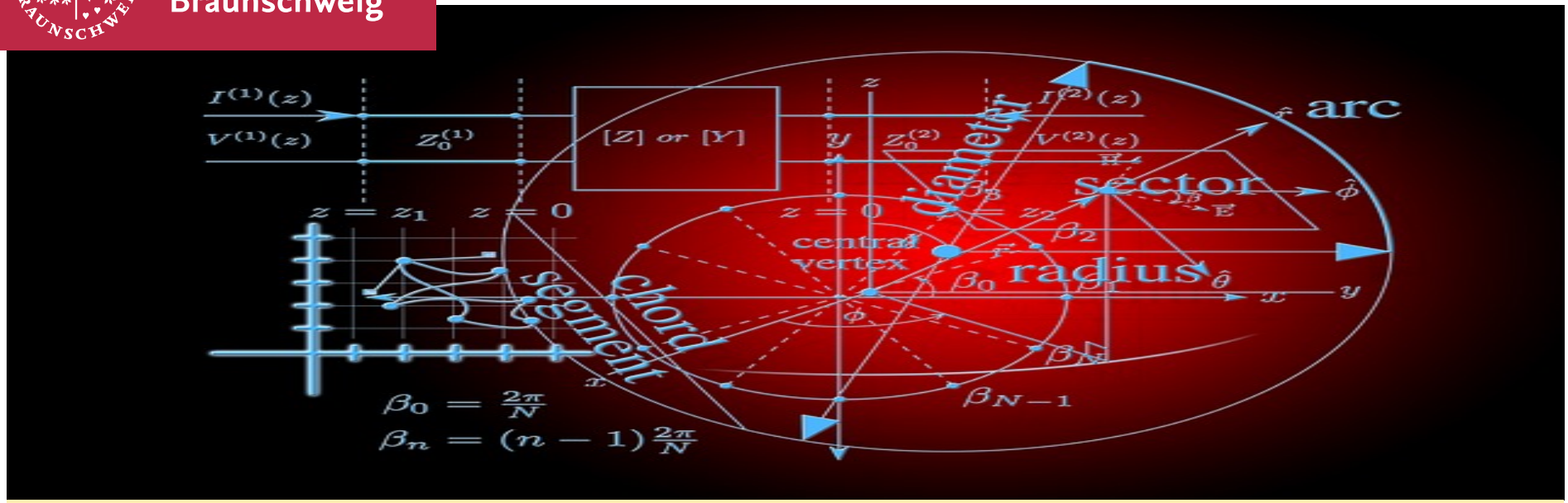
Technische Universität Braunschweig



Introduction to Scientific Computing

Consistency and convergence

Bojana Rosić, 3. Februar 2016

Last lecture: Linear multistep methods

In general linear multistep methods can be written in a form of:

$$\sum_{l=0}^{k} a_l x_{n+l} = h \sum_{l=0}^{k} b_l f(t_{n+l}, x_{n+l})$$

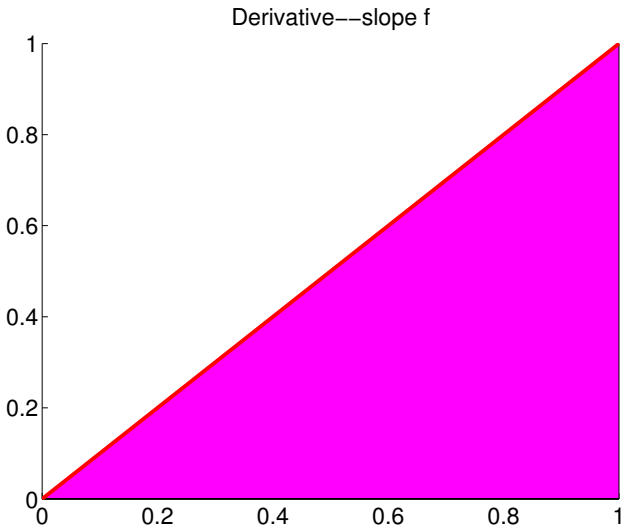
We have studied that these methods require several starting points (either given or predicted by one step method). The local error of these methods is defined via

$$\epsilon_{loc} = x_a(t) - x_n(t) \Rightarrow \| \frac{\epsilon_{loc}}{h} \| \leqslant Ch^p$$

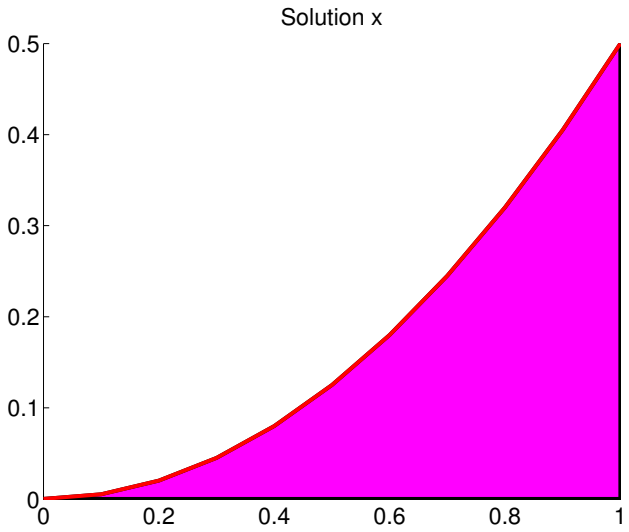
in which $x_a(t)$ is exact and $x_n(t)$ is numerical solution in one time step starting from the exact one. Thus, the local error defines consistency condition (error decreases with the step size going to zero).

