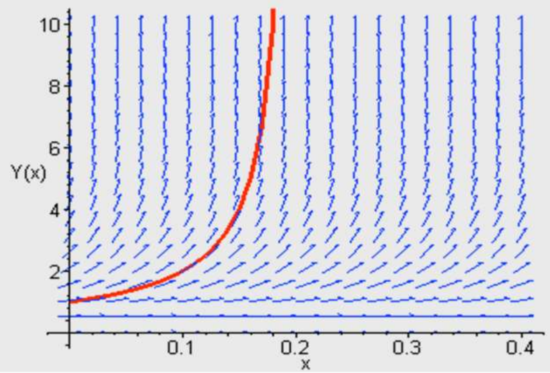
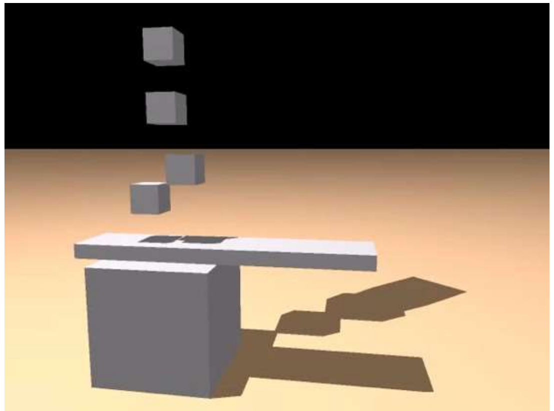
Differential Equations



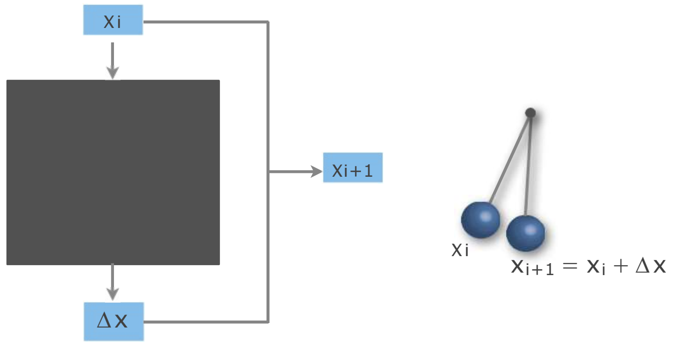


- Overview of differential equation
- Initial value problem
- Explicit numeric methods
- Implicit numeric methods
- Modular implementation

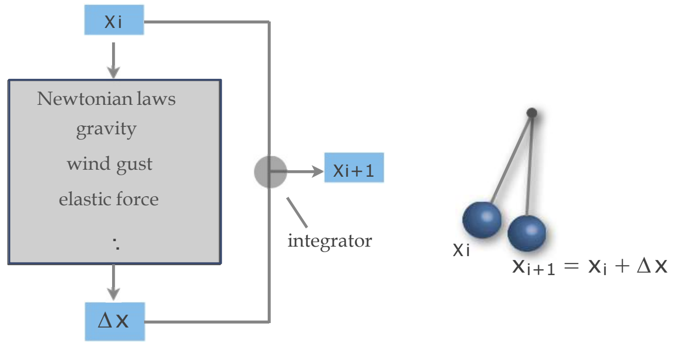
Physics-based simulation

- It's an algorithm that produces a sequence of states over time under the laws of physics
- What is a state?

Physics-based simulation



Physics-based simulation



Differential equations

- What is a differential equation?
  - It describes the relation between an unknown function and its derivatives
- Ordinary differential equation (ODE)
  - is the relation that contains functions of only one independent variable and its derivatives

Ordinary differential equations

An ODE is an equality equation involving a function and its derivatives

known function

$$\dot{x}(t) = f(x(t))$$

time derivative of the unknown function

unknown function that evaluates the state given time

What does it mean to "solve" an ODE?

