000 + 0.5 \times 1.000 = 0.500.
\end{aligned}
$$

$$
\begin{aligned}
y(1.0) \approx w_2 &= w_1 + hf(t_1, w_1) \\
&= 0.500 + 0.5 \times f(0.5, 0.500) \\
&= 0.5000 + 0.5 \times 0.357 = 0.678.
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.000) \\
&= e^{-0.0} - 0.000^2 \\
&= 1.000
\end{aligned}
$$

$$
\begin{aligned}
f(t_1, w_1) &= f(0.5, 0.500) \\
&= e^{-0.5} - 0.500^2 \\
&= 0.607 - 0.250 \\
&= 0.357
\end{aligned}
$$

Euler's method

Example Solve $\mathrm{d}y/\mathrm{d}t = f(t,y) := e^{-t} - y^2$ with $y(0) = 0$ up to time 1.

Take $n = 2$ steps, each with step size $h = 0.5$.

Times $t_0 = 0$, $t_1 = t_0 + h = 0.5$, $t_2 = t_1 + h = 1.0$.

Initialise $w_0 = y(t_0) = y(0) = 0.000$. Solution is $y(1) = y(t_2) \approx w_2$

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y(0.5) \approx w_1 &= w_0 + h f(t_0, w_0) \\
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&= e^{-0.0} - 0.000^2 \\
&= 1.000
\end{aligned}
$$

$$
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f(t_1, w_1) &= f(0.5, 0.500) \\
&= e^{-0.5} - 0.500^2 \\
&= 0.607 - 0.250 \\
&= 0.357
\end{aligned}
$$

Better approximation, absolute error ≈ 0.17; relative error 35%.

Euler's method

Example   Use fixed step size $h = 0.2$:

i	t_i	w_i	$f(t_i, w_i)$	$w_i + h f(t_i, w_i)$
0	0.00000	0.00000	1.00000	0.20000
1	0.20000	0.20000	0.77873	0.35575
2	0.40000	0.35575	0.54376	0.46450
3	0.60000	0.46450	0.33305	0.53111
4	0.80000	0.53111	0.16725	0.56456
5	1.00000	0.56456		

Better approximation; absolute error $|w_5 - y(1.0)| \approx 0.061$, relative error 12%.

With step size $h = 0.1$, find $y(1.0) \approx w_{10} = 0.5329$, relative error 5.8%.

Error approximately halves on halving the step-size: first order method!

Error of Euler's method (Non-examinable)

Error estimate   By Taylor's theorem, $y(t + h) = y(t) + h\dot{y}(t) + \frac{1}{2}h^2\ddot{y}(\tau)$.

The first derivative of y is given by the differential equation $\dot{y}(t) = f(t, y(t))$.

The second derivative of y is given by

$$\ddot{y}(t) = \frac{d}{\mathrm{d}t}\dot{y}(t) = \frac{d}{\mathrm{d}t}f(t, y(t)) = \frac{\partial f(t, y)}{\partial t} + \frac{\partial f(t, y)}{\partial y}\frac{dy(t)}{\mathrm{d}t}$$

$$= \frac{\partial f(t, y)}{\partial t} + \frac{\partial f(t, y)}{\partial y}\, f(t, y)$$

Using notation $f_{,t} = \partial f / \partial t$ and $f_{,y} = \partial f / \partial y$ we have

$$\ddot{y}(t) = f_{,t}(t, y(t)) + f_{,y}(t, y(t))\, f(t, y(t)).$$

Obtain local error estimate

$$\left| y(t_1) - w_1 \right| = \left| \left(\cancel{y(t_0)} + \cancel{h_0\dot{y}(t_0)} + \tfrac{1}{2}h_0^2\ddot{y}(\tau) \right) - \left(\cancel{w_0} + \cancel{h_0 f(t_0, w_0)} \right) \right|$$

$$= \left| \tfrac{1}{2}h_0^2\ddot{y}(\tau) \right| = \frac{h_0^2}{2}\left| f_{,t}(\tau, y(\tau)) + f_{,y}(\tau, y(\tau))f(\tau, y(\tau)) \right|$$

$$= \frac{h_0^2}{2}\left| f_{,t}(\tau, \eta) + f_{,y}(\tau, \eta)f(\tau, \eta) \right| \text{ for some } \tau, \eta.$$

Euler's method

Theorem (Local error bound for Euler's method)   Let y be the solution of the differential equation $\mathrm{d}y/\mathrm{d}t = f(t, y)$, and let

$$w_{i+1} = y(t_i) + h_i f(t_i, y(t_i))$$

be given by Euler's method.

Suppose $w_i = y(t_i)$ is exact.

Then there exists $\tau \in [t_i, t_{i+1}]$ such that

$$\left| w_{i+1} - y(t_{i+1}) \right| = \frac{1}{2} \left| f_{,t}(\tau, y(\tau)) + f_{,y}(\tau, y(\tau)) \, f(\tau, y(\tau)) \right| h_i^2.$$

In particular, if $y(t) \in [y_{\min}, y_{\max}]$ for all $t \in [t_i, t_{i+1}]$, and

$$\left| f_{,t}(\tau, \eta) + f_{,y}(\tau, \eta) \, f(\tau, \eta) \right| \leq M$$

for all $\tau \in [t_i, t_{i+1}]$ and $\eta \in [y_{\min}, y_{\max}]$, then

$$\left| w_{i+1} - y(t_{i+1}) \right| \leq \frac{M}{2} h_i^2 = O(h_i^2).$$

Euler's method

Growth of global errors   Need to approximate y at some *fixed* time t_f.

For steps size h, require $N = (t_f - t_0)/h$ steps.

For $i \geq 1$, $y(t_i) \neq w_i$, so error $w_{i+1} - y(t_{i+1})$ contains errors *accumulated* from previous time steps.

If $f_{,y}(\tau, \eta) \leq L$, then error e_i at time t_i satisfies $|e_{i+1}| \leq e^{-h_i L} |e_i|$ *if the step is exact.*

Theorem (Error bound for Euler's method)   If
$$f_{,y}(\tau, \eta) \leq L \text{ and } \left| f_{,t}(\tau, \eta) + f_{,y}(\tau, \eta)\, f(\tau, \eta) \right| \leq M$$
for all $\tau \in [0, T]$ and $\eta \in [y_{\min}, y_{\max}]$, then for a fixed step size $h = T/N$ and for all $i \leq N$,
$$|w_i - y(t_i)| \leq h\, \frac{M}{2}\, \frac{\exp(LT) - 1}{L}\,.$$
Although *local* (single-step) error is $O(h^2)$, *global* error (up to a fixed time) is $O(h)$, since we require $O(1/h)$ steps.

Second-order Taylor method (Non-examinable)

Second-order Taylor method   Use second-order term in Taylor expansion to improve Euler's method.

$$y(t + h) \approx y(t) + hf(t, y) + \tfrac{1}{2}h^2\big(f_{,t}(t, y) + f_{,y}(t, y)f(t, y)\big),$$

so take

$$w_{i+1} = w_i + h_i f(t_i, w_i) + \tfrac{1}{2}h_i^2\big(f_{,t}(t_i, w_i) + f_{,y}(t_i, w_i)f(t_i, w_i)\big).$$

Second-order Taylor method (Non-examinable)

Example   Let $f(t, y) = e^{-t} - y^2$, so $f_{,t}(t, y) = -e^{-t}$ and $f_{,y}(t, y) = -2y$. Initial condition $y(0) = 0$.

For step size $h = 1.0$,
$$f(0.0, 0.000) = 1.000, \quad f_{,t}(0.0, 0.000) = -1.000, \quad f_{,y}(0.0, 0.000) = 0.000;$$
$$y(1.0) \approx w_1 = w_0 + hf(t_0, w_0) + \tfrac{1}{2}h^2\big(f_{,t}(t_0, w_0) + f_{,y}(t_0, w_0)f(t_0, w_0)\big)$$
$$= 0.0000 + 1.0 \times 1.0000 + \tfrac{1}{2} \times 1.0^2 \times (-1.0000 + 0.0000 \times 1.0000)$$
$$= 0.0000 + 1.0000 - 0.5000 = 0.5000$$

Relative error 0.7%, much better!

Second-order Taylor method (Non-examinable)

Example Let $f(t, y) = e^{-t} - y^2$, so $f_{,t}(t, y) = -e^{-t}$ and $f_{,y}(t, y) = -2y$. Initial condition $y(0) = 0$.

For step size $h = 0.5$,

$$
\begin{aligned}
y(0.5) \approx w_1 &= w_0 + hf(t_0, w_0) + \tfrac{1}{2}h^2\big(f_{,t}(t_0, w_0) + f_{,y}(t_0, w_0)f(t_0, w_0)\big) \\
&= 0.0000 + 0.5 \times 1.0000 + \tfrac{1}{2} \times 0.5^2 \times \big(-1.0000 + 0.0000 \times 1.0000\big) \\
&= 0.3750.
\end{aligned}
$$

$$
\begin{aligned}
y(1.0) \approx w_2 &= w_1 + hf(t_1, w_1) + \tfrac{1}{2}h^2\big(f_{,t}(t_1, w_1) + f_{,y}(t_1, w_1)f(t_1, w_1)\big) \\
&= 0.3750 + 0.5 \times 0.4659 + \tfrac{1}{2} \times 0.5^2 \times \big(-0.6065 - 0.7500 \times 0.4659\big) \\
&= 0.4885.
\end{aligned}
$$

Relative error 3%, still much better than Euler's method.

For $h = 0.2$, $y(1.0) \approx w_5 = 0.500708$, with relative error 0.52%.
For $h = 0.1$, $y(1.0) \approx w_{10} = 0.502675$, with relative error 0.13%.

Halving the step size multiplies the error by a quarter, so method is *second* order; global error $O(h^2)$.

Higher-order Taylor methods (Non-examinable)

Higher-order derivatives   Consider (for simplicity) the *autonomous* differential equation $\dot{y} = f(y)$.

Then

$$\dot{y} = f(y);$$
$$\ddot{y} = f'(y)f(y);$$
$$\dddot{y} = f''(y)f(y)^2 + f'(y)^2 f(y);$$
$$\ddddot{y} = f'''(y)f(y)^3 + 4f''(y)f'(y)f(y)^2 + f'(y)^3 f(y);$$
$$\dddddot{y} = f''''(y)f(y)^4 + 7f'''(y)f'(y)f(y)^3 + 4f''(y)^2 f(y)^3$$
$$+ 11f''(y)f'(y)^2 f(y)^2 + f'(y)^4 f(y).$$

Higher-order Taylor methods   Higher order Taylor methods can be constructed from these derivatives. e.g. third-order

$$w_{i+1} = w_i + h_i f(w_i) + \frac{h_i^2}{2} f'(w_i)f(w_i) + \frac{h_i^3}{6}\big(f''(w_i)f(w_i)^2 + f'(w_i)^2 f(w_i)\big).$$

Higher-order Taylor methods (Non-examinable)

Advantages and disadvantages of Taylor methods

Taylor methods require the computation of partial derivatives, which is inconvenient.

Taylor methods can be used to give *rigorous* bounds on local and global errors.

e.g. For the second-order Taylor method applied to $\dot{y} = f(y)$, obtain local error

$$|w_1 - y(t_1)| \leq \frac{h^3}{6} \sup_{\tau \in [t_0, t_1]} \left| \dddot{y}(\tau) \right|$$

$$\leq \frac{h^3}{6} \sup_{\eta \in [y_{\min}, y_{\max}]} \left| f''(\eta) f(\eta)^2 + f'(\eta)^2 f(\eta) \right|,$$

and global error $O(h^2)$.

Runge-Kutta Methods

Midpoint method

Midpoint method

Midpoint method   Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Midpoint method

Midpoint method Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show

$$y(t+h) = y(t) + h\,\dot{y}(t) + O(h^2); \qquad y(t+h) = y(t) + h\,\dot{y}(t+\tfrac{h}{2}) + O(h^3).$$

Midpoint method

Midpoint method   Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show

$$y(t+h) = y(t) + h\,\dot{y}(t) + O(h^2); \qquad y(t+h) = y(t) + h\,\dot{y}(t+\tfrac{h}{2}) + O(h^3).$$

Would like to use approximation

$$y(t + h) \approx y(t) + h f(t + \tfrac{h}{2}, y(t + \tfrac{h}{2})).$$

Midpoint method

Midpoint method Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show
$$y(t+h) = y(t)+h\,\dot{y}(t)+O(h^2); \qquad y(t+h) = y(t)+h\,\dot{y}(t+\tfrac{h}{2})+O(h^3).$$
Would like to use approximation
$$y(t + h) \approx y(t) + hf(t + \tfrac{h}{2}, y(t + \tfrac{h}{2})).$$
Problem: Don't know $y(t + \frac{h}{2})$.

