THE UNIVERSITY OF TEXAS AT DALLAS

ERIK JONSSON SCHOOL OF ENGINEERING & COMPUTER SCIENCE

ORDINARY DIFFERENTIAL EQUATIONS

Notes prepared for EE 6481

by

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ORDINARY DIFFERENTIAL EQUATIONS (1)

- Solution of an ordinary differential equation (ODE)
  - ▷ The differential equation determines a family of functions
  - ▷ Boundary or initial conditions pick out one function from the family
- Classes of ODEs
  - ▷ Order of an ODE: The order of the highest derivative
  - ▷ Initial-value problem: An order-m ODE for which the values of the unknown function and its first $m-1$ derivatives are given at x_0
    - ∘ Example of an initial-value problem:

$$\text{Equation: } \frac{dy}{dx} = 5y \qquad \text{Initial condition: } y(0) = 10$$

$$\text{Solution: } y(x) = 10e^{5x}$$

  - ▷ Boundary-value problem: An ODE for an unknown function, plus prescribed values of the function on the boundary of its domain

ORDINARY DIFFERENTIAL EQUATIONS (2)

- We'll study intial-value problems involving ODEs of the form

$$\frac{dy}{dx} = f(x, y)$$

  where f is not necessarily linear

  - ▷ Limiting ourselves to first-order equations is not very restrictive
  - ▷ An order-m ODE is equivalent to a system of 1st-order ODEs
    - Example for $m = 2$: The ODE

$$\frac{d^2y}{dx^2} = g(x, y)$$

      is equivalent to the system of two 1st-order ODEs

$$\frac{dy}{dx} = y'$$
$$\frac{dy'}{dx} = g(x, y)$$

EULER'S METHOD (1)

- Introduction to Euler's method for solving $y' = f(x, y)$:
  - ▷ Textbook definition of derivative:

$$\frac{dy}{dx}(x) = \lim_{h \to 0} \frac{y(x+h) - y(x)}{h}$$

- ◦ Approximation using a difference quotient:

$$\frac{y(x+h) - y(x)}{h} \approx \text{numerical estimate of derivative}$$
$$\approx f(x, y(x))$$

- ◦ Algorithm for computing an approximate value for $y(x_n + h)$ given c_n = computed value of $y(x_n)$ (**Euler's method**):

$$\boxed{c_{n+1} = c_n + h f(x_n,\, c_n)}$$

- ◦ Euler's algorithm is *explicit* (the value to be computed, c_{n+1}, does not appear in f)

EULER'S METHOD (2)

- Analysis of the accuracy of Euler's method for solving $y' = f(x, y)$:
  - ▷ The accuracy of a computed solution depends on the function f
  - ▷ Since

$$f(x,\, y) = f(x,\, y_0) + (y - y_0)\frac{\partial f}{\partial y} + O((y - y_0)^2)$$

    a **test problem** for studying the growth of the computed solution is

$$f(x, y) = ay(x) \;\Rightarrow\; f(x_n, c_n) = ac_n$$

    - ◦ We know the exact solution of the initial-value problem: $y(x) = y(0)\, e^{ax}$
    - ◦ The solution c_{n+1}, for one step, computed using Euler's method given the value c_n at the beginning of the step, is determined by the equation

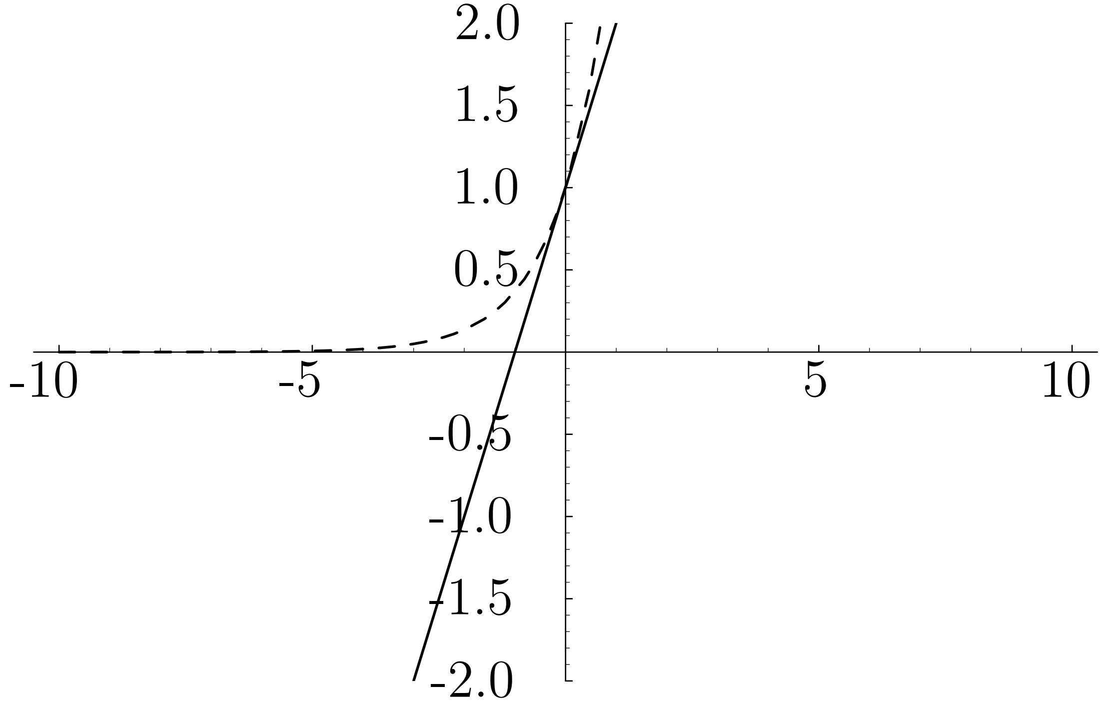
$$c_{n+1} = c_n + hf(x_n, c_n) = c_n(1 + ha) \Rightarrow c_{n+1} = (1 + ha)\, c_n$$

  - ▷ **Local truncation error** of Euler's method = computed − exact:

$$T_1 = (1 + ha) - e^{ha} \approx -\frac{1}{2}(ha)^2$$

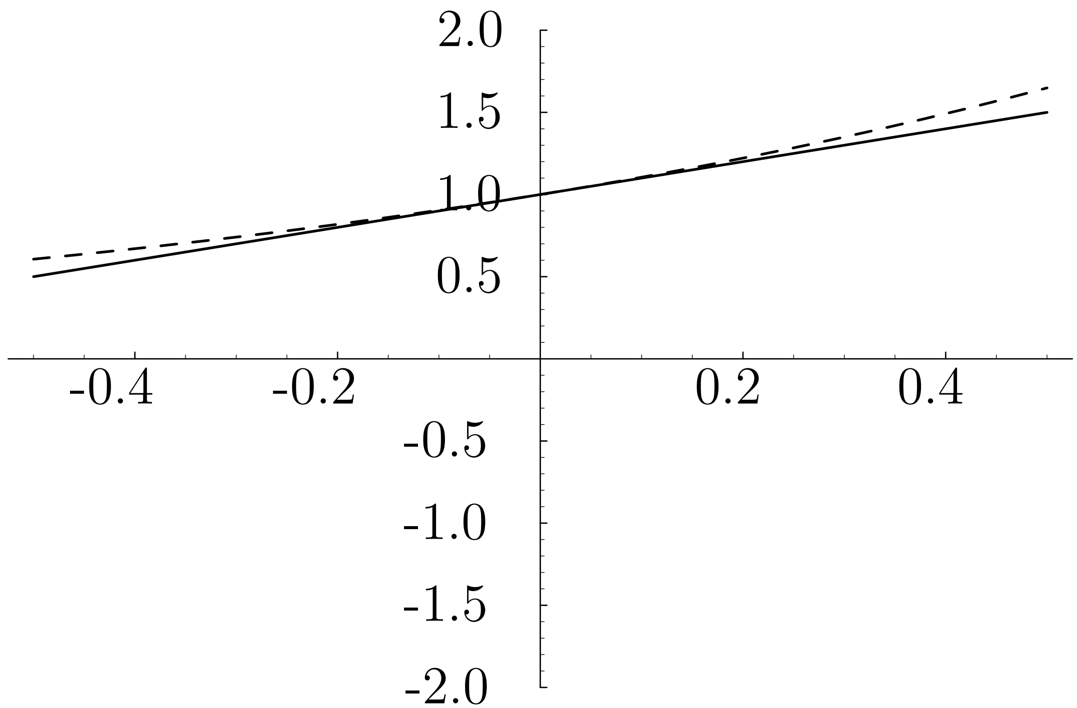
ACCURACY OF EULER'S METHOD (1)

- Plot shows $1 + ha$ (solid line) and e^{ha} (dashed line) vs. real values of ha



ACCURACY OF EULER'S METHOD (2)

- Plot shows $1 + ha$ (solid line) and e^{ha} (dashed line) vs. real values of ha



EULER'S METHOD (3)

- Global solution of the test problem $y' = ay$ obtained using Euler's method:

$$\boxed{c_{n+1} = (1 + ha)^{n+1}\, c_0}$$

  - ▷ **Global truncation error** after N steps (after an interval $L = Nh$):

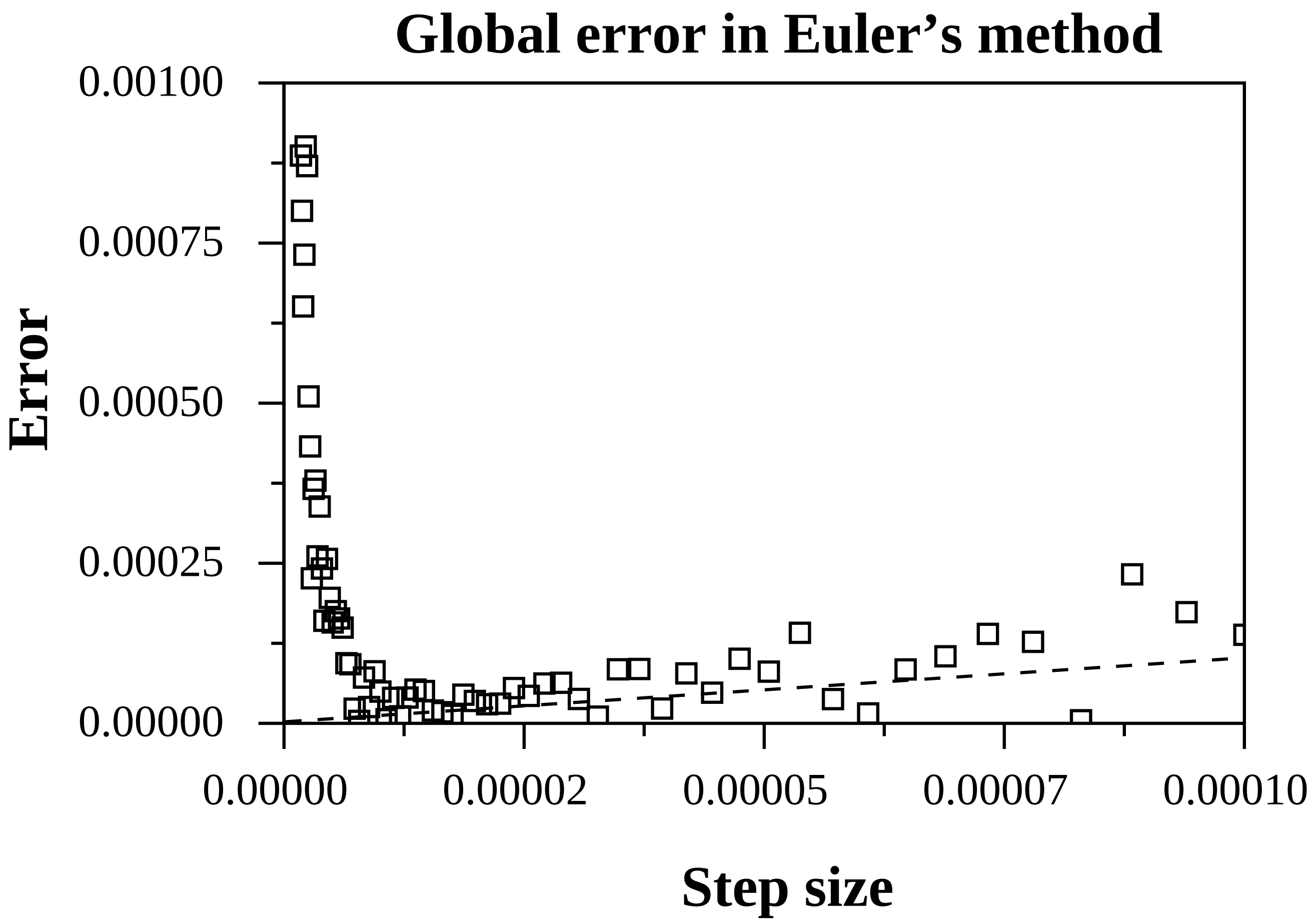
$$T_N = (1 + ha)^N - e^{Nha} \approx -\frac{1}{2}a^2 Lh$$

  - ▷ Regardless of the value of a,

$$\lim_{h \to 0} T_N = 0$$

    - ◦ This equation establishes mathematically that the computed solution of the test problem $y' = ay$ approaches the exact solution as $h \longrightarrow 0$ (**convergence**: A necessary but not sufficient condition for accuracy)
    - ◦ This limit is correct mathematically, but not necessarily numerically; see the next slide

OPTIMAL STEP SIZE FOR EULER'S METHOD



EULER'S METHOD (4)

- Stability analysis of the computed solution:
  - ▷ A system is called **stable** if a bounded input produces a bounded output
    - ◦ A system described by the ODE $y' = ay$ is stable if and only if

$$\mathrm{Re}(a) < 0$$

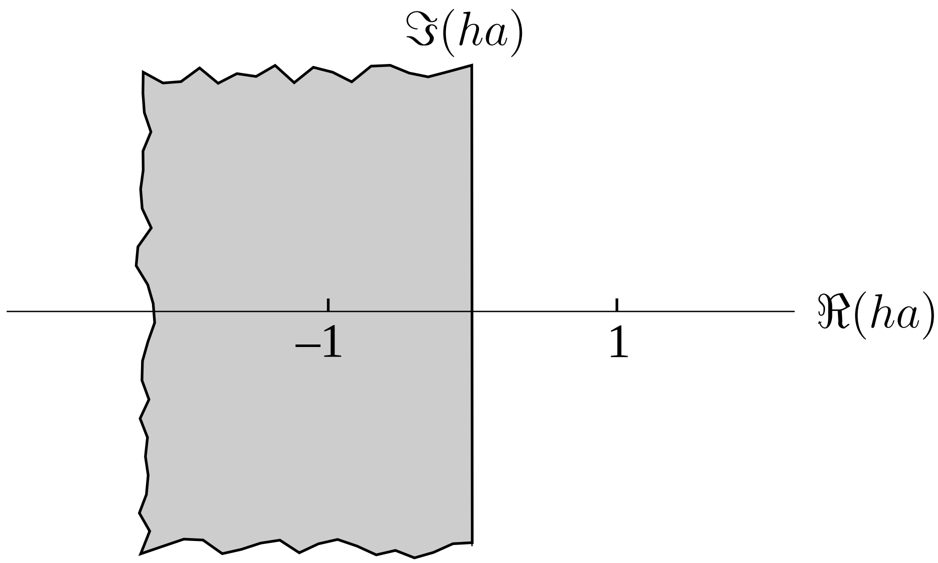
because the exact solution is $y(x) = y(0)e^{ax}$