Last lecture: Consistency

Let us integrate the ODE $\dot{x} = t$ in time interval $[0, 1]$ by taking whole interval as one step



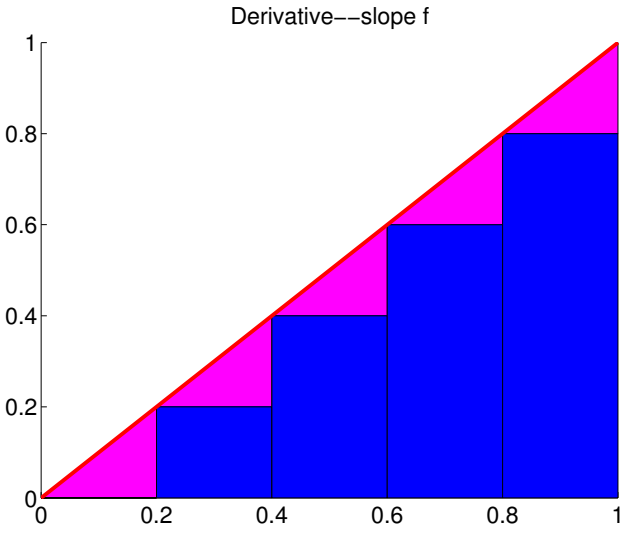
a) error in slope



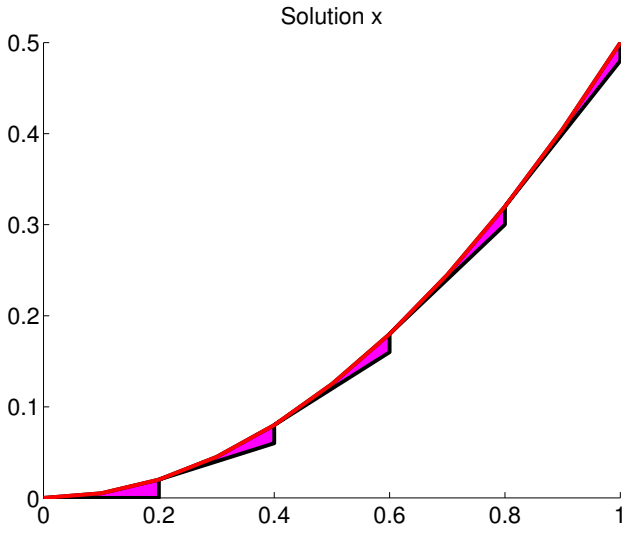
b) error in solution (local error) $= 0.5$

Last lecture: Consistency

or let us cut the time interval into several substeps



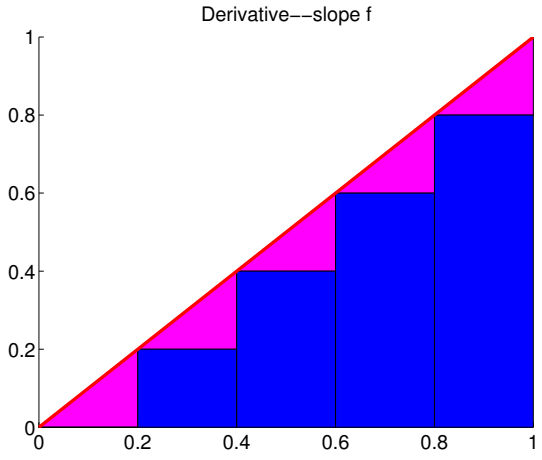
a) error in slope



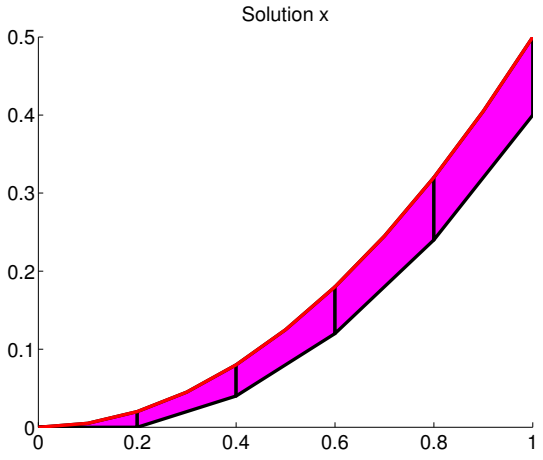
b) error in solution (local error)$\approx$ 0.02

Is consistency enough?

In order to see this, let us compute numerically the solution x_1 in one step starting from x_0 (which is analytical (**exact**)). Then, let us compute the next step starting from the **last** numerical solution x_1 to obtain x_2 etc. Finally, let us compute the total error between **full** numerical solution and analytical one over some time interval.



a) error in slope [a]

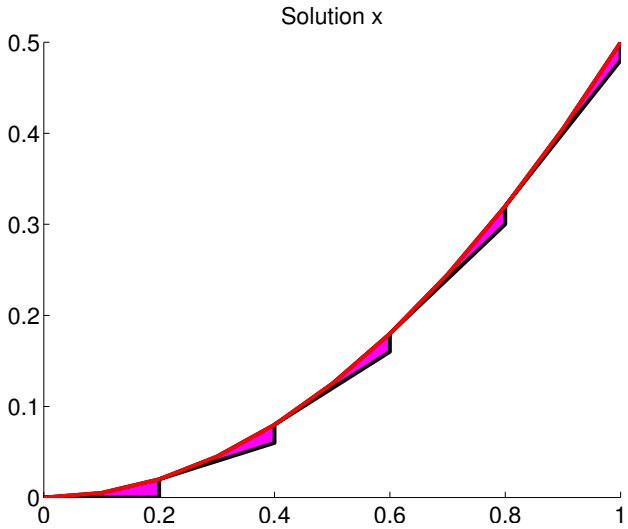


b) error in solution (global error)≈ 0.1

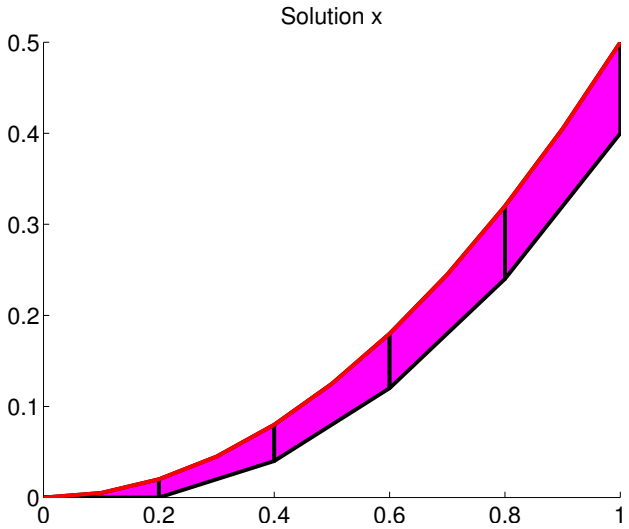
[a] same as before as f does not depend on x

Is consistency enough?

By comparing both of figures, we may see that the full numerical solution gives us bigger error (This is to expect as local error gets integrated over time. Also, the left picture is not realistic as usually one does not know the exact solution).



