MA3227 Numerical Analysis II

Lecture 6: Runge-Kutta Methods

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Runge-Kutta Methods

Problem statement

Given

$$f : \mathbb{R}^n \to \mathbb{R}^n, \qquad y_0 \in \mathbb{R}^n \qquad \text{and} \qquad T > 0,$$

determine $y : [0, T) \to \mathbb{R}^n$ such that

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

$\dot{y}$ is a shorthand notation for $\dot{y} = \frac{dy}{dt}$.

Terminology: Ordinary differential equations (ODEs)

Problems of the above form are known as *ordinary differential equations*.

ODEs are typically used to model time-evolution phenomena. For this reason, y_0 is called the *initial condition*, and T is called the *final time*.

Outlook

The following slides will illustrate the above problem statement by discussing several example ODEs.

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Example 1

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

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

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

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

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Example 2

Consider the problem of finding $y : [0, \frac{1}{y_0}) \to \mathbb{R}$ such that

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

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

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

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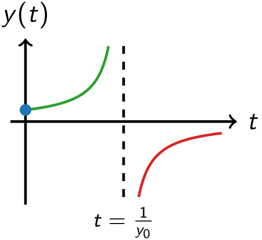
Example 2 (continued)

Note that the above solution diverges as t approaches $\frac{1}{y_0}$,

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



Example 2 is hence different from Example 1 in that the above $y(t)$ diverges already after a finite time $\frac{1}{y_0}$ while the solution in Example 1, namely

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

is finite for all $t \in [0, \infty)$.

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Example 3

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

$$x(0) = 1, \qquad \dot{x}(0) = 0 \qquad \text{and} \qquad \ddot{x} = -x.$$

The solution to this equation is given by

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

since this function satisfies

$$x(0) = \cos(0) = 1, \quad \dot{x}(0) = -\sin(0) = 0$$

and

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

Example 3 (continued)

The ODE $\ddot{x} = -x$ is not of the form $\dot{y} = f(y)$, but it can be reduced to this form by setting

$$y = \begin{pmatrix} x \\ \dot{x} \end{pmatrix} \qquad \text{and} \qquad f(y) = \begin{pmatrix} y_2 \\ -y_1 \end{pmatrix}$$

since then

$$\dot{y} = \begin{pmatrix} \dot{x} \\ \ddot{x} \end{pmatrix} = \begin{pmatrix} y_2 \\ -y_1 \end{pmatrix} = f(y).$$

This trick can be generalised to reduce ODEs with arbitrarily high derivatives to a system of ODEs involving only first-order derivatives.

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Real-world example: Newton's law of motion

A famous real-world example of an ODE is Newton's law of motion

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

This equation relates the acceleration $\ddot{x}$ of a point particle of mass m to the forces $F\big(x(x)\big)$ acting on the particle at the current position $x(t)$.

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ODEs vs PDEs

ODEs are similar to PDEs in the sense that the problem is to find a function $y(t)$ given an equation in terms of $y(t)$ and its derivatives.

Formally, the difference between ODEs and PDEs is the following.

- In an ODE, the unknown $y(t)$ depends on a single scalar variable and hence the derivatives are *ordinary* derivatives.
- In a PDE, the unknown $u(x_1, \ldots, x_d)$ depends on several variables and hence the derivatives are *partial* derivatives.

The terms "ODE" and "PDE" are hardly ever used in this way, 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 closer in spirit to e.g. the higher-dimensional Poisson equation $-\Delta u = f$ than to Newton's law of motion $m\,\ddot{x} = F(x)$.

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Outlook

Our main goal in this lecture is of course to develop numerical algorithms for evaluating the ODE map

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

However, before doing so it is advisable to first study the conditions under which this map is well defined, i.e. the conditions which guarantee that the above problem has precisely one solution.

It turns out that these conidtions are fairly simple: all we need is that $f(y)$ is Lipschitz continuous. The following slides will explain further.

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Def: (Global) Lipschitz continuity

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

$$\left\| f(y_1) - f(y_2) \right\| \;\leq\; L \, \|y_1 - y_2\|.$$

A function which is Lipschitz continuous with some unspecified Lipschitz constant $L > 0$ is called simply *Lipschitz continuous*.

Picard-Lindelöf theorem, global version

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

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

Proof. Beyond the scope of this module.

Runge-Kutta Methods

The Picard-Lindelöf theorem indicates that understanding Lipschitz continuity is important for understanding ODEs.

The following result provides a convenient tool for establishing Lipschitz continuity of a given function $f(y)$.

Thm: Global Lipschitz continuity and differentiability

A differentiable function $f : \mathbb{R}^n \to \mathbb{R}^n$ is Lipschitz continuous if $\|\nabla f\|$ is bounded.

Proof (not examinable). Immediate corollary of the result on the next slide (which I will skip in class).

Example

Recall from Example 1 on slide 3 the ODE

$$y(0) = y_0, \qquad \dot{y} = \lambda y.$$

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 $t \geq 0$.

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Lemma: Lipschitz constants and derivatives (not examinable)

Assume $f : \mathbb{R}^n \to \mathbb{R}^n$ has a bounded derivative. Then,

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

Proof.

$$\|f(y_1) - f(y_2)\| = \left\| \int_0^1 \frac{d}{dt}\Big(f\left(y_1 + t\left(y_2 - y_1\right)\right)\Big)\, dt \right\|$$

(fundamental theorem of calculus)

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

(chain rule)

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

($\| \int f(t)\, dt\| \leq \int \|f(t)\|\, dx$ and matrix norm definition)

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

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The Picard-Lindelöf theorem on slide 12 assumes that $f(y)$ is globally Lipschitz but in return guarantees existence and uniqueness of the solution for all $t \geq 0$. There is also a version of the Picard-Lindelöf theorem which assumes that $f(y)$ is only *locally Lipschitz continuous* (see below) but in return guarantees existence and uniqueness of the solution only over some potentially finite interval $[0, T)$.

Def: Local Lipschitz continuity

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

$$\|y_1 - y_2\| \leq \delta \qquad \Longrightarrow \qquad \big\|f(y_1) - f(y_2)\big\| \leq L\,\|y_1 - y_2\|.$$

Picard-Lindelöf theorem, local version

Assume $f : \mathbb{R}^n \to \mathbb{R}^n$ is locally Lipschitz continuous and $y_0 \in \mathbb{R}^n$. Then, there exists a $T > 0$ and a unique function $y : [0, T) \to \mathbb{R}^n$ such that

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

Proof. Beyond the scope of this module.

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Local Lipschitz continuity is again related to differentiability.

Thm: Local Lipschitz continuity and differentiability

A differentiable function $f : \mathbb{R}^n \to \mathbb{R}^n$ is locally Lipschitz continuous.

Proof (not examinable). Corollary of the result on slide 14.

Comparing the above against the analogous theorem for global Lipschitz continuity on slide 13, we conclude that the difference between local and global Lipschitz continuity is whether $\|\nabla f(y)\|$ is bounded.

Runge-Kutta Methods

Example

Recall from Example 2 on slide 4 the ODE

$$y(0) = y_0, \qquad \dot{y} = y^2.$$

Since $f'(y) = 2y$ exists but is unbounded, $f(y) = y^2$ is locally but not globally Lipschitz continuous and hence solutions may exist only over some finite interval $[0, T]$.

Indeed, we have observed previously that the solution

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

exists as a function $y : \mathbb{R} \to \mathbb{R}$ only on $[0, \frac{1}{y_0})$.

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Continuity of the ODE map

To approximate the ODE map $\big(f(y), y_0, T\big) \mapsto y(t)$ numerically, we need this map to be not only well defined but also continuous with respect to the initial conditions; otherwise any small perturbation in y_0 (e.g. rounding errors) may lead to arbitrarily large errors in the solution $y(t)$.

Fortunately, it turns out that Lipschitz continuity of $f(y)$ guarantees not existence and uniqueness of solutions but also that these solutions are a Lipschitz continuous function of the initial conditions y_0.

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 $y_1, y_2 : [0, T) \to \mathbb{R}^n$ are two solutions to the same ODE $\dot{y}_k = f(y_k)$ but with different initial conditions $y_1(0)$ and $y_2(0)$. Then,

$$\|y_1(t) - y_2(t)\| \ \le \ \exp(Lt)\, \|y_1(0) - y_2(0)\| \qquad \text{for any } t < T.$$

Proof (not examinable). See the following slides (which I will skip in class).

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Lipschitz continuity of the ODE map is a consequence of the following auxiliary result.

Lemma: Gronwall's inequality (not examinable)

$$\dot{y}(t) \le \lambda\, y(t) \qquad \Longrightarrow \qquad y(t) \le \exp(\lambda t)\, y(0).$$

Proof (not examinable).
Consider $z(t) = \exp(-\lambda t)\, y(t)$. Then, $z(0) = y(0)$ and

$$\begin{aligned} \dot{z}(t) &= -\lambda \exp(-\lambda t)\, y(t) + \exp(-\lambda t)\, \dot{y}(t) \\ &\le -\lambda \exp(-\lambda t)\, y(t) + \exp(-\lambda t)\, \lambda\, y(t) = 0; \end{aligned}$$

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

Proof of the theorem on slide 18 (not examinable).

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

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

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

$$\begin{aligned}
\frac{d}{dt}\|y_2(t) - y_1(t)\| &\leq \|\dot{y}_2(t) - \dot{y}_1(t)\| \\
&= \|f(y_2(t)) - f(y_1(t))\| \\
&\leq L\,\|y_2(t) - y_1(t)\|.
\end{aligned}$$

The claim then follows by Gronwall's inequality.

Runge-Kutta Methods

Interpretation of the ODE continuity

In the above bound

$$\|y_1(t) - y_2(t)\| \;\leq\; \exp(Lt)\;\|y_1(0) - y_2(0)\|,$$

$y_1(t)$ typically represents the exact solution and $y_2(t)$ represents an approximation to $y_1(t)$ resulting from a slightly perturbed initial condition $y_2(0)$. In this context, the above bound is both a blessing and a curse:

- Good: The error at time t is proportional to the error at time 0.
- Bad: The constant of proportionality is $\exp(Lt)$ and hence grows very rapidly once $t > \frac{1}{L}$.

The second point implies that solving ODEs over time spans longer than one over the Lipschitz constant is essentially impossible.

It is the mathematical foundation of phenomena like the butterfly effect, i.e. the claim that the occurrence of a tornado may depend on whether a butterfly flaps its wings.

Runge-Kutta Methods

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 solving ODEs.

It turns out that solving ODEs is in some sense equivalent to evaluating integrals, namely we have

$$y(0) = y_0, \quad \dot{y} = f(y) \qquad \Longleftrightarrow \qquad y(t) = y_0 + \int_0^t f(y(\tau))\, d\tau.$$

Numerically computing integrals is known as *quadrature*, and it is a problem that we already know how to solve. The following slides will recapitulate the basics.

