Chapter 8

Initial Value Problems

Definition 8.1. A *system of ordinary differential equations* (ODEs) of dimension N is a set of differential equations of the form

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t), t), \tag{8.1}$$

where t is time, $\mathbf{u} \in \mathbb{R}^N$ is the evolutionary variable, and the RHS function has the signature $\mathbf{f} : \mathbb{R}^N \times (0, +\infty) \to \mathbb{R}^N$. In particular, (8.1) is an ODE for $N = 1$.

Definition 8.2. A system of ODEs is *linear* if its RHS function can be expressed as $\mathbf{f}(\mathbf{u}, t) = \alpha(t)\mathbf{u} + \boldsymbol{\beta}(t)$, and *nonlinear* otherwise; it is *homogeneous* if it is linear and $\boldsymbol{\beta}(t) = \mathbf{0}$; it is *autonomous* if $\mathbf{f}$ does not depend on t explicitly; and *nonautonomous* otherwise.

Example 8.3. For the simple pendulum shown above, the moment of inertial and the torque are

$$I = m\ell^2, \ \tau = -mg\ell \sin\theta,$$

and the equation of motion can be derived from Newton's second law $\tau = I\theta''(t)$ as

$$\theta''(t) = -\frac{g}{\ell}\sin\theta, \tag{8.2}$$

which admits a unique solution if we impose two initial conditions

$$\theta(0) = \theta_0, \ \theta'(0) = \omega_0.$$

Alternatively, (8.2) can be derived by the consideration that the total energy remains a constant with respect to time.

$$L = \frac{1}{2}m(\ell\theta')^2 + mg\ell(1 - \cos\theta);$$

$$\frac{\mathrm{d}L}{\mathrm{d}t} = 0 \Rightarrow \ m\ell^2\theta'\theta'' + mg\ell\theta' \sin\theta = 0.$$

The ODE (8.2) is second-order, nonlinear, and autonomous; it can be reduced to a first-order system as follows,

$$\omega = \theta', \ \mathbf{u} = \begin{pmatrix} \theta \\ \omega \end{pmatrix} \ \Rightarrow \ \mathbf{u}'(t) = f(u) := \begin{pmatrix} \omega \\ -\frac{g}{\ell}\sin\theta \end{pmatrix}.$$

Definition 8.4. Given $T > 0$, $\mathbf{f} : \mathbb{R}^N \times [0, T] \to \mathbb{R}^N$, and $\mathbf{u}_0 \in \mathbb{R}^N$, the *initial value problem* (IVP) is to find $\mathbf{u}(t) \in \mathcal{C}^1$ such that

$$\begin{cases} \mathbf{u}(0) &= \mathbf{u}_0, \\ \mathbf{u}'(t) &= \mathbf{f}(\mathbf{u}(t), t), \ \forall t \in [0, T]. \end{cases} \tag{8.3}$$

Definition 8.5. The IVP in Definition 8.4 is *well-posed* if

(i) it admits a unique solution for any fixed $t > 0$,

(ii) $\exists c > 0$, $\hat{\epsilon} > 0$ s.t. $\forall \epsilon < \hat{\epsilon}$, the perturbed IVP

$$\mathbf{v}' = \mathbf{f}(\mathbf{v}, t) + \boldsymbol{\delta}(t), \qquad \mathbf{v}(0) = \mathbf{u}_0 + \boldsymbol{\epsilon}_0 \tag{8.4}$$

satisfies

$$\forall t \in [0, T], \begin{cases} \|\boldsymbol{\epsilon}_0\| < \epsilon \\ \|\boldsymbol{\delta}(t)\| < \epsilon \end{cases} \ \Rightarrow \ \|\mathbf{u}(t) - \mathbf{v}(t)\| \le c\epsilon. \tag{8.5}$$

8.1 Lipschitz continuity

Definition 8.6. A function $\mathbf{f} : \mathbb{R}^N \times [0, +\infty) \to \mathbb{R}^N$ is *Lipschitz continuous* in its first variable over some domain

$$\mathcal{D} = \{(\mathbf{u}, t) : \|\mathbf{u} - \mathbf{u}_0\| \le a, t \in [0, T]\} \tag{8.6}$$

if

$$\exists L \ge 0 \text{ s.t. } \forall (\mathbf{u}, t), (\mathbf{v}, t) \in \mathcal{D}, \ \|\mathbf{f}(\mathbf{u}, t) - \mathbf{f}(\mathbf{v}, t)\| \le L\|\mathbf{u} - \mathbf{v}\|. \tag{8.7}$$

Example 8.7. If $\mathbf{f}(\mathbf{u}, t) = \mathbf{f}(t)$, then $L = 0$.

