

MA5233 Computational Mathematics

Lecture 16: Explicit Runge-Kutta Methods

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Explicit Runge-Kutta Methods

Ordinary differential equation (ODE)

Given $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $y_0 \in \mathbb{R}^n$, find differentiable $y : [0, T] \rightarrow \mathbb{R}^n$ such that

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

ODEs are also called *initial value problems*.

$\dot{y}(t) := \frac{dy}{dt}(t)$ is a shorthand for the time derivative.

Example: Newton's law of motion $m\ddot{x} = F(x)$.

This can be written in above form by setting

$$y := \begin{pmatrix} x \\ \dot{x} \end{pmatrix}, \quad f(y) := \begin{pmatrix} y_2 \\ \frac{1}{m} F(y_1) \end{pmatrix}$$

such that

$$\dot{y} = \begin{pmatrix} \dot{x} \\ \ddot{x} \end{pmatrix} = \begin{pmatrix} \dot{x} \\ \frac{1}{m} F(x) \end{pmatrix} = \begin{pmatrix} y_2 \\ \frac{1}{m} F(y_1) \end{pmatrix} = f(y).$$

Explicit Runge-Kutta Methods

Picard-Lindelöf theorem

Assume $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is Lipschitz continuous, i.e. there exists a constant $L > 0$ such that for all $y_1, y_2 \in \mathbb{R}^n$ we have

$$\|f(y_2) - f(y_1)\| \leq L \|y_2 - y_1\|. \quad (1)$$

Then, there exists a unique differentiable $y : [0, \infty) \rightarrow \mathbb{R}^n$ such that

$$y(0) = y_0 \quad \text{and} \quad \dot{y}(t) = f(y(t)) \quad \text{for all } t \in [0, \infty). \quad (2)$$

Alternatively, assume f is locally Lipschitz continuous at y_0 , i.e. there exist $L > 0$ and $\varepsilon > 0$ such that (1) holds for $y_1, y_2 \in \{y \mid \|y - y_0\| \leq \varepsilon\}$. Then, the solution to (2) may be defined only on $[0, T)$ for some $T < \infty$.

Examples

- ▶ $f(y) = y$ is Lipschitz with $L = 1$.
Solution $y(t) = y_0 \exp(t)$ is defined on $[0, \infty)$.
- ▶ $f(y) = y^2$ is locally Lipschitz but not globally Lipschitz.
Solution $y(t) = \frac{y_0}{1 - y_0 t}$ is defined only on $[0, \frac{1}{y_0})$.

Explicit Runge-Kutta Methods

Conditioning of initial value problems

Assume $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is Lipschitz continuous with constant L , and $(y_i : [0, T) \rightarrow \mathbb{R}^n)_{i \in \{1,2\}}$ satisfy the two ODEs

$$y_i(0) = s_i, \quad \dot{y}_i = f(y_i).$$

Then,

$$\|y_2(t) - y_1(t)\| \leq e^{Lt} \|s_2 - s_1\| \quad \text{for all } t \in [0, T).$$

Interpretation

The map $s \mapsto y(t)$ is Lipschitz continuous, but the Lipschitz constant deteriorates exponentially for $t \rightarrow \infty$.

Real-world consequences:

- ▶ Weather prediction is difficult for large t .
- ▶ Shooting a rocket to Mars requires course corrections.

Explicit Runge-Kutta Methods

Solving ODEs via quadrature

The solution to the ODE $\dot{y} = f(y)$ is given by

$$y(t) = y(0) + \int_0^t f(y(\tau)) d\tau.$$

Observation: ODEs can be solved via quadrature!

Problem: We don't know $f(y(\tau_k))$ for quadpoints $\tau_k > 0$.

Solution 1: Use left-point rule: (This is known as Euler's method)

$$\tilde{y}(t) := y(0) + f(y(0)) t.$$

Solution 2: Use midpoint rule, and use left-point rule to estimate $y(\frac{t}{2})$:

$$\tilde{y}(t) := y(0) + f(\tilde{y}(\frac{t}{2})) t, \quad \tilde{\tilde{y}}(\frac{t}{2}) := y(0) + f(y(0)) \frac{t}{2}.$$

Solution 3: Use trapezoidal rule, and use left-point rule to estimate $y(t)$:

$$\tilde{y}(t) := y(0) + \left(f(y(0)) + f(\tilde{\tilde{y}}(t)) \right) \frac{t}{2}, \quad \tilde{\tilde{y}}(t) := y(0) + f(y(0)) t.$$

Explicit Runge-Kutta Methods

Solving ODEs via quadrature (continued)

Above schemes deliver poor accuracy since they use only few quadpoints.

Two ways to improve accuracy:

- ▶ Increase number of quadpoints \rightarrow s -stage Runge-Kutta methods.
- ▶ Use composite quadrature.

There are limits to how far the first approach can be pushed.

All practical schemes use composite quadrature, which in this context amounts to the following.

