Outline

Differential Equations

- Differential equations involve derivatives of unknown solution function
- *Ordinary differential equation* (ODE): all derivatives are with respect to single independent variable, often representing time
- Solution of differential equation is *function* in infinite-dimensional space of functions
- Numerical solution of differential equations is based on finite-dimensional approximation
- Differential equation is replaced by algebraic equation whose solution approximates that of given differential equation

Single ODE (IVP) Examples:

- First-order derivative in time - *initial value problem*.
- $y' \;=\; \frac{1}{2}y, \quad y(0) = 1: \qquad y(t) \;=\; e^{\frac{1}{2}t}.$
- $y' \;=\; -2 \;-\; y + y^2 \;\; + \;\; \text{I.C.s}$ (Ricatti Equation example)
- $y' \;=\; \sin(t) \;\; + \;\; \text{I.C.s}$
- $y' \;=\; \lambda\, y \; + \; \cos(t) \;\; + \;\; \text{I.C.s}$
- $y' \;=\; e^{-y} \;\; + \;\; \text{I.C.s}$
- etc.

System of ODEs

$$\begin{bmatrix} \frac{dy_1}{dt} \\ \frac{dy_2}{dt} \end{bmatrix} = \begin{bmatrix} f_1(t, y_1, y_2) \\ f_2(t, y_1, y_2) \end{bmatrix} = \mathbf{f}(t, \mathbf{y})$$

$$\mathbf{y}' := \frac{d\mathbf{y}}{dt} = \mathbf{f}(t, \mathbf{y})$$

$$\begin{bmatrix} \frac{dy_1}{dt} \\ \frac{dy_2}{dt} \end{bmatrix}_{t_k} = \begin{bmatrix} f_1(t, y_1, y_2) \\ f_2(t, y_1, y_2) \end{bmatrix}_{t_k} = \mathbf{f}(t_k, \mathbf{y}(t_k))$$

System of ODEs: Solved Numerically

Given data at t_k, find solution at t_{k+1}.

One example,

$$\left.\frac{d\mathbf{y}}{dt}\right|_{t_k} \approx \frac{\mathbf{y}_{k+1} - \mathbf{y}_k}{h_{(k)}} \approx \mathbf{f}(t_k, \mathbf{y}_k)$$

Yields Euler's method (a.k.a. Euler forward, "EF"):

$$\begin{aligned} \mathbf{y}_{k+1} &= \mathbf{y}_k + h_{(k)}\mathbf{f}_k \\ &= \mathbf{y}_k + h\mathbf{f}_k \qquad \text{(constant step-size case)} \end{aligned}$$

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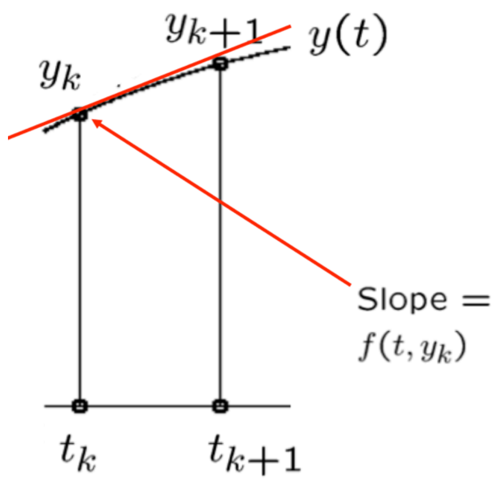

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Matlab Example: orbit.m, orbit1.m

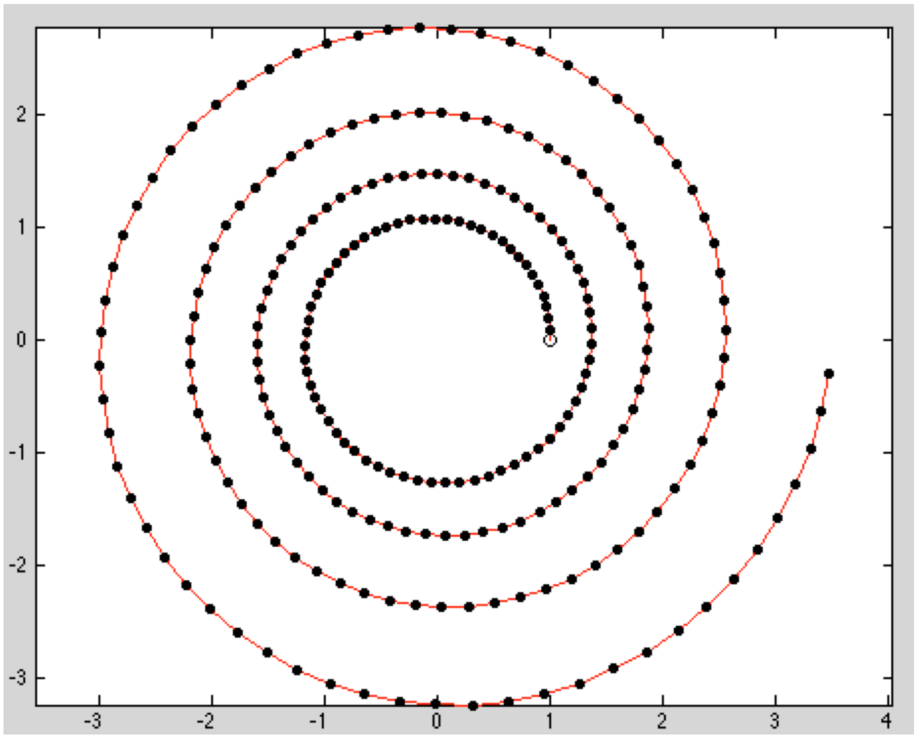
```
T = 2*pi; dt = T/n;  % Tfinal and dt

A = [ 0 -1 ; 1 0 ]; I=eye(2);

y0 = [ 1 ; 0 ]; % INITIAL CONDITION

y=y0;

io=floor(1+n/100);
for k=1:n;
   y=y + dt*(A*y);
   plot(y(1),y(2),'r.'); axis equal;hold on
end;
plot(y(1),y(2),'kx'); axis equal; hold on
```



Order of ODE

- *Order* of ODE is determined by highest-order derivative of solution function appearing in ODE
- ODE with higher-order derivatives can be transformed into equivalent first-order system *(For Initial Value Problems…)*
- We will discuss numerical solution methods only for first-order ODEs
- Most ODE software is designed to solve only first-order equations

Higher-Order ODEs, continued

- For k-th order ODE

$$y^{(k)}(t) = f(t, y, y', \dots, y^{(k-1)})$$

define k new unknown functions

$$u_1(t) = y(t),\ u_2(t) = y'(t),\ \dots,\ u_k(t) = y^{(k-1)}(t)$$

- Then original ODE is equivalent to first-order system

$$\begin{bmatrix} u_1'(t) \\ u_2'(t) \\ \vdots \\ u_{k-1}'(t) \\ u_k'(t) \end{bmatrix} = \begin{bmatrix} u_2(t) \\ u_3(t) \\ \vdots \\ u_k(t) \\ f(t, u_1, u_2, \dots, u_k) \end{bmatrix}$$

Converting Higher Order ODEs to First Order

Consider example:

$$y^{iv} = f(t, y, y', y'', y''')$$

Let $y_1 = y$, $y_2 = y'$, $y_3 = y''$, and $y_4 = y'''$.

$$\frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 0 & 1 & & \\ & 0 & 1 & \\ & & 0 & 1 \\ & & & 0 \end{bmatrix}\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ f \end{bmatrix}$$

$$\frac{d\mathbf{y}}{dt} = A\mathbf{y} + \mathbf{f}$$

Example: Newton's Second Law

- Newton's Second Law of Motion, $F = ma$, is second-order ODE, since acceleration a is second derivative of position coordinate, which we denote by y

- Thus, ODE has form

$$y'' = F/m$$

  where F and m are force and mass, respectively

- Defining $u_1 = y$ and $u_2 = y'$ yields equivalent system of two first-order ODEs

$$\begin{bmatrix} u_1' \\ u_2' \end{bmatrix} = \begin{bmatrix} u_2 \\ F/m \end{bmatrix}$$

Example, continued

- We can now use methods for first-order equations to solve this system
- First component of solution u_1 is solution y of original second-order equation
- Second component of solution u_2 is velocity y'

Ordinary Differential Equations

- General first-order system of ODEs has form

  $$\boldsymbol{y}'(t) = \boldsymbol{f}(t, \boldsymbol{y})$$

  where $\boldsymbol{y}\colon \mathbb{R} \to \mathbb{R}^n$, $\boldsymbol{f}\colon \mathbb{R}^{n+1} \to \mathbb{R}^n$, and $\boldsymbol{y}' = d\boldsymbol{y}/dt$ denotes derivative with respect to t,

  $$\begin{bmatrix} y_1'(t) \\ y_2'(t) \\ \vdots \\ y_n'(t) \end{bmatrix} = \begin{bmatrix} dy_1(t)/dt \\ dy_2(t)/dt \\ \vdots \\ dy_n(t)/dt \end{bmatrix}$$

- Function $\boldsymbol{f}$ is given and we wish to determine unknown function $\boldsymbol{y}$ satisfying ODE

- For simplicity, we will often consider special case of single scalar ODE, $n = 1$

Initial Value Problems

- By itself, ODE $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ does not determine unique solution function
- This is because ODE merely specifies *slope* $\boldsymbol{y}'(t)$ of solution function at each point, but not actual value $\boldsymbol{y}(t)$ at any point
- Infinite family of functions satisfies ODE, in general, provided $\boldsymbol{f}$ is sufficiently smooth
- To single out particular solution, value $\boldsymbol{y}_0$ of solution function must be specified at some point t_0

***y**$_0$ is the **initial condition**.*

Initial Value Problems, continued

- Thus, part of given problem data is requirement that $\boldsymbol{y}(t_0) = \boldsymbol{y}_0$, which determines unique solution to ODE
- Because of interpretation of independent variable t as time, think of t_0 as initial time and $\boldsymbol{y}_0$ as initial value
- Hence, this is termed *initial value problem*, or *IVP*
- ODE governs evolution of system in time from its initial state $\boldsymbol{y}_0$ at time t_0 onward, and we seek function $\boldsymbol{y}(t)$ that describes state of system as function of time

Example: Initial Value Problem

- Consider scalar ODE

$$y' = y$$

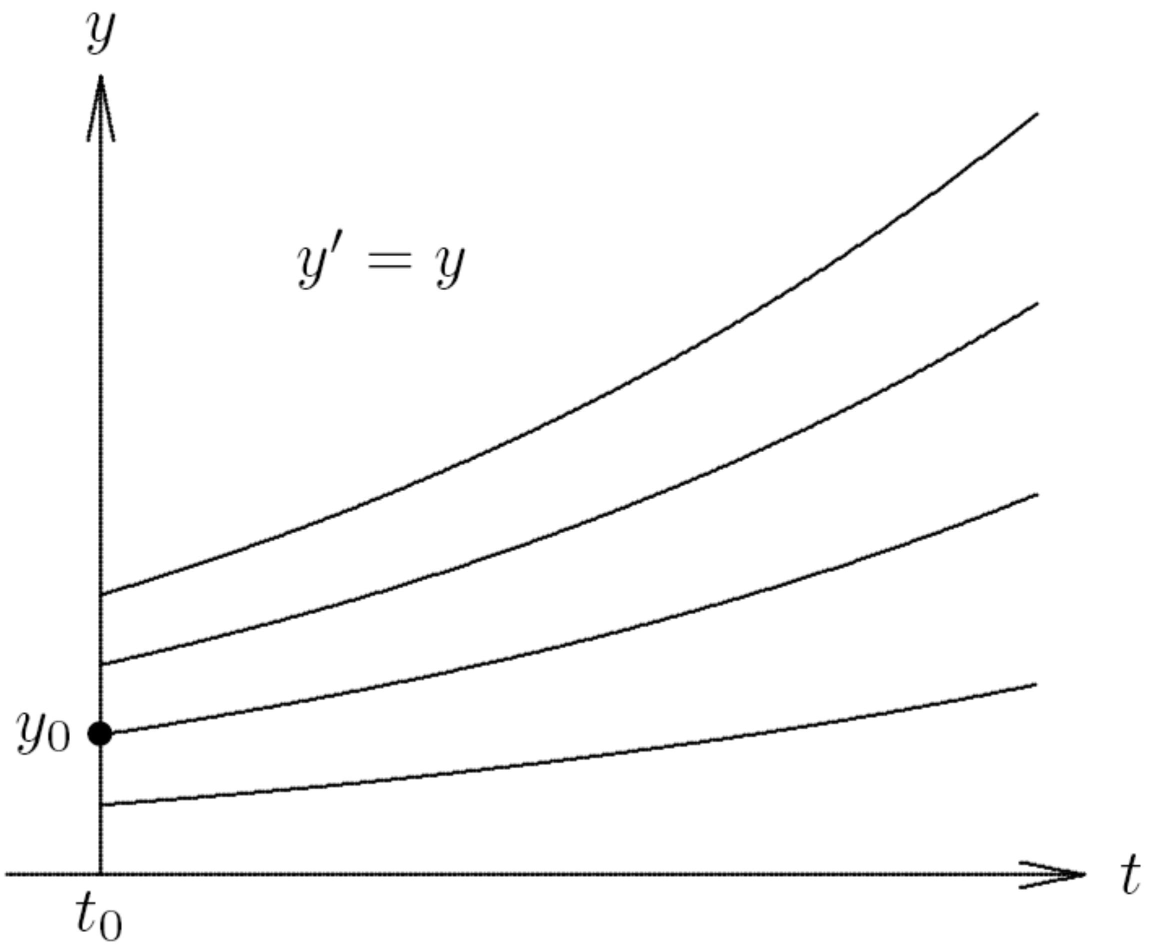
- Family of solutions is given by $y(t) = c\,e^t$, where c is any real constant

- Imposing initial condition $y(t_0) = y_0$ singles out unique particular solution

- For this example, if $t_0 = 0$, then $c = y_0$, which means that solution is $y(t) = y_0 e^t$

Example: Initial Value Problem

Family of solutions for ODE $y' = y$



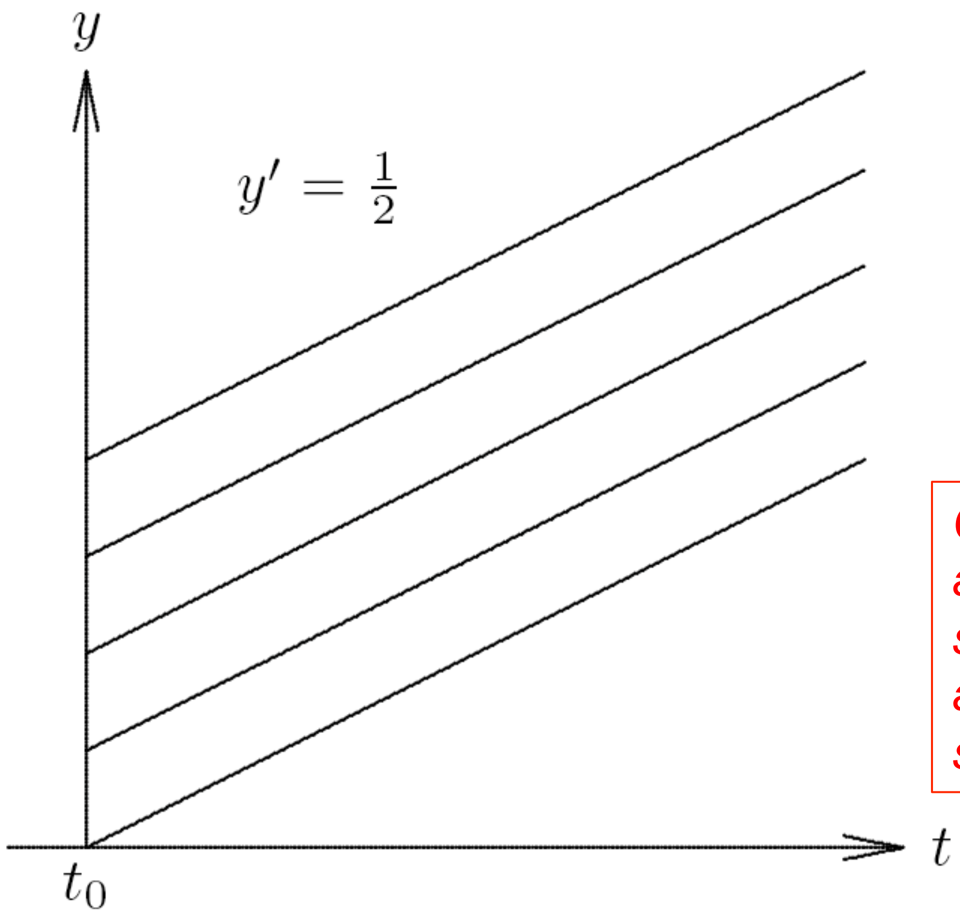
Stability of Solutions

Solution of ODE is

- *Stable* if solutions resulting from perturbations of initial value remain close to original solution
- *Asymptotically stable* if solutions resulting from perturbations converge back to original solution
- *Unstable* if solutions resulting from perturbations diverge away from original solution without bound