Example 8.8. If $\mathbf{f} \notin \mathcal{C}^0$, then $\mathbf{f}$ is not Lipschitz.

Definition 8.9. A subset of $S \subset \mathbb{R}^n$ is *star-shaped* with respect to a point $p \in S$ if for each $x \in S$ the line segment from p to x lies in S.

Theorem 8.10. Let $S \subset \mathbb{R}^n$ be star-shaped with respect to $p = (p_1, p_2, \ldots, p_n) \in S$. For a continuously differentiable function $f : S \to \mathbb{R}^m$, there exist continuously differentiable functions $g_1(\mathbf{x}), g_2(\mathbf{x}), \ldots, g_n(\mathbf{x})$ such that

$$f(\mathbf{x}) = f(p) + \sum_{i=1}^{n}(x_i - p_i)g_i(\mathbf{x}), \quad g_i(p) = \frac{\partial f}{\partial x_i}(p). \tag{8.8}$$

Proposition 8.11. If $\mathbf{f}(\mathbf{u}, t)$ is continuously differentiable on some compact convex set $\mathcal{D} \subseteq \mathbb{R}^{N+1}$, then $\mathbf{f}$ is Lipschitz on $\mathcal{D}$ with

$$L = \max_{i,j}\left|\frac{\partial f_i}{\partial u_j}\right|.$$

Lemma 8.12. Let (M, ρ) denote a complete metric space and $\phi : M \to M$ a contractive mapping in the sense that

$$\exists c \in [0, 1) \text{ s.t. } \forall \eta, \zeta \in M,\ \rho(\phi(\eta), \phi(\zeta)) \le c\rho(\eta, \zeta). \quad (8.9)$$

Then there exists a unique $\xi \in M$ such that $\phi(\xi) = \xi$.

Theorem 8.13 (Fundamental theorem of ODEs)**.** If $\mathbf{f}(\mathbf{u}(t), t)$ is Lipschitz continuous in $\mathbf{u}$ and continuous in t over some region $\mathcal{D} = \{(\mathbf{u}, t) : \|\mathbf{u} - \mathbf{u}_0\| \le a, t \in [0, T]\}$, then there is a unique solution to the IVP problem as in Definition 8.4 at least up to time $T^* = \min(T, \frac{a}{S})$ where $S = \max_{(\mathbf{u},t)\in\mathcal{D}} \|\mathbf{f}(\mathbf{u}, t)\|$.

Theorem 8.14. If $\mathbf{f}(\mathbf{u}, t)$ is Lipschitz in $\mathbf{u}$ and continuous in t on $\mathcal{D} = \{(\mathbf{u}, t) : \mathbf{u} \in \mathbb{R}^N, t \in [0, T]\}$, then the IVP in Definition 8.4 is well-posed for all initial data.

Example 8.15. Consider $N = 1$, $u'(t) = \sqrt{u(t)}$, $u(0) = 0$.

$$\lim_{u\to 0} f'(u) = \lim_{u\to 0} \frac{1}{2\sqrt{u}} = +\infty.$$

Hence $f(u)$ is not Lipschitz near $u = 0$. However, $u(t) \equiv 0$ and $u(t) = \frac{1}{4}t^2$ are both solutions. Hence the Lipschitz condition is not necessary for existence.

Example 8.16. Consider the IVP $u'(t) = u^2$, $u_0 = \eta > 0$. The slope $f'(u) = 2u \to +\infty$ as $u \to \infty$. So there is no unique solution on $[0, +\infty)$, but there might exist T^* such that unique solutions are guaranteed on $[0, T^*]$.

In fact, $u(t) = \frac{1}{\eta^{-1}-t}$ is a solution, but blows up at $t = 1/\eta$. According to Theorem 8.13, $f(u) = u^2$ and we would like to maximize a/S. Since $S = \max_{\mathcal{D}} |f(u)| = (\eta + a)^2$, it is equivalent to find $\min_{a>0}(\eta + a)^2/a$:

$$(\eta + a)^2/a = 2\eta + a + \eta^2\frac{1}{a} \ge 2\eta + 2\sqrt{\eta^2} = 4\eta.$$

Hence $T^* = \frac{1}{4\eta}$. The estimation of T^* in Theorem 8.13 is thus quite conservative for this case.

