MA579H Scientific Computing

Numerics of first order ODEs - I

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Lecture outline

- Numerical differentiation
- Euler method for ODE

Numerical differentiation

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- Differentiation is inherently sensitive, as small perturbations in data can cause large changes in result.
- If a function is known only at discrete set of points, then a good approach is to fit some smooth function to given data and then differentiate the approximating function.

Finite difference approximations

Let $h > 0$. Consider the expansions

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(\xi) \text{ for some } x < \xi < x+h, \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2} f''(\eta) \text{ for some } x-h < \eta < x. \end{aligned}$$

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Forward difference approximation:

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\frac{f(x+h) - f(x)}{h} = f'(x) + \underbrace{\frac{h}{2}f''(\xi)}_{\text{truncation error}} = f'(x) + \mathcal{O}(h).
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Backward difference approximation:

$$\frac{f(x) - f(x-h)}{h} = f'(x) - \underbrace{\frac{h}{2} f''(\xi)}_{\text{truncation error}} = f'(x) + \mathcal{O}(h).$$

Finite difference approximations (cont.)

Assuming that f is C^3, we have the expansions

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\xi), \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(\eta). \end{aligned}$$

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Centered difference approximation:

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \underbrace{\frac{h^2}{6}f'''(\theta)}_{\text{truncation error}} = f'(x) + \mathcal{O}(h^2).$$

Finite difference approximations (cont.)

Now assume that f is C^4 and consider the expansions

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi), \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\eta). \end{aligned}$$

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Then we have 3-point centered difference approximation of f'':

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \underbrace{\frac{h^2}{12}f^{(4)}(\theta)}_{\text{truncation error}} = f''(x) + \mathcal{O}(h^2).$$

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- Software packages are available implementing automatic differentiation (AD) of functions.

Example

Consider $f(x) = e^x$. Then $f'(0) = 1$. Forward difference approximation and centered difference approximation of $f'(0)$ is given in the following table.

h	$\frac{e^h - 1}{h} - 1$	$\frac{e^h - e^{-h}}{2h} - 1$
10^{-1}	5.17×10^{-2}	1.6×10^{-3}
10^{-2}	5.02×10^{-3}	1.67×10^{-5}
10^{-3}	5.0×10^{-4}	1.6×10^{-7}
10^{-4}	$5.0 \times 1o^{-5}$	1.67×10^{-9}
10^{-5}	5.0×10^{-6}	1.21×10^{-11}

Effect of rounding error

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$$|h| \text{ small } \implies E(x,h) \text{ is small.}$$

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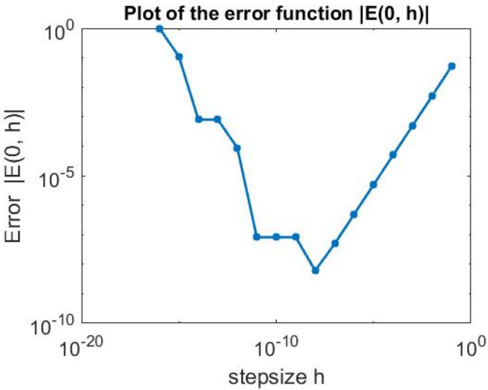

Ordinary differential equations (ODEs)

Consider the initial value problem (IVP) associated with a first order ODE

$$\frac{dy}{dx} = f(x, y), \; y(x_0) = y_0,$$

where $x_0 \in [a, b]$ and $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$.

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The direction or slope field of the ODE is obtained by affixing an arrow representing the vector $\left(\frac{1}{\sqrt{1+(f(x,y))^2}}, \frac{f(x,y)}{\sqrt{1+(f(x,y))^2}}\right)$ at each point (x, y) on a grid with $x \in [a, b]$. It is a graphical tool to analyze the solution of the IVP.

