

Lipschitz condition

Definition: function $f(t, y)$ satisfies a **Lipschitz condition** in the variable y on a set $D \subset \mathbf{R}^2$ if a constant $L > 0$ exists with

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

whenever $(t, y_1), (t, y_2)$ are in D . L is Lipschitz constant.

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- ▶ **Example 2:** $f(t, y) = t y^2$ satisfies Lipschitz condition on the region

$$D = \{(t, y) \mid 0 \leq t \leq T, \quad -Y \leq y \leq Y\}.$$

What is going on with $f(t, y) = t y^2$?

Initial value problem

$$y'(t) = t y^2(t), \quad y(t_0) = \alpha > 0$$

has unique, but unbounded solution

$$y(t) = \frac{2\alpha}{2 + \alpha(t_0^2 - t^2)},$$

the denominator of which vanishes at

$$t = \sqrt{\frac{2}{\alpha} + t_0^2}.$$

- ▶ for $|t_0| < T$, ODE has unique solution on

$$D = \{(t, y) \mid 0 \leq t \leq T, \quad -Y \leq y \leq Y\}.$$

- ▶ for $\sqrt{\frac{2}{\alpha} + t_0^2} < T$ ODE solution breaks down at $t = \sqrt{\frac{2}{\alpha} + t_0^2}$
on

$$D = \{(t, y) \mid 0 \leq t \leq T\}.$$

Well-posed problem

Definition in English: ODE is well-posed if

- ▶ A unique ODE solution exists, and
- ▶ Small changes (perturbation) to ODE imply small changes to solution.

Well-posed problem

The initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha, \quad (5.2)$$

is said to be a **well-posed problem** if:

- A unique solution, $y(t)$, to the problem exists, and
- There exist constants $\varepsilon_0 > 0$ and $k > 0$ such that for any ε , with $\varepsilon_0 > \varepsilon > 0$, whenever $\delta(t)$ is continuous with $|\delta(t)| < \varepsilon$ for all t in $[a, b]$, and when $|\delta_0| < \varepsilon$, the initial-value problem

$$\frac{dz}{dt} = f(t, z) + \delta(t), \quad a \leq t \leq b, \quad z(a) = \alpha + \delta_0, \quad (5.3)$$

has a unique solution $z(t)$ that satisfies

$$|z(t) - y(t)| < k\varepsilon \quad \text{for all } t \text{ in } [a, b]. \quad \blacksquare$$

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Theorem

Suppose $D = \{(t, y) \mid a \leq t \leq b \text{ and } -\infty < y < \infty\}$. If f is continuous and satisfies a Lipschitz condition in the variable y on the set D , then the initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha$$

is well-posed. ■

Well-posed problem, example

Show that the initial-value problem

$$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5. \quad (5.4)$$

is well posed on $D = \{(t, y) \mid 0 \leq t \leq 2 \text{ and } -\infty < y < \infty\}$.

Solution: Because

$$\frac{\partial f}{\partial y}(t, y) = 1, \quad \left| \frac{\partial f}{\partial y}(t, y) \right| = 1.$$

$f(t, y) = y - t^2 + 1$ satisfies a Lipschitz condition in y on D with Lipschitz constant 1. Therefore this ODE is well-posed. In fact,

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

Euler's Method: Initial value ODE to solve

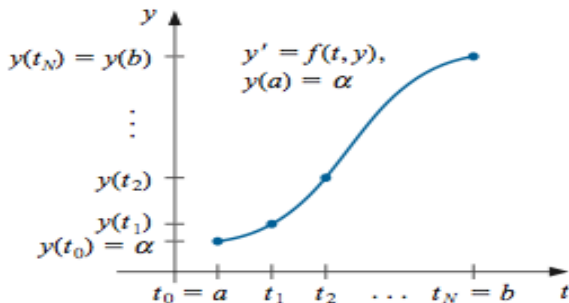
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- ▶ Choose positive integer N , and select mesh points

$$t_j = a + j h, \quad \text{for } j = 0, 1, 2, \dots, N, \quad \text{where } h = (b - a)/N.$$



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- ▶ For each j , do 2-term Taylor expansion

$$y(t_{j+1}) = y(t_j) + h y'(t_j) + \frac{h^2}{2} y''(\xi_j), \quad j = 0, 1, \dots, N - 1.$$

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- ▶ Ignore error term, set $w_0 = \alpha$,

$$w_{j+1} = w_j + h f(t_j, w_j), \quad j = 0, 1, \dots, N - 1.$$

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 $t_j = a + j h$, for $j = 0, 1, 2, \dots, N$, where $h = (b - a)/N$.