Symbolic solutions

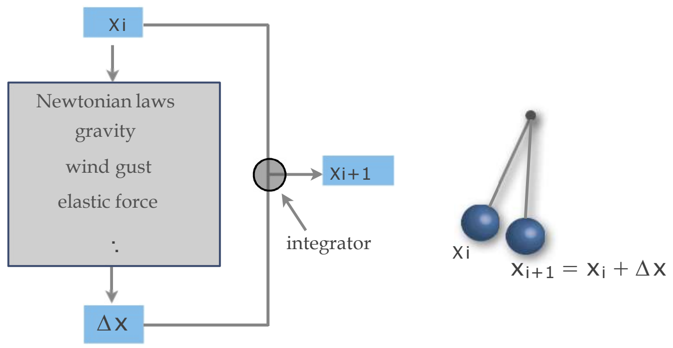
- Standard introductory differential equation courses focus on finding solutions analytically
- Linear ODEs can be solved by integral transforms
- Use `DSolve[eqn,x,t]` in Mathematica

Differential equation: $\dot{x}(t) = -kx(t)$
Solution: $x(t) = e^{-kt}$

Numerical solutions

- In this class, we will be concerned with numerical solutions
- Derivative function *f* is regarded as a black box
- Given a numerical value x and t, the black box will return the time derivative of x

Physics-based simulation



- Overview of differential equation
- Initial value problem
- Explicit numeric methods
- Implicit numeric methods
- Modular implementation

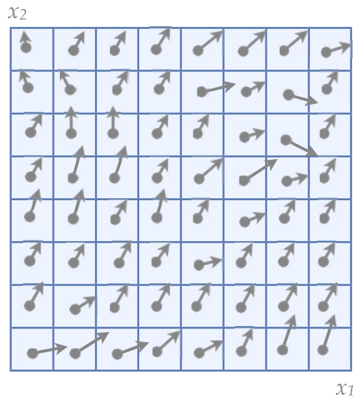
Initial value problems

In a canonical initial value problem, the behavior of the system is described by an ODE and its initial condition:

$$\dot{x} = f(x,t)$$
$$x(t_0) = x_0$$

To solve $x(t)$ numerically, we start out from x_0 and follow the changes defined by f thereafter

