

Set 18: Ordinary Differential Equations: Basic Concepts

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Foundations of Computational Math 2

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Sources and References

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The Initial Value Problem

Let $y(t) \in \mathbb{R}^n$ be a vector whose components are scalar functions of $t \in \mathbb{R}$, i.e., one independent variable.

Let $y'(t) \in \mathbb{R}^n$ be a vector whose components are the derivatives of the components of $y(t) \in \mathbb{R}^n$.

Let $f(y, t) \in \mathbb{R}^n$ be a vector whose components are scalar functions of time and the components of the vector $y(t) \in \mathbb{R}^n$ such that

$$y'_i(t) = \frac{dy_i}{dt}(t) = f_i(y, t)$$

The initial value problem is to find $y(t)$ given that

$$y'(t) = f(y, t) \quad \text{and} \quad y(0) = y_0$$

The Applications

ODEs are used to present the evolution over time of discrete interacting quantities interconnected via, e.g.,

- discrete interconnection network
 - circuit or power systems simulation
 - mechanical systems, e.g., spring-mass
- a “field” effect
 - molecular dynamics
 - electromagnetics
- discrete interaction laws
 - predator-prey
 - chemical reactions
- discrete quantities may represent a discretization of continuous quantities

Lipschitz Continuity

Definition 18.1. The function $f(y, t): \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ is Lipschitz continuous on $\mathcal{D} = |y| < \infty \times [a, b]$ if $\exists L$ such that for all (t, y) and (t, \hat{y}) in \mathcal{D}

$$|f(t, y) - f(t, \hat{y})| \leq L|y - \hat{y}|$$

If f is differentiable in y then L can be taken as a bound on the norm of the Jacobian matrix, $J = f_y(y, t)$.

Well-posed Form

If f is Lipschitz continuous then given the initial value problem

$$y'(t) = f(y, t) \quad \text{and} \quad y(0) = y_0$$

- There exists a unique differentiable solution on $[a, b]$ for each y_0 .
- The solution depends continuously on y_0 , i.e.,

$$|y(t) - \hat{y}(t)| \leq e^{Lt} |y(0) - \hat{y}(0)|$$

- The solution of a bounded perturbation of the ODE

$$\hat{y}'(t) = f(\hat{y}, t) + r(\hat{y}, t) \quad \hat{y}(0) = \hat{y}_0, \quad \|r\| \leq M$$

$$|y(t) - \hat{y}(t)| \leq e^{Lt} |y(0) - \hat{y}(0)| + \frac{M}{L} (e^{Lt} - 1)$$

Example: Simple Oscillator

- Derivative

$$f = \begin{pmatrix} f_1(y_1, y_2) \\ f_2(y_1, y_2) \end{pmatrix} = \begin{pmatrix} \omega y_2 \\ -\omega y_1 \end{pmatrix} = \begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = Ay$$

- Solution

$$\begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} 0 \\ \gamma \end{pmatrix} \quad \begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix} = \begin{pmatrix} \gamma \sin(\omega t) \\ \gamma \cos(\omega t) \end{pmatrix}$$

- linear, time-invariant, autonomous system

Example: Simple Predator-Prey System (Petzold)

- Derivative

$$f = \begin{pmatrix} f_1(y_1, y_2) \\ f_2(y_1, y_2) \end{pmatrix} = \begin{pmatrix} \alpha y_1 - \beta y_1 y_2 \\ \gamma y_2 - \delta y_1 y_2 \end{pmatrix}$$

- Parameters

- $[y_1(t), y_2(t)]$ population of [prey, predator].
- $\alpha > 0$ prey's birthrate minus natural deathrate
- $1 > \beta > 0$ probability of predator and prey meeting
- $\gamma < 0$ predator natural growth rate without prey
- δ increase in growth rate if predator and prey meet

- periodic solutions – stable but not constant populations
- nonlinear and autonomous

