# 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.

# Runge-Kutta Methods

**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

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

# Runge-Kutta Methods

**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

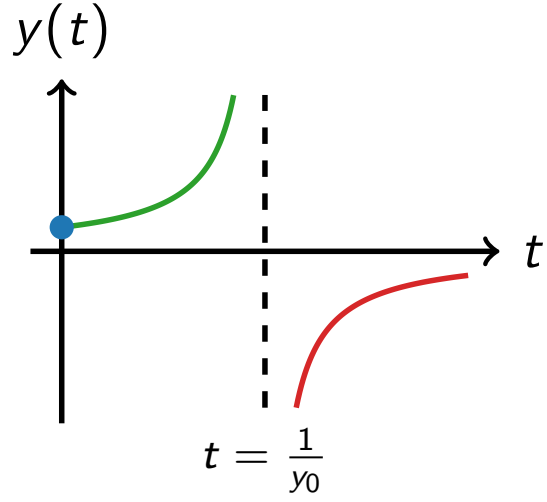
$$y(0) = \frac{y_0}{1 - y_0\, 0} = y_0 \qquad \text{and} \qquad \dot{y}(t) = \frac{y_0^2}{(1 - y_0 t)^2} = y(t)^2.$$

# Runge-Kutta Methods

**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 $t \in [0, \infty)$.

# Runge-Kutta Methods

**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

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

# Runge-Kutta Methods

**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.

# Runge-Kutta Methods

**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 $x(t)$.

# Runge-Kutta Methods

**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*.

# Runge-Kutta Methods

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

# Runge-Kutta Methods

**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.

# Runge-Kutta Methods

**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 $t \geq 0$.

# Runge-Kutta Methods

**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.*

$$\begin{aligned}
\|f(y_1) - f(y_2)\| &= \left\| \int_0^1 \frac{d}{dt} \Big( f\big(y_1 + t\,(y_2 - y_1)\big) \Big)\, dt \right\| \\
&\quad \uparrow \text{(fundamental theorem of calculus)} \\
&= \left\| \int_0^1 \nabla f\big(y_1 + t\,(y_2 - y_1)\big)\,(y_2 - y_1)\, dt \right\| \\
&\quad \uparrow \text{(chain rule)} \\
&\leq \int_0^1 \left\| \nabla f\big(y_1 + t\,(y_2 - y_1)\big) \right\| \left\| y_2 - y_1 \right\| dt \\
&\quad \uparrow \text{($\|\int f(t)\,dt\| \leq \int \|f(t)\|\,dx$ and matrix norm definition)} \\
&\leq \left( \sup_{y \in D} \|\nabla f(y)\| \right) \left\| y_2 - y_1 \right\|.
\end{aligned}$$

# Runge-Kutta Methods

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.

# Runge-Kutta Methods

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 $[0, \frac{1}{y_0})$.

# Runge-Kutta Methods

**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,

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

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

# Runge-Kutta Methods

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

**Lemma: Gronwall's inequality (not examinable)**

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

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

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

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

# Runge-Kutta Methods

*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

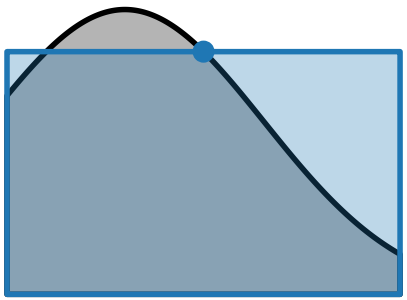
**Def: Quadrature rule**

A formula of the form

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

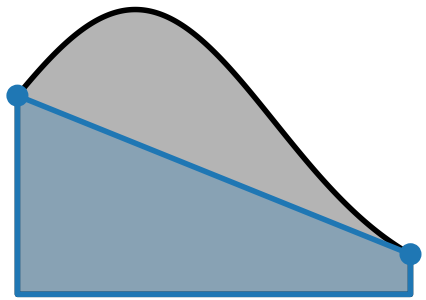
is called a *quadrature rule for* $[a, b]$. The parameters $(x_k \in \mathbb{R})_{k=1}^n$ and $(w_k \in \mathbb{R})_{k=1}^n$ are called *quadrature points* and *quadrature weights*, respectively.