- ▶ Assume we want to compute $\tilde{y}(T) \approx y(T)$.
- ▶ Introduce partition $0 = t_0 < t_1 < \dots < t_m = T$.
- ▶ Use any of the schemes on previous slide to iteratively compute

$$y(0) = \tilde{y}(t_0) \rightarrow \tilde{y}(t_1) \rightarrow \dots \rightarrow \tilde{y}(t_m) = \tilde{y}(T).$$

See `16_ordinary_differential_equations.jl`.

Explicit Runge-Kutta Methods

Abstract time-stepping scheme

A single step of Euler's / midpoint / trapezoidal rule can be interpreted as a function $\tilde{\Phi}_t : y(0) \rightarrow \tilde{y}(t)$.

Composite scheme is then given by

$$\tilde{y}(T) = \tilde{\Phi}_{t_m - t_{m-1}}(\dots \tilde{\Phi}_{t_2 - t_1}(\tilde{\Phi}_{t_1 - t_0}(y(0))))).$$

$\tilde{\Phi}_t$ is an approximation to $\Phi_t : y(0) \mapsto y(t)$.

Terminology:

- ▶ $\tilde{\Phi}_t(y)$: numerical propagator.
- ▶ $\Phi_t(y)$: exact propagator.

Goal: error estimate

$$\|\tilde{y}(T) - y(T)\| = \mathcal{O}(f(m))$$

assuming equispaced partition $(t_k := T \frac{k}{m})_{k=0}^m$.

Explicit Runge-Kutta Methods

Error analysis for abstract time-stepping scheme

Assumptions on numerical propagator:

- Consistency: $\|\tilde{\Phi}_t(y) - \Phi_t(y)\| = \mathcal{O}(t^{p+1})$ for some $p > 0$.
- Stability: $\|\tilde{\Phi}_t(y_2) - \tilde{\Phi}_t(y_1)\| \leq (1 + \tilde{L} t) \|y_2 - y_1\|$ for some $\tilde{L} > 0$.

Then,

$$\|\tilde{y}(T) - y(T)\| = \mathcal{O}(m^{-p}) \quad \text{for } m \rightarrow \infty.$$

Observe: consistency & stability \implies convergence.

Proof. For notational convenience, we set

$$\Phi(y) := \Phi_{T/m}(y), \quad \tilde{\Phi}(y) := \tilde{\Phi}_{T/m}(y), \quad y_k := y\left(\frac{Tk}{m}\right), \quad \tilde{y}_k := \tilde{y}\left(\frac{Tk}{m}\right).$$

Explicit Runge-Kutta Methods

Proof (continued). We compute

$$\begin{aligned}\|\tilde{y}(T) - y(T)\| &= \|\tilde{\Phi}(\tilde{y}_{m-1}) - \Phi(y_{m-1})\| \\&\leq \|\tilde{\Phi}(\tilde{y}_{m-1}) - \tilde{\Phi}(y_{m-1})\| + \|\tilde{\Phi}(y_{m-1}) - \Phi(y_{m-1})\| \\&\leq \left(1 + \frac{\tilde{L}T}{m}\right) \|\tilde{y}_{m-1} - y_{m-1}\| + \mathcal{O}(m^{-p-1}) \\&\leq \left(1 + \frac{\tilde{L}T}{m}\right)^2 \|\tilde{y}_{m-2} - y_{m-2}\| + \left(1 + \left(1 + \frac{\tilde{L}T}{m}\right)\right) \mathcal{O}(m^{-p-1}) \\&\leq \dots \\&\leq \left(1 + \frac{\tilde{L}T}{m}\right)^m \|\tilde{y}_0 - y_0\| + \left(\sum_{k=0}^{m-1} \left(1 + \frac{\tilde{L}T}{m}\right)^k\right) \mathcal{O}(m^{-p-1}) \\&\leq 0 + \left(1 + \frac{\tilde{L}T}{m}\right)^{m-1} \mathcal{O}(m^{-p})\end{aligned}$$

Claim follows after observing that since $1 + x \leq \exp(x)$, we have

$$\left(1 + \frac{\tilde{L}T}{m}\right)^{m-1} \leq \exp\left(\tilde{L} T \frac{m-1}{m}\right) \leq \exp(\tilde{L} T).$$

Explicit Runge-Kutta Methods

Consistency of Euler's, midpoint and trapezoidal method

Assuming y (and equivalently f) has sufficiently many derivatives, the consistency error $\tilde{y}(t) - y(t)$ can be estimated using Taylor series.

- Euler's method:

$$\begin{aligned}\tilde{y}(t) &= y(0) + f(y(0)) t \\ y(t) &= y(0) + \dot{y}(0) t + \mathcal{O}(t^2)\end{aligned}$$

Since $\dot{y}(0) = f(y(0))$, we have $\tilde{y}(t) - y(t) = \mathcal{O}(t^2)$.