    - ◦ The region of stability of the ODE is the left half-plane
  - ▷ A solution computed using Euler's method cannot be stable unless

$$\boxed{|1 + ha| \leq 1}$$

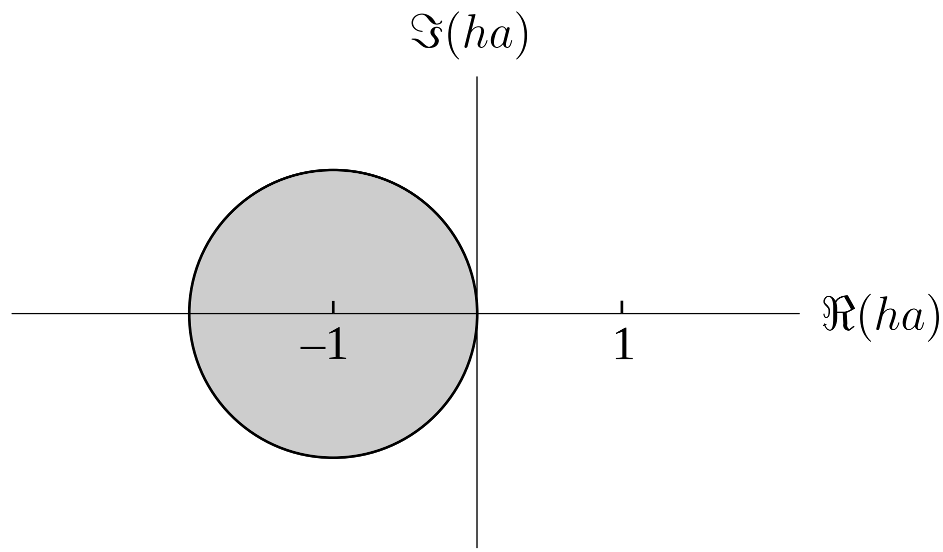
  - ▷ Since a can be complex, the set of values of ha for which the computed solution is stable lies within a disk of radius 1 centered at $ha = -1$ in the complex plane
    - ◦ The stability region of Euler's method is a subset of the left half-plane
    - ◦ Euler's method is unstable if a is purely imaginary ($a = i\mu$)

REGION OF STABILITY FOR $y' = ay$



$$y' = ay$$

REGION OF STABILITY FOR EULER'S METHOD

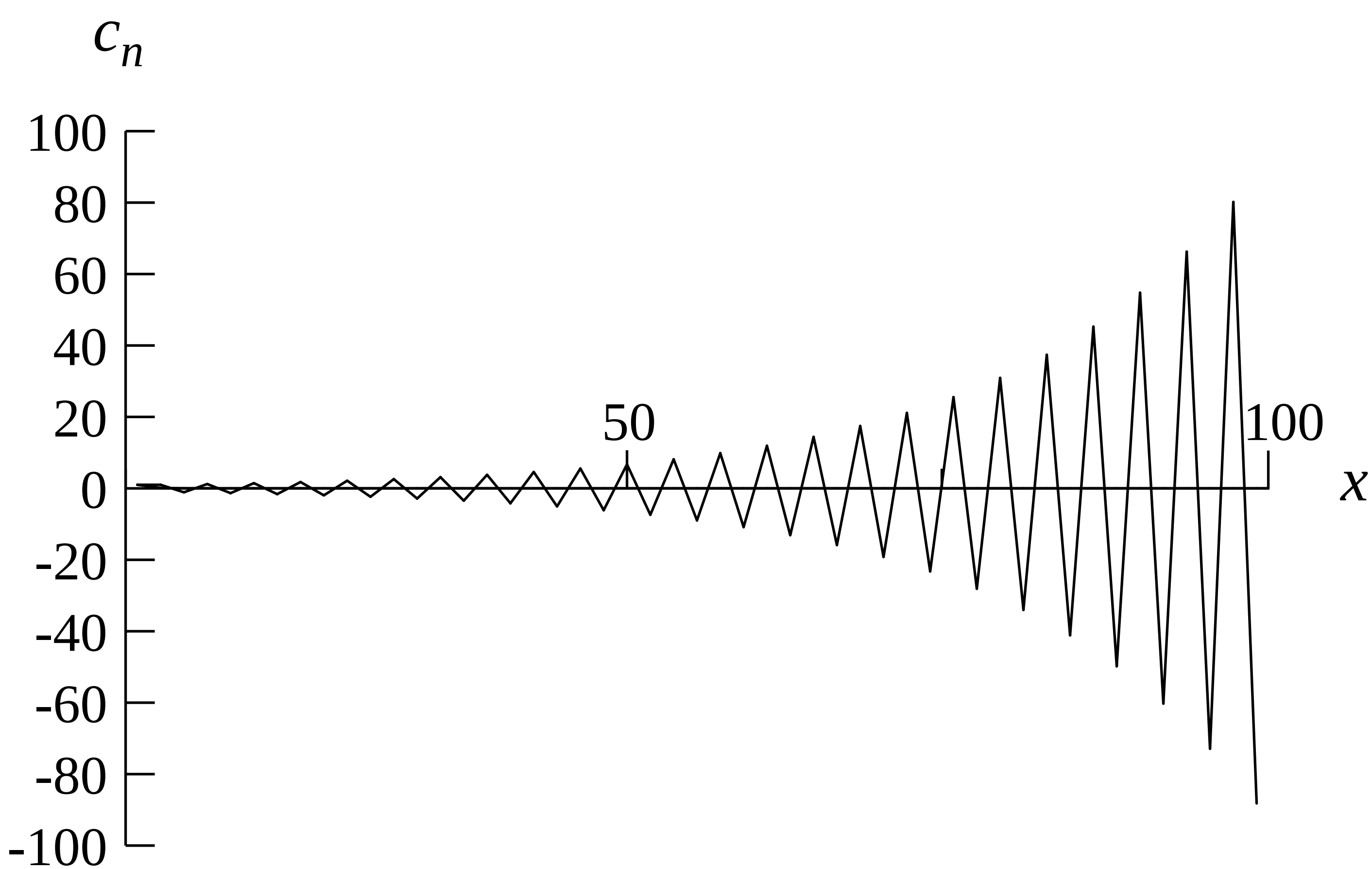


$$y' = ay$$

$$c_{n+1} = (1 + ha)\, c_n$$

EULER'S METHOD WITH AN UNSTABLE STEP SIZE

- Solution of $y' = -y$ computed using $h = 2.1 \Rightarrow ha = -2.1$



TRANSFER FUNCTION OF A FINITE-DIFFERENCE METHOD (1)

- Discretize by sampling at points $x_n = nh$
  - ▷ Let $y_n := y(x_n) =$ discretized exact solution, $c_n =$ computed solution
- Linear, multistep **difference equation** which approximates $dy/dx = f(x,\, y) = y'$:

$$\begin{aligned} c_{n+1} =& \alpha_1 c_n + \alpha_2 c_{n-1} + \cdots + \alpha_k c_{n-k+1} \\ & + h[\beta_0 f(x_{n+1}, c_{n+1}) + \beta_1 f(x_n, c_n) + \cdots + \beta_k f(x_{n-k+1}, c_{n-k+1})] \end{aligned}$$

- The difference equation above is a recursive digital filter
  - ▷ The transfer function of this digital filter provides a way to assess the global accuracy of the solution of the difference equation as an approximation to the solution of $y' = f(x,\, y)$

TRANSFER FUNCTION OF A FINITE-DIFFERENCE METHOD (2)

- The general finite-difference method for solving $y' = f(x, y)$,

$$c_{n+1} = \alpha_1 c_n + \alpha_2 c_{n-1} + \cdots + \alpha_k c_{n-k+1} + h[\beta_0 f(x_{n+1}, c_{n+1}) + \beta_1 f(x_n, c_n) + \cdots + \beta_k f(x_{n-k+1}, c_{n-k+1})]$$

is a recursive digital filter in which

$$\text{output at } x_n = c_n = \text{generalization of } y$$

$$\text{input at } x_n = f(x_n, c_n) = \text{generalization of } y'$$

- At each frequency ω,

$$\text{input at } x_n = A_I e^{in\omega h}$$
$$\text{output at } x_n = A_O e^{in\omega h}$$

and the transfer function is

$$A(\omega) = \frac{A_O}{A_I}$$

TRANSFER FUNCTION OF A FINITE-DIFFERENCE METHOD (3)

- To obtain the characteristic polynomial for the test problem $y' = ay$, for the finite-difference method

$$\begin{aligned} c_{n+1} =& \alpha_1 c_n + \alpha_2 c_{n-1} + \cdots + \alpha_k c_{n-k+1} \\ &+ h[\beta_0 f(x_{n+1}, c_{n+1}) + \beta_1 f(x_n, c_n) + \cdots + \beta_k f(x_{n-k+1}, c_{n-k+1})] \end{aligned}$$

  substitute $c_n = \xi^n c_0,\ f(x_n, c_n) = ac_n = a\xi^n c_0$

- Characteristic polynomial for the test problem $y' = ay$ [where $\alpha_0 := -1$]:

$$\begin{aligned} \phi(\xi) &= \sum_{l=0}^{k} \alpha_l \xi^{k-l} + ha \sum_{l=0}^{k} \beta_l \xi^{k-l} \\ &= \rho(\xi) + ha\,\sigma(\xi) \end{aligned}$$

- To obtain the transfer function, substitute $c_n = A_O \xi^n c_0$, $f(x_n, c_n) = A_I \xi^n c_0$, where $\xi = e^{i\omega h}$

TRANSFER FUNCTION OF A FINITE-DIFFERENCE METHOD (4)

- Calculation of the transfer function (where $\xi = e^{i\omega h}$):

$$\begin{aligned} A_O \xi^{n+1} =& A_O(\alpha_1 \xi^n + \alpha_2 \xi^{n-1} + \cdots + \alpha_k \xi^{n-k+1}) \\ & + hA_I[\beta_0 \xi^{n+1} + \beta_1 \xi^n + \cdots + \beta_k \xi^{n-k+1}] \end{aligned}$$

Divide by $A_I \xi^{n-k+1}$:

$$-\frac{A_O}{A_I}\rho(\xi) = h\sigma(\xi)$$

- The resulting transfer function is

$$A(\omega) = \frac{h\sum_{l=0}^{k} \beta_l \, e^{i(k-l)\omega h}}{\sum_{l=0}^{k} \alpha_l e^{i(k-l)\omega h}} = -\frac{h\sigma(e^{i\omega h})}{\rho(e^{i\omega h})}$$

TRANSFER FUNCTION OF A FINITE-DIFFERENCE METHOD (5)

- Transfer function of an ideal integrator:

$$A_{\text{ideal}}(\omega) = \frac{1}{i\omega}$$

because $y = e^{i\omega x}$ implies $y' = i\omega e^{i\omega x}$

- Ratio of the transfer function of the finite-difference method to the transfer function of an ideal integrator:

$$\frac{A(\omega)}{A_{\text{ideal}}(\omega)} := R(\omega)$$

- Characteristic polynomial for the test problem $y' = ay$ [where $\alpha_0 := -1$]:

$$\begin{aligned} \phi(\xi) &= \sum_{l=0}^{k} \alpha_l \xi^{k-l} + ha \sum_{l=0}^{k} \beta_l \xi^{k-l} \\ &= \rho(\xi) + ha\, \sigma(\xi) \end{aligned}$$

TRANSFER FUNCTION OF A FINITE-DIFFERENCE METHOD (6)

- The transfer function of the finite-difference method

$$\begin{aligned} c_{n+1} =& \alpha_1 c_n + \alpha_2 c_{n-1} + \cdots + \alpha_k c_{n-k+1} \\ & + h[\beta_0 f(x_{n+1}, c_{n+1}) + \beta_1 f(x_n, c_n) + \cdots + \beta_k f(x_{n-k+1}, c_{n-k+1})] \end{aligned}$$

is

$$A(\omega) = \frac{h \sum_{l=0}^{k} \beta_l \, e^{i(k-l)\omega h}}{\sum_{l=0}^{k} \alpha_l e^{i(k-l)\omega h}} = -\frac{h\sigma(e^{i\omega h})}{\rho(e^{i\omega h})}$$

▷ The ratio of the transfer function of the finite-difference method to the transfer function of an ideal integrator is

$$R(\omega) = -\frac{i\omega h\sigma(e^{i\omega h})}{\rho(e^{i\omega h})}$$

▷ Plots show $|R(\omega)|$ versus ω/ω_N

EULER'S METHOD (5)

- Transfer-function ratio of Euler's method:
  - ▷ Parameters:

$$\alpha_0 = -1,\ \alpha_1 = 1,\ \beta_1 = 1,\ \text{others} = 0$$

  - ▷ Then

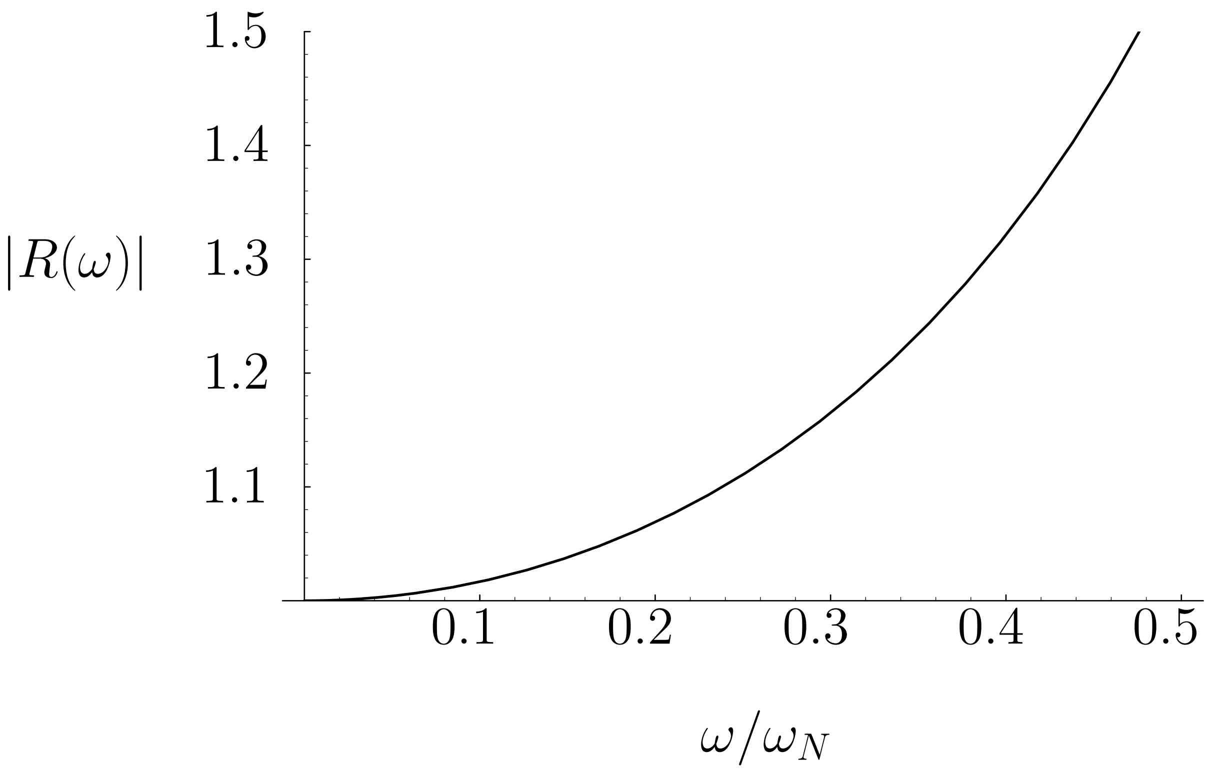
$$\sigma(e^{i\omega h}) = 1,\ \rho(e^{i\omega h}) = -e^{i\omega h} + 1$$