Direction fields of ODEs

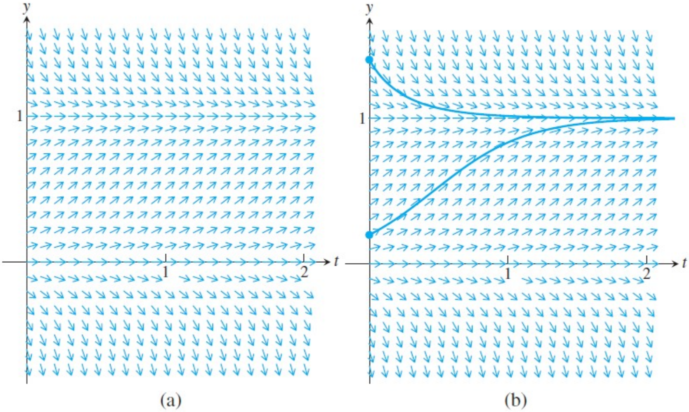


Figure : Direction field for the autonomous ODE $\frac{dy}{dt} = y(1-y)$ showing (a) no variation with t and (b) plotted with two solutions.

Direction fields of ODEs

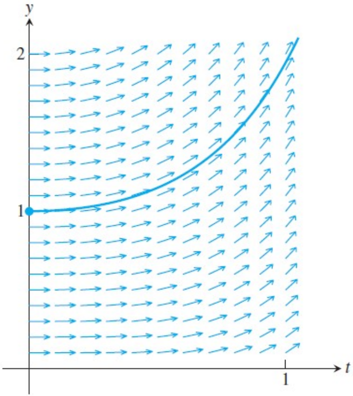
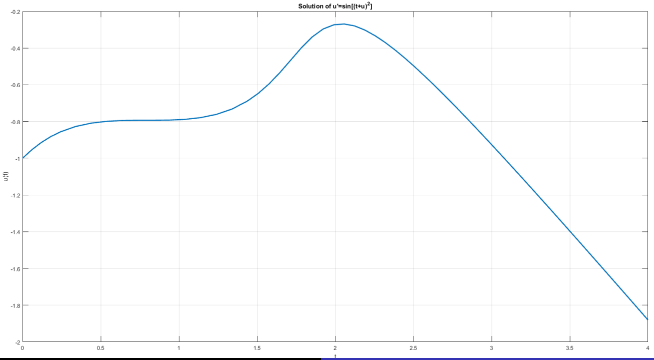


Figure : Direction field for the non-autonomous ODE $\frac{dy}{dt} = ty + y^3$ showing the solution $y(t) = 3e^{t^2/2} - t^2 - 2$ satisfying $y(0) = 1$.

Example

Consider the equation $u' = \sin((u+t)^2), u(0) = -1$. The MATLAB built-in function ode45 solves the ode numerically.

```
f = @(t,u) sin( (t+u).^2 );
[t,u] = ode45(f,[0,4],-1);
plot(t,u, 'LineWidth', 2), grid on
xlabel('t'), ylabel('u(t)')
title('Solution of u'' = sin[(t+u)^2]')
```



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$$\frac{dy}{dx} = f(x, y), \; y(x_0) = y_0,$$

has a unique solution if $|f(x, y_1) - f(x, y_2)| \leq K|y_1 - y_2|$ for all $a \leq x \leq b$, where K is a constant independent of x.

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- It is not expected to determine the solution y of the IVP as a function of x. Instead, we construct a table of function values

x_0	x_1	x_2	$\dots$	x_m
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Most numerical methods for solving ODEs produce such a table.

Example

Compute solution of $u' = sin((u+t)^2), u(0) = -1$ at data points

```
f = @(t,u) sin( (t+u).^2 );
t = linspace(0,4,60)';
[t,u] = ode45(f,t,-1);
plot(t,u,'o'), hold on
xlabel('t'), ylabel('u(t)')
title('Solution at 60 points')
```

Also, we can create a callable function for the solution. This is essentially a high-quality interpolant of the computed values.

```
u = @(t) deval( ode45(f,[0,4],-1), t );
fplot(u,[0,4], 'LineWidth', 2)
xlabel('t'), ylabel('u(t)')
title('Solution as a callable function')
```

