10.34: Numerical Methods Applied to Chemical Engineering

Lecture 13:
ODE-IVP and Numerical Integration

Recap

- Constrained optimization
- Method of Lagrange multipliers
- Interior point methods

Recap

- Example:
  - minimize: $\exp(-x_1^2 - x_2^2)$
  - subject to: $x_1^2 + x_2^2 - 1 = 0$
    - Can you solve this problem?

$$\begin{pmatrix} \nabla f - \lambda \nabla c \\ c \end{pmatrix} = \begin{pmatrix} -2x_1 e^{-x_1^2 - x_2^2} - 2x_1\lambda \\ -2x_2 e^{-x_1^2 - x_2^2} - 2x_2\lambda \\ x_1^2 + x_2^2 - 1 \end{pmatrix} = 0$$

$$\lambda = e^{-1}$$

Dynamic Models

- Most physical processes are dynamic in nature. This means that first principles models describing those processes can be depicted as differential equations:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t; \boldsymbol{\theta})$$

$$\mathbf{x}(t_0) = \mathbf{x}_0$$

  - $\mathbf{x}(t)$ is often called the state vector and is the set of dynamic variables for which we want to solve.
  - t is time
  - $\mathbf{u}(t)$ is a time dependent input that we specify
  - $\boldsymbol{\theta}$ is a vector of time independent parameters.
  - $\mathbf{x}_0$ is the initial value of the state vector at

Dynamic Models

- Usually, the solution we are interested in is values of the state vector within some time domain: $t \in [t_0, t_f]$
- The initial value problem can be rewritten as:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t) \quad \forall t \in [t_0, t_f]$$

$$\mathbf{x}(t_0) = \mathbf{x}_0$$

- By convention, the initial time, t_0, is often set to be zero.
- Since $\mathbf{f}(\mathbf{x}(t), t)$, can be an arbitrary nonlinear function of the state vector, a closed form, analytical solution rarely exists.
- Numerically, we will solve this equation by finding the state vector at a finite number of points within the time domain.
    - We will need to characterize the accuracy and stability of solution methods to these problems.

Dynamic Models

- Higher order differential equations can always be rewritten as systems of first order equations
- Consider the force balance on a driven mass-spring-damper:

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = f(t)$$

- Let: $v = \dfrac{dx}{dt}$
- Then: $\dfrac{dx}{dt} = v$
- And: $m\dfrac{dv}{dt} + bv + kx = f(t)$

Dynamic Models

- Higher order differential equations can always be rewritten as systems of first order equations
- Consider the force balance on a driven mass-spring-damper:

$$\frac{dx}{dt} = v \qquad\qquad m\frac{dv}{dt} + bv + kx = f(t)$$

- Collecting a state vector, $\begin{pmatrix} x(t) \\ v(t) \end{pmatrix}$, gives:

$$\frac{d}{dt}\underbrace{\begin{pmatrix} x(t) \\ v(t) \end{pmatrix}}_{\mathbf{x}} = \underbrace{\begin{pmatrix} v(t) \\ (f(t) - bv(t) - kx(t))/m \end{pmatrix}}_{\mathbf{f}(\mathbf{x}(t),\mathbf{u}(t),t) \text{ or } \mathbf{f}(\mathbf{x}(t),t)}$$

$$\mathbf{x}(t_0) = \begin{pmatrix} x(t_0) \\ \frac{dx}{dt}(t_0) \end{pmatrix}.$$

Existence and Uniqueness

- Example:
  - Use separation of variables to solve:

$$\frac{dx}{dt} = x^2$$

$$x(0) = x_0$$

  - Does a solution exist for all times? Is the solution unique?

$$\frac{dx}{x^2} = dt \Rightarrow \left(\frac{1}{x_0} - \frac{1}{x(t)}\right) = t \Rightarrow x(t) = \frac{1}{\frac{1}{x_0} - t}$$

Existence and Uniqueness

- Example:
  - Use separation of variables to solve:

$$\frac{dx}{dt} = x^3$$

$$x(0) = x_0$$

  - Does a solution exist for all times? Is the solution unique?

$$\frac{dx}{x^3} = dt \Rightarrow \frac{1}{2}\left(\frac{1}{x_0^2} - \frac{1}{x(t)^2}\right) = t \Rightarrow x(t)^2 = \frac{1}{\frac{1}{x_0^2} - 2t}$$