Example: Stable Solutions

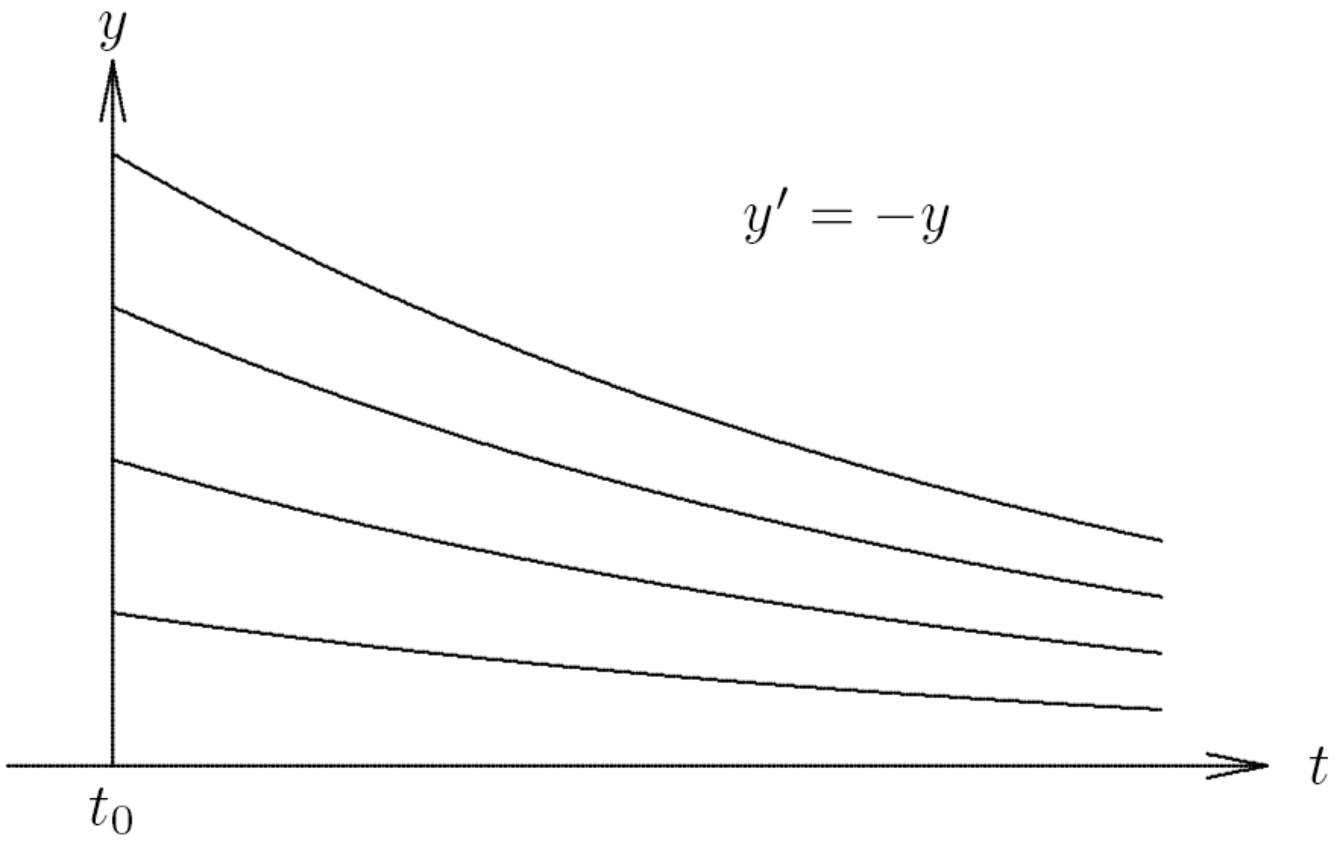
Family of solutions for ODE $y' = \frac{1}{2}$



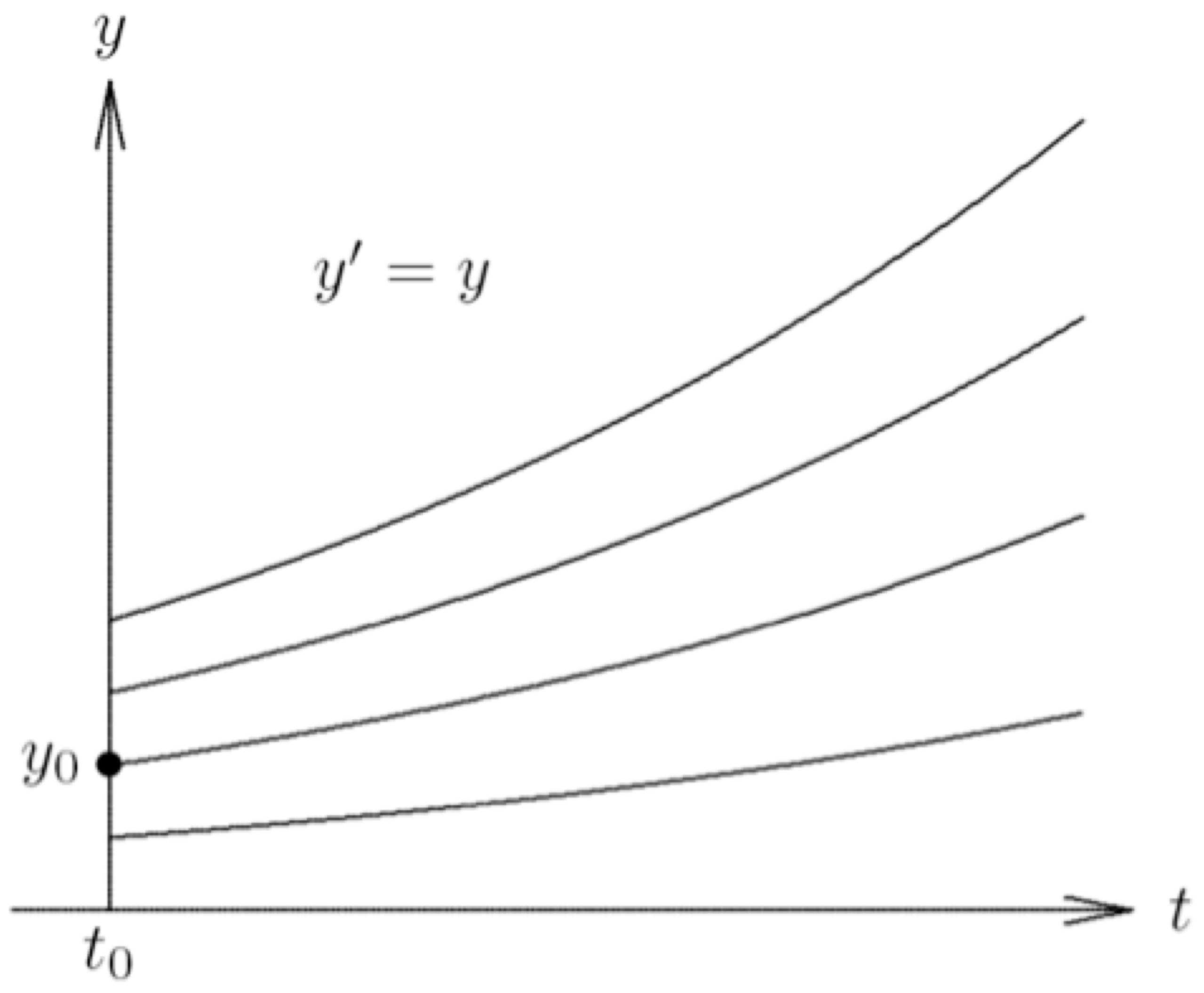
***Closed Orbits** are another example of stable, but not asymptotically stable ODEs.*

Example: Asymptotically Stable Solutions

Family of solutions for ODE $y' = -y$



Unstable ODE Example



Example: Stability of Solutions

- Consider scalar ODE $y' = \lambda y$, where λ is constant.
- Solution is given by $y(t) = y_0 \, e^{\lambda t}$, where $t_0 = 0$ is initial time and $y(0) = y_0$ is initial value
- For real λ
  - $\lambda > 0$: all nonzero solutions grow exponentially, so every solution is unstable
  - $\lambda < 0$: all nonzero solutions decay exponentially, so every solution is not only stable, but asymptotically stable
- For complex λ
  - $\mathrm{Re}(\lambda) > 0$: unstable
  - $\mathrm{Re}(\lambda) < 0$: asymptotically stable
  - $\mathrm{Re}(\lambda) = 0$: stable but not asymptotically stable

Most Important Model Problem

- $\dfrac{dy}{dt} = \lambda y, \qquad y(t=0) = y_0.$

- Exact solution: $y(t) = y_0 e^{\lambda t}$.

- Note that, $y_n = y_0 e^{\lambda n \Delta t}$, so

$$\begin{aligned} y_n &= y_0 e^{\lambda(t_{n-1}+\Delta t)} = y_0 e^{\lambda t_{n-1}}\, e^{\lambda \Delta t} \\ &= e^{\lambda \Delta t}\, y_{n-1}. \\ &= \tilde{G}\, y_{n-1}, \end{aligned}$$

where $\tilde{G}$ is a constant, referred to as the (analytical) *growth factor*.

Example: Linear System of ODEs

- Linear, homogeneous system of ODEs with constant coefficients has form
$$\boldsymbol{y}' = \boldsymbol{A}\boldsymbol{y}$$
where $\boldsymbol{A}$ is $n \times n$ matrix, and initial condition is $\boldsymbol{y}(0) = \boldsymbol{y}_0$

- Suppose $\boldsymbol{A}$ is diagonalizable, with eigenvalues λ_i and corresponding eigenvectors $\boldsymbol{v}_i$, $i = 1, \ldots, n$

- Express $\boldsymbol{y}_0$ as linear combination $\boldsymbol{y}_0 = \sum_{i=1}^{n} \alpha_i \boldsymbol{v}_i$
- Then
$$\boldsymbol{y}(t) = \sum_{i=1}^{n} \alpha_i \boldsymbol{v}_i e^{\lambda_i t}$$
is solution to ODE satisfying initial condition $\boldsymbol{y}(0) = \boldsymbol{y}_0$

Here, linearity implies A is a constant matrix A ≠ A(y). (Actually, that is also implied by the "constant coefficients" qualifier.)

Eigenvalues and ODEs

$$\frac{d\mathbf{y}}{dt} = J\mathbf{y} + \mathbf{f}(t)$$

Assume $J = \textit{constant}$ and there exist n eigenvectors $\mathbf{v}_j$ such that

$$J\mathbf{v}_j = \lambda_j \mathbf{v}_j$$

$$JV = V\Lambda = (\mathbf{v}_1\,\mathbf{v}_2 \ldots \mathbf{v}_n) \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Then, there exists a set of coefficients $\hat{y}_j(t)$ such that

$$\mathbf{y} = \sum_{j=1}^{n} \mathbf{v}_j \hat{y}_j \iff \mathbf{y} = V\hat{\mathbf{y}} \iff \hat{\mathbf{y}} = V^{-1}\mathbf{y}$$

$$J\mathbf{y} = \sum_{j=1}^{n} J\mathbf{v}_j \hat{y}_j = \sum_{j=1}^{n} \lambda_j \mathbf{v}_j \hat{y}_j = \sum_{j=1}^{n} \mathbf{v}_j \lambda_j \hat{y}_j = V\Lambda\hat{\mathbf{y}}.$$

Eigenvalues and ODEs

Inserting the expansion $\mathbf{y} = V\hat{\mathbf{y}}$ into our ODE...

$$\begin{aligned} \frac{d\mathbf{y}}{dt} &= J\mathbf{y} + \mathbf{f} \\ \frac{d}{dt}V\hat{\mathbf{y}} &= JV\hat{\mathbf{y}} + V\hat{\mathbf{f}} \\ &= V\Lambda\hat{\mathbf{y}} + V\hat{\mathbf{f}} \end{aligned}$$

Multiply through by V^{-1}:

$$\frac{d\hat{\mathbf{y}}}{dt} = \Lambda\hat{\mathbf{y}} + \hat{\mathbf{f}}$$

Eigenvalues and ODEs

$$\frac{d}{dt}\begin{pmatrix}\hat{y}_1\\ \vdots \\ \hat{y}_n\end{pmatrix} = \begin{bmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{bmatrix}\begin{pmatrix}\hat{y}_1\\ \vdots \\ \hat{y}_n\end{pmatrix} + \begin{pmatrix}\hat{f}_1\\ \vdots \\ \hat{f}_n\end{pmatrix}$$

$$= \begin{pmatrix}\lambda_1\hat{y}_1\\ \vdots \\ \lambda_n\hat{y}_n\end{pmatrix} + \begin{pmatrix}\hat{f}_1\\ \vdots \\ \hat{f}_n\end{pmatrix}$$

$$\frac{d\hat{y}_i}{dt} = \lambda_i\hat{y}_i + \hat{f}_i, \;\; i = 1, \ldots, n$$

- We now have n *decoupled* systems.
- Numerically, we solve these as the coupled system $\mathbf{y} = J\mathbf{y} + \mathbf{f}$.
- The behavior, however, is the same as this decoupled system, which is easier to understand.
- In particular, stability is governed by the maximum real part of the λ_is.

Example, continued

- Eigenvalues of $\boldsymbol{A}$ with positive real parts yield exponentially growing solution components
- Eigenvalues with negative real parts yield exponentially decaying solution components
- Eigenvalues with zero real parts (i.e., pure imaginary) yield oscillatory solution components
- Solutions stable if $\mathrm{Re}(\lambda_i) \le 0$ for every eigenvalue, and asymptotically stable if $\mathrm{Re}(\lambda_i) < 0$ for every eigenvalue, but unstable if $\mathrm{Re}(\lambda_i) > 0$ for any eigenvalue

Stability of Solutions, continued

- For general nonlinear system of ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$, determining stability of solutions is more complicated

- ODE can be linearized locally about solution $\boldsymbol{y}(t)$ by truncated Taylor series, yielding linear ODE

$$\boldsymbol{z}' = \boldsymbol{J}_f(t, \boldsymbol{y}(t))\, \boldsymbol{z}$$

  where $\boldsymbol{J}_f$ is Jacobian matrix of $\boldsymbol{f}$ with respect to $\boldsymbol{y}$

- Eigenvalues of $\boldsymbol{J}_f$ determine stability locally, but conclusions drawn may not be valid globally

Numerical Solution of ODEs

- Analytical solution of ODE is closed-form formula that can be evaluated at any point t
- Numerical solution of ODE is table of approximate values of solution function at discrete set of points
- Numerical solution is generated by simulating behavior of system governed by ODE
- Starting at t_0 with given initial value $\boldsymbol{y}_0$, we track trajectory dictated by ODE
- Evaluating $\boldsymbol{f}(t_0, \boldsymbol{y}_0)$ tells us slope of trajectory at that point
- We use this information to predict value $\boldsymbol{y}_1$ of solution at future time $t_1 = t_0 + h$ for some suitably chosen time increment h

Numerical Solution of ODEs, continued

- Approximate solution values are generated step by step in increments moving across interval in which solution is sought
- In stepping from one discrete point to next, we incur some error, which means that next approximate solution value lies on *different* solution from one we started on
- Stability or instability of solutions determines, in part, whether such errors are magnified or diminished with time

- Two types of stability to consider:
    - Stability of ODE
    - Stability of numerical method

Developing Numerical Solution Approaches for ODEs (IVPs)

- Principal considerations:
  - Deriving a **computable formula** for $\boldsymbol{y}_{k+1}$, given $\boldsymbol{y}_k$, $\boldsymbol{f}(\boldsymbol{y}_k,t_k)$ (and perhaps, $\boldsymbol{f}(\boldsymbol{y}_{k-1},t_{k-1})$, …).
  - Understanding **accuracy** as a function of stepsize, *h*, and function f.
  - Understanding **stability** as a function of stepsize, *h*, and function f.

Developing Numerical Solution Approaches for ODEs (IVPs)

- Some methods we'll encounter:
  - Euler's method (aka Forward Euler)
  - Backward Euler
  - Trapezoid Method
  - Backward difference formulae of order k (BDFk)
  - kth-order Runge-Kutta methods
  - …
- These methods are characterized by
  - Implicit, explicit, semi-implicit
  - Stability properties
  - Accuracy
  - ***Cost***

Developing Numerical Solution Approaches for ODEs (IVPs)

- Some methods we'll encounter:

Euler's method (aka Forward Euler)	*$O(h)$*
Backward Euler	*$O(h)$*
Trapezoid Method	*$O(h^2)$ – **not L-stable**☹*
Backward difference formulae of order k (BDFk)	*$O(h^k)$*
kth-order Runge-Kutta methods	*$O(h^k)$*
…	

- These methods are characterized by
  - Implicit, explicit, semi-implicit
  - Stability properties
  - Accuracy
  - ***Cost***

Euler's Method

- For general system of ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$, consider Taylor series

$$\begin{aligned}\boldsymbol{y}(t+h) &= \boldsymbol{y}(t) + h\boldsymbol{y}'(t) + \frac{h^2}{2}\boldsymbol{y}''(t) + \cdots \\ &= \boldsymbol{y}(t) + h\boldsymbol{f}(t, \boldsymbol{y}(t)) + \frac{h^2}{2}\boldsymbol{y}''(t) + \cdots\end{aligned}$$

- *Euler's method* results from dropping terms of second and higher order to obtain approximate solution value

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + h_k \boldsymbol{f}(t_k, \boldsymbol{y}_k)$$

- Euler's method advances solution by extrapolating along straight line whose slope is given by $\boldsymbol{f}(t_k, \boldsymbol{y}_k)$
- Euler's method is *single-step* method because it depends on information at only one point in time to advance to next point

Example: Euler's Method

- Applying Euler's method to ODE $y' = y$ with step size h, we advance solution from time $t_0 = 0$ to time $t_1 = t_0 + h$

