A-Stability

example: chemical reactions (Robertson 1966)

- catalytic reactions:

$$
\begin{aligned}
A &\rightarrow B \\
2B &\rightarrow B + C \\
B + C &\rightarrow A + C
\end{aligned}
$$

autocatalytic

- A converts to B which converts to C which drives conversion of B to A
- kinetic rate equations:

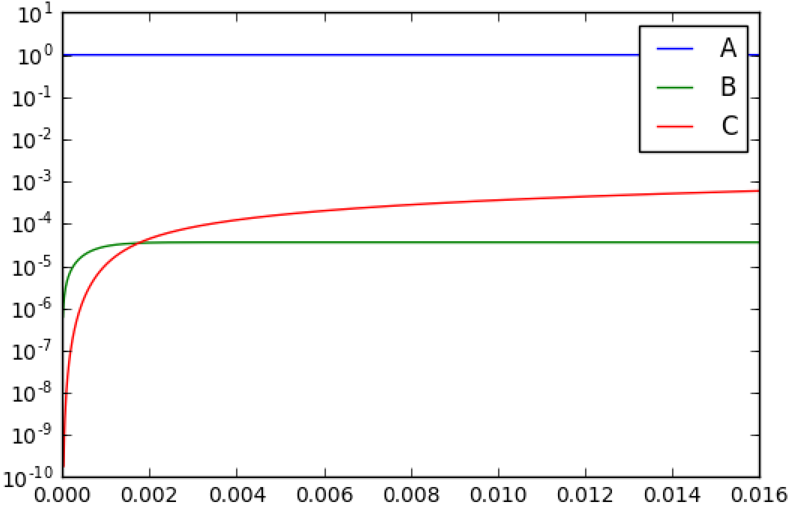
$$
\begin{aligned}
\frac{du_1}{dt} &= -0.04u_1 + 10^4 u_2 u_3 \\
\frac{du_2}{dt} &= 0.04u_1 - 3 \cdot 10^7 u_2^2 - 10^4 u_2 u_3 \\
\frac{du_3}{dt} &= 3 \cdot 10^7 u_2^2
\end{aligned}
$$

u_1, u_2 and u_3 are concentrations of A, B and C, respectively

numerical solution – short time T and small step h

```
def f(t,u): # Robertson reaction
    du = u.copy()
    du[0] = -0.04*u[0]                    + 10**4*u[1]*u[2]
    du[1] =  0.04*u[0] -3*10**7*u[1]**2 - 10**4*u[1]*u[2]
    du[2] =             3*10**7*u[1]**2
    return(du)
phi = f  # Euler
n  = 1024; T=0.016; h = T/n
tk = np.linspace(0,T,n+1)
uk = np.zeros((n+1,3))
uk[0,0] = 1.0
for j in range(n):
    uk[j+1,:] = uk[j,:] + h*phi(j*h,uk[j,:])
```

```
plt.semilogy(tk,uk[:,0],label='A')
plt.semilogy(tk,uk[:,1],label='B')
plt.semilogy(tk,uk[:,2],label='C')
plt.axis(ymax=10)
plt.legend();
```