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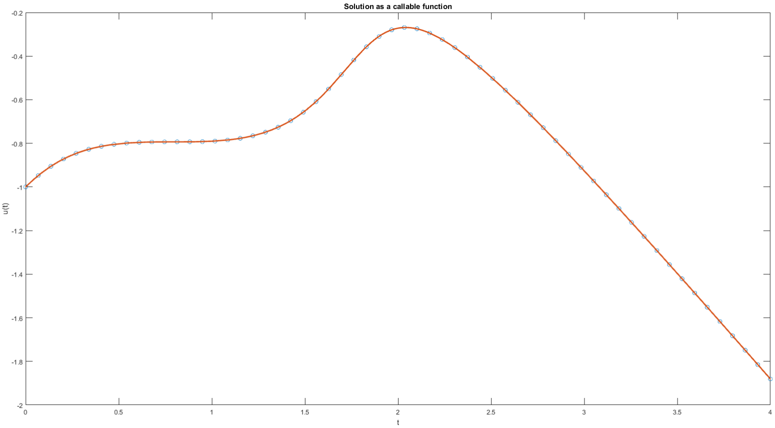

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Example

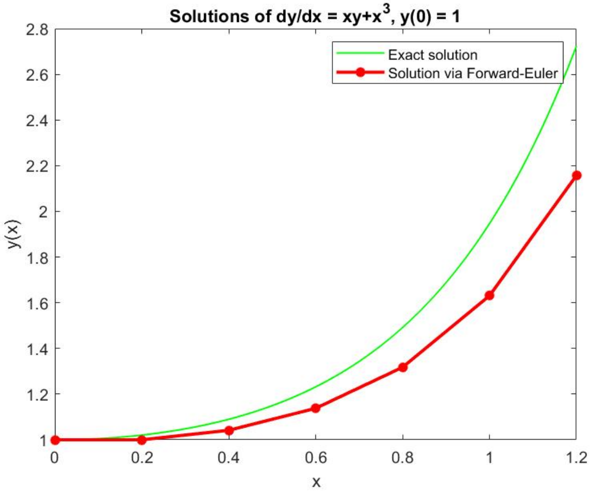

Figure : Plot of exact solution $y(x) = 3e^{x^2/2} - x^2 - 2$ of the non-autonomous ODE $\frac{dy}{dx} = xy + x^3$ satisfying $y(0) = 1$ along with solution via forward Euler method with $h = 0.2$.

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In backward Euler's method, we have to solve the nonlinear equation $y_{j+1} = y_j + hf(x_{j+1}, y_{j+1})$ for y_{j+1}, which would require extra work.

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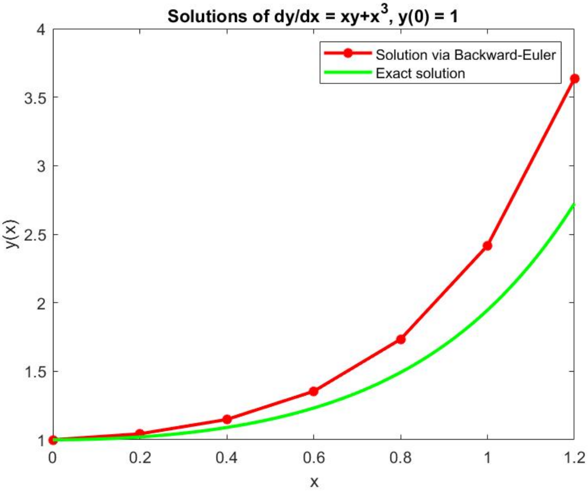
The first step in backward Euler's method yields $y_1 = y_0 + 2\sin(x_1 y_1)$. To compute y_1, solve $y_0 + 2\sin(x_1 y_1) - y_1 = 0$ by a root finding method.

Example



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Forward Euler's method via quadrature

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Integrating $y' = f(x, y)$ in $[x_j, x_{j+1}]$, we have

$$y(x_{j+1}) - y(x_j) = \int_{x_j}^{x_{j+1}} f(t, y(t))dt.$$

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This yields the forward Euler's method

$$y_{j+1} = y_j + hf(x_j, y_j), \;\; j = 0 : n-1.$$

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