Example: Driven System

- Derivative

$$\dot{y} = A(y - F(t)) + F'(t), \quad y(0) = y_0$$

- Solution

$$y(t) = (y_0 - F(0))e^{At} + F(t)$$

- time-invariant and linear (in y), nonautonomous system

Example: Van der Pol Oscillator

- Derivative

$$f = \begin{pmatrix} f_1(y_1, y_2) \\ f_2(y_1, y_2) \end{pmatrix} = \begin{pmatrix} y_2 \\ \mu(1 - y_1^2)y_2 - y_1 + \alpha \sin(\omega t) \end{pmatrix}$$

- from harmonic oscillator to damped rapidly changing oscillation
- nonlinear and nonautonomous

A Simple Method

Discretize the differential equation to solve it numerically,

$$y'(t) - f(y, t) = 0 \quad \text{and} \quad y(0) = y_0$$

Forward Euler Method

$$\frac{y_n - y_{n-1}}{h_n} - f(t_{n-1}, y_{n-1}) = 0$$

$$h_n = t_n - t_{n-1} \quad f_{n-1} = f(t_{n-1}, y_{n-1})$$

where y_i are the numerical solution values defined on the mesh induced by the h_i values, $t_0 < \dots < t_n < \dots < t_N$.

Forward Euler

- Evaluate recurrence to solve: $y_0 = c$ given, $y_n = y_{n-1} + h_n f_{n-1}$.
- Each step requires evaluation of $f(t_{n-1}, y_{n-1})$; not a solution of an equation with $f(t, y)$.
- A nonlinear recurrence due to dependence of f on y but has overall structure of a linear recurrence.

$$\begin{array}{l} y_1 = y_0 + hf_0 \\ y_2 = y_1 + hf_1 \\ y_3 = y_2 + hf_2 \end{array} \Leftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} c \\ hf_0 \\ hf_1 \\ hf_2 \end{pmatrix}$$

Difference Operator

Numerical methods replace a differential equation with a difference equation.

For example, Forward Euler has the difference operator,

$$\mathcal{N}_{h_n}[u(t_n)] = \frac{u(t_n) - u(t_{n-1})}{h_n} - f(t_{n-1}, u(t_{n-1}))$$

for any function $u(t)$ valid at mesh points.

- Forward Euler has a simple difference operator.
- Much more complicated forms are possible.
- All numerical methods for ODEs of interest can be expressed in terms of this type of operator.

Numerical Solutions

The numerical solution to the ODE is given by a set of equations and initial conditions.

For an s –step method, $s \geq 1$, the numerical solution y_n is

$$\begin{aligned} y_n &= c_n, \quad 0 \leq n < s \\ \mathcal{N}_{h_n}[y_n] &= 0 \quad s \leq n \leq N \end{aligned}$$

- This does not say anything about finite precision or approximate solutions.
- Shorthand for entire sequence and inverse mapping:

$$\mathcal{N}_{h_n}[y_*] = 0 \quad \text{and} \quad \mathcal{N}_{h_n}^{-1}[0] = y_*$$

Topics

- Convergence – Does the solution of the difference equation converge to the solution of the differential equation?
- Discretization Error (Consistency) – How well does the difference equation represent the differential equation?
- Stability – How sensitive is the solution to the difference equation to perturbations due to, e.g., finite precision computation or inexact data?

Discretization Error and Consistency

The solution to the differential equation **does not solve** the difference equation.

$$y' = \lambda y, \quad y(0) = y_0, \quad y(t) = y_0 e^{\lambda t}, \quad \text{IVP}$$

$$y' - \lambda y = 0 \quad \text{Differential equation}$$

$$\frac{y_n - y_{n-1}}{h_n} - \lambda y_{n-1} = 0 \quad \text{Difference equation}$$

$$\text{Let } \lambda = -1, \quad t_{n-1} = 1, \quad t_n = 2$$

$$\begin{aligned} \frac{y(t_n) - y(t_{n-1})}{h_n} - \lambda y(t_{n-1}) &= \frac{e^{-2} - e^{-1}}{2 - 1} + e^{-1} \\ &= e^{-2} \approx -0.097208875 \end{aligned}$$