Example 8.17. For the simple pendulum in Example 8.3, we have

$$|\sin\theta - \sin\theta^*| \le |\theta - \theta^*| \le \|\mathbf{u} - \mathbf{u}^*\|_\infty$$

since $\cos\theta^* \le 1$. In addition, we have $|\omega - \omega^*| \le \|\mathbf{u} - \mathbf{u}^*\|_\infty$.

$$\begin{aligned}\|\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v})\|_\infty &= \max\left(|\omega - \omega^*|, \frac{g}{\ell}|\sin\theta - \sin\theta^*|\right)\\ &\le \max(\frac{g}{\ell}, 1)\|\mathbf{u} - \mathbf{u}^*\|_\infty.\end{aligned}$$

Therefore, $\mathbf{f}$ is Lipschitz continuous with $L = \max(g/l, 1)$.

8.2 Duhamel's principle

Definition 8.18. Two matrices A and B are *similar* if there exists a nonsingular matrix S such that

$$B = S^{-1}AS, \quad (8.10)$$

and $S^{-1}AS$ is called a *similarity transformation* of A.

Theorem 8.19. Two similar matrices A and B have the same set of eigenvalues.

Definition 8.20. $A \in \mathbb{C}^{m\times m}$ is *diagonalizable* if there exists a similarity transformation that maps A to a diagonal matrix Λ, i.e.,

$$\exists \text{ invertible } R \text{ s.t. } R^{-1}AR = \Lambda. \quad (8.11)$$

Definition 8.21. Let $A \in \mathbb{C}^{m\times m}$, then the *matrix exponential* e^{At} is defined by

$$e^{At} := I + At + \frac{1}{2!}A^2t^2 + \cdots = \sum_{j=0}^{\infty} \frac{1}{j!}A^jt^j. \quad (8.12)$$

Proposition 8.22. If A is diagonalizable, i.e., (8.11) holds, then

$$\begin{aligned}e^{At} &= RR^{-1} + R\Lambda R^{-1}t + \frac{1}{2!}R\Lambda R^{-1}R\Lambda R^{-1}t^2 + \cdots\\ &= R\sum_{j=0}^{\infty} \frac{t^j}{j!}\Lambda^j R^{-1} = Re^{\Lambda t}R^{-1}.\end{aligned}$$

Theorem 8.23. For a linear IVP $\mathbf{f}(\mathbf{u}, t) = A(t)\mathbf{u} + \mathbf{g}(t)$ with a constant matrix $A(t) = A$, the solution is

$$\mathbf{u}(t) = e^{At}\mathbf{u}_0 + \int_0^t e^{A(t-\tau)}\mathbf{g}(\tau)\mathrm{d}\tau. \quad (8.13)$$

Example 8.24. Many linear problems are naturally formulated in the form of a single high-order ODE

$$v^{(m)}(t) - \sum_{j=1}^{m} c_j(t)v^{(m-j)} = \phi(t). \quad (8.14)$$

By setting $u_j(t) = v^{(j-1)}$ and $\mathbf{u} = [u_1, u_2, \ldots, u_m]^T$, we can rewrite (8.14) as

$$\mathbf{u}'(t) = A(t)\mathbf{u} + \mathbf{g}(t), \quad (8.15)$$

where $\mathbf{g}(t) = [0, \ldots, 0, \phi(t)]^T$ and

$$a_{ij}(t) = \begin{cases} 1 & \text{if } i = j - 1,\\ c_{m+1-j}(t) & \text{if } i = m,\\ 0 & \text{otherwise.}\end{cases}$$

Theorem 8.25 (Superposition principle)**.** If $\hat{\mathbf{u}}$ is a solution to the IVP

$$\mathbf{u}'(t) = A(t)\mathbf{u} + \mathbf{g}(t), \qquad \mathbf{u}(0) = \mathbf{u}_0 \quad (8.16)$$

and $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_k$ are solutions to the homogeneous IVP $\mathbf{u}'(t) = A(t)\mathbf{u}$, $\mathbf{u}(0) = \mathbf{0}$, then for any constants $\alpha_1, \alpha_2, \ldots, \alpha_k$, the function

$$\mathbf{U}(t) = \hat{\mathbf{u}}(t) + \sum_{i=1}^{k} \alpha_i\mathbf{v}_i(t) \quad (8.17)$$

is a solution to (8.16).