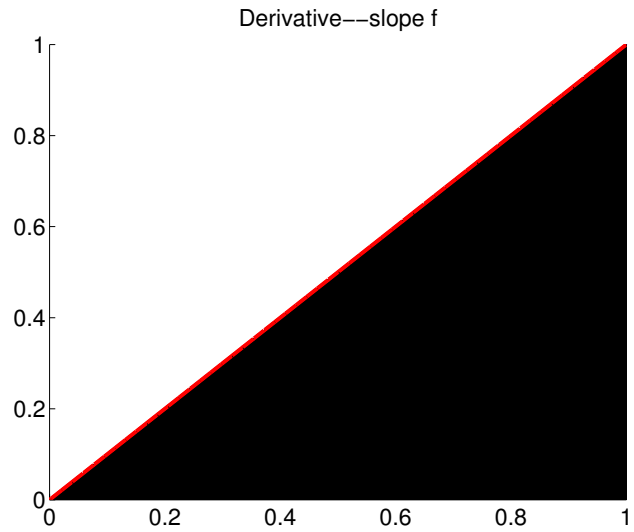
a) local error ≈ 0.02



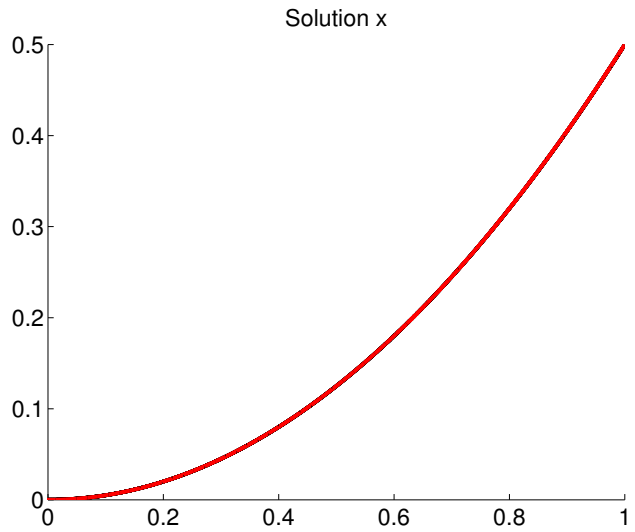
b) global error ≈ 0.1

Is consistency enough?

To reduce the error, one has to reduce the time step size. Hence, let us make the step size 100 times smaller, then we get



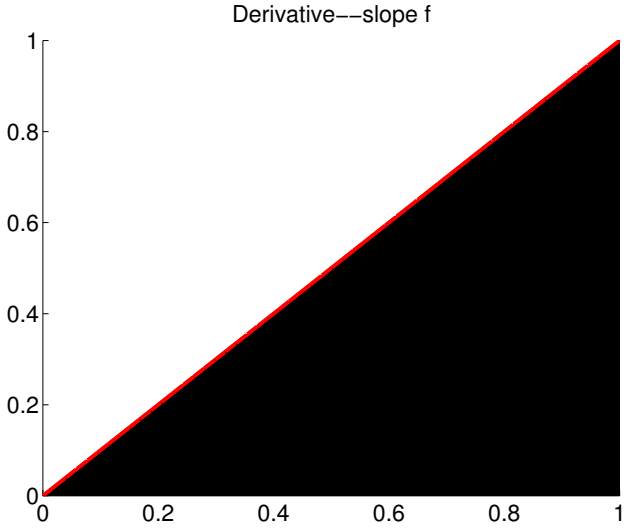
a) error in slope very small

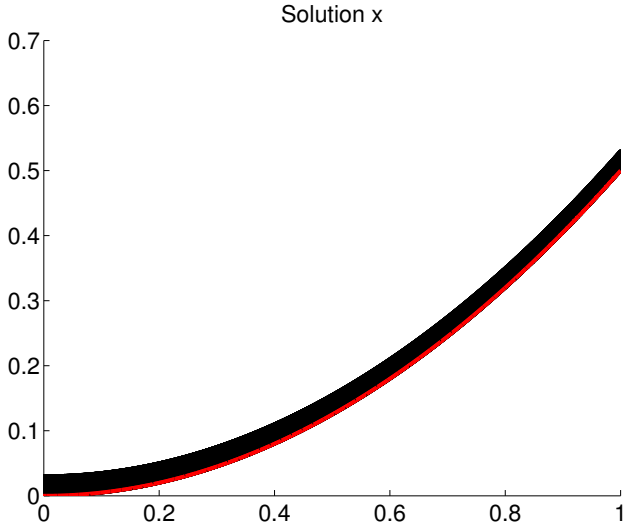


b) error in solution very small

But, the initial condition is...

maybe not exact (think about multistep method and only one starting point, or unknown initial condition)...Let us make inexact initial condition by perturbing it a bit (for a value 0.03)





a) error in slope very small [a] b) error in solution not very small!!

[a] because the slope does not depend on x in this example, i.e. $f = t$

Thus,

in order that the numerical scheme gives us the exact solution (i.e. convergent solution), following requirements have to satisfied

- the method has to be consistent,
- as well as stable on perturbation of initial conditions (i.e. zero stability)

convergence=consistency+zero stability

Convergence

Linear multistep method is known to be convergent if

$$\max_{t_n \in T} \|\epsilon_{glob}(t_n, h)\| \to 0, \quad h \to 0$$

The order of convergence is q if

$$\max_{t_n \in T} \|\epsilon_{glob}(t_n, h)\| \leqslant Ch^q$$

where

- the global error is
$$\epsilon_{glob} = x_a(t) - x(t)$$
- $x_a(t)$ is the exact solution of the differential equation $\dot{x} = f(t, x)$
- $x(t)$ is the approximate solution
- C is a constant independent of h

Convergence

Convergence implies consistency. Consistency does not imply convergence.