Existence and Uniqueness

- A unique solution exists if $\mathbf{f}(\mathbf{x}, t)$, is Lipschitz continuous.
  - Lipschitz continuity within some domain D means that:

$$\|\mathbf{f}(\mathbf{x}, t) - \mathbf{f}(\mathbf{z}, t)\|_p \leq m\|\mathbf{x} - \mathbf{z}\|_p \quad \mathbf{x}, \mathbf{z} \in D$$

  - This is stronger than regular continuity:

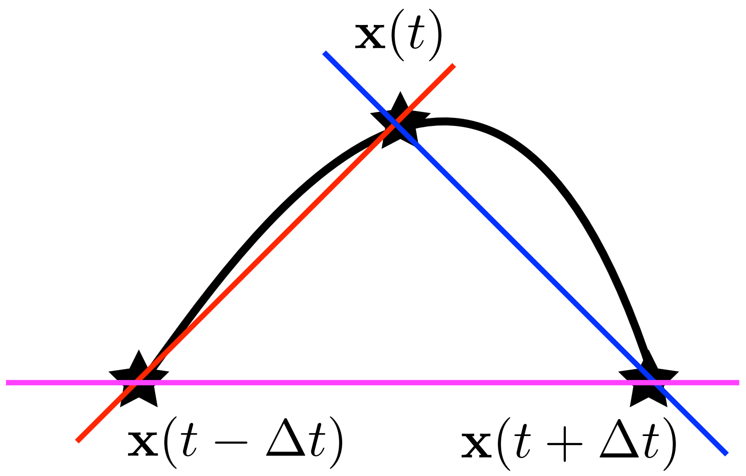
$$\lim_{\mathbf{x} \to \mathbf{z}} \|\mathbf{f}(\mathbf{x}, t) - \mathbf{f}(\mathbf{z}, t)\|_p \to 0$$

- For existence and uniqueness to be guaranteed, $\mathbf{f}(\mathbf{x}, t)$, needs to be Lipschitz continuous over the whole domain of $\mathbf{x}$ and in the time domain of interest.

- Examples:
  - Is $f(x) = x$ continuous? Is it uniformly Lipschitz cont.?
  - Is $f(x) = x^2$ continuous? Is it uniformly Lipschitz cont.?

Finite Differences

- One way to solve differential equations numerical is to approximate the derivatives and turn the differential equation into a sequence of algebraic equations.
  - Finite differences are a typical method for this approximation:



- Forward difference:

$$\frac{d}{dt}\mathbf{x}(t) \approx \frac{1}{\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t))$$

- Backward difference:

$$\frac{d}{dt}\mathbf{x}(t) \approx \frac{1}{\Delta t}(\mathbf{x}(t) - \mathbf{x}(t-\Delta t))$$

- Central difference:

$$\frac{d}{dt}\mathbf{x}(t) \approx \frac{1}{2\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t-\Delta t))$$

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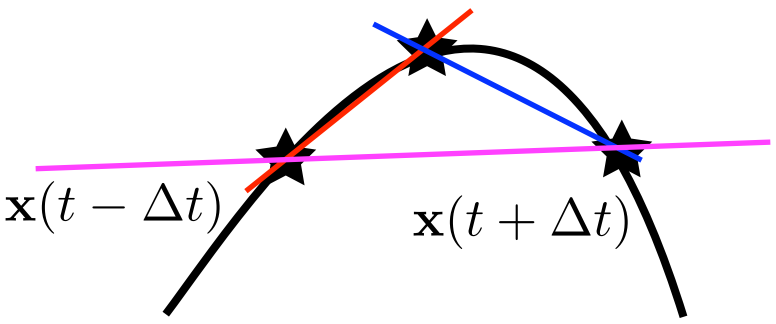

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- Central difference:

$$\frac{d}{dt}\mathbf{x}(t) \approx \frac{1}{2\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t-\Delta t))$$

Finite Differences

- Taylor expansions can be used to evaluate the accuracy of finite difference approximations:

$$\mathbf{x}(t+\Delta t) = \mathbf{x}(t) + \Delta t \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{2!}\frac{d^2}{dt^2}\mathbf{x}(t) + \frac{(\Delta t)^3}{3!}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^4),$$

$$\mathbf{x}(t-\Delta t) = \mathbf{x}(t) - \Delta t \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{2!}\frac{d^2}{dt^2}\mathbf{x}(t) - \frac{(\Delta t)^3}{3!}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^4),$$