Midpoint method

Midpoint method   Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show

$$y(t+h) = y(t) + h\,\dot{y}(t) + O(h^2); \qquad y(t+h) = y(t) + h\,\dot{y}(t+\tfrac{h}{2}) + O(h^3).$$

Would like to use approximation

$$y(t + h) \approx y(t) + hf(t + \tfrac{h}{2}, y(t + \tfrac{h}{2})).$$

Problem: Don't know $y(t + \frac{h}{2})$.

Solution: Estimate $y(t + \frac{h}{2})$ by Euler's method!

Midpoint method

Midpoint method   Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show

$$y(t+h) = y(t) + h\,\dot{y}(t) + O(h^2); \qquad y(t+h) = y(t) + h\,\dot{y}(t+\tfrac{h}{2}) + O(h^3).$$

Would like to use approximation

$$y(t + h) \approx y(t) + hf(t + \tfrac{h}{2}, y(t + \tfrac{h}{2})).$$

Problem: Don't know $y(t + \frac{h}{2})$.

Solution: Estimate $y(t + \frac{h}{2})$ by Euler's method!

$$y(t + \tfrac{h}{2}) \approx y(t) + \tfrac{h}{2} f(t, y(t))$$

Midpoint method

Midpoint method   Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show

$$y(t+h) = y(t) + h\,\dot{y}(t) + O(h^2); \qquad y(t+h) = y(t) + h\,\dot{y}(t+\tfrac{h}{2}) + O(h^3).$$

Would like to use approximation

$$y(t + h) \approx y(t) + hf(t + \tfrac{h}{2}, y(t + \tfrac{h}{2})).$$

Problem: Don't know $y(t + \frac{h}{2})$.

Solution: Estimate $y(t+\frac{h}{2})$ by Euler's method!

$$y(t+\tfrac{h}{2}) \approx y(t) + \tfrac{h}{2}f(t, y(t))$$

Then

$$y(t + h) \approx y(t) + hf\!\left(t + \tfrac{h}{2}, y(t) + \tfrac{h}{2}f(t, y(t))\right).$$

Midpoint method

Midpoint method   Expect derivative $\dot{y}(t + \frac{h}{2})$ at midpoint of interval $[t, t + h]$ to give a better approximation to the average change $\frac{1}{h}(y(t + h) - y(t))$ than derivative $\dot{y}(t)$ at left endpoint.

Can show

$$y(t+h) = y(t) + h\,\dot{y}(t) + O(h^2); \qquad y(t+h) = y(t) + h\,\dot{y}(t+\tfrac{h}{2}) + O(h^3).$$

Would like to use approximation

$$y(t + h) \approx y(t) + hf(t + \tfrac{h}{2}, y(t + \tfrac{h}{2})).$$

Problem: Don't know $y(t + \frac{h}{2})$.

Solution: Estimate $y(t+\frac{h}{2})$ by Euler's method!

$$y(t+\tfrac{h}{2}) \approx y(t) + \tfrac{h}{2}f(t, y(t))$$

Then

$$y(t + h) \approx y(t) + hf\left(t + \tfrac{h}{2}, y(t) + \tfrac{h}{2}f(t, y(t))\right).$$

Obtain midpoint method:

$$w_{i+1} = w_i + h_i f(t_i + \tfrac{1}{2}h_i,\ w_i + \tfrac{1}{2}h_i f(t_i, w_i)).$$

Midpoint method

Example   Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Midpoint method

Example Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Times $t_0 = 0.0$, $t_1 = 0.5$, $t_2 = 1.0$. $w_0 = y(t_0) = 0.000$. Solution $y(1) = y(t_2) \approx w_2$.

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$$w_1 = w_0 + hf(t_0 + \tfrac{1}{2}h, \; w_0 + \tfrac{1}{2}hf(t_0, w_0))$$

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\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.0000))
\end{aligned}
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\end{aligned}
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\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000
\end{aligned}
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Midpoint method

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&= w_0 + hf(0.0 + \tfrac{1}{2}{\times}0.5, \ 0.0000 + \tfrac{1}{2}{\times}0.5{\times}1.0000)
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&= w_0 + hf(0.25, 0.2500)
\end{aligned}
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f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000
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w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h,\ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
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&= w_0 + hf(0.25, 0.2500)
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000 \\[4pt]
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) & \\
&= f(0.25, 0.2500) \\
&= e^{-0.2500} - 0.2500^2 \\
&= 0.7788 - 0.0625 \\
&= 0.7163
\end{aligned}
$$

Midpoint method

Example   Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Times $t_0 = 0.0$, $t_1 = 0.5$, $t_2 = 1.0$. $w_0 = y(t_0) = 0.000$. Solution $y(1) = y(t_2) \approx w_2$.

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w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
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\end{aligned}
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\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000 \\[2mm]
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= f(0.25, 0.2500) \\
&= e^{-0.2500} - 0.2500^2 \\
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&= w_0 + hf(0.25, 0.2500) = 0.0000 + 0.5 \times 0.7163 \\
&= 0.3582
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000 \\[1em]
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= f(0.25, 0.2500) \\
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&= 0.3582 \\[2mm]
w_2 &= w_1 + hf(t_1 + \tfrac{1}{2}h,\ w_1 + \tfrac{1}{2}hf(t_1, w_1))
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f(t_0, w_0) &= f(0.0, 0.0000) \\
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f(t_0 + \tfrac{1}{2}h&, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
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f(t_1, w_1) &= f(0.5, 0.3582) \\
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Midpoint method

Example Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

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f(t_1, w_1) &= f(0.5, 0.3582) \\
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Midpoint method

Example Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

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&= w_1 + hf(0.5 + \tfrac{1}{2}\times 0.5, \ 0.3582 + \tfrac{1}{2}\times 0.5\times 0.4783) \\
&= w_1 + hf(0.75, 0.4777)
\end{aligned}
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\begin{aligned}
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&= 1.0000
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Midpoint method

Example Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Times $t_0 = 0.0$, $t_1 = 0.5$, $t_2 = 1.0$. $w_0 = y(t_0) = 0.000$. Solution $y(1) = y(t_2) \approx w_2$.

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w_2 &= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
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&= w_1 + hf(0.75, 0.4777)
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000
\end{aligned}
$$

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\begin{aligned}
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= f(0.25, 0.2500) \\
&= e^{-0.2500} - 0.2500^2 \\
&= 0.7788 - 0.0625 \\
&= 0.7163
\end{aligned}
$$

$$
\begin{aligned}
f(t_1, w_1) &= f(0.5, 0.3582) \\
&= 0.4783
\end{aligned}
$$

$$
\begin{aligned}
f(t_1 + \tfrac{1}{2}h, w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
&= f(0.75, 0.4777) \\
&= 0.2442
\end{aligned}
$$

Midpoint method

Example   Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Times $t_0 = 0.0$, $t_1 = 0.5$, $t_2 = 1.0$. $w_0 = y(t_0) = 0.000$. Solution $y(1) = y(t_2) \approx w_2$.

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&= w_0 + hf(0.25, 0.2500) = 0.0000 + 0.5 \times 0.7163 \\
&= 0.3582
\end{aligned}
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w_2 &= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
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&= w_1 + hf(0.75, 0.4777) = 0.3582 + 0.5 \times 0.2442
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000
\end{aligned}
$$

$$
\begin{aligned}
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
= f(0.25, 0.2500) \\
= e^{-0.2500} - 0.2500^2 \\
= 0.7788 - 0.0625 \\
= 0.7163
\end{aligned}
$$

$$
\begin{aligned}
f(t_1, w_1) &= f(0.5, 0.3582) \\
&= 0.4783
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$$

$$
\begin{aligned}
f(t_1 + \tfrac{1}{2}h, w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
= f(0.75, 0.4777) \\
= 0.2442
\end{aligned}
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Midpoint method

Example Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Times $t_0 = 0.0$, $t_1 = 0.5$, $t_2 = 1.0$. $w_0 = y(t_0) = 0.000$. Solution $y(1) = y(t_2) \approx w_2$.

$$
\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.0000)) \\
&= w_0 + hf(0.0 + \tfrac{1}{2}\times 0.5, \ 0.0000 + \tfrac{1}{2}\times 0.5 \times 1.0000) \\
&= w_0 + hf(0.25, 0.2500) = 0.0000 + 0.5 \times 0.7163 \\
&= 0.3582
\end{aligned}
$$

$$
\begin{aligned}
w_2 &= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
&= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(0.5, 0.3582)) \\
&= w_1 + hf(0.5 + \tfrac{1}{2}\times 0.5, \ 0.3582 + \tfrac{1}{2}\times 0.5 \times 0.4783) \\
&= w_1 + hf(0.75, 0.4777) = 0.3582 + 0.5 \times 0.2442 \\
&= 0.4802.
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000 \\[4pt]
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= f(0.25, 0.2500) \\
&= e^{-0.2500} - 0.2500^2 \\
&= 0.7788 - 0.0625 \\
&= 0.7163 \\[4pt]
f(t_1, w_1) &= f(0.5, 0.3582) \\
&= 0.4783 \\[4pt]
f(t_1 + \tfrac{1}{2}h, w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
&= f(0.75, 0.4777) \\
&= 0.2442
\end{aligned}
$$

Midpoint method

Example   Solve $\dot{y} = e^{-t} - y^2$ with $y(0) = 0$ up to $t = 1$ using $h = 0.5$.

Times $t_0 = 0.0$, $t_1 = 0.5$, $t_2 = 1.0$. $w_0 = y(t_0) = 0.000$. Solution $y(1) = y(t_2) \approx w_2$.

$$
\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.0000)) \\
&= w_0 + hf(0.0 + \tfrac{1}{2} \times 0.5, \ 0.0000 + \tfrac{1}{2} \times 0.5 \times 1.0000) \\
&= w_0 + hf(0.25, 0.2500) = 0.0000 + 0.5 \times 0.7163 \\
&= 0.3582
\end{aligned}
$$

$$
\begin{aligned}
w_2 &= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
&= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(0.5, 0.3582)) \\
&= w_1 + hf(0.5 + \tfrac{1}{2} \times 0.5, \ 0.3582 + \tfrac{1}{2} \times 0.5 \times 0.4783) \\
&= w_1 + hf(0.75, 0.4777) = 0.3582 + 0.5 \times 0.2442 \\
&= 0.4802.
\end{aligned}
$$

$$
\begin{aligned}
f(t_0, w_0) &= f(0.0, 0.0000) \\
&= 1.0000 \\[4pt]
f(t_0 + \tfrac{1}{2}h, w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= f(0.25, 0.2500) \\
&= e^{-0.2500} - 0.2500^2 \\
&= 0.7788 - 0.0625 \\
&= 0.7163 \\[4pt]
f(t_1, w_1) &= f(0.5, 0.3582) \\
&= 0.4783 \\[4pt]
f(t_1 + \tfrac{1}{2}h, w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
&= f(0.75, 0.4777) \\
&= 0.2442
\end{aligned}
$$

Exact value $y(1) = 0.503347$ (6 sf).

Relative error 4.5%, better than 12% for Euler's method with $h = 0.2$.

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:
$$w_1 = w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0))$$

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:

$$w_1 = w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0))$$
$$= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.00000))$$

Midpoint method

Example For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:

$$
\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \; w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \; w_0 + \tfrac{1}{2}hf(0.0, 0.00000)) \\
&= w_0 + hf(0.0 + \tfrac{1}{2}\times 0.1, \; 0.00000 + \tfrac{1}{2}\times 0.1 \times 1.0000)
\end{aligned}
$$

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:

$$
\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.00000)) \\
&= w_0 + hf(0.0 + \tfrac{1}{2} \times 0.1, \ 0.00000 + \tfrac{1}{2} \times 0.1 \times 1.0000) \\
&= w_0 + hf(0.05, 0.05000)
\end{aligned}
$$

Midpoint method

Example For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:

$$
\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.00000)) \\
&= w_0 + hf(0.0 + \tfrac{1}{2}\times 0.1, \ 0.00000 + \tfrac{1}{2}\times 0.1 \times 1.0000) \\
&= w_0 + hf(0.05, 0.05000) \\
&= 0.0000 + 0.1 \times 0.9487 = 0.09487
\end{aligned}
$$

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.