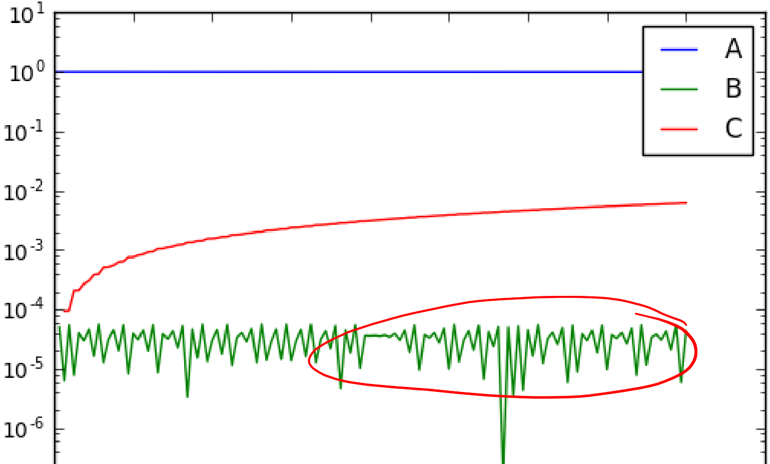
larger time T and step size h

- larger step size to reduce computational time

```
n  = 128; T=0.16; h = T/n
tk = np.linspace(0,T,n+1)
uk = np.zeros((n+1,3))
uk[0,0] = 1.0
for j in range(n):
    uk[j+1,:] = uk[j,:] + h*phi(j*h,uk[j,:])
```

- larger step sizes introduce (numerical) fluctuations

```
plt.semilogy(tk,uk[:,0],label='A')
plt.semilogy(tk,abs(uk[:,1]),label='B')
plt.semilogy(tk,uk[:,2],label='C')
plt.axis(ymax=10)
plt.legend();
```



Stability of solutions of ODEs

- ODE

$$\frac{du}{dt} = f(t, u)$$

Definition (stable solution)
A solution $u(t)$ of the ODE is stable if for some $\epsilon > 0$ and all solutions $v(t)$ of the ODE with $\|v(0) - u(0)\| \leq \epsilon$ the difference $v(t) - u(t)$ is bounded.
Example For $t \in \mathbb{R}_+$ and the differential equation

$$\frac{du}{dt} = -u \qquad u(t) = u_0 e^{-t}$$

any solution $u(t)$ is stable.

Definition (unstable solution)
A solution $u(t)$ of the ODE is unstable if for all $\epsilon > 0$ there exists a solution $v(t)$ of the ODE with $\|v(0) - u(0)\| \leq \epsilon$ such that the difference $v(t) - u(t)$ is unbounded.
Example For $t \in \mathbb{R}_+$ and the differential equation

$$\frac{du}{dt} = u$$

any solution $u(t)$ is unstable.
Definition (asymptotically stable solution) *A solution $u(t)$ of the ODE is asymptotically stable if for some $\epsilon > 0$ and all solutions $v(t)$ of the ODE with $\|v(0) - u(0)\| \leq \epsilon$ one has* $\lim_{t\to\infty}\|u(t) - v(t)\| = 0$.

perturbation analysis of stable solutions of ODEs

- consider a family of solutions $u_\epsilon(t) = u(t) + \epsilon v(t)$ which all satisfy the same ODE

$$\frac{du_\epsilon}{dt} = f(t, u_\epsilon) \qquad \frac{du}{dt} = f(t,u)$$

  where u is an asymptotically stable solution
- as $v(t)$ is bounded one has, for twice continuously differentiable f the Taylor expansion

$$f(t, u_\epsilon) = f(t, u) + \epsilon f_u(t, u) v + O(\epsilon^2)$$

- it follows that v satisfies approximately the linear ODE

$$\boxed{\frac{dv}{dt} = f_u(t, u) v}$$

Jacobi matrix

  and consequently, the solutions of this ODE with sufficiently small initial values have to be bounded if the solution $u(t)$ is stable

- if for $t \to \infty$ one has $f_u(t,u) \to \lambda$ then all solutions of

$$\boxed{\frac{dv}{dt} = \lambda v}$$

  have to be asymptotically stable and thus $\lambda < 0$
- when considering multiple variables $f_u(t,u)$ is the Jacobi matrix then think of λ as a (complex) eigenvalue and $u(t) \in \mathbb{C}$
- this motivates the study of the numerical solution of

$$du/dt = \lambda u$$

  and $u(t) \in \mathbb{C}$

$$u(t) = e^{\lambda t} u(0)$$

amplification factor

- consider family of complex ODEs with $\boxed{f(t,u) = \lambda u}$

$$\boxed{\frac{du}{dt} = \lambda u} \quad (*)$$

- all one-step methods considered construct $\phi(t,u)$ through compositions of linear combinations of evaluations of f
- it follows that for for the family of ODEs considered one has