  - ▷ The transfer-function ratio is

$$R(\omega) = -\frac{i\omega h\sigma(e^{i\omega h})}{\rho(e^{i\omega h})} = \frac{\omega h/2}{\sin(\omega h/2)} e^{-i\omega h/2}$$

    - ∘ Because the phase of $R(\omega)$ is proportional to ω, Euler's method shifts the x origin of the computed solution in signal space by $h/2$ per step
    - ∘ This implies that, with each step, Euler's method lands on a different solution curve in the family of solutions to $y' = ay$

TRANSFER-FUNCTION RATIO OF EULER'S METHOD



MIDPOINT METHOD (1)

- Midpoint method:
  - ▷ The integral equation

$$y(x+h) = y(x-h) + \int_{x-h}^{x+h} f(x', y(x'))\, dx'$$

is equivalent to the ODE $y' = f(x, y)$ with the initial value $y(x-h)$

  - ▷ Evaluating the integral using the midpoint (centered rectangle) rule gives

$$\boxed{c_{n+1} = 2hf(x_n,\, c_n) + c_{n-1}}$$

  - ▷ For the test problem $y' = ay$, assume a solution of the form $c_n = c_0\xi^n$:

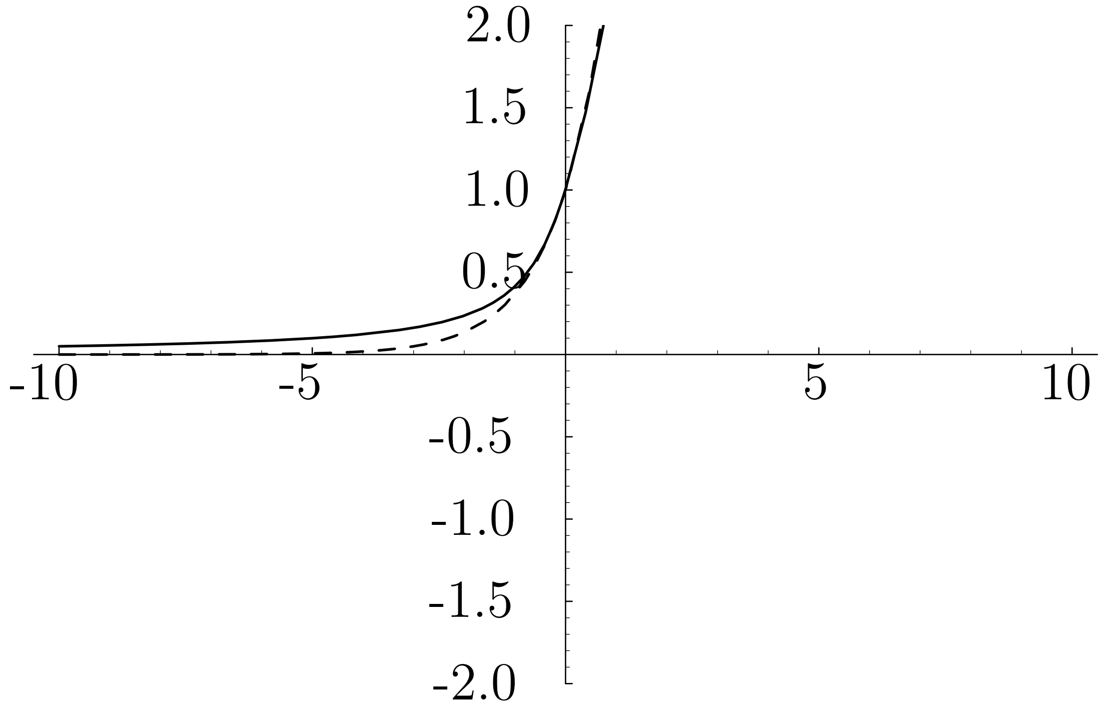
$$\xi^{n+1} = 2ha\xi^n + \xi^{n-1} \Rightarrow \xi^2 - 2ha\xi - 1 = 0 \Rightarrow \boldsymbol{\xi = ha \pm \sqrt{1 + (ha)^2}}$$

    - ∘ There are two roots:

$$\xi_1 = 1 + ha + \frac{(ha)^2}{2} + O((ha)^3) = e^{ha} + O((ha)^3) \quad \text{and} \quad \xi_2 = -\frac{1}{\xi_1}$$

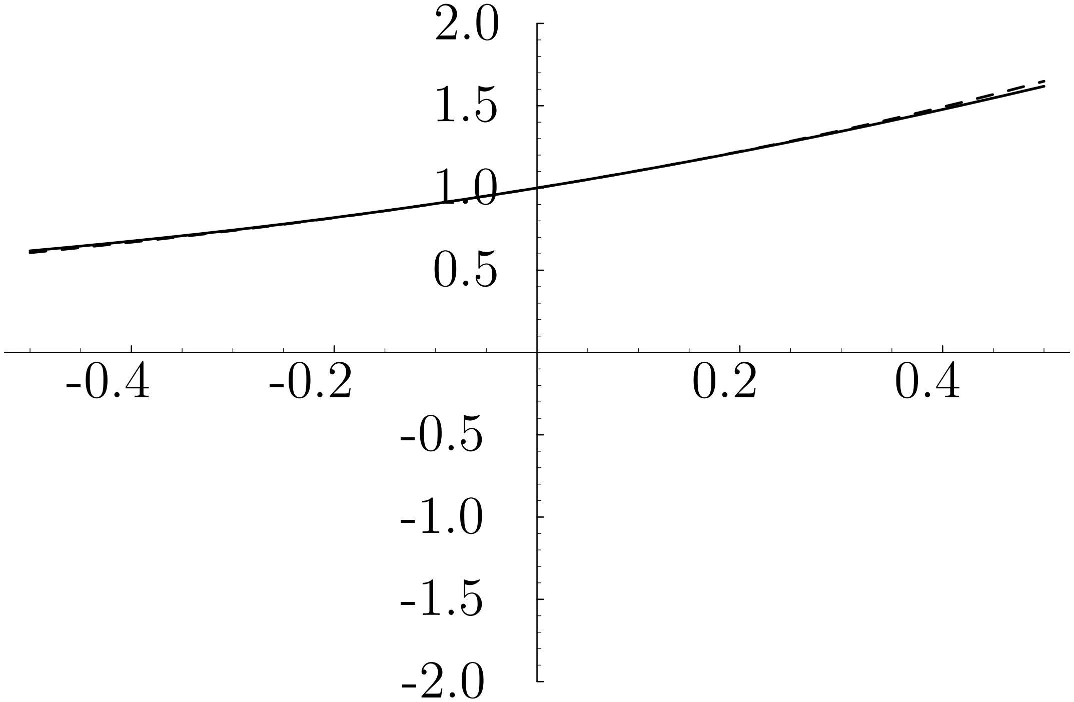
ACCURACY OF THE MIDPOINT METHOD (1)

- Plot shows $ha + \sqrt{1 + (ha)^2}$ (solid line) and e^{ha} (dashed line) vs. real values of ha



ACCURACY OF THE MIDPOINT METHOD (2)

- Plot shows $ha + \sqrt{1 + (ha)^2}$ (solid line) and e^{ha} (dashed line) vs. real values of ha



MIDPOINT METHOD (2)

- A multistep method is one in which the finite-difference equation contains computed points in addition to c_{n+1} and c_n
  - ▷ Example: The midpoint method is a 2-step method, because it uses c_{n+1}, c_n and c_{n-1} (3 points define 2 steps)
    - ◦ The root that is closest to e^{ha}, ξ_1, is the **principal characteristic root**
    - ◦ The other root, ξ_2, is the **parasitic root**
    - ◦ The general solution of the midpoint difference equation is a linear combination of powers of the two characteristic roots (if $\xi_2 \neq \xi_1$):

$$c_n = \alpha \xi_1^n + \beta \xi_2^n$$

    - ◦ For the initial condition $c_0 = y_0$, use a one-step method to get c_1
    - ◦ Then α and β are determined by the equations

$$c_0 = \alpha + \beta$$
$$c_1 = \alpha \xi_1 + \beta \xi_2$$

MIDPOINT METHOD (3)

- Example of weak instability in the midpoint method when ha is real:
  - ▷ Solve $y' = -y$ with initial condition $y(0) = 1$ and step size $h = 0.1$

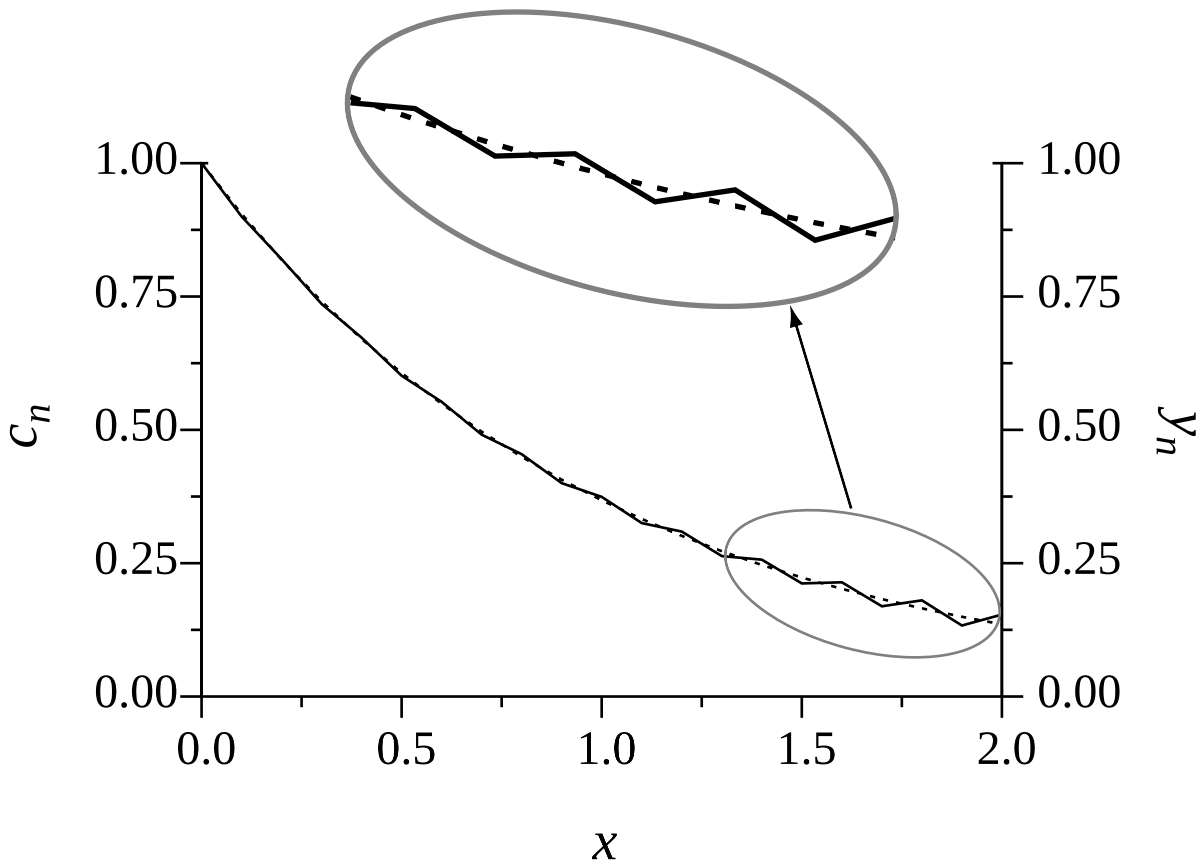
$$\xi_1 = ha + \sqrt{1 + (ha)^2} = -0.1 + \sqrt{1.01} \approx 0.9050$$

$$\xi_2 = -\frac{1}{\xi_1} \approx -1.1050$$

$$\alpha \approx 0.9975, \quad \beta \approx 0.0025$$

  - ▷ Because $|\xi_2| > 1$ and $|\xi_1| < 1$ (**weak instability**), the contribution of the parasitic root eventually overwhelms the contribution of the principal root

WEAK INSTABILITY OF THE MIDPOINT METHOD



MIDPOINT METHOD (4)

- Stability region of the midpoint method:
  - ▷ We require

$$|\xi_1| = |ha + \sqrt{1+(ha)^2}| \le 1 \quad \text{and} \quad |\xi_2| = |ha - \sqrt{1+(ha)^2}| \le 1$$