8.3 Some basic numerical methods

Notation 8. In the following, we shall use k to denote the time step, and thus $t_n = nk$.

To numerically solve the IVP (8.3), we are given initial data $\mathbf{U}^0 = \mathbf{u}_0$, and want to compute approximations $\mathbf{U}^1, \mathbf{U}^2, \ldots$ such that

$$\mathbf{U}^n \approx \mathbf{u}(t_n).$$

Definition 8.26. The *(forward) Euler's method* solves the IVP (8.3) by

$$\mathbf{U}^{n+1} = \mathbf{U}^n + k\mathbf{f}(\mathbf{U}^n, t_n), \tag{8.18}$$

which is based on replacing $\mathbf{u}'(t_n)$ with the forward difference $(\mathbf{U}^{n+1} - \mathbf{U}^n)/k$ and $\mathbf{u}(t_n)$ with $\mathbf{U}^n$ in $\mathbf{f}(\mathbf{u}, t)$.

Definition 8.27. The *backward Euler's method* solves the IVP (8.3) by

$$\mathbf{U}^{n+1} = \mathbf{U}^n + k\mathbf{f}(\mathbf{U}^{n+1}, t_{n+1}), \tag{8.19}$$

which is based on replacing $\mathbf{u}'(t_{n+1})$ with the backward difference $(\mathbf{U}^{n+1} - \mathbf{U}^n)/k$ and $\mathbf{u}(t_{n+1})$ with $\mathbf{U}^{n+1}$ in $\mathbf{f}(\mathbf{u}, t)$.

Definition 8.28. The *trapezoidal method* is

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \frac{k}{2}\left(\mathbf{f}(\mathbf{U}^n, t_n) + \mathbf{f}(\mathbf{U}^{n+1}, t_{n+1})\right). \tag{8.20}$$

Definition 8.29. The *midpoint (or leapfrog) method* is

$$\mathbf{U}^{n+1} = \mathbf{U}^{n-1} + 2k\mathbf{f}(\mathbf{U}^n, t_n). \tag{8.21}$$

Example 8.30. Applying Euler's method (8.18) with step size $k = 0.2$ to solve the IVP

$$u'(t) = u, \quad u(0) = 1, \quad t \in [0, 1],$$

yields the following table:

n	U^n	$kf(U^n, t_n)$
0	1	0.2
1	1.2	$0.2 \times 1.2 = 0.24$
2	1.44	$0.2 \times 1.44 = 0.288$
3	1.728	$0.2 \times 1.728 = 0.3456$
4	2.0736	$0.2 \times 2.0736 = 0.41472$
5	2.48832	

8.4 Accuracy and convergence

Definition 8.31. The *local truncation error*(LTE) is the error caused by replacing continuous derivatives with finite difference formulas.

Example 8.32. For the leapfrog method, the local truncation error is

$$\begin{aligned}
\boldsymbol{\tau}^n &= \frac{\mathbf{u}(t_{n+1}) - \mathbf{u}(t_{n-1})}{2k} - \mathbf{f}(\mathbf{u}(t_n), t_n) \\
&= \left[\mathbf{u}'(t_n) + \frac{1}{6}k^2\mathbf{u}'''(t_n) + O(k^4)\right] - \mathbf{u}'(t_n) \\
&= \frac{1}{6}k^2\mathbf{u}'''(t_n) + O(k^4).
\end{aligned}$$

Definition 8.33. For a numerical method of the form

$$\mathbf{U}^{n+1} = \boldsymbol{\phi}(\mathbf{U}^{n+1}, \mathbf{U}^n, \ldots, \mathbf{U}^{n-m}),$$

the *one-step error* is defined by

$$\mathcal{L}^n := \mathbf{u}(t_{n+1}) - \boldsymbol{\phi}(\mathbf{u}(t_{n+1}), \mathbf{u}(t_n), \ldots, \mathbf{u}(t_{n-m})). \tag{8.22}$$

Example 8.34. For the leapfrog method, the one-step error is

$$\begin{aligned}
\mathcal{L}^n &= \mathbf{u}(t_{n+1}) - \mathbf{u}(t_{n-1}) - 2k\mathbf{f}(\mathbf{u}(t_n), t_n) \\
&= \frac{1}{3}k^3\mathbf{u}'''(t_n) + O(k^5) \\
&= 2k\boldsymbol{\tau}^n.
\end{aligned}$$