Runge-Kutta Methods

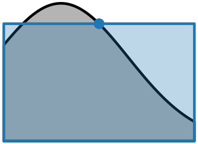
Def: Quadrature rule

A formula of the form

$$\sum_{k=1}^{n} f(x_k)\, w_k \approx \int_a^b f(x)\, dx$$

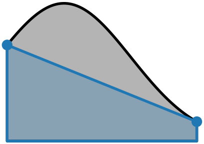
is called a *quadrature rule for* $[a, b]$. The parameters $(x_k \in \mathbb{R})_{k=1}^{n}$ and $(w_k \in \mathbb{R})_{k=1}^{n}$ are called *quadrature points* and *quadrature weights*, respectively.

Example quadrature rules $\quad (m = \frac{a+b}{2})$



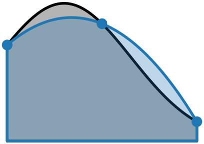
Midpoint rule

$(b-a)\, f(m)$



Trapezoidal rule

$\frac{b-a}{2}\, \big(f(a) + f(b)\big)$



Simpson's rule

$\frac{b-a}{6}\, \big(f(a) + 4\, f(m) + f(b)\big)$

Runge-Kutta Methods

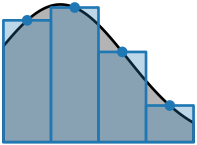
Composite quadrature

Quadrature rules generally become more accurate the larger the number of quadrature points. A simple way to construct quadrature rules with many points is to split the original integral into many small integrals,

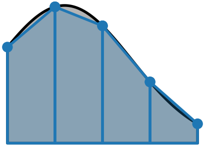
$$\int_a^b f(x)\,dx \;=\; \sum_{k=1}^{n} \int_{c_{k-1}}^{c_k} f(x)\,dx$$

and then apply a simple quadrature rule to each of these small integrals. This trick is known as *composite quadrature*.

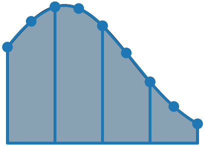
Example composite quadrature rules



Composite midpoint



Composite trapezoidal



Composite Simpson

Runge-Kutta Methods

Solving ODEs using quadrature (continued)

Let us now return to the problem of evaluating the ODE integral

$$y(t) = y_0 + \int_0^t f(y(\tau))\, d\tau.$$

The first challenge that we face when trying to apply quadrature to this integral is that the integration interval $[0, t]$ is of variable rather than fixed width. This circumstance can be remedied by substituting $\tau = xt$, which yields

$$y(t) = y_0 + \int_0^1 f(y(xt))\, t\, dx.$$

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

$$y(t) \approx y_0 + \sum_{k=1}^{s} f\big(y(x_k t)\big)\, w_k t.$$

Runge-Kutta Methods

Solving ODEs using quadrature (continued)

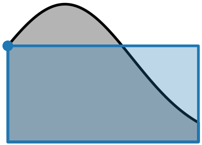
The second challenge is that the highlighted values in

$$y(t) \approx y_0 + \sum_{k=1}^{s} f\big(y(x_k t)\big)\, w_k t$$

are available only if $x_k = 0$.

The only admissible quadrature rule is hence the *left-point rule* given by

$$x_1 = 0, \qquad w_1 = 1 \qquad \longleftrightarrow$$



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This quadrature rule leads us to the approximation

$$y(t) \approx y(0) + f\big(y(0)\big)\, t$$

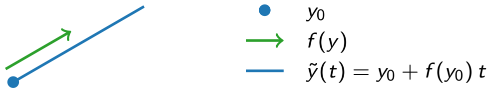
which is known as an *Euler step*.

Runge-Kutta Methods

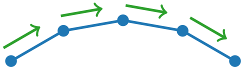
Visual interpretation of Euler's method

The right-hand side $f(y)$ in the ODE $\dot{y} = f(y)$ can be interpreted as the direction in which $y(t)$ should move given its current position.

In this mental model, the Euler step formula corresponds to looking at the direction once and then moving in this direction forever.



It is clear that this procedure will not lead to good approximations. We can obtain better approximations by using the Euler step formula to extrapolate only some small distance into the future and then update the direction $f(y)$.



This procedure is analogous to the composite quadrature idea and known as *Euler's method*.

Runge-Kutta Methods

Def: Euler's method

Approximating the solution to $y(0) = y_0$, $\dot{y} = f(y)$ using

$$\tilde{y}(0) = y_0, \qquad \tilde{y}\big(t_k\big) = \tilde{y}(t_{k-1}) + f\big(\tilde{y}(t_{k-1})\big)\,\big(t_k - t_{k-1}\big)$$

is known as *Euler's method*.

The t_k in this formula refer to a sequence of time points

$$0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T.$$

Such a sequence is called a *temporal mesh*.

For much of this lecture, I will be using the equispaced temporal mesh

$$\Big(\ t_k = \tfrac{T}{n}\,k\ \Big)_{k=0}^{n},$$

but it will occasionally be useful to also consider more general meshes.

Numerical demonstration

See `euler_step()`, `propagate()` and `example()`.

Runge-Kutta Methods

Runtime and Convergence of Euler's method

In addition to the ODE parameters $f(y)$, y_0, and T, Euler's method requires us to also choose a temporal mesh $(t_k)_{k=0}^{n}$.

We intuitively expect that choosing a mesh with a larger number of points n will lead to smaller errors but longer runtimes. Choosing a temporal mesh hence amounts to striking a balance between accuracy and performance.

As usual, the best way to quantify this error is to analyse separately how the runtime and accuracy depends on the number of time steps n.

This will be tackled on the following slides.

Runge-Kutta Methods

Thm: Runtime of Euler's method

n steps of Euler's method require n evaluations of $f(y)$ and $O(n)$ other operations.

Proof. Immediate consequence of the recursion equation

$$\tilde{y}(t_k) = \tilde{y}(t_{k-1}) + f\big(\tilde{y}(t_{k-1})\big)\,\big(t_k - t_{k-1}\big).$$

Note that I count exactly the number of ODE-right-hand-side evaluations $f(y)$ but I count only in the big O sense the number of other operations. The reason for this is that evaluating $f(y)$ is usually by far the most time-consuming part of any ODE solver; hence it is usually fair to say that an algorithm which performs x times as many $f(y)$ evaluations is also x times slower.

Runge-Kutta Methods

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,

$$\big\|\tilde{y}(T) - y(T)\big\| = O\Big(\exp(LT)\,\tfrac{T^2}{n}\Big) \qquad \text{for both } n, T \to \infty,$$

assuming $f(y)$ is Lipschitz continuous with Lipschitz constant L.
Proof. See the following slides.

Numerical demonstration
See `convergence()`.

Runge-Kutta Methods

Verifying the above result requires us to first put into place quite a bit of mathematical machinery.

For starters, we need the notion of time propagators defined as follows.

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

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

Simply put, time propagators are functions which take in the current state y_0 and a time span t, and produce the (approximate) solution at time t in the future.

We have seen on slide 18 that the ODE solution $y(t)$ is a Lipschitz continuous function of the initial condition y_0.

This fact can be expressed in terms of the time propagator as follows.

Thm: Lipschitz continuity of the exact time propagator

If $f(y)$ is Lipschitz continuous with Lipschitz constant L, then $\Phi(y_0, t)$ is Lipschitz continuous in y_0 with Lipschitz constant $\exp(Lt)$, i.e.

$$\big\|\Phi(y_1, t) - \Phi(y_2, t)\big\| \;\le\; \exp(Lt)\,\big\|y_1 - y_2\big\|.$$

Proof. Immediate consequence of the result on slide 18.

Runge-Kutta Methods

Shorthand notations

I will use the shorthand notations

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

and

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

in the following. As usual, $(t_k)_k$ denotes some temporal mesh specified by the context.

With this, we now have all the pieces in place to derive an error estimate for Euler's method.

Runge-Kutta Methods

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 by Euler's method with temporal mesh $(t_k)_{k=0}^{n}$. Then,

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

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

Proof.

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

Runge-Kutta Methods

The factor $\left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\|$ on the right-hand side of the above error estimate is known under several names.

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

The above bound

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

can hence 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 $\Phi(y, t)$ (see slide 18).

Runge-Kutta Methods

The above bound shows that the total error $\|\tilde{y}_n - y_n\|$ vanishes if all the local errors $\left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\|$ vanish as the time steps $t_k - t_{k-1}$ go to zero. The following result shows that this is indeed the case.

Lemma: Consistency of Euler time propagator

The Euler time propagator $\tilde{\Phi}(y_0, t)$ satisfies

$$\left\|\tilde{\Phi}(y_0, t) - \Phi(y_0, t)\right\| = O(t^2) \qquad \text{for } t \to 0.$$

Proof.

$$\begin{aligned}
\Phi(y_0, t) &= y(0) + \dot{y}(0)\, t + O(t^2) && \text{(apply Taylor)} \\
&= y_0 + f(y_0)\, t + O(t^2) && \text{(use } y(0) = y_0 \text{ and } \dot{y} = f(y)\text{)} \\
&= \tilde{\Phi}(y_0, t) + O(t^2) && \text{(definition of } \tilde{\Phi}(y_0, t)\text{)}
\end{aligned}$$

Runge-Kutta Methods

The above property has a special name.

Terminology: pth-order consistency

A numerical time propagator $\tilde{\Phi}(y_0, t)$ such that

$$\left\|\tilde{\Phi}(y_0, t) - \Phi(y_0, t)\right\| = O(t^p) \qquad \text{for } t \to 0$$

is said to be pth-order consistent.

We can now finally verify the claimed order of convergence of Euler's method by combining the above error bound and consistency result.

Proof of convergence of Euler's method (slide 31).

$$\begin{aligned}
\left\|\tilde{y}_n - y_n\right\| &\leq \sum_{k=1}^{n} \exp\big(L\,(t_n - t_k)\big)\left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\| \\
&\leq n \exp\big(L\,(t_n - t_0)\big)\, O\Big(\big(\tfrac{T}{n}\big)^2\Big) \\
&= \exp\big(L\,(t_n - t_0)\big)\, O\big(\tfrac{T^2}{n}\big)
\end{aligned}$$

Runge-Kutta Methods

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 $O\big(n^{-2}\big)$; 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

$$\big\|\tilde{y}(T) - y(T)\big\| = O\Big(\exp(LT)\,\tfrac{T^2}{n}\Big) \leq \tau$$

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

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

See `nsteps()` for numerical demonstration.

Runge-Kutta Methods

Improving Euler's method

The theorem on slide 31 establishes that Euler's method

$$\tilde{y}(0) = y(0), \qquad \tilde{y}\big(t_k\big) = \tilde{y}\big(t_{k-1}\big) + f\big(\tilde{y}\big(t_{k-1}\big)\big)\,\big(t_k - t_{k-1}\big)$$

converges to the exact solution $y(t)$, but it also shows that the rate of convergence is only

$$\big\|\tilde{y}(T) - y(T)\big\| = O\big(n^{-1}\big).$$

This slow convergence is ultimately due to the fact that Euler's method is based on the very poor quadrature approximation

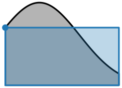
$$\int_0^t f(y(\tau))\,d\tau \;\approx\; f(y(0))\,t;$$

hence the question arises whether we can improve the speed of convergence by choosing a more accurate quadrature rule.