Work to machine precision, display w_i to 4 dp:

$$
\begin{aligned}
w_1 &= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(t_0, w_0)) \\
&= w_0 + hf(t_0 + \tfrac{1}{2}h, \ w_0 + \tfrac{1}{2}hf(0.0, 0.00000)) \\
&= w_0 + hf(0.0 + \tfrac{1}{2}{\times}0.1, \ 0.00000 + \tfrac{1}{2}{\times}0.1{\times}1.0000) \\
&= w_0 + hf(0.05, 0.05000) \\
&= 0.0000 + 0.1 \times 0.9487 = 0.09487 \\
w_2 &= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(t_1, w_1)) \\
&= w_1 + hf(t_1 + \tfrac{1}{2}h, \ w_1 + \tfrac{1}{2}hf(0.1, 0.09487)) \\
&= w_1 + hf(0.1 + \tfrac{1}{2}{\times}0.1, \ 0.09487 + \tfrac{1}{2}{\times}0.1{\times}0.89584) \\
&= w_1 + hf(0.15, 0.13966) \\
&= 0.09487 + 0.1 \times 0.8412 = 0.17899.
\end{aligned}
$$

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, take step-size $h = 0.1$.
Let $t_{i+\frac{1}{2}} = t_i + \frac{1}{2}h$, $\hat{w}_{i+\frac{1}{2}} = w_i + \frac{1}{2}hf(t_i, w_i)$, $w_{i+1} = w_i + hf(t_{i+\frac{1}{2}}, \hat{w}_{i+\frac{1}{2}})$.
Work to machine precision, display w_i to 5 decimal places:

i	t_i	w_i	$f(t_i, w_i)$	$t_{i+\frac{1}{2}}$	$\hat{w}_{i+\frac{1}{2}}$	$f(t_{i+\frac{1}{2}}, \hat{w}_{i+\frac{1}{2}})$	w_{i+1}
0	0.0	0.00000	1.0000	0.05	0.05000	0.9487	0.09487
1	0.1	0.09487	0.8958	0.15	0.13966	0.8412	0.17899
2	0.2	0.17899	0.7867	0.25	0.21833	0.7311	0.25211
3	0.3	0.25211	0.6773	0.35	0.28597	0.6229	0.31440
4	0.4	0.31440	0.5715	0.45	0.34297	0.5200	0.36640
5	0.5	0.36640	0.4723	0.55	0.39001	0.4248	0.40888
6	0.6	0.40888	0.3816	0.65	0.42796	0.3389	0.44277
7	0.7	0.44277	0.3005	0.75	0.45780	0.2628	0.46905
8	0.8	0.46905	0.2293	0.85	0.48052	0.1965	0.48870
9	0.9	0.48870	0.1677	0.95	0.49709	0.1396	0.50267
10	1.0	0.50267					

Exact value $y(1) = 0.503347$; relative error 0.13%.

Midpoint method

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, approximating $y(1) = 0.503347\,(6\,\text{sf})$ with different step-sizes gives

n	1	2	5	10
h	1.0	0.5	0.2	0.1
$y(1.0) \approx w_n$	0.356531	0.480228	0.500418	0.502666
error	29%	4.6%	0.58%	0.14%

The midpoint method is *second-order*, with global errors $O(h^2)$.

Modified Euler (trapezoid) method

Modified Euler (trapezoid) method   Trapezoid rule gives

$$y(t+h) = y(t) + \tfrac{h}{2}\big(\dot{y}(t) + \dot{y}(t+h)\big) + O(h^3).$$

Estimate $y(t+h)$ by Euler's method, $y(t+h) \approx y(t) + hf(t, y(t))$.
Then

$$y(t+h) \approx y(t) + \tfrac{1}{2}h\big(f(t, y(t)) + f(t+h, y(t)+hf(t, y(t)))\big).$$

Obtain *modified Euler* (trapezoid) method:

$$w_{i+1} = w_i + \tfrac{1}{2}h_i\big(f(t_i, w_i) + f(t_i+h_i, w_i+h_i f(t_i, w_i))\big).$$

Example   For $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, approximating $y(1) = 0.503347\,(6\,\text{sf})$
with different step-sizes gives

n	1	2	5	10
h	1.0	0.5	0.2	0.1
w_n	0.183940	0.468458	0.499972	0.502639
error	63%	6.9%	0.67%	0.14%

Second-order Runge-Kutta methods

General second-order Runge-Kutta method

$$y(t + h) \approx y(t) + h\big(a_1 f(t, y(t)) + a_2 f(t + \alpha h, y(t) + \beta h f(t, y(t)))\big)$$

Differentiate with respect to h:

$$\dot{y}(t + h) = \big(a_1 f(t, y(t)) + a_2 f(t + \alpha h, y(t) + \beta h f(t, y(t)))\big)$$
$$+ h a_2 \big(\alpha f_{,t}(t + \alpha h, y + \beta h f(t, y)) + \beta f_{,y}(t + \alpha h, y + \beta h f(t, y)) f(t, y)\big)$$

Hence

$$\dot{y}(t) = a_1 f(t, y) + a_2 f(t, y) = (a_1 + a_2) f(t, y)$$
$$\ddot{y}(t) = 2 a_2 \big(\alpha f_{,t}(t, y) + \beta f_{,y}(t, y) f(t, y)\big)$$

From Taylor's theorem,

$$\dot{y}(t) = f(t, y); \quad \ddot{y}(t) = f_{,t}(t, y) + f_{,y}(t, y) f(t, y).$$

Comparing coefficients gives $a_1 + a_2 = 1$ and $2 a_2 \alpha = 2 a_2 \beta = 1$, so

$$\beta = \alpha \quad \text{and} \quad a_1 = 1 - 1/2\alpha, \ a_2 = 1/2\alpha.$$

Obtain method

$$w_{i+1} = w_i + h_i \big((1 - \tfrac{1}{2\alpha}) f(t_i, w_i) + \tfrac{1}{2\alpha} f(t_i + \alpha h_i, w_i + \alpha h_i f(t_i, w_i))\big)$$

Ralston's method

General second-order Runge-Kutta method

$$w_{i+1} = w_i + h_i\big((1 - \tfrac{1}{2\alpha})f(t_i, w_i) + \tfrac{1}{2\alpha}f(t_i + \alpha h_i, w_i + \alpha h_i f(t_i, w_i))\big)$$

Midpoint and modified Euler methods

Taking $\alpha = \tfrac{1}{2}$ gives the midpoint method with $a_1 = 0$, $a_2 = 1$.

Taking $\alpha = 1$ gives the modified Euler method with $a_1 = a_2 = \tfrac{1}{2}$.

Ralston's Method

Taking $\alpha = \tfrac{2}{3}$ gives $a_2 = \tfrac{3}{4}$, $a_1 = \tfrac{1}{4}$ and

$$w_{i+1} = w_i + \tfrac{1}{4}h_i\big(f(t_i, w_i) + 3f(t_i + \tfrac{2}{3}h_i, w_i + \tfrac{2}{3}h_i f(t_i, w_i))\big)$$

This can be written in a standard form for Runge-Kutta methods:

$$k_{i,1} = h_i f(t_i, w_i);$$
$$k_{i,2} = h_i f(t_i + \tfrac{2}{3}h_i, w_i + \tfrac{2}{3}k_{i,1});$$
$$w_{i+1} = w_i + \tfrac{1}{4}\big(k_{i,1} + 3k_{i,2}\big) = w_i + \tfrac{1}{4}k_{i,1} + \tfrac{3}{4}k_{i,2}$$
$$= w_i + k_i \text{ where } k_i = \tfrac{1}{4}k_{i,1} + \tfrac{3}{4}k_{i,2}.$$

Runge-Kutta Methods

Example $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$. Step size $h = 0.1$.

	$y(0.1)$	$y(1.0)$
Euler	0.100000000000000	0.53290486346010
Midpoint	0.0948729424500714	0.502665926212565
Trapezoid	0.0947418709017980	0.50263870657163
Ralston	0.0948296905440380	0.502658823715687
Exact	$0.094854320\cdots$	$0.5033467\cdots$

Third-order Runge-Kutta methods

Heun's third-order method

$$k_{i,1} = h_i f(t_i, w_i);$$
$$k_{i,2} = h_i f(t_i + \tfrac{1}{3}h_i, w_i + \tfrac{1}{3}k_{i,1});$$
$$k_{i,3} = h_i f(t_i + \tfrac{2}{3}h_i, w_i + \tfrac{2}{3}k_{i,2});$$

$$w_{i+1} = w_i + \tfrac{1}{4}\big(k_{i,1} + 3k_{i,3}\big).$$

Local error $O(h^4)$, global error $O(h^3)$.

Kutta's third-order method

$$k_{i,1} = h_i f(t_i, w_i);$$
$$k_{i,2} = h_i f(t_i + \tfrac{1}{2}h_i, w_i + \tfrac{1}{2}k_{i,1});$$
$$k_{i,3} = h_i f(t_i + h_i, w_i - k_{i,1} + 2k_{i,2});$$

$$w_{i+1} = w_i + \tfrac{1}{6}\big(k_{i,1} + 4k_{i,2} + k_{i,3}\big).$$

Third-order Runge-Kutta methods

General third-order method (Non-examinable)

$$k_{i,1} = h_i f(t_i, w_i);$$

$$k_{i,2} = h_i f(t_i + c_2 h_i, w_i + a_{21} k_{i,1});$$

$$k_{i,3} = h_i f(t_i + c_3 h_i, w_i + a_{31} k_{i,1} + a_{32} k_{i,2});$$

$$w_{i+1} = w_i + \left(b_1 k_{i,1} + b_2 k_{i,2} + b_3 k_{i,3} \right).$$

where

$$b_1 + b_2 + b_3 = 1; \ c_2 b_2 + c_3 b_2 = \tfrac{1}{2}; \ c_2^2 b_2 + c_3^2 b_3 = \tfrac{1}{3};$$

$$c_2 = a_{21}; \ c_3 = a_{31} + a_{32}; \ c_2 b_3 a_{32} = \tfrac{1}{6}.$$

Can choose c_2, c_3 freely. Then

$$b_3 = (3c_2 - 2)/6c_3(c_2 - c_3), \ b_2 = (3c_3 - 2)/6c_2(c_3 - c_2), \ b_1 = 1 - b_2 - b_3,$$

$$a_{32} = 1/6c_2 b_3, \ a_{31} = c_3 - a_{32}, \ a_{21} = c_2.$$

Classical fourth-order Runge-Kutta method

Classical fourth-order Runge-Kutta method

$$k_{i,1} = h_i f(t_i, w_i);$$

$$k_{i,2} = h_i f(t_i + \tfrac{1}{2} h_i, w_i + \tfrac{1}{2} k_{i,1});$$

$$k_{i,3} = h_i f(t_i + \tfrac{1}{2} h_i, w_i + \tfrac{1}{2} k_{i,2});$$

$$k_{i,4} = h_i f(t_i + h_i, w_i + k_{i,3});$$

$$w_{i+1} = w_i + \tfrac{1}{6}(k_{i,1} + 2k_{i,2} + 2k_{i,3} + k_{i,4})$$

Local error $O(h^5)$, global error $O(h^4)$.

May set $k_i = \tfrac{1}{6}(k_{i,1} + 2k_{i,2} + 2k_{i,3} + k_{i,4})$, so $w_{i+1} = w_i + k_i$.

Often drop the subscript i:

$$k_1 = h f(t, w); \qquad k_2 = h f(t + \tfrac{1}{2} h, w + \tfrac{1}{2} k_1);$$

$$k_3 = h f(t + \tfrac{1}{2} h, w + \tfrac{1}{2} k_2); \qquad k_4 = h f(t + h, w + k_3);$$

$$w' = w + \tfrac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Fourth-order Runge-Kutta methods

Fourth-order Runge-Kutta method

$$k_{i,1} = h_i f(t_i, w_i);$$
$$k_{i,2} = h_i f(t_i + \tfrac{1}{3} h_i, w_i + \tfrac{1}{3} k_{i,1});$$
$$k_{i,3} = h_i f(t_i + \tfrac{2}{3} h_i, w_i - \tfrac{1}{3} k_{i,1} + k_{i,2});$$
$$k_{i,4} = h_i f(t_i + h_i, w_i + k_{i,1} - k_{i,2} + k_{i,3});$$
$$w_{i+1} = w_i + \tfrac{1}{8}(k_{i,1} + 3k_{i,2} + 3k_{i,3} + k_{i,4})$$

Local error $O(h^5)$, global error $O(h^4)$.

May set $k_i = \tfrac{1}{8}(k_{i,1} + 3k_{i,2} + 3k_{i,3} + k_{i,4})$, so $w_{i+1} = w_i + k_i$.

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Fourth-order Runge-Kutta methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Initialise $t_0 = 0.0,\ w_0 = y(t_0) = y(0) = 0.0000$.

