

MA3227 Numerical Analysis II

Lecture 18: Implicit Runge-Kutta Methods

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Implicit Runge-Kutta Methods

Introduction

Recall from Lecture 17 that adaptive time-stepping applied to the ODE $\dot{y} = \lambda y$ with $\lambda < 0$ failed to increase the time step Δt beyond a certain upper bound even though theory tells us that we should be able to choose Δt arbitrarily large for t large enough.

The ODE $\dot{y} = \lambda y$ is simple enough that we can determine explicit formulae for the Euler and midpoint steps:

► Euler: $\tilde{y}(t) = y_0 + f(y_0) t = y_0 + \lambda y_0 t = (1 + \lambda t) y_0.$

► Midpoint:

$$\begin{aligned}\tilde{y}(t) &= y_0 + f\left(y_0 + f(y_0) \frac{t}{2}\right) t \\ &= y_0 + \lambda \left(y_0 + \frac{1}{2} \lambda y_0 t\right) t \\ &= \left(1 + \lambda t + \frac{(\lambda t)^2}{2}\right) y_0.\end{aligned}$$

Conclusion: after k steps with constant step size Δt , the Runge-Kutta solution is given by

$$\tilde{y}(k \Delta t) = R(\lambda \Delta t)^k y(0) \quad \text{where} \quad R(z) = \begin{cases} 1 + z & \text{(Euler),} \\ 1 + z + \frac{z^2}{2} & \text{(midpoint).} \end{cases}$$

Implicit Runge-Kutta Methods

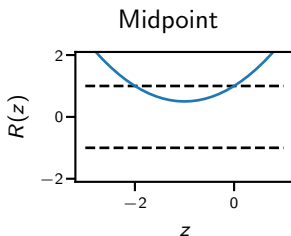
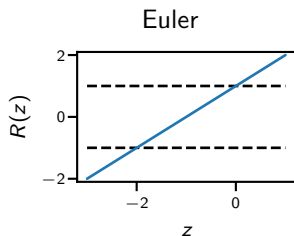
Introduction (continued)

We know that since $\lambda < 0$, the exact solution $y(t) = \exp(\lambda t)$ satisfies

$$\lim_{k \rightarrow \infty} y(k \Delta t) = \lim_{k \rightarrow \infty} \exp(\lambda k \Delta t) = 0.$$

It follows from the equation on the previous slide that the numerical solution $\tilde{y}(k \Delta t)$ has the same limit if and only if $|R(\lambda \Delta t)| < 1$, and plots of $R(z)$ reveal that

$$|R(\lambda \Delta t)| < 1 \iff -2 < \lambda \Delta t < 0 \iff \Delta t < \frac{2}{-\lambda}.$$



Implicit Runge-Kutta Methods

Introduction (continued)

The above explains our observations in Lecture 17: if $\Delta t > \frac{2}{-\lambda}$, then the numerical solution diverges from the exact solution. The step-size control detects this and makes sure Δt never exceeds $\frac{2}{-\lambda}$.

The discrepancy between our expectations and the numerical results arises because our expectations are based on a wrong interpretation of Taylor series. We have seen that Euler's method satisfies

$$\tilde{\Phi}_k(\tilde{y}_{k-1}) - \Phi_k(\tilde{y}_{k-1}) = \ddot{y}(t_{k-1}) \frac{\Delta t_k^2}{2} + \mathcal{O}(\Delta t_k^3),$$

and we have assumed that if the Δt_k^2 -term is small, then all higher-order terms must be even smaller. This is indeed the case if Δt_k is small, but in adaptive time-stepping we are interested in making Δt_k as large as possible, so eventually this Taylor-series argument will break down.

Implicit Runge-Kutta Methods

Linearisation of ODEs

The discussion so far was specific to the ODE $\dot{y} = \lambda y$

However, it turns out that our conclusions are relevant for generic ODEs $\dot{y} = f(y)$ as long as there is a partially attractive fixed point, i.e. a y_F such that $f(y_F) = 0$ and $\nabla f(y_F)$ has at least one eigenvalue λ with $\operatorname{Re}(\lambda) < 0$.