Last lecture: Proof

The approximation scheme has the form

$$\frac{1}{h}\sum_{i=0}^{k} a_i x_{n+i} = F(t, x_n, \ldots, x_{n+k}, h).$$

If the method converges to a solution z of the ODE for $h \to 0$, we obtain

$$x_n = x(nh) = x(t) \to z(t), \ldots, x_{n+k} = x(t+kh) \to z(t).$$

Last lecture: Proof

From this, it follows that for $h \to 0$

$$\sum_{i=0}^{k} a_i z(t) = \lim_{h \to 0} hF(t, x_n, \ldots, x_{n+k}, h) = 0,$$

and thus $\sum_{i=0}^{k} a_i = 0$. Also, one may conclude that

$$\sum_{i=0}^{k} a_i (x_{n+i} - x_n) = \sum_{i=0}^{k} a_i x_{n+i} - x_n \sum_{i=0}^{k} a_i = \sum_{i=0}^{k} a_i x_{n+i}$$

Hence, the original LMM can be rewritten as

$$\Longrightarrow \quad \frac{1}{h} \sum_{i=0}^{k} \frac{i}{i} a_i \left(x(t + ih) - x(t) \right) = F(t, x_n, \ldots, x_{n+k}, h).$$

Last lecture: Proof

Putting ih into the substruction one has

$$\Longrightarrow \quad \sum_{i=0}^{k} i a_i \frac{(x(t+ih) - x(t))}{ih} = F(t, x_n, \ldots, x_{n+k}, h).$$

Note that

$$\lim_{h \to 0} \frac{x(t+ih) - x(t)}{ih} = \dot{z}(t) = f(z, t).$$

Hence, for $h \to 0$ one obtains LMM

$$\sum_{i=0}^{k} a_i i \dot{z}(t) = \dot{z}(t) \sum_{i=0}^{k} a_i i = \dot{z}(t) \rho'(1) = F(t, z(t), \ldots, z(t), 0)$$

Last lecture: Proof

Following this one obtains consistency conditions:

$$\dot{\mathbf{z}}(t) = \mathbf{f}(t, \mathbf{z}(t)) = \mathbf{F}(t, \mathbf{z}(t), \ldots, \mathbf{z}(t), 0)/\rho'(1).$$

$$\sum_{i=0}^{k} a_i = \rho(1) = 0$$

Hence, the convergent method is also consistent.

Theorem

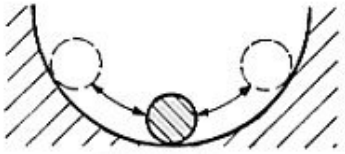
Theorem

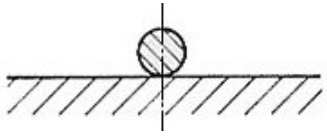
An integration scheme is convergent if and only if it is consistent and zero stable, and in case it is convergent, the order of consistency and the order of convergence are equal.

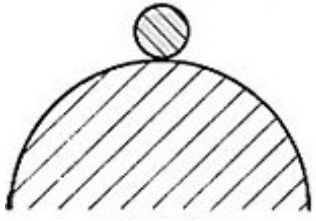
Zero stability

Assume that a system is in an equilibrium. If the system is now disturbed a little, one of the following may happen:

- The system might immediately return to the equilibrium. In this case, the equilibrium is called asymptotically stable.
- Or the system might move around in a neighborhood of the old equilibrium without returning to it but without moving far away neither. In this case, the equilibrium is stable but not asymptotically stable.
- The system might move far away from the old equilibrium. In this case, the equilibrium is instable.







Equilibria of first order ODE

The dynamical system is in equilibrium state x_* when the change of its state in time is equal to zero:

$$\frac{dx}{dt} = 0$$

The stability of x_* is judged according to the behaviour of intergal curves

$$x(t) = x(t_0) + \int_{t_0}^{t} x'(s)ds = x(t_0) + \int_{t_0}^{t} f(x(s), s)ds$$

obtained from the initial conditions x_0 which are in close vicinity of the equilibrium point $x_0 = x_* + \delta$ where δ is small perturbation.

Linear first order ODE

The equilibrium point of

$$\frac{dx}{dt} = ax, \quad x(t_0) = x_0$$

is

- stable and attractive if $a < 0$
- stable if $a = 0$
- unstable if $a > 0$
- in case of nonlinear ODE compute Jacobian and apply previous rules

Approximated ODE

As we studied before, ODE is sometimes difficult to solve algebraically. By applying numerical method to the ODE one obtains approximation, and hence the stability conditions change.

Example: linear multistep method

$$\sum_{j=0}^{k} a_j x_{n+j} = h \sum_{j=0}^{k} b_j f(t_{n+j}, x_{n+j}), \quad n = 0, \ldots, N-k$$

applied on ODE $\dot{x} = f(t, x)$ gives the stability condition

$$\dot{x} = 0 \rightarrow \sum_{j=0}^{k} a_j x_{n+j} = 0$$

which is **linear homogeneous difference equation.**

Linear homogeneous difference equation

The difference equation

$$\sum_{j=0}^{k} a_j x_{n+j} = 0$$

has for a general solution:

$$u_n = \sum_{i=1}^{r} p_i \xi_i^n,$$

where ξ_i are the roots of first characteristic polynomial

$$\rho(\xi) = \sum_{i=0}^{k} a_i \xi^i.$$

Hence, we need to study stability of difference equiation with respect to the zero (initial) conditions.

Stability of difference equation

Consider: general difference equation of order 1 and dimension d

$$\mathbf{x}_{n+1} = F(\mathbf{x}_n), \qquad \mathbf{x}_n \in \mathbb{R}^d,\ n \in \mathbb{N}.$$

Definition: An equilibrium point of the dynamical system

$$\mathbf{x}_{n+1} = F(\mathbf{x}_n), \qquad \mathbf{x}_n \in \mathbb{R}^d,\ n \in \mathbb{N}$$

is a state–vector $\mathbf{x}_* \in \mathbb{R}^d$ such that

$$F(\mathbf{x}_*) = \mathbf{x}_*$$

holds.

Stability of difference equation

Stability criteria: of $x_{n+1} = Ax_n$

- If all λ_i of A have absolute value smaller than one: $(\forall i = 1, \ldots, d : |\lambda_i| < 1)$, then for every $x_0 \in \mathbb{R}^d$ the sequence $x_n \overset{n\to\infty}{\longrightarrow} 0$, and x_* is asymptotically stable.
- If any λ_i of A has absolute value greater than one: $(\exists i : |\lambda_i| > 1)$ then there exist $x_0 \in \mathbb{R}^d$ such that the sequence $x_n \overset{n\to\infty}{\longrightarrow} \infty$, and x_* is unstable.
- If all λ_i of A have absolute value smaller or equal than one: $(\forall i = 1, \ldots, d : |\lambda_i| \leqslant 1)$ and if there are λ_j's with $|\lambda_j| = 1$, then we cannot decide whether or not x_* is stable.
- if the system is nonlinear then compute Jacobian and apply previous rules

Zero stability of approximated ODE

Another way of investigating stability of

$$\sum_{l=0}^{k} a_l x_{m+l} = 0$$

is to look at general solution:

$$u_m = \sum_{i=1}^{r} p_i \xi_i^m,$$

where ξ_i are the roots of ρ.