- Midpoint method: $\tilde{y}(t) = y(0) + f(y(0) + f(y(0))\frac{t}{2}) t$

$$\begin{aligned}\tilde{y}(t) &= y(0) + f(y(0)) t + f'(y(0)) f(y(0)) \frac{t^2}{2} + \mathcal{O}(t^3) \\ y(t) &= y(0) + \dot{y}(0) t + \ddot{y}(0) \frac{t^2}{2} + \mathcal{O}(t^3)\end{aligned}$$

Since $\dot{y}(0) = f(y(0))$ and $\ddot{y}(0) = f'(y(0)) \dot{y}(0) = f'(y(0)) f(y(0))$, we have $\tilde{y}(t) - y(t) = \mathcal{O}(t^3)$.

- Trapezoidal method: analogous. Result is $\tilde{y}(t) - y(t) = \mathcal{O}(t^3)$.

Explicit Runge-Kutta Methods

Stability of Euler's, midpoint and trapezoidal method

Assuming $f(y)$ is Lipschitz continuous, $\|f(y_2) - f(y_1)\| \leq L \|y_2 - y_1\|$, we can estimate the stability as follows.

- Euler's method: $\tilde{\Phi}_t(y) = y + f(y) t$.

$$\begin{aligned}\|\tilde{\Phi}_t(y_2) - \tilde{\Phi}_t(y_1)\| &\leq \|y_2 - y_1\| + t \|f(y_2) - f(y_1)\| \\ &\leq (1 + tL) \|y_2 - y_1\|.\end{aligned}$$

- Midpoint method: $\tilde{\Phi}_t(y) = y + f(y + f(y) \frac{t}{2}) t$.

$$\begin{aligned}\|\tilde{\Phi}_t(y_2) - \tilde{\Phi}_t(y_1)\| &\leq \|y_2 - y_1\| + t \|f(y_2 + f(y_2) \frac{t}{2}) - f(y_1 + f(y_1) \frac{t}{2})\| \\ &\leq (1 + tL) \|y_2 - y_1\| + \frac{t^2}{2} L \|f(y_2) - f(y_1)\| \\ &\leq (1 + tL + \frac{(tL)^2}{2}) \|y_2 - y_1\|.\end{aligned}$$

- Trapezoidal method: analogous.

Conclusion

Euler: error = $\mathcal{O}(m^{-1})$, midpoint & trapezoidal: error = $\mathcal{O}(m^{-2})$.

Explicit Runge-Kutta Methods

General Runge-Kutta methods

Assume we have quadrature points x_i and a sequence of quadrature weights w_{ij} with $i \in \{0, \dots, s\}$ and $j \in \{0, \dots, i-1\}$ such that

$$x_0 = 0, \quad x_s = 1,$$

and

$$\int_0^{x_i} f(x) dx \approx \sum_{j=0}^{i-1} w_{ij} f(x_j) \quad \text{for all } i \in \{0, \dots, s\}.$$

Then, we can compute an approximate solution to $\dot{y} = f(y)$ through

$$\tilde{y}(t) := y(0) + t \sum_{j=0}^s w_{sj} f_j \approx y(t)$$

where

$$f_i := f\left(y(0) + t \sum_{j=0}^i w_{ij} f_j\right) \approx f(y(t x_i))$$

Algorithms of this form are known as *s-stage Runge-Kutta methods*.

Explicit Runge-Kutta Methods

Butcher's tableau

The parameters x_i and w_{ij} of Runge-Kutta methods can be conveniently represented in a *Butcher's tableau*:

0					
x_1	w_{10}				
x_2	w_{20}	w_{21}			
\vdots	\vdots	\vdots	\ddots		
x_{s-1}	$w_{s-1,0}$	$w_{s-1,1}$	\cdots	$w_{s-1,s-2}$	
	$w_{s,0}$	$w_{s,1}$	\cdots	$w_{s,s-2}$	$w_{s,s-1}$

Examples

Euler

0		
	1	

Midpoint

0		
$\frac{1}{2}$	$\frac{1}{2}$	
	0	1

Trapezoidal

0		
1	1	
	$\frac{1}{2}$	$\frac{1}{2}$

Explicit Runge-Kutta Methods

Error analysis for Runge-Kutta schemes

The analysis from slides 7-11 works for arbitrary Runge-Kutta method.

In particular, it can be used to determine x_i, w_{ij} such that consistency error is $\mathcal{O}(t^{p+1})$ with p as large as possible.

Bad: calculations get tedious very quickly for increasing s .

Good: others have done the work for us:

https://en.wikipedia.org/wiki/List_of_Runge-Kutta_methods.

Interesting observation: minimal number of stages s to achieve error $\mathcal{O}(m^{-p})$ grows faster than p .

p	1	2	3	4	5	6	7	8
min s	1	2	3	4	6	7	9	11

Explicit Runge-Kutta Methods

References and further reading

- ▶ E. Suli and D. F. Mayers. *An Introduction to Numerical Analysis*. Cambridge University Press (2003), doi:10.1017/CB09780511801181
Can be accessed online for free via the library website!