Discretization Error and Consistency

Definition 18.2. The discretization error or local truncation error of a method is the residual when the difference operator is applied to the exact solution of the ODE, $y(t)$.

$$\mathcal{N}_{h_n}[y(t_n)] = d_n \quad s < n \leq N$$

$$\mathcal{N}_{h_n}[y(t_*)] = d_*, \quad \mathcal{N}_{h_n}^{-1}[d_*] = y(t_*)$$

Definition 18.3. A method is consistent of order $p > 0$ if

$$d_n = \mathcal{N}_{h_n}[y(t_n)] = C_{p+1} h_n^p y^{(p+1)}(\xi_n) = \mathcal{O}(h_n^p) \quad s < n \leq N$$

$$d_* = \mathcal{N}_h[y(t_*)] = \mathcal{O}(h^p)$$

The difference equation becomes an increasingly good approximation of the differential equation as $h \rightarrow 0$.

Forward Euler

Lemma. *Forward Euler is consistent.*

Proof. Suppose $y(t)$ solves the initial value problem and has Taylor expansion at all relevant points. Substituting the expansions yields

$$y(t_n) = y(t_{n-1}) + h_n y'(t_{n-1}) + \frac{h_n^2}{2} y''(\xi)$$

$$= y(t_{n-1}) + h_n f(t_{n-1}, y(t_{n-1})) + \mathcal{O}(h_n^2)$$

$$y(t_n) - y(t_{n-1}) - h_n f(t_{n-1}, y(t_{n-1})) = \mathcal{O}(h_n^2)$$

$$\mathcal{N}_{h_n}[y(t_n)] = \frac{y(t_n) - y(t_{n-1})}{h_n} - f(t_{n-1}, y(t_{n-1})) = \mathcal{O}(h_n)$$

\therefore Forward Euler is consistent. □

Convergence

What about the solutions of the difference and differential equations?

Definition 18.4. Given h_i values and the mesh they induce, $t_0 < \dots < t_n < \dots < t_N$ with t_0 and t_N fixed as $h_i \rightarrow 0$, the global error is defined on the mesh as

$$e_n = y_n - y(t_n), \quad \text{with } e_0 = 0.$$

A difference method \mathcal{N}_h is convergent of order k if

$$e_n = \mathcal{O}(h^k) \quad \text{where } \forall i, h > h_i$$

Convergence Forward Euler

Scalar Forward Euler on the fixed interval $[t_0, t_N]$.

$$y_{n+1} = y_n + hf_n$$

$$y(t_{n+1}) = y(t_n) + hf(t_n, y(t_n)) + hd_n$$

$$e_{n+1} = e_n + h(f(t_n, y(t_n)) - f_n) + hd_n$$

$$\text{by MVT } |f(t_n, y(t_n)) - f_n| \leq L_n |y(t_n) - y_n|$$

$$|e_{n+1}| \leq (1 + hL_n)|e_n| + |hd_n|$$

Convergence Forward Euler

$$|e_{n+1}| \leq (1 + hL_n)|e_n| + |hd_n|$$

Take for a fixed h the bounds $L_n \leq L$, $|hd_n| \leq h\delta$

$$|e_{n+1}| \leq (1 + hL)|e_n| + h\delta$$

$$|e_{n+1}| \leq (1 + hL)^{n+1}|e_0| + h\delta \sum_{i=0}^n (1 + hL)^i$$

$$e_0 = 0 \rightarrow |e_N| \leq h\delta \frac{(1 + hL)^N - 1}{hL} = \delta \frac{(1 + hL)^N - 1}{L}$$