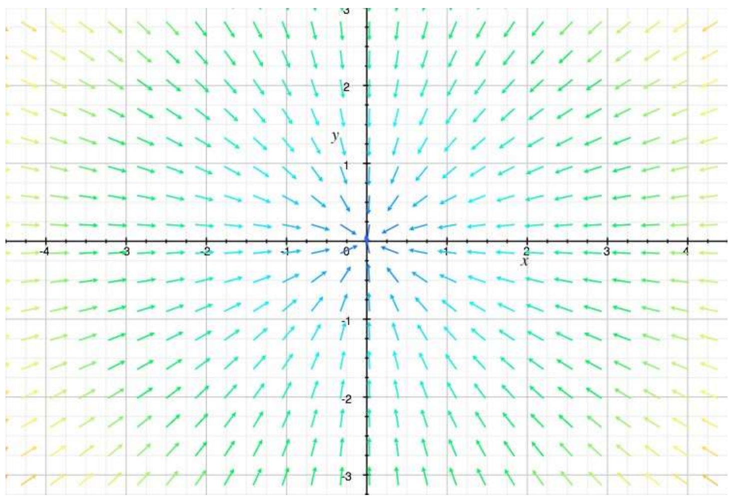
Vector field

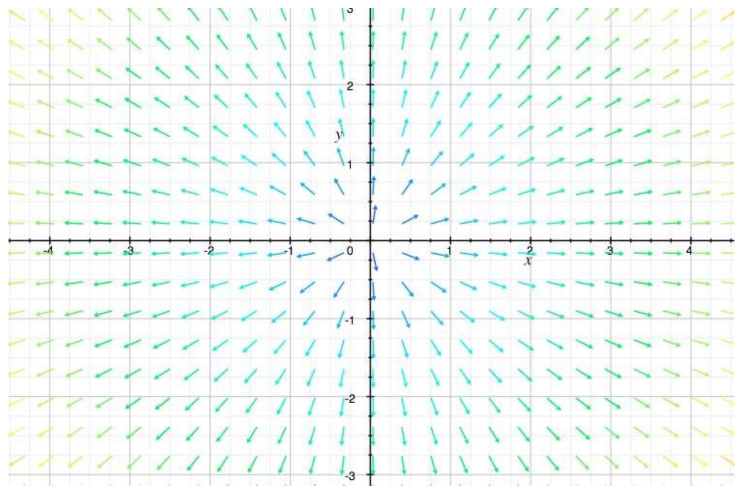


The differential equation can be visualized as a vector field

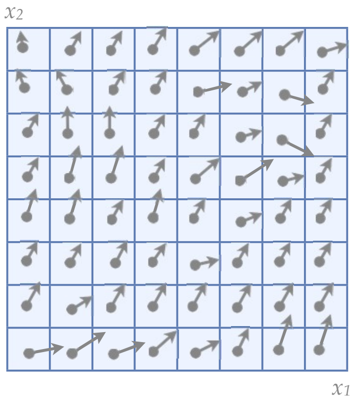
$$\dot{\mathbf{x}} = f(\mathbf{x}, t)$$

$x(t)$: a moving point
$f(x,t)$: x's velocity





Vector field

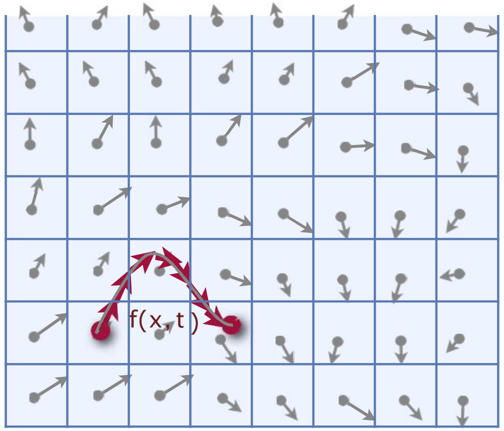


The differential equation can be visualized as a vector field

$$\dot{\mathbf{x}} = f(\mathbf{x}, t)$$

How does the vector field look like if *f* depends directly on time?

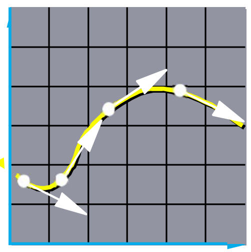
Integral curves



$$\int_{t_0} f(\mathbf{x}, t)dt$$

Integral Curves

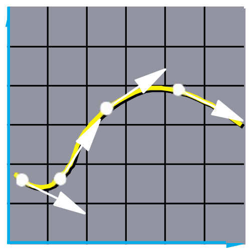
Start Here



Pick any starting point, and follow the vectors.

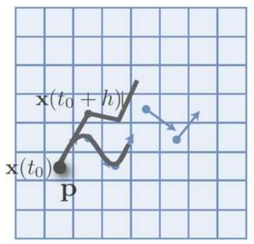
Initial Value Problem

Given the starting point, follow the integral curve.



- Overview of differential equation
- Initial value problem
- Explicit numeric methods
- Implicit numeric methods
- Modular implementation

Explicit Euler method



How do we get to the next state from the current state?

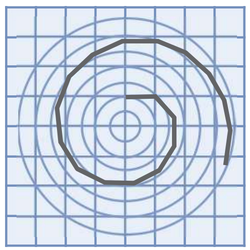
$$\mathbf{x}(t_0+h) = \mathbf{x}_0 + h\dot{\mathbf{x}}(t_0)$$

Instead of following real integral curve, $\mathbf{p}$ follows a polygonal path

Discrete time step h determines the errors

Problems of Euler method

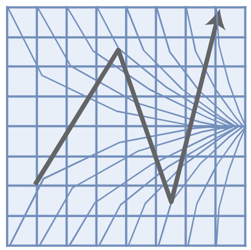
Inaccuracy



The circle turns into a spiral no matter how small the step size is

Problems of Euler method

Instability



$\dot{\mathbf{x}} = -k\mathbf{x}$

Symbolic solution: $x(t) = e^{-kt}$

Oscillation:

Divergence:

How small the step size has to be?