Definition 8.35. The *solution error* of a numerical method for solving the IVP in Definition 8.4 is

$$\mathbf{E}^N := \mathbf{U}^{T/k} - \mathbf{u}(T); \qquad \mathbf{E}^n = \mathbf{U}^n - \mathbf{u}(t_n). \tag{8.23}$$

Definition 8.36. A numerical method is *convergent* for a family of IVPs if the application of it to any IVP with $\mathbf{f}(\mathbf{u}, t)$ Lipschitz continuous in $\mathbf{u}$ and continuous in t yields

$$\lim_{\substack{k\to 0 \\ Nk=T}} \mathbf{U}^N = \mathbf{u}(T) \tag{8.24}$$

for every fixed $T > 0$.

8.5 Analysis of Euler's methods

8.5.1 Linear IVPs

In this section, we consider the convergence of Euler's method for solving linear IVPs of the form

$$\begin{cases} \mathbf{u}'(t) = \lambda\mathbf{u}(t) + \mathbf{g}(t), \\ \mathbf{u}(0) = \mathbf{u}_0, \end{cases} \tag{8.25}$$

where λ is either a scalar or a diagonal matrix.

Lemma 8.37. For the linear IVP (8.25), the solution errors and the local truncation error of Euler's method satisfy

$$\mathbf{E}^{n+1} = (1 + k\lambda)\mathbf{E}^n - k\boldsymbol{\tau}^n. \tag{8.26}$$

Lemma 8.38. For the linear IVP (8.25), the solution error and the local truncation errors of Euler's method satisfy

$$\mathbf{E}^n = (1 + k\lambda)^n\mathbf{E}^0 - k\sum_{m=1}^{n}(1 + k\lambda)^{n-m}\boldsymbol{\tau}^{m-1}. \tag{8.27}$$

Theorem 8.39. Euler's method is convergent for solving the linear IVP (8.25).

8.5.2 Nonlinear IVPs

Lemma 8.40. Consider a nonlinear IVP of the form

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t), t),$$

where $\mathbf{f}(\mathbf{u}, t)$ is continuous in t and is Lipschitz continuous in $\mathbf{u}$ with L as the Lipschitz constant. Euler's method satisfies

$$\|\mathbf{E}^{n+1}\| \le (1 + kL)\|\mathbf{E}^n\| + k\|\boldsymbol{\tau}^n\|. \tag{8.28}$$

Theorem 8.41. For the nonlinear IVP in Lemma 8.40, Euler's method is convergent.

8.5.3 Zero stability and absolute stability

Example 8.42. Consider the scalar IVP

$$u'(t) = \lambda(u - \cos t) - \sin t,$$

with $\lambda = -2100$ and $u(0) = 1$. The exact solution is clearly

$$u(t) = \cos t.$$

The following table shows the error at time $T = 2$ when Euler's method is used with various values of k.

k	$E(T)$
2.00e-4	1.48e-8
4.00e-4	3.96e-8
8.00e-4	7.92e-8
9.50e-4	3.21e-7
9.76e-4	5.88e+35
1.00e-3	1.45e+76

The first three lines confirm the first-order accuracy of Euler's method, but something dramatic happens between $k = 9.76\text{e-}4$ and $k = 9.50\text{e-}4$. What's going on?

Definition 8.43. The Euler's method

$$U^{n+1} = (1 + k\lambda)U^n$$

for solving the scalar IVP

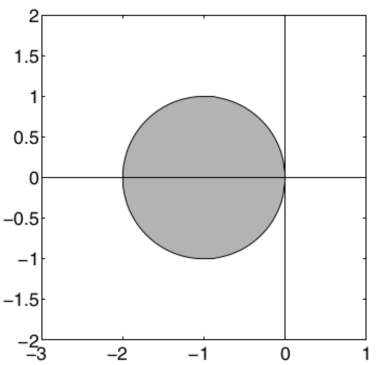
$$u'(t) = \lambda u(t) \tag{8.29}$$

is *absolutely stable* if

$$|1 + k\lambda| \le 1. \tag{8.30}$$

Definition 8.44. The *region of absolute stability* for Euler's method applied to (8.29) is the set of all points