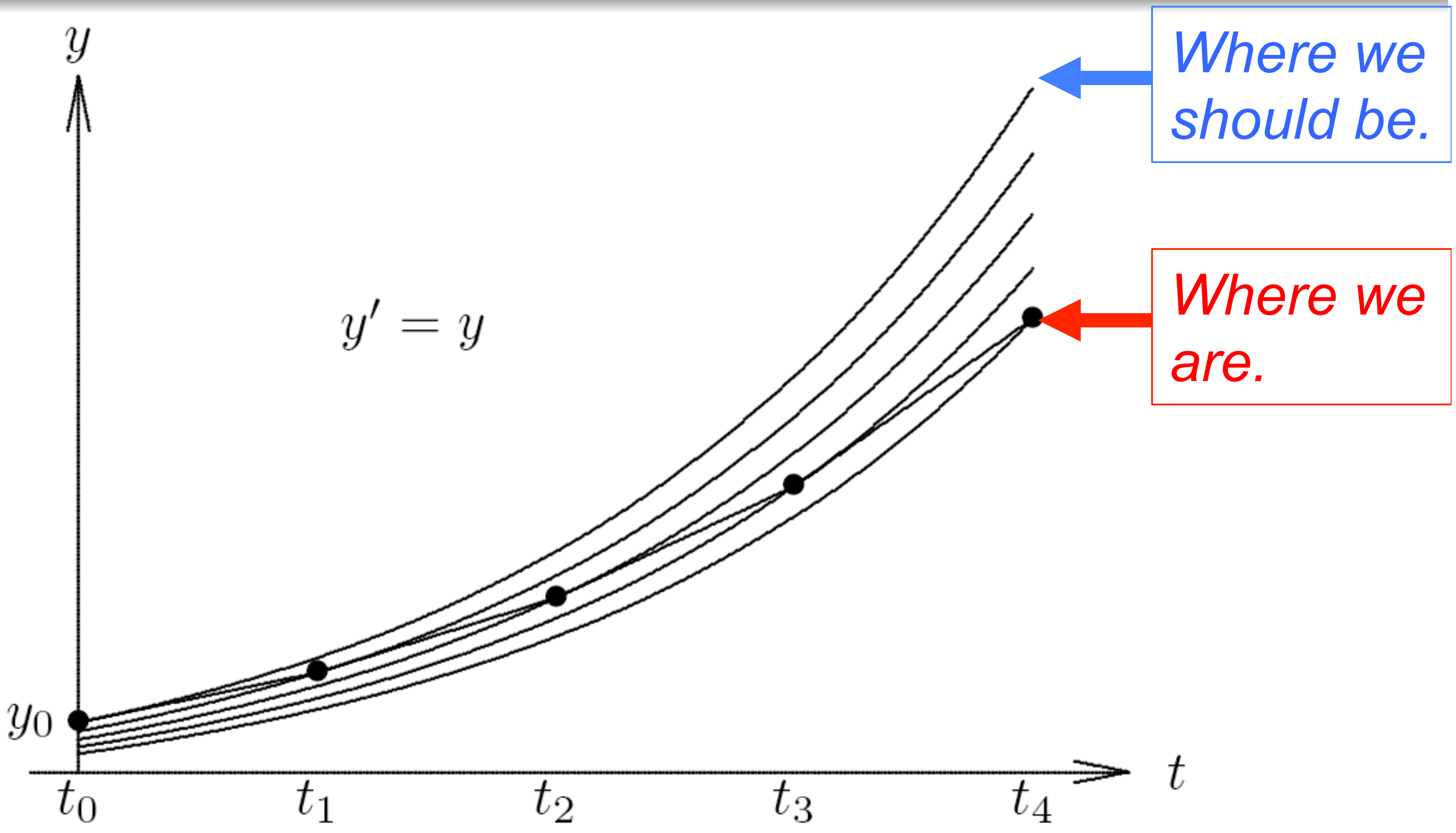
$$y_1 = y_0 + hy_0' = y_0 + hy_0 = (1+h)y_0$$

- Value for solution we obtain at t_1 is not exact, $y_1 \neq y(t_1)$
- For example, if $t_0 = 0$, $y_0 = 1$, and $h = 0.5$, then $y_1 = 1.5$, whereas exact solution for this initial value is $y(0.5) = \exp(0.5) \approx 1.649$
- Thus, y_1 lies on different solution from one we started on

Example, continued

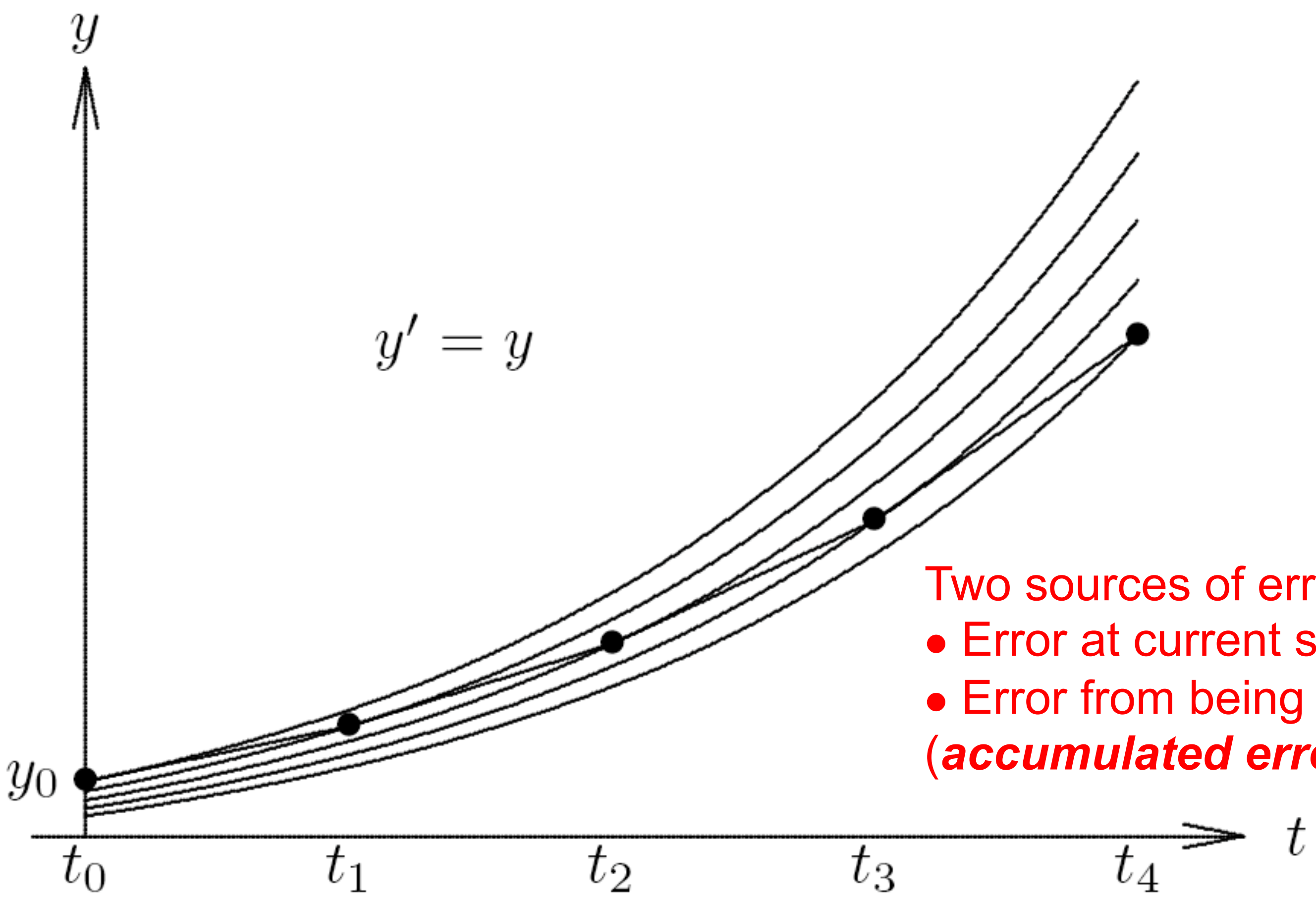
- To continue numerical solution process, we take another step from t_1 to $t_2 = t_1 + h = 1.0$, obtaining $y_2 = y_1 + hy_1 = 1.5 + (0.5)(1.5) = 2.25$
- Now y_2 differs not only from true solution of original problem at $t = 1$, $y(1) = \exp(1) \approx 2.718$, but it also differs from solution through previous point (t_1, y_1), which has approximate value 2.473 at $t = 1$
- Thus, we have moved to still another solution for this ODE

Example, continued



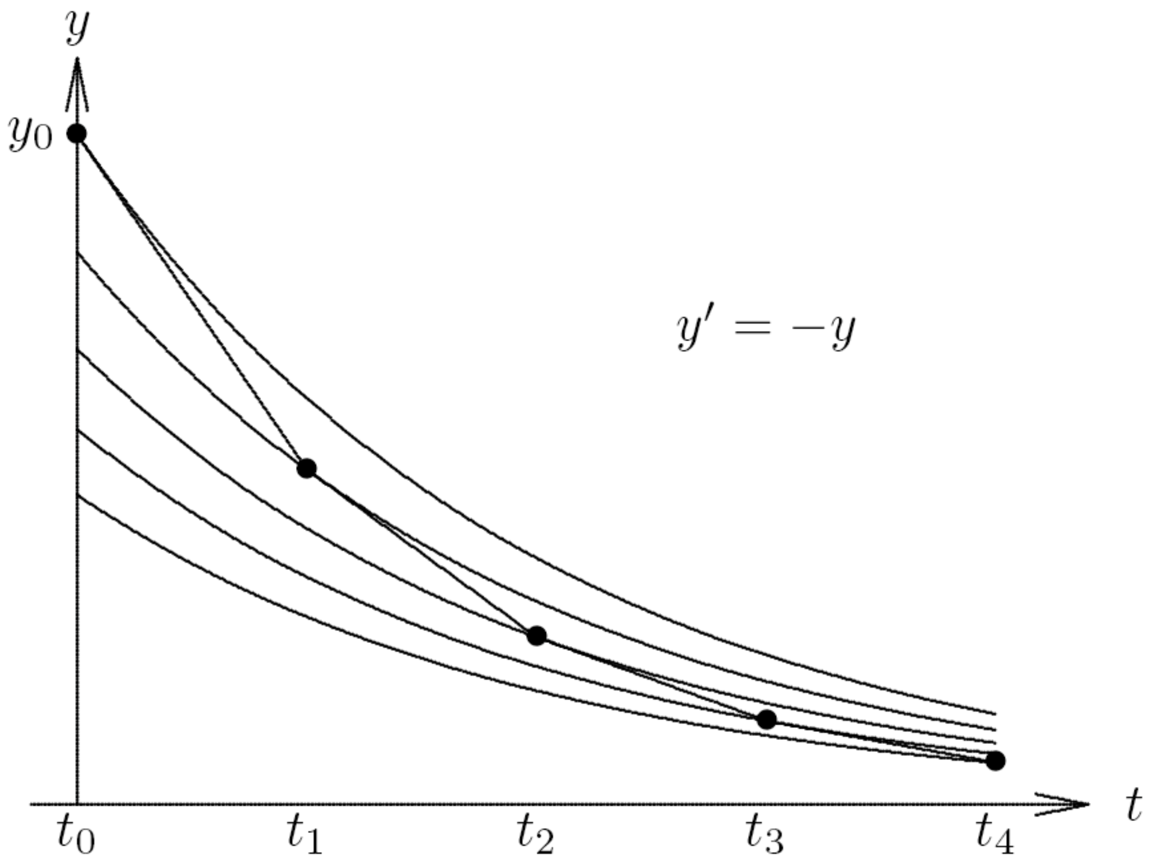
For unstable solutions, errors in numerical solution grow with time

Example, continued



Two sources of error:
- Error at current step (***local error***)
- Error from being on the wrong trajectory (***accumulated error***)

Example, continued



For stable solutions, errors in numerical solution may diminish with time *(Local errors are suppressed.)*

Errors in Numerical Solution of ODEs

- Numerical methods for solving ODEs incur two distinct types of error
  - *Rounding error*, which is due to finite precision of floating-point arithmetic
  - *Truncation error* (*discretization error*), which is due to approximation method used and would remain even if all arithmetic were exact
- In practice, truncation error is dominant factor determining accuracy of numerical solutions of ODEs, so we will henceforth ignore rounding error

(Keep in mind, however, that even with a perfect algorithm, round-off is an ever-present source of noise in the system – e.g., we must assume that all eigenmodes are present, so any unstable mode will grow.)

Global Error and Local Error

Truncation error at any point t_k can be broken down into

- *Global error*: difference between computed solution and true solution $\boldsymbol{y}(t)$ passing through initial point $(t_0, \boldsymbol{y}_0)$

$$\boldsymbol{e}_k = \boldsymbol{y}_k - \boldsymbol{y}(t_k)$$

- *Local error*: error made in one step of numerical method

$$\boldsymbol{\ell}_k = \boldsymbol{y}_k - \boldsymbol{u}_{k-1}(t_k)$$

where $\boldsymbol{u}_{k-1}(t)$ is true solution passing through previous point $(t_{k-1}, \boldsymbol{y}_{k-1})$

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GTE – Global Truncation Error

- *Local error*: error made in one step of numerical method

$$\boldsymbol{\ell}_k = \boldsymbol{y}_k - \boldsymbol{u}_{k-1}(t_k)$$

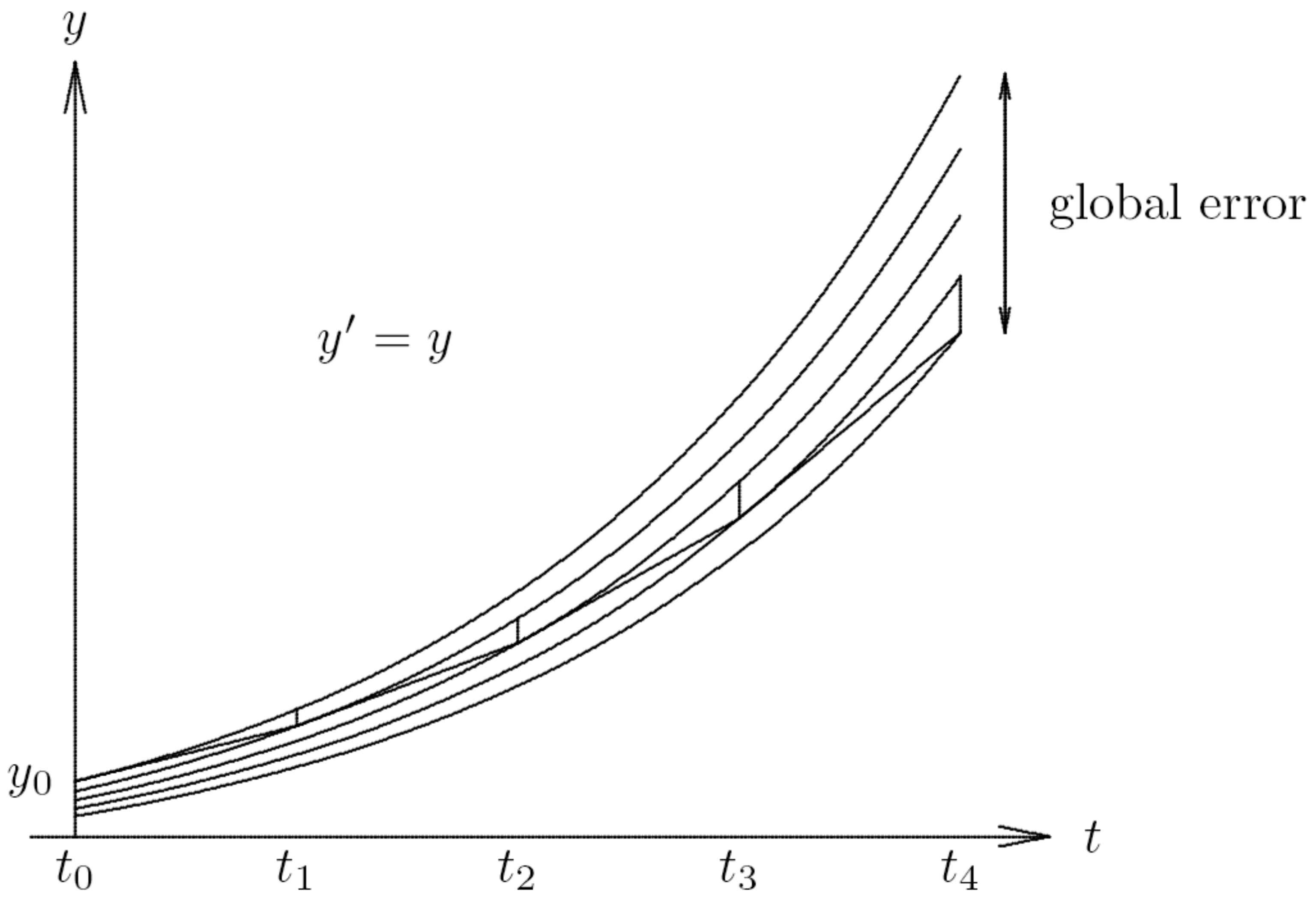
LTE – Local Truncation Error

where $\boldsymbol{u}_{k-1}(t)$ is true solution passing through previous point $(t_{k-1}, \boldsymbol{y}_{k-1})$