“Proof”. For y close to y_F , we obtain

$$\begin{aligned}\frac{d}{dt}(y(t) - y_F) &= f(y(t)) \\ &= \underbrace{f(y_F)}_{=0} + \nabla f(y_F) (y(t) - y_F) + \mathcal{O}(\|y(t) - y_F\|^2).\end{aligned}$$

Let us assume that $\nabla f(y_F)$ has eigendecomposition $\nabla f(y_F) = V\Lambda V^{-1}$. Ignoring the \mathcal{O} -term and introducing $w(t) = V^{-1}(y(t) - y_F)$, we then obtain

$$V\dot{w}(t) = \frac{d}{dt}Vw(t) = \nabla f(y_F)Vw(t) = V\Lambda w(t) \quad \Longleftrightarrow \quad \dot{w} = \Lambda w.$$

The last equation is a system of n decoupled ODEs of precisely the form $\dot{w}_i = \lambda w_i$; hence the above discussion applies for $y(t)$ close enough to y_F .

Implicit Runge-Kutta Methods

Discussion

The discussion on the previous slide shows that for general $f(y)$, we are interested in the behaviour of Runge-Kutta methods applied to the ODE $\dot{y} = \lambda y$ where λ is an eigenvalue of $\nabla f(y_F)$.

The Jacobian $\nabla f(y_F)$ is generally a non-symmetric matrix, so the eigenvalues λ can be complex. The solution to $\dot{y} = \lambda y$ is still

$$y(t) = y_0 \exp(\lambda t) = y_0 \exp(\operatorname{Re}(\lambda) t) \left(\cos(\operatorname{Im}(\lambda) t) + i \sin(\operatorname{Im}(\lambda) t) \right);$$

hence we conclude that $\operatorname{Re}(\lambda)$ indicates whether $y(t)$ converges to zero ($\operatorname{Re}(\lambda) < 0$) or diverges ($\operatorname{Re}(\lambda) > 0$), and $\operatorname{Im}(\lambda)$ indicates whether the solution oscillates.

Similarly, the Runge-Kutta solutions still satisfy $\tilde{y}(k \Delta t) = R(\lambda \Delta t)^k$, and we conclude that these solutions have the right convergence / divergence behaviour if

$$\operatorname{Re}(z) < 0 \quad \Longleftrightarrow \quad |R(z)| < 1.$$

This motivates the definitions on the next slide.

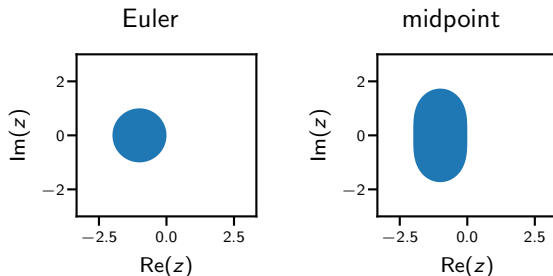
Implicit Runge-Kutta Methods

Terminology

- ▶ The functions $R(z)$ introduced above are called the stability function of the Runge-Kutta method.
- ▶ The set $\{z \in \mathbb{C} \mid |R(z)| < 1\}$ is called the stability domain of the Runge-Kutta method.

Example

The stability domains of the Euler and midpoint methods are:



Implicit Runge-Kutta Methods

Example

Consider the ODE $\ddot{x} = -x$, $x(0) = 1$, $\dot{x}(0) = 0$, or equivalently

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

We have $\nabla f = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ with eigenvalues $\lambda = \pm i$.

These eigenvalues are purely imaginary; hence the solution oscillates but does neither converge nor diverge. This is indeed the case since the exact solution is $x(t) = \cos(t)$.

We conclude from the domains of stability shown above that both Euler and midpoint methods have $|R(z)| > 1$ for purely imaginary z ; hence they diverge when applied to the above ODE.