Fourth-order Runge-Kutta methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Initialise $t_0 = 0.0$, $w_0 = y(t_0) = y(0) = 0.0000$.

First step $h_0 = h = 0.5$, $t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Initialise $t_0 = 0.0$, $w_0 = y(t_0) = y(0) = 0.0000$.

First step $h_0 = h = 0.5$, $t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

$$
\begin{aligned}
k_{0,1} &= h_0 f(t_0, w_0) = 0.5 f(0.00, 0.0000) \\
&= 0.5 \times f(0.00, 0.0000) = 0.5 \times 1.0000 = 0.5000
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Initialise $t_0 = 0.0, \ w_0 = y(t_0) = y(0) = 0.0000$.

First step $h_0 = h = 0.5, \ t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

$$
\begin{aligned}
k_{0,1} &= h_0 f(t_0, w_0) = 0.5 f(0.00, 0.0000) \\
&= 0.5 \times f(0.00, 0.0000) = 0.5 \times 1.0000 = 0.5000 \\
k_{0,2} &= h_0 f(t_0 + \tfrac{1}{2} h_0, w_0 + \tfrac{1}{2} k_{0,1}) = 0.5 f(0.0 + \tfrac{1}{2} \times 0.5, 0.0000 + \tfrac{1}{2} \times 0.5000) \\
&= 0.5 \times f(0.25, 0.2500) = 0.5 \times 0.7163 = 0.3582
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Initialise $t_0 = 0.0, \ w_0 = y(t_0) = y(0) = 0.0000$.

First step $h_0 = h = 0.5, \ t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

$$
\begin{aligned}
k_{0,1} &= h_0 f(t_0, w_0) = 0.5 f(0.00, 0.0000) \\
&= 0.5 \times f(0.00, 0.0000) = 0.5 \times 1.0000 = 0.5000 \\
k_{0,2} &= h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,1}) = 0.5 f(0.0 + \tfrac{1}{2} \times 0.5, 0.0000 + \tfrac{1}{2} \times 0.5000) \\
&= 0.5 \times f(0.25, 0.2500) = 0.5 \times 0.7163 = 0.3582 \\
k_{0,3} &= h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,2}) = 0.5 f(0.0 + \tfrac{1}{2} \times 0.5, 0.0000 + \tfrac{1}{2} \times 0.3582) \\
&= 0.5 \times f(0.25, 0.1791) = 0.5 \times 0.7467 = 0.3734
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

Initialise $t_0 = 0.0$, $w_0 = y(t_0) = y(0) = 0.0000$.

First step $h_0 = h = 0.5$, $t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

$$
\begin{aligned}
k_{0,1} &= h_0 f(t_0, w_0) = 0.5 f(0.00, 0.0000) \\
&= 0.5 \times f(0.00, 0.0000) = 0.5 \times 1.0000 = 0.5000 \\
k_{0,2} &= h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,1}) = 0.5 f(0.0 + \tfrac{1}{2}\times 0.5, 0.0000 + \tfrac{1}{2}\times 0.5000) \\
&= 0.5 \times f(0.25, 0.2500) = 0.5 \times 0.7163 = 0.3582 \\
k_{0,3} &= h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,2}) = 0.5 f(0.0 + \tfrac{1}{2}\times 0.5, 0.0000 + \tfrac{1}{2}\times 0.3582) \\
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k_{0,4} &= h_0 f(t_0 + h_0, w_0 + k_{0,3}) = 0.5 f(0.0 + 0.5, 0.0000 + 0.3734) \\
&= 0.5 \times f(0.50, 0.3734) = 0.5 \times 0.4671 = 0.2336
\end{aligned}
$$

Fourth-order Runge-Kutta methods

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Initialise $t_0 = 0.0$, $w_0 = y(t_0) = y(0) = 0.0000$.

First step $h_0 = h = 0.5$, $t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

$$k_{0,1} = h_0 f(t_0, w_0) = 0.5 f(0.00, 0.0000)$$
$$= 0.5 \times f(0.00, 0.0000) = 0.5 \times 1.0000 = 0.5000$$
$$k_{0,2} = h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,1}) = 0.5 f(0.0 + \tfrac{1}{2} \times 0.5, 0.0000 + \tfrac{1}{2} \times 0.5000)$$
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$$= 0.5 \times f(0.50, 0.3734) = 0.5 \times 0.4671 = 0.2336$$
$$k_0 = \tfrac{1}{6}(k_{0,1} + 2k_{0,2} + 2k_{0,3} + k_{0,4})$$
$$= \tfrac{1}{6}(0.5000 + 2 \times 0.3582 + 2 \times 0.3734 + 0.2336) = 0.3661$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

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First step $h_0 = h = 0.5, \ t_1 = t_0 + h_0 = 0.0 + 0.5 = 0.5$.

$$
\begin{aligned}
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k_{0,2} &= h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,1}) = 0.5 f(0.0 + \tfrac{1}{2}\times 0.5, 0.0000 + \tfrac{1}{2}\times 0.5000) \\
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k_0 &= \tfrac{1}{6}(k_{0,1} + 2k_{0,2} + 2k_{0,3} + k_{0,4}) \\
&= \tfrac{1}{6}(0.5000 + 2\times 0.3582 + 2\times 0.3734 + 0.2336) = 0.3661 \\
w_1 &= w_0 + k_0 = 0.0000 + 0.3661 = 0.3661
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

First step gave $t_1 = 0.5, \ w_1 = 0.3661$.

Fourth-order Runge-Kutta methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

First step gave $t_1 = 0.5, \; w_1 = 0.3661$.

Second step $h_1 = h = 0.5, \; t_2 = t_1 + h_1 = 0.5 + 0.5 = 1.0$.

Fourth-order Runge-Kutta methods

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$$
\begin{aligned}
k_{1,1} = h_1 f(t_1, w_1) &= 0.5 f(0.50, 0.3661) \\
&= 0.5 \times f(0.50, 0.3661) = 0.5 \times 0.4725 = 0.2363
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Fourth-order Runge-Kutta methods

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First step gave $t_1 = 0.5, \ w_1 = 0.3661$.

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k_{1,2} &= h_1 f(t_1 + \tfrac{1}{2}h_1, w_1 + \tfrac{1}{2}k_{1,1}) = 0.5 f(0.5 + \tfrac{1}{2} \times 0.5, 0.3661 + \tfrac{1}{2} \times 0.2363) \\
&= 0.5 \times f(0.75, 0.4842) = 0.5 \times 0.2379 = 0.1189
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

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&= 0.5 \times f(0.75, 0.4256) = 0.5 \times 0.2913 = 0.1456
\end{aligned}
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Fourth-order Runge-Kutta methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

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k_{1,4} &= h_1 f(t_1 + h_1, w_1 + k_{1,3}) = 0.5 f(0.5 + 0.5, 0.3661 + 0.1456) \\
&= 0.5 \times f(1.00, 0.5117) = 0.5 \times 0.1060 = 0.0530
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

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k_1 &= \tfrac{1}{6}(k_{1,1} + 2k_{1,2} + 2k_{1,3} + k_{1,4}) \\
&= \tfrac{1}{6}(0.2363 + 2 \times 0.1189 + 2 \times 0.1456 + 0.0530) = 0.1365
\end{aligned}
$$

Fourth-order Runge-Kutta methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$ with $y(0) = 0$ using $h = 0.5$.

First step gave $t_1 = 0.5$, $w_1 = 0.3661$.

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k_{1,2} &= h_1 f(t_1 + \tfrac{1}{2} h_1, w_1 + \tfrac{1}{2} k_{1,1}) = 0.5 f(0.5 + \tfrac{1}{2} \times 0.5, 0.3661 + \tfrac{1}{2} \times 0.2363) \\
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k_1 &= \tfrac{1}{6}(k_{1,1} + 2k_{1,2} + 2k_{1,3} + k_{1,4}) \\
&= \tfrac{1}{6}(0.2363 + 2 \times 0.1189 + 2 \times 0.1456 + 0.0530) = 0.1365
\end{aligned}
$$

$$
y(1) \approx w_2 = w_1 + k_1 = 0.3661 + 0.1365 = 0.5025
$$

Fourth-order Runge-Kutta methods

Example $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$. Take $h = 0.5$. Take two steps. Calulate:

i	t_i	w_i	$k_{i,1}$	$k_{i,2}$	$k_{i,3}$	$k_{i,4}$	k_i
0	0.0	0.000000	0.500000	0.358150	0.373366	0.233564	0.366100
1	0.5	0.366100	0.236251	0.118946	0.145627	0.053008	0.136401
2	1.0	0.502501					

Exact value $y(1) = 0.503347\,(6\,\text{dp})$; relative error 0.17%.

Fourth-order Runge-Kutta methods

Example   Take $h = 0.2$.

$$k_{0,1} = h_0 f(t_0, w_0)$$
$$= 0.2 f(0.0, 0.00000) = 0.2 \times 1.00000 = 0.20000$$
$$k_{0,2} = h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,1})$$
$$= 0.2 f(0.1, 0.10000) = 0.2 \times 0.89484 = 0.17897$$
$$k_{0,3} = h_0 f(t_0 + \tfrac{1}{2}h_0, w_0 + \tfrac{1}{2}k_{0,2})$$
$$= 0.2 f(0.1, 0.08948) = 0.2 \times 0.89683 = 0.17937$$
$$k_{0,4} = h_0 f(t_0 + h_0, w_0 + k_{0,3}) = 0.5 f(0.2, 0.17937)$$
$$= 0.2 \times 0.78656 = 0.15731$$
$$k_0 = \tfrac{1}{6}(k_{0,1} + 2k_{0,2} + 2k_{0,3} + k_{0,4})$$
$$= \tfrac{1}{6}(0.20000 + 2 \times 0.17897 + 2 \times 0.17937 + 0.15731)$$
$$= 0.17900$$
$$w_1 = w_0 + k_0 = 0.0000 + 0.17900 = 0.17900$$

Fourth-order Runge-Kutta methods

Example   Take $h = 0.2$.

i	t_i	w_i	$k_{i,1}$	$k_{i,2}$	$k_{i,3}$	$k_{i,4}$	k_i
0	0.0	0.00000	0.20000	0.17897	0.17937	0.15731	0.17900
1	0.2	0.17900	0.15734	0.13489	0.13602	0.11422	0.13556
2	0.4	0.31456	0.11427	0.09367	0.09519	0.07618	0.09470
3	0.6	0.40925	0.07626	0.05929	0.06079	0.04568	0.06035
4	0.8	0.46960	0.04576	0.03281	0.03407	0.02284	0.03373
5	1.0	0.50333					

Higher-order Runge-Kutta methods

Low order methods   For $n = 1, 2, 3, 4$, there are methods of order n requiring n function evaluations per time step.

Higher order methods   At least *six* function evaluations are needed for a *fifth* order method.

Even more evaluations are needed for higher orders.

Choice of order   Fourth-order methods usually provide a good balance between accuracy and efficiency.

Comparison of Runge-Kutta methods

Comparison $\dot{y}(t) = e^{-t} - y^2, y(0) = 0.$

	h	$y(0.1)$	$y(1.0)$	N_f	e_{rel}
Euler	0.2		0.564559864473071	5	1.2×10^{-1}
Ralston2	0.2		0.500286600094707	10	6.1×10^{-3}
Heun3	0.2		0.503415367048022	15	1.4×10^{-4}
RK4	0.2		0.503328891202093	20	3.6×10^{-5}
Euler	0.1	0.100000000000000	0.532904863460103	10	5.9×10^{-2}
Ralston2	0.1	0.094829690544380	0.502658823715687	20	1.3×10^{-3}
Heun3	0.1	0.094851904260542	0.503354541136427	30	1.5×10^{-5}
RK4	0.1	0.094854151051763	0.50334561387307	40	2.8×10^{-6}
Euler	0.025	0.096146975265123	0.510557320425266	40	1.4×10^{-2}
Ralston2	0.05	0.094849139693260	0.503183407918572	40	1.6×10^{-4}
Heun3	0.077		0.503350170836445	39	6.3×10^{-6}
RK4	0.1	0.094854151051763	0.50334561387307	40	1.0×10^{-6}
Exact		$0.094854320\cdots$	$0.5033467\cdots$		

Multistep Methods

Multistep methods

Idea Use information from previous (t_j, w_j).

Stages An n-stage multistep method computes w_{i+1} using $w_i, \ldots, w_{i-n+1}$.