Accuracy of Euler method

- At each step, $\mathbf{x}(t)$ can be written in the form of Taylor series:

$$\mathbf{x}(t_0+h)=\mathbf{x}(t_0)+h\dot{\mathbf{x}}(t_0)+\frac{h^2}{2!}\ddot{\mathbf{x}}(t_0)+\frac{h^3}{3!}\dddot{\mathbf{x}}(t_0)+\ldots+\frac{h^n}{n!}\frac{\partial^n\mathbf{x}}{\partial t^n}+\ldots$$

- What is the order of the error term in Euler method?
- The cost per step is determined by the number of evaluations per step

Taylor series is a representation of a function as an infinite sum of terms calculated using the derivatives at a particular point

Stability of Euler method

- Assume the derivative function is linear

$$\frac{d}{dt}\mathbf{x}=\mathbf{A}\mathbf{x}$$

- Look at $\mathbf{x}$ parallel to the largest eigenvector of $\mathbf{A}$

$$\frac{d}{dt}\mathbf{x}=\lambda\mathbf{x}$$

- Note that eigenvalue λ can be complex

The test equation

- Test equation advances x by

$$x_{n+1}=x_n+h\lambda x_n$$

- Solving gives

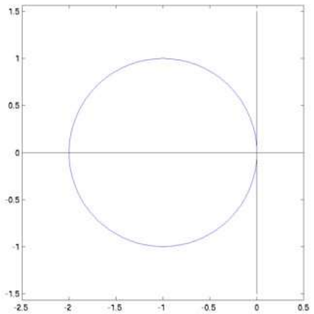
$$x_n=(1+h\lambda)^n x_0$$

- Condition of stability

$$|1+h\lambda|\le 1$$

Stability region

- Plot all the values of $h\lambda$ on the complex plane where Euler method is stable



Real eigenvalue

- If eigenvalue is real and negative, what kind of the motion does **x** correspond to?
  - a damping motion smoothly coming to a halt
- The threshold of time step

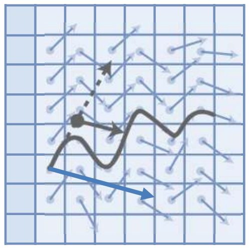
$$h \le \frac{2}{|\lambda|}$$

- What about the imaginary axis?

Imaginary eigenvalue

- If eigenvalue is pure imaginary, Euler method is unconditionally unstable
- What motion does **x** look like if the eigenvalue is pure imaginary?
  - an oscillatory or circular motion
- We need to look at other methods

The midpoint method



1. Compute an Euler step

$$\Delta x = hf(x(t_0))$$

2. Evaluate *f* at the midpoint

$$f_{mid} = f\left(x(t_0) + \frac{\Delta x}{2}\right)$$

3. Take a step using f_{mid}

$$x(t_0 + h) = x(t_0) + hf_{mid}$$

$$\mathbf{x}(t+h) = \mathbf{x}_0 + hf(\mathbf{x}_0 + \frac{h}{2}f(\mathbf{x}_0))$$

Accuracy of midpoint

Prove that the midpoint method is correct within $O(h^3)$

$$\mathbf{x}(t+h) = \mathbf{x}_0 + hf(\mathbf{x}_0 + \frac{h}{2}f(\mathbf{x}_0))$$

$$\Delta\mathbf{x} = \frac{h}{2}f(\mathbf{x}_0)$$

$$f(\mathbf{x}_0 + \Delta\mathbf{x}) = f(\mathbf{x}_0) + \Delta x\frac{\partial f(\mathbf{x}_0)}{\partial \mathbf{x}} + O(\mathbf{x}^2)$$

$$\mathbf{x}(t+h) = \mathbf{x}_0 + hf(\mathbf{x}_0) + \frac{h^2}{2}f(\mathbf{x}_0)\frac{\partial f(\mathbf{x}_0)}{\partial \mathbf{x}} + hO(x^2)$$

$$\mathbf{x}(t+h) = \mathbf{x}_0 + h\dot{\mathbf{x}}_0 + \underset{RK2}{\frac{h^2}{2}\ddot{\mathbf{x}}_0} + O(h^3)$$