Moreover, knowing $R(z)$ allows us to precisely predict the rate with which they diverge, see `harmonic_oscillator_divergence()`.

Implicit Runge-Kutta Methods

Discussion

The above shows that when we are integrating an ODE near a partially attractive fixed-point y_F , then we must choose Δt such that $|R(\lambda \Delta t)| < 1$ in order to avoid spurious exponential blow-up in the numerical solution.

This constraint may be harmless because we need to choose a small Δt anyway e.g. for accuracy reasons, but it can also be very restrictive. In the latter case, the ODE is called stiff.

Note that stiffness is a qualitative term and not one with a mathematically rigorous definition. We will see real-world examples of stiff equations later which will help clarify the concept.

The above shows that how well a given Runge-Kutta scheme can handle stiff equations is determined by the stability function $R(z)$. Our next goals are therefore to determine a formula for $R(z)$ for arbitrary Runge-Kutta methods, and figuring out how to construct Runge-Kutta methods which do not have a step size constraint when applied to stiff equations.

Implicit Runge-Kutta Methods

Stability function for abstract Runge-Kutta method

Consider a general Runge-Kutta scheme with Butcher tableau

$$\left(\begin{array}{c|c} \theta & V \\ \hline & w^T \end{array} \right).$$

When applied to the ODE $\dot{y} = \lambda y$, the numerical solution $\tilde{y}(t)$ after a single step is given by

$$\tilde{y}(t) = y_0 + w^T \mathbf{f} t \quad \text{where} \quad \mathbf{f} = \lambda (y_0 + V \mathbf{f} t).$$

You can verify the above formula by comparing it against the formula provided in the summary of Lecture 16.

Solving the second formula for \mathbf{f} yields ($\mathbf{1}$ denotes the vector of all ones)

$$\mathbf{f} = \lambda (I - \lambda t V)^{-1} \mathbf{1} y_0,$$

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

$$\tilde{y}(t) = \left(1 + \lambda t w^T (I - \lambda t V)^{-1} \mathbf{1} \right) y(0).$$

Implicit Runge-Kutta Methods

Stability function for abstract Runge-Kutta method (continued)

Replacing all instances of λt with z in the above formula, we conclude that the stability function for the abstract Runge-Kutta scheme

$$\left(\begin{array}{c|c} \theta & V \\ \hline & w^T \end{array} \right)$$

is given by

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

Example: stability function for Euler method

Butcher tableau:

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

Stability function:

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

Implicit Runge-Kutta Methods

Example: stability function for midpoint method

Butcher tableau:

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

Stability function:

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

Implicit Runge-Kutta Methods

Discussion

Recall the formula for the stability function given above:

$$\left(\begin{array}{c|c} \theta & V \\ \hline & w^T \end{array} \right) \longrightarrow R(z) = 1 + z w^T (I - z V)^{-1} \mathbf{1}.$$

We observe that $R(z)$ is a rational function for all V and w , and one can easily show that $R(z)$ is a polynomial if V is strictly lower triangular using Cramer's rule.

All Runge-Kutta methods that we have seen so far have a strictly lower-triangular V . This is for a good reason, as the example on the next slide shows.

Implicit Runge-Kutta Methods

Example: Implicit Euler

Consider the Runge-Kutta method with Butcher tableau

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

The corresponding one-step equations are

$$\tilde{y}(t) = y_0 + f_1 t, \quad f_1 = f(y_0 + f_1 t) \quad \Longleftrightarrow \quad \tilde{y}(t) = y_0 + f(\tilde{y}(t)) t.$$

This method is called the implicit Euler method because the one-step equation has the same form as the (explicit) Euler method that we have seen before, but the argument to $f(y)$ is now $\tilde{y}(t)$ rather than y_0 .

In quadrature terms, explicit Euler corresponds to a left-point rule while implicit Euler corresponds to a right-point rule.