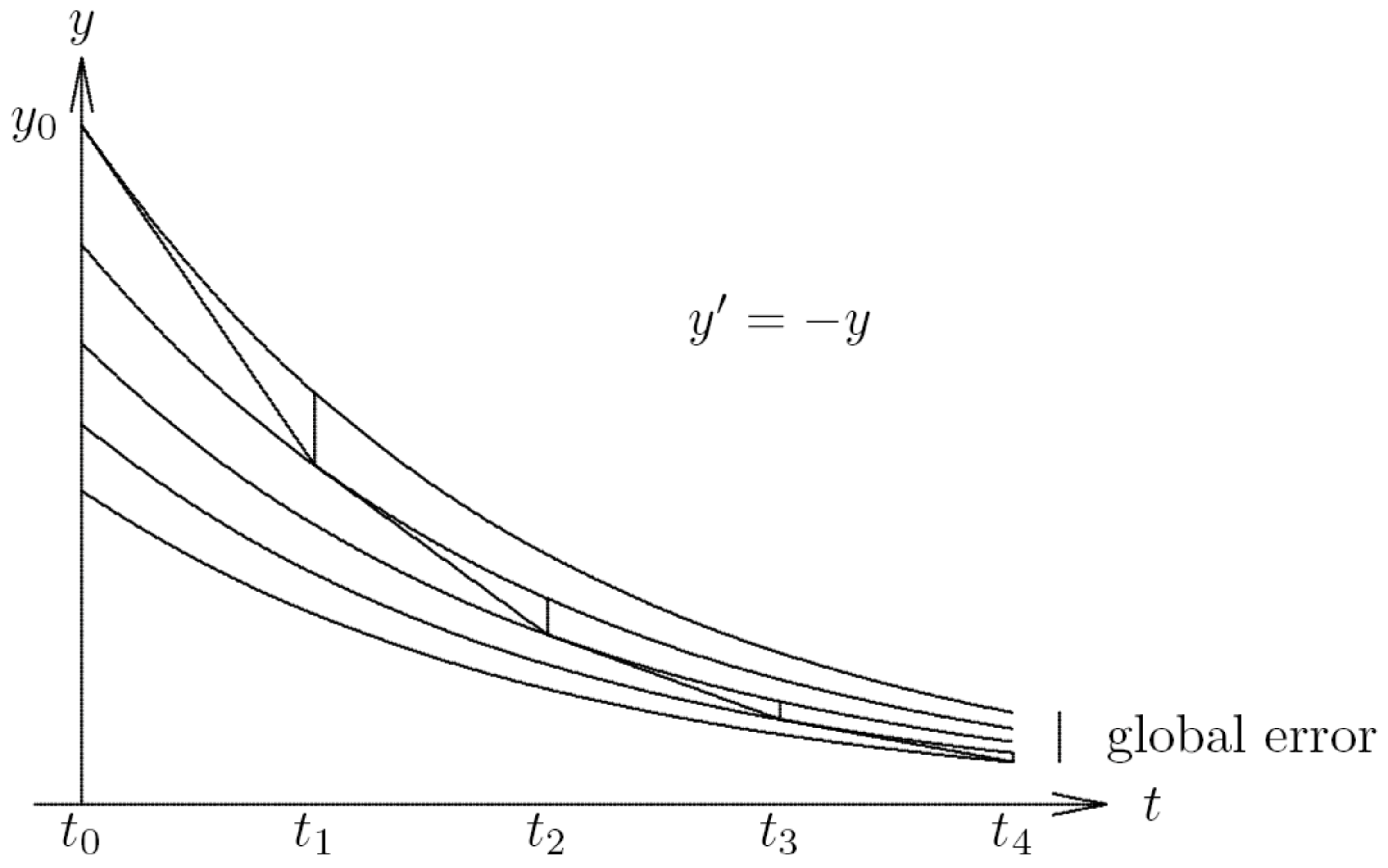
Global Error and Local Error, continued

- Global error is not necessarily sum of local errors
- Global error is generally greater than sum of local errors if solutions are unstable, but may be less than sum if solutions are stable
- Having small global error is what we want, but we can control only local error directly

Global Error and Local Error, continued



Global and Local Error, continued



Order of Accuracy

- *Order of accuracy* of numerical method is p if

$$\boldsymbol{\ell}_k = \mathcal{O}(h_k^{p+1})$$

- Then local error per unit step, $\boldsymbol{\ell}_k / h_k = \mathcal{O}(h_k^p)$
- Under reasonable conditions, $\boldsymbol{e}_k = \mathcal{O}(h^p)$, where h is average step size

GTE – Global Truncation Error ~ $O(h^p)$

LTE – Local Truncation Error ~ $O(h^{p+1})$

Global Truncation Error is what you expect after final time $T = n \cdot h$, where n=number of steps.

Making n local errors of size $O(h^{p+1})$, expect $e(T) = O(nh^{p+1}) = T\,O(h^p)$.

Stability

- Numerical method is *stable* if small perturbations do not cause resulting numerical solutions to diverge from each other without bound
- Such divergence of numerical solutions could be caused by instability of solution to ODE, but can also be due to numerical method itself, even when solutions to ODE are stable

***Stability**, **Accuracy** and **Cost** of the numerical scheme are the primary considerations in the development of ODE solvers.*

Determining Stability and Accuracy

- Simple approach to determining stability and accuracy of numerical method is to apply it to scalar ODE $y' = \lambda y$, where λ is (possibly complex) constant
- Exact solution is given by $y(t) = y_0 e^{\lambda t}$, where $y(0) = y_0$ is initial condition
- Determine stability of numerical method by characterizing growth of numerical solution
- Determine accuracy of numerical method by comparing exact and numerical solutions

Example: Euler's Method

- Applying Euler's method to $y' = \lambda y$ using fixed step size h,

$$y_{k+1} = y_k + h\lambda y_k = (1 + h\lambda) y_k$$

which means that

$$y_k = (1 + h\lambda)^k y_0$$

- If $\mathrm{Re}(\lambda) < 0$, exact solution decays to zero as t increases, as does computed solution if

$$|1 + h\lambda| < 1$$

which holds if $h\lambda$ lies inside circle in complex plane of radius 1 centered at -1

$\boxed{\text{Here, } (1 + \lambda h) \text{ is the } \textit{growth factor.}}$

Recall Eigenvalues and ODEs, Analytical Case

$$\frac{d\mathbf{y}}{dt} = J\mathbf{y} + \mathbf{f}(t)$$

Assume $J = \textit{constant}$ and there exist n eigenvectors $\mathbf{v}_j$ such that

$$J\mathbf{v}_j = \lambda_j \mathbf{v}_j$$

$$JV = V\Lambda = (\mathbf{v}_1\,\mathbf{v}_2 \ldots \mathbf{v}_n)\begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Then, there exists a set of coefficients $\hat{y}_j(t)$ such that

$$\mathbf{y} = \sum_{j=1}^{n} \mathbf{v}_j \hat{y}_j \iff \mathbf{y} = V\hat{\mathbf{y}} \iff \hat{\mathbf{y}} = V^{-1}\mathbf{y}$$

$$J\mathbf{y} = \sum_{j=1}^{n} J\mathbf{v}_j \hat{y}_j = \sum_{j=1}^{n} \lambda_j \mathbf{v}_j \hat{y}_j$$

Recall, Eigenvalues and ODEs, Analytical Case

Inserting this expansion into our ODE...

$$\begin{aligned}
\frac{d\mathbf{y}}{dt} &= J\mathbf{y} + \mathbf{f} \\
\frac{d}{dt}V\hat{\mathbf{y}} &= JV\hat{\mathbf{y}} + V\hat{\mathbf{f}} \\
&= V\Lambda\hat{\mathbf{y}} + V\hat{\mathbf{f}}
\end{aligned}$$

Multiply through by V^{-1}:

$$\frac{d\hat{\mathbf{y}}}{dt} = \Lambda\hat{\mathbf{y}} + \hat{\mathbf{f}}$$

Eigenvalues and ODEs, Analytical Case

$$\frac{d}{dt}\begin{pmatrix}\hat{y}_1\\ \vdots\\ \hat{y}_n\end{pmatrix} = \begin{bmatrix}\lambda_1 & & \\ & \ddots & \\ & & \lambda_n\end{bmatrix}\begin{pmatrix}\hat{y}_1\\ \vdots\\ \hat{y}_n\end{pmatrix} + \begin{pmatrix}\hat{f}_1\\ \vdots\\ \hat{f}_n\end{pmatrix}$$

$$= \begin{pmatrix}\lambda_1\hat{y}_1\\ \vdots\\ \lambda_n\hat{y}_n\end{pmatrix} + \begin{pmatrix}\hat{f}_1\\ \vdots\\ \hat{f}_n\end{pmatrix}$$

$$\frac{d\hat{y}_i}{dt} = \lambda_i\hat{y}_i + \hat{f}_i, \quad i = 1,\dots,n$$

- We now have n *decoupled* systems.
- We solve these (numerically) in a coupled fashion.
- The behavior, however, is the same as this decoupled system, which is easier to understand.

Discrete Case: Euler Forward Example

$$\frac{\mathbf{y}_{k+1} - \mathbf{y}_k}{\Delta t} \;=\; J\mathbf{y}_k \;+\; \mathbf{f}_k \qquad (h := \Delta t)$$

$$V^{-1} \times \left[\frac{\mathbf{y}_{k+1} - \mathbf{y}_k}{\Delta t} \;=\; J\mathbf{y}_k \;+\; \mathbf{f}_k\right]$$

$$\Longrightarrow \frac{\hat{\mathbf{y}}_{k+1} - \hat{\mathbf{y}}_k}{\Delta t} \;=\; \Lambda\hat{\mathbf{y}}_k \;+\; \hat{\mathbf{f}}_k$$

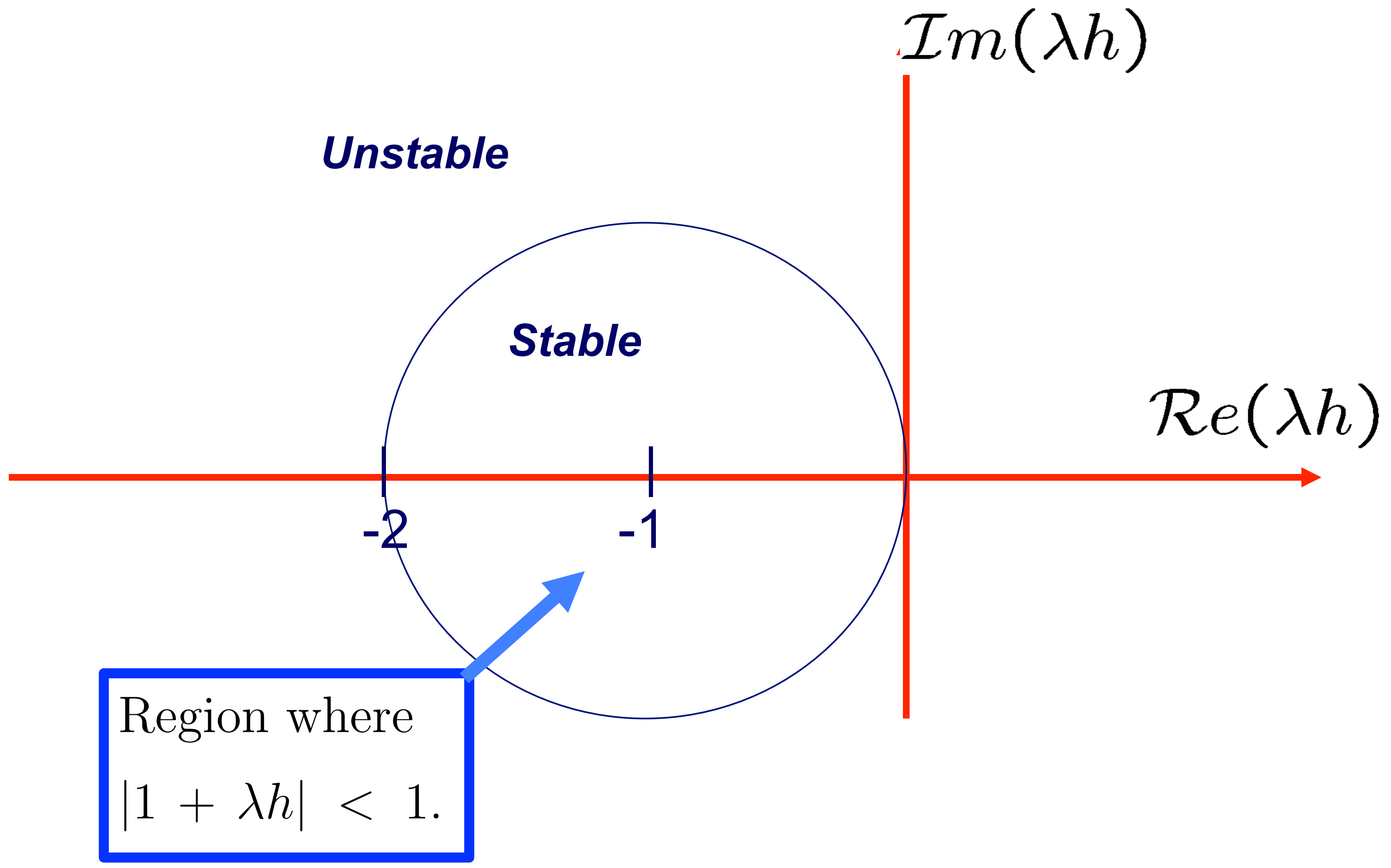
$$\hat{\mathbf{y}}_{k+1} \;=\; \hat{\mathbf{y}}_k + \Delta t\Lambda\hat{\mathbf{y}}_k \;+\; \Delta t\hat{\mathbf{f}}_k$$

$$\hat{y}_{j,k+1} \;=\; (1 + \Delta t\lambda_j)\hat{y}_{j,k} \;+\; \Delta t\hat{f}_{j,k}$$

Therefore, forward Euler stability requires

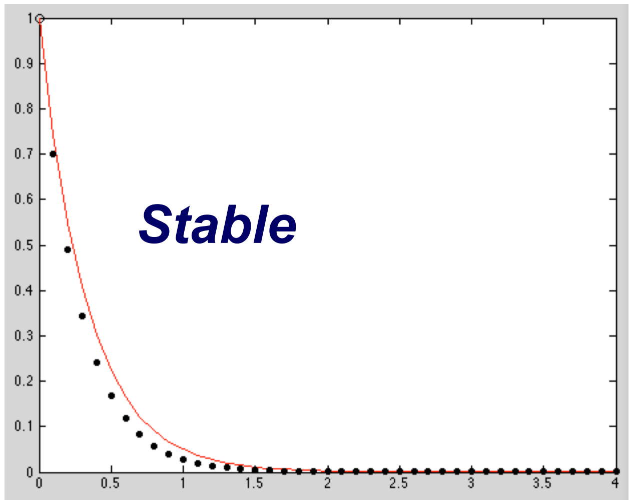
$$|1 + \Delta t\lambda_j| \;<\; 1, \qquad j = 1, \ldots, n$$

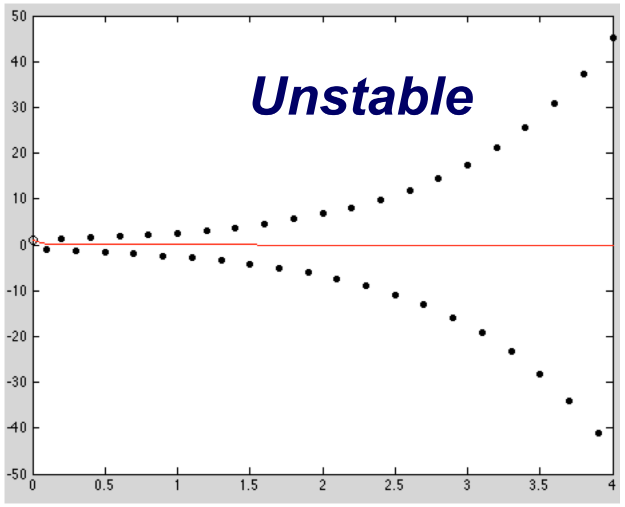
Stability Region for Euler's Method



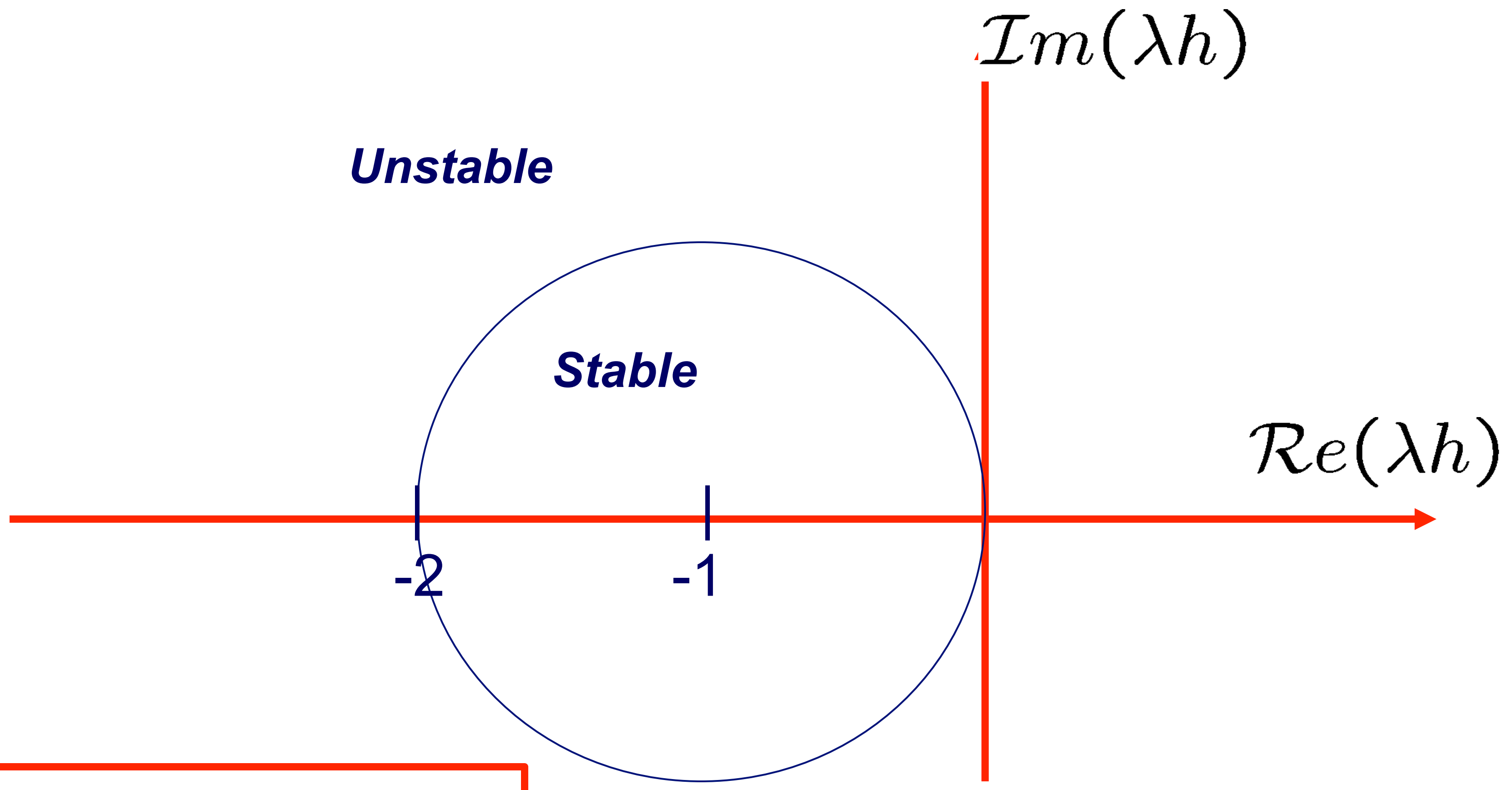
MATLAB EXAMPLE: Euler for y' = λ y (ef1.m)

```
%% A simple Euler forward integrator
%
%  Typical Usage:  h=.01; lambda=3; ef1
%

tfinal = 4; nsteps=ceil(tfinal/h); h=tfinal/nsteps;

x=zeros(nsteps+1,1);t=x;

t=h*(0:nsteps);

hold off; x(1)=1; plot(t(1),x(1),'ko'); hold on;

xe=x(1)*exp(lambda*t); plot(t,xe,'r-')

for k=1:nsteps;

    fx = lambda*x(k);

    x(k+1)=x(k) + h*fx;
    t(k+1)=k*h;

    plot(t(k+1),x(k+1),'k.'); drawnow;

end;
```





Stability Region for Euler's Method



Why complex plane?