Runge-Kutta Methods

Improving Euler's method (continued)

The reason why we settled for the "left-point rule"

$$x_1 = 0, \qquad w_1 = 1 \qquad \longleftrightarrow$$  .

on slide 26 was that we assumed that we do not know $y(t)$ at times $t > 0$ and hence we cannot have quadrature points $x_k > 0$.

However, this constraint no longer applies now that we know how to (approximately) propagate $y(0)$ into the future using Euler steps.

For example, we can use an Euler step to estimate

$$\tilde{y}_2(t) \; = \; y(0) + f\big(y(0)\big)\, t,$$

and then we can use a trapezoidal rule approximation

$$\tilde{y}(t) = y(0) + \Big(f\big(y(0)\big) + f\big(\tilde{y}_2(t)\big) \Big)\, \tfrac{t}{2},$$

to improve this estimate. This idea is known as the trapezoidal rule.

Runge-Kutta Methods

Def: Trapezoidal rule

Approximating the solution to $y(0) = y_0$, $\dot{y} = f(y)$ using

$$\begin{aligned} \tilde{y}(0) &= y_0 \\ \tilde{y}_2(t_k) &= \tilde{y}(t_{k-1}) + f\left(\tilde{y}(t_{k-1})\right)\left(t_k - t_{k-1}\right), \\ \tilde{y}(t_k) &= \tilde{y}(t_{k-1}) + \Big(f\left(\tilde{y}(t_{k-1})\right) + f\left(\tilde{y}_2(t_k)\right)\Big)\,\tfrac{t_k - t_{k-1}}{2}, \end{aligned}$$

is known as the trapezoidal rule method.

The pictorial interpretation of a trapezoidal step is as follows.

Runge-Kutta Methods

Terminology: Quadrature rules vs. ODE solvers

It is common to refer to both the above ODE solver as well as the quadrature rule from which it is derived as the "trapezoidal rule".

This is not a problem since we can usually deduce from context whether the ODE solver or the quadrature rule is meant.

Notation: Distinguishing approximations to the same value

Note that the trapezoidal rule computes two different numerical approximation $\tilde{y}_2(t_k)$ and $\tilde{y}(t_k)$ to the same value $y(t_k)$.

Here and throughout this lecture, I will distinguish these approximations by writing $\tilde{y}_i(t_k)$, $i = 1, 2, 3, \ldots$, for the auxiliary approximations, and $\tilde{y}(t_k)$ without a subscript for the final approximation.

Runge-Kutta Methods

Implementation of the trapezoidal rule

See `trapezoidal_step()` and `integrate()`.

Note that `f1 = t * f(y0)` is used both in

`f2 = t * f(y0 + f1)` and `y0 + (f1 + f2)/2` .

Introducing `f1` hence avoids having to evaluate `t * f(y0)` twice.

Runge-Kutta Methods

Runtime and convergence of the trapezoidal rule

We now have two algorithms for solving the same problem, namely Euler's method and the trapezoidal rule.

To compare these methods, I will next repeat for the trapezoidal rule what we have already done for Euler's method, namely I will study the scaling of the runtime and accuracy as a function of the number of time steps n.

Thm: Runtime of the trapezoidal rule

n steps of the trapezoidal rule require $2n$ evaluations of $f(y)$ and $O(n)$ other operations.

Proof. Immediate consequence of the recursion equations

$$\begin{aligned} \tilde{y}_2(t_k) &= \tilde{y}(t_{k-1}) + f\big(\tilde{y}(t_{k-1})\big)\,\big(t_k - t_{k-1}\big), \\ \tilde{y}(t_k) &= \tilde{y}(t_{k-1}) + \Big(f\big(\tilde{y}(t_{k-1})\big) + f\big(\tilde{y}_2(t_k)\big)\Big)\,\tfrac{t_k - t_{k-1}}{2}. \end{aligned}$$

Runge-Kutta Methods

Thm: Convergence of the trapezoidal rule

Denote by $y(t)$ the solution to $\dot{y} = f(y)$ and by $\tilde{y}(t)$ the numerical approximation obtained using the trapezoidal rule with the equispaced temporal mesh $(t_k = \frac{k}{n}\,T)_{k=0}^{n}$.

Then,

$$\big\|\tilde{y}(T) - y(T)\big\| = O\Big(\exp(LT)\,\tfrac{T^3}{n^2}\Big) \qquad \text{for both } n, T \to \infty,$$

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

Proof. See the following slides.

Runge-Kutta Methods

Proof of convergence of the trapezoidal rule.

We have seen on slides 31 and following that the first-order convergence of Euler's method is a consequence of the error bound

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

and the second-order consistency of the Euler time propagator.

Looking back at the proofs of these results, we realise that both the above bound and the claim

$$(p+1)\text{th order consistency} \quad\implies\quad p\text{-order convergence}$$

are in fact not specific to Euler's method but rather hold for any numerical time propagator $\tilde{\Phi}_k(y_0, t)$.

All that is needed to show second-order convergence of the trapezoidal rule is hence to introduce the numerical time propagator associated with the trapezoidal rule and show that this propagator is third-order consistent.

This will be tackled on the following slides.

Runge-Kutta Methods

Def: Trapezoidal rule time propagator

The *trapezoidal rule time propagator* associated with $f : \mathbb{R}^n \to \mathbb{R}^n$ is given by

$$\tilde{\Phi}(y_0, t) = y_0 + \big(f(y_0) + f(y_2)\big)\,\tfrac{t}{2} \qquad \text{where} \qquad y_2 = y_0 + f(y_0)\,t,$$

or equivalently,

$$\tilde{\Phi}(y_0, t) = y_0 + f(y_0)\,\tfrac{t}{2} + f\big(y_0 + f(y_0)\,t\big)\,\tfrac{t}{2}.$$

Runge-Kutta Methods

Lemma: Consistency of trapezoidal rule

The trapezoidal rule time propagator $\tilde\Phi(y_0, t)$ satisfies

$$\left\|\tilde\Phi(y_0,t) - \Phi(y_0,t)\right\| = O(t^3) \qquad \text{for } t \to 0.$$

Proof. As on slide 37, the proof amounts to showing that the Taylor series of $\tilde y(t) = \tilde\Phi(y_0, t)$ agrees with the Taylor series of $y(t) = \Phi(y_0, t)$ up to and including the second-order term.

I therefore compute

$$\begin{aligned}
\tilde y(t) &= y_0 \;+\; f(y_0)\,\tfrac{t}{2} \;+\; f\big(y_0 + f(y_0)\,t\big)\,\tfrac{t}{2} \\
\dot{\tilde y}(t) &= f(y_0)\,\tfrac{1}{2} \;+\; f'\big(y_0 + f(y_0)\,t\big)\,f(y_0)\,\tfrac{t}{2} \;+\; f\big(y_0 + f(y_0)\,t\big)\,\tfrac{1}{2} \\
\ddot{\tilde y}(t) &= f''\big(y_0 + f(y_0)\,t\big)\,f(y_0)^2\,\tfrac{t}{4} \;+\; 2\,f'\big(y_0 + f(y_0)\,t\big)\,f(y_0)\,\tfrac{1}{2}
\end{aligned}$$

and conclude that we indeed have

$$\tilde y(0) = y_0 = y(0), \quad \dot{\tilde y}(0) = f(y_0) = \dot y(0), \quad \ddot{\tilde y}(0) = f'(y_0)\,f(y_0) = \ddot y(0),$$

where for the second-order term I used that

$$\dot y(t) = f(y(t)) \quad \Longrightarrow \quad \ddot y(t) = f'\big(y(t)\big)\,\dot y(t) = f'\big(y(t)\big)\,f\big(y(t)\big).$$

Runge-Kutta Methods

Euler vs trapezoidal method

We can summarise the performance characteristics of Euler's method and the trapezoidal rule as follows.

	$f(y)$ evals	Error
Euler	n	$O(n^{-1})$
Trapezoidal	$2n$	$O(n^{-2})$

In practice, this means that Euler's method tends to be faster for moderate accuracy requirements but is eventually outperformed by the trapezoidal rule as the error tolerance decreases.

See `convergence()` (uncomment the `"trapezoidal"` line).

Runge-Kutta Methods

General Runge-Kutta methods

Given the above, one may wonder whether we can invest even more work per time step to achieve an even better order of convergence and hence a smaller runtime in the limit $\tau \to 0$.

The answer is yes, and in fact we can do so simply by continuing the procedure which led us to the trapezoidal rule.

Algorithms derived from this idea are known as *Runge-Kutta methods*.

Runge-Kutta Methods

Def: Runge-Kutta method

An algorithm which approximates the solution to $y(0) = y_0$, $\dot{y} = f(y)$ using

```
ỹ(0) = y_0,
for k = 1, ..., n do
    for i = 1, ..., s do
        ỹ_i = ỹ(t_{k-1}) + Σ_{j=1}^{s} f(ỹ_j) W_{ij} (t_k - t_{k-1})
    end for
    ỹ(t_k) = ỹ(t_{k-1}) + Σ_{j=1}^{s} f(ỹ_j) w_j (t_k - t_{k-1})
end for
```

$$\tilde{y}(0) = y_0,$$

for $k = 1, \dots, n$ **do**

  for $i = 1, \dots, s$ **do**

$$\tilde{y}_i = \tilde{y}(t_{k-1}) + \sum_{j=1}^{s} f\left(\tilde{y}_j\right) W_{ij} \left(t_k - t_{k-1}\right)$$

  end for

$$\tilde{y}(t_k) = \tilde{y}(t_{k-1}) + \sum_{j=1}^{s} f\left(\tilde{y}_j\right) w_j \left(t_k - t_{k-1}\right)$$

end for

is called an *s-stage Runge-Kutta method*.

The parameters $w \in \mathbb{R}^s$ and $W \in \mathbb{R}^{s \times s}$ can be interpreted as the quadrature weights of the following quadrature rules:

- $(x_j, w_j)_{j=1}^s$ is a quadrature rule for $[0, 1]$.
- $(x_i, W_{ij})_{i=1}^s$ is a quadrature rule for $[0, x_j]$.

Runge-Kutta Methods

The parameters $x \in \mathbb{R}^s$, $W \in \mathbb{R}^{s \times s}$ and $w \in \mathbb{R}^s$ introduced in the above definition are most conveniently represented in a tabular form known as a *Butcher tableau*.

Def: Butcher tableau

The representation of the Runge-Kutta parameters $x \in \mathbb{R}^s$, $W \in \mathbb{R}^{s \times s}$ and $w \in \mathbb{R}^s$ given by

$$\begin{array}{c|ccc} x_1 & W_{11} & \dots & W_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ x_s & W_{s1} & \dots & W_{ss} \\ \hline & w_1 & \dots & w_s \end{array}$$

is called a *Butcher tableau*.