Implicit Runge-Kutta Methods

Discussion

We conclude that if V is not strictly lower triangular, then the one-step equations become implicit, i.e. $\tilde{y}(t)$ can no longer be computed by simply evaluating a given formula, but rather we have to solve a potentially nonlinear equation or maybe even system of equations.

This motivates the following terminology.

- ▶ A RK scheme is called *explicit* if V is strictly lower triangular.
- ▶ A RK scheme is called *implicit* if V is not strictly lower triangular.

It depends on the context whether implicit one-step equations are a problem. For example, if $f(y) = Ay$ for some $A \in \mathbb{R}^{n \times n}$, the implicit Euler equation becomes

$$\tilde{y}(t) = y_0 + A\tilde{y}(t)t \quad \Longleftrightarrow \quad \tilde{y}(t) = (I - At)^{-1}y_0.$$

If n is small, we can solve $(I - At)^{-1}y_0$ reliably and cheaply using the LU factorisation. If n is large, we may have to use iterative methods like Krylov or multigrid, which can become expensive since we have to solve a new linear system $(I - At)^{-1}y_0$ for every time step.

Implicit Runge-Kutta Methods

Implicit Runge-Kutta methods (continued)

Also, recall that iterative methods may fail to converge, which can be frustrating if your ODE solver breaks down due to a failure of the nested iterative solver.

Of course, the above remarks regarding iterative linear solvers also apply if $f(y)$ is nonlinear and we have to solve

$$\tilde{y}(t) - y_0 - f(\tilde{y}(t)) t = 0$$

using an iterative nonlinear solver like Newton's method.

We conclude that going from explicit to implicit Runge-Kutta methods may or may not introduce difficulties depending on the properties of $f(y)$. Next, let us look into why we are interested in implicit Runge-Kutta methods in the first place.

Implicit Runge-Kutta Methods

Stability functions of explicit Runge-Kutta methods

Recall the formula for the stability function given above:

$$\left(\begin{array}{c|c} \theta & V \\ \hline & w^T \end{array} \right) \longrightarrow R(z) = 1 + z w^T (I - z V)^{-1} \mathbf{1}.$$

We have seen:

- ▶ Explicit Runge-Kutta methods have a strictly lower-triangular V .
- ▶ Strictly lower-triangular V implies $R(z)$ is a polynomial.

For polynomial $R(z)$, we necessarily have

$$|z| \rightarrow \infty \implies |R(z)| \rightarrow \infty.$$

This implies that the stability domain $\{z \in \mathbb{C} \mid |R(z)| < 1\}$ is bounded, which in turn implies that all explicit Runge-Kutta methods have a stability-induced step-size constraint.

By contrast, $R(z)$ is a rational function if V is arbitrary. Rational functions can be bounded for $|z| \rightarrow \infty$; hence implicit Runge-Kutta methods can avoid the step size constraint of explicit Runge-Kutta methods. This is the one and only reason why implicit Runge-Kutta methods are used in practice.

Implicit Runge-Kutta Methods

Discussion

I will next determine the stability function and domain of stability for the implicit Euler method introduced on slide 14, and for the implicit midpoint method which I will introduce later.

The following remark will be useful for this purpose.

Remark: determining stability functions

Stability functions can be determined in either of two ways.

- Write down the Butcher tableau and use the formula given above,

$$\left(\begin{array}{c|c} \theta & V \\ \hline & w^T \end{array} \right) \longrightarrow R(z) = 1 + z w^T (I - z V)^{-1} \mathbf{1}.$$

- Write down the one-step equations for $\dot{y} = y$ and rearrange them into the form $\tilde{y}(t) = R(t) y_0$.

The first approach is convenient if you have a computer to do the linear algebra for you, the second approach is easier if you have to do the calculations by hand.