Convergence Forward Euler

$$|e_N| \leq h\delta \frac{(1 + hL)^N - 1}{hL}$$

- Two terms: first is based on difference equation and the second is based on the differential equation.
- L can be taken as the Lipschitz constant for $f(t, y)$ which is independent of h .
- As $h \rightarrow 0$ and $N \rightarrow \infty$ consistency implies $d_n \rightarrow 0$ therefore the bound can be taken as a function of h with $\delta \rightarrow 0$.
- convergence follows, i.e., $|e_N| \rightarrow 0$. and $|e_N| = \mathcal{O}(h)$.
- consistency is necessary for convergence, i.e., convergence implies consistency.

Convergence and Consistency

Lemma. *Convergence implies consistency.*

Question: Let $h \rightarrow 0$.

Does $\|d_*\| = \mathcal{O}(h^p) \Rightarrow \|e_*\| = \|y_* - y(t_*)\| = \mathcal{O}(h^p)$?

Answer: Yes, if \mathcal{N}_h^{-1} is Lipschitz continuous uniformly with respect to h .

Note. We need better ways to characterize convergent methods!

Computed Numerical Solutions

In practice, due to inexact arithmetic, perturbations to data (coefficients, initial conditions etc.) and approximate solutions of equations we do not have

$$\mathcal{N}_{h_n}[y_*] = 0 \quad \text{and} \quad \mathcal{N}_{h_n}^{-1}[0] = y_*$$

Computed numerical solutions satisfy

$$\mathcal{N}_{h_n}[\hat{y}_*] = \hat{\delta}_* \quad \text{and} \quad \mathcal{N}_{h_n}^{-1}[\hat{\delta}_*] = \hat{y}_*$$

Stability of Forward Euler Method

Apply Forward Euler to solve $y' = f(y, t)$, $y(0) = c$.

Suppose that due to finite precision when evaluating $f(y, t)$ and computing y_n we introduce errors.

Denoting the computed solution to the difference equation z_n , we have

$$z_0 = c + \delta_0, \quad z_n = z_{n-1} + hf(t_{n-1}, z_{n-1}) + h\delta_n$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} z_0 \\ z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} c + \delta_0 \\ hf_0 + h\delta_1 \\ hf_1 + h\delta_2 \\ hf_2 + h\delta_3 \end{pmatrix}$$

Stability of Forward Euler Method

Suppose $\mathcal{N}_{h_n}[\tilde{z}_*] = \tilde{\delta}_*$ and $\mathcal{N}_{h_n}[z_*] = \delta_*$ for Forward Euler applied to a differential equation $y' = f(y, t)$, $y(0) = c$ with Lipschitz constant L .

$$z_0 = c + \delta_0, \quad z_n = z_{n-1} + hf(t_{n-1}, z_{n-1}) + h\delta_n$$

$$\tilde{z}_0 = c + \tilde{\delta}_0, \quad \tilde{z}_n = \tilde{z}_{n-1} + hf(t_{n-1}, \tilde{z}_{n-1}) + h\tilde{\delta}_n$$

The following very loose bound can be proven

$$\|\tilde{z}_* - z_*\| \leq \left[\frac{e^{L(t_N - t_0)} - 1}{L} + e^{L(t_N - t_0)} \right] \|\tilde{\delta}_* - \delta_*\|$$

- difference solution is stable, i.e., bounded response to perturbations
- not useful for error estimation

Stability of Numerical Difference Methods

Definition 18.5. The numerical method defined by \mathcal{N}_{h_n} is *0-stable* for each differential equation satisfying the Lipschitz condition if $\exists h_0 > 0$ and $K > 0$, independent of h , such that for any two solutions z_* and \tilde{z}_* with $\mathcal{N}_{h_n}[\tilde{z}_*] = \tilde{\delta}_*$ and $\mathcal{N}_{h_n}[z_*] = \delta_*$ we have

$$\|\tilde{z}_* - z_*\| \leq K \|\tilde{\delta}_* - \delta_*\|$$

for all $h < h_0$, where the norm $\|\delta_* - \hat{\delta}_*\|$ includes the initial conditions specified for each sequence.