The examples on the next slide might help you to better understand the definition of Runge-Kutta schemes and Butcher tableaus.

Runge-Kutta Methods

Example 1: Euler's method

Tableau

$$\begin{array}{c|c} 0 & \\ \hline & 1 \end{array}$$

Interpretation

$$\begin{array}{r} \tilde{y}_1(t_{k-1}) = \tilde{y}(t_{k-1}) \\ \hline \tilde{y}(t_k) = \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,(t_k - t_{k-1}) \end{array}$$

Example 2: Trapezoidal rule

Tableau

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Interpretation

$$\begin{array}{r} \tilde{y}_1(t_{k-1}) = \tilde{y}(t_{k-1}) \\ \tilde{y}_2(t_k) = \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,(t_k - t_{k-1}) \\ \hline \tilde{y}(t_k) = \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,\frac{t_k - t_{k-1}}{2} + f(\tilde{y}_2)\,\frac{t_k - t_{k-1}}{2} \end{array}$$

Optimal Runge-Kutta methods

The above definition allows us to turn any set of parameters x, W and w into a Runge-Kutta method, but of course not all methods constructed in this way are equally interesting.

Specifically, there is no point considering a particular Runge-Kutta method if there is another method with same number of $f(y)$ evaluations per time step but better accuracy.

Combining this insight with the observation that the number of $f(y)$ evaluation per step is equal to the number of stages s, we conclude that a particular Runge-Kutta method is interesting only if its order of convergence is as large as possible for the given s.

Runge-Kutta Methods

Convergence theory of Runge-Kutta methods

Determining Runge-Kutta methods with maximal order of convergence is straightforward.

- Like Euler's method and the trapezoidal rule, Runge-Kutta methods construct an approximate solution $\tilde{y}(t)$ by repeatedly applying a particular numerical time propagator $\tilde{\Phi}(y_0, t)$;
- Any Runge-Kutta solution $\tilde{y}(t_n)$ hence satisfies the bound

$$\left\|\tilde{y}(t_n) - y(t_n)\right\| \;\leq\; \sum_{k=1}^{n} \exp\big(L\,(t_n - t_k)\big)\; \left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\|$$

  derived on slide 35.
- The order of convergence is thus maximised if we choose x, W and w such that the Taylor series of the Runge-Kutta time propagator $\tilde{\Phi}(y_0, t)$ agrees with the one of the exact time propagator $\Phi(y_0, t)$ as far as possible.

Convergence theory of Runge-Kutta methods (continued)

The "only" obstacle in the above procedure is that computing derivatives of $\Phi(y_0, t)$ and $\tilde{\Phi}(y_0, t)$ becomes more and more tedious as the order of the derivative and the number of stages of the Runge-Kutta method increase.

Fortunately, you will hardly ever have to do these computations yourself, because other people have already done them and they have catalogued their findings for us. See

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

In practice, determining a suitable Runge-Kutta method is hence as simple as skimming the appropriate Wikipedia list.

Runge-Kutta Methods

Example

Runge-Kutta ODE solvers are named after two German mathematicians who proposed the following scheme and showed that it is a fourth-order method.

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & & \frac{1}{2} & & \\
1 & & & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

I demonstrate in `rk4_step()` how to implement this scheme and in `convergence()` that it is indeed a fourth-order method.

Runge-Kutta Methods

Number of stages vs. order of convergence

We have now seen three particular Runge-Kutta methods.

Method	# stages	Convergence
Euler	1	$O(n^{-1})$
Trapezoidal	2	$O(n^{-2})$
RK4	4	$O(n^{-4})$

Based on this table, you might expect but that optimal s-stage Runge-Kutta schemes achieve $O(n^{-s})$ convergence, but this is not true; it can be shown that the optimal order of convergence p as a function of the number of stages s is given by

$$\begin{array}{c|ccccccccccc} s & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & \dots \\ \hline p & 1 & 2 & 3 & 4 & 4 & 5 & 6 & 6 & 7 & 8 & \dots \end{array}.$$

For this reason, Runge-Kutta schemes with $s > 4$ stages are rarely used.

Runge-Kutta Methods

Adaptive time-stepping

The definition of Runge-Kutta methods on slide 52 depends on the physical / mathematical parameters $f(y)$ and y_0, but in addition it also depends on two types of numerical parameters, namely

- the quadrature weights $W \in \mathbb{R}^{s \times s}$ and $w \in \mathbb{R}^s$, and
- the temporal mesh $(t_k)_{k=0}^n$.

The above slides discussed the various criteria affecting our choice of quadrature weights. Next, I would like to turn our attention towards the temporal mesh $(t_k)_{k=0}^n$, and specifically I would like to study how the accuracy depends on the mesh points t_k for a fixed mesh size n.

This study complements our earlier convergence results where we fixed the mesh $t_k = \frac{T}{n}\,k$ to be equispaced and instead studied the limit of increasingly larger mesh sizes n.

Adaptive time-stepping (continued)

The motivation for studying accuracy as a function of the mesh points t_k is that the runtime of Runge-Kutta methods depends on only the number of time steps n but not on their spacing, and thus varying the mesh points t_k without increasing their number n gives us a means to improve accuracy without increasing the computational workload.

As soon as we understand how the temporal mesh affects the accuracy, we will therefore also be looking into how we can optimise the mesh such that the error is as small as possible for the given number of mesh points.

The algorithm which will result from this analysis is known as *adaptive time-stepping*.

Runge-Kutta Methods

Adaptive time-stepping (continued)

It turns out that all we have to do to understand the impact of the temporal mesh on accuracy is to repeat the earlier convergence analysis but fill in a bit more detail. Specifically:

1. On slide 35, we have seen that the error of a Runge-Kutta scheme $\tilde{y}(t)$ with associated time propagator $\tilde{\Phi}(y_0, t)$ is bounded by

$$\left\|\tilde{y}(t_n) - y(t_n)\right\| \;\leq\; \sum_{k=1}^{n} \exp\bigl(L\,(t_n - t_k)\bigr)\; \left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\|.$$

2. If we had used the Taylor theorem with remainder in our consistency analyses on slides 37 and 49, then we would have found that the local errors are bounded by

$$\left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\| \;\leq\; \tfrac{1}{p!}\,\bigl(t_k - t_{k-1}\bigr)^p \max_{t \in [t_{k-1}, t_k]} \left\|\tilde{y}^{(p)}(t) - y^{(p)}(t)\right\|,$$

   where p denotes the order of consistency (e.g. $p = 2$ for Euler's method and $p = 3$ for the trapezoidal rule).

Runge-Kutta Methods

Adaptive time-stepping (continued)

The above results readily answer the question of how the step lengths impact accuracy, but they are a bit inconvenient to work with. Let us therefore make the following simplifying assumptions:

- $\exp\bigl(L\,(t_n - t_k)\bigr) \approx 1.$

  Justification: We have seen earlier that solving ODEs over time spans $T \gg \frac{1}{L}$ is generally not advisable

- $\max\limits_{t \in [t_{k-1}, t_k]} \bigl\|\tilde{y}^{(p)}(t) - y^{(p)}(t)\bigr\| \;\approx\; \bigl\|\tilde{y}^{(p)}(t_{k-1}) - y^{(p)}(t_{k-1})\bigr\|.$

  Justification: The step sizes $t_k - t_{k-1}$ are typically small enough such that the objective function is essentially constant over $[t_{k-1}, t_k]$.

We then obtain the approximate error bound

$$\bigl\|\tilde{y}(t_n) - y(t_n)\bigr\| \;\lesssim\; \sum_{k=1}^{n} \tfrac{1}{p!}\, \bigl(t_k - t_{k-1}\bigr)^p \;\bigl\|\tilde{y}^{(p)}(t_{k-1}) - y^{(p)}(t_{k-1})\bigr\|.$$

This answers the question of how the temporal mesh impacts the error.

Runge-Kutta Methods

Adaptive time-stepping (continued)

Next, let us consider how we can optimise the mesh such that the error is as small as possible, i.e. let us consider the constrained optimisation problem

$$\min_{(\Delta t_k)_{k=1}^n} \sum_{k=1}^n c_k \, \Delta t_k^p \quad \text{subject to} \quad \sum_{k=1}^n \Delta t_k - T = 0$$

where I introduced the abbreviations

$$\Delta t_k = t_k - t_{k-1} \qquad \text{and} \qquad c_k = \tfrac{1}{p!} \left\| \tilde{y}^{(p)}(t_{k-1}) - y^{(p)}(t_{k-1}) \right\|.$$

According to the Lagrangian multiplier trick, the solution to this problem is such that the derivatives of the objective function

$$F\big((\Delta t_k)_k, \lambda\big) = \sum_{k=1}^n c_k \, \Delta t_k^p \; + \; \lambda \left(\sum_{k=1}^n \Delta t_k - T \right)$$

with respect to all Δt_k and λ are zero.

Runge-Kutta Methods

Adaptive time-stepping (continued)

This in particular implies that

$$\frac{\partial F}{\partial \Delta t_k} \;=\; p\, c_k\, \Delta t_k^{p-1} + \lambda \;=\; 0;$$

hence the mesh $(t_k)_k$ is optimal if

$$\Delta t_k^{p-1} \left\| \tilde{y}^{(p)}(t_{k-1}) - y^{(p)}(t_{k-1}) \right\| \;=\; \tau,$$

where $\tau \;=\; -(p-1)!\,\lambda \;\in\; [0, \infty)$ represents some local error tolerance independent of k.

This condition may look cryptic at first, but actually its meaning is both simple and intuitive, see next slide.

Runge-Kutta Methods

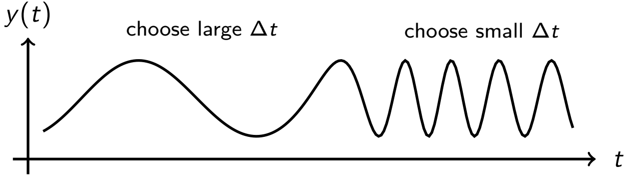
Adaptive time-stepping (continued)

It turns out that for many Runge-Kutta methods, we have

$$\left\|\tilde{y}^{(p)}(t_{k-1}) - y^{(p)}(t_{k-1})\right\| \approx \left\|y^{(p)}(t_{k-1})\right\|.$$

The right-hand side in this approximate identity can be interpreted as a measure for the curvature in $y(t)$, and hence the above finding can be summarised as follows.

The optimal step size Δt_k is small if the curvature is large, and large if the curvature is small.



Runge-Kutta Methods

Adaptive time-stepping (continued)

The condition

$$\Delta t_k^{p-1} \left\| \tilde{y}^{(p)}(t_{k-1}) - y^{(p)}(t_{k-1}) \right\| = \tau$$

tells us on a theoretical level what a good mesh should like, but it does not quite tell us yet how to determine such a mesh in practice because we are missing a tool to estimate the purple factor.

This missing tool is provided by the result on the next slide.