Recall: Orbit Example

$$\frac{d}{dt}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = A\,\mathbf{y}.$$

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

$$\begin{aligned} \left|A - \lambda I\right| &= \begin{vmatrix} -\lambda & -1 \\ 1 & -\lambda \end{vmatrix} \\ &= \lambda^2 + 1 = 0 \end{aligned}$$

$$\lambda = \pm i$$

- ***Even though ODE involves only reals, the behavior can be governed by complex eigenvalues.***

Euler's Method, continued

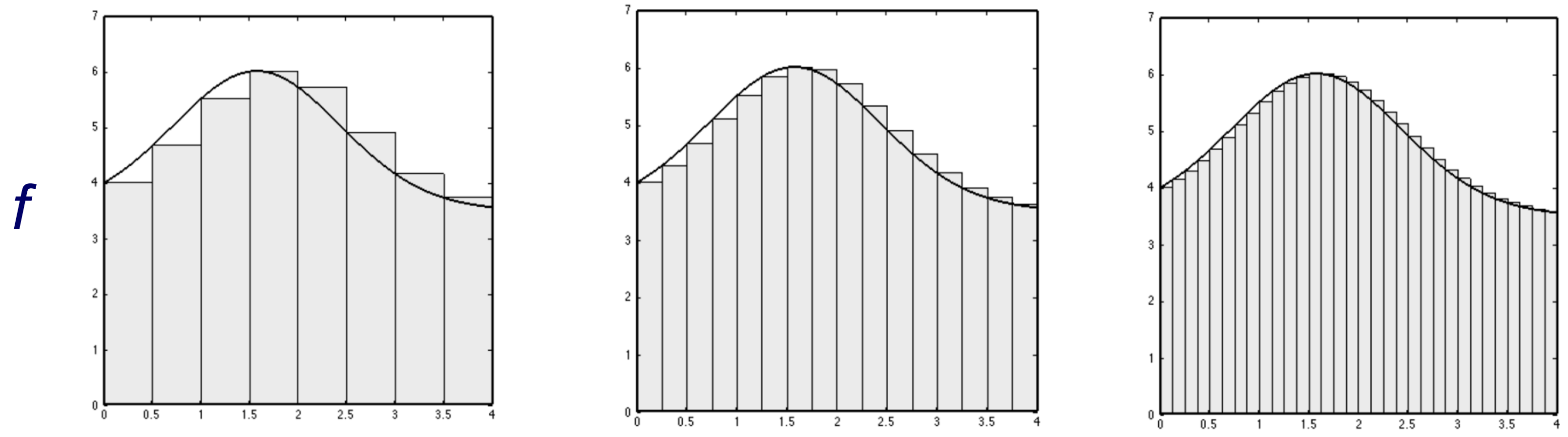
- If λ is real, then $h\lambda$ must lie in interval $(-2, 0)$, so for $\lambda < 0$, we must have
$$h \leq -\frac{2}{\lambda}$$
for Euler's method to be stable

- *Growth factor* $1 + h\lambda$ agrees with series expansion
$$e^{h\lambda} = 1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{6} + \cdots$$
through terms of first order in h, so Euler's method is first-order accurate

LTE is O(h^2) !

GTE is O(h) !

Relationship between LTE and GTE



$$y_n \;=\; y_0 + \int_0^T f(t,y)\,dt$$

- If LTE $= O(\Delta t^2)$, then commit $O(\Delta t^2)$ error on each step.
- Interested in final error at time $t = T = n\Delta t$.
- Interested in the final error $e_n := y(t_n) - y_n$ in the limit $n \longrightarrow \infty$, $n\Delta t = T$ *fixed.*
- Nominally, the final error will be proportional to the sum of the local errors,

$$e_n \;\sim\; C\,n \cdot \text{LTE} \sim C\,n\Delta t^2 \sim C\,(n\Delta t)\Delta t \sim C\,T\Delta t$$

- GTE $\sim$ LTE $/\Delta t$

Stability of Numerical Methods for ODEs

In general, growth factor depends on

- Numerical method, which determines form of growth factor
- Step size h
- Jacobian $\boldsymbol{J}_f$, which is determined by particular ODE

Implicit Methods

- Euler's method is *explicit* in that it uses only information at time t_k to advance solution to time t_{k+1}
- This may seem desirable, but Euler's method has rather limited stability region
- Larger stability region can be obtained by using information at time t_{k+1}, which makes method *implicit*
- Simplest example is *backward Euler method*

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + h_k \boldsymbol{f}(t_{k+1}, \boldsymbol{y}_{k+1})$$

- Method is implicit because we must evaluate $\boldsymbol{f}$ with argument $\boldsymbol{y}_{k+1}$ before we know its value

Implicit Methods, continued

- This means that we must solve algebraic equation to determine $\boldsymbol{y}_{k+1}$
- Typically, we use iterative method such as Newton's method or fixed-point iteration to solve for $\boldsymbol{y}_{k+1}$
- Good starting guess for iteration can be obtained from explicit method, such as Euler's method, or from solution at previous time step

< interactive example >

Implicit Methods, continued

- Given extra trouble and computation in using implicit method, one might wonder why we bother
- Answer is that implicit methods generally have significantly larger stability region than comparable explicit methods
- Increased stability implies we can take (many) fewer steps, assuming that accuracy is not compromised by the larger stepsize, h.

Backward Euler Method

- To determine stability of backward Euler, we apply it to scalar ODE $y' = \lambda y$, obtaining

$$y_{k+1} = y_k + h\lambda y_{k+1}$$
$$(1 - h\lambda) y_{k+1} = y_k$$
$$y_k = \left(\frac{1}{1 - h\lambda}\right)^k y_0$$

- Thus, for backward Euler to be stable we must have

$$\left|\frac{1}{1 - h\,\lambda}\right| \le 1$$

which holds for *any* $h > 0$ when $\mathrm{Re}(\lambda) < 0$

- So stability region for backward Euler method includes entire left half of complex plane, or interval $(-\infty, 0)$ if λ is real

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Growth Factor, G

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Backward Euler Method, continued

- Growth factor

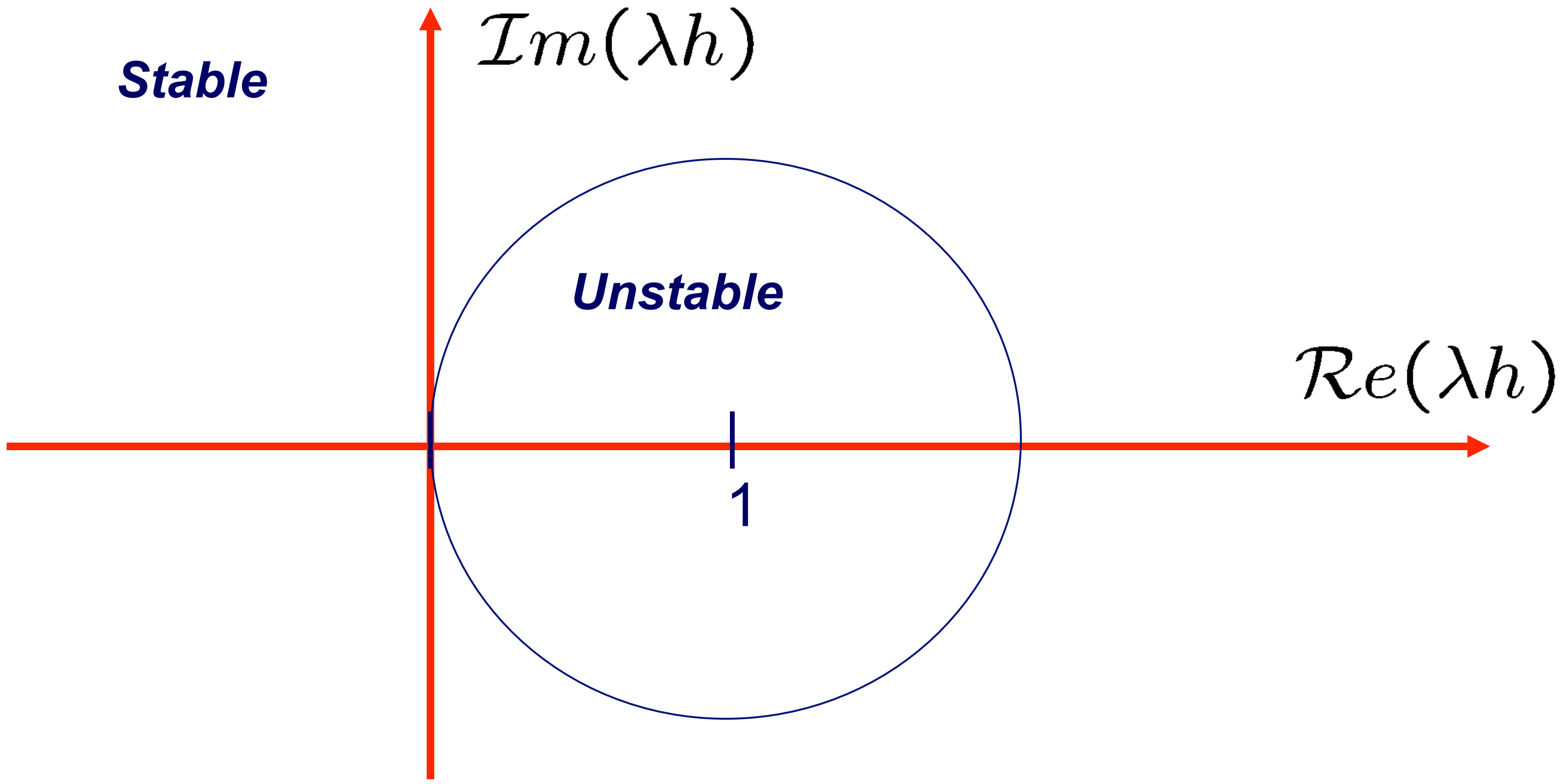
$$\frac{1}{1-h\lambda} = 1 + h\lambda + (h\lambda)^2 + \cdots$$

  agrees with expansion for $e^{\lambda h}$ through terms of order h, so backward Euler method is first-order accurate

- Growth factor of backward Euler method for general system of ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$ is $(\boldsymbol{I} - h\boldsymbol{J}_f)^{-1}$, whose spectral radius is less than 1 provided all eigenvalues of $h\boldsymbol{J}_f$ lie outside circle in complex plane of radius 1 centered at 1

- Thus, stability region of backward Euler for general system of ODEs is entire left half of complex plane

Stability Region for Backward Euler Method



Unconditionally Stable Methods

- Thus, for computing stable solution backward Euler is stable for any positive step size, which means that it is *unconditionally* stable
- Great virtue of unconditionally stable method is that desired accuracy is only constraint on choice of step size
- Thus, we may be able to take much larger steps than for explicit method of comparable order and attain much higher overall efficiency despite requiring more computation per step
- Although backward Euler method is unconditionally stable, its accuracy is only of first order, which severely limits its usefulness

Trapezoid Method

- Higher-order accuracy can be achieved by averaging Euler and backward Euler methods to obtain implicit *trapezoid method*

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + h_k \left(\boldsymbol{f}(t_k, \boldsymbol{y}_k) + \boldsymbol{f}(t_{k+1}, \boldsymbol{y}_{k+1}) \right) /2$$

- To determine its stability and accuracy, we apply it to scalar ODE $y' = \lambda y$, obtaining

$$y_{k+1} = y_k + h\,(\lambda y_k + \lambda y_{k+1})\,/2$$

$$y_k = \left(\frac{1 + h\lambda/2}{1 - h\lambda/2} \right)^k y_0$$

- Method is stable if

$$\left| \frac{1 + h\lambda/2}{1 - h\lambda/2} \right| < 1$$

which holds for any $h > 0$ when $\mathrm{Re}(\lambda) < 0$

Trapezoid Method, continued

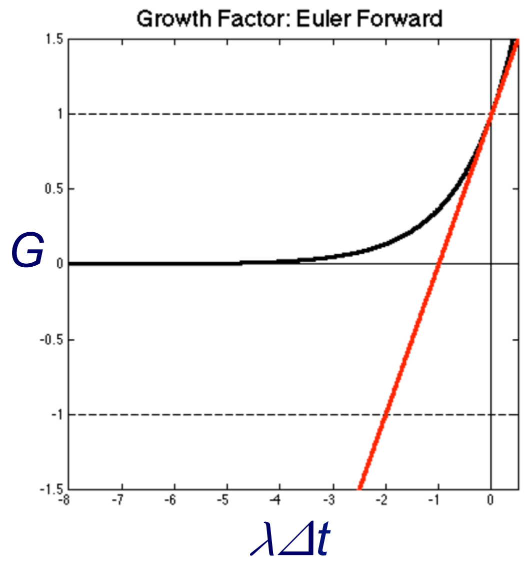
- Thus, trapezoid method is unconditionally stable
- Its growth factor

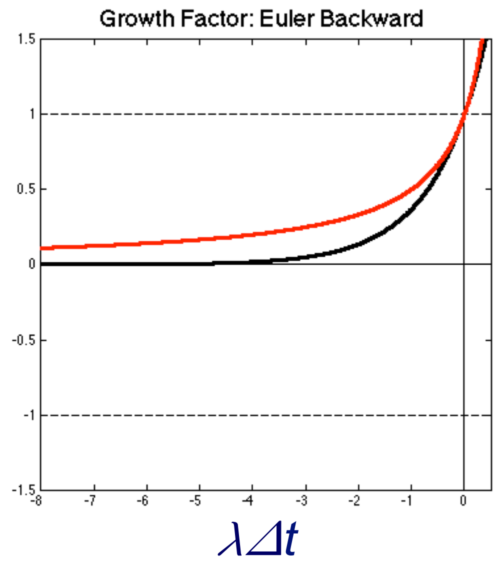
$$\begin{aligned}\frac{1+h\lambda/2}{1-h\lambda/2} &= \left(1+\frac{h\lambda}{2}\right)\left(1+\frac{h\lambda}{2}+\left(\frac{h\lambda}{2}\right)^2+\left(\frac{h\lambda}{2}\right)^3+\cdots\right)\\ &= 1+h\lambda+\frac{(h\lambda)^2}{2}+\frac{(h\lambda)^3}{4}+\cdots\end{aligned}$$

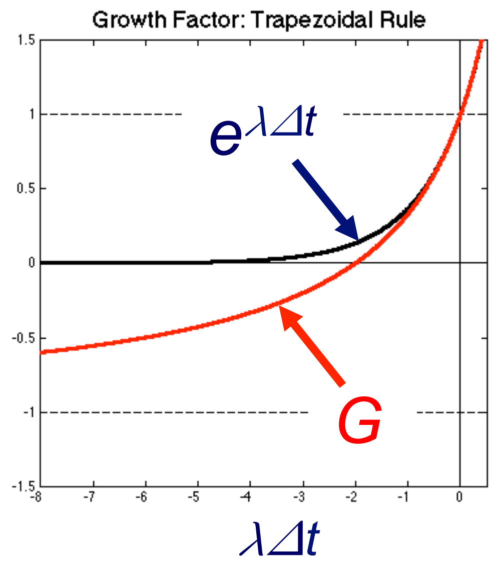
  agrees with expansion of $e^{h\lambda}$ through terms of order h^2, so trapezoid method is second-order accurate

- For general system of ODEs $\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y})$, trapezoid method has growth factor $(\boldsymbol{I} + \frac{1}{2}h\boldsymbol{J}_f)(\boldsymbol{I} - \frac{1}{2}h\boldsymbol{J}_f)^{-1}$, whose spectral radius is less than 1 provided eigenvalues of $h\boldsymbol{J}_f$ lie in left half of complex plane

Growth Factors for Real λ







- Each growth factor approximates $e^{\lambda \Delta t}$ for $\lambda \Delta t \rightarrow 0$
- For EF, $|G|$ is not bounded by 1
- For Trapezoidal Rule, local (small $\lambda \Delta t$) approximation is $O(\lambda \Delta t^2)$, but $|G| \rightarrow -1$ as $\lambda \Delta t \rightarrow -\infty$. [Trapezoid method is not ***L-stable.***]
- BDF2 will give 2nd-order accuracy, stability, and $|G| \rightarrow 0$ as $\lambda \Delta t \rightarrow -\infty$.