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



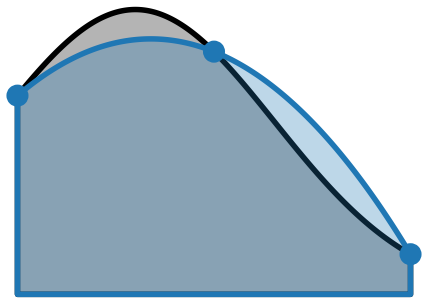
Midpoint rule

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



Trapezoidal rule

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



Simpson's rule

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

# Runge-Kutta Methods

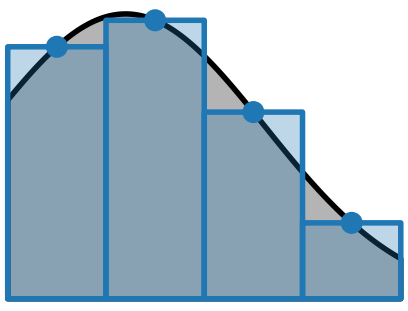
## Composite quadrature

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,

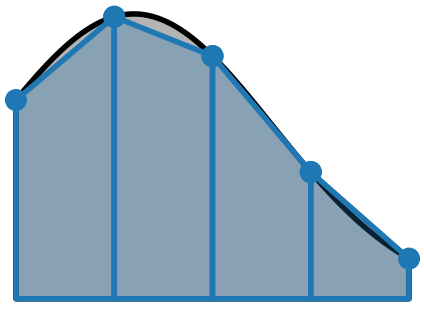
$$\int_a^b f(x)\,dx = \sum_{k=1}^{n} \int_{c_{k-1}}^{c_k} f(x)\,dx$$

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

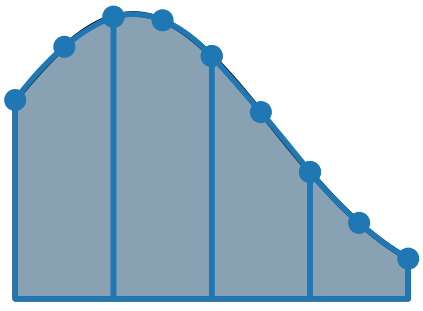
## Example composite quadrature rules



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)**

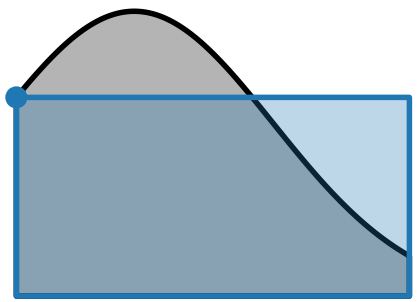
The second challenge is that the highlighted values in

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

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

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

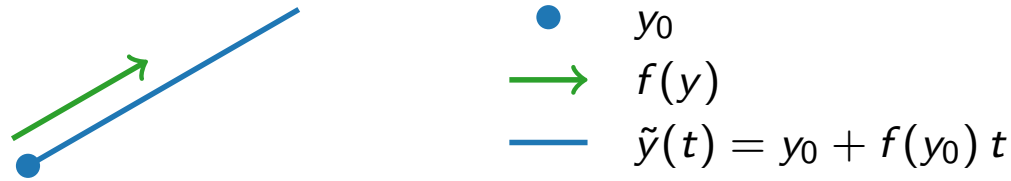
which is known as an *Euler step*.

# Runge-Kutta Methods

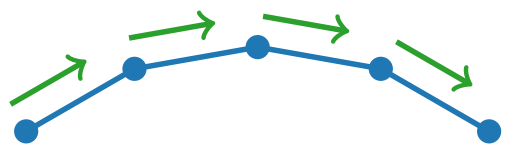
**Visual interpretation of Euler's method**

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

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

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

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

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

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

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,

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

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.