Runge-Kutta Methods

Thm: Estimating curvature by comparing methods

Let $\tilde{\Phi}(y_0, t)$, $\tilde{\Phi}_{\text{ref}}(y_0, t)$ be two Runge-Kutta time propagators with orders of consistency p and $p_{\text{ref}} > p$, respectively. We then have

$$\left\|\tilde{\Phi}(y_0, t) - \tilde{\Phi}_{\text{ref}}(y_0, t)\right\| = \left\|\tilde{y}^{(p)}(0) - y^{(p)}(0)\right\| \tfrac{t^p}{p!} + O(t^{p+1}),$$

i.e. we can estimate the curvature by comparing in each time step two approximate solutions $\tilde{y}(t)$ and $\tilde{y}_{\text{ref}}(t)$ computed using two Runge-Kutta steps of different orders of consistency $p < p_{\text{ref}}$.

Proof. According to Taylor's theorem, we have

$$\begin{aligned}
\tilde{\Phi}(y_0, t) &= y(0) + \ldots + y^{(p-1)}(0) \tfrac{t^{p-1}}{(p-1)!} + \tilde{y}^{(p)}(0) \tfrac{t^p}{p!} + O\big(t^{p+1}\big), \\
\tilde{\Phi}_{\text{ref}}(y_0, t) &= y(0) + \ldots + y^{(p-1)}(0) \tfrac{t^{p-1}}{(p-1)!} + y^{(p)}(0) \tfrac{t^p}{p!} + O\big(t^{p+1}\big), \\
\Phi(y_0, t) &= y(0) + \ldots + y^{(p-1)}(0) \tfrac{t^{p-1}}{(p-1)!} + y^{(p)}(0) \tfrac{t^p}{p!} + O\big(t^{p+1}\big).
\end{aligned}$$

Therefore,

$$\tilde{\Phi}(y_0, t) - \tilde{\Phi}_{\text{ref}}(y_0, t) \;=\; \Big(\tilde{y}^{(p)}(0) - y^{(p)}(0)\Big) \tfrac{t^p}{p!} + O\big(t^{p+1}\big).$$

Runge-Kutta Methods

Adaptive Runge-Kutta methods (continued)

We now have all the mathematical tools needed to determine good temporal meshes. What is needed next is some clever mathematical engineering to translate these tools into a simple and fast adaptive time-stepping algorithm.

The next slide will present a big-picture outline of this algorithm, and the slides after that will fill in a few details.

Runge-Kutta Methods

The adaptive time-stepping algorithm

Set $t_0 = 0$, $\tilde{y}(t_0) = y_0$, and until we have $t_k = T$, repeat the following:

1. Compute the two Runge-Kutta estimates $\tilde{y}$ and $\tilde{y}_{\text{ref}}$ for the solution at the next time point t_k using a trial step size Δt.
2. Estimate what the optimal step size would have been by solving for Δt_{opt} the two equations

$$\|\tilde{y} - \tilde{y}_{\text{ref}}\| \approx \|\tilde{y}^{(p)} - y^{(p)}\| \, \frac{\Delta t^p}{p!} \quad \text{and} \quad \|\tilde{y}^{(p)} - y^{(p)}\| \, \frac{\Delta t_{\text{opt}}^{p-1}}{p!} = \tau,$$

   i.e. by computing

$$\Delta t_{\text{opt}} = \left(\frac{\tau \, \Delta t^p}{\|\tilde{y} - \tilde{y}_{\text{ref}}\|} \right)^{1/(p-1)} .$$

3. If the trial step size is less than the optimal step size, $\Delta t < \Delta t_{\text{opt}}$, then we set $t_k = t_{k-1} + \Delta t$ and $\tilde{y}(t_k) = \tilde{y}_{\text{ref}}$ and move on to the next step $t_k \to t_{k+1}$.

   Otherwise, we update the trial step size to $\Delta t = 0.9 \, \Delta t_{\text{opt}}$ and restart from step 1.

   The 0.9 in this formula is a safety factor intended to increase the chances that we accept the new trial step size.

Runge-Kutta Methods

As promised, I will next look at a few details of the above algorithm.

Embedded Runge-Kutta schemes

At first sight, it may seem that computing both $\tilde{y}$ and $\tilde{y}_{\text{ref}}$ in step 1 of the above algorithm would take roughly twice as long as computing just one of these trial solutions.

This factor of 2 can be avoided by choosing the two Runge-Kutta schemes such that the lower-order method uses only $f(y)$ values which must be computed anyway when evaluating the higher-order method.

Such pairs of Runge-Kutta schemes are called *embedded*.

Example. The trapezoidal step

$$\tilde{y}_{\text{Euler}}(t_k) = \tilde{y}(t_{k-1}) + f\left(\tilde{y}(t_{k-1})\right)\left(t_k - t_{k-1}\right),$$

$$\tilde{y}_{\text{trap}}(t_k) = \tilde{y}(t_{k-1}) + \left(f\left(\tilde{y}(t_{k-1})\right) + f\left(\tilde{y}_{\text{Euler}}(t_k)\right)\right)\frac{t_k - t_{k-1}}{2}$$

already evaluates the Euler step formula; thus the runtime of using the trapezoidal rule to estimate the accuracy of an Euler step is exactly equal to that of just evaluating a trapezoidal step. See `embedded_ET_step()`.

Embedded Runge-Kutta schemes (continued)

Further examples of embedded Runge-Kutta schemes can be found under

`https://en.wikipedia.org/wiki/List_of_Runge-Kutta_methods#Embedded_methods`.

Implementation of adaptive time-stepping

See `propagate_adaptive()` and `step_example()`.

Note that this code determines a good temporal mesh for the less accurate Runge-Kutta scheme $\tilde{\Phi}$ but then returns the approximations computed according to the more accurate scheme $\tilde{\Phi}_{\mathsf{ref}}$ as "the" ODE solution (see the `push!(y,yref)` statement).

The rationale for this abuse of the higher-order scheme is that it seems silly to compute a more accurate result and then not use it.

Runge-Kutta Methods

Adaptive time-stepping applied to $\dot{y} = \lambda y$

Encouraged by our observations in `step_example()`, I next apply adaptive time-stepping to the ODE

$$y(0) = 1, \quad \dot{y} = \lambda y \quad \iff \quad y(t) = \exp(\lambda\, t) \quad \text{where} \quad \lambda < 0$$

in `decay_example()`.

Since the solution to this ODE converges to a constant, one might expect that our adaptive time-stepping scheme would choose increasingly larger step sizes as $t \to \infty$, but we empirically observe that this is not the case.

Choosing small step sizes even in regions where the solution $y(t)$ barely changes feels like a waste of computational resources. Let us therefore investigate why our step selection routine refuses to increase the step size beyond some upper bound Δt_{max}.

Runge-Kutta Methods

Runge-Kutta methods applied to $\dot{y} = \lambda y$

The key to answering the above question is to observe that both Euler's method and the trapezoidal rule applied to $\dot{y} = \lambda y$ take a very simple form: the numerical time propagator for Euler's method is given by

$$\tilde{\Phi}(y_0, t) \;=\; y_0 + f(y_0)\, t \;=\; y_0 + \lambda y_0 t \;=\; (1 + \lambda t)\, y_0, \qquad \text{(Euler)}$$

and the numerical time propagator for the trapezoidal rule is given by

$$\begin{aligned} \tilde{\Phi}(y_0, t) &= y_0 + \Big(f(y_0) + f\big(y_0 + f(y_0)\, t\big) \Big) \tfrac{t}{2} \\ &= y_0 + \Big(\lambda y_0 + \lambda \big(y_0 + \lambda y_0 t\big) \Big) \tfrac{t}{2} \qquad \text{(trapezoidal)} \\ &= \big(1 + \lambda t + \tfrac{\lambda^2 t^2}{2}\big)\, y_0. \end{aligned}$$

The numerical solutions $\tilde{y}(t)$ after k steps with constant step size Δt are hence given by

$$\tilde{y}(k\,\Delta t) = R(\lambda\,\Delta t)^k\, y(0)$$

where

$$R(z) = \begin{cases} 1 + z & \text{for Euler's method, and} \\ 1 + z + \frac{z^2}{2} & \text{for the trapezoidal rule.} \end{cases}$$

Runge-Kutta Methods

Runge-Kutta methods applied to $\dot{y} = \lambda y$ (continued)

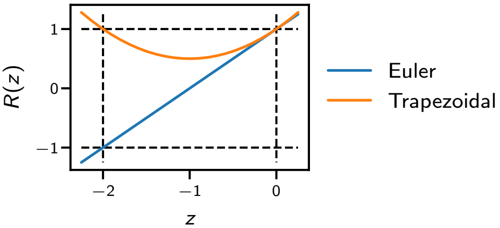
The Runge-Kutta solutions $\tilde{y}(t)$ therefore

- grow exponentially if $|R(\lambda\,\Delta t)| > 1$,
- are constant or oscillate if $|R(\lambda\,\Delta t)| = 1$, and
- decay exponentially if $|R(\lambda\,\Delta t)| < 1$.

In the case

$$y(0) = 1, \quad \dot{y} = \lambda y \quad \Longleftrightarrow \quad y(t) = \exp(\lambda\, t) \quad \text{where} \quad \lambda < 0,$$

we know that the exact solution decays exponentially and hence we want our numerical solutions to do the same, i.e. we want $|R(\lambda \Delta t)| < 1$. Looking at the below plots of $R(z)$, we conclude that this is the case if and only if $-2 < \lambda\,\Delta t < 0$.



Runge-Kutta Methods

We may summarise these findings as follows.

Thm: Step size constraint for $\dot{y} = \lambda y$

Euler's method and the trapezoidal rule applied to $\dot{y} = \lambda y$ with an equispaced temporal mesh $(t_k = k\,\Delta t)_{k=1}^{\infty}$ produce numerical solutions $\tilde{y}(t)$ such that $\lim_{t\to\infty} \tilde{y}(t) = 0$ if and only if $\Delta t < -2/\lambda$.

Terminology: Step size constraint and largest admissible step size

Bounds of the form $\Delta t < \Delta t_{\max}$ are called *step size constraints*, and the upper bound $\Delta t_{\max}$ is called the *largest admissible step size*.

Numerical demonstration

`stepsize()` shows that our adaptive time-stepping routine was able to detect the step size constraint and choose Δt accordingly.

Furthermore, `stability_example()` shows that $\tilde{y}(t)$ indeed converges to 0 only if $\Delta t < -2/\lambda$.

Runge-Kutta Methods

Why step size constraints for $\dot{y} = \lambda y$ matter

The above findings are specific to the simple ODE $\dot{y} = \lambda y$ whose solution can be determined analytically. At first sight, it may therefore seem that these findings have little practical value, but actually the opposite is true. The reason for this is the following.

The issues described above at the example of $\dot{y} = \lambda y$ arise whenever we apply Runge-Kutta methods to ODEs with attractive fixed points.

The term "fixed point" in this statement refers to the following definition.