Implicit Methods, continued

- We have now seen two examples of implicit methods that are unconditionally stable, but not all implicit methods have this property
- Implicit methods generally have larger stability regions than explicit methods, but allowable step size is not always unlimited
- Implicitness alone is not sufficient to guarantee stability

Example: backward difference formula of order 3 or higher

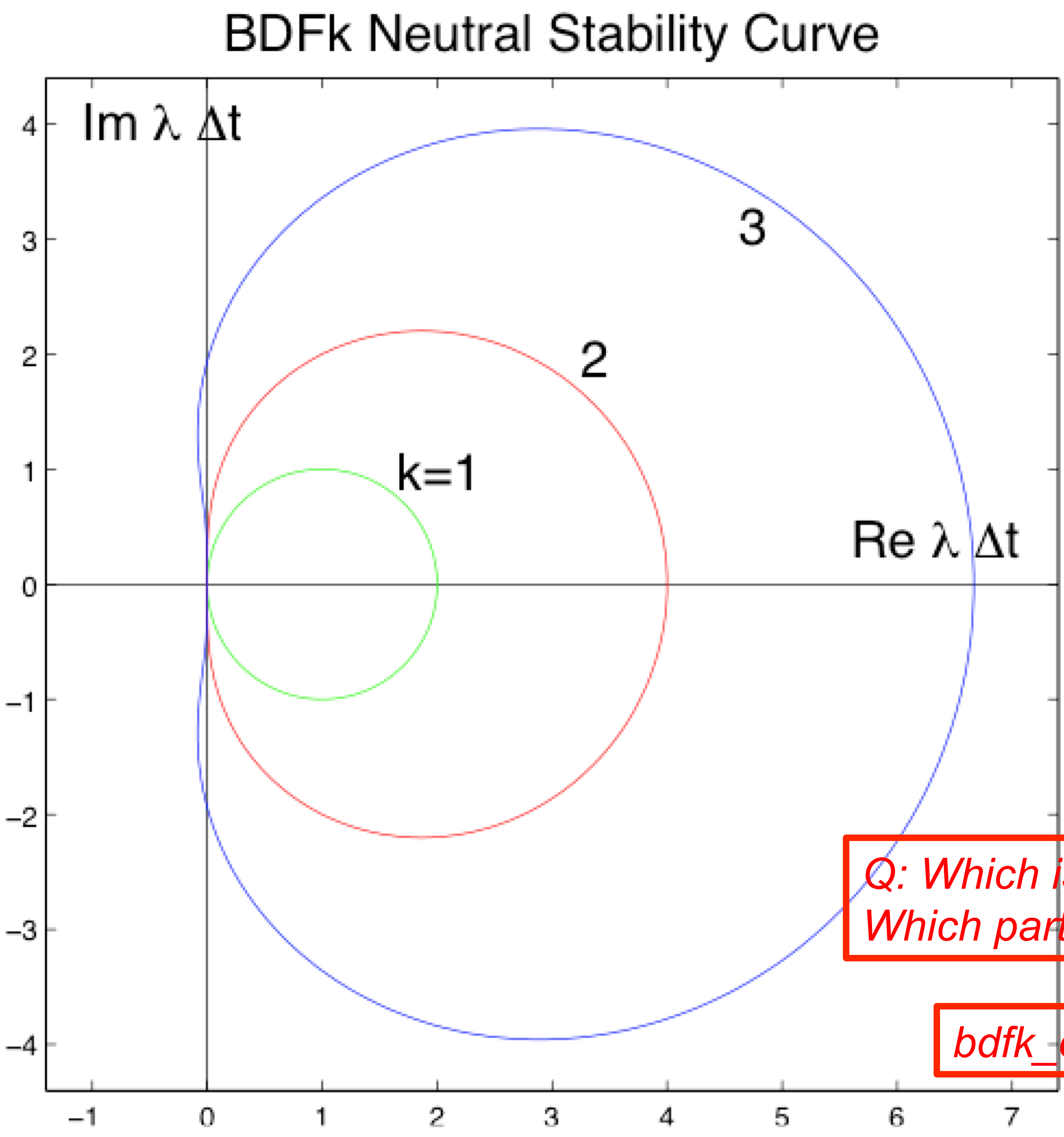
BDFk Formulas: GTE = O(h^k)

$$\text{BDF1:}\quad \left.\frac{\partial u}{\partial t}\right|_{t^n} = \frac{u^n - u^{n-1}}{\Delta t} + O(\Delta t)$$

$$\text{BDF2:}\quad \left.\frac{\partial u}{\partial t}\right|_{t^n} = \frac{3u^n - 4u^{n-1} + u^{n-2}}{2\Delta t} + O(\Delta t^2)$$

$$\text{BDF3:}\quad \left.\frac{\partial u}{\partial t}\right|_{t^n} = \frac{11u^n - 18u^{n-1} + 9u^{n-2} - 2u^{n-3}}{6\Delta t} + O(\Delta t^3).$$

- Unlike the trapezoidal rule, these methods are L-stable:
  - |G|→0 as $\lambda\Delta$t → -∞
- k-th order accurate
- Implicit
- Unconditionally stable only for k $\leq$ 2   (here, k := order of method)
- Multi-step: require data from previous timesteps

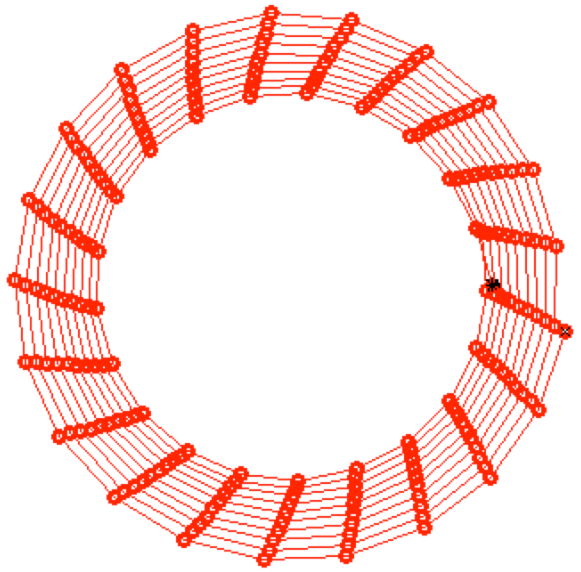


Q: Which is stable?
Which part is unstable?

bdfk_orbit.m

Implicit Orbit Example

```
%  BDFk-Orbit: Typical Usage:  dt=.1; bdfk_orbit

T = 2*pi; n=ceil(T/dt); dt = T/n;  n=10*n; % Tfinal and dt; 10 orbits

A = [ 0 -1 ; 1 0 ]; I=eye(2);

y0 = [ 1 ; 0 ]; % INITIAL CONDITION

y=y0; y2=y; y1=y; y3=y;

xk=zeros(n+1,1); yk=xk;
for k=1:n;

    xk(k)=y(1); yk(k)=y(2);
    y3=y2; y2=y1;y1=y;

    if k==1;                           % BDF 1 for 1st step
       E = I - dt*A;
       y = E\y1;
    elseif k==2;                       % BDF 2 for 2nd step
       E = 1.5*I - dt*A;
       y = E\((4*y1-y2)/2);
    else                               % BDF 3 for step > 2
       E = (11/6)*I - dt*A;
       y = E\((18*y1-9*y2+2*y3)/6);
    end

end;
xk(end)=y(1); yk(end)=y(2);
plot(xk,yk,'r-'); axis equal;hold on
plot(xk(1),yk(1),'k*'); axis equal; hold on
plot(y(1),y(2),'kx'); axis equal; hold on
```



Explicit High-Order Methods

- High-order explicit methods are of interest for several reasons:
  - Lower cost per step than implicit (but possibly many steps if system has disparate timescales, i.e., is stiff --- spring-mass example).
  - More accuracy
  - For k > 2, encompass part of the imaginary axis near zero, so stable for systems having purely imaginary eigenvalues, ***provided h is sufficiently small.***
  - We'll look at three classes of high-order explicit methods:
    - BDFk / Ext k
    - kth-order Adams Bashforth
    - Runge-Kutta methods
  - Each has pros and cons…

Higher-Order Explicit Timesteppers: BDFk/EXTk

- Idea: evaluate left-hand and right-hand sides at t_{k+1} to accuracy $O(\Delta t^k)$.

$$\left.\frac{dy}{dt}\right|_{t_{k+1}} = \left. f(t,y)\right|_{t_{k+1}}$$

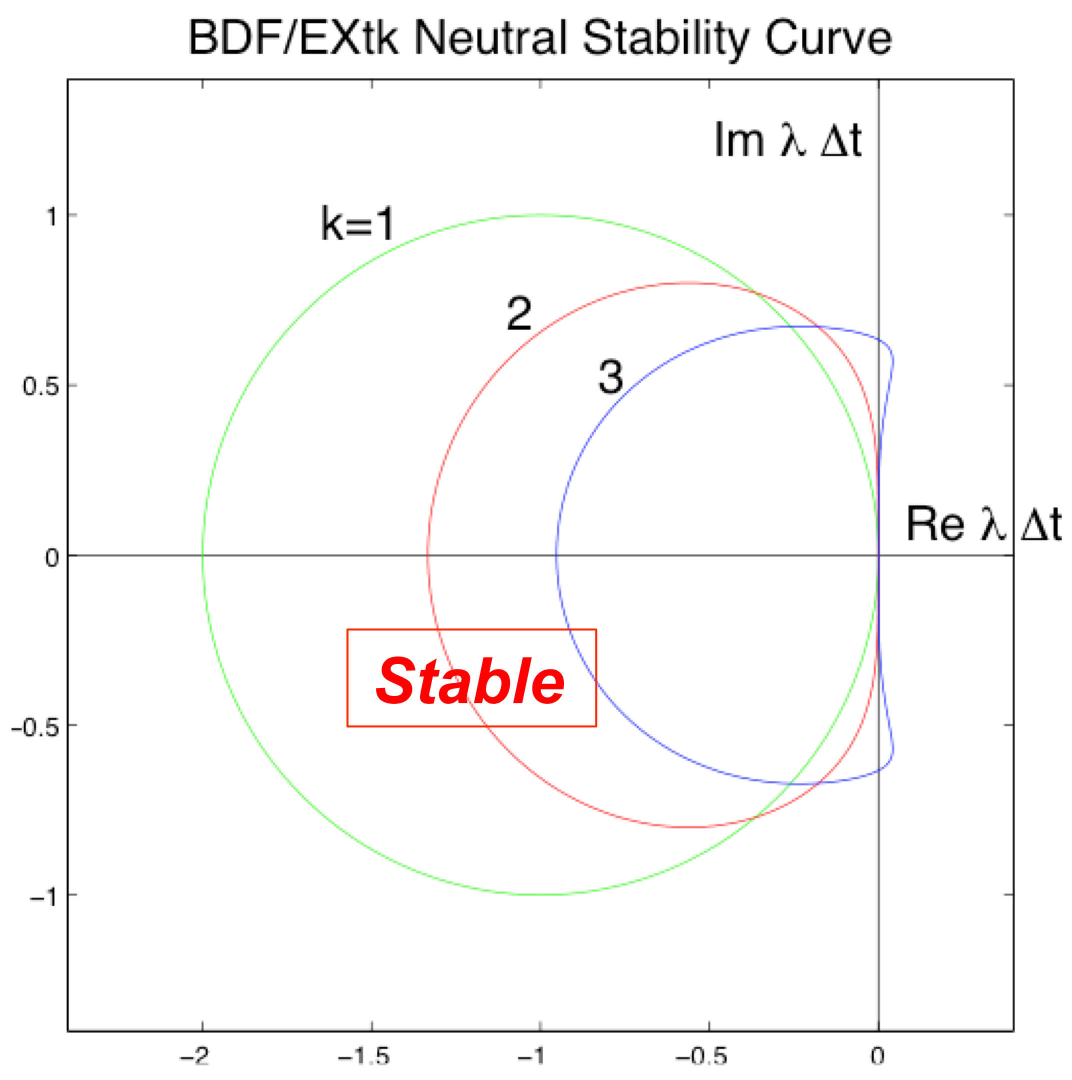
- Can treat term on the right via kth-order extrapolation.
- For example, for $k=2$,

$$\frac{3y_{k+1} - 4y_k + y_{k-1}}{2\Delta t} + O(\Delta t^2) = 2f_k - f_{k-1} + O(\Delta t^2)$$

- Solve for y_{k+1} in terms of known quantities on the right:

$$y_{k+1} = \frac{2}{3}\left[\frac{4y_k - y_{k-1}}{2} + \Delta t(2f_k - f_{k-1})\right] + O(\Delta t^3)$$

- Note that LTE is $O(\Delta t^3)$, GTE=$O(\Delta t^2)$.



- Here we see that the k=3 curve encompasses part of the imaginary axis near the origin of the $\lambda\Delta$t plane, which is important for stability of non-dissipative systems.

Higher-Order Explicit Timesteppers: kth-order Adams-Bashforth

- Adams-Bashforth methods are a somewhat simpler alternative to BDFk/EXTk.
- Time advancement via integration:

$$\mathbf{y}_{k+1} \;=\; \mathbf{y}_k \;+\; \int_{t_k}^{t_{k+1}} \mathbf{f}(t,\mathbf{y})\,dt$$

- AB1:

$$\int_{t_k}^{t_{k+1}} f(t,\mathbf{y})\,dt \;=\; h_k f_k \;+\; O(h^2)$$

- AB2:

$$\begin{aligned}\int_{t_k}^{t_{k+1}} \mathbf{f}(t,\mathbf{y})\,dt \;&=\; h_k\mathbf{f}_k \;+\; \frac{h_k^2}{2}\left[\frac{\mathbf{f}_k-\mathbf{f}_{k-1}}{h_{k-1}}\right] \;+\; O(h^3)\\ &=\; h\left(\frac{3}{2}\mathbf{f}_k \;-\; \frac{1}{2}\mathbf{f}_{k-1}\right) \;+\; O(h^3) \text{ (if } h \text{ is constant)}\end{aligned}$$

- AB3:

$$\int_{t_k}^{t_{k+1}} \mathbf{f}(t,\mathbf{y})\,dt \;=\; h\left(\frac{23}{12}\mathbf{f}_k \;-\; \frac{16}{12}\mathbf{f}_{k-1} \;+\; \frac{5}{12}\mathbf{f}_{k-2}\right) \;+\; O(h^4) \text{ (if } h \text{ is constant)}$$

- LTE for ABm is $O(h^{m+1})$. GTE for ABm is $O(h^m)$.

Stability of Various Timesteppers

- Derived from model problem $\frac{du}{dt} = \lambda u$
- Stability regions shown in the λΔt plane (stable *inside* the curves)

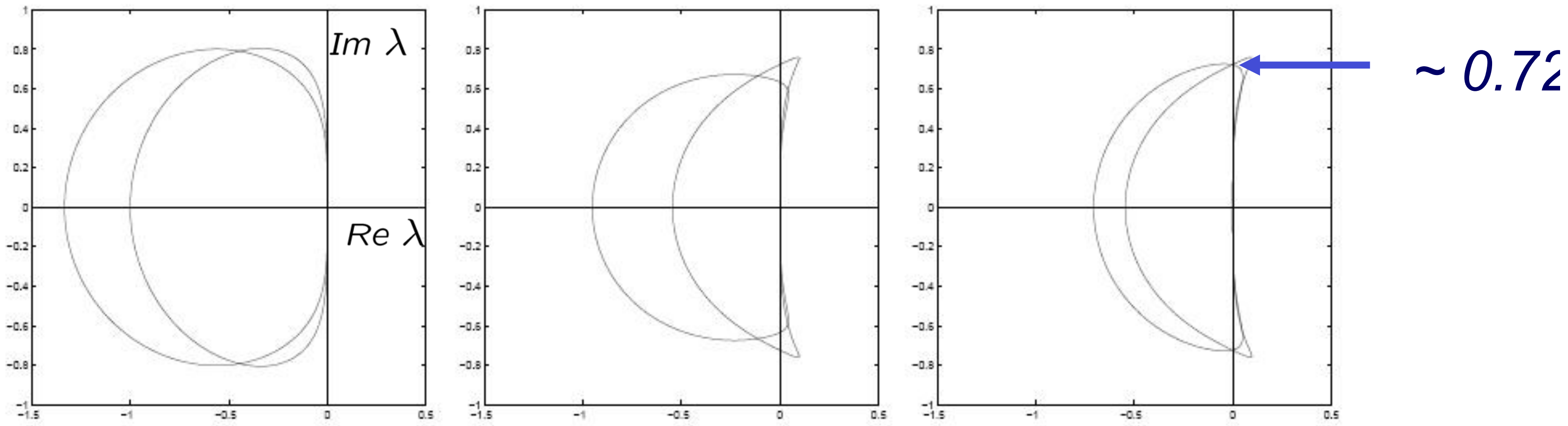


Figure 1: Stability regions for (left) AB2 and BDF2/EXT2, (center) AB3 and BDF3/EXT3, and (right) AB3 and BDF2/EXT2a.