$O(h^5)$ RK4

Stability region

$$\mathbf{x}_{n+1} = \mathbf{x}_n + h\lambda\mathbf{x}_{n+\frac{1}{2}} = \mathbf{x}_n + h\lambda(\mathbf{x}_n + \frac{1}{2}h\lambda\mathbf{x}_n)$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n(1 + h\lambda + \frac{1}{2}(h\lambda)^2)$$

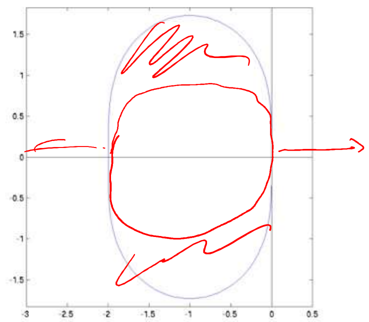
$$h\lambda = x + iy$$

$$\left\| \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} x \\ y \end{bmatrix} + \frac{1}{2}\begin{bmatrix} x^2 - y^2 \\ 2xy \end{bmatrix} \right\| \leq 1$$

$$\left\| \begin{bmatrix} 1 + x + \frac{x^2 - y^2}{2} \\ y + xy \end{bmatrix} \right\| \leq 1$$

Stability of midpoint

- Midpoint method has larger stability region, but still unstable on the imaginary axis



Runge-Kutta method

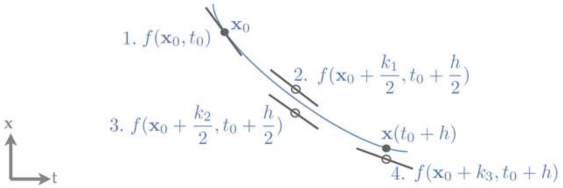
- Runge-Kutta is a numeric method of integrating ODEs by evaluating the derivatives at a few locations to cancel out lower-order error terms
- Also an explicit method: $\mathbf{x}_{n+1}$ is an explicit function of $\mathbf{x}_n$

Runge-Kutta method

- q-stage p-order Runge-Kutta evaluates the derivative function q times in each iteration and its approximation of the next state is correct within $O(h^{p+1})$
- What order of Runge-Kutta does midpoint method correspond to?

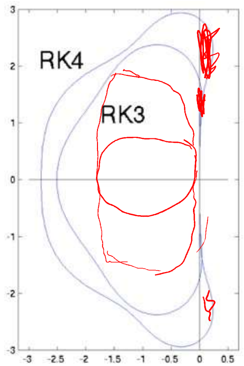
4-stage 4th order Runge-Kutta

$$
\begin{aligned}
k_1 &= hf(\mathbf{x}_0, t_0)\\
k_2 &= hf(\mathbf{x}_0 + \tfrac{k_1}{2}, t_0 + \tfrac{h}{2})\\
k_3 &= hf(\mathbf{x}_0 + \tfrac{k_2}{2}, t_0 + \tfrac{h}{2})\\
k_4 &= hf(\mathbf{x}_0 + k_3, t_0 + h)\\
\mathbf{x}(t_0 + h) &= \mathbf{x}_0 + \tfrac{1}{6}k_1 + \tfrac{1}{3}k_2 + \tfrac{1}{3}k_3 + \tfrac{1}{6}k_4
\end{aligned}
$$



High order Runge-Kutta

- RK3 and up are include part of the imaginary axis



Stage vs. order

p	1	2	3	4	5	6	7	8	9	10
$q_{min}(p)$	1	2	3	4	6	7	9	11	12-17	13-17

The minimum number of stages necessary for an explicit method to attain order p is still an open problem

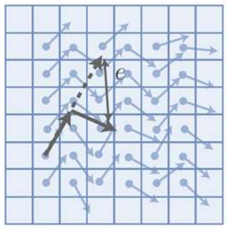
Why is fourth order the most popular Runge Kutta method?