# Runge-Kutta Methods

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.

$$\left\|\Phi(y_1, t) - \Phi(y_2, t)\right\| \;\leq\; \exp(Lt)\left\|y_1 - y_2\right\|.$$

*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.*

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

# 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: $p$th-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 $p$th-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 $O\left(n^{-2}\right)$; 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

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

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

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

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

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

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

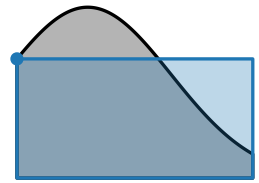
hence the question arises whether we can improve the speed of convergence by choosing a more accurate quadrature rule.

# 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

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

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

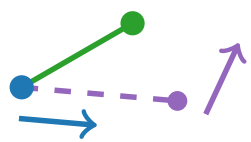
**Def: Trapezoidal rule**

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

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

is known as the trapezoidal rule method.

The pictorial interpretation of a trapezoidal step is as follows.



$y(t_\ell)$

$f(y_\ell)$

# 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

$$\tilde{y}_2(t_k) = \tilde{y}(t_{k-1}) + f\left(\tilde{y}(t_{k-1})\right)\left(t_k - t_{k-1}\right),$$

$$\tilde{y}(t_k) = \tilde{y}(t_{k-1}) + \left(f\left(\tilde{y}(t_{k-1})\right) + f\left(\tilde{y}_2(t_k)\right)\right)\frac{t_k - t_{k-1}}{2}.$$

# 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,

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

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

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

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

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

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

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

*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

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

# 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

1: $\tilde{y}(0) = y_0$,
2: **for** $k = 1, \ldots, n$ **do**
3: **for** $i = 1, \ldots, s$ **do**
4: $$\tilde{y}_i = \tilde{y}(t_{k-1}) + \sum_{j=1}^{s} f\left(\tilde{y}_j\right) W_{ij} \left(t_k - t_{k-1}\right)$$
5: **end for**
6: $$\tilde{y}(t_k) = \tilde{y}(t_{k-1}) + \sum_{j=1}^{s} f\left(\tilde{y}_j\right) w_j \left(t_k - t_{k-1}\right)$$
7: **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

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

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

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

**Example 2: Trapezoidal rule**

Tableau

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

Interpretation

$$\begin{aligned} \tilde{y}_1(t_{k-1}) &= \tilde{y}(t_{k-1}) \\ \tilde{y}_2(t_k) &= \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,(t_k - t_{k-1}) \\ \hline \tilde{y}(t_k) &= \tilde{y}(t_{k-1}) + f(\tilde{y}_1)\,\tfrac{t_k - t_{k-1}}{2} + f(\tilde{y}_2)\,\tfrac{t_k - t_{k-1}}{2} \end{aligned}$$

# Runge-Kutta Methods

**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 stp 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

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

  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.

# Runge-Kutta Methods

**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

| $s$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | ... |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $p$ | 1 | 2 | 3 | 4 | 4 | 5 | 6 | 6 | 7 | 8 | ... |

.

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

# Runge-Kutta Methods

**Adaptive Runge-Kutta methods**

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 $n$.

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.

# Runge-Kutta Methods

**Adaptive Runge-Kutta methods (continued)**

Now that I have established what the following slides are about, let me dive right in: we have seen on slide 35 that the global error of a given Runge-Kutta scheme is upper-bounded by

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

and 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

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

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 Runge-Kutta methods (continued)**

Assuming $\exp\big(L\,(t_n - t_k)\big) \approx 1$, which is motivated by our earlier observation that solving ODEs over time spans $T \gg \frac{1}{L}$ is generally not advisable, we hence have

$$\big\|\tilde{y}(t_n) - y(t_n)\big\| \;\lesssim\; \sum_{k=1}^{n} \big(t_k - t_{k-1}\big)^p \max_{t\in[t_{k-1},t_k]} \big\|\tilde{y}^{(p)}(t) - y^{(p)}(t)\big\|,$$

i.e. the total error is approximately upper-bounded by

$$[\,\text{step size}\,] \;\times\; [\,\text{variation in } y(t)\,],$$

summed over all time steps $k = 1, \ldots, n$.