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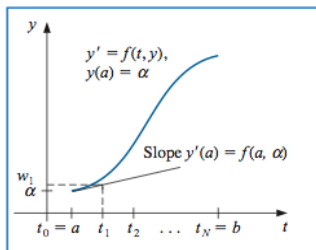
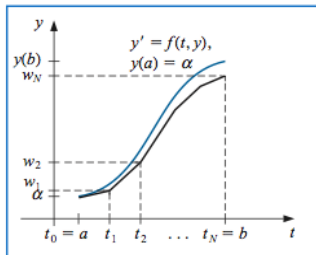


Figure 5.4



Euler's Method: example

Initial Value ODE $\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$
exact solution $y(t) = (1 + t)^2 - 0.5 e^t.$

- ▶ Choose positive integer $N = 10$, so

$$h = 0.2, \quad t_j = 0.2j, \quad \text{for } j = 0, 1, 2, \dots, 10.$$

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

Error Bounds for Euler's Method

$$D = \{(t, y) \mid 0 \leq t \leq T, \quad -Y \leq y \leq Y\}.$$

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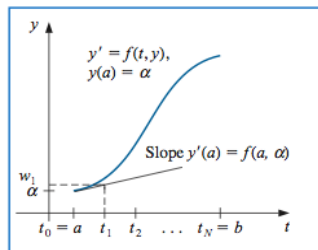
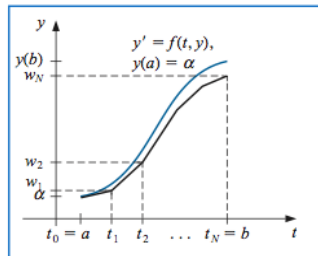


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Theorem: Suppose that in the initial value ODE,

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$$|y(t_j) - w_j| \leq \frac{hM}{2L} \left(e^{L(t_j-a)} - 1 \right),$$

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- ▶ **Bad News:** N may have to be impossibly large:

$$e^{L(t_N-a)} = e^{L(b-a)} > 10^{43} \quad \text{if} \quad L > 10 \quad \text{and} \quad b - a > 10.$$

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Proof of **Theorem 1**

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$$\begin{aligned} y(t_{j+1}) &= y(t_j) + h y'(t_j) + \frac{h^2}{2} y''(\xi_j) \\ &= y(t_j) + h f(t_j, y(t_j)) + \frac{h^2}{2} y''(\xi_j), \quad j = 0, 1, \dots, N - 1. \end{aligned}$$

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- ▶ Subtraction of two equations:

$$y(t_{j+1}) - w_{j+1} = y(t_j) - w_j + h (f(t_j, y(t_j)) - f(t_j, w_j)) + \frac{h^2}{2} y''(\xi_j).$$

Proof of **Theorem II**

- ▶ Difference of two equations:

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- ▶ This implies a linear recursion:

$$\begin{aligned} |y(t_{j+1}) - w_{j+1}| &\leq |y(t_j) - w_j| + h |f(t_j, y(t_j)) - f(t_j, w_j)| + \frac{h^2}{2} |y''(\xi_j)| \\ &\leq |y(t_j) - w_j| + hL |y(t_j) - w_j| + \frac{h^2}{2} M \\ &= (1 + hL) |y(t_j) - w_j| + \frac{h^2}{2} M. \end{aligned}$$

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- ▶ Further simplification for $j = 0, \dots, N - 1$,

$$\begin{aligned} |y(t_{j+1}) - w_{j+1}| + \frac{hM}{2L} &\leq (1 + hL) |y(t_j) - w_j| + \frac{h^2}{2} M + \frac{hM}{2L} \\ &= (1 + hL) \left(|y(t_j) - w_j| + \frac{hM}{2L} \right). \end{aligned}$$

Proof of Theorem III

- ▶ Solving linear recursion:

$$\begin{aligned} |y(t_{j+1}) - w_{j+1}| + \frac{hM}{2L} &\leq (1 + hL) \left(|y(t_j) - w_j| + \frac{hM}{2L} \right) \\ &\leq (1 + hL)^2 \left(|y(t_{j-1}) - w_{j-1}| + \frac{hM}{2L} \right) \\ &\quad \vdots \\ &\leq (1 + hL)^{j+1} \left(|y(t_0) - w_0| + \frac{hM}{2L} \right). \end{aligned}$$

- ▶ Since $y(t_0) = w_0 = \alpha$,

$$|y(t_{j+1}) - w_{j+1}| + \frac{hM}{2L} \leq (1 + hL)^{j+1} \frac{hM}{2L},$$

it follows that

$$\begin{aligned} |y(t_{j+1}) - w_{j+1}| &\leq \frac{hM}{2L} \left((1 + hL)^{j+1} - 1 \right) \\ &\leq \frac{hM}{2L} \left(e^{L(t_{j+1}-a)} - 1 \right). \end{aligned}$$

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- ▶ Set $w_0 = 0.5$. For $j = 0, 1, \dots, 9$,

$$\begin{aligned} w_{j+1} &= w_j + h(w_j - t_j^2 + 1) = w_j + 0.2(w_j - 0.04j^2 + 1) \\ &= 1.2w_j - 0.008j^2 + 0.2. \end{aligned}$$

Since $y''(t) = 2 - 0.5 e^t, \quad \frac{\partial f}{\partial y}(t, y) = 1,$

it follows that $|y''(t)| \leq 0.5 e^2 - 2 \stackrel{\text{def}}{=} M, \quad L = 1.$

Euler's Method: example (II)

Initial Value ODE $\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$
exact solution $y(t) = (1 + t)^2 - 0.5 e^t.$

- ▶ Therefore $M = 0.5 e^2 - 2, L = 1,$

$$|y(t_i) - w_i| \leq \frac{hM}{2L} \left(e^{L(t_i-a)} - 1 \right) = 0.1 (0.5 e^2 - 2) (e^{t_i} - 1).$$