RK4

Adaptive step size

- Ideally, we want to choose h as large as possible, but not so large as to give us big error or instability
- We can vary h as we march forward in time
  - Step doubling
  - Embedding estimate
  - Variable step, variable order

Step doubling



Estimate $\mathbf{x}_a$ by taking a full Euler step

$$\mathbf{x}_a = \mathbf{x}_0 + hf(\mathbf{x}_0, t_0)$$

Estimate $\mathbf{x}_b$ by taking two half Euler steps

$$\mathbf{x}_{temp} = \mathbf{x}_0 + \frac{h}{2}f(\mathbf{x}_0, t_0)$$

$$\mathbf{x}_b = \mathbf{x}_{temp} + \frac{h}{2}f(\mathbf{x}_{temp}, t_0 + \frac{h}{2})$$

$e = |\mathbf{x}_a - \mathbf{x}_b|$ is bound by $O(h^2)$

Given error tolerance ϵ, what is the optimal step size? $\left(\frac{\epsilon}{e}\right)^{\frac{1}{2}} h$

Embedding estimate

- Also called Runge-Kutta-Fehlberg
- Compare two estimates of $x(t_0 + h)$
  - Fifth order Runge-Kutta with 6 stages
  - Forth order Runge-Kutta with 6 stages

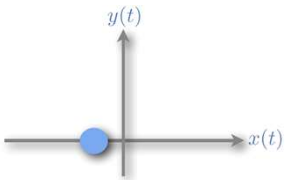
Variable step, variable order

- Change between methods of different order as well as step based on obtained error estimates
- These methods are currently the last work in numerical integration

Problems of explicit methods

- Do not work well with stiff ODEs
  - Simulation blows up if the step size is too big
  - Simulation progresses slowly if the step size is too small

Example: a bead on the wire



$$\mathbf{Y}(t) = (x(t), y(t))$$

$$\dot{\mathbf{Y}} = \frac{d}{dt}\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} -x(t) \\ -ky(t) \end{pmatrix}$$

Explicit Euler's method:

$$\mathbf{Y}_{new} = \mathbf{Y}_0 + h\dot{\mathbf{Y}}(t_0) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} + h\begin{pmatrix} -x(t) \\ -ky(t) \end{pmatrix}$$

$$\mathbf{Y}_{new} = \begin{pmatrix} (1-h)x(t) \\ (1-kh)y(t) \end{pmatrix} \qquad h \leq \frac{2}{|\lambda|}$$

Stiff equations

- Stiffness constant: k
- Step size is limited by the largest k
- Systems that has some big k's mixed in are called "stiff system"

- Overview of differential equation
- Initial value problem
- Explicit numeric methods
- **Implicit numeric methods**
- Modular implementation

Implicit methods

Explicit Euler: $Y_{new} = Y_0 + hf(Y_0)$

Implicit Euler: $Y_{new} = Y_0 + hf(Y_{new})$

Solving for Y_{new} such that f, at time $t_0 + h$, points directly back at Y_0

Implicit methods

Our goal is to solve for Y_{new} such that

$$Y_{new} = Y_0 + hf(Y_{new})$$

Approximating $f(Y_{new})$ by linearizing $f(Y)$

$$f(Y_{new}) = f(Y_0) + \Delta Y f'(Y_0), \text{ where } \Delta Y = Y_{new} - Y_0$$

$$Y_{new} = Y_0 + hf(Y_0) + h\Delta Y f'(Y_0)$$

$$\Delta Y = \left(\frac{1}{h}I - f'(Y_0)\right)^{-1} f(Y_0)$$

$$f(Y,t) = \dot{Y}(t)$$

$$f'(Y,t) = \frac{\partial f}{\partial Y}$$

Example: A bead on the wire

Apply the implicit Euler method to the bead-on-wire example

$$\Delta Y = \left(\frac{1}{h}I - f'(Y_0)\right)^{-1} f(Y_0)$$

$$f(Y(t)) = \begin{pmatrix} -x(t) \\ -ky(t) \end{pmatrix}$$

$$f'(Y(t)) = \frac{\partial f(Y(t))}{\partial Y} = \begin{pmatrix} -1 & 0 \\ 0 & -k \end{pmatrix}$$