$$\boxed{u_{k+1} = \rho(\lambda h) u_k}$$

where $\rho(z)$ is a polynomial with real coefficients and $\rho(0) = 1$ for the (explicit) one-step methods
- in the following we will also consider *implicit methods* for which $\rho(z)$ is a rational function
- $\rho(\lambda h)$ is the *amplification factor* and

$$\boxed{u_k = \rho(\lambda h)^k u_0}$$

A-stability

- the ODEs considered are asymptotically stable if $\boxed{\mathrm{Re}(\lambda) < 0}$ and in this case the exact solution $u(t)$ satisfies

$$\boxed{u(t) \to 0, \quad t \to \infty}$$

$e^{\lambda t} = e^{\lambda_R t} \cdot e^{i\lambda_I t}$

- we say that a one-step method is *A-stable* if

$$\boxed{u_k \to 0, \quad k \to \infty}$$

$\left(\frac{1}{4}\right)^k \to 0$

and this is the case

$$\boxed{|\rho(\lambda h)| < 1}$$

$\left(\frac{1}{4} \cdot i\right)^k \to 0$

- the *region of A-stability* of a one-step method is

$$\Omega = \{z \in \mathbb{C} \mid |\rho(z)| < 1\}$$

$z = \lambda h$

A-stability of Euler's method

- Euler's method for the ODEs considered gives

$$u_{k+1} = (1 + \lambda h)u_k = u_k + h\underbrace{f(t,u)}_{= \lambda u}$$

- amplification factor for Euler

$$\rho(z) = 1 + z$$

- region of A-stability

$$\Omega = \{z \mid |1 + z| < 1\}$$

is a circle in the complex plane with radius 1 and centre -1

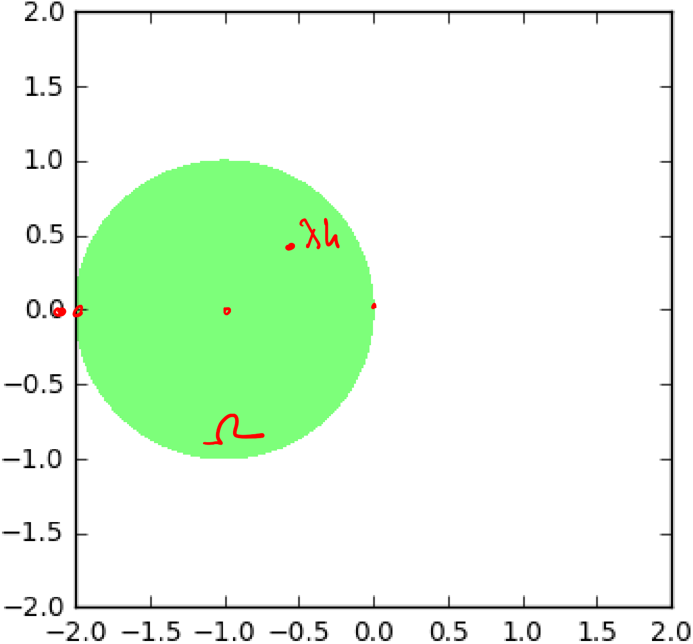
plotting the region of A-stability of Euler's method

```
xg = np.linspace(-2,2,100)
yg = np.linspace(-2,2,100)
X, Y = np.meshgrid(xg,yg)
Rho = np.sqrt((1+X)**2 + Y**2)
```

