MA5233 Computational Mathematics

Lecture 10: Runge-Kutta Methods

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Introduction

The aim of this lecture is to develop numerical methods for solving problems of the following form.

Def: Ordinary differential equation (ODE)

Given $f: \mathbb{R}^n \to \mathbb{R}^n$, $y_0 \in \mathbb{R}^n$ and T > 0, find $y: [0, T) \to \mathbb{R}^n$ such that

$$y(0) = y_0$$
 and $\dot{y}(t) = f(y(t))$ for all $t \in [0, T)$.

 $\dot{y}=y'=rac{dy}{dt}$ is a shorthand notation for taking derivatives of a function $y:\mathbb{R} o\mathbb{R}^n$.

Outlook

The following slides illustrate the above definition by discussing three example ODEs. These ODEs will reappear later in this lecture, so pay attention even if you are already familiar with ODEs.

Example 1

Consider the problem of finding $y:[0,\infty)\to\mathbb{R}$ such that

$$y(0) = y_0$$
 and $\dot{y}(t) = \lambda y(t)$

for some given $y_0, \lambda \in \mathbb{R}$.

The solution to this problem is given by

$$y(t) = y_0 \exp(\lambda t)$$

because this function satisfies

$$y(0) = y_0 \exp(\lambda 0) = y_0$$
 and $\dot{y}(t) = y_0 \exp(\lambda t) \lambda = \lambda y(t)$.

Example 2

Consider the problem of finding $y:[0,\frac{1}{v_0})\to\mathbb{R}$ such that

$$y(0) = y_0$$
 and $\dot{y}(t) = y(t)^2$

for some given $y_0 \in \mathbb{R}$.

The solution to this problem is given by

$$y(t) = \frac{y_0}{1 - y_0 t}$$

because this function satisfies

$$y(0) = \frac{y_0}{1 - y_0 \cdot 0} = y_0$$
 and $\dot{y}(t) = \frac{y_0^2}{(1 - y_0 t)^2} = y(t)^2$.

Note that this y(t) is undefined for $t = \frac{1}{y_0}$. This shows that unlike the solution of Example 1, the solution to this ODE has a finite domain of definition $[0, \frac{1}{y_0})$.

The formula for y(t) is well defined for $t > \frac{1}{y_0}$, but this part of the solution has no mathematical meaning since it is disconnected from the starting point t = 0.

Example 3

Consider the problem of finding $x:[0,\infty)\to\mathbb{R}$ such that

$$x(0) = 1$$
 and $\ddot{x} = -x$.

The solution to this equation is given by

$$x(t) = \cos(t)$$

since this function satisfies $x(0) = \cos(0) = 1$ and

$$\ddot{x}(t) = \frac{d^2}{dt^2}\cos(t) = -\frac{d}{dt}\sin(t) = -\cos(t) = -x(t).$$

 $\ddot{x} = -x$ is not of the form $\dot{y} = f(y)$, but it can easily be reduced to this form: if we set

$$y = \begin{pmatrix} x \\ \dot{x} \end{pmatrix}$$
 and $f(y) = \begin{pmatrix} y[2] \\ -y[1] \end{pmatrix}$,

then this y(t) and f(y) indeed satisfy

$$\dot{y} = \begin{pmatrix} \dot{x} \\ \ddot{x} \end{pmatrix} = \begin{pmatrix} y[2] \\ -y[1] \end{pmatrix} = f(y).$$

This shows that considering ODEs involving only first-order derivatives is enough to cover ODEs involving arbitrarily high derivatives.

Real-world example: Newton's law of motion

Consider a point particle of mass m > 0 subject to a force $F(x) \in \mathbb{R}^3$ which depends on the location $x \in \mathbb{R}^3$ of the particle.