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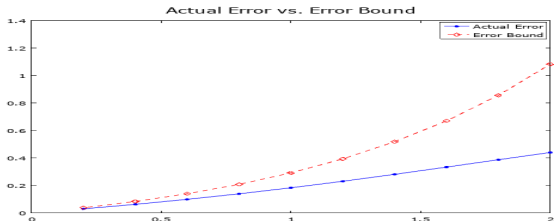
t_i	w_i	$y_i = y(t_i)$	$ y_i - w_i $
0.0	0.5000000	0.5000000	0.0000000
0.2	0.8000000	0.8292986	0.0292986
0.4	1.1520000	1.2140877	0.0620877
0.6	1.5504000	1.6489406	0.0985406
0.8	1.9884800	2.1272295	0.1387495
1.0	2.4581760	2.6408591	0.1826831
1.2	2.9498112	3.1799415	0.2301303
1.4	3.4517734	3.7324000	0.2806266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

$$|y(t_i) - w_i| \leq 0.1 (0.5 e^2 - 2) (e^{t_i} - 1)$$

t_i	Actual Error	Error Bound
0.200000	0.029300	0.037520
0.400000	0.062090	0.083340
0.600000	0.098540	0.139310
0.800000	0.138750	0.207670
1.000000	0.182680	0.291170
1.200000	0.230130	0.393150
1.400000	0.280630	0.517710
1.600000	0.333360	0.669850
1.800000	0.387020	0.855680
2.000000	0.439690	1.082640

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0.200000	0.029300	0.037520
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1.600000	0.333360	0.669850
1.800000	0.387020	0.855680
2.000000	0.439690	1.082640



Euler's Method in Finite Precision, I

- ▶ Mesh points

$$t_j = a + j h, \quad \text{for } j = 0, 1, 2, \dots, N, \quad \text{where } h = (b - a)/N.$$

Euler's Method in Finite Precision, I

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$$t_j = a + j h, \quad \text{for } j = 0, 1, 2, \dots, N, \quad \text{where } h = (b - a)/N.$$

- ▶ For each j , we have 2-term Taylor expansion

$$\begin{aligned} y(t_{j+1}) &= y(t_j) + h y'(t_j) + \frac{h^2}{2} y''(\xi_j) \\ &= y(t_j) + h f(t_j, y(t_j)) + \frac{h^2}{2} y''(\xi_j), \quad j = 0, 1, \dots, N - 1. \end{aligned}$$

Euler's Method in Finite Precision, I

- ▶ Mesh points

$$t_j = a + j h, \quad \text{for } j = 0, 1, 2, \dots, N, \quad \text{where } h = (b - a)/N.$$

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- ▶ Euler's method for each j , in finite precision

$$u_{j+1} = u_j + h f(t_j, u_j) + \delta_{j+1},$$

where $|\delta_{j+1}| \leq \delta$.

Euler's Method in Finite Precision, I

- ▶ Mesh points

$$t_j = a + j h, \quad \text{for } j = 0, 1, 2, \dots, N, \quad \text{where } h = (b - a)/N.$$

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$$u_{j+1} = u_j + h f(t_j, u_j) + \delta_{j+1},$$

where $|\delta_{j+1}| \leq \delta$.

- ▶ Subtraction of two equations:

$$y(t_{j+1}) - u_{j+1} = y(t_j) - u_j + h (f(t_j, y(t_j)) - f(t_j, u_j)) + \frac{h^2}{2} y''(\xi_j) - \delta_{j+1}.$$

Euler's Method in Finite Precision, II

- ▶ Difference of two equations:

$$y(t_{j+1}) - u_{j+1} = y(t_j) - u_j + h(f(t_j, y(t_j)) - f(t_j, u_j)) + \frac{h^2}{2} y''(\xi_j) - \delta_{j+1}.$$

Euler's Method in Finite Precision, II

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- ▶ This implies a linear recursion:

$$\begin{aligned} |y(t_{j+1}) - u_{j+1}| &\leq |y(t_j) - u_j| + h |f(t_j, y(t_j)) - f(t_j, u_j)| + \frac{h^2}{2} |y''(\xi_j)| + |\delta_{j+1}| \\ &\leq |y(t_j) - u_j| + hL |y(t_j) - u_j| + \frac{h^2}{2} M + \delta \\ &= (1 + hL) |y(t_j) - u_j| + \frac{h^2}{2} M + \delta. \end{aligned}$$

Euler's Method in Finite Precision, II

- ▶ Difference of two equations:

$$y(t_{j+1}) - u_{j+1} = y(t_j) - u_j + h(f(t_j, y(t_j)) - f(t_j, u_j)) + \frac{h^2}{2} y''(\xi_j) - \delta_{j+1}.$$

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- ▶ Further simplification for $j = 0, \dots, N-1$,

$$\begin{aligned} |y(t_{j+1}) - u_{j+1}| + \frac{hM}{2L} + \frac{\delta}{hL} &\leq (1 + hL) |y(t_j) - u_j| + \frac{h^2}{2} M + \frac{hM}{2L} + \delta + \frac{\delta}{hL} \\ &= (1 + hL) \left(|y(t_j) - u_j| + \frac{hM}{2L} + \frac{\delta}{hL} \right). \end{aligned}$$