This answers the question of how the temporal mesh $(t_k)_k$ impacts the error. Next, let us consider how we can optimise the mesh such that the error is as small as possible.

# Runge-Kutta Methods

## Adaptive Runge-Kutta methods (continued)

Optimising the error amounts to solving

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

where I introduced

$$c_k = \max_{t \in [t_{k-1}, t_k]} \left\| \tilde{y}^{(p)}(t) - y^{(p)}(t) \right\|.$$

I ignore here that the coefficients $c_k$ depend on the mesh points $t_k$ and hence the step sizes $\Delta t_k$, and I recommend you do the same for now. The justification for this ignorance will become clear later when I discuss how we construct optimal meshes.

Using the Lagrangian multiplier technique, this problem can be solved by determining $(\Delta t_k)_k$ and $\lambda$ 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 $\Delta t_k$ and $\lambda$ are zero.

# Runge-Kutta Methods

**Adaptive Runge-Kutta methods (continued)**

The derivative of $F\big((\Delta t_k)_k, \lambda\big)$ with respect to $\Delta t_k$ is

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

Setting this derivative equal to zero, we hence conclude that the mesh $(t_k)_k$ is optimal if the step sizes $\Delta t_k = t_k - t_{k-1}$ satisfy

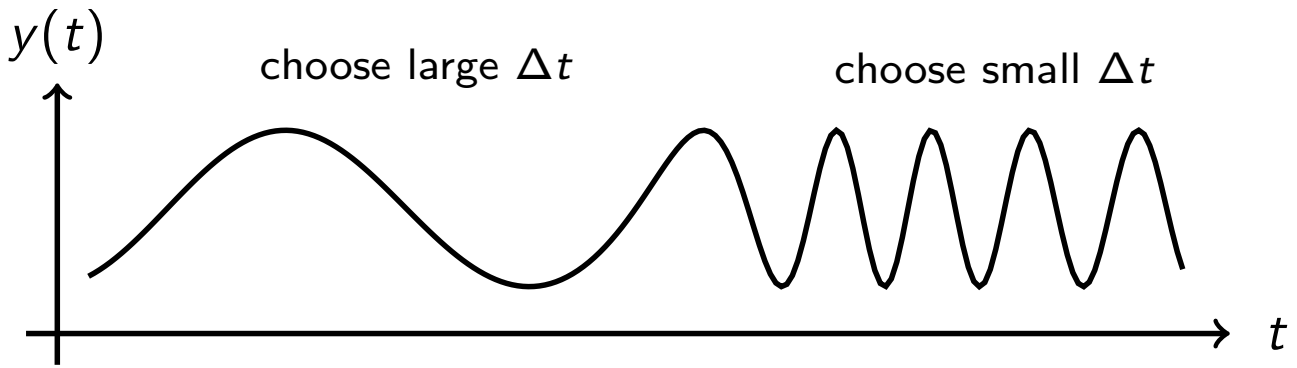
$$\Delta t_k^{p-1} \max_{t \in [t_{k-1}, t_k]} \big\| \tilde{y}^{(p)}(t) - y^{(p)}(t) \big\| \;=\; \text{const independent of } k.$$

# Runge-Kutta Methods

**Adaptive Runge-Kutta methods (continued)**

If we interpret the above purple factor as a measure for the "variation" in $y(t)$, then we can put this finding into words as follows:

The optimal step size $\Delta t_k$ is small if the variation in $y(t)$ is large, and large if the variation in $y(t)$ is small.



# Runge-Kutta Methods

[To be continued]