Newton's law of motion then states that the trajectory $x(t) \in \mathbb{R}^3$ of this particle satisfies

$$m\ddot{x}(t) = F(x(t)).$$

This equation is again not of the form $\dot{y} = f(y)$ but can reduced to this form by setting

$$y = \begin{pmatrix} x \\ \dot{x} \end{pmatrix}, \qquad f(y) = \begin{pmatrix} y[2] \\ \frac{1}{m} F(y[1]) \end{pmatrix}$$

such that

$$\dot{y} = \begin{pmatrix} \dot{x} \\ \ddot{x} \end{pmatrix} = \begin{pmatrix} \dot{x} \\ \frac{1}{m}F(x) \end{pmatrix} = \begin{pmatrix} y[2] \\ \frac{1}{m}F(y[1]) \end{pmatrix} = f(y).$$

Time-dependent ODEs

Many textbooks allow the ODE-defining function f(y,t) to also depend on the time variable t. I omit this generality here because it is rarely needed in applications and it significantly complicates the analysis.

ODEs vs PDEs

ODEs are similar to PDEs in that the problem is to find a function y(t) given an equation in terms of y(t) and its derivatives which is to hold at every point in the domain.

Historically / formally, the defining property of an ODE is that the unknown y(t) depends on only a single variable and hence the derivatives in the differential equations are *ordinary* derivatives.

By contrast, the unknown $u(x_1, ..., x_d)$ in a PDE depends on several variables and hence the derivatives are *partial* derivatives.

The terms "ODE" and "PDE" are hardly ever used in this way anymore, however.

In modern terminology, the defining property of an ODE is that fixed values for y(t) and its derivatives are specified at a single point t_0 . For this reason, ODEs are also called *initial value problems*.

The defining property of a PDE is that fixed values of u(x) and its derivatives are specified at two or more points $x \in \partial \Omega$. For this reason, PDEs are also called *boundary value problems*.

Example: ODEs vs PDEs

The one-dimensional Poisson equation -u''(x) = f(x) is an ODE in the formal sense because there is only a single independent variable x. However, this equation is usually called a PDE because it is almost always paired with boundary conditions rather than initial conditions and hence it is much more similar to e.g. the higher-dimensional Poisson equation $-\Delta u = f$ than to Newton's law of motion $m\ddot{x} = F(x)$.

Discussion

As mentioned earlier, our goal in this lecture is to develop numerical algorithms which approximate the map

$$(f(y), y_0, T) \mapsto y(t)$$
 such that $y(0) = y_0, \dot{y}(t) = f(y(t)).$

However, it is advisable to first establish that this map is well defined and well conditioned, since otherwise we might end up constructing (and trusting!) numerical solutions $\tilde{y}(t)$ which have no meaning.

It turns out that the key condition guaranteeing the existence of solutions y(t) is Lipschitz continuity as defined on the next slide.

Def: (Global) Lipschitz continuity

A function $f: D \to \mathbb{R}^n$ with $D \subset \mathbb{R}^n$ is called *(globally) Lipschitz* continuous with Lipschitz constant L > 0 if for all $y_1, y_2 \in D$ we have

$$||f(y_1)-f(y_2)|| \leq L ||y_1-y_2||.$$

Note that whether a function f(y) is Lipschitz continuous does not depend on the choice of norm due to norm equivalence in finite dimensions. However, the Lipschitz constant L may depend on the choice of norm.

Def: Local Lipschitz continuity

A function $f: \mathbb{R}^n \to \mathbb{R}^n$ is called *locally Lipschitz continuous* if for every $y_0 \in \mathbb{R}^n$ there exists a pair $\delta, L > 0$ such that for all $y_1, y_2 \in \mathbb{R}^n$ we have

$$||y_k - y_0|| \le \delta$$
 \Longrightarrow $||f(y_1) - f(y_2)|| \le L ||y_1 - y_2||.$

Discussion

Lipschitz continuity of a function f(y) is usually most conveniently verified using the following result.

Corollary

Assume $D \subset \mathbb{R}^n$ is convex and $f: D \to \mathbb{R}^n$ is differentiable everywhere in D. Then, f(y) is locally Lipschitz continuous, and it is globally Lipschitz continuous if $\|\nabla f\|$ is bounded.