General form The general form of an n-stage *linear* multistep method is

$$w_{i+1} = \sum_{j=0}^{n-1} a_j w_{i-k} + h \sum_{j=0}^{n-1} b_j f(t_{i-j}, w_{i-j}).$$

Adams-Bashforth methods

Derivation

$$y(t_i + h_i) = y(t_i) + \int_{t_i}^{t_i+h_i} \dot{y}(\tau)\, d\tau = y(t_i) + \int_{t_i}^{t_i+h_i} f(\tau, y(\tau))\, d\tau$$

Find a polynomial $p(\tau)$ approximating $f(\tau, y(\tau))$ over $[t_i, t_i + h_i]$.
Estimate $p(\tau)$ by interpolating $f(\tau, y(\tau))$ at $\tau = t_i, t_{i-1}, t_{i-2}, \ldots, t_{i-k+1}$.

Linear interpolation at (t_i, w_i) and (t_{i-1}, w_{i-1}) gives

$$p(\tau) = f(t_i, w_i) + \frac{(\tau - t_i)}{h_{i-1}}\big(f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Then for equally-sized steps,

$$y(t_{i+1}) \approx w_{i+1} = w_i + \int_{t_i}^{t_i+h} f(t_i, w_i) + \frac{(\tau - t_i)}{h}\big(f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)\, d\tau$$

$$= w_i + hf(t_i, w_i) + \tfrac{1}{2}h\big(f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

$$= w_i + \tfrac{1}{2}h\big(3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Adams-Bashforth methods

Two-stage Adams-Bashforth method

$$w_{i+1} = w_i + \tfrac{1}{2}h\big(3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big).$$

Local error $E = \frac{5}{12}h^3 y^{(3)}(\tau)$ for some $\tau \in (t_{i-1}, t_{i+1})$.
Global error $O(h^2)$; second-order.

Three-stage Adams-Bashforth method

$$w_{i+1} = w_i + \tfrac{1}{12}h\big(23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})\big).$$

Local error $E = \frac{3}{8}h^4 y^{(4)}(\tau)$ for some $\tau \in (t_{i-2}, t_{i+1})$.
Global error $O(h^3)$; third-order.

Four-stage Adams-Bashforth method

$$w_{i+1} = w_i + \tfrac{1}{24}h\big(55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1})$$
$$+ 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})\big).$$

Local error $E = \frac{251}{720}h^5 y^{(5)}(\tau)$. Global error $O(h^4)$; fourth-order.

Bootstrapping multistep methods

Bootstrapping   The first step(s) of a multistep method require w_i for $i < 0$ which is not available.

e.g.Two-stage Adams-Bashforth:
$$w_1 = w_0 + \tfrac{1}{2}h\big(3f(t_0, w_0) - f(t_{-1}, w_{-1})\big)$$
Use a Runge-Kutta method *of the same order* (or higher) to start the multistep method.

Multistep methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$ at $t = 1$ using the two-stage Adams-Bashforth method with $h = 0.5$. Booststrap using a second-order method.

Multistep methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$ at $t = 1$ using the two-stage Adams-Bashforth method with $h = 0.5$. Booststrap using a second-order method.

Bootstrap using Ralston's second-order method:

Multistep methods

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Bootstrap using Ralston's second-order method:
$$f(t_0, w_0) = f(0.0, 0.0000) = 1.0000,$$

Multistep methods

Example Solve $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$ at $t = 1$ using the two-stage Adams-Bashforth method with $h = 0.5$. Booststrap using a second-order method.

Bootstrap using Ralston's second-order method:

$$f(t_0, w_0) = f(0.0, 0.0000) = 1.0000,$$

$$f\left(t_0 + \tfrac{2}{3}h_0, w_0 + \tfrac{2}{3}h_0 f(t_0, w_0)\right) = f(0.\dot{3}, 0.3333) = 0.6054,$$

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$$= 0.3520 + \tfrac{1}{2} \times 0.5 \times (3 \times 0.48260 - 1.0000) = 0.4640.$$

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Take one step of the Adams-Bashforth method to find w_2:

$$y(1.0) \approx w_2 = w_1 + \tfrac{1}{2}h\left(3f(t_1, w_1) - f(t_0, w_0)\right)$$
$$= 0.3520 + \tfrac{1}{2}\times 0.5\times (3\times f(0.5, 0.3520) - f(0.0, 0.0000))$$
$$= 0.3520 + \tfrac{1}{2}\times 0.5\times (3\times 0.48260 - 1.0000) = 0.4640.$$

Solution $y(1) \approx 0.4640$ has absolute error 0.039, relative error 7.8%.

Multistep methods

Example   Solve $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$ at $t = 1$ using the two-stage Adams-Bashforth method with $h = 0.1$.

Booststrap using Ralston's second-order method:

$$w_1 = w_0 + \tfrac{1}{4}h_0\left(f(t_0, w_0) + 3f(t_0 + \tfrac{2}{3}h_0, w_0 + \tfrac{2}{3}h_0 f(t_0, w_0))\right).$$

Continue with the two-stage Adams-Bashforth method

$$w_{i+1} = w_i + \tfrac{1}{2}h\left(3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\right).$$

t_i	w_i	$f_i = f(t_i, w_i)$	t_i	w_i	$f_i = f(t_i, w_i)$
0.0	0.000000	1.000000	0.5	0.366485	0.472220
0.1	0.094830	0.895845	0.6	0.408752	0.381734
0.2	0.179206	0.786616	0.7	0.442401	0.300867
0.3	0.252407	0.677109	0.8	0.468444	0.229889
0.4	0.314642	0.571320	0.9	0.487884	0.168539
			1.0	0.501670	

So $y(1.0) \approx w_{10} = 0.501670$.

Absolute error 0.0017, relative error 0.33%.

Implicit Methods

Implicit methods

Idea   Use an extra *forward* interpolation condition $\dot{y}(t_{i+1}) = f(t_{i+1}, w_{i+1}))$.

Formula for w_{i+1} then depends on $f(t_{i+1}, w_{i+1})$, leading to an algebraic equation for w_{i+1} which has to be solved.

Adams-Moulton methods

Two-stage interpolation Interpolate $(t_{i-1}, f(t_{i-1}, w_{i-1}))$, $(t_i, f(t_i, w_i))$ and $(t_{i+1}, f(t_{i+1}, w_{i+1}))$. Assume equal step-size h.

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

$$+ \frac{(\tau - t_i)^2}{2h^2}\big(f(t_{i+1}, w_{i+1}) - 2f(t_i, w_i) + f(t_{i-1}, w_{i-1})\big)$$

Then

$$w_i + \int_{t_i}^{t_i+h} p(\tau)\,d\tau = w_i + hf(t_i, w_i) + \tfrac{1}{4}h\big(f(t_{i+1}, w_{i+1}) - f(t_{i-1}, w_{i-1})\big)$$

$$+ \tfrac{1}{6}h\big(f(t_{i+1}, w_{i+1}) - 2f(t_i, w_i) + f(t_{i-1}, w_{i-1})\big)$$

so

$$w_{i+1} = w_i + \tfrac{1}{12}h\big(5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Adams-Moulton methods

Two-stage implicit Adams-Moulton method

$$w_{i+1} = w_i + \tfrac{1}{12}h\big(5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Local error $E = -\tfrac{1}{24}h^4 y^{(4)}(\tau)$ for some $\tau \in (t_{i-1}, t_{i+1})$.
Global error $O(h^3)$; third-order.

Three-stage implicit Adams-Moulton method

$$w_{i+1} = w_i + \tfrac{1}{24}h\big(9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})\big)$$

Local error $E = -\tfrac{19}{720}h^5 y^{(5)}(\tau)$ for some $\tau \in (t_{i-2}, t_{i+1})$.
Global error $O(h^4)$; fourth-order.

Explicit versus implicit methods   Implicit multistep methods have higher accuracy than explicit methods of the same order. e.g.

Adams-Bashforth three-stage method local error:
$$E = \tfrac{3}{8}y^{(4)}(\tau)h^4 \text{ for some } \tau \in (t_{i-2}, t_{i+1}).$$

Adams-Moulton two-stage method local error:
$$E = -\tfrac{1}{24}y^{(4)}(\tau)h^4 \text{ for some } \tau \in (t_{i-1}, t_{i+1}).$$

Predictor-corrector approach (Advanced)

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Use an *estimate* $\tilde{w}_{i+1}$ on the right-hand side of the Adams-Moulton formula.

e.g. $\qquad w_{i+1} = w_i + \frac{1}{12}h\big(5f(t_{i+1}, \tilde{w}_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$

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Typically use an explicit Adams-Bashforth method to obtain $\tilde{w}_{i+1}$ with the same number of stages (and lower order).

$$\text{e.g.} \quad \tilde{w}_{i+1} = w_i + \tfrac{1}{2}h\big(3f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big).$$

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Theorem The combination of an n-stage Adams-Bashforth method (order n) as a predictor with an n-stage Adams-Mouton method (order $n+1$) as a corrector has order $n+1$.

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Alternatively, can use an $(n+1)$-stage Adams-Bashforth method and an n-stage Adams-Mouton method to estimate the error.

e.g. $\qquad \tilde{w}_{i+1} = w_i + \frac{1}{12}h\big(23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})\big).$

Predictor-corrector approach (Advanced)

Predictor-corrector approach

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May iterate corrector formula to improve accuracy, but improvement is usually not worth the additional effort.

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Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$. Assume $y(0.1) \approx 0.09485432$.

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Times $t_0 = 0.0$, $t_1 = 0.1$, $t_2 = 0.2, \ldots$ with $w_0 = 0.0$ and $w_1 = 0.09485432$.

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Predictor from two-stage Adams-Bashforth method:
$$\tilde{w}_2 = w_1 + \tfrac{1}{2}h\big(3f(t_1, w_1) - f(t_0, w_0)\big) = 0.17923033.$$

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$$w_{i+1} = w_i + \tfrac{1}{12}h\big(5f(t_{i+1}, \tilde{w}_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

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Corrector
$$w_2 = w_1 + \tfrac{1}{12}h\big(5f(t_2, \tilde{w}_2) + 8f(t_1, w_1) - f(t_0, w_0)\big)$$

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Times $t_0 = 0.0$, $t_1 = 0.1$, $t_2 = 0.2$, ... with $w_0 = 0.0$ and $w_1 = 0.09485432$.

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$$w_2 = w_1 + \tfrac{1}{12}h\big(5f(t_2, \tilde{w}_2) + 8f(t_1, w_1) - f(t_0, w_0)\big)$$
$$= 0.0949 + \tfrac{1}{12}\,0.1\big(5f(0.2, 0.1792) + 8f(0.1, 0.0949) - f(0.0, 0.0000)\big)$$

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$$\begin{aligned}
w_2 &= w_1 + \tfrac{1}{12}h\big(5f(t_2, \tilde{w}_2) + 8f(t_1, w_1) - f(t_0, w_0)\big) \\
&= 0.0949 + \tfrac{1}{12}\,0.1\big(5f(0.2, 0.1792) + 8f(0.1, 0.0949) - f(0.0, 0.0000)\big) \\
&= 0.0949 + \tfrac{1}{12} \times 0.1 \times \big(5 \times 0.7866 + 8 \times 0.8958 - 1.0000\big)
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&= 0.0949 + \tfrac{1}{12}\times 0.1\times\big(5\times 0.7866 + 8\times 0.8958 - 1.0000\big)\\
&= 0.17901896.
\end{aligned}$$

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Example Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Assume $y(0.1) \approx 0.09485432$.

Times $t_0 = 0.0$, $t_1 = 0.1$, $t_2 = 0.2$, ... with $w_0 = 0.0$ and $w_1 = 0.09485432$.

Predictor from two-stage Adams-Bashforth method:

$$\tilde{w}_2 = w_1 + \tfrac{1}{2}h\big(3f(t_1, w_1) - f(t_0, w_0)\big) = 0.17923033.$$

Adams-Moulton formula

$$w_{i+1} = w_i + \tfrac{1}{12}h\big(5f(t_{i+1}, \tilde{w}_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Corrector

$$
\begin{aligned}
w_2 &= w_1 + \tfrac{1}{12}h\big(5f(t_2, \tilde{w}_2) + 8f(t_1, w_1) - f(t_0, w_0)\big) \\
&= 0.0949 + \tfrac{1}{12}\,0.1\big(5f(0.2, 0.1792) + 8f(0.1, 0.0949) - f(0.0, 0.0000)\big) \\
&= 0.0949 + \tfrac{1}{12}\times 0.1\times\big(5\times 0.7866 + 8\times 0.8958 - 1.0000\big) \\
&= 0.17901896.
\end{aligned}
$$

Applying the corrector again gives 0.17902212.

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Assume $y(0.1) \approx 0.09485432$.