- *To make effective use of this plot, we need to know something about the eigenvalues λ of the Jacobian.*
- *But first, How are these plots generated?*

Determining the Neutral-Stability Curve

Consider BDF2/EXT2, and apply it to $\dfrac{du}{dt} = \lambda u$:

$$3u^m - 4u^{m-1} + u^{m-2} = 2\lambda\Delta t \left(2u^{m-1} - u^{m-2}\right).$$

Seek solutions of the form $u^m = (z)^m$, $z \in C$:

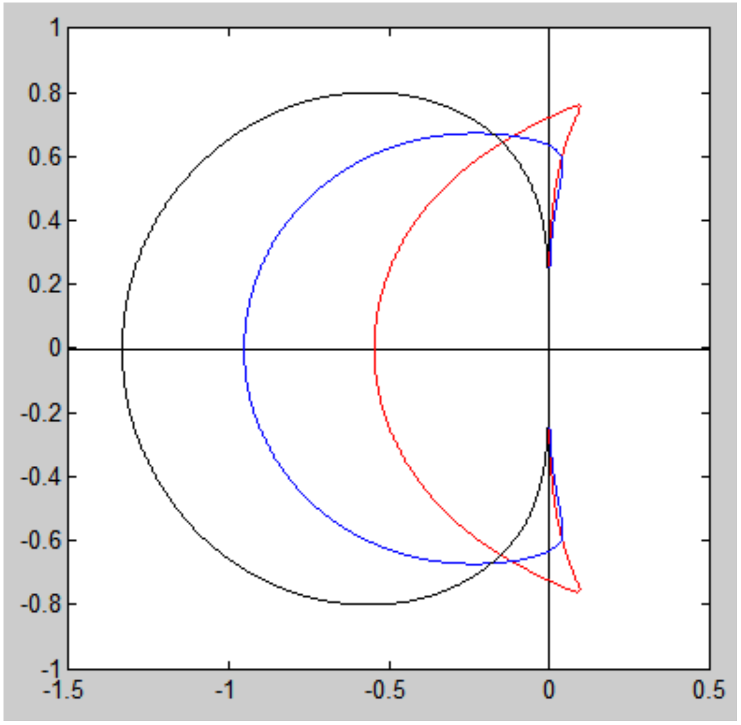
$$\begin{aligned} 3z^m - 4z^{m-1} + z^{m-2} &= 2\lambda\Delta t \left(2z^{m-1} - z^{m-2}\right). \\ 3z^2 - 4z + 1 &= 2\lambda\Delta t\,(2z-1)\,. \end{aligned}$$

Set $z = e^{i\theta}$, $\theta \in [0, 2\pi]$, and solve for $\lambda\Delta t$:

$$\lambda\Delta t = \frac{3e^{i2\theta} - 4e^{i\theta} + 1}{2\left(2e^{i\theta} - 1\right)}.$$

Matlab Code: stab.m

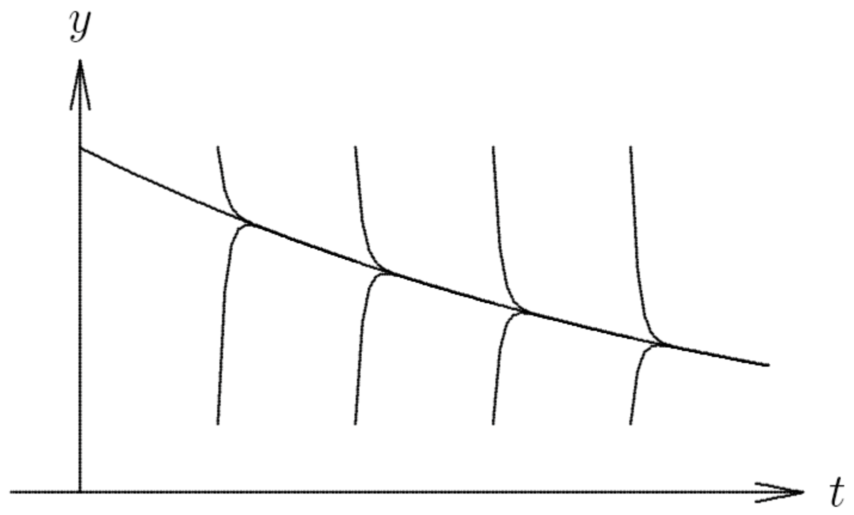
```
ymax=1; ep=1.e-13; yaxis=[-ymax*ii ymax*ii]';  % Plot axes
xaxis=[-2.0+ep*ii 2.0+ep*ii]';
hold off; plot (yaxis,'k-'); hold on; plot (xaxis,'k-');
axis square; axis([-ymax-.5 ymax-.5 -ymax ymax]);

ii=sqrt(-1); th=0:.001:2*pi;  th=th'; ith=ii*th; ei=exp(ith);
E = [ ei 1+0*ei 1./ei 1./(ei.*ei) 1./(ei.*ei.*ei)];


ab0   = [1 0.0 0.0 0. 0.]';
ab1   = [0 1.0 0.0 0. 0.]';
ab2   = [0 1.5 -.5 0. 0.]';
ab3   = [0 23./12. -16./12. 5./12. 0.]';
bdf1  = (([ 1.  -1.   0.   0. 0.])/1.)';
bdf2  = (([ 3.  -4.   1.   0. 0.])/2.)';
bdf3  = (([11. -18.   9. -2. 0.])/6.)';
exm   = [1 0   0 0 0]';
ex1   = [0 1   0 0 0]';
ex2   = [0 2 -1 0 0]';
ex3   = [0 3 -3 1 0]';
du    = [1. -1. 0. 0. 0.]';
```



```
ldtab3 =(E*du)./(E*ab3);   plot (ldtab3 ,'r-');  % AB3
bdf3ex3=(E*bdf3)./(E*ex3); plot (bdf3ex3,'b-');  % BDF3/EXT3
bdf2ex2=(E*bdf2)./(E*ex2); plot (bdf2ex2,'k-');  % BDF2/EXT2
```

Stiff Differential Equations

- Asymptotically stable solutions converge with time, and this has favorable property of damping errors in numerical solution
- But if convergence of solutions is too rapid, then difficulties of different type may arise
- Such ODE is said to be *stiff*



Stiff System Examples

- Spring-mass system

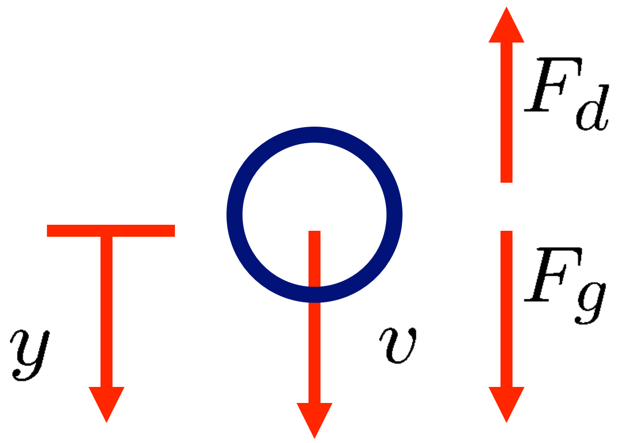
$$M\mathbf{y}'' \; = \; -K\mathbf{y}$$

- Nonlinear ODE

$$y' \; = \; -1000y \; + \; cos(y^3)$$

- Falling Particle in a viscous fluid

Stiffness Example: Drag on a Falling Particle



$$F_g = gm$$

$$\begin{pmatrix} \frac{dy}{dt} \\ \frac{dv}{dt} \end{pmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & s \end{bmatrix} \begin{pmatrix} y \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ g \end{pmatrix}$$

Stokes drag for small particles:

$$F_d = -6\pi\mu r v$$

$$\frac{1}{m} F_d = -\frac{6\pi\mu r v}{\frac{4}{3}\pi r^3 \rho_p} = -\frac{18\mu}{\rho_p d^2} v =: sv, \qquad d = 2r = 2 \times \text{ radius}$$

Stiffness Example: Drag on a Falling Particle

- Consider acceleration of falling particle,

$$\begin{aligned} y &= \text{position} \\ v = \frac{dy}{dt} &= \text{velocity} \\ \frac{1}{m}F_{\text{net}} = \frac{dv}{dt} &= \text{acceleration} \end{aligned}$$

- Equation of motion:

$$\begin{pmatrix} \frac{dy}{dt} \\ \frac{dv}{dt} \end{pmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & s \end{bmatrix} \begin{pmatrix} y \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ g \end{pmatrix}$$

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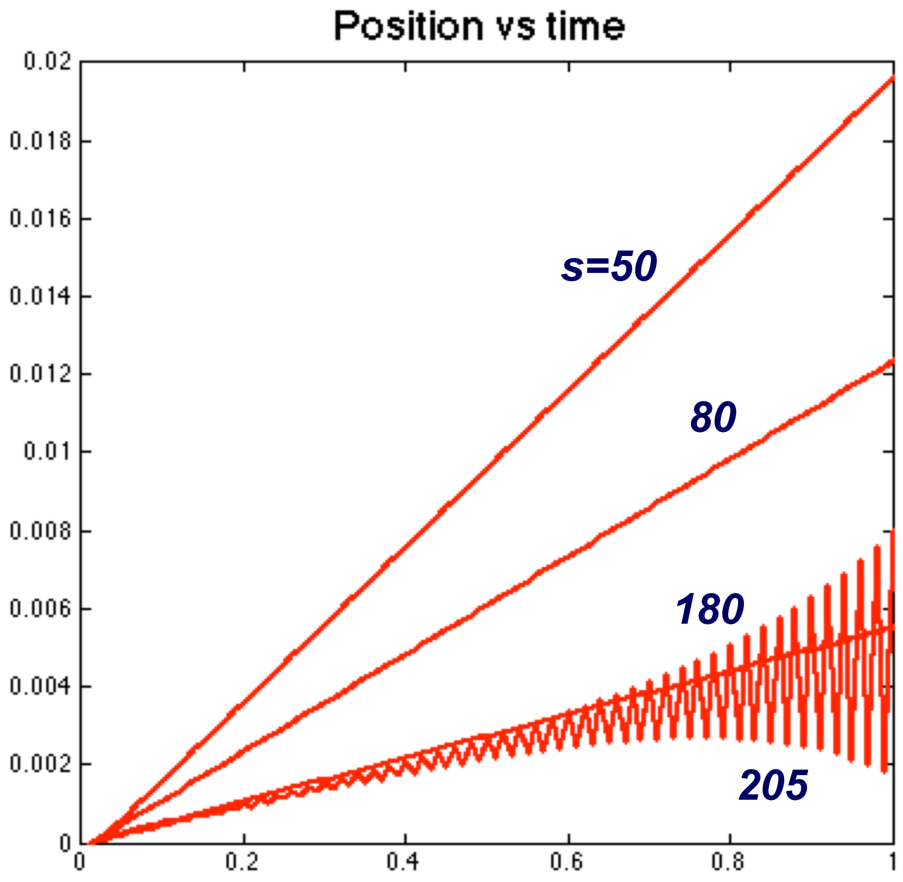
where $d = 2r =$ particle diameter.

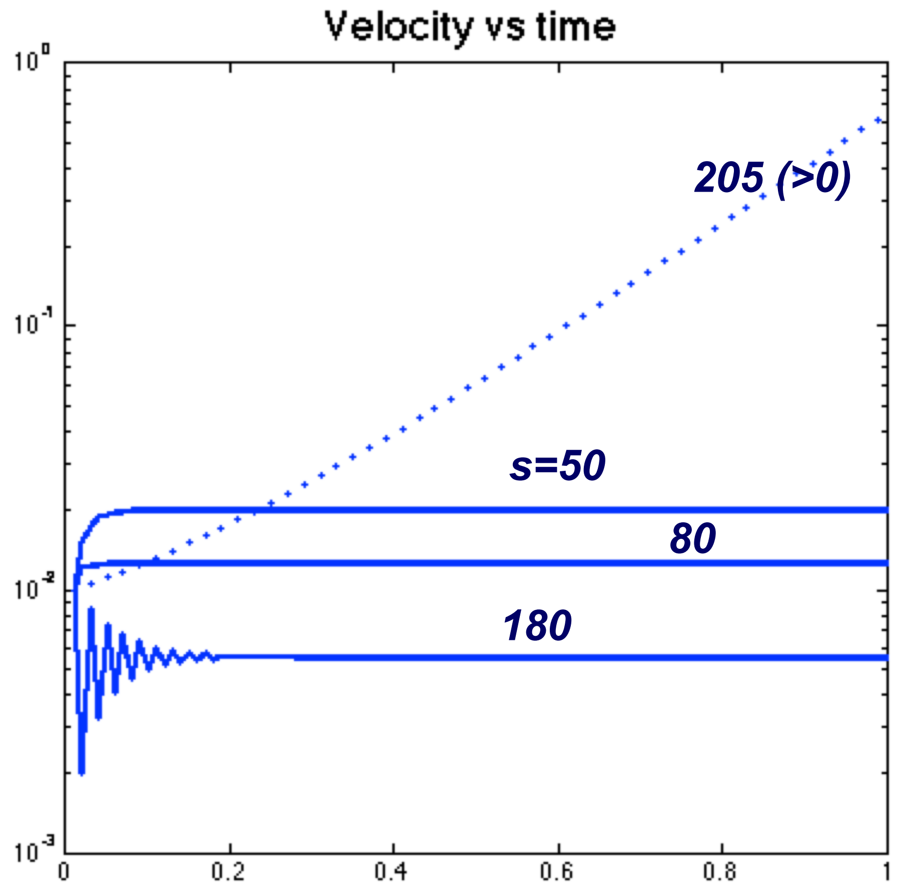
- Eigenvalues of the system:

$$\begin{aligned} 0 &= |J - I\lambda| = \begin{vmatrix} -\lambda & 1 \\ 0 & s-\lambda \end{vmatrix} = \lambda(\lambda - s) \\ \lambda &= 0, \quad \boxed{\lambda = s.} \end{aligned}$$

Falling Particle Using Euler Forward

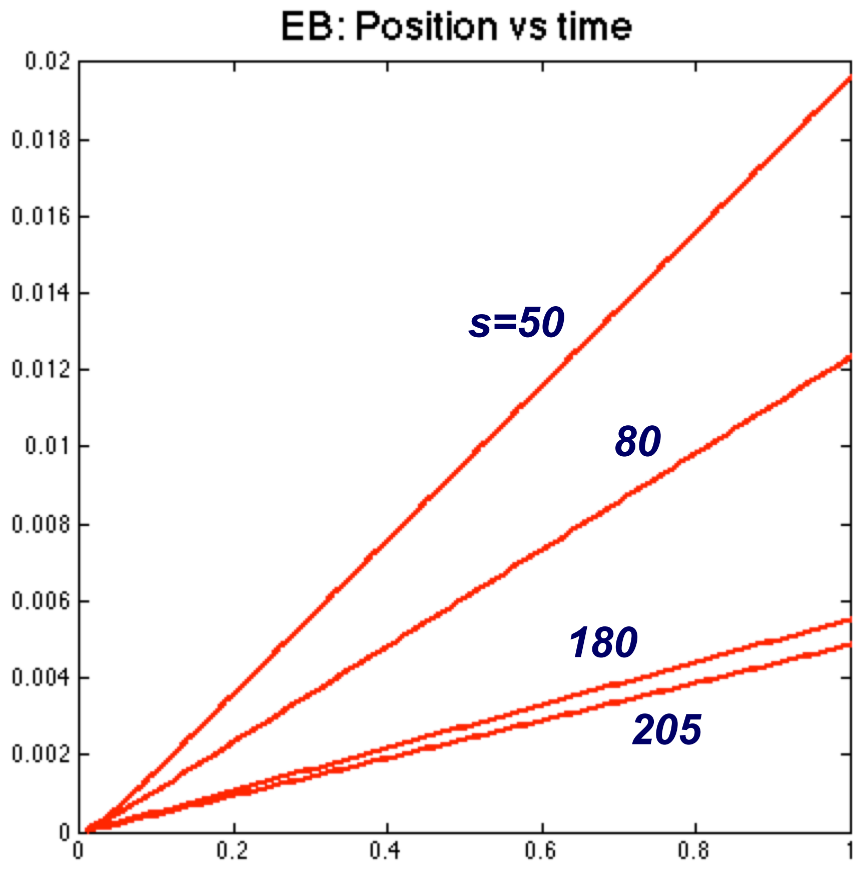
stokeseb.m

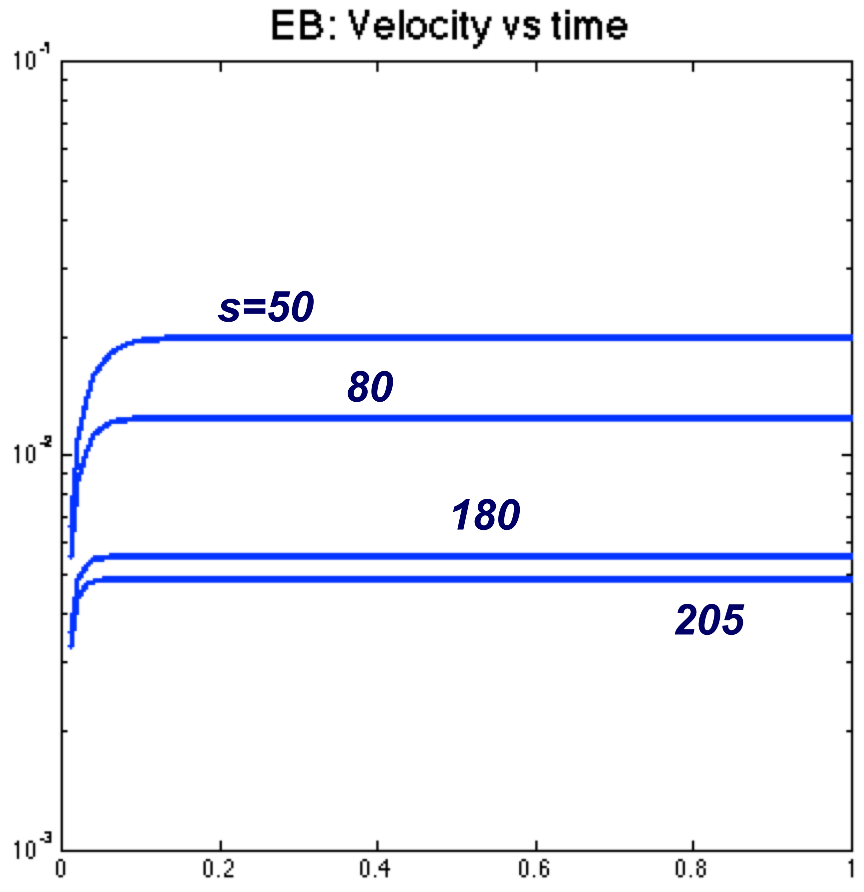




Q: What must the h value be, in this case?

Falling Particle Using Euler Backward





Note: Still only O(h) accurate. Trapezoid or BDF2 would be O(h^2)

Semi-Implicit Methods for Stiff ODEs

- Recall, for general system of ODES,

$$\mathbf{y}' \;=\; \mathbf{f}(t, \mathbf{y}),$$

  growth factor for EB is spectral radius ($\max |\lambda_j|$) of $(I - hJ)^{-1}$

- Recall our basic timesteppers for model problem $\mathbf{y}' = J\mathbf{y}$:
  - EF: $\quad \mathbf{y}_{k+1} \;=\; (I + hJ)\mathbf{y}_k$
  - EB: $\quad (I - hJ)\mathbf{y}_{k+1} \;=\; \mathbf{y}_k$
  - Trap: $\quad (I - \frac{h}{2}J)\mathbf{y}_{k+1} \;=\; (1 + \frac{h}{2}J)\mathbf{y}_k$
- We see that the trapezoidal rule is just a splitting of the Jacobian J.
- We can effect other splittings to get stable schemes that are easier to solve than the fully-implicit systems (where $J = J(\mathbf{y}_{k+1})$, in general).