Note. We need better ways to characterize stable methods!

Convergence

Theorem 18.1. (Henrici) *If the method \mathcal{N}_{h_n} is consistent of order p and 0–stable then it is convergent of order p :*

$$\|e_n\| \leq K \max_j \|d_j\| = \mathcal{O}(h^p)$$

- consistency and 0–stability \Rightarrow convergence
- necessary and sufficient for some classes of methods
- consistency is related to size of local errors and stability is related to how they propagate.
- d_n is not the local error

Local Error

The local error is the difference between the numerical solution y_n and the solution of the IVP using the numerical solution value y_{n-1} as an initial condition at t_{n-1} .

If $u(t_{n-1}) = y_{n-1}$, $u'(t) = f(t, u(t))$ then $\ell_n = y_n - u(t_n)$

global error $e_n = y(t_n) - y_n$

Local Error

The local truncation error for local solution $u(t)$ can be used to estimate local error:

$$\|d_n\| = \|\mathcal{N}_h[u(t_n)]\| + \mathcal{O}(h^{p+1})$$

$$h_n \|\mathcal{N}_h[u(t_n)]\| = \|\ell_n\|(1 + \mathcal{O}(h_n))$$

- Therefore, $h_n \|d_n\|$ and $\|\ell_n\|$ are closely related local error estimators.
- Both can be related to the global error.

Local Error

Consider the simple example of forward Euler and the local truncation error for the local solution $u(t)$:

$$\begin{aligned}\mathcal{N}_h[u(t_n)] &= \frac{u(t_n) - u(t_{n-1})}{h} - f(t_{n-1}, u(t_{n-1})) \\ &= \frac{u(t_n) - y_{n-1}}{h} - f(t_{n-1}, y_{n-1})\end{aligned}$$

$$\begin{aligned}h\mathcal{N}_h[u(t_n)] &= u(t_n) - y_{n-1} - hf(t_{n-1}, y_{n-1}) \\ &= u(t_n) - (y_{n-1} + hf(t_{n-1}, y_{n-1})) = u(t_n) - y_n \\ &= \ell_n\end{aligned}$$

- $h_n\mathcal{N}_h[u(t_n)] = \ell_n$ is true for one-step methods of interest.
- For s -step methods use the more general forms on the previous slide.

Implicit Methods

- Forward Euler is an explicit method – no solution of a nonlinear equation required to take a step.
- Implicit methods are often superior from some points of view.
- The numerical difference operator \mathcal{N}_h defining y_n involves $f(t_n, y_n)$.
- This requires the solution of an equation possibly nonlinear to determine y_n
- Solutions via functional iteration, Newton's method, etc.
- Two examples Backward Euler, trapezoidal rule.

Examples

Backward Euler:

$$\mathcal{N}_{h_n}[y_n] = \frac{y_n - y_{n-1}}{h_n} - f(t_n, y_n) = 0 \Rightarrow y_n = y_{n-1} + h_n f(t_n, y_n)$$

$$\begin{aligned} y_1 &= y_0 + h f_1 \\ y_2 &= y_1 + h f_2 \\ y_3 &= y_2 + h f_3 \end{aligned} \Leftrightarrow \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} c \\ h f_1 \\ h f_2 \\ h f_3 \end{pmatrix}$$

Computing y_n requires solving the nonlinear equation

$$F(z) = \frac{z - y_{n-1}}{h_n} - f(t_n, z) = 0$$

Examples

Trapezoidal Rule:

$$\mathcal{N}_{h_n}[y_n] = \frac{y_n - y_{n-1}}{h_n} - \frac{1}{2}(f(t_n, y_n) + f(t_{n-1}, y_{n-1})) = 0$$

$$y_1 = y_0 + \frac{h}{2}(f_1 + f_0), \quad y_2 = y_1 + \frac{h}{2}(f_2 + f_1), \quad y_3 = y_2 + \frac{h}{2}(f_3 + f_2)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} c \\ \frac{h}{2}(f_1 + f_0) \\ \frac{h}{2}(f_2 + f_1) \\ \frac{h}{2}(f_3 + f_2) \end{pmatrix}$$