Def: Fixed point / steady state

$y_F \in \mathbb{R}^n$ is called a *fixed point* or a *steady state* of $\dot{y} = f(y)$ if $f(y_F) = 0$.

Example. $y_F = 0$ is a fixed point of the ODE $\dot{y} = \lambda y$.

In the case $\dot{y} = \lambda y$, the "attractive" part refers to the fact that $\lambda < 0$ which implies that $y(t)$ converges to the fixed point $y_F = 0$. A more general definition of "attractive" will follow in due time.

A mathematical justification for the above claim is provided by the result on the next slide.

Runge-Kutta Methods

Thm: Linearisation of ODEs

Assume $y(t)$ solves the ODE $\dot{y} = f(y)$ which has a fixed point $y_F \in \mathbb{R}^n$, and assume the Jacobian $\nabla f(y_F)$ has the eigenvalue decomposition

$$\nabla f(y_F) = V \Lambda V^{-1}.$$

We then have

$$w(t) = V^{-1}\big(y(t) - y_F\big) \qquad \Longrightarrow \qquad \dot{w}_k = \lambda_k w_k + O\big(\|w\|^2\big),$$

i.e. $\dot{y} = f(y)$ reduces to $\dot{w}_k = \lambda_k w_k$ for values $y(t)$ close to y_F.

Proof. We have

$$\begin{aligned}
\tfrac{d}{dt}\big(y(t) - y_F\big) &= f\big(y(t)\big) - 0 \\
&= f(y_F) + \nabla f(y_F)\,\big(y(t) - y_F\big) + O\big(\|y(t) - y_F\|^2\big) \\
&= 0 + V\Lambda V^{-1}\,\big(y(t) - y_F\big) + O\big(\|y(t) - y_F\|^2\big).
\end{aligned}$$

Multiplying from the left with V^{-1}, we thus have

$$\tfrac{d}{dt} V^{-1}\big(y(t) - y_F\big) = \Lambda\, V^{-1}\big(y(t) - y_F\big) + O\Big(\big\|y(t) - y_F\big\|^2\Big).$$

Runge-Kutta Methods

The above result is known under a special name.

Terminology: Linearisation

$\dot{w} = \Lambda w$ is called the *linearisation* of $\dot{y} = f(y)$ because it is derived from the linear approximation

$$f(y) \;\approx\; f(y_F) + \nabla f(y_F)\,(y - y_F).$$

The above result shows that our findings for the ODE $\dot{y} = \lambda y$ are relevant for arbitrary ODEs because close enough to a fixed point any ODE will "look like" $\dot{y} = \lambda y$.

It also shows that our earlier characterisation of "attractiveness" (0 is an attractive fixed point for $\dot{y} = \lambda y$ if $\lambda < 0$) was more general than what one might have expected. Specifically, we can characterise "attractiveness" of a fixed point y_F as follows.

Def: Attractive fixed point

A fixed point y_F of $\dot{y} = f(y)$ is said to be *attractive* if all eigenvalues of $\nabla f(y_F)$ have a negative real part.

Runge-Kutta Methods

Eigenvalues of the Jacobian

Attractiveness is not the only property which can be read off from the eigenvalues of $\Delta f(y_F)$: the solution to the linearised ODE $\dot{w} = \lambda w$ is given by

$$\begin{aligned} w(t) &= w_0 \exp(\lambda t) \\ &= w_0 \exp\big(\mathrm{Re}(\lambda)\, t\big) \Big(\cos\big(\mathrm{Im}(\lambda)\, t\big) + i \sin\big(\mathrm{Im}(\lambda)\, t\big)\Big)' \end{aligned}$$

and hence we conclude:

- $y(t)$ converges to y_F if all eigenvalues of $\nabla f(y_F)$ have a negative real part $\mathrm{Re}(\lambda) < 0$, and it diverges from y_F if at least one eigenvalue has a positive real part $\mathrm{Re}(\lambda) > 0$.
- $y(t)$ oscillates if $\mathrm{Im}(\lambda) \neq 0$, and $y(t)$ is monotonous if $\mathrm{Im}(\lambda) = 0$.

Note that $\nabla f(y_F)$ is not a symmetric matrix and hence its eigenvalues can be complex even if $\nabla f(y_F)$ is real.

Runge-Kutta Methods

Example: Complex eigenvalues indicates oscillation

Recall from slide 6 the ODE $\ddot{x} = -x$, or equivalently

$$\dot{y} = \begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} y_2 \\ -y_1 \end{pmatrix} = f(y) \qquad \text{with} \qquad \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} x \\ \dot{x} \end{pmatrix}.$$

The eigenvalues of

$$\nabla f = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

are $\lambda = \pm i$. We therefore expect the solution to this ODE oscillate but neither grow nor decrease in magnitude.

This of course agrees with the solution

$$y(t) = \begin{pmatrix} \cos(t) \\ -\sin(t) \end{pmatrix}$$

determined on slide 6.

Runge-Kutta Methods

Intermediate summary

Our main insight on slides 73 until now is the following.

Euler's method and the trapezoidal rule applied to an ODE with attractive fixed points exhibit a step size constraint which may force them to invest compute time in regions where we should not be investing compute time.

The mathematical literature has a special term for such ODEs.

Terminology: Stiffness

ODEs for which some[1] Runge-Kutta methods require small time steps even in regions where there is virtually no change in the solution are called *stiff*.

[1] Specifically, stiff ODEs are ODEs for which *explicit* Runge-Kutta methods require small time steps. The notion of explicit and implicit Runge-Kutta methods will be introduced later.

The importance of stiffness

Managing stiffness is perhaps the single most important source of complications when solving ODEs in practice.

In simple cases like the $\dot{y} = \lambda y$ example discussed above, "managing stiffness" amounts to recognising that we should stop the Runge-Kutta solver once we reach a time T such that $f(\tilde{y}(T)) \approx 0$ and set $\tilde{y}(t) = \tilde{y}(T)$ for all $T > t$.

However, this work-around breaks down once we move to more complicated ODEs like the one discussed on the next slide.

Runge-Kutta Methods

Example: Separation of time scales

Consider the problem of finding $y : [0, \infty) \to \mathbb{R}^2$ such that

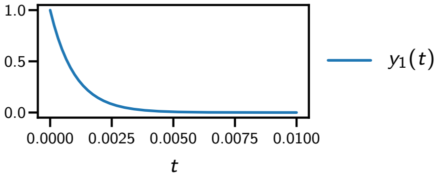
$$\dot{y}_1 = -1000\, y_1, \qquad \dot{y}_2 = -y_2.$$

Since $\lambda_1 = -1000$ is very negative, the Euler / trapezoidal rule solution will remain bounded only if we use a very small time step $\Delta t < \frac{2}{1000}$.

This would not be a problem if the ODE consisted of only y_1, because a large λ_1 also means that $y_1(t)$ converges to the steady state quickly and hence the minimal number of time steps

$$n \geq \frac{[\text{time scale of interest}]}{[\text{largest admissible time step}]} \approx \frac{1/1000}{1/1000} \approx 1$$

would still be manageable for the single ODE $\dot{y}_1 = -1000\, y_1$.



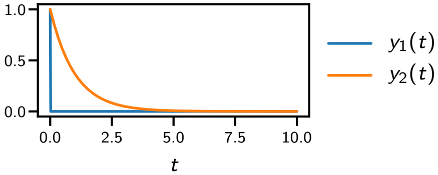
Runge-Kutta Methods

Example: Separation of time scales (continued)

However, once we add the relatively slowly converging $\dot{y}_2 = -y_2$ to the simulation, then the time scale of interest will change to ≈ 1 and thus the lower bound on the number of time steps becomes

$$n \geq \frac{\text{[time scale of interest]}}{\text{[largest admissible time step]}} \approx \frac{1}{1/1000} \approx 1000.$$

This may be more than we can handle.



Runge-Kutta Methods

Separation of time scales

An ODE $\dot{y} = f(y)$ like the above where some components converge / oscillate very rapidly while others converge / oscillate very slowly is said to exhibit a *separation of time scales*.

Separation of time scales is a common feature in our everyday lives. Some examples include:

- Weather (fast) vs climate (slow).
- Car (slow) with rotating wheels (fast).
- Monthly spending (fast) vs wealth generation (slow).

Separation of time scales is the primary reason why stiffness is a problem: the rapidly moving components force us to take very small time steps while the slowly moving components prevent us from terminating the simulation once the former components converge.

Separation of time scales (continued)

It is sometimes possible to eliminate a separation-of-time-scales-induced loss in performance by splitting the overall ODE into one ODE for the rapidly oscillating components and another ODE for the slowly oscillating components, but this approach is often cumbersome and may not work at all.

We would therefore prefer to simulate ODEs exhibiting separation of time scales using just a single Runge-Kutta method which does not suffer from a time step constraint when applied to stiff ODEs.

We have seen that neither Euler's method nor the trapezoidal rule satisfy this criterion, so the question arises whether we can design special Runge-Kutta schemes which do.

The answer is yes, but to describe how I first need to introduce a few abstract concepts.

Runge-Kutta Methods

Def: Stability function

The *stability function* associated with a Runge-Kutta scheme is the function $R : \mathbb{C} \to \mathbb{C}$ such that the numerical time propagator for the equation $\dot{y} = \lambda y$ is given by

$$\tilde{\Phi}(y_0, t) = R(\lambda t)\, y_0.$$

Def: Stability domain

The *stability domain* associated with a Runge-Kutta method is the set

$$\Big\{ z \in \mathbb{C} \;\Big|\; |R(z)| < 1 \Big\}.$$

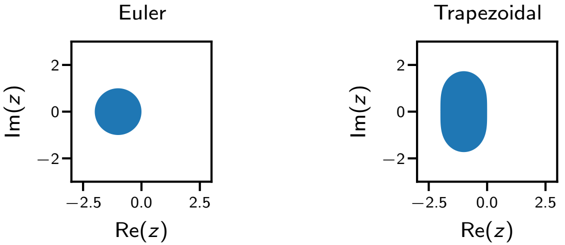
Runge-Kutta Methods

Example

We have derived on slide 74 two examples of stability functions, namely

- $R(z) = 1 + z$ for Euler's method, and
- $R(z) = 1 + z + \frac{z^2}{2}$ for the trapezoidal rule.

Plugging these functions into a plotting tool, we obtain the following stability domains.



Runge-Kutta Methods

Example (continued)

The stability domain for Euler's method can also be determined using pen-and-paper analysis: the set

$$\left\{ z \in \mathbb{C} \;\middle|\; |R(z)| = |1 + z| < 1 \right\}$$

is simply a ball of radius 1 centred at $z = -1$.

Determining the stability domain of the trapezoidal rule using pen-and-paper analysis would be more complicated. I will therefore leave it at the plot presented on the previous slide.