$$= \mathrm{abs}(\underbrace{X+iY}_{z})$$

$$|1+z|$$

```
plt.contourf(X,Y,Rho,[0.0,1.0,]); plt.axis('square');
```



A-stability and choice of h for $du/dt = \lambda u$ with $\lambda < 0$

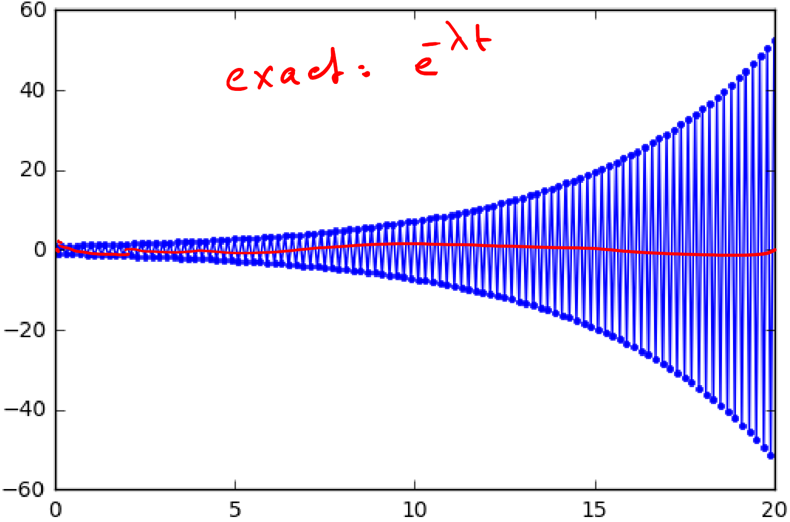
- convergence for small h and unstability for large h

```
f = lambda t, u, lam=-20.2 : lam*u
phi = f # Euler
n = 200; h=0.1; T = n*h;
tk = np.linspace(0,T,n+1)
uk = np.ones(n+1)
for k in range(0,n):
    uk[k+1] = uk[k] + h*phi(k,uk[k])
```

$h\lambda = -2.02$

- $\lambda h = -2.02$ (just) outside region of A-stability

```
plt.plot(tk,uk,'.-');
```



backward Euler method

- also implicit Euler method as rhs depends on u_{k+1}

$$u_{k+1} = u_k + hf(t_{k+1}, u_{k+1})$$

- numerical solution, typically iterative method

$$\begin{aligned} u_{k+1}^0 &= u_k \\ u_{k+1}^{j+1} &= \alpha u_{k+1}^j + (1-\alpha)(u_k + hf(t_{k+1}, u_{k+1}^j)), \quad j = 0, \dots, m \end{aligned}$$

- for the iteration we choose a relaxed fixed point iteration (sometimes called corrector) with $\alpha \in [0, 1]$

$\alpha = 0.5$ 0.9

amplification factor for backward Euler

- one-step for model problem

$$u_{k+1} = u_k + \lambda h u_{k+1}$$

$h f(t_{k+1}, u_{k+1}) = h \lambda u_{k+1}$

- solve

$$u_{k+1} = \frac{1}{1 - \lambda h} u_k$$

- amplification factor

$$\boxed{\rho(z) = \frac{1}{1 - z}}$$

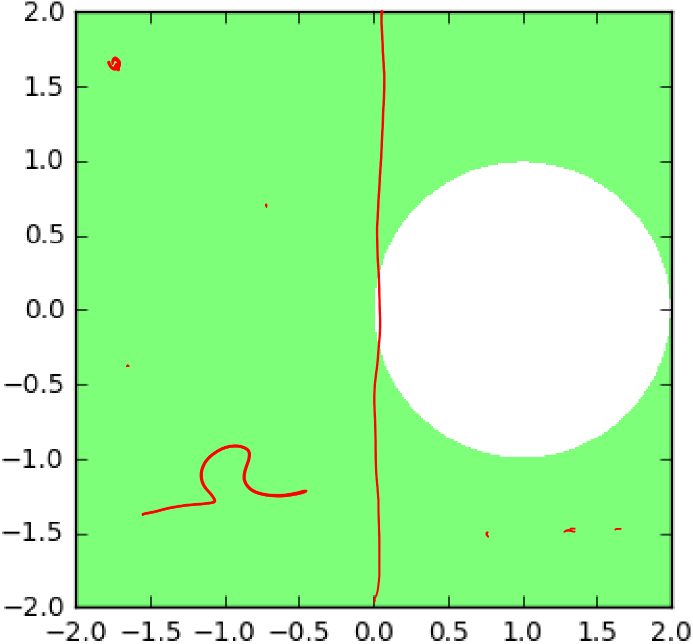
- the iterative solver gives a slightly different amplification factor which should be investigated ...