Zero stability of approximated ODE

A scheme satisfies the root condition (is zero stable) if every root ξ_i of the first characteristic polynomial ρ

$$\rho(\xi) = \sum_{i=0}^{k} a_i \xi^i.$$

has magnitude smaller than one, $|\xi_i| \leqslant 1$, and if every root ξ_i with $|\xi_i| = 1$ is a simple root of ρ.

Definition

Definition

In order for a consistent scheme to be convergent, a stability property has to be fulfilled:

A scheme satisfies the root condition (is zero stable) if every root ξ_i of the first characteristic polynomial ρ has magnitude smaller than one, $|\xi_i| \leqslant 1$, and if every root ξ_i with $|\xi_i| = 1$ is a simple root of ρ.

Theorem

Theorem

An integration scheme is convergent if and only if it is consistent and zero stable, and in case it is convergent, the order of consistency and the order of convergence are equal.

Exercise

The method

$$x_{n+1} = x_n + h\left(\frac{5}{12}f_{n+1} + \frac{8}{12}f_n - \frac{1}{12}f_{n-1}\right)$$

applied on

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

gives the stability condition

$$x_{n+1} - x_n = 0$$

i.e. characteristic equation

$$\xi - 1 = 0$$

The single root is equal to 1. Hence, the method is zero stable but not attractive.

Is zero-stability enough?

The next question to ask is if zero-stability is enough to obtain convergence and accuracy (**namely, the method can converge, but to the wrong solution!!**). Let us observe the numerical integration of the following two systems by explicit Euler method:

$$\dot{x} = -2000x, \quad x(0) = 1$$

and

$$\dot{x} = -x, \quad x(0) = 1$$

with the time step size $h = 10^{-3}$ in the time interval $[0, 2]$.

Convergence

Before integration let us check if the method is

1. consistent:

$$\rho(\xi) = \xi - 1 \Rightarrow \rho(1) = 0, \rho'(1) = 1$$

,

$$F = f_n \Rightarrow f = \frac{F}{\rho'(1)}$$

2. zero stable

$$\rho(\xi) = \xi - 1 = 0 \Rightarrow \xi = 1$$

Hence, the method is consistent and zero stable, and thus the method is convergent when $h \to 0$.

Convergence

By comparing numerical results one obtains

Case	Truth	Numerical	Relative error
Case I	0.1353	0.1352	0.001
Case II	1.383e-87	3.055e-92	0.999

This table shows that even the step size was taken to be almost equal to zero, the relative error can be still huge (99% in second case). But the method is convergent?

Convergence

The method is convergent as can be seen in the following table because the error goes to zero when the time step size decreases.

Case	Case I	Case II
h=1	1	7.08e+90
h=0.1	0.1017	8.78e+105
h=1e-3	0.001	0.9999
h=1e-6	$\approx$1e-6	0.00995

Since one cannot adopt too small h, the question is now:

When to stop? Which step size is small enough to give us desried accuracy?

Global convergence

To answer this one, first the global error has to be studied:

$$\epsilon_{glob}^{n+1} = x_a(t_{n+1}) - x(t_{n+1})$$

in which x_a is analytical and x full numerical solution. Having in mind that

$$x(t_{n+1}) = x(t_n) + hf(t_n, x_n) = x(t_n) + h\lambda x_n, \quad n = 0, 1, 2, \ldots$$

one may write

$$\epsilon_{glob}^{n+1} = x_a(t_{n+1}) - x(t_n) - h\lambda x_n$$

Global convergence

Expanding x_a into Taylor serie

$$x_a(t_{n+1}) = x_a(t_n) + h\dot{x}_a(t_n) + \frac{h^2}{2}\ddot{x}_a + h.o.t.$$

one obtains

$$\epsilon_{glob}^{n+1} = x_a(t_n) + h\dot{x}_a(t_n) + \frac{h^2}{2}\ddot{x}_a - x_n - h\lambda x_n$$

Here, the first derivative is known from given ODE

$$\dot{x}_a(t_n) = \lambda x_a(t_n)$$

Global convergence

This finally gives expression for the global error

$$\epsilon_{glob}^{n+1} = x_a(t_n) + h\lambda x_a(t_n) + \frac{h^2}{2}\ddot{x}_a - x_n - h\lambda x_n + h.o.t.$$

Collecting terms together one obtains

$$\epsilon_{glob}^{n+1} = (1 + h\lambda)(x_a(t_n) - x_n) + \frac{h^2}{2}\ddot{x}_a + h.o.t.$$

$$\epsilon_{glob}^{n+1} = (1 + h\lambda)\epsilon_{glob}^{n} + \frac{h^2}{2}\ddot{x}_a$$

Note that in last relation the term $\frac{h^2}{2}\ddot{x}_a$ represents the local error

$$\epsilon_{loc} = \frac{h^2}{2}\ddot{x}_a$$

Global convergence

Looking at

$$\epsilon_{glob}^{n+1} = (1 + h\lambda)\epsilon_{glob}^{n} + \epsilon_{loc}$$

one may conclude that the global error in $n+1$ step does not only dependend on the currecnt local error ϵ_{loc} but also on the propagated error from the previous step $(1 + h\lambda)\epsilon_{glob}^{n}$. This error gets multiplied by $(1 + h\lambda)$, and hence the behaviour of ϵ_{glob} in time will be driven by λ (given model we cannot change) and the step size h (one can modify). After n steps the global error is proportional to

$$(1 + h\lambda)^n$$

and is driven by power law of n.