  - ▷ Because

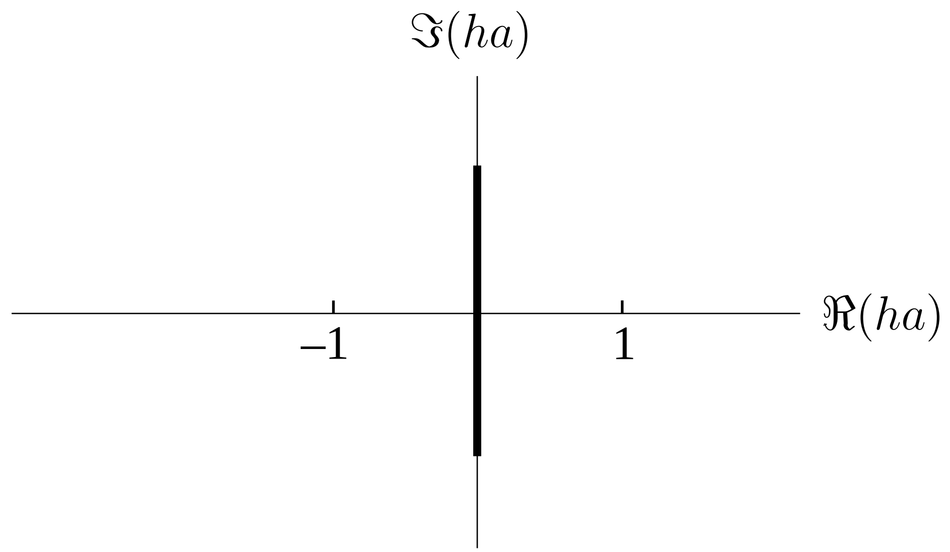
$$\xi_2 = -\frac{1}{\xi_1} \Rightarrow |\xi_2| = \frac{1}{|\xi_1|}$$

    the moduli of both characteristic roots can be ≤ 1 iff $|\xi_1| = |\xi_2| = 1$
  - ▷ But $|\xi_1| = 1 \Rightarrow \xi_1^* = 1/\xi_1$; then $\xi_2 = -1/\xi_1 = -\xi_1^*$
  - ▷ The characteristic equation $\xi^2 - 2ha\xi - 1 = 0$ implies $ha = \frac{1}{2}(\xi_1 + \xi_2)$
  - ▷ Then $ha = \frac{1}{2}(\xi_1 - \xi_1^*) \Rightarrow ha$ is purely imaginary $\Rightarrow \boldsymbol{ha = ih\mu}$
  - ▷ From $\xi_2 = -\xi_1^*$ and the quadratic formula,

$$ha - \sqrt{1+(ha)^2} = -(ha)^* - \left(\sqrt{1+(ha)^2}\right)^* \Rightarrow \sqrt{1-(h\mu)^2} \text{ is real}$$

  - ▷ Since $h\mu$ is real, $\sqrt{1-(h\mu)^2}$ is real iff $\boldsymbol{h\mu \in [-1, 1]}$

REGION OF STABILITY OF THE MIDPOINT METHOD



$$y' = ay$$

$$c_{n+1} = \left(ha + \sqrt{1 + (ha)^2}\right) c_n$$

MIDPOINT METHOD (5)

- Transfer-function ratio of the midpoint method:
  - ▷ Parameters:

$$\alpha_0 = -1,\ \alpha_2 = 1,\ \beta_1 = 2,\ \text{others} = 0$$

  - ▷ Then

$$\sigma(e^{i\omega h}) = 2e^{i\omega h},\ \rho(e^{i\omega h}) = -e^{2i\omega h} + 1$$

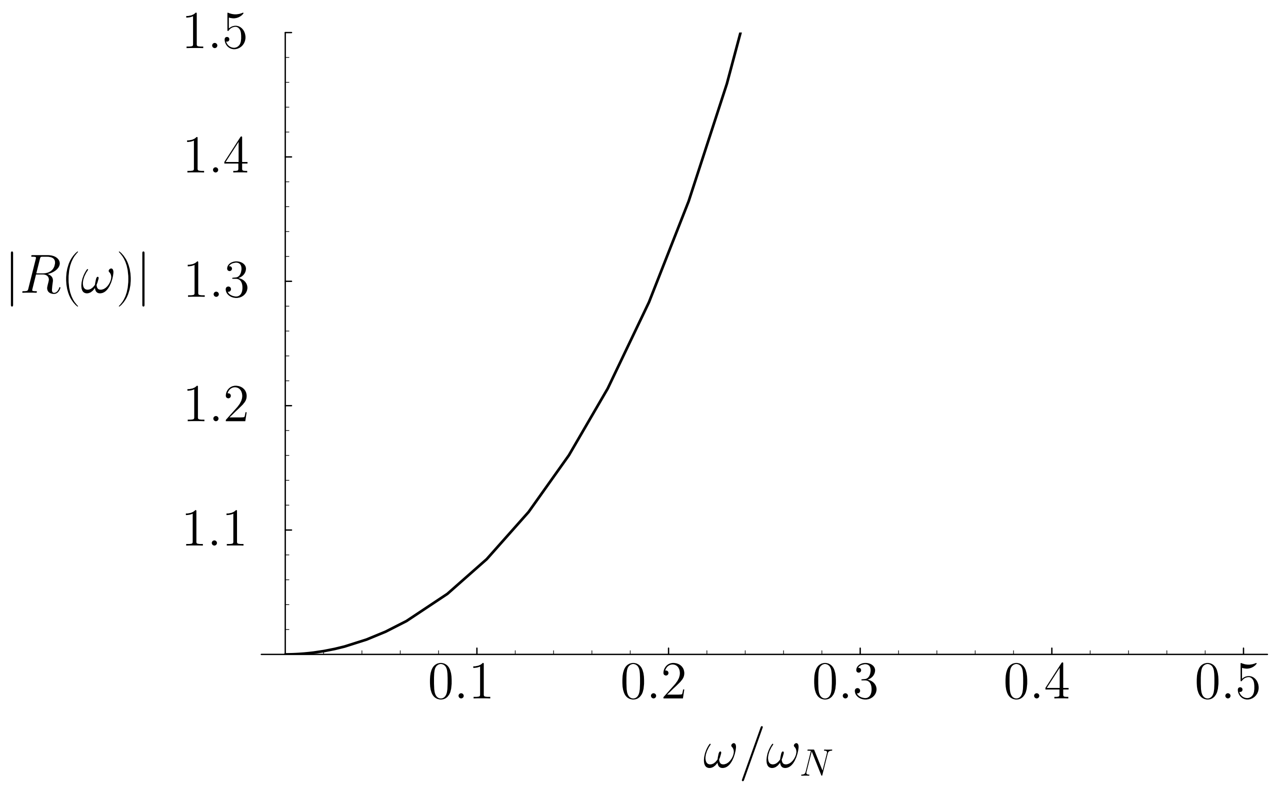
  - ▷ The transfer-function ratio is

$$R(\omega) = -\frac{i\omega h \sigma(e^{i\omega h})}{\rho(e^{i\omega h})} = \frac{\omega h}{\sin(\omega h)}$$

    - ∘ Evidently $R(\omega)$ has a pole at

$$\omega h = \frac{2\pi\omega}{\omega_N} = \pi \Rightarrow \omega = \omega_N/2$$

TRANSFER-FUNCTION RATIO OF THE MIDPOINT METHOD



MIDPOINT METHOD (6)

- Phase error of the midpoint method for the test problem $y' = ay$:
  - ▷ Since the midpoint method is stable when a is purely imaginary, $a = i\mu$, it is useful to know the method's phase accuracy
  - ▷ The phase of the computed solution for one step,

$$\xi_1 = ih\mu + \sqrt{1 - (h\mu)^2} = e^{i\theta},$$

    is

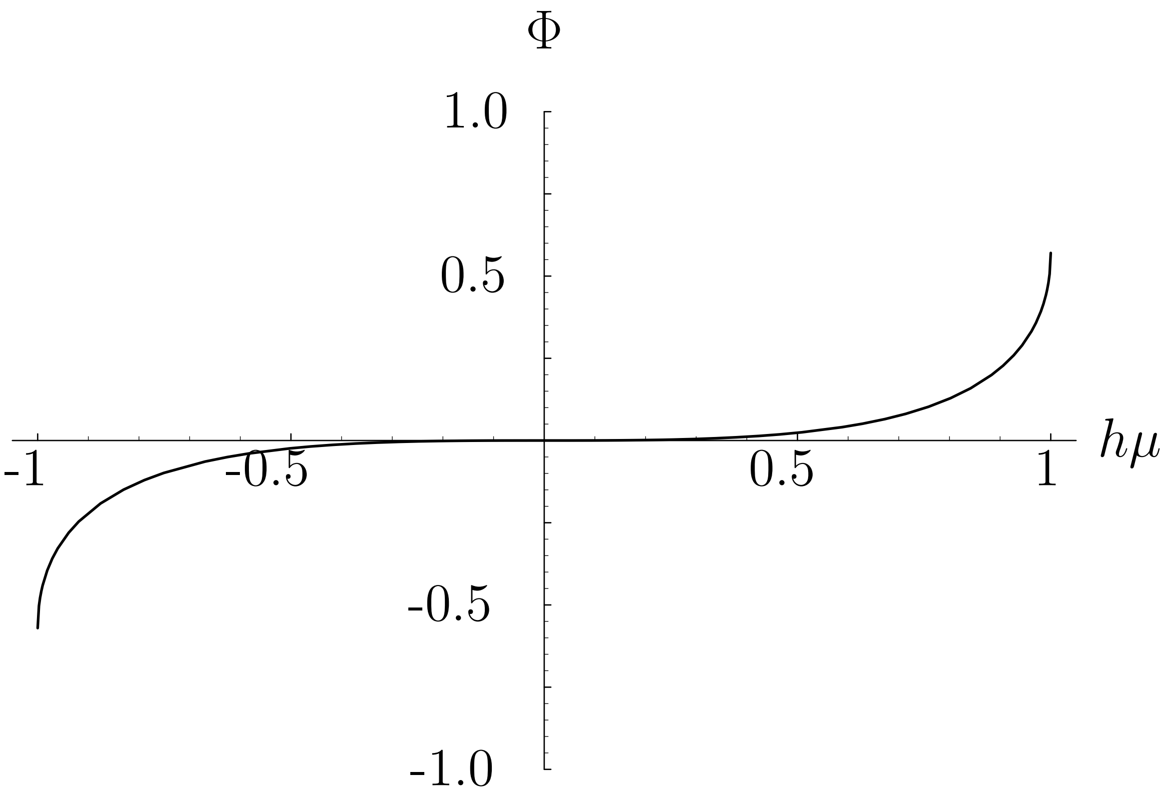
$$\theta = \tan^{-1} \frac{h\mu}{\sqrt{1 - (h\mu)^2}}$$

  - ▷ The phase of the exact solution for one step, $e^{ih\mu}$, is $h\mu$
  - ▷ The **phase error** is the computed phase minus the exact phase:

$$\Phi = \tan^{-1} \frac{h\mu}{\sqrt{1 - (h\mu)^2}} - h\mu$$

  - ▷ Plot shows Φ (in radians) vs. $h\mu$

PHASE ERROR OF THE MIDPOINT METHOD



ABSOLUTE AND RELATIVE STABILITY

- For many problems, stability is not enough
- Test problem:

$$y' = ay$$

where a may be complex

- ▷ Expect different behavior when a is real > 0, real < 0 or purely imaginary
- ▷ **Absolute stability**: No characteristic root has a modulus > 1
  - ∘ For all i, $|\xi_i| \leq 1$
  - ∘ The **region of absolute stability** of a finite-difference method is the region in the complex ha-plane for which the method is absolutely stable
- ▷ **Relative stability**: No parasitic root has a modulus greater than the modulus of the principal characteristic root
  - ∘ For all $i > 1$, $|\xi_i| \leq |\xi_1|$

TRAPEZOIDAL METHOD (1)

- **Trapezoidal method:**

$$c_{n+1} = c_n + \frac{h}{2}(f(x_{n+1}, c_{n+1}) + f(x_n, c_n)) \quad \text{(implicit)}$$

Characteristic root:

$$\xi_1 = \frac{1 + ha/2}{1 - ha/2}$$

▷ If $\mathrm{Re}[a] \leq 0$, then $|\xi_1| \leq 1$

- The trapezoidal method is absolutely stable whenever the differential equation $y' = ay$ is stable (*i.e.*, for all ha in the left half-plane)
- If $a = i\mu$, then $|\xi_1| = 1$ **(exact unitarity for all $|ha|$)**

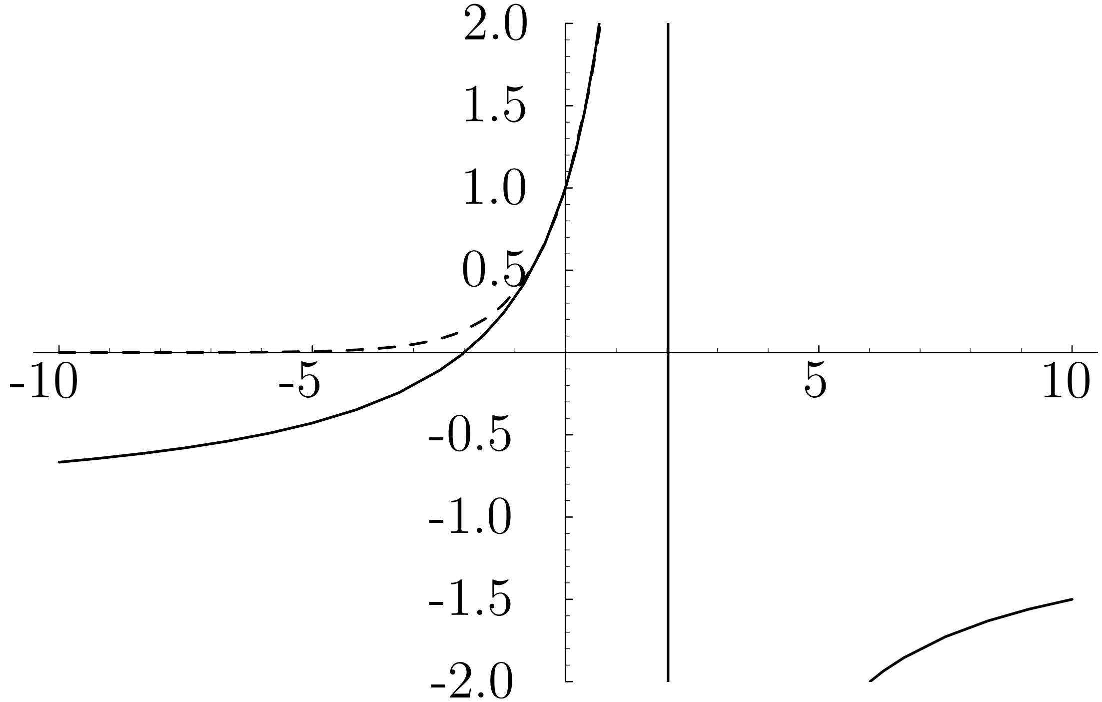
▷ Bad news: as $|ha| \to \infty$ in the complex plane,

$$\xi_1 \to -1$$

(creates oscillations at the Nyquist frequency when ha is large)