Absolute Stability

- 0–stability is related to perturbations and $h \rightarrow 0$
- instability in that sense, relates to blowing up of small local errors to overwhelm the solution
- setting h should allow the numerical difference method to mimic the behavior of the solution when $h \neq 0$
- test equation for $\lambda \in \mathbb{C}$ and $c \in \mathbb{R}$

$$y' = \lambda y \quad y(0) = c \Rightarrow y(t) = ce^{\lambda t}$$

- behavior of solution:
 - $\operatorname{Re}(\lambda) < 0 \Rightarrow |y(t)| \rightarrow 0$ (damped)
 - $\operatorname{Re}(\lambda) > 0 \Rightarrow |y(t)| \rightarrow \infty$ (increasing)
 - $\operatorname{Re}(\lambda) = 0 \Rightarrow |y(t)| = c$ (oscillatory)

Absolute Stability

Definition 18.6. The region of absolute stability for a numerical difference method \mathcal{N}_h is the region in the complex plane

$$\{h\lambda \mid y' = \lambda y, \mathcal{N}_h[y_*] = 0, \forall n \mid |y_n| < K\}$$

That is, the numerical solution of the test equation remains bounded.

Ideally we want the numerical solution

- bounded in entire left-half plane like the true solution (A-stable)
- unstable in the right-half plane near the origin
- stable/unstable/don't care in rest of right-half plane depending on the application

Examples

Forward Euler:

$$y_n = y_{n-1} + hf(t_n, y_{n-1}) \rightarrow y_n = y_{n-1} + h\lambda y_{n-1}$$

$$y_n = (1 + h\lambda)y_{n-1} = \cdots = (1 + h\lambda)^n y_0$$

$$|y_n| \leq |(1 + h\lambda)^n| |y_0|$$

$$|(1 + h\lambda)^n| \leq 1 \Leftrightarrow |1 + h\lambda| \leq 1$$

Absolute stability region: $\{h\lambda : |h\lambda + 1| \leq 1\}$

Stable only in circle around -1 with radius 1.

Examples

Backward Euler:

$$y_n = y_{n-1} + hf(t_n, y_n) \rightarrow y_n = y_{n-1} + h\lambda y_n$$

$$y_n = (1 - h\lambda)^{-1} y_{n-1} = \cdots = (1 - h\lambda)^{-n} y_0$$

$$|y_n| \leq |(1 - h\lambda)^{-n}| |y_0|$$

$$|(1 - h\lambda)^{-n}| \leq 1 \Leftrightarrow |1 - h\lambda| \geq 1$$

Absolute stability region: $\{h\lambda : 1 \leq |h\lambda - 1|\}$

Unstable only within circle around 1 with radius 1

A-stable method and superstable in right-half plane

Examples

Trapezoidal Rule:

$$\frac{y_n - y_{n-1}}{h} - \frac{1}{2}(f(t_n, y_n) + f(t_{n-1}, y_{n-1})) = 0$$

$$\frac{y_n - y_{n-1}}{h} - \frac{1}{2}(\lambda y_n + \lambda y_{n-1}) = 0$$

$$(1 - \frac{h\lambda}{2})y_n = (1 + \frac{h\lambda}{2})y_{n-1}$$

$$|y_n| \leq \left(\frac{|2 + h\lambda|}{|2 - h\lambda|} \right)^n |y_0|$$

Absolute stability region: $\{h\lambda : |h\lambda + 2| \leq |h\lambda - 2|\}$

A-stable method and unstable in right-half plane