  - Forward difference:

$$\begin{aligned}\frac{d}{dt}\mathbf{x}(t) &\approx \frac{1}{\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t)) \\ &= \frac{1}{\Delta t}\left(\mathbf{x}(t) + \Delta t \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{2!}\frac{d^2}{dt^2}\mathbf{x}(t) + \frac{(\Delta t)^3}{3!}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^4) - \mathbf{x}(t)\right) \\ &= \frac{d}{dt}\mathbf{x}(t) + \frac{\Delta t}{2}\frac{d^2}{dt^2}\mathbf{x}(t) + \frac{(\Delta t)^2}{6}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^3),\end{aligned}$$

  - Central difference:

$$\begin{aligned}\frac{d}{dt}\mathbf{x}(t) &\approx \frac{1}{2\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t-\Delta t)) \\ &= \frac{1}{2\Delta t}\Bigg(\mathbf{x}(t) + \Delta t \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{2}\frac{d^2}{dt^2}\mathbf{x}(t) + \frac{(\Delta t)^3}{3!}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^4) \\ &\qquad -\left(\mathbf{x}(t) - \Delta t \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{2!}\frac{d^2}{dt^2}\mathbf{x}(t) - \frac{(\Delta t)^3}{3!}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^4)\right)\Bigg) \\ &= \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{6}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^3).\end{aligned}$$

Finite Differences

- The order of accuracy of a finite difference approximation is given by the leading order error in the Taylor expansion.
  - For example:

$$
\begin{aligned}
\frac{d}{dt}\mathbf{x}(t) &\approx \frac{1}{\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t)) \\
&= \frac{1}{\Delta t}\left(\mathbf{x}(t) + \Delta t \frac{d}{dt}\mathbf{x}(t) + \frac{(\Delta t)^2}{2!}\frac{d^2}{dt^2}\mathbf{x}(t) + \frac{(\Delta t)^3}{3!}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^4) - \mathbf{x}(t)\right) \\
&= \frac{d}{dt}\mathbf{x}(t) + \boxed{\frac{\Delta t}{2}\frac{d^2}{dt^2}\mathbf{x}(t)} + \frac{(\Delta t)^2}{6}\frac{d^3}{dt^3}\mathbf{x}(t) + \mathrm{O}((\Delta t)^3),
\end{aligned}
$$

    - is said to be a first order accurate approximation.
  - If the error in the approximation is: $E(\Delta t) \sim (\Delta t)^p$, then the approximation is pth-order accurate
- The order of accuracy can be determined by calculating the error in the solution method after one step and plotting:

$$\log|E(\Delta t)| \approx \log c + p \log \Delta t$$

Explicit Methods for IVPs

- Explicit (or Forward) Euler method:
  - Approximate the derivative with forward differences:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t)$$
$$\frac{1}{\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t)) \approx \mathbf{f}(\mathbf{x}(t), t)$$
$$\mathbf{x}(t+\Delta t) \approx \mathbf{x}(t) + (\Delta t)\mathbf{f}(\mathbf{x}(t), t),$$

- This gives a sequence of approximations for the solution at different time points:

$$\begin{aligned}
\mathbf{x}(t_0) &= \mathbf{x}_0 \\
\mathbf{x}(t_0+\Delta t) &\approx \mathbf{x}(t_0) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0), t_0) = \mathbf{x}_0 + (\Delta t)\mathbf{f}(\mathbf{x}_0, t_0) \\
\mathbf{x}(t_0+2\Delta t) &\approx \mathbf{x}(t_0+\Delta t) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0+\Delta t), t_0+\Delta t) \\
\mathbf{x}(t_0+3\Delta t) &\approx \mathbf{x}(t_0+2\Delta t) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0+2\Delta t), t_0+2\Delta t) \\
&\vdots \\
\mathbf{x}(t_0+(k+1)\Delta t) &\approx \mathbf{x}(t_0+k\Delta t) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0+k\Delta t), t_0+k\Delta t) \\
&\vdots
\end{aligned}$$

Explicit Methods for IVPs

- Explicit Euler method:
  - Approximate the derivative with forward differences:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t)$$

$$\frac{1}{\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t)) \approx \mathbf{f}(\mathbf{x}(t), t)$$

$$\mathbf{x}(t+\Delta t) \approx \mathbf{x}(t) + (\Delta t)\mathbf{f}(\mathbf{x}(t), t)$$