Euler's Method in Finite Precision, III

- ▶ Solving linear recursion:

$$\begin{aligned} |y(t_{j+1}) - u_{j+1}| + \frac{hM}{2L} + \frac{\delta}{hL} &\leq (1 + hL) \left(|y(t_j) - u_j| + \frac{hM}{2L} + \frac{\delta}{hL} \right) \\ &\vdots \\ &\leq (1 + hL)^{j+1} \left(|y(t_0) - u_0| + \frac{hM}{2L} + \frac{\delta}{hL} \right). \end{aligned}$$

- ▶ Assume $|y(t_0) - u_0| = |\alpha - u_0| \leq \delta$,

$$|y(t_{j+1}) - u_{j+1}| + \frac{hM}{2L} + \frac{\delta}{hL} \leq (1 + hL)^{j+1} \left(\delta + \frac{hM}{2L} + \frac{\delta}{hL} \right),$$

it follows that

$$\begin{aligned} |y(t_{j+1}) - u_{j+1}| &\leq \frac{1}{L} \left(\frac{hM}{2} + \frac{\delta}{h} \right) \left((1 + hL)^{j+1} - 1 \right) + \delta (1 + hL)^{j+1} \\ &\leq \frac{1}{L} \left(\frac{hM}{2} + \frac{\delta}{h} \right) \left(e^{L(t_{j+1}-a)} - 1 \right) + \delta e^{L(t_{j+1}-a)}. \end{aligned}$$

Euler's Method in Finite Precision, IV

- ▶ Error bound in finite precision

$$|y(t_{j+1}) - u_{j+1}| \leq \frac{1}{L} \left(\frac{hM}{2} + \frac{\delta}{h} \right) \left(e^{L(t_{j+1}-a)} - 1 \right) + \delta e^{L(t_{j+1}-a)}.$$

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- ▶ Value of h can't be too small:

$$\lim_{h \rightarrow 0} \left(\frac{hM}{2} + \frac{\delta}{h} \right) = \infty.$$

Euler's Method in Finite Precision, IV

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$$\lim_{h \rightarrow 0} \left(\frac{hM}{2} + \frac{\delta}{h} \right) = \infty.$$

- ▶ "Optimal" value of h

$$h_{\text{opt}} = \sqrt{\frac{2\delta}{M}}, \quad \text{and} \quad \left(\frac{h_{\text{opt}}M}{2} + \frac{\delta}{h_{\text{opt}}} \right) = \sqrt{2\delta M}.$$

Euler's Method in Finite Precision, IV

- ▶ Error bound in finite precision

$$|y(t_{j+1}) - u_{j+1}| \leq \frac{1}{L} \left(\frac{hM}{2} + \frac{\delta}{h} \right) \left(e^{L(t_{j+1}-a)} - 1 \right) + \delta e^{L(t_{j+1}-a)}.$$

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- ▶ "Practical" value of $h \gg h_{\mathbf{opt}}$.

Midterm Scope

- ▶ First 5 Chapters of Text Book.
- ▶ **Chapter 1:** Calculus, Computer Math.
- ▶ **Chapter 2:** Solve $f(x) = 0$.
- ▶ **Chapter 3:** Approximate given functions.
- ▶ **Chapter 4:** Derivatives, integrals.
- ▶ **Chapter 5:** Initial value ODEs, up to Section 5.3.

Review: Midterm rules

- ▶ No calculators.
- ▶ one-sided one-page cheat sheet.
- ▶ exam problems are mostly (modified) from exercises in textbook.
- ▶ free to use results in the proper text, but not anything else.

Chapter 1

- ▶ **Calculus**
 - ▶ Extreme Value Theorem
 - ▶ Mean Value Theorem
 - ▶ Intermediate Value Theorem
- ▶ **Machine Precision**
 - ▶ Round-off errors
 - ▶ Stable quadratic roots
 - ▶ Numerical stability
- ▶ **Rate of convergence: the Big O**

Root finders

- ▶ **Bisection**
- ▶ **Fixed Point Iteration**
- ▶ **Newton's Method**
- ▶ **Order of convergence**
- ▶ **Polynomial roots**
- ▶ **Multiple roots**

Able to develop, use, and analyze methods

Interpolation and Polynomial Approximation

- ▶ **Interpolation and the Lagrange Polynomial**
- ▶ **Error Analysis**
- ▶ **Divided Differences**
- ▶ **Hermite Interpolation**
- ▶ **Cubic Spline Interpolation**

Able to develop and analyze approximation methods

Numerical Differentiation and Integration

- ▶ **Numerical Differentiation**
- ▶ **Extrapolation**
- ▶ **Trapezoidal/Simpson rules, DoP**
- ▶ **Composite Numerical Integration**
- ▶ **Adaptive Quadrature, error bounds vs. estimates**
- ▶ **Gaussian Quadrature**
- ▶ **Multiple/Improper Integrals**

Able to develop and analyze basic integration methods

Initial-Value Problems for ODEs

- ▶ **Elementary Theory of Initial-Value Problems, Lipschitz conditions**
- ▶ **Euler's Method**
- ▶ **Higher-Order Taylor Methods**