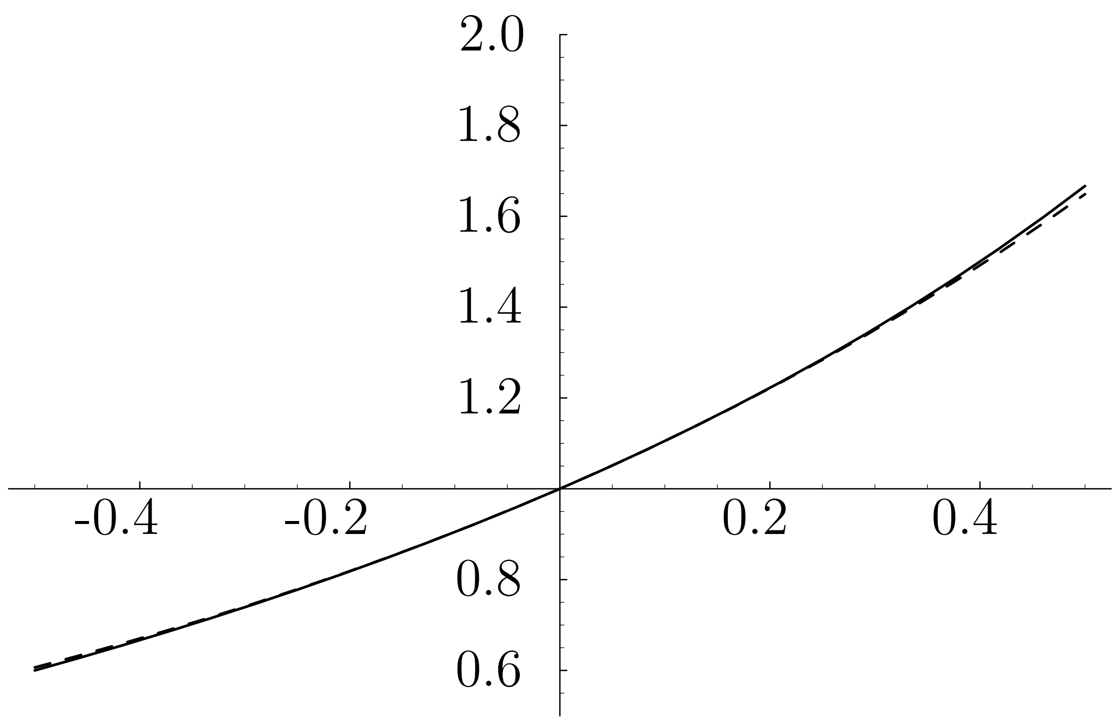
ACCURACY OF THE TRAPEZOIDAL METHOD (1)

- Plot shows $(1 + \frac{1}{2}ha)/(1 - \frac{1}{2}ha)$ (solid line) and e^{ha} (dashed line) vs. real values of ha

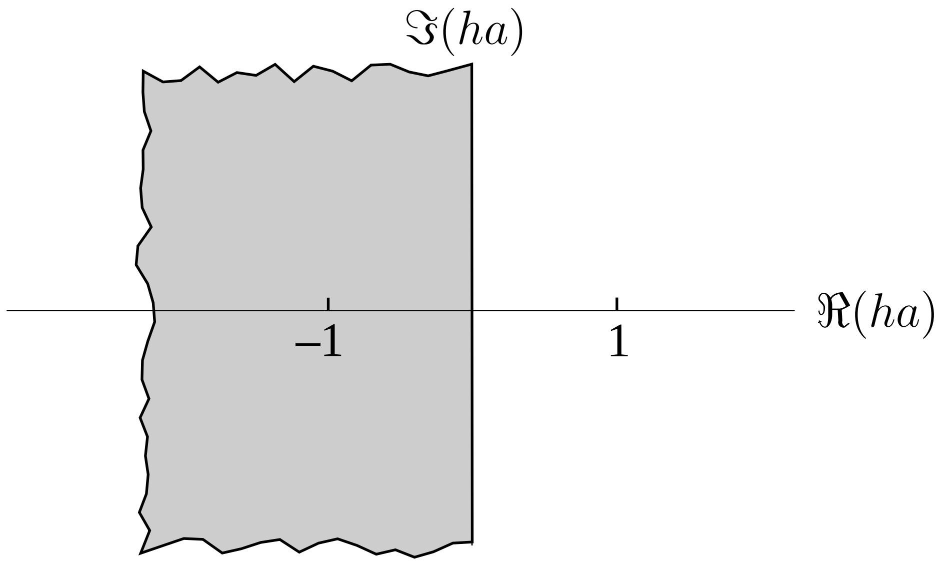


ACCURACY OF THE TRAPEZOIDAL METHOD (2)

- Plot shows $(1 + \frac{1}{2}ha)/(1 - \frac{1}{2}ha)$ (solid line) and e^{ha} (dashed line) vs. real values of ha



REGION OF STABILITY OF THE TRAPEZOIDAL METHOD



$$y' = ay$$

$$c_{n+1} = \left(\frac{1 + ha/2}{1 - ha/2} \right) c_n$$

TRAPEZOIDAL METHOD (2)

- Transfer-function ratio of the trapezoidal method:
  - ▷ Parameters:

$$\alpha_0 = -1,\ \alpha_1 = 1,\ \beta_0 = \tfrac{1}{2},\ \beta_1 = \tfrac{1}{2},\ \text{others} = 0$$

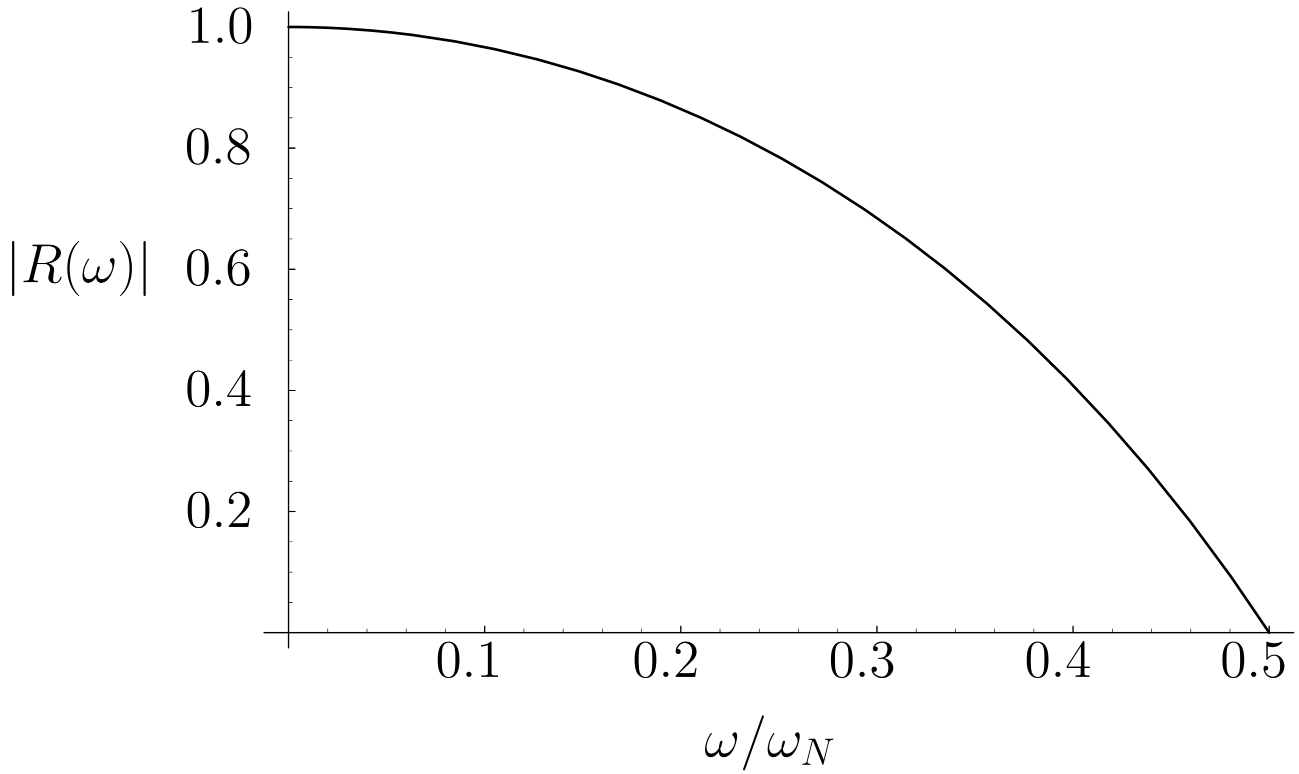
  - ▷ Then

$$\sigma(e^{i\omega h}) = \beta_0 e^{i\omega h} + \beta_1 = \tfrac{1}{2}(e^{i\omega h} + 1)$$
$$\rho(e^{i\omega h}) = \alpha_0 e^{i\omega h} + \alpha_1 = -e^{i\omega h} + 1$$

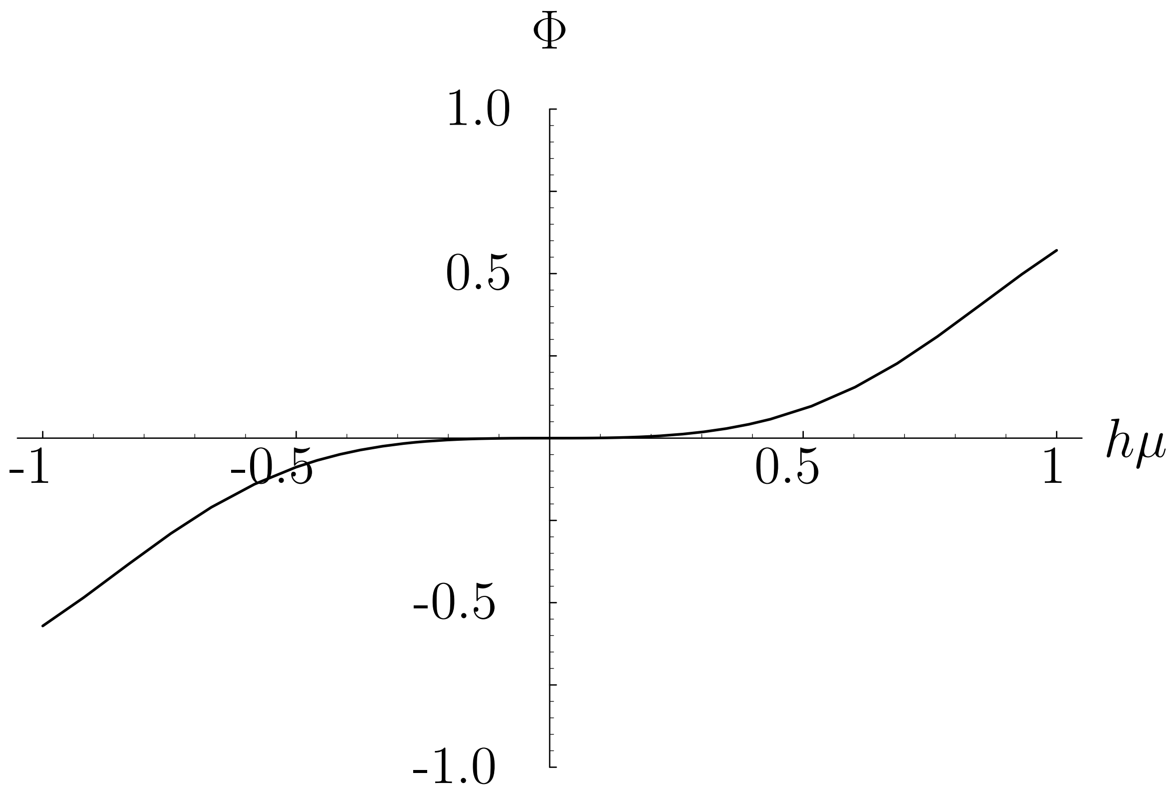
  - ▷ The transfer-function ratio is

$$R(\omega) = -\frac{i\omega h \sigma(e^{i\omega h})}{\rho(e^{i\omega h})} = (\omega h/2)\cot(\omega h/2)$$

TRANSFER-FUNCTION RATIO OF THE TRAPEZOIDAL METHOD



PHASE ERROR OF THE TRAPEZOIDAL METHOD



MIDPOINT-TRAPEZOIDAL METHOD (1)

- **Midpoint-trapezoidal predictor-corrector:**

$$p_{n+1} = c_{n-1} + 2hf(x_n, c_n) \quad \text{(predict)}$$

$$c_{n+1} = c_n + \frac{h}{2}(f(x_{n+1}, p_{n+1}) + f(x_n, c_n)) \quad \text{(correct)}$$

▷ Characteristic roots:

$$\xi_1 = \tfrac{1}{2}\left[1 + \frac{ha}{2} + (ha)^2\right] + \tfrac{1}{2}\left\{\left[1 + \frac{ha}{2} + (ha)^2\right]^2 + 2ha\right\}^{1/2}$$

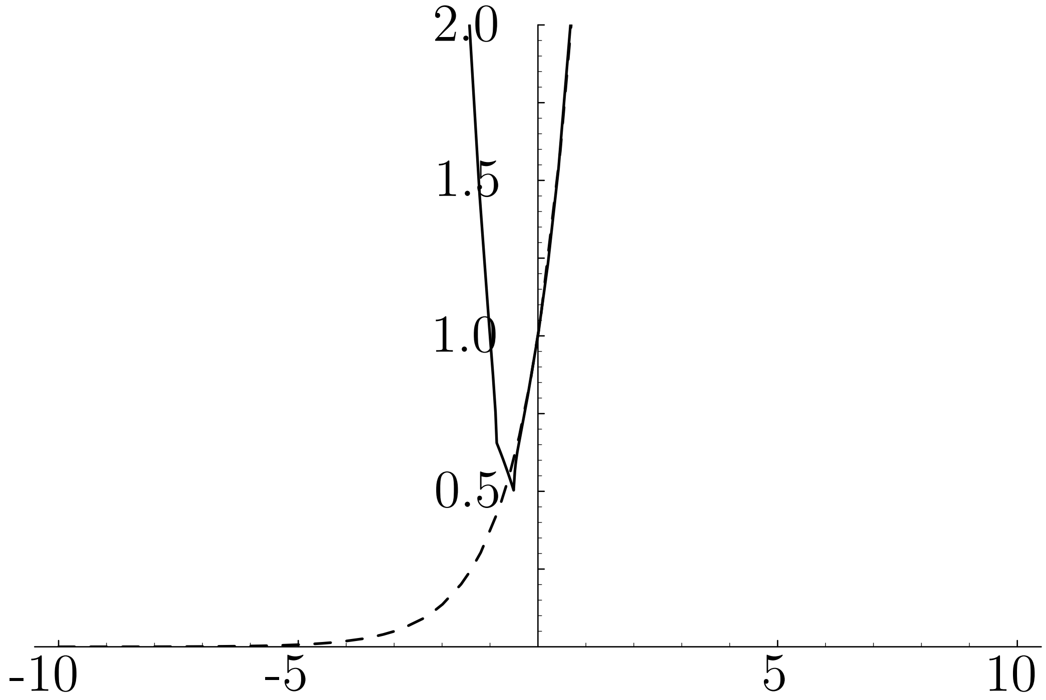
$$= e^{ha} + O(h^3) \quad \text{(principal root)}$$

$$\xi_2 = \tfrac{1}{2}\left[1 + \frac{ha}{2} + (ha)^2\right] - \tfrac{1}{2}\left\{\left[1 + \frac{ha}{2} + (ha)^2\right]^2 + 2ha\right\}^{1/2}$$

(parasitic root)