Times $t_0 = 0.0$, $t_1 = 0.1$, $t_2 = 0.2, \ldots$ with $w_0 = 0.0$ and $w_1 = 0.09485432$.

Predictor from two-stage Adams-Bashforth method:

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$$w_{i+1} = w_i + \tfrac{1}{12}h\big(5f(t_{i+1}, \tilde{w}_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Corrector

$$
\begin{aligned}
w_2 &= w_1 + \tfrac{1}{12}h\big(5f(t_2, \tilde{w}_2) + 8f(t_1, w_1) - f(t_0, w_0)\big) \\
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&= 0.17901896.
\end{aligned}
$$

Applying the corrector again gives 0.17902212.
Repeated application of the corrector converges to 0.17902207.

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Assume $y(0.1) \approx 0.09485432$.

Times $t_0 = 0.0$, $t_1 = 0.1$, $t_2 = 0.2$, ... with $w_0 = 0.0$ and $w_1 = 0.09485432$.

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$$w_{i+1} = w_i + \tfrac{1}{12}h\big(5f(t_{i+1}, \tilde{w}_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)$$

Corrector

$$
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w_2 &= w_1 + \tfrac{1}{12}h\big(5f(t_2, \tilde{w}_2) + 8f(t_1, w_1) - f(t_0, w_0)\big) \\
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&= 0.0949 + \tfrac{1}{12}\times 0.1 \times \big(5 \times 0.7866 + 8 \times 0.8958 - 1.0000\big) \\
&= 0.17901896.
\end{aligned}
$$

Applying the corrector again gives 0.17902212.
Repeated application of the corrector converges to 0.17902207.

The exact value is $y(0.2) = 0.17900201$ (8 sf).

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.

Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.

Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1,\ w_1 = 0.0949,\ f(t_1, w_1) = 0.8958, t_2 = 0.2,\ w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!
$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1,\ w_1 = 0.0949,\ f(t_1, w_1) = 0.8958, t_2 = 0.2,\ w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\begin{aligned}
\tilde{w}_3 &= w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big) \\
&= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big) \\
&= 0.1790 + \tfrac{1}{2}\times 0.1 \times (3\times 0.7867 - 0.8958)
\end{aligned}$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$
\begin{aligned}
\tilde{w}_3 &= w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big) \\
&= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big) \\
&= 0.1790 + \tfrac{1}{2}\times 0.1\times (3\times 0.7867 - 0.8958) = 0.25222940.
\end{aligned}
$$

Predictor-corrector approach

Example Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{2}\times 0.1\times(3\times 0.7867 - 0.8958) = 0.25222940.$$

$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{2}\times 0.1\times(3\times 0.7867 - 0.8958) = 0.25222940.$$

$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{12}\,0.1\big(5f(0.3, 0.2522) + 8f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$

Predictor-corrector approach

Example Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

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$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{2} \times 0.1 \times (3 \times 0.7867 - 0.8958) = 0.25222940.$$

$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
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Predictor-corrector approach

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Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

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$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{2}\times 0.1 \times (3\times 0.7867 - 0.8958) = 0.25222940.$$

$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{12}0.1\big(5f(0.3, 0.2522) + 8f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{12}\times 0.1 \times \big(5\times 0.6772 + 8\times 0.7867 - 0.8958\big) = 0.25221576.$$
$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$

Predictor-corrector approach

Example Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

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$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$
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Predictor-corrector approach

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$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{12}0.1\big(5f(0.3, 0.2522) + 8f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
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$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{2}0.1\big(3f(0.3, 0.2522) - f(0.2, 0.1790)\big) = 0.31446243$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{2}0.1\big(3f(0.3, 0.2522) - f(0.2, 0.1790)\big) = 0.31446243$$

$$w_4 = w_3 + \tfrac{1}{12}h\big(5f(t_4, \tilde{w}_4) + 8f(t_3, w_3) - f(t_2, w_2)\big)$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

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$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
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$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{2}0.1\big(3f(0.3, 0.2522) - f(0.2, 0.1790)\big) = 0.31446243$$

$$w_4 = w_3 + \tfrac{1}{12}h\big(5f(t_4, \tilde{w}_4) + 8f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{12}0.1\big(5f(0.4, 0.3144) + 8f(0.3, 0.2522) - f(0.2, 0.1790)\big)$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{2}\times 0.1 \times (3 \times 0.7867 - 0.8958) = 0.25222940.$$

$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
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$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{2}0.1\big(3f(0.3, 0.2522) - f(0.2, 0.1790)\big) = 0.31446243$$

$$w_4 = w_3 + \tfrac{1}{12}h\big(5f(t_4, \tilde{w}_4) + 8f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{12}0.1\big(5f(0.4, 0.3144) + 8f(0.3, 0.2522) - f(0.2, 0.1790)\big)$$
$$= 0.2522 + \tfrac{1}{12}\times 0.1 \times \big(5 \times 0.5714 + 8 \times 0.6772 - 0.7867\big)$$

Predictor-corrector approach

Example   Solve $\dot{y} = e^{-t} - y^2$, with $y(0) = 0$ using $h = 0.1$.
Continue using $t_1 = 0.1$, $w_1 = 0.0949$, $f(t_1, w_1) = 0.8958$, $t_2 = 0.2$, $w_2 = 0.1790$.

Important: Use the *corrected* value w_2 to compute further in both $\tilde{w}_3$ and w_3!

$$\tilde{w}_3 = w_2 + \tfrac{1}{2}h\big(3f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{2}0.1\big(3f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
$$= 0.1790 + \tfrac{1}{2}\times0.1\times(3\times0.7867 - 0.8958) = 0.25222940.$$

$$w_3 = w_2 + \tfrac{1}{12}h\big(5f(t_3, \tilde{w}_3) + 8f(t_2, w_2) - f(t_1, w_1)\big)$$
$$= 0.1790 + \tfrac{1}{12}0.1\big(5f(0.3, 0.2522) + 8f(0.2, 0.1790) - f(0.1, 0.0949)\big)$$
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$$\tilde{w}_4 = w_3 + \tfrac{1}{2}h\big(3f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{2}0.1\big(3f(0.3, 0.2522) - f(0.2, 0.1790)\big) = 0.31446243$$

$$w_4 = w_3 + \tfrac{1}{12}h\big(5f(t_4, \tilde{w}_4) + 8f(t_3, w_3) - f(t_2, w_2)\big)$$
$$= 0.2522 + \tfrac{1}{12}0.1\big(5f(0.4, 0.3144) + 8f(0.3, 0.2522) - f(0.2, 0.1790)\big)$$
$$= 0.2522 + \tfrac{1}{12}\times0.1\times\big(5\times0.5714 + 8\times0.6772 - 0.7867\big) = 0.31461683.$$

Predictor-corrector approach

Example   Solve $\dot{y}(t) = e^{-t} - y^2$, $y(0) = 0$ at $t = 1$ using the two-stage Adams-Bashforth-Moulton predictor-corrector method with $h = 0.1$.

t_i	$\tilde{w}_i$	$\tilde{f}_i = f(t_i, \tilde{w}_i)$	w_i	$f_i = f(t_i, w_i)$
0.0			0.00000000	1.00000000
0.1			0.09485432	0.89584008
0.2	0.17923033	0.78660724	0.17901896	0.78668296
0.3	0.25222940	0.67719855	0.25221576	0.67720543
0.4	0.31446243	0.57143343	0.31461683	0.57133630
0.5	0.36645700	0.47223993	0.36673920	0.47203302
0.6	0.40897734	0.38154917	0.40934481	0.38124846
0.7	0.44293043	0.30039794	0.44334435	0.30003109
0.8	0.46928659	0.22909906	0.46971515	0.22869665
0.9	0.48901809	0.16743097	0.48943762	0.16702048
1.	0.503055859	0.11481424	0.50345044	

$y(1.0) \approx w_{10} = 0.503450$. Absolute error 0.00010, relative error 0.021%.

Fully-implicit approach (Non-examinable)

Fully-implicit approach

Try to solve the implicit equation for w_{i+1} exactly. Need to solve for $z = w_{i+1}$ in

$$z = w_i + \tfrac{1}{12} h \big(5 f(t_{i+1}, z) + 8 f(t_i, w_i) - f(t_{i-1}, w_{i-1}) \big)$$

or equivalantly

$$g_{i+1}(z) = \tfrac{5}{12} h f(t_{i+1}, z) - z + w_i + \tfrac{1}{12} h \big(8 f(t_i, w_i) - f(t_{i-1}, w_{i-1}) \big) = 0.$$

Typically use the secant method, starting with w_i and $\tilde{w}_{i+1}$, or Newton's method, which requires computing $f_{,y}$ since $g'(z) = \tfrac{5}{12} h f_{,y}(t_{i+1}, z) - 1$.

Gear's method (Non-examinable)

Gear's method Fit a polynomial p to data (t_j, w_j) for $j = i - k + 1, \dots, i, i + 1$.
Solve the equation $\dot{p}(t_{i+1}) = f(t_{i+1}, p(t_{i+1}))$.

Backward-difference method For $k = 2$, equally-sized steps h, have

$$p(\tau) = w_i + \frac{\tau - t_i}{2h}(w_{i+1} - w_{i-1}) + \frac{(\tau - t_i)^2}{2h^2}(w_{i+1} - 2w_i + w_{i-1})$$

so

$$\dot{p}(\tau) = \frac{1}{2h}(w_{i+1} - w_{i-1}) + \frac{\tau - t_i}{h^2}(w_{i+1} - 2w_i + w_{i-1}).$$

Taking $\tau = t_{i+1} = t_i + h$ gives

$$\dot{p}(t_{i+1}) = \frac{1}{2h}(w_{i+1} - w_{i-1}) + \frac{1}{h}(w_{i+1} - 2w_i + w_{i-1}) = \frac{1}{2h}(3w_{i+1} - 4w_i + w_{i-1}).$$

So Gear's method is

$$\frac{1}{2h}(3w_{i+1} - 4w_i + w_{i-1}) = f(t_{i+1}, w_{i+1}).$$

Rearranging gives

$$w_{i+1} = \tfrac{4}{3}w_i - \tfrac{1}{3}w_{i-1} + \tfrac{2}{3}hf(t_{i+1}, w_{i+1}).$$

Gear's methods (Non-examinable)

Two-stage Gear's (backward-difference) method

$$w_{i+1} = \tfrac{4}{3}w_i - \tfrac{1}{3}w_{i-1} + \tfrac{2}{3}hf(t_{i+1}, w_{i+1}).$$

Three-stage Gear's (backward-difference) method

$$w_{i+1} = \tfrac{18}{11}w_i - \tfrac{9}{11}w_{i-1} + \tfrac{2}{11}w_{i-2} + \tfrac{6}{11}hf(t_{i+1}, w_{i+1}).$$

Four-stage Gear's (backward-difference) method

$$w_{i+1} = \tfrac{48}{25}w_i - \tfrac{36}{25}w_{i-1} + \tfrac{16}{25}w_{i-2} - \tfrac{3}{25}w_{i-3} + \tfrac{12}{25}hf(t_{i+1}, w_{i+1}).$$

Gear's method (Non-examinable)

Exercise   Take $f(t, y) = e^{-t} - y^2$, $h = 0.1$, $w_0 = 0.0$, $w_1 = 0.09485432$.

Find w_2 using the backward-difference method.

Gear's method (Non-examinable)

Exercise Take $f(t, y) = e^{-t} - y^2$, $h = 0.1$, $w_0 = 0.0$, $w_1 = 0.09485432$.
Find w_2 using the backward-difference method.

Solve for $w_2 = z$ in

$$g_2(z) = \tfrac{4}{3}w_1 - \tfrac{1}{3}w_0 + \tfrac{2}{3}hf(t_2, z) - z = 0$$

Stability

Stability analysis (Advanced)

Example   Consider $\dot{y} = \lambda y$ with step size h.

Exact solution has

$$y(t + h) = e^{\lambda h} y(t).$$

For $\lambda < 0$, the exact solution is monotonic decreasing.

Euler's method gives

$$w_{i+1} = w_i + h f(w_i) = w_i + h \lambda w_i = (1 + h\lambda) w_i.$$

For $-1 < h\lambda < 0$, Euler's method is monotonic decreasing.
For $-2 < h\lambda < -1$, Euler's method oscillates and decreases.
For $-\infty < h\lambda < -2$, Euler's method oscillates and grows.

Say Euler's method is *monotonically stable* for $-1 < h\lambda < 0$, *stable* for $-2 < h\lambda < 0$ and *unstable* for $h\lambda < -2$.

Stability analysis

Linear stability analysis   Consider $\dot{y} = \lambda y$ with step size h; set $\alpha = \lambda h$.