Local Truncation Error for a general difference method

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

Definition: The difference method

$$\begin{aligned} w_0 &= \alpha, \\ w_{j+1} &= w_j + h\phi(t_j, w_j), \quad \text{for } j = 0, 1, \dots, N-1 \end{aligned}$$

has **local truncation error**

$$\begin{aligned} \tau_{j+1}(h) &\stackrel{\text{def}}{=} \frac{y(t_{j+1}) - (y(t_j) + h\phi(t_j, y(t_j)))}{h} \\ &= \frac{y(t_{j+1}) - y(t_j)}{h} - \phi(t_j, y(t_j)). \end{aligned}$$

Local Truncation Error for Euler's method

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

Euler's method

$$\begin{aligned} w_0 &= \alpha, \\ w_{j+1} &= w_j + hf(t_j, w_j), \quad \text{for } j = 0, 1, \dots, N-1 \end{aligned}$$

has **local truncation error**

$$\begin{aligned} \tau_{j+1}(h) &= \frac{y(t_{j+1}) - y(t_j)}{h} - f(t_j, y(t_j)) \\ &= \frac{y(t_{j+1}) - y(t_j)}{h} - y'(t_j) = \frac{h}{2} y''(\xi_j), \quad \xi_j \in (t_j, t_{j+1}). \end{aligned}$$

This implies

$$|\tau_{j+1}(h)| \leq \frac{h}{2} \max_{t \in [a, b]} |y''(t)| \stackrel{\text{def}}{=} \frac{hM}{2}, \quad \text{a first order method.}$$

n -th Order Taylor Methods:

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

n -th Order Taylor Methods:

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- ▶ $(n + 1)$ -term Taylor expansion

$$\begin{aligned} y(t_{j+1}) = & y(t_j) + hy'(t_j) + \frac{h^2}{2}y''(t_j) + \cdots + \frac{h^n}{n!}y^{(n)}(t_j) \\ & + \frac{h^{n+1}}{(n+1)!}y^{(n+1)}(\xi_j). \end{aligned}$$

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- ▶ On the other hand,

$$\begin{aligned} y'(t_j) &= f(t_j, y(t_j)), \quad y''(t_j) = f'(t_j, y(t_j)), \cdots \\ y^{(n)}(t_j) &= f^{(n-1)}(t_j, y(t_j)). \end{aligned}$$

n -th Order Taylor Method:

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

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► $(n + 1)$ -term Taylor expansion

$$y(t_{j+1}) = y(t_j) + hf(t_j, y(t_j)) + \frac{h^2}{2}f'(t_j, y(t_j)) + \cdots + \frac{h^n}{n!}f^{(n-1)}(t_j, y(t_j)) \\ + \frac{h^{n+1}}{(n+1)!}f^{(n)}(\xi_j, y(\xi_j)).$$

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- ▶ $(n + 1)$ -term Taylor expansion

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- ▶ n -th order Taylor method

$$w_0 = \alpha,$$

$$w_{j+1} = w_j + h\mathbf{T}^{(n)}(t_j, w_j), \quad j = 0, 1, \dots, N-1,$$

where $\mathbf{T}^{(n)}(t_j, w_j) = f(t_j, w_j) + \frac{h}{2}f'(t_j, w_j) + \cdots + \frac{h^{n-1}}{n!}f^{(n-1)}(t_j, w_j).$

Example: Second Order Taylor Method:

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

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- ▶ Second order Taylor method

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$$w_{j+1} = w_j + h\mathbf{T}^{(2)}(t_j, w_j), \quad j = 0, 1, \dots, N-1,$$

$$\text{where } \mathbf{T}^{(2)}(t_j, w_j) = f(t_j, w_j) + \frac{h}{2}f'(t_j, w_j) \quad \text{with}$$

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$$\begin{aligned} f'(t, y(t)) &= \frac{d}{dt}f(t, y(t)) = \frac{\partial f}{\partial t}(t, y(t)) + \frac{\partial f}{\partial y}(t, y(t))y'(t) \\ &= \frac{\partial f}{\partial t}(t, y(t)) + \frac{\partial f}{\partial y}(t, y(t))f(t, y(t)). \end{aligned}$$

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- ▶ Second order Taylor method in explicit form

$$w_{j+1} = w_j + h \left(f(t_j, w_j) + \frac{h}{2} \left(\frac{\partial f}{\partial t}(t_j, w_j) + \frac{\partial f}{\partial y}(t_j, w_j) f(t_j, w_j) \right) \right).$$

Example: Second Order Taylor Method:

$$\frac{dy}{dt} = f(t, y), \quad f(t, y) = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5.$$

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$$\frac{dy}{dt} = f(t, y), \quad f(t, y) = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5.$$

► Second order Taylor method

$$w_{j+1} = w_j + h \left(f(t_j, w_j) + \frac{h}{2} \left(\frac{\partial f}{\partial t}(t_j, w_j) + \frac{\partial f}{\partial y}(t_j, w_j) f(t_j, w_j) \right) \right).$$

$$\frac{\partial f}{\partial t}(t, y(t)) = -2t, \quad \frac{\partial f}{\partial y}(t, y(t)) = 1.$$

Thus,

$$\begin{aligned} w_{j+1} &= w_j + h \left(w_j - t_j^2 + 1 + \frac{h}{2} (-2t_j + w_j - t_j^2 + 1) \right) \\ &= \left(1 + h + \frac{h^2}{2} \right) w_j + \left(h + \frac{h^2}{2} \right) (1 - t_j^2) - h^2 t_j. \end{aligned}$$