plotting the region of A-stability for backward Euler

- backward Euler is unconditionally (for all h) A-stable for all λ with $\mathrm{Re}(\lambda) < 0$

```
xg = np.linspace(-2,2,100)
yg = np.linspace(-2,2,100)
X, Y = np.meshgrid(xg,yg)
Rho = 1.0/np.sqrt((1-X)**2 + Y**2)
```

```python
plt.contourf(X,Y,Rho,[0.0,1.0,]); plt.axis('square');
```



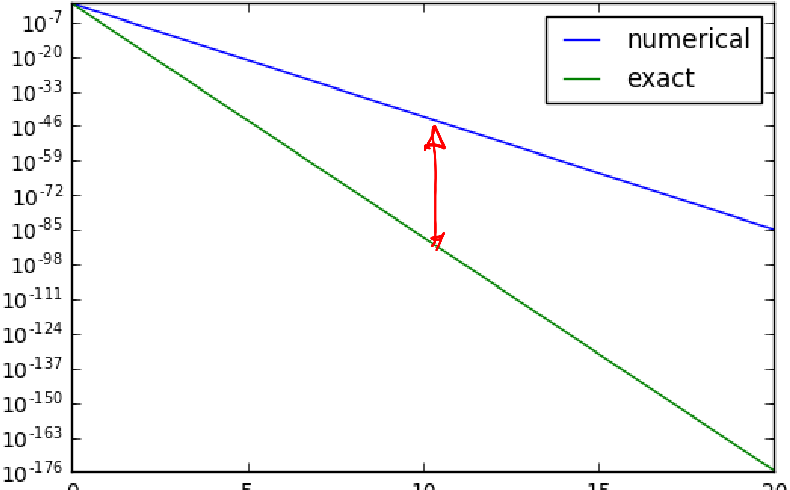
previous example with backward Euler

- convergence for small h and unstability for large h

```
lam=-20.2
f = lambda t, u, lam = lam : lam*u
phi = f # Euler forward
n = 200; h=0.1; T = n*h; m=4; alpha=0.5
tk = np.linspace(0,T,n+1)
uk = np.ones(n+1)
for k in range(0,n):
    ukp1 = uk[k]
    for j in range(m): # corrector: relaxed fixpoint
        ukp1 = alpha*ukp1 + (1-alpha)*(uk[k] + h*phi(k,ukp1
    uk[k+1] = ukp1
```

- solution decreasing (with error)

```
plt.semilogy(tk,uk, label='numerical')
plt.semilogy(tk,np.exp(lam*tk), label='exact')
plt.legend();
```



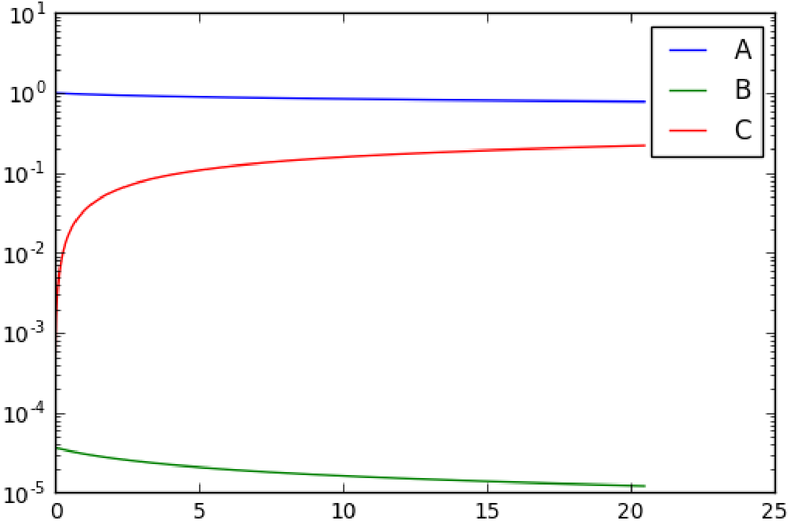
backward Euler for Robertson example

```
def f(t,u): # Robertson reaction
    du = u.copy()
    du[0] = -0.04*u[0]                       + 10**4*u[1]*u[2]
    du[1] =  0.04*u[0] -3*10**7*u[1]**2 - 10**4*u[1]*u[2]
    du[2] =             3*10**7*u[1]**2
    return(du)
phi = f  # Euler
s=128; n  = s*32; T=s*0.16; h = T/n
m = 10; alpha = 0.1
tk = np.linspace(0,T,n+1)
uk = np.zeros((n+1,3))
uk[0,0] = 1.0
for j in range(n):
    ukp1 = uk[j,:]
    for i in range(m):
        ukp1 = (1-alpha)*ukp1 + alpha*(uk[j,:] + h*phi(j*h
    uk[j+1,:] = uk[j,:] + h*phi(j*h,ukp1)
```