Implicit Runge-Kutta Methods

Example: stability function for the implicit Euler method

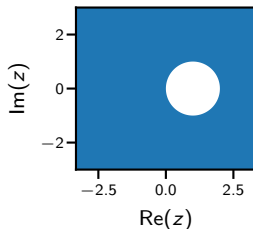
The one-step equation for implicit Euler is $\tilde{y}(t) = y_0 + f(\tilde{y}(t)) t$.
Inserting $f(y) = y$ yields

$$\tilde{y}(t) = y_0 + \tilde{y}(t) t \quad \Longleftrightarrow \quad \tilde{y}(t) = \frac{y_0}{1 - t};$$

hence the stability function is $R(z) = \frac{1}{1-z}$, and the stability domain is

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

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



Implicit Runge-Kutta Methods

Example: implicit midpoint method

Recall: the midpoint method is based on the midpoint quadrature rule and uses the explicit Euler method to approximate $y(\frac{t}{2})$,

$$\tilde{y}(t) = y_0 + f(\tilde{y}(\frac{t}{2})) t, \quad \tilde{y}(\frac{t}{2}) = y_0 + f(y_0) \frac{t}{2}.$$

This method can be turned into an implicit scheme by replacing the explicit Euler with the implicit Euler method,

$$\tilde{y}(t) = y_0 + f(\tilde{y}(\frac{t}{2})) t, \quad \tilde{y}(\frac{t}{2}) = y_0 + f(\tilde{y}(\frac{t}{2})) \frac{t}{2}.$$

The Butcher tableau for this method is

$$\left(\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array} \right) \longleftrightarrow \begin{cases} f_1 = f(y_0 + f_1 \frac{t}{2}), \\ \tilde{y}(t) = y_0 + f_1 t. \end{cases}$$

Implicit Runge-Kutta Methods

Example: implicit midpoint method (continued)

To determine the stability function, we set $f(y) = y$ and rearrange,

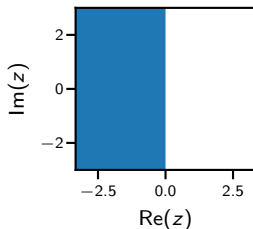
$$\tilde{y}\left(\frac{t}{2}\right) = y_0 + \tilde{y}\left(\frac{t}{2}\right) \frac{t}{2} \quad \Longleftrightarrow \quad \tilde{y}\left(\frac{t}{2}\right) = \frac{y_0}{1 - \frac{t}{2}},$$

$$\tilde{y}(t) = y_0 + \tilde{y}\left(\frac{t}{2}\right) t = \left(1 + \frac{t}{1 - \frac{t}{2}}\right) y_0 = \frac{1 + \frac{t}{2}}{1 - \frac{t}{2}} y_0 = \frac{2 + t}{2 - t} y_0.$$

The stability function is thus $R(z) = \frac{2+z}{2-z}$, and the stability domain is

$$\{z \mid |R(z)| < 1\} = \{z \mid \left|\frac{2+z}{2-z}\right| < 1\} = \{z \mid |2+z| < |2-z|\}.$$

This is the set of all points which are closer to -2 than they are to 2 , i.e. the set $\{z \mid \operatorname{Re}(z) < 0\}$.



Implicit Runge-Kutta Methods

Discussion

We have seen that the stability domains of the implicit Euler and implicit midpoint methods include the entire left half-plane $\{z \mid \operatorname{Re}(z) < 0\}$.

This means that these methods will not encounter a step-size constraint when applied to the ODE $\dot{y} = \lambda y$ with $\operatorname{Re}(\lambda) < 0$ (which as we have seen is representative of the local behaviour for ODEs with fixed points).

See `plot_stepsize()` for demonstration.

Remark

Runge-Kutta methods with stability domains including the left half-plane $\{z \mid \operatorname{Re}(z) < 0\}$ are sometimes called A-stable in the literature. I will not use this term and I will not ask for it in the exam, since the definition is easy enough that whenever I do need this property I can simply describe it.

Implicit Runge-Kutta Methods

Discussion

The above demonstrates that implicit Runge-Kutta methods allow us to take arbitrarily large steps without risking spurious exponential blow-up in the numerical solution. This is the one and only advantage of implicit methods over explicit methods, and it comes at the cost that for each time step we now have to solve a potentially nonlinear equation or system of equations.