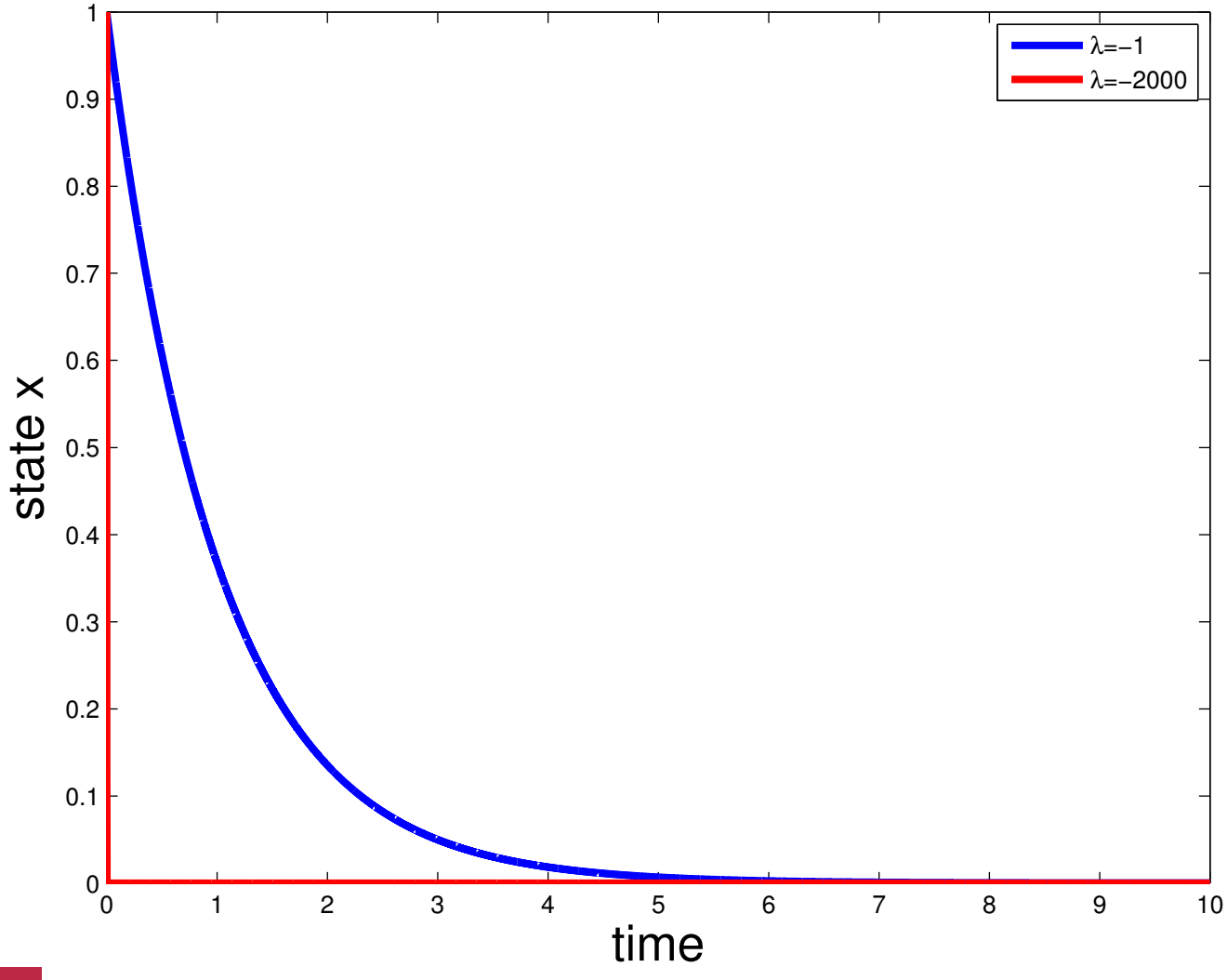
Global convergence

In our examples this means

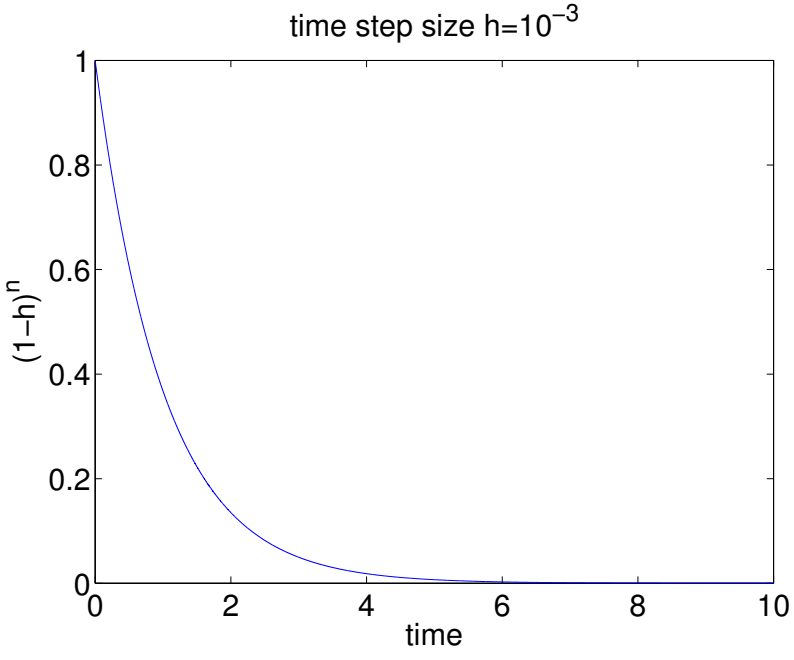
$$(1 + h\lambda)^n \Rightarrow (1 - h)^n \quad \text{or} \quad (1 - 2000h)^n$$