- fluctuations in B disappear even for large T

```
def plotting():
    plt.semilogy(tk,uk[:,0],label='A')
    plt.semilogy(tk,abs(uk[:,1]),label='B')
    plt.semilogy(tk,uk[:,2],label='C')
    plt.axis(ymax=10)
    plt.legend();
```

plotting()



amplification factor for Runge-Kutta

- recall: 2 stages of Runge-Kutta
  - stage 1:

$$U_k^j = u_k + h \sum_{i=1}^{m} b_{ji}\, f(s_i, U_k^i), \quad j = 1, \ldots, m$$

  - stage 2:

$$u_{k+1} = u_k + h \sum_{j=1}^{m} c_j\, \cancel{U_k^j}\, f(s_j, U_k^j)$$

- stage 1: define $\rho_j(z)$ for every U_k^j:

$$\rho_j(z) = 1 + z \sum_{i=1}^{m} b_{ji}\, \rho_i(z)$$

  - one needs to solve this system of equations for ρ_j
- stage 2:

$$\rho(z) = 1 + z \sum_{j=1}^{m} c_j\, \rho_j(z)$$

example 2: Heun's method

$$B = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad c^T = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}$$

- first stage
  - $\rho_1(z) = 1$ and $\rho_2(\lambda h) = 1 + z$
- second stage

$$\rho(z) = 1 + 0.5z + 0.5z(1 + z) = 1 + z + z^2/2$$

example 3: midpoint method

$$B = \begin{bmatrix} 0 & 0 \\ 0.5 & 0 \end{bmatrix}, \quad c^T = \begin{bmatrix} 0 & 1 \end{bmatrix}$$

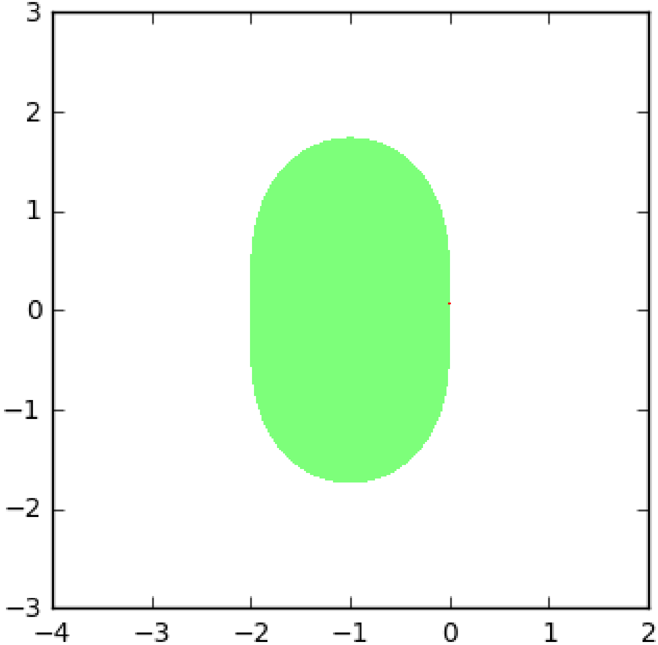
- first stage
  - $\rho_1(z) = 1$ and $\rho_2(z) = 1 + z/2$
- second stage