Of course, in practice we not only want to avoid spurious blow-up of the numerical solution, but we also want that the numerical solution converges to the exact solution as the fineness of the temporal mesh $(t_k)_k$ goes to zero.

This can be shown using the abstract convergence theory from Lecture 16, which only requires us to show that the Runge-Kutta scheme is consistent. The following slides demonstrate how to determine the order of consistency for implicit Runge-Kutta methods at the example of the implicit Euler and implicit midpoint methods.

Implicit Runge-Kutta Methods

Consistency of implicit Euler method

By repeatedly differentiating the one-step equation for the implicit Euler method, we obtain

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

$$\dot{\tilde{y}}(t) = f'(\tilde{y}(t)) \dot{\tilde{y}}(t) t + f(\tilde{y}(t)),$$

$$\ddot{\tilde{y}}(t) = f''(\tilde{y}(t)) (\dot{\tilde{y}}(t))^2 t + f'(\tilde{y}(t)) \ddot{\tilde{y}}(t) t + 2 f'(\tilde{y}(t)) \dot{\tilde{y}}(t).$$

Setting $t = 0$, we conclude

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

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

We observe that the zeroth and first derivatives of $\tilde{y}(t)$ and $y(t)$ match, but the second derivative does not. Hence we conclude that implicit Euler is second-order consistent and first-order convergent like the explicit Euler method.

Implicit Runge-Kutta Methods

Consistency of implicit midpoint method

By repeatedly differentiating the one-step equation for the implicit midpoint method, we obtain

$$\tilde{y}(t) = y_0 + f(\tilde{y}(\tfrac{t}{2})) t,$$

$$\dot{\tilde{y}}(t) = f'(\tilde{y}(\tfrac{t}{2})) \dot{\tilde{y}}(\tfrac{t}{2}) \tfrac{t}{2} + f(\tilde{y}(\tfrac{t}{2})),$$

$$\ddot{\tilde{y}}(t) = f''(\tilde{y}(\tfrac{t}{2})) (\dot{\tilde{y}}(\tfrac{t}{2}))^2 \tfrac{t}{4} + f'(\tilde{y}(\tfrac{t}{2})) \ddot{\tilde{y}}(\tfrac{t}{2}) \tfrac{t}{2} + 2 f'(\tilde{y}(\tfrac{t}{2})) \dot{\tilde{y}}(\tfrac{t}{2}) \tfrac{1}{2}.$$

Setting $t = 0$ and using that $\tilde{y}(\tfrac{t}{2})$ is determined using the implicit Euler method which we have seen to be second-order consistent on the previous slide, we conclude

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

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

We observe that the zeroth, first and second derivatives of $\tilde{y}(t)$ and $y(t)$ match. Hence we conclude that implicit midpoint is at least third-order consistent and second-order convergent like the explicit midpoint method. We could verify by computing $\ddot{\tilde{y}}(0)$ that the order of the method is not higher than this, but we omit doing so because the required computations are quite lengthy.

Implicit Runge-Kutta Methods

Numerics

See `implicit_euler_step()` and `implicit_midpoint_step()` for details regarding the numerical implementation of these methods.

`convergence()` demonstrates that both Euler methods are indeed first-order convergent, and both midpoint methods are second-order convergent.

Moreover, we observe that the accuracy of the explicit methods first deteriorates before the asymptotic behaviour for $n \rightarrow \infty$ sets in. This is precisely due to the instability of these methods for large step sizes.

Implicit Runge-Kutta Methods

Summary

- ▶ Stability function: $R(z)$ such that

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

- ▶ Domain of stability $\{z \in \mathbb{C} \mid |R(z)| < 1\}$.
- ▶ Pro of implicit methods: no step-size constraint.
Con of implicit methods: we have to solve equations in every step.
- ▶ Order of consistency of implicit methods can be determined by comparing derivatives of the numerical and exact solution.