$$\{z \in \mathbb{C} : |1 + z| \le 1\}. \tag{8.31}$$

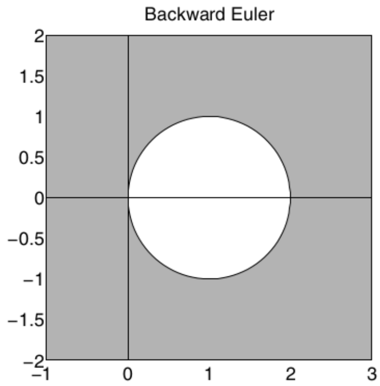


Example 8.45. The backward Euler's method applied to (8.29) reads

$$U^{n+1} = U^n + k\lambda U^{n+1} \Rightarrow U^{n+1} = \frac{1}{1 - k\lambda}U^n.$$

Hence the region of absolute stability for backward Euler's method is

$$\{z \in \mathbb{C} : |1 - z| \ge 1\}. \tag{8.32}$$



Lemma 8.46. Consider an autonomous, homogeneous, and linear system of IVPs

$$\mathbf{u}'(t) = A\mathbf{u} \tag{8.33}$$

where $\mathbf{u} \in \mathbb{R}^N$, $N > 1$, and A is diagonalizable with eigenvalues as λ_i's. Euler's method is absolutely stable if each $z_i := k\lambda_i$ is within the stability region (8.31).

Definition 8.47. The *law of mass action* states that the rate of a chemical reaction is proportional to the product of the concentration of the reacting substances, with each concentration raised to a power equal to the coefficient that occurs in the reaction.

Example 8.48. For the reaction

$$\alpha\mathrm{A} + \beta\mathrm{B} \underset{\mathrm{k}_-}{\overset{\mathrm{k}_+}{\rightleftharpoons}} \sigma\mathrm{S} + \tau\mathrm{T},$$

the forward reaction rate is $k_+[A]^\alpha[B]^\beta$ and the backward reaction rate is $k_-[S]^\sigma[T]^\tau$.

Example 8.49. Consider

$$\mathrm{A} + \mathrm{B} \underset{\mathrm{c}_2}{\overset{\mathrm{c}_1}{\rightleftharpoons}} \mathrm{AB}.$$

Let

$$\mathbf{u} := \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} [A] \\ [B] \\ [AB] \end{bmatrix}.$$

Then we have

$$\begin{aligned} u_1' &= -c_1u_1u_2 + c_2u_3; \\ u_2' &= -c_1u_1u_2 + c_2u_3; \\ u_3' &= c_1u_1u_2 - c_2u_3, \end{aligned}$$

which can be written more compactly as

$$\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}).$$

Let $\mathbf{v}(t) := \mathbf{u}(t) - \bar{\mathbf{u}}$ with $\bar{\mathbf{u}}$ independent on time. Then

$$\begin{aligned} \mathbf{v}'(t) = \mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t)) &= \mathbf{f}(\mathbf{v} + \bar{\mathbf{u}}) \\ &= \mathbf{f}(\bar{\mathbf{u}}) + \mathbf{f}'(\bar{\mathbf{u}})\mathbf{v}(t) + O(\|\mathbf{v}\|^2), \end{aligned}$$

and hence

$$\mathbf{v}'(t) = A\mathbf{v}(t) + \mathbf{b},$$

where $A = \mathbf{f}'(\bar{\mathbf{u}})$ is the Jacobian, i.e.,

$$A = \begin{bmatrix} -c_1u_2 & -c_1u_1 & c_2 \\ -c_1u_2 & -c_1u_1 & c_2 \\ c_1u_2 & c_1u_1 & -c_2 \end{bmatrix},$$

with eigenvalues $\lambda_1 = -c_1(u_1+u_2) - c_2$ and $\lambda_2 = \lambda_3 = 0$. Since $u_1 + u_2$ is simply the total concentration of species A and B present, they can be bounded by $u_1(0)+u_2(0)+u_3(0)$.

Example 8.50. For the reaction

$$\mathrm{A} \underset{c_2}{\overset{c_1}{\rightleftharpoons}} \mathrm{B},$$

we obtain the linear IVPs

$$\begin{cases} u_1' = -c_1u_1 + c_2u_2; \\ u_2' = c_1u_1 - c_2u_2. \end{cases}$$

8.5.4 Review of Jordan canonical form

Theorem 8.51 (Factorization of a polynomial over $\mathbb{C}$)**.** If $p \in \mathcal{P}(\mathbb{C})$ is a nonconstant polynomial, then p has a unique factorization (except for the order of the factors) of the form

$$p(z) = c(z-\lambda_1)\cdots(z-\lambda_m), \tag{8.34}$$

where $c, \lambda_1, \ldots, \lambda_m \in \mathbb{C}$.