Stability criteria

Method is *unconditionally-stable* if $w_i \to 0$ as $i \to \infty$ for all $h\lambda < 0$.

Method is *limit-stable* if $w_{i+1}/w_i \to 0$ as $h\lambda \to -\infty$.

Stability analysis

Stability analyses   Euler's method has

$$w_{i+1} = (1+\alpha)w_i,$$

so is monotone and stable for $-1 \le \alpha \le 0$, oscillatory and stable for $-2 < \alpha \le -1$, unstable for $\alpha < -2$.

Ralston's method is stable for $-2 \le \alpha < 0$, since

$$w_{i+1} = w_i + \tfrac{1}{4}h(\lambda w_i + 3\lambda(w_i + \tfrac{2}{3}\lambda h w_i)) = w_i + \alpha w_i + \tfrac{1}{2}\alpha^2 w_i = (1 + \alpha + \tfrac{1}{2}\alpha^2)w_i.$$

Midpoint and modified Euler methods are also stable for $-2 \le \alpha < 0$.

Third-order Runge-Kutta methods are stable for $-2.51 \le \alpha < 0$.
Classical fourth-order Runge-Kutta method is stable for $-2.78 \le \alpha < 0$.

The two-stage Adams-Bashforth method has

$$w_{i+1} = w_i + \tfrac{1}{2}h(3\lambda w_i - \lambda w_{i-1}) = (1 + \tfrac{3}{2}\alpha)w_i - \tfrac{1}{2}\alpha w_{i-1}.$$

Assuming $w_i = \beta^i w_0$ gives $\beta^2 - (1 + \tfrac{3}{2}\alpha)\beta + \tfrac{1}{2}\alpha = 0$.
Stable for $-0.8 < \alpha < 0$ when $|\beta| < 1$ for all solutions.

Stability analysis

Backward Euler method $w_{i+1} = w_i + hf(t_{i+1}, w_{i+1})$.

Have $w_{i+1} = w_i + h\lambda w_{i+1} = w_i + \alpha w_{i+1}$, so $(1 - \alpha)w_{i+1} = w_i$, giving

$$w_{i+1} = \frac{1}{1 - \alpha} \, w_i.$$

Unconditionally stable, nonoscillating.

Trapezoid (Crank-Nicolson) method

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

Then $w_{i+1} = w_i + \frac{1}{2}h(\lambda w_i + \lambda w_{i+1}) = w_i + \frac{1}{2}\alpha w_i + \frac{1}{2}\alpha w_{i+1}$, so $(1 - \alpha/2)w_{i+1} = (1 + \alpha/2)w_i$. Hence

$$w_{i+1} = \frac{1 + \alpha/2}{1 - \alpha/2} \, w_i.$$

Unconditionally stable, oscillates if $\alpha < -2$, ratio $w_{i+1}/w_i \to 1$ as $i \to \infty$.

Stability analysis

Backward-difference method (Non-examinable)

$$w_{i+1} = \tfrac{4}{3}w_i - \tfrac{1}{3}w_{i-1} + \tfrac{2}{3}hf(t_{i+1}, w_{i+1}).$$

Stability $w_i = \beta^i w_0$ yields

$$\beta = \tfrac{4}{3} - \tfrac{1}{3}\beta^{-1} + \tfrac{2}{3}\alpha\beta$$

Hence $(3 + 2\alpha)\beta^2 - 4\beta + 1 = 0$, so

$$\beta = \frac{4 \pm \sqrt{16 - 4(3 + 2\alpha)}}{3 + 2\alpha} = \frac{2 \pm \sqrt{1 - 2\alpha}}{3 + 2\alpha} = \frac{1}{2 \mp \sqrt{1 - 2\alpha}}$$

with $|\beta| < 1$ for $\alpha < 0$.

Unconditionally stable.

Stability analysis

Implicit Adams-Moulton (Non-examinable)

Suppose $w_i = \beta^i w_0$. $f(t, y) = \lambda y$ with $h\lambda = \alpha$. Then

$$\beta w_i = w_i + \tfrac{1}{12}\left(5\alpha\beta w_i + 8\alpha w_i - \alpha w_i/\beta\right).$$

Simplifying gives

$$(12 - 5\alpha)\beta^2 - (12 + 8\alpha)\beta + \alpha = 0.$$

Hence

$$\beta = \frac{(12 + 8\alpha) \pm \sqrt{(12 + 8\alpha)^2 - 4\alpha(12 - 5\alpha)}}{2(12 - 5\alpha)}.$$

This has a positive stable branch and a negative branch which becomes unstable.

If $w_{i-1} = w_i/\gamma$ with $\gamma > 0$, and $w_{i+1} = \beta w_i$, then

$$\beta = \frac{12 + 8\alpha + \alpha/\gamma}{12 - 5\alpha}.$$

In practise, little danger of instability if w_1 is chosen correctly.

Explicit vs implicit methods

Theorem   No explicit Runge-Kutta or multistep method is unconditionally stable.

Theorem (Dahlquist barrier)   An implicit multistep method can only be unconditionally stable if its order is at most 2.

Stiff systems

Idea   A *stiff system* contains *fast* and *stable* variables, which behave similarly to $\dot{y}_i = \lambda y_i$ for $\lambda \ll 0$.

These variables converge quickly to a *pseudo-equilibrium*, after which the dynamics is determined by the *slow* variables.

Explicit methods are unstable for moderate step sizes, requiring either implicit methods, or small step sizes.

Stiff systems

Example   Consider the system

$$\dot{y} = 1 - ty.$$

Eventually, any explicit method becomes unstable for any fixed step size!

Example   The Fitzhugh-Nagumo equations are

$$\dot{v} = (v - v^3/3 - w + I_{\text{ext}})\tau;$$
$$\dot{w} = (v + a - bw);$$

with parameters

$$I_{\text{ext}} = 0.5; \; a = 0.7; \; b = 0.8; \; \tau = 12.5;$$

The parameter τ describes the *time-scale separation*; the variable v changes quickly and w comparitively slowly.

The Fitzhugh-Nagumo equations are stiff, exhibiting oscillations starting around $h = 0.04$.

Multivariable Systems

Multivariable systems

Example   Predator-prey system with rabbits (r) and stoats (s) satisfying

$$\dot{r} = r(3 - s); \quad \dot{s} = s(r - 2);$$

with initial conditions

$$r(0) = 5; \quad s(0) = 2.$$

To solve in Matlab, write the system in vector form. Introduce the *state vector* $\mathbf{y}$ with components $y_1 = r$ and $y_2 = s$.

Write in vector form:

$$\dot{\mathbf{y}} = \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} \dot{r} \\ \dot{s} \end{pmatrix} = \begin{pmatrix} r(3 - s) \\ s(r - 2) \end{pmatrix} = \begin{pmatrix} y_1(3 - y_2) \\ y_2(y_1 - 2) \end{pmatrix} =: f(t, \mathbf{y}).$$

The initial conditions are

$$\mathbf{y}(0) = \begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} r(0) \\ s(0) \end{pmatrix} = \begin{pmatrix} 5 \\ 2 \end{pmatrix} =: \mathbf{y}_0.$$

Multivariable systems

Example   Predator-prey system with rabbits (r) and stoats (s) satisfying

$$\dot{r} = r(3 - s); \quad \dot{s} = s(r - 2); \qquad r(0) = 5, \; s(0) = 2.$$

Vector form

$$\mathbf{y} = \begin{pmatrix} r \\ s \end{pmatrix}; \quad \dot{\mathbf{y}} = \begin{pmatrix} r(3 - s) \\ s(r - 2) \end{pmatrix} = \begin{pmatrix} y_1(3 - y_2) \\ y_2(y_1 - 2) \end{pmatrix} =: f(t, \mathbf{y}); \quad \mathbf{y}_0 = \begin{pmatrix} 5 \\ 2 \end{pmatrix}.$$

In Matlab,

```
f=@(t,y)[y(1)*(3-y(2));y(2)*(y(1)-2)]
t0=0, tf=?
y0=[5;2]
```

Solve up to time `tf`:

```
ode45(f,[t0,tf],y0)
```

Alternatively, set up r and s rate equations separately and combine:

```
dotr=@(r,s)r*(3-s), dots=@(r,s)s*(r-2), r0=5, s0=2
f=@(t,y)[dotr(y(1),y(2));dots(y(1),y(2))], y0=[r0;s0]
```

Second-order systems (Advanced)

Example   Damped driven pendulum

$$ml^2\ddot{s} + \delta l\dot{s} + mgl\sin(s) = A\cos(\omega t)$$

New variable $v = \dot{s}$ gives equations

$$\dot{s} = v; \quad \dot{v} = \ddot{s} = -(\delta/ml)v - (g/l)\sin(s) + (A/ml^2)\cos(\omega t).$$

Write in vector form $y_1 = s$, $y_2 = v$:

$$\mathbf{y} = \begin{pmatrix} s \\ v \end{pmatrix}; \quad \dot{\mathbf{y}} = \mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} y_2 \\ (A/ml^2)\cos(\omega t) - (g/l)\sin(y_1) - (\delta/ml)y_2 \end{pmatrix}$$

Run simulation with $m = g = l = 1$, $\omega = 1$,

$$\dot{y}_1 = y_2; \quad \dot{y}_2 = A\cos(\omega t) - \sin(y_1) - \delta y_2.$$

With $A = 0$, $\delta = 1/4$, $s_0 = 0$, $v_0 = 2$, get damping, slowly varying period.
With $A = 3$, $\delta = 1/4$, $s_0 = 0$ and $v_0 = 2$ get chaos.

Second-order systems

General formulation Suppose

$$\ddot{x} = g(t, x, \dot{x}); \quad x(0) = x_0, \; \dot{x}_0 = v_0.$$

Introduce new variable $v = \dot{x}$ with $\dot{v} = \ddot{x}$ to obtain system

$$\dot{x} = v; \quad \dot{v} = g(t, x, v)$$

Write in vector form with $y_1 = x, \; y_2 = v$ and $\mathbf{y} = \begin{pmatrix} y_1 & y_2 \end{pmatrix}^T$ to obtain

$$\dot{\mathbf{y}} = \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} v \\ g(t, x, v) \end{pmatrix} = \begin{pmatrix} y_2 \\ g(t, y_1, y_2) \end{pmatrix} =: \mathbf{f}(t, \mathbf{y}).$$

Formulation in Matlab

```
g = @(t,x,v) ...
x0=..., v0=...
f = @(t,y) [y(2); g(t,y(1),y(2))]
y0 = [x0;v0]
odeXX(f,[t0,tf],y0)
```

Second-order multivariable systems

Example The motion of a small satellite around a planet of mass M is defined by the differential equation

$$\ddot{\mathbf{x}} = -\frac{GM}{\|\mathbf{x}\|^3}\mathbf{x} =: \mathbf{g}(\mathbf{x})$$

Second-order multivariable systems

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Introduce the velocity $\mathbf{v} = \dot{\mathbf{x}}$.

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Introduce the velocity $\mathbf{v} = \dot{\mathbf{x}}$. The *state* vector $\mathbf{y}$ is given by $\mathbf{y} = \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix}$.

Second-order multivariable systems

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Introduce the velocity $\mathbf{v} = \dot{\mathbf{x}}$. The *state* vector $\mathbf{y}$ is given by $\mathbf{y} = \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix}$.

In components,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}; \quad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix}; \quad \mathbf{y} = \begin{pmatrix} x_1 \\ x_2 \\ v_1 \\ v_2 \end{pmatrix}.$$

Second-order multivariable systems

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The evolution of $\mathbf{y}$ is given by

$$\dot{\mathbf{y}} = \begin{pmatrix} \dot{\mathbf{x}} \\ \dot{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} \mathbf{v} \\ \mathbf{g}(\mathbf{x}) \end{pmatrix}$$

Second-order multivariable systems

Example The motion of a small satellite around a planet of mass M is defined by the differential equation

$$\ddot{\mathbf{x}} = -\frac{GM}{\|\mathbf{x}\|^3}\mathbf{x} =: \mathbf{g}(\mathbf{x})$$

Introduce the velocity $\mathbf{v} = \dot{\mathbf{x}}$. The *state* vector $\mathbf{y}$ is given by $\mathbf{y} = \begin{pmatrix} \mathbf{x} \\ \mathbf{v} \end{pmatrix}$.