Runge-Kutta Methods

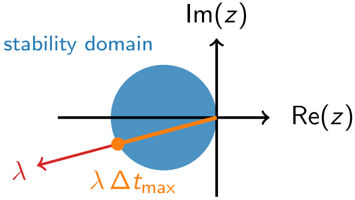
Determining step size constraints using stability domains

The purpose of the stability domain is to allow us to visually estimate the range of admissible time steps Δt such that the numerical solution

$$\tilde{y}(k\,\Delta t) = R(\lambda\,\Delta t)^k y_0$$

to $\dot{y} = \lambda y$ does not blow up: this range is proportional to the intersection between the stability domain $\{|R(z)| < 1\}$ and the ray $\lambda\,[0,\infty)$.

Furthermore, the largest admissible time step $\Delta t_{\max}$ is proportional to the point of maximum modulus in this intersection.



Runge-Kutta Methods

Unbounded stability domains

We have seen on slide 80 that the exact solution to $\dot{y} = \lambda y$ converges to 0 whenever $\mathrm{Re}(\lambda) < 0$, and that we want our numerical solutions to exhibit the same asymptotic behaviour.

Combined with the insights from the previous slide, this means that a given Runge-Kutta scheme will suffer from a time step constraint unless its stability domain involves the entire left half plane $\{\mathrm{Re}(z) < 0\}$.

Devising a Runge-Kutta scheme with unbounded stability domain $\{|R(z)| < 1\}$ will be easier once we have a formula for the stability function of a generic Runge-Kutta scheme.

Runge-Kutta Methods

Thm: Stability function formula

The stability function of a Runge-Kutta scheme with Butcher tableau

$$\begin{array}{c|c} \theta & W \\ \hline & w^T \end{array} \qquad \text{is given by} \qquad R(z) = 1 + zw^T\left(I - zW\right)^{-1}\mathbf{1},$$

where $\mathbf{1}$ denotes the vector of all ones.

Proof. The time propagator for the above Butcher tableau and the ODE $\dot{y} = \lambda y$ is given by ($\mathbf{1}$ denotes the vector of all ones)

$$\tilde{\Phi}(y_0, t) = y_0 + \lambda t\, w^T \tilde{y} \qquad \text{where} \qquad \tilde{y} = y_0\,\mathbf{1} + \lambda t\, W\tilde{y}.$$

Solving the second equation for the vector of auxiliary variables $\tilde{y}$, we obtain

$$\tilde{y} = y_0\,(I - \lambda t\, W)^{-1}\,\mathbf{1},$$

and inserting this expression into the formula for $\tilde{\Phi}(y_0, t)$ yields

$$\tilde{\Phi}(y_0, t) = \left(1 + \lambda t\, w^T(I - \lambda t\, W)^{-1}\,\mathbf{1}\right) y_0 = R(\lambda t)\, y_0.$$

Runge-Kutta Methods

Example: Stability function for Euler's method

Butcher tableau:

$$\left(\begin{array}{c|c} 0 & \\ \hline & 1 \end{array}\right)$$

Stability function:

$$R(z) = 1 + z\,1\,(1-0)^{-1}\,1 = 1 + z.$$

Runge-Kutta Methods

Example: stability function for the trapezoidal rule

Butcher tableau:

$$\left(\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}\right)$$

Stability function:

$$\begin{aligned} R(z) &= 1 + z \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \left(I - z \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \right)^{-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= 1 + z \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -z & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ &= 1 + z \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 1 + z \end{pmatrix} \\ &= 1 + z \left(1 + \frac{z}{2} \right) \\ &= 1 + z + \frac{z^2}{2}. \end{aligned}$$

Runge-Kutta Methods

Now that we have a general formula for the stability function $R(z)$, let us look into what this formula tells us about the possible shapes of the stability domain.

The following result will be useful for this endeavour.

Lemma

$$R(z) = 1 + zw^T \left(I - zW\right)^{-1} \mathbf{1}$$

is a rational function of z in general, and it is a polynomial in z if W is strictly lower triangular (i.e. $i \leq j \implies W_{ij} = 0$).

Proof. $(I - zW)^{-1}\,\mathbf{1}$ can be evaluated using LU factorisation and back substitution. These algorithms involve only addition, multiplication and division; hence every entry of $(I - zW)^{-1}\,\mathbf{1}$ is a rational function of z, and thus $R(z)$ is a rational function.

If W is strictly lower triangular, then $I - zW$ is a triangular matrix and hence we can skip the LU factorisation. Furthermore, all diagonal entries of $I - zW$ are 1 and thus back substitution does not involve any divisions. Every entry of $(I - zW)^{-1}\,\mathbf{1}$ is hence a polynomial in z, and $R(z)$ is a polynomial in this case.

Runge-Kutta Methods

Stability domains for polynomial and rational stability functions

The above result is important because if $R(z)$ is a polynomial, then we must necessarily have $\lim_{|z|\to\infty} |R(z)| = \infty$ and hence the stability domain $\{|R(z)| < 1\}$ is bounded and the Runge-Kutta method suffers from a step size constraint.

By contrast, if $R(z)$ is rational, then $\lim_{|z|\to\infty} |R(z)| < \infty$ is possible and hence the stability domain may be unbounded.

All the Butcher tableaus so far were strictly lower triangular.

$$\text{Euler:} \quad \begin{array}{c|c} 0 & \\ \hline & 1 \end{array}, \qquad \text{Trap:} \quad \begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad \text{RK4:} \quad \begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & & \frac{1}{2} & & \\ 1 & & & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array}.$$

The example on the next slide will discuss the simplest Runge-Kutta scheme with a not-lower-triangular Butcher tableau.

Runge-Kutta Methods

Example: Implicit Euler method

Consider the Runge-Kutta scheme

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \qquad \longleftrightarrow \qquad \begin{array}{c} \tilde{y}_1(t) = y_0 + f\big(\tilde{y}_1(t)\big)\, t \\ \hline \tilde{y}(t) = y_0 + f\big(\tilde{y}_1(t)\big)\, t \end{array}$$

The formulae for $\tilde{y}_1(t)$ and $\tilde{y}(t)$ are exactly the same; hence we have $\tilde{y}_1(t) = \tilde{y}(t)$, and the formula for $\tilde{y}(t)$ can be reduced to

$$\tilde{y}(t) = y_0 + f\big(\tilde{y}(t)\big)\, t.$$

Aiming to compute the stability function $R(z)$, I insert $f(y) = \lambda y$, solve for $\tilde{y}(t)$,

$$\tilde{y}(t) = y_0 + \lambda\, \tilde{y}(t)\, t \qquad \Longleftrightarrow \qquad \tilde{y}(t) = \tfrac{y_0}{1-\lambda t},$$

and conclude that $R(z) = \frac{1}{1-z}$.

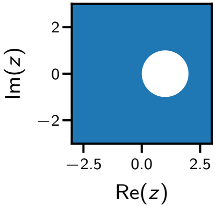
Runge-Kutta Methods

Example: Implicit Euler method (continued)

The stability domain is hence given by

$$\{z \mid |R(z)| < 1\} = \{z \mid \tfrac{1}{|1-z|} < 1\} = \{z \mid |1-z| > 1\},$$

which is the complement of the ball of radius 1 around $z = 1$.



This stability domain includes the entire left half plane; thus the above scheme does not impose a time step constraint.

Numerical demonstration

See `implicit_euler_step()`, `stability_example()`.

Example: Implicit Euler method (continued)

The above demonstrates that avoiding time step constraints is possible, but it also indicates that doing so comes at a price of having to solve the nonlinear and potentially high-dimensional system of equations

$$\tilde{y}(t) = y_0 + f\big(\tilde{y}(t)\big)\, t.$$

I will discuss the consequences of this fact later. For now, I would like to instead point out that the above equation agrees with the Euler step formula except that y_0 is replaced with $\tilde{y}(t)$. This motivates the following terminology.

Def: Implicit Euler method

Approximating the solution to $y(0) = y_0$, $\dot{y} = f(y)$ using

$$\tilde{y}(0) = y(0), \qquad \tilde{y}\big(t_k\big) = \tilde{y}(t_{k-1}) + f\big(\tilde{y}(t_k)\big)\,\big(t_k - t_{k-1}\big)$$

is known as the implicit Euler method.

The earlier Euler method is sometimes also called the *explicit* Euler method to emphasise the difference to the above method.

Runge-Kutta Methods

More generally, one can show that Runge-Kutta schemes cannot be evaluated using simple forward substitution whenever W is not strictly lower triangular. The explicit / implicit terminology for Euler's method therefore generalises as follows.

Terminology: Explicit and implicit Runge-Kutta schemes

A Runge-Kutta scheme with Butcher tableau

$$\begin{array}{c|c} x & W \\ \hline & w^T \end{array}$$

is called *explicit* if W is strictly lower triangular, and *implicit* otherwise.

Runge-Kutta Methods

Convergence of implicit Euler method

We have now seen that the implicit Euler method allows us to take arbitrarily large time steps without risking spurious blow-up of the numerical solution.

Being able to choose large time steps when appropriate is certainly valuable, but of course we also want that the numerical solution converges to the exact solution as the time step goes to zero, i.e. we want that the implicit Euler method converges in the limit $\max_k |t_k - t_{k-1}| \to 0$.

Using the bound

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

from slide 35, we can once again reduce the problem of showing convergence to that of showing that the local consistency errors satisfy

$$\lim_{t\to 0}\,\left\|\tilde{\Phi}(y_0,t) - \Phi_k(y_0,t)\right\| = 0.$$

Runge-Kutta Methods

Lemma: Consistency of implicit Euler time propagator

The implicit Euler time propagator $\tilde{\Phi}(y_0, t)$ satisfies

$$\left\|\tilde{\Phi}(y_0, t) - \Phi(y_0, t)\right\| = O(t^2) \qquad \text{for } t \to 0.$$

Proof. We obtain by repeatedly differentiating the one-step equation for the implicit Euler method that

$$\begin{aligned}
\tilde{y}(t) &= y_0 + f\left(\tilde{y}(t)\right) t, \\
\dot{\tilde{y}}(t) &= f'\left(\tilde{y}(t)\right) \dot{\tilde{y}}(t)\, t + f\left(\tilde{y}(t)\right), \\
\ddot{\tilde{y}}(t) &= f''\left(\tilde{y}(t)\right) \left(\dot{\tilde{y}}(t)\right)^2 t + f'\left(\tilde{y}(t)\right) \ddot{\tilde{y}}(t)\, t + 2\, f'\left(\tilde{y}(t)\right) \dot{\tilde{y}}(t).
\end{aligned}$$

Setting $t = 0$, we conclude

$$\tilde{y}(0) = y_0 = y(0), \quad \dot{\tilde{y}}(0) = f(y_0) = \dot{y}(0), \quad \ddot{\tilde{y}}(0) = 2\, f'(y_0)\, f(y_0) = 2\, \ddot{y}(0).$$

We observe that the zeroth and first derivatives of $\tilde{y}(t)$ and $y(t)$ match, but the second derivatives differ by a factor 2. Hence the implicit Euler method is second-order consistent like the explicit Euler method.