Definition 8.52. Let $A \in \mathbb{C}^{m\times m}$, then the *characteristic polynomial* of A is

$$p_A(z) = \det(zI - A). \tag{8.35}$$

Proposition 8.53. Let $A \in \mathbb{C}^{m\times m}$, then λ is an eigenvalue of A iff λ is a root of the characteristic polynomial of A.

Exercise 8.54. Show that

$$p_M(z) = z^r + \sum_{j=0}^{r-1} \alpha_j z^j.$$

is the characteristic polynomial of

$$M = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ -\alpha_0 & -\alpha_1 & \cdots & -\alpha_{r-2} & -\alpha_{r-1} \end{bmatrix} \in \mathbb{C}^{r\times r}. \tag{8.36}$$

Definition 8.55. If the characteristic polynomial $p_A(z)$ has a factor $(z-\lambda)^n$, then λ is said to have *algebraic multiplicity* $m_a(\lambda) = n$.

Definition 8.56. Let λ be an eigenvalue of $A \in \mathbb{C}^{m\times m}$, the *eigenspace* of A corresponding to λ is

$$\begin{aligned} \mathcal{N}(A-\lambda I) &= \{\mathbf{u} \in \mathbb{C}^m : (A-\lambda I)\mathbf{u} = \mathbf{0}\} \\ &= \{\mathbf{u} \in \mathbb{C}^m : A\mathbf{u} = \lambda\mathbf{u}\}. \end{aligned} \tag{8.37}$$

The dimension of $\mathcal{N}(A-\lambda I)$ is the *geometric multiplicity* $m_g(\lambda)$ of λ.

Proposition 8.57. Geometric multiplicity and algebraic multiplicity satisfy

$$1 \le m_g(\lambda) \le m_a(\lambda). \tag{8.38}$$

Definition 8.58. An eigenvalue λ of A is *defective* if

$$m_g(\lambda) < m_a(\lambda). \tag{8.39}$$

A is *defective* if A has one or more defective eigenvalues.

Proposition 8.59. A nondefective matrix A is diagnolizable, i.e.,

$$\exists \text{ nonsingular } R \text{ s.t. } R^{-1}AR = \Lambda \text{ is diagonal.} \tag{8.40}$$

Theorem 8.60 (Schur decomposition)**.** For each square matrix A, there exists a unitary matrix Q such that

$$A = QUQ^{-1}, \tag{8.41}$$

where U is upper triangular.

Definition 8.61. A *Jordan block* of order k has the form

$$J(\lambda, k) = \lambda I_k + S_k, \tag{8.42}$$

where

$$(S_k)_{i,j} = \begin{cases} 1, & i = j-1, \\ 0, & \text{otherwise.} \end{cases}$$

Example 8.62. The Jordan blocks of orders 1, 2, and 3 are

$$J(\lambda,1) = \lambda, \quad J(\lambda,2) = \begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix}, \quad J(\lambda,3) = \begin{bmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{bmatrix}.$$

Theorem 8.63 (Jordan canonical form)**.** Every square matrix A can be expressed as

$$A = RJR^{-1}, \tag{8.43}$$

where R is invertible and J is a block diagonal matrix of the form

$$J = \begin{bmatrix} J(\lambda_1,k_1) & & & \\ & J(\lambda_2,k_2) & & \\ & & \ddots & \\ & & & J(\lambda_s,k_s) \end{bmatrix}. \tag{8.44}$$

Each $J(\lambda_i, k_i)$ is a Jordan block of some order k_i and $\sum_{i=1}^{s} k_i = m$. If λ is an eigenvalue of A with algebraic multiplicity m_a and geometric multiplicity m_g, then λ appears in m_g blocks and the sum of the orders of these blocks is m_a.

