Chapter 5
Initial Value Problems for ODEs: One-Step Methods

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Differential Equations

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

Order of ODE

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

ODEs

- Initial Value Problem (IVP) for First-oder ODE:

$$\frac{dy}{dx} = f(x, y) \tag{1}$$

for $x \in [a, b]$ with an initial condition $y(a) = y_0$.

- IVP for a system of first-order ODEs:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}) \tag{2}$$

for $x \in [a, b]$ with an initial condition $\mathbf{y}(a) = \mathbf{y}_0$, where

$$\mathbf{y} = [y^1, \ldots, y^d]^T, \mathbf{f} = [f^1, \ldots, f^d]^T, \mathbf{y}_0 = [y_0^1, \ldots, y_0^d]^T$$

Higher-Order ODEs

- IVP for a dth-order ODE:

$$y^{(d)} = f(x, y, y', \ldots, y^{(d-1)})$$

for $x \in [a, b]$ with an initial condition $y^{(i)}(a) = y_0^i,\ i = 0, 1, \ldots, d-1.$

- Define d new unknown functions

$$y^1(x) = y(x), y^2(x) = y'(x), \ldots, y^d(x) = y^{(d-1)}(x)$$

- Original dth-order ODE is equivalent to a system of first-order ODEs:

$$\begin{bmatrix} (y^1)'(x) \\ (y^2)'(x) \\ \vdots \\ (y^{d-1})'(x) \\ (y^d)'(x) \end{bmatrix} = \begin{bmatrix} y^2(x) \\ y^3(x) \\ \vdots \\ y^d(x) \\ f(x, y^1, y^2, \ldots, y^d) \end{bmatrix}, \begin{bmatrix} y^1(a) = y_0^0 \\ y^2(a) = y_0^1 \\ \vdots \\ y^{d-1}(a) = y_0^{d-2} \\ y^d(a) = y_0^{d-1} \end{bmatrix}$$

Example

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

$$y'' = F/m$$

  where F and m are force and mass, respectively
- Defining $y^1 = y$ and $y^2 = y'$ yields equivalent system of two first-order ODEs

$$\begin{bmatrix} (y^1)' \\ (y^2)' \end{bmatrix} = \begin{bmatrix} y^2 \\ F/m \end{bmatrix}$$

- We can now use methods for first-order equations to solve this system
- First component of solution y^1 is solution y of original second-order equation
- Second component of solution y^2 is velocity y'

Example: IVP

- Consider scalar ODE
$$y' = y$$
- Family of solutions is given by $y(x) = ce^x$, where c is any real constant
- Imposing initial condition $y(a) = y_0$ singles out unique particular solution
- For this example, if $a = 0$, then $c = y_0$, which means that solution is $y(x) = y_0 e^x$

Lipschitz Condition and Convexity

Definition

A function $f(x, y)$ is said to satisfy a Lipschitz condition in the variable y on a set $D \in \mathbf{R}^2$ if a constant $L > 0$ exists with

$$|f(x, y_1) - f(x, y_2)| \leqslant L|y_1 - y_2|,$$

whenever $(x, y_1), (x, y_2) \in D$. The constant L is called a Lipschitz constant for f.

Definition

A set $D \subset \mathbf{R}^2$ is said to be convex if whenever (x_1, y_1) and (x_2, y_2) belong to D and λ is in $[0, 1]$, the point $((1 - \lambda)x_1 + \lambda x_2, (1 - \lambda)y_1 + \lambda y_2)$ also belongs to D.

Existence and Uniqueness

Theorem

Suppose $f(x, y)$ *is defined on a convex set* $D \subset \mathbf{R}^2$. *If a constant* $L > 0$ *exists with*

$$|\frac{\partial f}{\partial y}(x, y)| \leqslant L, \forall (x, y) \in D,$$

then f *satisfies a Lipschitz condition on* D *in the variable* y *with Lipschitz condition* L.

Theorem

Suppose that $D = \{(x, y) | a \leqslant x \leqslant b, -\infty \leqslant y \leqslant \infty\}$ *and that* $f(x, y)$ *is continuous on* D. *If* f *satisfies a Lipschitz condition on* D *in the variable* y, *then the initial-value problem*

$$y'(x) = f(x, y), a \leqslant x \leqslant b, y(a) = y_0,$$

has a unique solution $y(x)$ *for* $a \leqslant x \leqslant b$.

Well-Posedness

Definition

The initial-value problem $\frac{dy}{dx} = f(x, y),\ a \leqslant x \leqslant b,\ y(a) = y_0$, is said to be a well-posed problem if:

- A unique solution, $y(x)$, to the problem exists, and
- There exists constants $\epsilon_0 > 0$ and $k > 0$ such that for any ϵ, with $\epsilon_0 > \epsilon > 0$, whenever $\delta(x)$ is continuous with $|\delta(x)| < \epsilon$ for all $x \in [a, b]$, and when $|\delta_0| < \epsilon$, the initial-value problem

  $$\frac{dz}{dx} = f(x, z) + \delta(x),\ a \leqslant x \leqslant b,\ z(a) = y_0 + \delta_0,$$

  has a unique solution $z(x)$ that satisfies

  $$|z(x) - y(x)| < k\epsilon, \forall x \in [a, b]$$

Well-Posedness

Theorem

Suppose $D = \{(x, y) | a \leqslant x \leqslant b, -\infty \leqslant y \leqslant \infty\}$*. If* f *is continuous and satisfies a Lipschitz condition in the variable* y *on the set* D*, then the initial-value problem*

$$\frac{dy}{dx} = f(x, y),\ a \leqslant x \leqslant b,\ y(a) = y_0$$

is well-posed.