Euler's Method vs. Second Order Taylor Method: $N = 10$

$$\frac{dy}{dt} = f(t, y), \quad f(t, y) = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5.$$

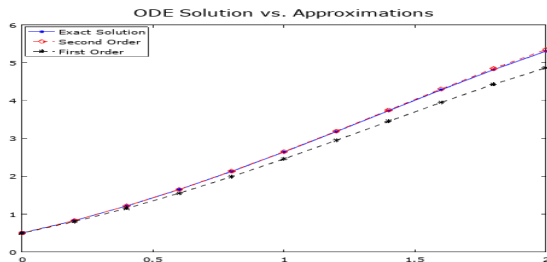
Euler's Method vs. Second Order Taylor Method: $N = 10$

$$\frac{dy}{dt} = f(t, y), \quad f(t, y) = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5.$$

t_i	Euler's Method	Taylor Method	Exact Solution
0.00000	0.50000	0.50000	0.50000
0.20000	0.80000	0.83000	0.82930
0.40000	1.15200	1.21580	1.21409
0.60000	1.55040	1.65208	1.64894
0.80000	1.98848	2.13233	2.12723
1.00000	2.45818	2.64865	2.64086
1.20000	2.94981	3.19135	3.17994
1.40000	3.45177	3.74864	3.73240
1.60000	3.95013	4.30615	4.28348
1.80000	4.42815	4.84630	4.81518
2.00000	4.86578	5.34768	5.30547

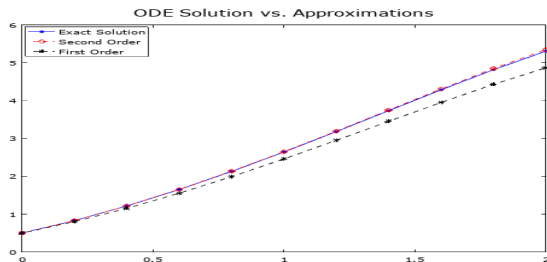
Euler's Method vs. Second Order Taylor Method: $N = 10$

- ▶ Second order method looks more accurate.

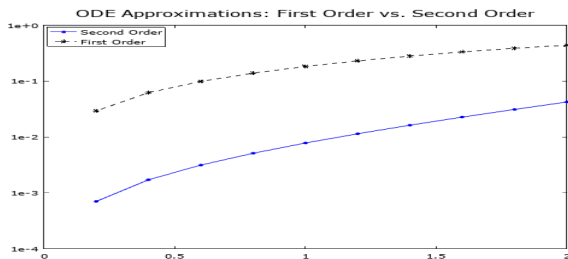


Euler's Method vs. Second Order Taylor Method: $N = 10$

- ▶ Second order method looks more accurate.



- ▶ Second order method has much smaller errors.



Runge-Kutta methods

With orders of Taylor methods yet without derivatives of $f(t, y(t))$

First order Taylor expansion in two variables

Theorem: Suppose that $f(t, y)$ and all its partial derivatives are

continuous on $D \stackrel{\text{def}}{=} \{(t, y) \mid a \leq t \leq b, \quad c \leq y \leq d.\}$

Let $(t_0, y_0), (t, y) \in D, \Delta_t = t - t_0, \Delta_y = y - y_0$. **Then**

$$f(t, y) = P_1(t, y) + R_1(t, y), \quad \text{where}$$

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$$P_1(t, y) = f(t_0, y_0) + \Delta_t \frac{\partial f}{\partial t}(t_0, y_0) + \Delta_y \frac{\partial f}{\partial y}(t_0, y_0),$$

$$R_1(t, y) = \frac{\Delta_t^2}{2} \frac{\partial^2 f}{\partial t^2}(\xi, \mu) + \Delta_t \Delta_y \frac{\partial^2 f}{\partial t \partial y}(\xi, \mu) + \frac{\Delta_y^2}{2} \frac{\partial^2 f}{\partial y^2}(\xi, \mu),$$

for some point $(\xi, \mu) \in D$.

Second order Taylor expansion in two variables

Theorem: Suppose that $f(t, y)$ and all its partial derivatives are

continuous on $D \stackrel{\text{def}}{=} \{(t, y) \mid a \leq t \leq b, c \leq y \leq d.\}$

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$$\begin{aligned} P_2(t, y) = & f(t_0, y_0) + \left(\Delta_t \frac{\partial f}{\partial t}(t_0, y_0) + \Delta_y \frac{\partial f}{\partial y}(t_0, y_0) \right) \\ & + \left(\frac{\Delta_t^2}{2} \frac{\partial^2 f}{\partial t^2}(t_0, y_0) + \Delta_t \Delta_y \frac{\partial^2 f}{\partial t \partial y}(t_0, y_0) + \frac{\Delta_y^2}{2} \frac{\partial^2 f}{\partial y^2}(t_0, y_0) \right), \end{aligned}$$

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$$R_2(t, y) = \frac{1}{3!} \left(\sum_{j=0}^3 \binom{3}{j} \Delta_t^{3-j} \Delta_y^j \frac{\partial^3 f}{\partial t^{3-j} \partial y^j}(\xi, \mu) \right)$$