  - This gives a sequence of approximations for the solution at different time points:

$$\begin{aligned}
\mathbf{x}(t_0) &= \mathbf{x}_0 \\
\mathbf{x}(t_0+\Delta t) &\approx \mathbf{x}(t_0) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0), t_0) = \mathbf{x}_0 + (\Delta t)\mathbf{f}(\mathbf{x}_0, t_0) \\
\mathbf{x}(t_0+2\Delta t) &\approx \mathbf{x}(t_0+\Delta t) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0+\Delta t), t_0+\Delta t) \\
\mathbf{x}(t_0+3\Delta t) &\approx \mathbf{x}(t_0+2\Delta t) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0+2\Delta t), t_0+2\Delta t) \\
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\mathbf{x}(t_0+(k+1)\Delta t) &\approx \mathbf{x}(t_0+k\Delta t) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0+k\Delta t), t_0+k\Delta t) \\
&\vdots
\end{aligned}$$

Explicit Methods for IVPs

- Explicit Euler method:
  - Approximate the derivative with forward differences:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t)$$

$$\frac{1}{\Delta t}(\mathbf{x}(t+\Delta t) - \mathbf{x}(t)) \approx \mathbf{f}(\mathbf{x}(t), t)$$

$$\mathbf{x}(t+\Delta t) \approx \mathbf{x}(t) + (\Delta t)\mathbf{f}(\mathbf{x}(t), t)$$

  - This gives a sequence of approximations for the solution at different time points:

$$\begin{aligned}
\mathbf{x}(t_0) &= \mathbf{x}_0 \\
\mathbf{x}(t_1) &\approx \mathbf{x}(t_0) + (\Delta t)\mathbf{f}(\mathbf{x}(t_0), t_0) \\
\mathbf{x}(t_2) &\approx \mathbf{x}(t_1) + (\Delta t)\mathbf{f}(\mathbf{x}(t_1), t_1) \\
\mathbf{x}(t_3) &\approx \mathbf{x}(t_2) + (\Delta t)\mathbf{f}(\mathbf{x}(t_2), t_2) \\
&\vdots \\
\mathbf{x}(t_{k+1}) &\approx \mathbf{x}(t_k) + (\Delta t)\mathbf{f}(\mathbf{x}(t_k), t_k) \\
&\vdots
\end{aligned}$$

$$t_k = t_0 + k\Delta t$$

$$k = 0, 1, 2, \ldots$$

Explicit Methods for IVPs

- Explicit Euler method:

```
f = @(x,t) % Does something

t0 = 0;
tf = 1;
dt = 0.01;

x0 = % Initial condition

t = [t0:dt:tf]
x = zeros( length( x0 ), length( t ) );

x( :, 1 ) = x0;

for i = 2:length( t )

  x( :, i ) = x( :, i - 1 ) + dt * f( x( :, i - 1 ), t( i - 1 ) );

end;
```

Explicit Methods for IVPs

- Explicit methods are termed explicit because the algebraic approximation to the IVP does not require a complicated solution method.
  - Higher order explicit methods can be derived by incorporating information about the solution at intermediate or past time points.
  - There are innumerable different methods by which this can be done. Some are more accurate, others are more stable, others still require fewer function evaluations.
- Example: explicit Runge-Kutta method

$$\mathbf{x}(t+\Delta t/2) = \mathbf{x}(t) + \frac{\Delta t}{2}\mathbf{f}(\mathbf{x}(t),t)$$
$$\mathbf{x}(t+\Delta t) = \mathbf{x}(t) + (\Delta t)\mathbf{f}(\mathbf{x}(t+\Delta t/2), t+\Delta t/2)$$

  - uses information at the midpoint of the step
  - requires twice as many function evaluations

Explicit Methods for IVPs

- Example:

$$\frac{dy}{dt} = -y, \quad y(0) = 1 \qquad\qquad y(t) = e^{-t}$$

- Forward Euler:

$$y(t + \Delta t) = y(t) - \Delta t y(t) = (1 - \Delta t) y(t)$$

$$y(\Delta t) = 1 - \Delta t$$

- Midpoint:

$$y(t + \Delta t/2) = y(t) - \frac{\Delta t}{2} y(t) = \left(1 - \frac{\Delta t}{2}\right) y(t)$$