Stability of Solutions

Solution of ODE is

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

Stable solution: e.g., $y' = 1/2$

Asymptotically Stable Solutions: e.g., $y' = -y$

Example

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

Example: Linear System of ODEs

- Linear, homogeneous system of ODEs with constant coefficients has form

$$\mathbf{y}' = \mathbf{A}\mathbf{y}$$

  where $\mathbf{A}$ is $d \times d$ matrix, and initial condition $\mathbf{y}(0) = \mathbf{y}_0$
- Suppose $\mathbf{A}$ is diagonalizable, with eigenvalues λ_i and corresponding eigenvectors $\mathbf{v}_i,\ i = 1, \dots, d$.
- Express $\mathbf{y}_0$ as linear combination $\mathbf{y}_0 = \sum_{i=1}^{d} \alpha_i \mathbf{v}_i$
- Then

$$\mathbf{y}(x) = \sum_{i=1}^{d} \alpha_i \mathbf{v}_i e^{\lambda_i x}$$

  is solution to ODE satisfying initial condition $\mathbf{y}(0) = \mathbf{y}_0$

Example, cont'ed

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

Stability of Solutions, cont'ed

- For general nonlinear system of ODEs $\mathbf{y}' = \mathbf{f}(x, \mathbf{y})$, determining stability of solutions is more complicated
- ODE can be linearized locally about solution $\mathbf{y}(x)$ by truncated Taylor series, yielding linear ODE

$$\mathbf{z}' = \mathbf{J}_f(x, \mathbf{y}(x))\mathbf{z}$$

  where $\mathbf{J}_f$ is Jacobian matrix of $\mathbf{f}$ with respect to $\mathbf{y}$
- Eigenvalues of $\mathbf{J}_f$ determine stability locally, but conclusions drawn may not be valid globally

Numerical Solution of ODEs

- Analytical solution of ODE is closed-form formula that can be evaluated at any point x
- Numerical solution of ODE is table of approximate values of solution function at discrete set of points
- Numerical solution is generated by simulating behavior of system governed by ODE
- Starting at $x_0 \equiv a$ with given initial value $\mathbf{y}_0$, we track trajectory dictated by ODE
- Evaluating $\mathbf{f}(a, \mathbf{y}_0)$ tells us slope of trajectory at that point
- We use this information to predict value $\mathbf{y}_1$ of solution at future time $x_1 = x_0 + h$ for some suitably chosen time increment h

Numerical Solution of ODEs, cont'ed

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

Numerical Methods for ODEs

- Approximation $\{\mathbf{u}_n \approx \mathbf{y}(x_n)\}$ at discrete points $\{x_n\}$: grid function $\{\mathbf{u}_n\}$ on a grid

$$a = x_0 < x_1 < \cdots < x-_{N-1} < x_N = b$$

- One-step method: $\mathbf{u}_{n+1}$ is determined solely from information at x_n, $\mathbf{u}_n$, and step size h with $x_{n+1} = x_n + h$
  - Local description:

$$(x, \mathbf{y}) \to (x + h, \mathbf{y}_{next})$$

  - Global description:

$$(x_n, \mathbf{u}_n) \to (x_{n+1}, \mathbf{u}_{n+1}), \text{ step } h_n = x_{n+1} - x_n$$

- Multistep method: in a k-step method, $\mathbf{u}_{n+1}$ is determined from information at $k-1$ points, $(x_{n-j}, \mathbf{u}_{n-j})$, $j = 1, \ldots, k-1$

Local Description of One-Step Methods

- For a generic point $(x, \mathbf{y})$, a single step of the one-step method:

$$\mathbf{y}_{next} = \mathbf{y} + h\mathbf{\Phi}(x, \mathbf{y}; h), h > 0,$$

  where $\mathbf{\Phi}$ is the approximate difference quotient that defines the method.

- Reference solution $\mathbf{u}(t)$ of local initial value problem

$$\frac{d\mathbf{u}}{dt} = \mathbf{f}(t, \mathbf{u}),\ x \leqslant t \leqslant x + h;\ \mathbf{u}(x) = \mathbf{y}.$$

Definition (Truncation Error)

The truncation error of the method $\mathbf{\Phi}$ at the point $(x, \mathbf{y})$ is defined by

$$\mathbf{T}(x, \mathbf{y}; h) = \frac{1}{h}[\mathbf{y}_{next} - \mathbf{u}(x+h)] \quad (\text{or } = \mathbf{\Phi}(x, \mathbf{y}; h) - \frac{1}{h}[\mathbf{u}(x+h) - \mathbf{u}(x)]).$$

Consistency; Order; Principal Error Function

Definition (Consistency)

The method $\boldsymbol{\Phi}$ is called consistent if $\mathbf{T}(x, \mathbf{y}; h) \to 0$, as $h \to 0$ uniformly for $(x, \mathbf{y}) \in [a, b] \times \mathbf{R}^d$.

Definition (Order of the Method)

The method $\boldsymbol{\Phi}$ is said to have order p if, for some vector norm $\| \cdot \|$, $\|\mathbf{T}(x, \mathbf{y}; h)\| \leqslant Ch^p$ uniformly on $[a, b] \times \mathbf{R}^d$, with a constant C not depending on $x, \mathbf{y}$, and h.

Definition

A function $\boldsymbol{\tau} : [a, b] \times \mathbf{R}^d \to \mathbf{R}^d$ that satisfies $\boldsymbol{\tau} \not\equiv 0$ and

$$\mathbf{T}(x, \mathbf{y}; h) = \boldsymbol{\tau}(x, \mathbf{y}) h^p + O(h^{p+1}), \ h \to 0,$$

is called the principal error function.