Example: Second order Taylor expansion in two variables

$$\begin{aligned} f(t, y) &= \mathbf{exp} \left(-\frac{(t-2)^2}{4} - \frac{(y-3)^2}{4} \right) \mathbf{cos}(2t + y - 7) \\ &= P_2(t, y) + R_2(t, y), \quad \text{with } (t_0, y_0) = (2, 3). \end{aligned}$$

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$$\text{Let } \Delta_t = t - 2, \Delta_y = y - 3,$$

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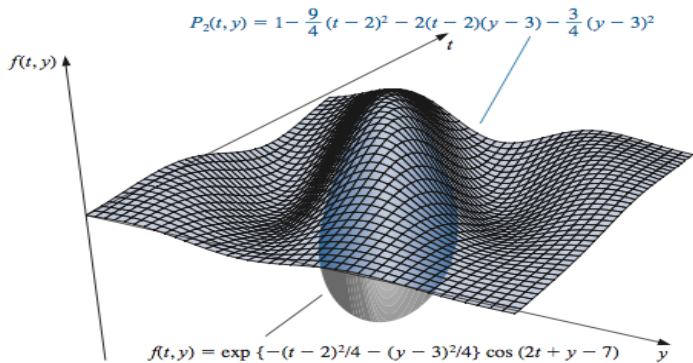
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$$\text{so } f(t, y) \approx P_2(t, y) = 1 - \frac{9}{4}(t-2)^2 - 2(t-2)(y-3) - \frac{3}{4}(y-3)^2.$$

$$\begin{aligned} f(t, y) &= \mathbf{exp} \left(-\frac{(t-2)^2}{4} - \frac{(y-3)^2}{4} \right) \mathbf{cos}(2t + y - 7) \\ &\approx 1 - \frac{9}{4}(t-2)^2 - 2(t-1)(y-3) - \frac{3}{4}(y-3)^2. \end{aligned}$$

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$$\approx 1 - \frac{9}{4}(t-2)^2 - 2(t-1)(y-3) - \frac{3}{4}(y-3)^2.$$



Approximation good near (2, 3), bad elsewhere

Taylor's Theorem in two variables

Theorem: Suppose that $f(t, y)$ and all its partial derivatives are continuous on $D \stackrel{\text{def}}{=} \{(t, y) \mid a \leq t \leq b, c \leq y \leq d.\}$

Let $(t_0, y_0), (t, y) \in D, \Delta_t = t - t_0, \Delta_y = y - y_0$. **Then** for $n \geq 1$,

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Runge-Kutta Method of Order Two (I)

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

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- ▶ Second order Taylor method

$$w_0 = \alpha,$$

$$w_{j+1} = w_j + h\mathbf{T}^{(2)}(t_j, w_j), \quad j = 0, 1, \dots, N-1, \quad \text{where}$$

$$\begin{aligned}\mathbf{T}^{(2)}(t, y) &= f(t, y) + \frac{h}{2}f'(t, y) \\ &= f(t, y) + \frac{h}{2} \left(\frac{\partial f}{\partial t}(t, y) + \frac{\partial f}{\partial y}(t, y) \frac{dy}{dt} \right) \\ &= f(t, y) + \frac{h}{2} \left(\frac{\partial f}{\partial t}(t, y) + \frac{\partial f}{\partial y}(t, y) f(t, y) \right) \\ &= f \left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y) \right) - R_1 \left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y) \right)\end{aligned}$$

Runge-Kutta Method of Order Two (II)

- ▶ Second order Taylor method

$$w_0 = \alpha,$$

$$w_{j+1} = w_j + h\mathbf{T}^{(2)}(t_j, w_j), \quad j = 0, 1, \dots, N-1, \quad \text{where}$$

$$\mathbf{T}^{(2)}(t, y) = f\left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y)\right) - R_1\left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y)\right),$$

- ▶ From first order Taylor expansion,

$$\begin{aligned} R_1\left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y)\right) &= \frac{h^2}{8} \frac{\partial^2 f}{\partial t^2}(\xi, \mu) + \frac{h^2 f(t, y)}{4} \Delta_t \Delta_y \frac{\partial^2 f}{\partial t \partial y}(\xi, \mu) \\ &+ \frac{h^2 f^2(t, y)}{8} \frac{\partial^2 f}{\partial y^2}(\xi, \mu) = O(h^2). \end{aligned}$$

Method remains second order after dropping $R_1\left(t + \frac{h}{2}, y + \frac{h}{2}f(t, y)\right)$

Runge-Kutta Method of Order Two (III)

► Midpoint Method

$$w_0 = \alpha,$$

$$w_{j+1} = w_j + hf \left(t_j + \frac{h}{2}, w_j + \frac{h}{2} f(t_j, w_j) \right), \quad j = 0, 1, \dots, N-1.$$

- Two function evaluations for each j ,
- Second order accuracy.

No need for derivative calculations

General 2nd order Runge-Kutta Methods

► $w_0 = \alpha$; for $j = 0, 1, \dots, N - 1$,

$$w_{j+1} = w_j + h (a_1 f(t_j, w_j) + a_2 f(t_j + \alpha_2, w_j + \delta_2 f(t_j, w_j))).$$

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- ▶ $w_0 = \alpha$; for $j = 0, 1, \dots, N - 1$,

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- ▶ Two function evaluations for each j ,
- ▶ Want to choose $a_1, a_2, \alpha_2, \delta_2$ for highest possible order of accuracy.