In components,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}; \quad \mathbf{v} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix}; \quad \mathbf{y} = \begin{pmatrix} x_1 \\ x_2 \\ v_1 \\ v_2 \end{pmatrix}.$$

The evolution of $\mathbf{y}$ is given by

$$\dot{\mathbf{y}} = \begin{pmatrix} \dot{\mathbf{x}} \\ \dot{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} \mathbf{v} \\ \mathbf{g}(\mathbf{x}) \end{pmatrix}$$

Formulation in Matlab

```
g=@(x) (-G*M/norm(x)^3)*x;
f=@(t,y) [y(3:4); g(y(1:2))];
x0=[?;?]; v0=[?;?]; y0=[x0;v0];
```

Adaptive Methods

Adaptive methods

Matlab   Matlab's `ode` methods are all *adaptive* methods. The `ode23` method is the *Bogacki-Shampine* method.

Estimating accuracy   Combine a order-n method $y(t + h) \approx y(t) + k$ with an order-$(n-1)$ method $y(t + h) \approx y(t) + \kappa$.

Expect
$$|y(t + h) - (y + k)| \ll |y(t + h) - (y + \kappa)| \approx |(y + k) - (y + \kappa)| = |k - \kappa|.$$

A *tolerance* of ϵ means that the error of a single step h should be at most ϵh.

A step is *of the embedded lower-order method* acceptable if
$$|k - \kappa| \le \epsilon h.$$

Adaptive methods

Adjusting step-size   If $|k-\kappa| > \epsilon h$, the step is rejected and a smaller step size qh is attepted instead.
If $|k - \kappa| \le \epsilon h$, the step is accepted, and a larger step size of $\max\{h, qh\}$ is used for the *next* step.

For an order-n method with step size qh, if the error for step-size h is approximately $|k - \kappa|$, expect single-step error $|k - \kappa|q^{n+1}$.
Require error for step size qh to be less than $qh\,\epsilon$, so $|k - \kappa|q^{n+1} \le qh\,\epsilon$.

When taking a step of size h, set

$$q = \left(\frac{\epsilon h}{s|k - \kappa|}\right)^{1/n} \le \left(\frac{\epsilon h}{|k - \kappa|}\right)^{1/n}$$

Here, s is a safety factor, typically $s = 2$.

Bogacki-Shampine method (Advanced)

Bogacki-Shampine method A third-order method with an embedded second-order method.

$$k_1 = hf(t, w);$$

$$k_2 = hf(t + \tfrac{1}{2}h, w + \tfrac{1}{2}k_1);$$

$$k_3 = hf(t + \tfrac{3}{4}h, w + \tfrac{3}{4}k_2);$$

$$k = \tfrac{2}{9}k_1 + \tfrac{3}{9}k_2 + \tfrac{4}{9}k_3;$$

$$k_4 = hf(t + h, w + \tfrac{2}{9}k_1 + \tfrac{3}{9}k_2 + \tfrac{4}{9}k_3) = hf(t + h, w + k);$$

$$\kappa = \tfrac{7}{24}k_1 + \tfrac{6}{24}k_2 + \tfrac{8}{24}k_3 + \tfrac{3}{24}k_4;$$

Error estimates

$$y(t + h) - (y(t) + k) = O(h^{3+1}), \qquad y(t + h) - (y(t) + \kappa) = O(h^{2+1}).$$

Note that

$$|\kappa - k| = \left| \tfrac{5}{72}k_1 - \tfrac{1}{12}k_2 - \tfrac{1}{9}k_3 + \tfrac{1}{8}k_4 \right| = \tfrac{1}{72}|5k_1 - 6k_3 - 8k_3 + 9k_4|.$$

Bogacki-Shampine method (Advanced)

Example $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, $\epsilon = 0.001$.

For $h = 1.0$, find

$k_{0,1} = hf(t_0, w_0) = hf(0.00, 0.0000) = 1.0 \times 1.0000 = 1.0000$;

$k_{0,2} = hf(t_0 + \frac{1}{2}h, w_0 + \frac{1}{2}k_{0,1}) = hf(0.50, 0.5000) = 1.0 \times 0.3565 = 0.3565$;

$k_{0,3} = hf(t_0 + \frac{3}{4}h, w_0 + \frac{3}{4}k_{0,2}) = hf(0.75, 0.2674) = 1.0 \times 0.4009 = 0.4009$;

$\begin{aligned} k_0 &= \frac{2}{9}k_{0,1} + \frac{3}{9}k_{0,2} + \frac{4}{9}k_{0,3} \\ &= \frac{2}{9} \times 1.0000 + \frac{3}{9} \times 0.3565 + \frac{4}{9} \times 0.4009 = 0.5192; \end{aligned}$

$k_{0,4} = hf(t_0 + h, w_0 + k_0) = hf(1.0, 0.5192) = 1.0 \times 0.0983 = 0.0983$;

$\begin{aligned} \kappa_0 &= \frac{7}{24}k_{0,1} + \frac{6}{24}k_{0,2} + \frac{8}{24}k_{0,3} + \frac{3}{24}k_{0,4} \\ &= \frac{7}{24} \times 1.0000 + \frac{6}{24} \times 0.3565 + \frac{8}{24} \times 0.4009 + \frac{3}{24} \times 0.0983 = 0.5267; \end{aligned}$

Then $|k_0 - \kappa_0| = |0.5192 - 0.5267| = 0.0075$ and $\epsilon h = 0.001$; reject step.

$q = \left(\frac{1}{2}\epsilon h / |k - \kappa|\right)^{1/2} = \left(\frac{1}{2} \times 0.001 \times 1.0 / 0.0075\right)^{1/2} = 0.067^{1/2} \approx 0.26$.

Try step size $\hat{h} = qh = 0.26 \times 1.00 = 0.26$.

Bogacki-Shampine method (Advanced)

Example $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, $\epsilon = 0.001$.

For $h = 0.26$, find

$k_{0,1} = hf(t_0, w_0) = hf(0.00, 0.0000) = 0.26 \times 1.0000 = 0.2686$;

$k_{0,2} = hf(t_0 + \frac{1}{2}h, w_0 + \frac{1}{2}k_{0,1}) = hf(0.13, 0.1293) = 0.26 \times 0.8620 = 0.2229$;

$k_{0,3} = hf(t_0 + \frac{3}{4}h, w_0 + \frac{3}{4}k_{0,2}) = hf(0.19, 0.1672) = 0.26 \times 0.7958 = 0.2058$;

$\quad k_0 = \frac{2}{9}k_{0,1} + \frac{3}{9}k_{0,2} + \frac{4}{9}k_{0,3}$

$\qquad = \frac{2}{9} \times 0.2686 + \frac{3}{9} \times 0.2229 + \frac{4}{9} \times 0.2058 = 0.2232$;

$k_{0,4} = hf(t_0 + h, w_0 + k_0) = hf(0.26, 0.2232) = 0.26 \times 0.7223 = 0.1868$;

$\quad \kappa_0 = \frac{7}{24}k_{0,1} + \frac{6}{24}k_{0,2} + \frac{8}{24}k_{0,3} + \frac{3}{24}k_{0,4}$

$\qquad = \frac{7}{24} \times 0.2686 + \frac{6}{24} \times 0.2229 + \frac{8}{24} \times 0.2058 + \frac{3}{24} \times 0.1868 = 0.2231$;

Then $|k_0 - \kappa_0| = |0.22321 - 0.22308| = 1.3 \times 10^{-4} \le \epsilon h = 2.6 \times 10^{-4}$; accept.

$\quad q = \left(\frac{1}{2}\epsilon h / |k - \kappa|\right)^{1/n} = \left(\frac{1}{2} \times 0.001 \times 0.26 / 0.00013\right)^{1/2} = 0.97^{1/2} \approx 0.98$.

Set $t_1 = t_0 + h_0 = 0.26$ and $w_1 = w_0 + k_0 = 0.2232$.

Try next step size $qh = 0.98 \times 0.26 = 0.25$.

Bogacki-Shampine method (Advanced)

Example $\dot{y} = e^{-t} - y^2$, $y(0) = 0$, $\epsilon = 0.001$.

With $t_1 = 0.26$ (2sf), $w_1 = 0.2232$ (4sf) and $h = 0.25$ (2sf), find

$k_{1,1} = hf(t_1, w_1) = hf(0.26, 0.2232) = 0.25 \times 0.7223 = 0.1837$;

$k_{1,2} = hf(t_1 + \frac{1}{2}h, w_1 + \frac{1}{2}k_{1,1}) = hf(0.39, 0.3150) = 0.25 \times 0.5807 = 0.1477$;

$k_{1,3} = hf(t_1 + \frac{3}{4}h, w_1 + \frac{3}{4}k_{1,2}) = hf(0.45, 0.3340) = 0.25 \times 0.5266 = 0.1339$;

$\quad k_1 = \frac{2}{9}k_{0,1} + \frac{3}{9}k_{0,2} + \frac{4}{9}k_{1,3}$

$\qquad = \frac{2}{9} \times 0.1837 + \frac{3}{9} \times 0.1477 + \frac{4}{9} \times 0.1339 = 0.1495$;

$k_{1,4} = hf(t_1 + h, w_1 + k_1) = hf(0.52, 0.3727) = 0.25 \times 0.4599 = 0.1169$;

$\quad \kappa_1 = \frac{7}{24}k_{1,1} + \frac{6}{24}k_{1,2} + \frac{8}{24}k_{1,3} + \frac{3}{24}k_{1,4}$

$\qquad = \frac{7}{24} \times 0.1837 + \frac{6}{24} \times 0.1477 + \frac{8}{24} \times 0.1339 + \frac{3}{24} \times 0.1169 = 0.1497$;

Then $|k_1 - \kappa_1| = |0.14954 - 0.14973| = 0.00019 < 0.00025 = \epsilon h$; accept.

$$q = \left(\epsilon h / |k - \kappa|\right)^{1/n} = \left(0.001 \times 0.25 / 0.00019\right)^{1/2} = 0.67^{1/2} \approx 0.82.$$

Set $t_2 = t_1 + h_1 = 0.52$, $w_2 = w_1 + k_1 = 0.2232 + 0.1495 = 0.3727$.

Next step $h = qh = 0.82 \times 0.25 = 0.21$.

Adaptive multistep methods (Non-examinable)

Changing step size in a multistep method

To halve the step size, in the two-stage Adams Bashforth method, use

$$
y(t + \tfrac{1}{2}h) \approx y(t) + \int_t^{t+h/2} f(t, y(t)) + \frac{(\tau - t)}{h}\big(f(t, y(t)) - f(t-h, y(t-h))\big)\mathrm{d}\tau
$$

$$
= y(t) + \tfrac{1}{2}hf(t, y(t)) + \tfrac{1}{8}h\big(f(t, y(t)) - f(t - h, y(t - h))\big)
$$

$$
= y(t) + \tfrac{1}{8}h\big(5f(t, y(t)) - f(t - h, y(t - h))\big)
$$

Hence

$$
t_{i+1} = t_i + h_i \text{ where } h_i = \tfrac{1}{2}h_{i-1}
$$

$$
w_{i+1} = w_i + \tfrac{1}{4}h_i\big(5f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)
$$

To double the step size, use

$$
t_{i+1} = t_i + h_i \text{ where } h_i = 2h_{i-1}
$$

$$
w_{i+1} = w_i + h_i\big(2f(t_i, w_i) - f(t_{i-1}, w_{i-1})\big)
$$

Global errors

Growth of global errors (Advanced)

Growth of global errors   If $\dot{y} = \lambda y$, then $y(t) = y(0)e^{\lambda t}$, so an error of size ϵ at time 0 becomes $\epsilon\, e^{\lambda t}$ at time t.

In general
$$\frac{\mathrm{d}}{\mathrm{d}t}\big(y_1(t) - y_2(t)\big) = f(t, y_1(t)) - f(t, y_2(t)) = f_{,y}(t, \eta)\big(y_1(t) - y_2(t)\big)$$

Error bound   Combine global growth of error with local error estimate:

Theorem   If $f_y(\tau, y(\tau)) \leq L$ and the local error is $C\, f^{(n)}(\tau, y(\tau))\, h^{n+1}$ then at times $t_n \in [0, T]$,
$$\big|w_n - y(t_n)\big| \leq CM\, \frac{\exp(LT) - 1}{L}\, h^n \text{ where } M = \sup_{\tau \in [0,T]} |f^{(n)}(\tau, y(\tau))|.$$

Growth of errors and chaos (Non-examinable)

Example Duffing oscillator

$$\ddot{x} + \delta\dot{x} + \alpha x + \beta x^3 = \gamma\cos(\omega t).$$

Take $\alpha = \beta = \gamma = \omega = 1,\ \delta = 0.1; x(0) = 1.5, \dot{x}(0) = 0.0.$

Uncontrollable growth of local errors and *chaotic* motion.