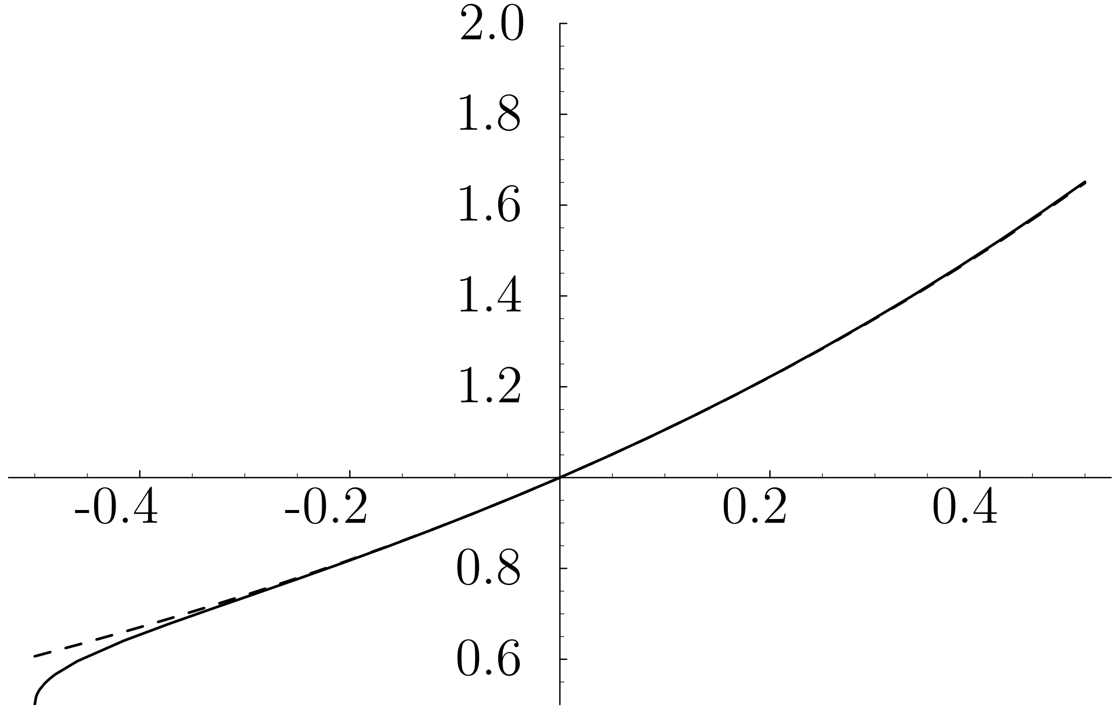
ACCURACY OF THE MID-TRAP METHOD (1)

- Plot shows $\max[\xi_1, \xi_2]$ (solid line) and e^{ha} (dashed line) vs. real values of ha



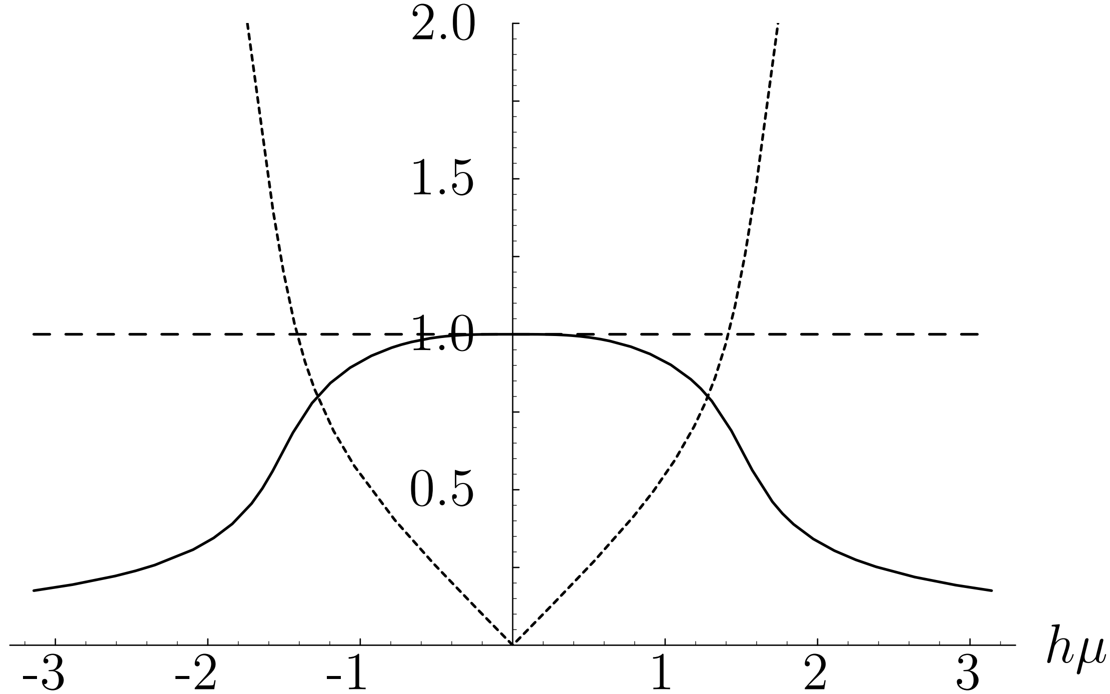
ACCURACY OF THE MID-TRAP METHOD (2)

- Plot shows $\max[\xi_1, \xi_2]$ (solid line) and e^{ha} (dashed line) vs. real values of ha

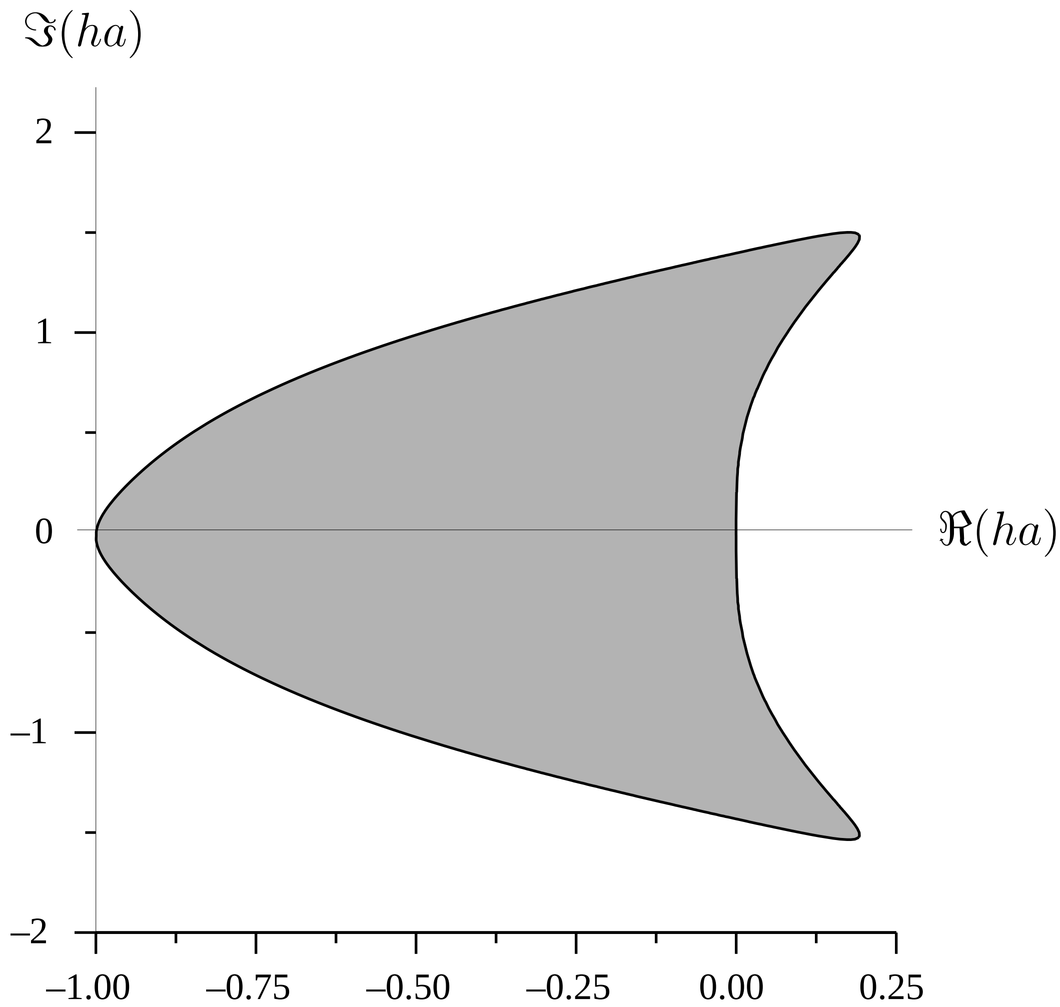


ACCURACY OF THE MID-TRAP METHOD (3)

- Plot shows $|\xi_1|$ (solid line), $|\xi_2|$ (dotted line), and $|e^{ih\mu}|$ (dashed line) vs. $h\mu$ for purely imaginary values of $a = i\mu$



MIDPOINT-TRAPEZOIDAL STABILITY REGION



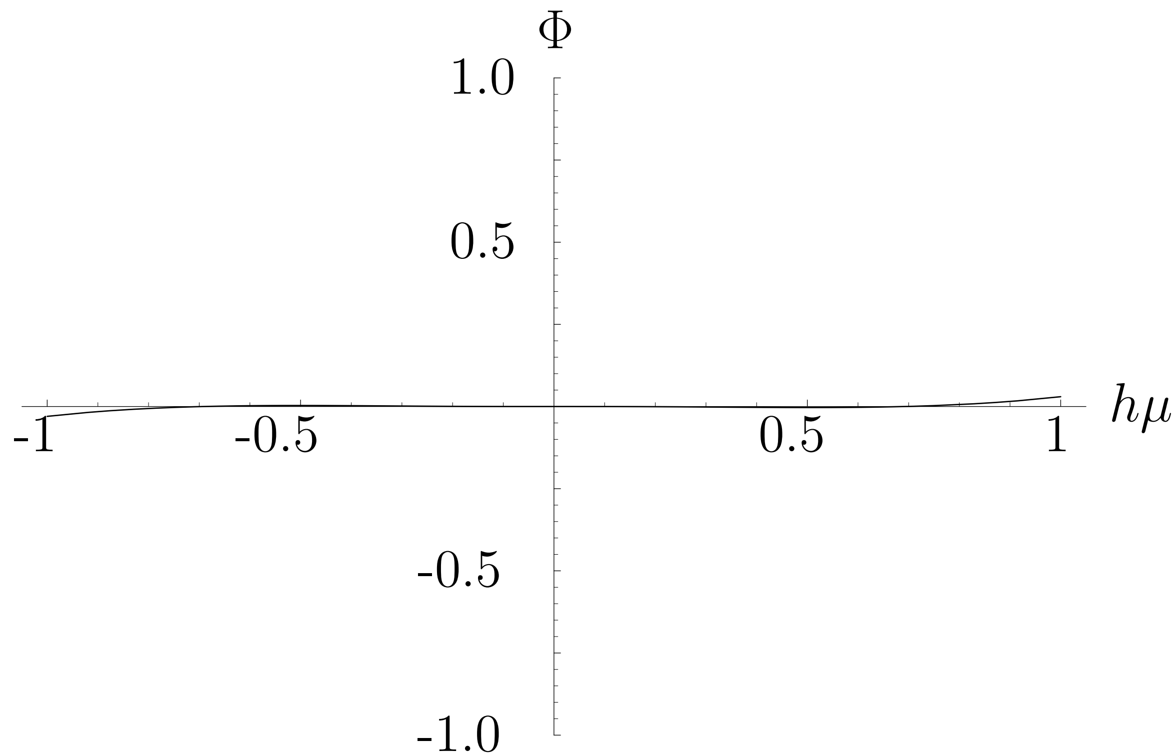
MIDPOINT-TRAPEZOIDAL METHOD (2)

- Transfer-function ratio of the midpoint-trapezoidal method:
  - ▷ The trapezoidal corrector determines the transfer function, because the input is predetermined as $f(x_n, c_n) = A_I e^{in\omega h}$
    - ◦ The input is unaffected by the predictor step
  - ▷ The transfer-function ratio is the same as for the trapezoidal method:

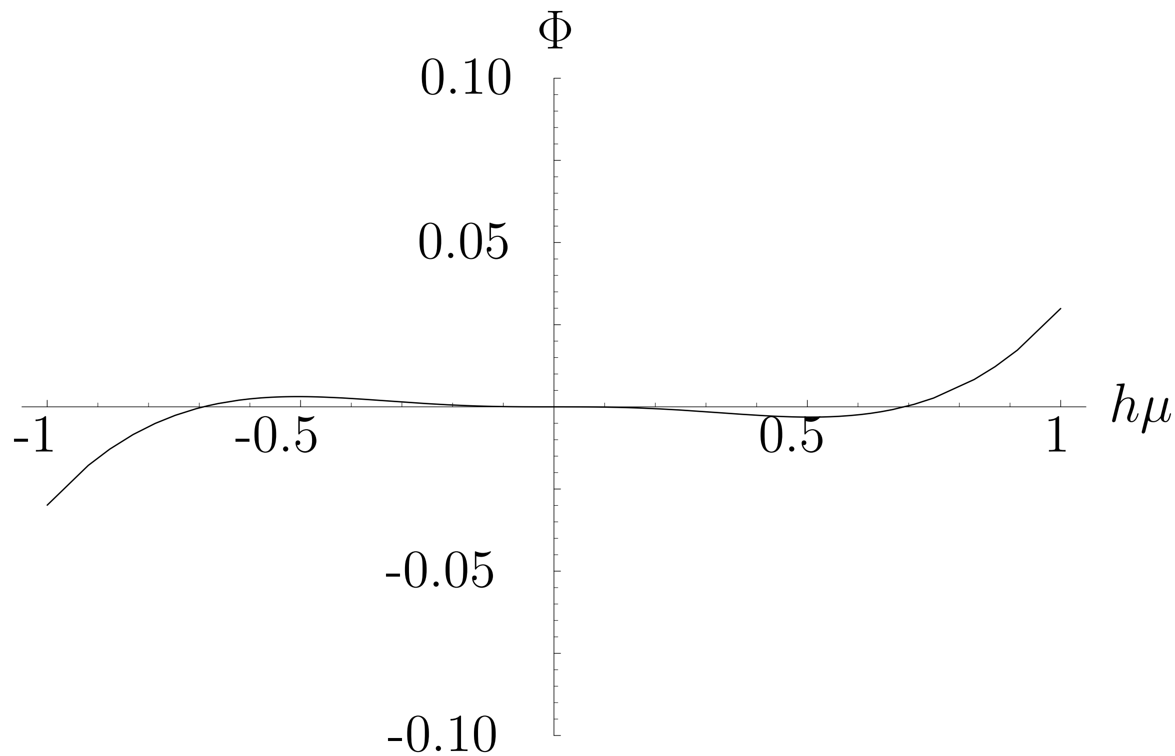
$$R(\omega) = (\omega h/2)\cot(\omega h/2)$$