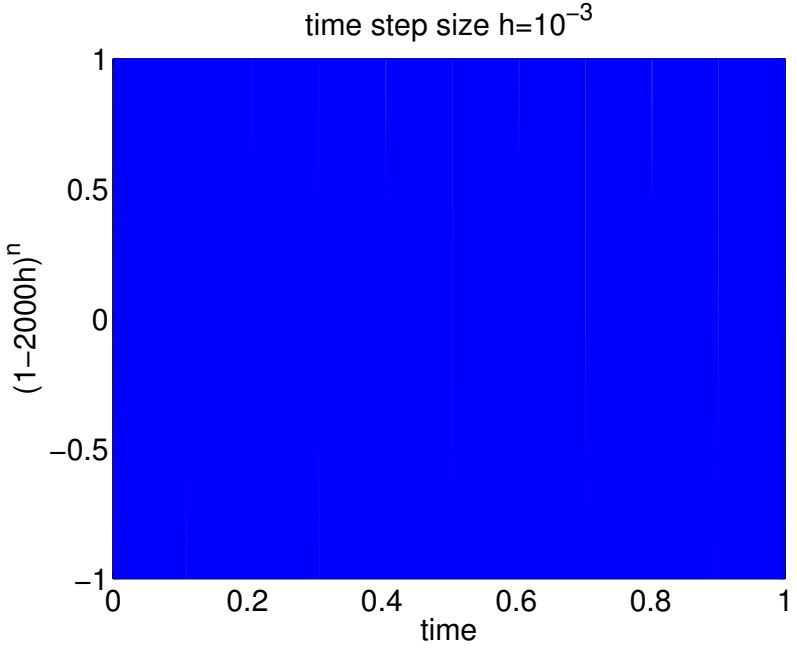
However, as both $1-h$ and $1-2000h$ are smaller than 1 by absolute value (for $h = 10^{-6}$), the global error will converge to zero (this corresponds to the exact solution) with $n \to \infty$. However, for $h = 10^{-3}$, the first term will converge to zero whereas the other not. Reason is higher value of λ in second ODE. One may show that the higher the value of λ is, the more difficult is to integrate. In other words ODE becomes stiffer. Unfortunately, most of practical examples are considered to be stiff. Due to this reason, this will be the main subject of ODE2!!

Non-stiff vs stiff - response

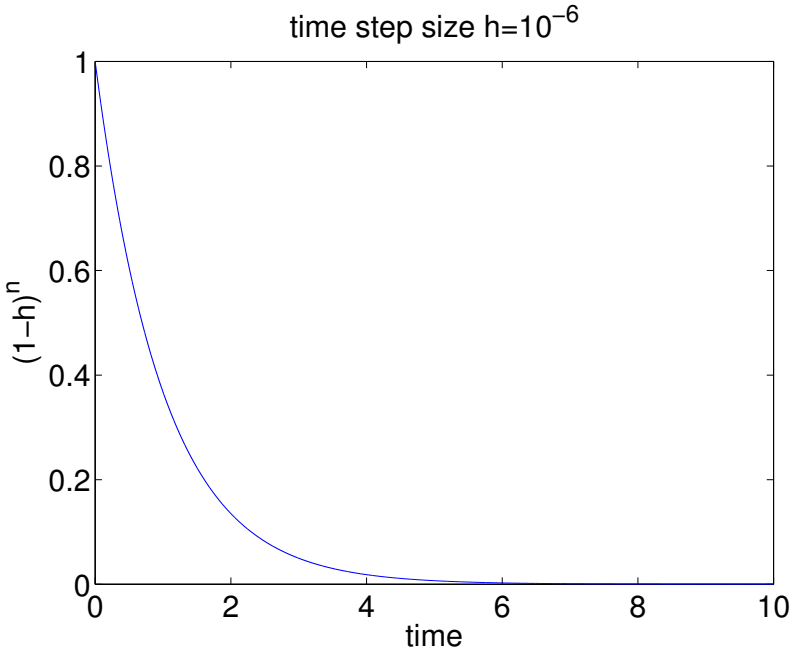


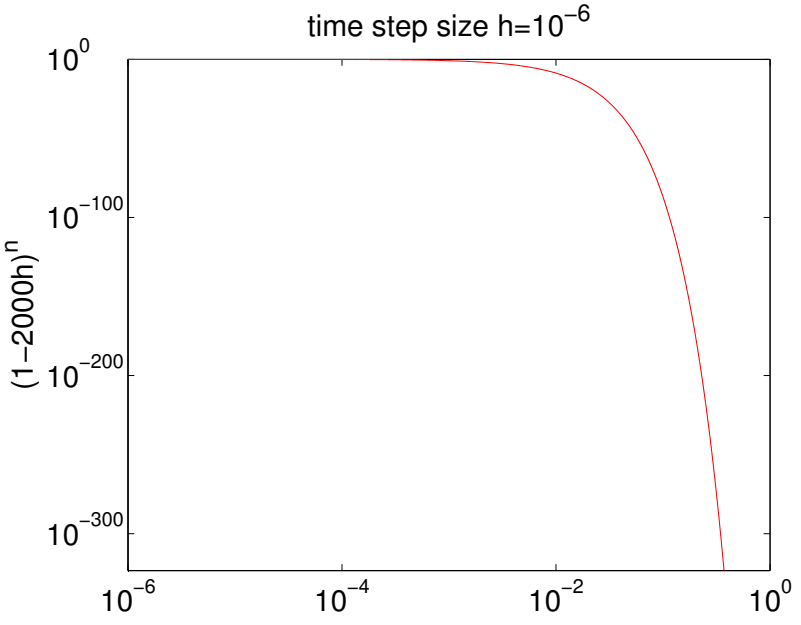
Non-stiff vs stiff $(1+\lambda h)^n$





Non-stiff vs stiff $(1+\lambda h)^n$





Global convergence

After previous observations have been made, one may give the following conclusion:

In order to get convergent and accurate method for some system ($\dot{x} = \lambda x$), one has to study its stability with respect to the time step size (i.e. stability of numerical method=difference equation)

Absolute Stability

To judge if the numerical method with the desired $h > 0$ is accurate enough, the term of absolute stability is introduced. This stability is tested on the Dahlquist problem:

$$\dot{x} = \lambda x, \quad x(0) = 1$$

whose exact solution is

$$x = \exp(\lambda t)$$

$$\lim_{t \to \infty} |x(t)| = \begin{cases} 0, & \text{if } \lambda < 0 \\ 1, & \text{if } \lambda = 0 \\ \infty, & \text{if } \lambda > 0 \end{cases}$$

We are interested in the case $\lambda < 0$. In this case the ODE is assymptotically stable.

Absolute Stability

Why we study Dahlquist problem?

Because any system can be represented as a linear system of ODEs. In case that you study nonlinear ODE then linearise and observe Jacobian.

Absolute Stability

If the previous ODE is solved by explicit Euler method, then one obtains numerical solution in a form

$$x_{n+1} = x_n + h\lambda x_n = (1 + h\lambda)x_n \Rightarrow x_n = (1 + h\lambda)^n x_0$$

This difference equation is stable when

$$|1 + h\lambda| \leqslant 1$$

Hence, one obtains restirction on the step size

$$-2 \leqslant h\lambda \leqslant 0$$

Absolute Stability

It is common practice to speak about absolute stability in the region of complex z plane

$$z = h\lambda$$

instead in terms of the step size. This allows λ to be complex.