Proof. Immediate corollary of the result on the next slide.

Lemma: Lipschitz constants and derivatives

Assume $D \subset \mathbb{R}^n$ is convex and $f: D \to \mathbb{R}^n$ has a bounded derivative. Then,

$$||f(y_1) - f(y_2)|| \le L ||y_1 - y_2||$$
 where $L = \sup_{y \in D} ||\nabla f(y)||$

Proof. According to the chain rule, we have that

$$\frac{d}{dt} \Big(f \big(y_1 + t \, (y_2 - y_1) \big) \Big) = \nabla f \big(y_1 + t \, (y_2 - y_1) \big) \, (y_2 - y_1)$$

and hence we conclude using the fundamental theorem of calculus that

$$||f(y_1) - f(y_2)|| = \left\| \int_0^1 \nabla f(y_1 + t(y_2 - y_1)) (y_2 - y_1) dt \right\|$$

$$\leq \int_0^1 \left\| \nabla f(y_1 + t(y_2 - y_1)) \right\| \left\| y_2 - y_1 \right\| dt$$

$$\leq \left(\sup_{y \in D} \|\nabla f(y)\| \right) \left\| y_2 - y_1 \right\|.$$

Discussion

Armed with the definition of Lipschitz continuity, we can now establish that the ODE function $(f(y), y_0, T) \mapsto y(t)$ is indeed well defined if f(y) is Lipschitz continuous.

Picard-Lindelöf theorem

Assume $f: \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz continuous. Then, there exists a unique function $y: [0, \infty) \to \mathbb{R}^n$ such that

$$y(0) = y_0$$
 and $\dot{y}(t) = f(y(t))$ for all $t \in [0, \infty)$.

Proof. Beyond the scope of this module.

Example

Consider the function $f(y) = \lambda y$ from the example on slide 3. Since $f'(y) = \lambda$ is bounded for all y, this function is globally Lipschitz continuous and hence the solution $y(t) = y_0 \exp(\lambda t)$ exists for all $t \ge 0$.

Discussion

The above result assumes global Lipschitz continuity of f(y) but in returns guarantees that the solution is well defined for all times $t \geq 0$. If f(y) is only local Lipschitz, then the following result establishes that the solution y(t) is well defined at least on some interval $[0,T] \subset [0,\infty)$.

Picard-Lindelöf theorem. local version

Assume $f: \mathbb{R}^n \to \mathbb{R}^n$ is locally Lipschitz continuous. Then, there exists a T>0 and a unique function $y:[0,T)\to \mathbb{R}^n$ such that

$$y(0) = y_0$$
 and $\dot{y}(t) = f(y(t))$ for all $t \in [0, T)$.

Proof. Beyond the scope of this module.

Example

Consider the function $f(y)=y^2$ from the example on slide 4. Since f'(y)=2y exists but is unbounded \mathbb{R} , this function is locally Lipschitz but not globally Lipschitz. Correspondingly, the solution $y(t)=\frac{y_0}{1-y_0t}$ is defined only on the finite interval $[0,\frac{1}{y_0})$ but not on all of $[0,\infty)$.

Discussion

In order to approximate the ODE map $(f(y), y_0, T) \mapsto y(t)$ numerically, we need this map to be not only well defined but also continuous with respect to y_0 ; if this is not the case, then any small perturbation in y_0 (e.g. floating-point rounding) may lead to arbitrarily large errors in the solution y(t).

We will see on the next slide that continuity is a simple consequence of the following auxiliary result.

Gronwall's inequality

$$\dot{y}(t) \le \lambda y(t) \implies y(t) \le \exp(\lambda t) y(0).$$

Proof. Consider $z(t) = \exp(-\lambda t) y(t)$. Then, z(0) = y(0) and

$$\dot{z}(t) = -\lambda \exp(-\lambda t) y(t) + \exp(-\lambda t) \dot{y}(t)$$

$$\leq -\lambda \exp(-\lambda t) y(t) + \exp(-\lambda t) \lambda y(t) = 0;$$

hence $z(t) \le y(0)$ and thus $y(t) \le y(0) \exp(\lambda t)$.