$$\rho(z) = 1 + z(1 + z/2) = 1 + z + z^2/2$$

region of A-stability for Heun and midpoint method

```
xg = np.linspace(-4,2,100)
yg = np.linspace(-3,3,100)
X, Y = np.meshgrid(xg,yg)
Rho = np.sqrt((1+X+(X*X-Y*Y)/2)**2 + (Y+X*Y)**2)
```

```
plt.contourf(X,Y,Rho,[0.0,1.0,]); plt.axis('square');
```



example 4: fourth order Runge Kutta method

$$B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad c^T = \frac{1}{6}\begin{bmatrix} 1 & 2 & 2 & 1 \end{bmatrix}$$

- first stage

$$\begin{aligned} \rho_1(z) &= 1 \\ \rho_2(z) &= 1 + z/2 \\ \rho_3(z) &= 1 + z/2 + z^2/4 \\ \rho_4(z) &= 1 + z + z^2/2 + z^3/4 \end{aligned}$$

- second stage

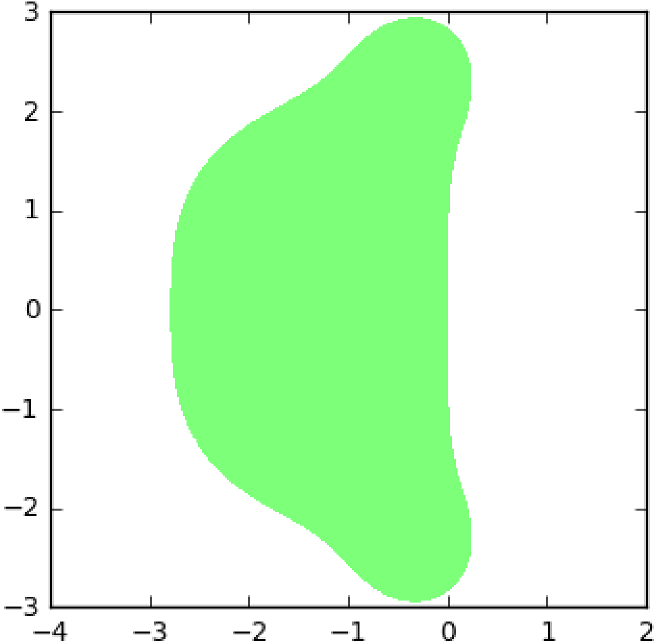
$$\rho(z) = 1 + z + z^2/2 + z^3/6 + z^4/24$$

plot A-stability region for Runge-Kutta

```
xg = np.linspace(-4,2,100)
yg = np.linspace(-3,3,100)
X, Y = np.meshgrid(xg,yg)
Z = X + Y*1j
Rho = abs(1+Z+Z**2/2+Z**3/6+Z**4/24)
```

Python $\sqrt{-1}$

```
plt.contourf(X,Y,Rho,[0.0,1.0,]); plt.axis('square');
```



example 5: trapezoidal rule

$$u(t_{k+1}) = u(t_k) + \int_{t_k}^{t_{k+1}} f(s, u(s))\,ds$$

$$\frac{h}{2}\left(f(t_k, u(t_k)) + f(t_{k+1}, u(t_{k+1}))\right)$$

- implicit method:

$$u_{k+1} = u_k + 0.5\lambda\, h(u_k + u_{k+1})$$

- solve

$$u_{k+1} = \frac{1 + \lambda h/2}{1 - \lambda h/2} u_k$$

- amplification factor

$$\rho(z) = \frac{1 + z/2}{1 - z/2}$$

- $|\rho(z)| < 1$ for all z with $\mathrm{Re}(z) < 0$ and larger than 1 else

plot A-stability region for (implicit) trapezoidal rule

```
xg = np.linspace(-4,2,100)
yg = np.linspace(-3,3,100)
X, Y = np.meshgrid(xg,yg)
Z = X + Y*1j
Rho = abs((1+Z/2)/(1-Z/2))
```

```
plt.contourf(X,Y,Rho,[0.0,1.0,]); plt.axis('square');
```