Runge-Kutta Methods

Corollary: Convergence of the implicit Euler rule

Denote by $y(t)$ the solution to $\dot{y} = f(y)$ and by $\tilde{y}(t)$ the numerical approximation obtained using the implicit Euler rule with the equispaced temporal mesh $(t_k = \frac{k}{n}\,T)_{k=0}^{n}$.

Then,

$$\left\|\tilde{y}(T) - y(T)\right\| = O\Big(\exp(LT)\,\tfrac{T^2}{n}\Big) \qquad \text{for both } n, T \to \infty,$$

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

Proof. Analogous to the one on slide 31.

Numerical demonstration

See `convergence()`.

Runge-Kutta Methods

Higher-order implicit schemes

We have now seen how we can avoid time step constraints for stiff ODEs by switching from the explicit to the implicit Euler method.

The same is also possible for higher-order schemes. For example, we can transform the (explicit) trapezoidal rule scheme from slide 42 into an implicit scheme by modifying it as follows.

Def: Implicit trapezoidal rule

Approximating the solution to $y(0) = y_0$, $\dot{y} = f(y)$ using $\tilde{y}(0) = y(0)$ and

$$\begin{aligned} \tilde{y}(0) &= y_0, \\ \tilde{y}(t_k) &= \tilde{y}(t_{k-1}) + \Big(f\big(\tilde{y}(t_{k-1})\big) + f\big(\tilde{y}(t_k)\big) \Big) \tfrac{t_k - t_{k-1}}{2}, \end{aligned}$$

is known as the implicit trapezoidal rule

Implementation of the implicit trapezoidal rule

See `implicit_trapezoidal_step()`.

Runge-Kutta Methods

Outlook

The following slides will discuss

- the Butcher tableau,
- the order of consistency and the order of convergence, and finally
- the stability function and stability domain

of the implicit trapezoidal rule.

Runge-Kutta Methods

Butcher tableau for the implicit trapezoidal rule

The Butcher tableau for the implicit trapezoidal rule is given by

$$\begin{array}{c|cc} 0 & & \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \qquad \begin{array}{r} \tilde{y}_1(t_{k-1}) = \tilde{y}(t_{k-1}) \\ \tilde{y}_2(t_k) = \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,\frac{t_k - t_{k-1}}{2} + f(\tilde{y}_2)\,\frac{t_k - t_{k-1}}{2} \\ \hline \tilde{y}(t_k) = \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,\frac{t_k - t_{k-1}}{2} + f(\tilde{y}_2)\,\frac{t_k - t_{k-1}}{2} \end{array}$$

These equations are indeed equivalent to the equation

$$\tilde{y}(t_k) = \tilde{y}(t_{k-1}) + \Big(f\big(\tilde{y}(t_{k-1})\big) + f\big(\tilde{y}(t_k)\big)\Big)\,\frac{t_k - t_{k-1}}{2}$$

given on slide 105 because the formulae for $\tilde{y}_2(t_k)$ and $\tilde{y}(t_k)$ are the same and hence $\tilde{y}(t_k) = \tilde{y}_2(t_k)$.

Runge-Kutta Methods

Lemma: Consistency of implicit trapezoidal rule time propagator
The implicit trapezoidal rule time propagator $\tilde{\Phi}(y_0, t)$ satisfies

$$\left\|\tilde{\Phi}(y_0, t) - \Phi(y_0, t)\right\| = O(t^3) \qquad \text{for } t \to 0.$$

Proof. We obtain by repeatedly differentiating the one-step equation for the implicit trapezoidal rule that

$$\begin{aligned}
\tilde{y}(t) &= y_0 + f(y_0)\,\tfrac{t}{2} + f\big(\tilde{y}(t)\big)\,\tfrac{t}{2}, \\
\dot{\tilde{y}}(t) &= f(y_0)\,\tfrac{1}{2} + f'\big(\tilde{y}(t)\big)\,\dot{\tilde{y}}(t)\,\tfrac{t}{2} + f\big(\tilde{y}(t)\big)\,\tfrac{1}{2}, \\
\ddot{\tilde{y}}(t) &= f''\big(\tilde{y}(t)\big)\,\big(\dot{\tilde{y}}(t)\big)^2\,\tfrac{t}{2} + f'\big(\tilde{y}(t)\big)\,\ddot{\tilde{y}}(t)\,\tfrac{t}{2} + 2\,f'\big(\tilde{y}(t)\big)\,\dot{\tilde{y}}(t)\,\tfrac{1}{2}.
\end{aligned}$$

Setting $t = 0$, we conclude

$$\tilde{y}(0) = y_0 = y(0), \quad \dot{\tilde{y}}(0) = f(y_0) = \dot{y}(0), \quad \ddot{\tilde{y}}(0) = f'(y_0)\,f(y_0) = \ddot{y}(0),$$

i.e. the zeroth to second derivatives of $\tilde{y}(t)$ and $y(t)$ match and hence the implicit trapezoidal rule is third-order consistent like the explicit trapezoidal rule.

Runge-Kutta Methods

Corollary: Convergence of the implicit trapezoidal rule

Denote by $y(t)$ the solution to $\dot{y} = f(y)$ and by $\tilde{y}(t)$ the numerical approximation obtained using the implicit trapezoidal rule with the equispaced temporal mesh $\left(t_k = \frac{k}{n}\,T\right)_{k=0}^{n}$.

Then,

$$\big\|\tilde{y}(T) - y(T)\big\| = O\Big(\exp(LT)\,\tfrac{T^3}{n^2}\Big) \qquad \text{for both } n, T \to \infty,$$

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

Proof. Analogous to the one on slide 31.

Numerical demonstration

See `convergence()`.

Runge-Kutta Methods

Stability function of the implicit trapezoidal rule

Inserting $f(y) = \lambda y$ into the one-step equation of the implicit trapezoidal rule, we obtain

$$\tilde{y}(t) = y_0 + \lambda y_0 \tfrac{t}{2} + \lambda \tilde{y}(t) \tfrac{t}{2} \qquad \Longleftrightarrow \qquad \tilde{y}(t) = \frac{1+\frac{\lambda t}{2}}{1-\frac{\lambda t}{2}} y_0.$$

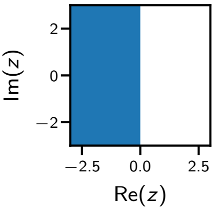
The stability function of the implicit trapezoidal rule is hence

$$R(z) = \tfrac{2+z}{2-z},$$

and the stability domain is

$$\left\{ \left| \tfrac{2+z}{2-z} \right| < 1 \right\} = \left\{ |2+z| < |2-z| \right\}.$$

This is the set of points which are closer to -2 than to $+2$, i.e. the left half plane $\{\mathrm{Re}(z) < 0\}$.



Runge-Kutta Methods

Step size constraint for the implicit trapezoidal rule

We conclude from the above that the implicit trapezoidal rule incurs no step size constraint. This is demonstrated in `stability_example()`.

Adaptive implicit time stepping

The implicit trapezoidal rule can be combined with a lower-order scheme to obtain an embedded method for step size selection. See `embedded_implicit_ET_step()`, `decay_example()` and `stepsize()`.

Runge-Kutta Methods

Explicit vs. implicit schemes

The key takeaways regarding implicit Runge-Kutta schemes are the following.

- Explicit Runge-Kutta schemes applied to an ODE with attractive fixed points impose a time step constraint.
- This constraint may significantly reduce performance if the ODE is stiff, i.e. if it exhibits a separation of time scales.
- Implicit Runge-Kutta schemes can avoid time step constraints, but they require solving a potentially nonlinear system of equations in each time step.

Given these points, we conclude that implicit schemes are a method of last resort to solve ODEs which would be hard to solve otherwise, but because solving nonlinear systems of equations is difficult we would like to avoid implicit Runge-Kutta schemes whenever possible.

Explicit vs. implicit schemes (continued)

In particular, if the separation of time scales is only small, then it is usually more efficient to use an explicit scheme with small time steps than to use an implicit scheme with larger time steps but a much longer runtime per time step.

Similarly, it is occasionally possible to eliminate the separation of time scales by eliminating the fast-moving component. We will see a real-world application of this trick in the next lecture.

Runge-Kutta Methods

Summary

Theory of ODEs:

- Picard-Lindelöf theorems: $\dot{y} = f(y)$ has a unique (local) solution if $f(y)$ is (locally) Lipschitz continuous.
- If $f(y)$ has Lipschitz constant L, then $y(t)$ is a Lipschitz continuous function of $y(0)$, but the Lipschitz constant is $\exp(Lt)$.

Runge-Kutta Methods

Summary

Runge-Kutta scheme:

$\tilde{y}(0) = y(0)$,

for $k = 1, 2, \ldots$ **do**

  for $i = 1, \ldots, s$ **do**

$$\tilde{y}_i^{(k)} = \tilde{y}(t_{k-1}) + \sum_{j=1}^{i-1} f\left(\tilde{y}_j^{(k)}\right) W_{ij}\left(t_k - t_{k-1}\right)$$

  end for

$$\tilde{y}(t_k) = \tilde{y}(t_{k-1}) + \sum_{j=1}^{s} f\left(\tilde{y}_j^{(k)}\right) w_j\left(t_k - t_{k-1}\right)$$

end for

Butcher tableau representation:

$$\begin{array}{c|ccc} x_1 & w_{11} & \ldots & w_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ x_s & w_{s1} & \ldots & w_{ss} \\ \hline & w_1 & \ldots & w_s \end{array}$$

Runge-Kutta Methods

Summary

Convergence theory:

- Global error is weighted sum of local errors,

$$\left\|\tilde{y}_n - y_n\right\| \;\leq\; \sum_{k=1}^{n} \exp\bigl(L\,(t_n - t_k)\bigr)\;\left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\|.$$

- Local / consistency errors $\left\|\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1})\right\|$ can be estimated using Taylor's theorem.

Adaptive time stepping:

- An efficient temporal mesh takes large steps if the curvature of the solution is small and small steps if the curvature is high.
- We can adaptively determine close-to-optimal step sizes with very little extra computations using embedded Runge-Kutta methods.

Runge-Kutta Methods

Summary

Stability and implicit Runge-Kutta methods

- Explicit Runge-Kutta schemes applied to ODEs with attractive fixed points lead to spurious blow-up of the solution unless the time step is less than some largest admissible time step $\Delta t_{\max}$.
- This phenomenon can be explained using linearisation, the stability function $R(z)$ and the stability domain $\big\{z \in \mathbb{C} \mid |R(z)| < 1\big\}$.
- Stability functions can be determined using either the formula

$$R(z) = 1 + z w^T \big(I - zW\big)^{-1} \mathbf{1}$$

  or the defining property

$$\dot{y} = \lambda y \quad \Longrightarrow \quad \tilde{y}(k\,\Delta t) = R(\lambda\,\Delta t)^k\, y_0.$$

  The first approach is useful if you have a computer to do the calculations for you, the second approach is more convenient if you have to do the arithmetic by hand.
- Implicit Runge-Kutta schemes can avoid time step constraints and the associated performance problems, but they require solving a potentially nonlinear equation in each time step.