Thm: Lipschitz continuity of the ODE map

Assume $f: \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz continuous with Lipschitz constant L, and assume $y_1, y_2: [0, T) \to \mathbb{R}^n$ satisfy $\dot{y}_k = f(y_k)$. Then,

$$||y_1(t) - y_2(t)|| \le \exp(Lt) ||y_1(0) - y_2(0)||$$
 for any $t < T$.

Proof. We have for any $y: \mathbb{R} \to \mathbb{R}^n$ that

$$\frac{d}{dt}\|y(t)\| = \lim_{\tilde{t}\to t} \frac{\|y(\tilde{t})\| - \|y(t)\|}{\tilde{t}-t} \le \lim_{\tilde{t}\to t} \frac{\|y(\tilde{t})-y(t)\|}{\tilde{t}-t} = \|\dot{y}(t)\|.$$

Combining the above with the Lipschitz continuity of f(y), we obtain

$$\frac{d}{dt} \|y_2(t) - y_1(t)\| \le \|\dot{y}_2(t) - \dot{y}_1(t)\|
= \|f(y_2(t)) - f(y_1(t))\|
\le L \|y_2(t) - y_1(t)\|$$

from which the claim follows by Gronwall's inequality.

Discussion

The bound on the previous slide is a two-sided coin:

- ▶ Good: error at time *t* is proportional to error at time 0.
- ▶ Bad: constant of proportionality is exp(Lt).

The exponential function has a noticeable two-stage character:

- ▶ For $t \leq \frac{1}{L}$, exp(Lt) is about 1.
- ► For $t \gtrsim \frac{1}{L}$, exp(Lt) grows very quickly.

In practice, this means that there is often a characteristic time-scale $\frac{1}{L}$ beyond which numerical simulations become unreliable.

For example, we can predict the weather fairly accurately for the next 2-3 days, but predictions beyond one week are virtually impossible.

Solving ODEs using quadrature

We have now established that if f(y) is Lipschitz continuous, then $\dot{y} = f(y)$ has a unique solution and this solution is a Lipschitz continuous function of the initial conditions y_0 .

Let us now move on to discuss numerical methods for approximating y(t).

According to the fundamental theorem of calculus, we have

$$\begin{array}{c} y(0) = y_0 \\ \dot{y} = f(y) \end{array} \right\} \qquad \Longleftrightarrow \qquad y(t) = y_0 + \int_0^t f(y(\tau)) d\tau.$$

Given a quadrature formula $(\theta_k, w_k)_{k=1}^s$ for [0, 1], we can hence compute a numerical approximation to y(t) using the formula

$$\tilde{y}(t) = y_0 + \sum_{k=1}^{s} f(y(\theta_k t)) w_k t.$$

The quadrature points θ_k and weights w_k are multiplied by t because we need to scale the quadrature rule from [0,1] to [0,t].

However, we need to be careful because we do not know y(t) for t > 0 and hence we cannot evaluate $f(y(\theta_k t))$ for quadrature points $\theta_k > 0$.

Solving ODEs using quadrature (continued)

The above suggests that we solve ODEs using the 1-point quadrature rule

$$heta_1=0, \qquad w_1=1 \qquad \longleftrightarrow$$

This yields the following ODE solver.

Def: Euler step

Approximate the solution to $\dot{y} = f(y)$ using

$$y(t) \approx y(0) + f(y(0)) t.$$

Discussion

The error of this formula is easily estimated using Taylor's theorem.