Allowing λ to be complex comes from the fact that in practice we are usually solving a system of ordinary differential equations (ODEs). In the linear case it is the eigenvalues of the coefficient matrix that are important in determining stability. In the nonlinear case we typically linearize and consider the eigenvalues of the Jacobian matrix. Hence λ represents a typical eigenvalue and these may be complex even if the matrix is real.

Absolute Stability

Thus, to get absolutely stable method it must be satisfied

$$|R(z)| \leqslant 1$$

in which

$$R(z) = 1 + z$$

What if we have general linear multistep method?

Absolute Stability

When general linear multistep method

$$\sum_{j=0}^{k} a_j x_{n+j} = h \sum_{j=0}^{k} b_j f(t_{n+j}, x_{n+j})$$

is applied on

$$\dot{x} = \lambda x$$

one obtains

$$\sum_{j=0}^{k} a_j x_{n+j} = h \sum_{j=0}^{k} b_j \lambda x_{n+j}$$

Absolute Stability

i.e.

$$\sum_{j=0}^{k} (a_j - h\lambda b_j) x_{n+j} = 0$$

which is difference equation. Its stability is given by the roots of characteristic polynomial

$$\rho(\xi) - z\sigma(\xi) = 0$$

in which

$$\rho(\xi) = \sum_{j=0}^{k} a_j \xi^j, \quad \sigma(\xi) = \sum_{j=0}^{k} b_j \xi^j$$

Absolute Stability

The difference equation is stable if roots

$$\rho(\xi) - z\sigma(\xi) = 0$$

are smaller by amplitude than 1, or eventually only one of them is equal to 1. With respect to this one defines

Definition

The region of absolute stability for the LMM is the set of points z in the complex plane for which the polynomial $\rho(\xi) - z\sigma(\xi) = 0$ satisfies the root condition.

$$G_s := \{z \in \mathbb{C} \ : \ |\xi(z)| \leqslant 1\}$$

Example

For Euler method

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

one has

$$x_{n+1} - x_n \Rightarrow \rho(\xi) = \xi - 1$$

and

$$h\lambda x_n \Rightarrow z\sigma(\xi) = z$$

Thus

$$\rho(\xi) - z\sigma(\xi) = 0$$

$$\xi - 1 - z = 0 \Rightarrow \xi_1 = 1 + z = R(z)$$

From this follows stability region

$$G_s := \{z \in \mathbb{C} \ : \ |1 + z| \leqslant 1\}$$

Example

To plot the previous region, one has to notice the following: z on boundary of the stability region gives the root ξ of absolute value equal to 1. In polar coordinates this means that

$$\xi = e^{i\theta}, \quad \theta \in [0, 2\pi]$$

Since this is the root of

$$\rho(\xi) - z\sigma(\xi) = 0$$

one has

$$\rho(e^{i\theta}) - z\sigma(e^{i\theta}) = 0$$

and hence

$$z = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}$$

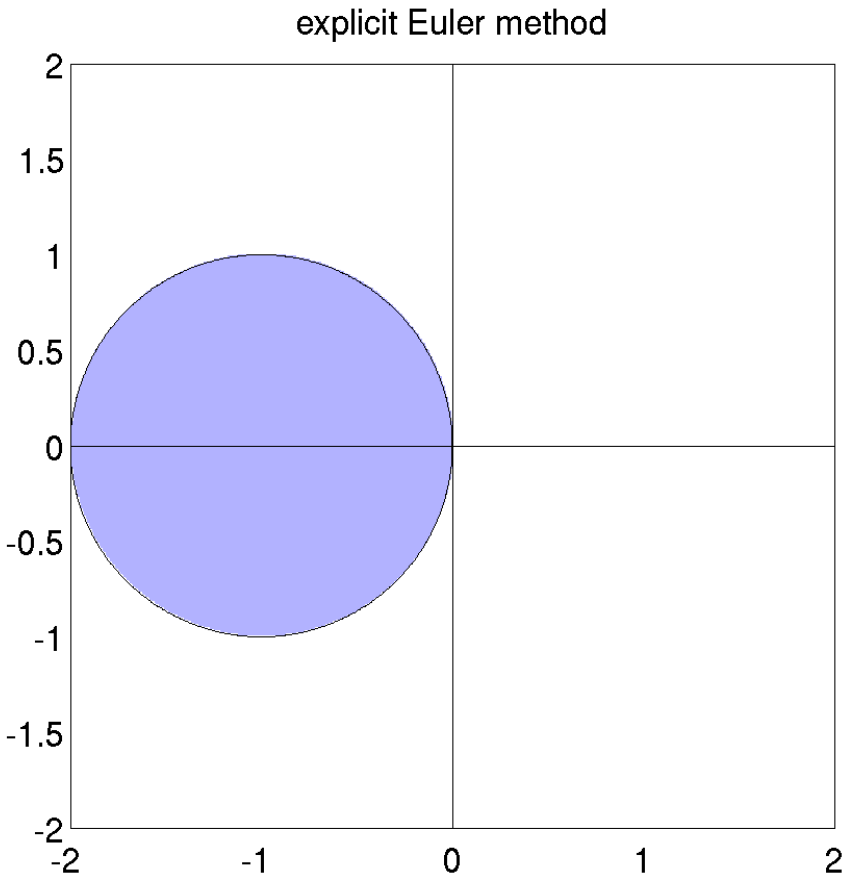
Example

Another way to draw this in Matlab is

```
nptsx = 501;
nptsy = 501;
x = linspace(xa,xb,nptsx);
y = linspace(ya,yb,nptsy);
[X,Y] = meshgrid(x,y);
Z = X + 1i*Y;
Rval = feval(R,Z);
```

in which $R(z) = \rho(\xi) - z\sigma(\xi)$.

Example



Example

For implicit Euler method

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

one has

$$x_{n+1} - x_n \Rightarrow \rho(\xi) = \xi - 1$$

and

$$h\lambda x_{n+1} \Rightarrow z\sigma(\xi) = z\xi$$

Thus

$$\rho(\xi) - z\sigma(\xi) = 0$$

$$\xi - 1 - z\xi = 0 \Rightarrow \xi_1 = \frac{1}{1-z} = R(z)$$

From this follows stability region

$$G_s := \{z \in \mathbb{C} \ : \ |\frac{1}{1-z}| \leqslant 1\}$$

Example