- In general, for predictor-corrector methods, the corrector step determines the transfer function

PHASE ERROR OF THE MID-TRAP METHOD (1)



PHASE ERROR OF THE MID-TRAP METHOD (2)



RUNGE-KUTTA METHODS

- A typical **fourth-order Runge-Kutta method:**

$$c_{n+1} = c_n + \tfrac{1}{6}[k_1 + 4k_2 + k_3]$$

where

$$k_1 = hf(x_n, c_n)$$

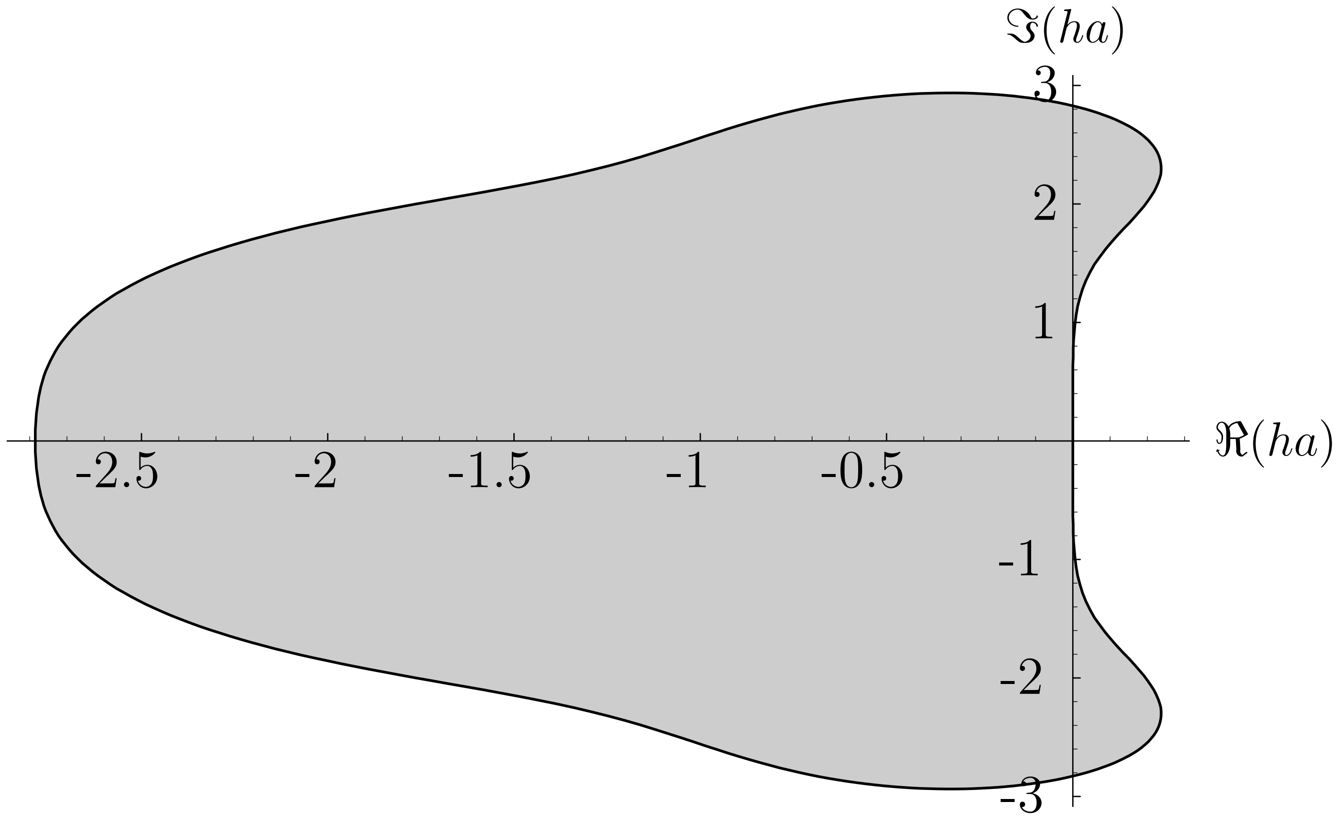
$$k_2 = hf(x_n + h/2, c_n + k_1/2)$$

$$k_3 = hf(x_n + h, c_n - k_1 + 2k_2)$$

▷ Characteristic root for the test problem $y' = ay$:

$$\xi_1 = 1 + ha + \frac{(ha)^2}{2} + \frac{(ha)^3}{6} + \frac{(ha)^4}{24}$$

STABILITY REGION OF 4th ORDER R-K METHOD



$$y' = ay$$

$$c_{n+1} = \left(1 + ha + \frac{(ha)^2}{2} + \frac{(ha)^3}{6} + \frac{(ha)^4}{24}\right) c_n$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (1)

- System of first-order ODEs:

$$\frac{d\mathbf{y}}{dx} = \frac{d}{dx}\begin{pmatrix} y^1 \\ \vdots \\ y^N \end{pmatrix} = \mathbf{y}' := \mathbf{f}(x,\, \mathbf{y}) = \begin{pmatrix} f^1 \\ \vdots \\ f^N \end{pmatrix} \text{ where } y^i = i^{\text{th}} \text{ component of } \mathbf{y}$$

- Linearize:

$$\mathbf{f}(x,\, \mathbf{y}) \approx \mathbf{f}(x,\, \mathbf{y}_0) + \mathbf{J}(\mathbf{f},\, \mathbf{y}_0)(\mathbf{y} - \mathbf{y}_0)$$

$\mathbf{J}(\mathbf{f},\, \mathbf{y}) = N \times N$ Jacobian matrix, $J^i_j = \partial f^i / \partial y^j$

- Why study a linearized system?
  - ▷ A numerical method for a system of nonlinear ODEs must at least be stable and accurate for the linearized system
  - ▷ The linearized system has the same local behavior as the nonlinear system
  - ▷ **The eigenvalues of $\mathbf{J}(\mathbf{f},\, \mathbf{y})$ determine which methods are locally most stable and accurate for a given set of ODEs**

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (2)

References

1. C. W. Gear, *Numerical Initial Value Problems in Ordinary Differential Equations,* Prentice-Hall, 1974
2. L. Lapidus and J. H. Seinfeld, *Numerical Solutions of Ordinary Differential Equations,* Academic Press, 1971
3. G. Dahlquist and A. Björck, *Numerical Methods,* Prentice-Hall, 1974
4. R. W. Hamming, *Digital Filters,* Third Edition, Prentice-Hall, 1989

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (3)

- For stability analysis, approximate a system of nonlinear ODEs locally by

$$\frac{d\mathbf{y}}{dx} = \mathbf{M}\mathbf{y}$$

  - ▷ $\mathbf{M}$ is constant or slowly varying in x
- Assume that $\mathbf{M}$ is a normal matrix (and therefore has an orthonormal basis of eigenvectors):

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

  - ▷ $\mathbf{v}_j$ = dressed state if $\mathbf{M} = -i\mathbf{H}$
  - ▷ $\mathbf{v}_i^* \cdot \mathbf{v}_j = \delta_{ij}$
  - ▷ m^{th} component of $\mathbf{y}_n = y_n^m$
  - ▷ 1-component vector is denoted y_n
- Exact solution of $d\mathbf{y}/dx = \mathbf{M}\mathbf{y}$ for constant $\mathbf{M}$:

$$\mathbf{y}(x) = \sum_{j=1}^{N} K_j \, e^{\lambda_j x} \, \mathbf{v}_j$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (4)

- Discretize by sampling at points $x_n = nh$
  - ▷ Let $\mathbf{y}_n := \mathbf{y}(x_n)$ = discretized exact solution, $\mathbf{c}_n$ = computed solution
- Linear, multistep **difference equation** which approximates $d\mathbf{y}/dx = \mathbf{f}(x, \mathbf{y}) = \mathbf{y}'$:

$$\begin{aligned}\mathbf{c}_{n+1} = &\alpha_1 \mathbf{c}_n + \alpha_2 \mathbf{c}_{n-1} + \cdots + \alpha_k \mathbf{c}_{n-k+1} \\ &+ h[\beta_0 \mathbf{f}(x_{n+1}, \mathbf{c}_{n+1}) + \beta_1 \mathbf{f}(x_n, \mathbf{c}_n) + \cdots + \beta_k \mathbf{f}(x_{n-k+1}, \mathbf{c}_{n-k+1})]\end{aligned}$$

  - ▷ $\beta_0 \neq 0 \Rightarrow$ **implicit** method $\Rightarrow$ iterative solution if $\mathbf{f}$ is nonlinear in $\mathbf{y}$
  - ▷ $\beta_0 = 0 \Rightarrow$ **explicit** method

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (5)

- Computed solution of the difference equation for $\mathbf{y}' = \mathbf{M}\mathbf{y}$:

$$\mathbf{c}_n = \sum_{j=1}^{N} \{d_1^{(j)}[\xi_1^{(j)}]^n + \cdots + d_k^{(j)}[\xi_k^{(j)}]^n\}\mathbf{v}_j$$

  - ▷ $d_1^{(j)}, \ldots, d_k^{(j)}$ = real or complex constants
  - ▷ $\xi_1^{(j)}, \ldots, \xi_k^{(j)}$ = roots of the **characteristic equation**

$$\begin{aligned}[\xi^{(j)}]^k =& \alpha_1[\xi^{(j)}]^k + \alpha_2[\xi^{(j)}]^{k-1} + \cdots + \alpha_k \\ &+ h\lambda_j\{\beta_0[\xi^{(j)}]^k + \beta_1[\xi^{(j)}]^{k-1} + \cdots + \beta_k\}\end{aligned}$$

  - ▷ If root $\xi_l^{(j)}$ is repeated r times: add a linear combination of $n[\xi_l^{(j)}]^n\mathbf{v}_j, \ldots, n^{r-1}[\xi_l^{(j)}]^n\mathbf{v}_j$ to above solution for $\mathbf{y}_n$

- **The characteristic roots determine the local stability and accuracy of the finite-difference method**

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (6)

- The k initial vectors $\mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{k-1}$ determine the constants $d_l^{(j)}$ which appear in the analytical solution of the difference equation
- Assume that:
  - ▷ The characteristic equation has k distinct roots
  - ▷ We are given (by some other method) $\mathbf{c}_n = \kappa_n^{(j)} \mathbf{v}_j$ for $n = 0, \ldots, k-1$ (usually we want the principal root $\Rightarrow j = 1$)
- The k equations

$$\kappa_n^{(j)} = \sum_{l=1}^{k} d_l^{(j)} [\xi_l^{(j)}]^n$$

for $n = 0, \ldots, k-1$ are a non-singular linear system which can be solved for $d_l^{(j)}$ in terms of $\kappa_n^{(j)}$

- In practice one just computes $\mathbf{c}_0, \mathbf{c}_1, \ldots, \mathbf{c}_{k-1}$ by a one-step method

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (7)

- Basic concepts of stability of a finite-difference method
  - ▷ The **principal characteristic root** approximates the exact solution:

$$[\xi_1^{(j)}]^n \approx e^{nh\lambda_j}$$

  - ▷ $\xi_2^{(j)}, \ldots, \xi_k^{(j)}$, which occur whenever $k > 1$, are **parasitic roots**
  - ▷ **Relative stability:**

$$|\xi_1| \geq |\xi_l|$$

    for $l = 2, \ldots, k \Rightarrow$ the parasitic part of the solution never exceeds the principal part
  - ▷ **Absolute stability,**

$$|\xi_l| \leq 1 \quad (l = 1, \ldots, k),$$

    is necessary when the exact solution of the ODE is damped or has a constant norm

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (8)

- Basic concepts pertaining to the accuracy of a finite-difference method:
  - ▷ **Local truncation error:**

$$T(\{\alpha\};\{\beta\};h\lambda) = \xi_1 - e^{h\lambda}$$

  - ▷ The **order** of the **local discretization error**

$$L_h[y(x)] = \sum_{l=0}^{k} [\alpha_l y(x - lh) + h\beta_l y'(x - lh)]$$

    (where $\alpha_0 = -1$) is the smallest r such that

$$L_h[y(x)] \sim O(h^{r+1})$$

    for every y with $r+1$ continuous derivatives
  - ▷ A finite-difference method is **consistent** with an ODE of order p if the order of L_h is at least p.
  - ▷ Consistency $\Rightarrow$ L_h approaches the correct differential operator as $h \longrightarrow 0$.

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (9)

- A quantitative expression for the effect of a finite-difference operator:
  - ▷ Apply Taylor's theorem to $L_h[y(x)]$:

$$L_h[y(x)] = \sum_{q=0}^{r+1} C_q h^q y^{[q]}(x) + O(h^{r+2})$$

$$C_0 = \sum_{l=0}^{k} \alpha_l$$

$$C_q = \sum_{l=0}^{k} \left[\frac{(-l)^q}{q!}\alpha_l + \frac{(-l)^{q-1}}{(q-1)!}\beta_l \right] \quad (q > 0)$$

  - ▷ If the method is consistent with a first-order ODE, then

$$C_0 = 0, \quad C_1 = 0$$

  - ▷ If the order of the finite-difference operator L_h is r, then

$$C_0 = C_1 = \cdots = C_r = 0$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (10)

- A quantitative expression for the local truncation error:
  - ▷ If $y' = \lambda y$ ($\Rightarrow$ exact solution is $e^{\lambda x}$) and if L_h is of order r, then

$$\begin{aligned} L_h[e^{\lambda x}] &= e^{\lambda(x-hk)}\phi(e^{h\lambda}) \\ &= C_{r+1}(h\lambda)^{r+1} + O(h^{r+2}) \end{aligned}$$

  - ▷ In terms of the characteristic polynomial, ϕ:

$$\phi(e^{h\lambda}) = \sum_{l=0}^{k}(\alpha_l + h\lambda\beta_l)\left[e^{h\lambda}\right]^{k-l}$$

$$\Rightarrow \phi(e^{h\lambda}) = C_{r+1}(h\lambda)^{r+1} + O(h^{r+2})$$

$$\Rightarrow \xi_1 = e^{h\lambda} - \frac{C_{r+1}(h\lambda)^{r+1}}{\sum_{l=0}^{k}\beta_l}$$

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (11)

- Common methods for ODEs which are *not* discretized PDEs:

Method	k	E	Type	Stiff Eqs?
Runge-Kutta	1	≥ 4	explicit	no
Adams-Bashforth (P)	≥ 4	1	explicit	no
Adams-Moulton (C)	≥ 4	1	implicit	no
Gear	≥ 4	1	implicit	yes

In the table:
P = predictor,
C = corrector,
k = no. of steps,
E = no. of evaluations of right-hand side per step,
"Type" = explicit or implicit

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (12)

- Common methods for discretized PDEs:

Method	k	E	Type	Stiff Eqs?
Midpoint (P)	2	1	explicit	no
Trapezoidal (C)	1	1	implicit	no
Backward Euler	1	1	implicit	yes

- In the above, P means a predictor method and C means a corrector method. The usual usage of a predictor-corrector set is PECE (predict, evaluate y', correct, evaluate y').