$$\Delta Y = \begin{pmatrix} \frac{1+h}{h} & 0 \\ 0 & \frac{1+kh}{h} \end{pmatrix}^{-1} \begin{pmatrix} -x_0 \\ -ky_0 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{h}{h+1} & 0 \\ 0 & \frac{h}{1+kh} \end{pmatrix} \begin{pmatrix} -x_0 \\ -ky_0 \end{pmatrix}$$

$$= -\begin{pmatrix} \frac{h}{h+1}x_0 \\ \frac{h}{1+kh}ky_0 \end{pmatrix}$$

Example: A bead on the wire

What is the largest step size the implicit Euler method can take?

$$\lim_{h\to\infty} \Delta Y = \lim_{h\to\infty} -\begin{pmatrix} \frac{h}{h+1}x_0 \\ \frac{h}{1+kh}ky_0 \end{pmatrix}$$

$$= -\begin{pmatrix} x_0 \\ \frac{1}{k}ky_0 \end{pmatrix} = -\begin{pmatrix} x_0 \\ y_0 \end{pmatrix}$$

$$Y_{new} = Y_0 + (-Y_0) = 0$$

Stability of implicit Euler

- Test equation shows stable when

$$|1 - h\lambda| \geq 1$$

- How does the stability region look like?

Problems of implicit Euler

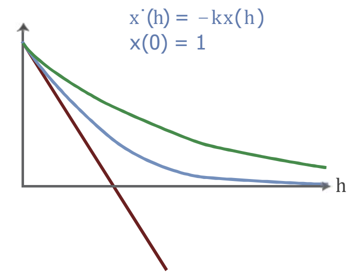
- Implicit Euler could be stable even when physics is not!
- Implicit Euler damps out motion unrealistically

Implicit vs. explicit

correct solution: $x(h) = e^{-hk}$

explicit Euler: $x(h) = 1 - hk$

implicit Euler: $x(h) = \frac{1}{1 + hk}$



Trapezoidal rule

- Take a half step of explicit Euler and a half step of implicit Euler

$$x_{n+1} = x_n + h(\frac{1}{2}f(x_n) + \frac{1}{2}f(x_{n+1}))$$

- Explicit Euler is under-stable, implicit Euler is over-stable, the combination is just right

Stability of Trapezoidal

- What is the test equation for Trapezoidal?

$$h\lambda \leq 0$$

- Where is the stability region?
  - negative half-plane
- Stability region is consistent with physics
- Good for pure rotation

Terminology

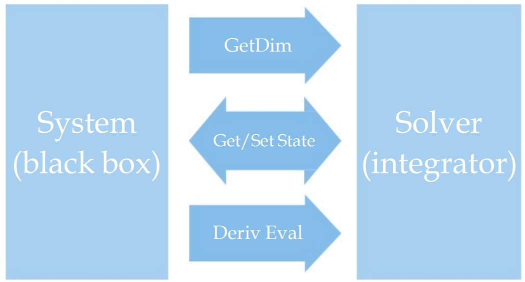
- Explicit Euler is also called forward Euler
- Implicit Euler is also called backward Euler

- Overview of differential equation
- Initial value problem
- Explicit numeric methods
- Implicit numeric methods
- Modular implementation

Modular implementation

- Write integrator in terms of
  - Reusable code
  - Simple system implementation
- Generic operations:
  - Get dim(x)
  - Get/Set x and t
  - Derivative evaluation at current (x, t)

Solver interface



Summary

- Explicit Euler is simple, but might not be stable; modified Euler may be a cheap alternative
- RK4 allows for larger time step, but requires much more computation
- Use implicit Euler for better stability, but beware of over-damp