Semi-Implicit Methods for Stiff ODEs

- For stiff problems can split Jacobian into fast and slow parts

$$J \;=\; \underset{\substack{\uparrow \\ \textit{fast} \\ \textit{part}}}{J_f} \;+\; \underset{\substack{\uparrow \\ \textit{slow} \\ \textit{part}}}{J_s}$$

$$(I \;-\; hJ_f)\mathbf{y}_{k+1} \;=\; (I \;+\; hJ_s)\mathbf{y}_k$$

- Growth factor is spectral radius

$$\rho\left[(I \;-\; hJ_f)^{-1}(I \;+\; hJ_s)\right]$$

- Often, J_f can be linear and diagonal or a linearization of the nonlinear system operator.

- J_s, treated explicitly, can be nonlinear, nonlocal, nonsymmetric, etc.

Semi-Implicit Methods for Stiff ODEs

- Method can be extended to high-order using BDFq/EXTq.
- For example, a 2nd-order BDF/EXT scheme would be:

$$\begin{aligned}\frac{d\mathbf{y}}{dt} &= \frac{3\mathbf{y}_{k+1} - 4\mathbf{y}_k + \mathbf{y}_{k-1}}{2h} + O(h^2) \\ &= J_f\mathbf{y}_{k+1} + (2q_k - q_{k-1}) + O(h^2)\end{aligned}$$

with $q_{k-j} := J_s(t_{k-j}, \mathbf{y}_{k-j})\mathbf{y}_{k-j}$.

- One can rearrange to solve for $\mathbf{y}_{k+1}$. The system is of the form

$$\left(3I + \frac{2h}{3}J_f\right)\mathbf{y}_{k+1} = \mathbf{g}$$

- This scheme can be relatively stable and 2nd-order accurate.

Runge-Kutta Methods

- *Runge-Kutta methods* are single-step methods similar in motivation to Taylor series methods, but they do not require computation of higher derivatives
- Instead, Runge-Kutta methods simulate effect of higher derivatives by evaluating $\boldsymbol{f}$ several times between t_k and t_{k+1}
- Simplest example is second-order *Heun's method*

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \frac{h_k}{2}(\boldsymbol{k}_1 + \boldsymbol{k}_2)$$

where

Essentially, "explicit" trapezoidal rule.

$$\begin{aligned}\boldsymbol{k}_1 &= \boldsymbol{f}(t_k, \boldsymbol{y}_k)\\ \boldsymbol{k}_2 &= \boldsymbol{f}(t_k + h_k, \boldsymbol{y}_k + h_k\boldsymbol{k}_1)\end{aligned}$$

Runge-Kutta Methods, continued

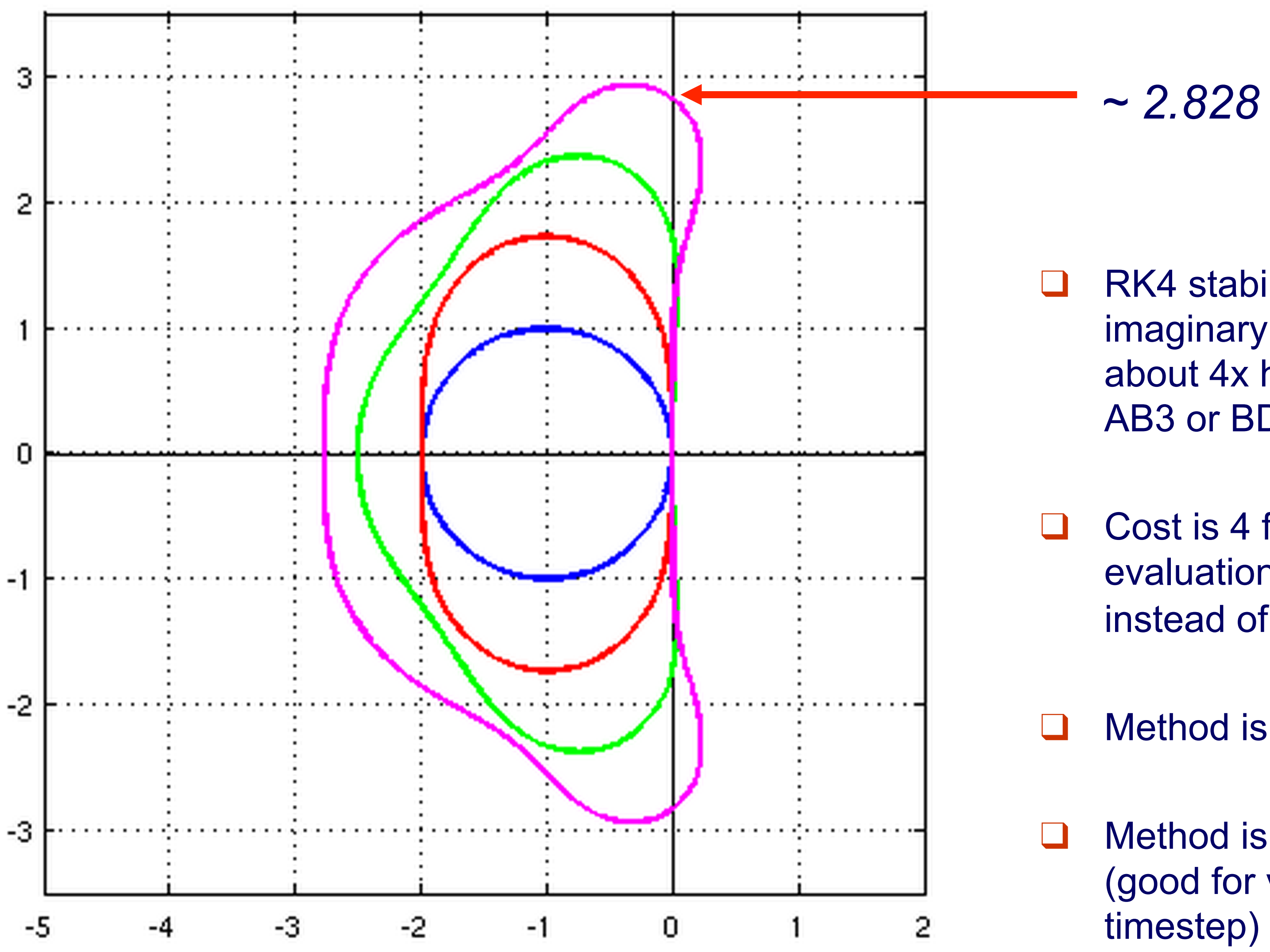
- Heun's method is analogous to implicit trapezoid method, but remains explicit by using Euler prediction $\boldsymbol{y}_k + h_k \boldsymbol{k}_1$ instead of $\boldsymbol{y}(t_{k+1})$ in evaluating $\boldsymbol{f}$ at t_{k+1}
- Best known Runge-Kutta method is classical fourth-order scheme

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \frac{h_k}{6}\left(\boldsymbol{k}_1 + 2\boldsymbol{k}_2 + 2\boldsymbol{k}_3 + \boldsymbol{k}_4\right)$$

where

$$\begin{aligned} \boldsymbol{k}_1 &= \boldsymbol{f}(t_k, \boldsymbol{y}_k) \\ \boldsymbol{k}_2 &= \boldsymbol{f}(t_k + h_k/2, \boldsymbol{y}_k + (h_k/2)\boldsymbol{k}_1) \\ \boldsymbol{k}_3 &= \boldsymbol{f}(t_k + h_k/2, \boldsymbol{y}_k + (h_k/2)\boldsymbol{k}_2) \\ \boldsymbol{k}_4 &= \boldsymbol{f}(t_k + h_k, \boldsymbol{y}_k + h_k\boldsymbol{k}_3) \end{aligned}$$

Stability Regions for RK1—4



- RK4 stability region on imaginary axis extends about 4x higher than for AB3 or BDF3/EXT3
- Cost is 4 function evaluations per step instead of 1
- Method is 4th order
- Method is self-starting (good for variable timestep)

Derivation of Stability Region

- Begin with $f(y) = \lambda y$.
- Expand all terms in the time advancement scheme.
- Gives the growth factor G.
- Set $G = e^{i\theta}$ and solve for λh.

Runge-Kutta Methods, continued

- To proceed to time t_{k+1}, Runge-Kutta methods require no history of solution prior to time t_k, which makes them *self-starting* at beginning of integration, and also makes it easy to change step size during integration
- These facts also make Runge-Kutta methods relatively easy to program, which accounts in part for their popularity
- Unfortunately, classical Runge-Kutta methods provide no error estimate on which to base choice of step size

Runge-Kutta Methods, continued

- Fehlberg devised *embedded Runge-Kutta* method that uses six function evaluations per step to produce both fifth-order and fourth-order estimates of solution, whose difference provides estimate for local error
- Another embedded Runge-Kutta method is due to Dormand and Prince
- This approach has led to automatic Runge-Kutta solvers that are effective for many problems, but which are relatively inefficient for stiff problems or when very high accuracy is required
- It is possible, however, to define *implicit* Runge-Kutta methods with superior stability properties that are suitable for solving stiff ODEs

Time Step Selection

- Assuming Δt satisfies the stability criteria, can also choose Δt based on accuracy by estimating the LTE at each step.
  - Common way to estimate with, say, RK4 scheme, is to take a step with size Δt and another pair of steps with size $\Delta t/2$.
  - The difference gives an estimate of LTE (for step size $\Delta t/2$).
  - If GTE ~ LTE*T/Δt, and LTE ~ C Δt^5, solve for Δt such that you will realize the desired final error.
- Self-starting (i.e., multistage) methods such as RK are well-suited to this strategy.

Summary of Methods / Properties

- Multistep methods of order > 2 require special starting procedures
- Multistage (e.g., RKq) methods are self-starting and easy to change stepsize h.
- Multistage methods are attractive for automated stepsize selection.
- Be sure to understand the stability diagrams of these methods.
  - Left, or right side of complex λh plane?
  - Does it include Im. axis? If so, where does it cut?
  - Where does it cut the real axis?

Method	Implementation	LTE	GTE	Comments
EF	$\mathbf{y}_{k+1} = \mathbf{y}_k + h\mathbf{f}_k$	$O(h^2)$	$O(h)$	explicit
EB	$\mathbf{y}_{k+1} = \mathbf{y}_k + h\mathbf{f}_{k+1}$	$O(h^2)$	$O(h)$	implicit/stable
Trap	$\mathbf{y}_{k+1} = \mathbf{y}_k + \frac{h}{2}(\mathbf{f}_k + \mathbf{f}_{k+1})$	$O(h^3)$	$O(h^2)$	implicit/stable (but *not* L-stable)
BDFq	interpolation of $\mathbf{y}_{k-j}$	$O(h^{q+1})$	$O(h^q)$	multistep, implicit,stable for $q < 3$
BDFq/EXTq	interpolation of $\mathbf{y}_{k-j}$, $\mathbf{f}_{k-j}$	$O(h^{q+1})$	$O(h^q)$	multistep, extends to semi-implicit
ABq	integration over $[t_k, t_{k+1}]$	$O(h^{q+1})$	$O(h^q)$	multistep, explicit, captures Im. axis for q=3
RKq	integration over $[t_k, t_{k+1}]$	$O(h^{q+1})$	$O(h^q)$	multistage explicit, easy to start
Extrapolation	extends methods above			implicit or explicit

Example: Stiff ODE

- Consider scalar ODE

$$y' = -100y + 100t + 101$$

  with initial condition $y(0) = 1$

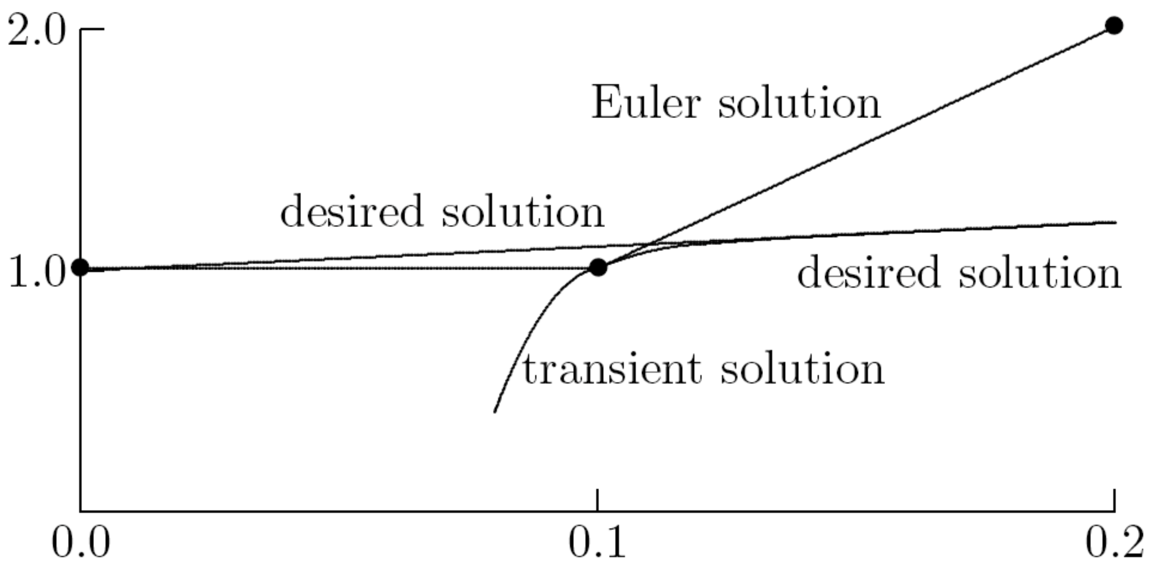
- General solution is $y(t) = 1 + t + ce^{-100t}$, and particular solution satisfying initial condition is $y(t) = 1 + t$ (i.e., $c = 0$)

- Since solution is linear, Euler's method is theoretically exact for this problem

- However, to illustrate effect of using finite precision arithmetic, let us perturb initial value slightly

Example, continued

- Euler's method bases its projection on derivative at current point, and resulting large value causes numerical solution to diverge radically from desired solution
- Jacobian for this ODE is $J_f = -100$, so stability condition for Euler's method requires step size $h < 0.02$,



Multistep Methods

- *Multistep methods* use information at more than one previous point to estimate solution at next point
- *Linear multistep* methods have form

$$\boldsymbol{y}_{k+1} = \sum_{i=1}^{m} \alpha_i \boldsymbol{y}_{k+1-i} + h \sum_{i=0}^{m} \beta_i \boldsymbol{f}(t_{k+1-i}, \boldsymbol{y}_{k+1-i})$$

- Parameters α_i and β_i are determined by polynomial interpolation
- If $\beta_0 = 0$, method is explicit, but if $\beta_0 \neq 0$, method is implicit
- Implicit methods are usually more accurate and stable than explicit methods, but require starting guess for $\boldsymbol{y}_{k+1}$

Examples: Multistep Methods

- Simplest second-order accurate explicit two-step method is

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \frac{h}{2}(3\boldsymbol{y}'_k - \boldsymbol{y}'_{k-1})$$

- Simplest second-order accurate implicit method is trapezoid method

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \frac{h}{2}(\boldsymbol{y}'_{k+1} + \boldsymbol{y}'_k)$$

- One of most popular pairs of multistep methods is explicit fourth-order Adams-Bashforth predictor

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \frac{h}{24}(55\boldsymbol{y}'_k - 59\boldsymbol{y}'_{k-1} + 37\boldsymbol{y}'_{k-2} - 9\boldsymbol{y}'_{k-3})$$

and implicit fourth-order Adams-Moulton corrector

$$\boldsymbol{y}_{k+1} = \boldsymbol{y}_k + \frac{h}{24}(9\boldsymbol{y}'_{k+1} + 19\boldsymbol{y}'_k - 5\boldsymbol{y}'_{k-1} + \boldsymbol{y}'_{k-2})$$

Examples: Multistep Methods

- *Backward differentiation formulas* form another important family of implicit multistep methods
- BDF methods, typified by popular formula

$$\boldsymbol{y}_{k+1} = \frac{1}{11}(18\boldsymbol{y}_k - 9\boldsymbol{y}_{k-1} + 2\boldsymbol{y}_{k-2}) + \frac{6h}{11}\boldsymbol{y}'_{k+1}$$

are effective for solving stiff ODEs

< interactive example >

Multistep Adams Methods

- Stability and accuracy of some Adams methods are summarized below
  - *Stability threshold* indicates left endpoint of stability interval for scalar ODE
  - *Error constant* indicates coefficient of h^{p+1} term in local truncation error, where p is order of method

Explicit Methods

Order	Stability threshold	Error constant
1	-2	$1/2$
2	-1	$5/12$
3	$-6/11$	$3/8$
4	$-3/10$	$251/720$

Implicit Methods

Order	Stability threshold	Error constant
1	$-\infty$	$-1/2$
2	$-\infty$	$-1/12$
3	-6	$-1/24$
4	-3	$-19/720$

- Implicit methods are both more stable and more accurate than corresponding explicit methods of same order

Properties of Multistep Methods

- They are not self-starting, since several previous values of $\boldsymbol{y}_k$ are needed initially
- Changing step size is complicated, since interpolation formulas are most conveniently based on equally spaced intervals for several consecutive points
- Good local error estimate can be determined from difference between predictor and corrector
- They are relatively complicated to program
- Being based on interpolation, they can efficiently provide solution values at output points other than integration points

Properties of Multistep, continued

- Implicit methods have much greater region of stability than explicit methods, but must be iterated to convergence to enjoy this benefit fully
  - PECE scheme is actually explicit, though in a somewhat complicated way
- Although implicit methods are more stable than explicit methods, they are still not necessarily unconditionally stable
  - No multistep method of greater than second order is unconditionally stable, even if it is implicit
- Properly designed implicit multistep method can be very effective for solving stiff ODEs

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