Thm: Error estimate for Euler step

Assume f(y) is differentiable, y(t) satisfies $\dot{y}=f(y)$, and t>0. Then, there exists $\xi\in(0,t)$ such that

$$y(t) \ = \ \underbrace{y(0) + f(y(0))\,t}_{\text{Euler step}} \ + \ \underbrace{\frac{1}{2}\,\nabla f(\xi)\,\dot{y}(\xi)\,t^2}_{\text{error}}.$$

Proof. According to Taylor's theorem, there exists $\xi \in (0, t)$ such that

$$y(t) = y(0) + \dot{y}(0) t + \frac{1}{2} \ddot{y}(\xi) t^{2}.$$

The claim follows by noting that since $\dot{y}(t) = f(y(t))$, we have

$$\dot{y}(0) = f(y(0))$$
 and $\ddot{y}(\xi) = \nabla f(y(\xi)) \dot{y}(\xi)$.

Discussion

The error estimate

$$y(t) = \underbrace{y(0) + f(y(0)) t}_{\text{Euler step}} + \underbrace{\frac{1}{2} \nabla f(\xi) \dot{y}(\xi) t^2}_{\text{error}}$$

gives us two important pieces of information.

The error is smaller the closer f(y) and y(t) are to being constant (i.e. the smaller their derivative).

This is not surprising since the quadrature rule $\theta_1 = 0$, $w_1 = 1$ is exact for constant integrands.

ightharpoonup The error is smaller for smaller times t.

This is again not surprising because for smaller t, the integral $\int_0^t f(y(\tau)) d\tau$ is both smaller and the integrand $f(y(\tau))$ is closer to being constant over the interval [0, t].

Both the ODE function f(y) and the time interval [0, T] are imposed on us by the application; hence the Euler step presented above gives us no means to improve the accuracy by investing more compute time.

This circumstance can be remedied using the composition idea presented on the next slide.

Def: Temporal mesh

An ordered sequence of points $0 = t_0 < t_1 < \dots$

Def: Euler's method

Approximate the solution to $\dot{y} = f(y)$ using

$$\tilde{y}(0) = y(0), \qquad \tilde{y}(t) = \tilde{y}(t_{k-1}) + f(\tilde{y}(t_{k-1})) t \quad \text{for } t \in (t_{k-1}, t_k],$$

where $(t_k)_k$ denotes a given temporal mesh.

Numerical demonstration

See euler_step(), integrate() and example().

Discussion

We intuitively expect that composing Euler steps into Euler's method yields a numerical approximation $\tilde{y}(t)$ which converges to the exact solution y(t) as the mesh width $\max_k |t_k - t_{k-1}|$ goes to 0.

I will next show that this is indeed the case, and I will do so using the notions of exact and Euler time propagators introduced on the next slide.

Def: (Exact) time propagator

The *(exact) time propagator* associated with $f: \mathbb{R}^n \to \mathbb{R}^n$ is the function

$$\Phi: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n, \qquad \Phi(y_0, t) = y(t)$$

where y(t) is the solution to $\dot{y} = f(y)$, $y(0) = y_0$.

Def: Euler time propagator

The *Euler time propagator* associated with $f: \mathbb{R}^n \to \mathbb{R}^n$ is the function

$$\tilde{\Phi}: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n, \qquad \tilde{\Phi}(y_0, t) = y_0 + f(y_0) t.$$

Shorthand notations

In the following, I will use the shorthand notations

$$y_k = y(t_k), \qquad \tilde{y}_k = \tilde{y}(t_k),$$

and

$$\Phi_k(y_0) = \Phi(y_0, t_k - t_{k-1}), \qquad \tilde{\Phi}_k(y_0) = \tilde{\Phi}(y_0, t_k - t_{k-1}),$$

where $(t_k)_k$ denotes some temporal mesh specified by the context.

Thm: Error estimate for Euler's method

Denote by y(t) the solution to $\dot{y} = f(y)$ and by $\tilde{y}(t)$ the numerical approximation obtained using Euler's method with mesh $(t_k)_{k=0}^n$. Then,

$$\|\tilde{y}_n - y_n\| \le \sum_{k=1}^n \exp(L(t_n - t_k)) \|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\|,$$

assuming f(y) is Lipschitz continuous with Lipschitz constant L.