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- ▶ Two function evaluations for each j ,
- ▶ Want to choose $a_1, a_2, \alpha_2, \delta_2$ for highest possible order of accuracy.

local truncation error

$$\begin{aligned} \tau_{j+1}(h) &= \frac{y(t_{j+1}) - y(t_j)}{h} - (a_1 f(t_j, y(t_j)) + a_2 f(t_j + \alpha_2, y(t_j) + \delta_2 f(t_j, y(t_j)))) \\ &= y'(t_j) + \frac{h}{2} y''(t_j) + O(h^2) \\ &\quad - \left((a_1 + a_2) f(t_j, y(t_j)) + a_2 \alpha_2 \frac{\partial f}{\partial t}(t_j, y(t_j)) \right. \\ &\quad \left. + a_2 \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \right). \end{aligned}$$

local truncation error

$$\begin{aligned}\tau_{j+1}(h) = & y'(t_j) + \frac{h}{2}y''(t_j) + O(h^2) \\ & - \left((a_1 + a_2) f(t_j, y(t_j)) + a_2 \alpha_2 \frac{\partial f}{\partial t}(t_j, y(t_j)) \right. \\ & \left. + a_2 \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \right).\end{aligned}$$

where $y'(t_j) = f(t_j, y(t_j))$,

local truncation error

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For any choice with

$$a_1 + a_2 = 1, \quad a_2 \alpha_2 = a_2 \delta_2 = \frac{h}{2},$$

we have a second order method

$$\tau_{j+1}(h) = O(h^2).$$

local truncation error

$$\begin{aligned}\tau_{j+1}(h) = & y'(t_j) + \frac{h}{2}y''(t_j) + O(h^2) \\ & - \left((a_1 + a_2) f(t_j, y(t_j)) + a_2 \alpha_2 \frac{\partial f}{\partial t}(t_j, y(t_j)) \right. \\ & \left. + a_2 \delta_2 f(t_j, y(t_j)) \frac{\partial f}{\partial y}(t_j, y(t_j)) + O(h^2) \right).\end{aligned}$$

where $y'(t_j) = f(t_j, y(t_j))$,

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For any choice with

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we have a second order method

$$\tau_{j+1}(h) = O(h^2).$$

Four parameters, three equations

General 2nd order Runge-Kutta Methods

$$w_0 = \alpha; \text{ for } j = 0, 1, \dots, N - 1,$$

$$w_{j+1} = w_j + h (a_1 f(t_j, w_j) + a_2 f(t_j + \alpha_2, w_j + \delta_2 f(t_j, w_j))).$$

$$a_1 + a_2 = 1, \quad a_2 \alpha_2 = a_2 \delta_2 = \frac{h}{2},$$

- ▶ **Midpoint method:** $a_1 = 0, a_2 = 1, \alpha_2 = \delta_2 = \frac{h}{2},$

$$w_{j+1} = w_j + h f \left(t_j + \frac{h}{2}, w_j + \frac{h}{2} f(t_j, w_j) \right).$$

- ▶ **Modified Euler method:** $a_1 = a_2 = \frac{1}{2}, \alpha_2 = \delta_2 = h,$

$$w_{j+1} = w_j + \frac{h}{2} (f(t_j, w_j) + f(t_{j+1}, w_j + h f(t_j, w_j))).$$

3rd order Runge-Kutta Method (rarely used in practice)

$$w_0 = \alpha;$$

for $j = 0, 1, \dots, N - 1,$

$$w_{j+1} = w_j + \frac{h}{4} \left(f(t_j, w_j) + 3f \left(t_j + \frac{2h}{3}, w_j + \frac{2h}{3} f \left(t_j + \frac{h}{3}, w_j + \frac{h}{3} f(t_j, w_j) \right) \right) \right)$$

$$\stackrel{\text{def}}{=} w_j + h \phi(t_j, w_j).$$

3rd order Runge-Kutta Method (rarely used in practice)

$$w_0 = \alpha;$$

for $j = 0, 1, \dots, N - 1,$

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local truncation error

$$\tau_{j+1}(h) = \frac{y(t_{j+1})y(t_j)}{h} - \phi(t_j, y(t_j)) = O(h^3).$$

4th order Runge-Kutta Method

$$w_0 = \alpha;$$

for $j = 0, 1, \dots, N - 1,$

$$k_1 = hf(t_j, w_j),$$

$$k_2 = hf\left(t_j + \frac{h}{2}, w_j + \frac{1}{2}k_1\right),$$

$$k_3 = hf\left(t_j + \frac{h}{2}, w_j + \frac{1}{2}k_2\right),$$

$$k_4 = hf(t_{j+1}, w_j + k_3),$$

$$w_{j+1} = w_j + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

4 function evaluations per step

Example

Initial Value ODE $\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$
exact solution $y(t) = (1 + t)^2 - 0.5 e^t.$

Example

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

Example

Initial Value ODE $\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$
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Example

Initial Value ODE $\frac{dy}{dt} = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$

exact solution $y(t) = (1 + t)^2 - 0.5 e^t.$