STABILITY OF FINITE-DIFFERENCE METHODS FOR ODEs (13)

- A **minimax approach** to designing a finite-difference method (Chu and Cantrell):
  - ▷ The **maximum local truncation error** is

    $$T_{\max}(\{\alpha\};\{\beta\};S) = \max_{h\lambda\in S} |T(\{\alpha\};\{\beta\};h\lambda)|$$

    where S is the region of stability (or some useful subset)
  - ▷ Choose the coefficients $\{\alpha\};\{\beta\}$ in L_h to minimize $T_{\max}(\{\alpha\};\{\beta\};S)$:

    $$T_{\text{minimax}}(S) = \min_{\{\alpha\};\{\beta\}} T_{\max}(\{\alpha\};\{\beta\};S)$$
  - ▷ Implementation of the minimax principle:
    - ◦ Expand the local truncation error in Chebyshev polynomials and make the first N Chebyshev coefficients vanish
    - ◦ Perform a numerical minimization

STIFF ORDINARY DIFFERENTIAL EQUATIONS (1)

- Example:

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

where

$$\mathbf{M} = \begin{pmatrix} 998 & -999 \\ -999 & -1999 \end{pmatrix}$$

Eigenvalues: $\lambda_1 = -1$, $\lambda_2 = -1000$

▷ Solution when

$$\mathbf{y}(0) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

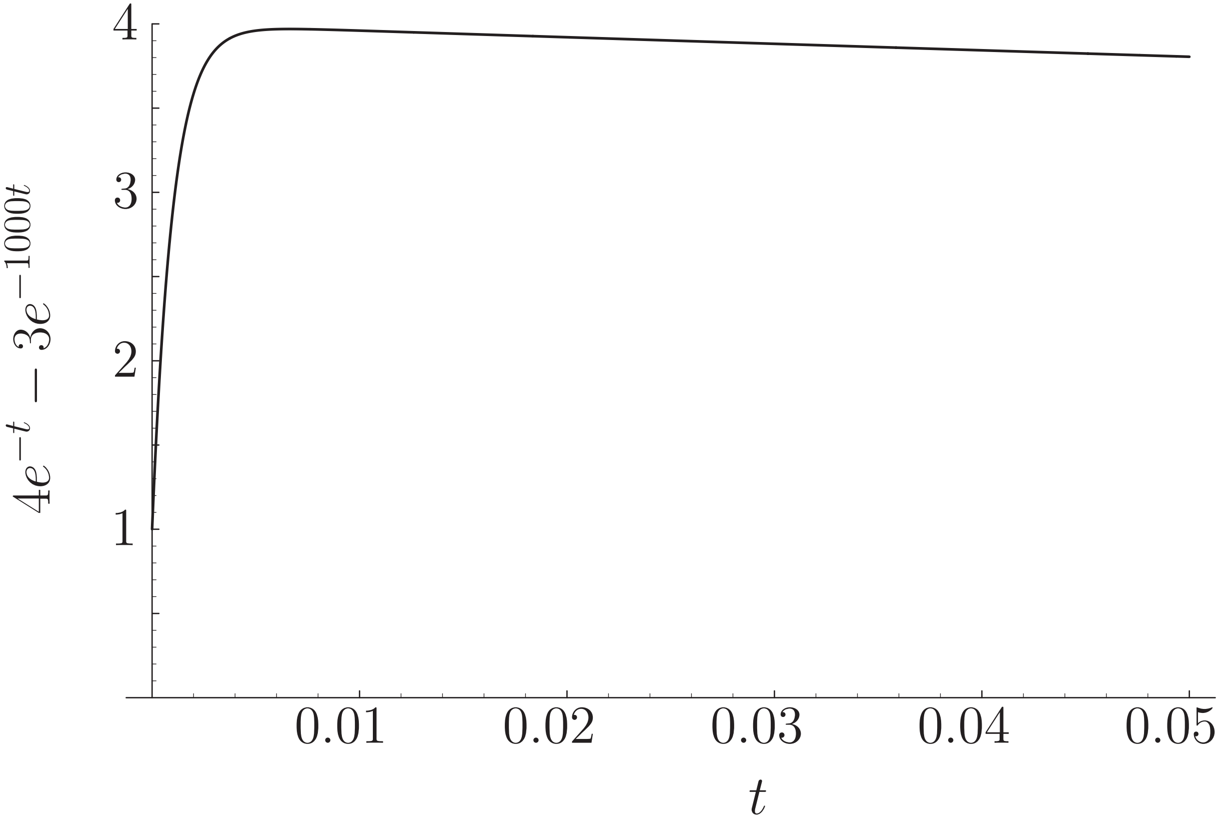
is

$$\mathbf{y}(t) = \begin{pmatrix} 4e^{-t} - 3e^{-1000t} \\ -2e^{-t} + 3e^{-1000t} \end{pmatrix}$$

▷ For most numerical methods, the e^{-1000t} part $\Rightarrow$ very small step size, even though $e^{-1000t} \ll e^{-t}$ for $t > 2 \times 10^{-3}$

"STIFF" TIME DEPENDENCE

- Plot shows one component of the solution of a set of stiff equations
  - ▷ The kink occurs because e^{-1000t} decays away rapidly, leaving only e^{-t}



STIFF ORDINARY DIFFERENTIAL EQUATIONS (2)

- A *system* of ODEs is called **stiff** if there exist eigenvalues λ, λ' of the Jacobian matrix $\mathbf{J}(\mathbf{f}, \mathbf{y})$ such that

$$|\operatorname{Re}[\lambda]| \gg |\operatorname{Re}[\lambda']|.$$

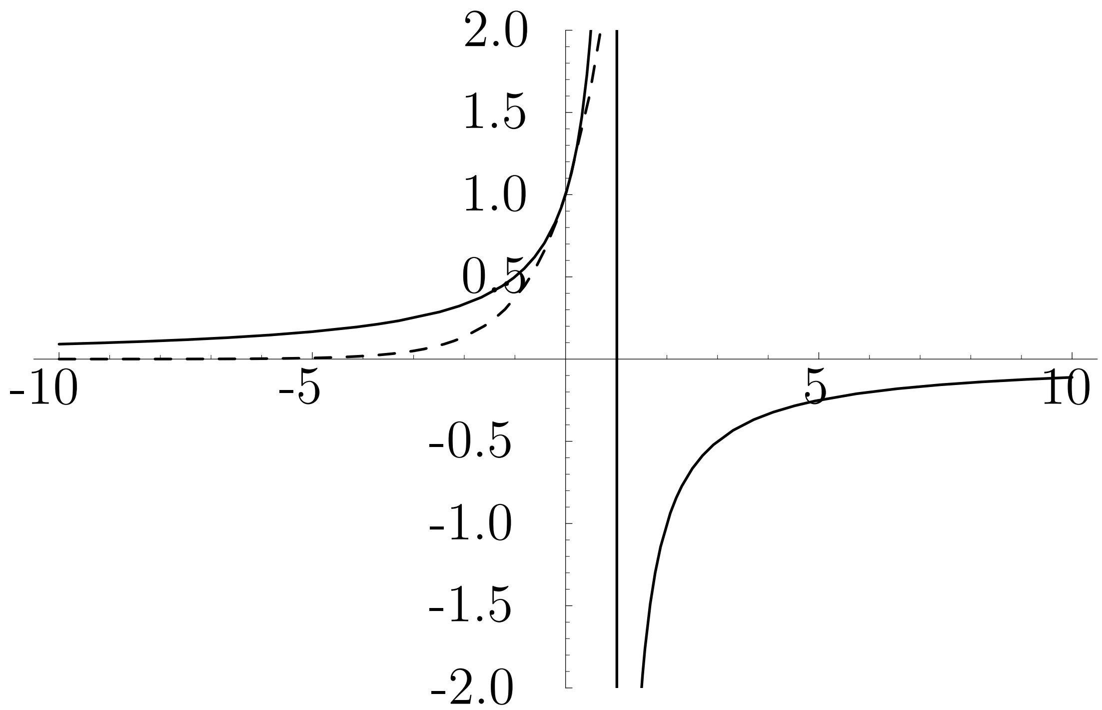
  - ▷ Methods in which the region of absolute stability is *inside* a closed curve require step sizes of order $K/|\lambda| \ll K/|\lambda'|$ to ensure that both $h\lambda$ and $h\lambda'$ are inside the region of stability.
  - ▷ The basic stiff method: the **backward Euler method**

$$\mathbf{c}_{n+1} = \mathbf{c}_n + h\mathbf{f}(x_{n+1}, \mathbf{c}_{n+1})$$

    - ○ Characteristic root $= 1/(h\lambda - 1)$
    - ○ Stable *outside* the circle $|h\lambda - 1| = 1$

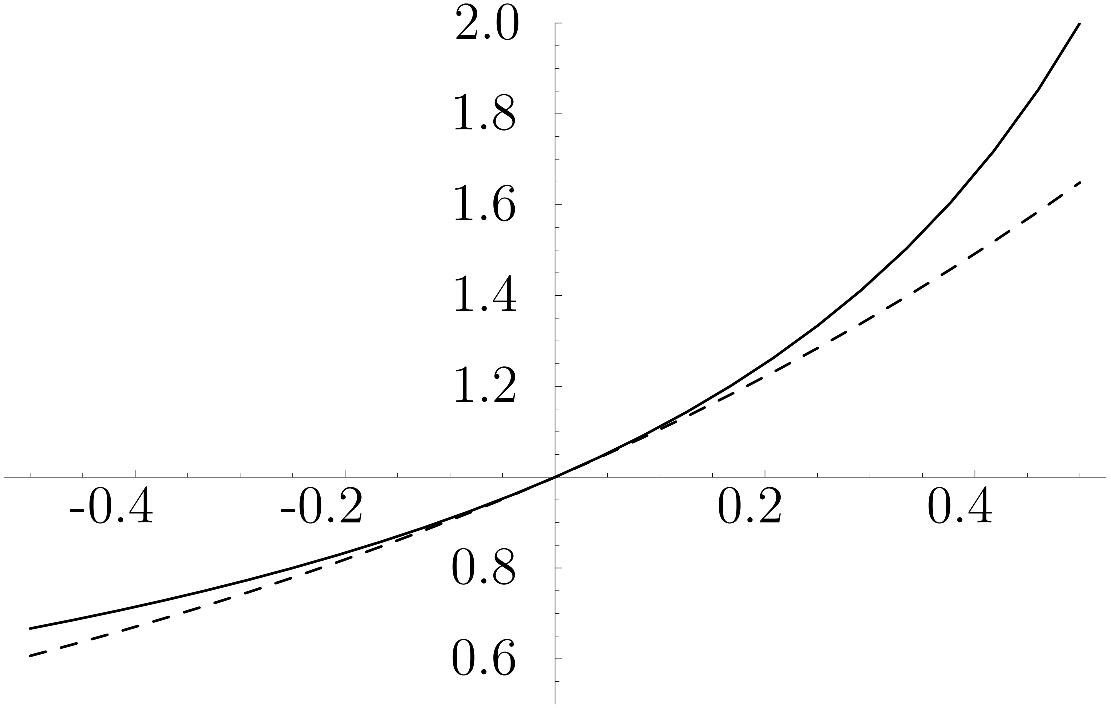
ACCURACY OF THE BACKWARD EULER METHOD (1)

- Plot shows $(1 - ha)^{-1}$ (solid line) and e^{ha} (dashed line) vs. real values of ha



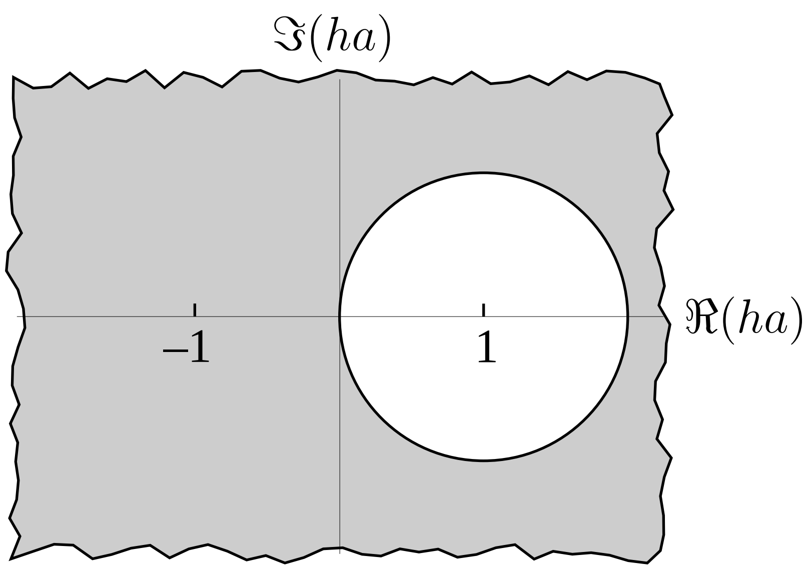
ACCURACY OF THE BACKWARD EULER METHOD (2)

- Plot shows $(1-ha)^{-1}$ (solid line) and e^{ha} (dashed line) vs. real values of ha



STIFF ORDINARY DIFFERENTIAL EQUATIONS (3)

- Region of absolute stability of the backward Euler method:



$$y' = ay$$

$$c_{n+1} = (1 - ha)^{-1}\, c_n$$

STIFF ORDINARY DIFFERENTIAL EQUATIONS (4)

- A finite-difference scheme for a *system* of ODEs is called **stiffly stable** if:
  - ▷ The scheme is absolutely stable for all $h\lambda$ such that $\mathrm{Re}[h\lambda] < D$
  - ▷ The scheme is accurate in a rectangular region of the $h\lambda$ plane such that $\mathrm{Re}[h\lambda] \in [D, \alpha]$ and $\mathrm{Im}[h\lambda] \in [-i\theta, i\theta]$

STIFF ORDINARY DIFFERENTIAL EQUATIONS (5)

- Coefficients for stiffly stable methods (calculated by C. W. Gear):

$$c_n = \sum_{i=1}^{k} \alpha_i c_{n-i} + h\beta_0 f_n$$

	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$
β_0	$\frac{2}{3}$	$\frac{6}{11}$	$\frac{12}{25}$	$\frac{60}{137}$	$\frac{60}{147}$
α_1	$\frac{4}{3}$	$\frac{18}{11}$	$\frac{48}{25}$	$\frac{300}{137}$	$\frac{360}{147}$
α_2	$-\frac{1}{3}$	$-\frac{9}{11}$	$-\frac{36}{25}$	$-\frac{300}{137}$	$-\frac{450}{147}$
α_3		$\frac{2}{11}$	$\frac{16}{25}$	$\frac{200}{137}$	$\frac{400}{147}$
α_4			$-\frac{3}{25}$	$-\frac{75}{137}$	$-\frac{225}{147}$
α_5				$\frac{12}{137}$	$\frac{72}{147}$
α_6					$-\frac{10}{147}$