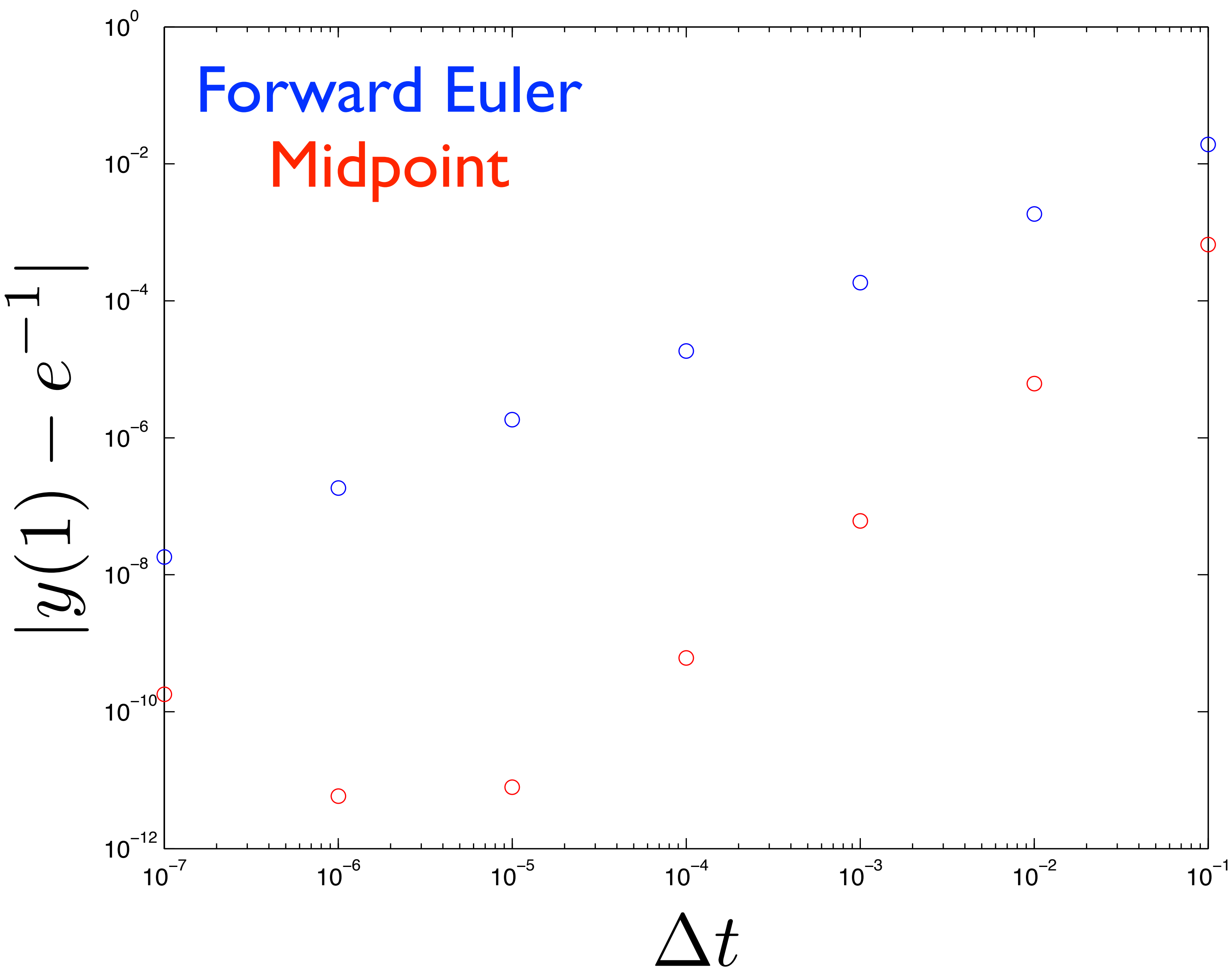
$$y(t + \Delta t) = y(t) - \Delta t y(t + \Delta t/2) = \left[1 - \Delta t \left(1 - \frac{\Delta t}{2}\right)\right] y(t)$$

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

Explicit Methods for IVPs

- Example:

$$\frac{dy}{dt} = -y, \quad y(0) = 1 \qquad\qquad y(t) = e^{-t}$$



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