Proof.

$$\begin{split} \|\tilde{y}_n - y_n\| &= \|\tilde{\Phi}_n(\tilde{y}_{n-1}) - \Phi_n(y_{n-1})\| & \text{(definition of time propagators)} \\ \text{(triangle ineq.)} &\leq \|\tilde{\Phi}_n(\tilde{y}_{n-1}) - \Phi_n(\tilde{y}_{n-1})\| + \|\Phi_n(\tilde{y}_{n-1}) - \Phi_n(y_{n-1})\| \\ \text{(Φ Lipschitz)} &\leq \|\tilde{\Phi}_n(\tilde{y}_{n-1}) - \Phi_n(\tilde{y}_{n-1})\| + \exp\left(L\left(t_n - t_{n-1}\right)\right)\|\tilde{y}_{n-1} - y_{n-1}\| \\ \text{(recursion)} &\leq \sum_{k=1}^n \exp\left(L\left(t_n - t_k\right)\right)\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\|. \end{split}$$

Terminology

 $\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\|$ is called the *local*, *consistency* or *truncation* error of the numerical time propagator $\tilde{\Phi}$.

Remark

The bound

$$\|\tilde{y}_{n} - y_{n}\| \le \sum_{k=1}^{n} \exp(L(t_{n} - t_{k})) \|\tilde{\Phi}_{k}(\tilde{y}_{k-1}) - \Phi_{k}(\tilde{y}_{k-1})\|$$

can be put into words as follows.

The error at the final time t_n is upper-bounded by the sum of the errors introduced in the time steps $(t_{k-1} \to t_k)_{k=1}^n$ multiplied by the Lipschitz constant of $\Phi(y,t)$ derived on slide 17.

Discussion

The bound

$$\|\tilde{y}_n - y_n\| \le \sum_{k=1}^n \exp(L(t_n - t_k)) \|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\|$$

shows that

$$\max_{k} |t_{k} - t_{k-1}| \to 0 \qquad \Longrightarrow \qquad \|\tilde{y}_{n} - y_{n}\| \to 0$$

as long as

$$|t_k - t_{k-1}| \to 0$$
 \Longrightarrow $\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\| \to 0.$ (1)

We have already seen on slide 21 that (1) is indeed the case. Specifically, we have seen that

$$\left\|\tilde{\Phi}(\tilde{y}_{k-1},t)-\Phi(\tilde{y}_{k-1},t)\right\|=O(t^2).$$

This observation immediately yields the following theorem.

Thm: Convergence of Euler's method

Denote by y(t) the solution to $\dot{y} = f(y)$ and by $\tilde{y}(t)$ the numerical approximation obtained using Euler's method with the equispaced temporal mesh $(t_k = \frac{k}{n} T)_{k=0}^n$.

Then,

$$\|\tilde{y}(T) - y(T)\| = O\left(\exp(LT)\frac{T^2}{n}\right),$$

assuming f(y) is Lipschitz continuous with Lipschitz constant L.

Proof.

$$\|\tilde{y}_n - y_n\| \le \sum_{k=1}^n \exp(L(t_n - t_k)) \|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\|$$

$$\le n \exp(L(t_n - t_0)) O\left(\left(\frac{T}{n}\right)^2\right)$$

$$= \exp(L(t_n - t_0)) O\left(\frac{T^2}{n}\right)$$

Numerical demonstration

See convergence().

Remark 1

Note that Euler's method is second-order consistent but only first-order convergent. The heuristic reason for this is that Euler's method makes n errors of magnitude $O(n^{-2})$; hence the total error is $n O(n^{-2}) = O(n^{-1})$.

Remark 2

The above convergence estimate indicates that the number of steps required to reach a fixed error tolerance

$$\|\tilde{y}(T) - y(T)\| = O\left(\exp(LT)\frac{T^2}{n}\right) \le \tau$$

is
$$n = O(\tau^{-1} T^2 \exp(LT))$$
.

This once again indicates that it is difficult to solve ODEs on time-scales larger than one over the Lipschitz constant.

This is demonstrated numerically in nsteps().

To be continued.