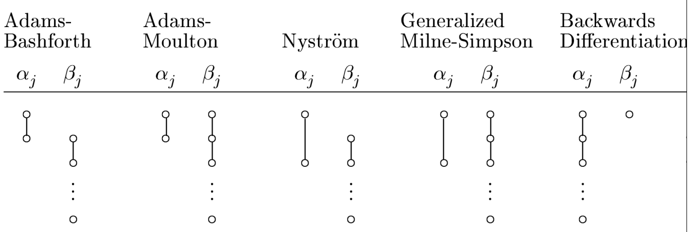
8.6 Linear multistep methods

Definition 8.64. For solving the IVP (8.3), an *s-step linear multistep method* (LMM) has the form

$$\sum_{j=0}^{s} \alpha_j \mathbf{U}^{n+j} = k \sum_{j=0}^{s} \beta_j \mathbf{f}(\mathbf{U}^{n+j}, t_{n+j}), \tag{8.45}$$

where $\alpha_s = 1$ is assumed WLOG.

Definition 8.65. An LMM method (8.45) is *explicit* if $\beta_s = 0$; otherwise it is *implicit*.



Definition 8.66. An *Adams formula* is an LMM of the form

$$\mathbf{U}^{n+s} = \mathbf{U}^{n+s-1} + k \sum_{j=0}^{s} \beta_j \mathbf{f}(\mathbf{U}^{n+j}, t_{n+j}), \tag{8.46}$$

whese β_j's are chosen to maximize the order of accuracy.

Definition 8.67. An *Adams-Bashforth formula* is an Adams formula with $\beta_s = 0$. An *Adams-Moulton formula* is an Adams formula with $\beta_s \neq 0$.

Example 8.68. Euler's method is the 1-step Adams-Bashforth formula with

$$s = 1,\ \alpha_1 = 1,\ \alpha_0 = -1,\ \beta_1 = 0,\ \beta_0 = 1.$$

Example 8.69. The trapezoidal method is the 1-step Adams-Moulton formula with

$$s = 1,\ \alpha_1 = 1,\ \alpha_0 = -1,\ \beta_1 = \beta_0 = \frac{1}{2}.$$

Definition 8.70. An *Nyström formula* is an LMM of the form

$$\mathbf{U}^{n+s} = \mathbf{U}^{n+s-2} + k \sum_{j=0}^{s-1} \beta_j \mathbf{f}(\mathbf{U}^{n+j}, t_{n+j}), \tag{8.47}$$

where β_j's are chosen to give order s.

Example 8.71. The midpoint method is the 2-step Nyström formula with

$$s = 2,\ \alpha_2 = 1,\ \alpha_1 = 0,\ \alpha_0 = -1,\ \beta_1 = 1,\ \beta_0 = 0.$$

Definition 8.72. A *backward differentiation formula* (BDF) is an LMM of the form

$$\sum_{j=0}^{s} \alpha_j \mathbf{U}^{n+j} = k\mathbf{f}(\mathbf{U}^{n+s}, t_{n+j}), \tag{8.48}$$

where α_j's are chosen to give order s.

Example 8.73. The backward Euler's method is the 1-step BDF with

$$s = 1,\ \alpha_1 = \beta_1 = 1,\ \alpha_0 = -1,\ \beta_0 = 0.$$

8.6.1 Accuracy

Definition 8.74. The *characteristic polynomials* or *generating polynomials* for the LMM (8.45) are

$$\rho(\zeta) = \sum_{j=0}^{s} \alpha_j \zeta^j; \qquad \sigma(\zeta) = \sum_{j=0}^{s} \beta_j \zeta^j. \tag{8.49}$$

Example 8.75. The forward Euler's method (8.18) has

$$\rho(\zeta) = \zeta - 1, \qquad \sigma(\zeta) = 1, \tag{8.50}$$

while the backward Euler's method (8.19) has

$$\rho(\zeta) = \zeta - 1, \qquad \sigma(\zeta) = \zeta. \tag{8.51}$$

Example 8.76. The trapezoidal method (8.20) has

$$\rho(\zeta) = \zeta - 1, \qquad \sigma(\zeta) = \frac{1}{2}(\zeta + 1), \tag{8.52}$$

and the midpoint method (8.21) has

$$\rho(\zeta) = \zeta^2 - 1, \qquad \sigma(\zeta) = 2\zeta. \tag{8.53}$$

Notation 9. Denote by Z a *time shift operator* that acts on both discrete functions according to

$$Z\mathbf{U}^n = \mathbf{U}^{n+1} \tag{8.54}$$

and on continuous functions according to

$$Z\mathbf{u}(t) = \mathbf{u}(t + k). \tag{8.55}$$

Definition 8.77. The *difference operator of an LMM* is an operator $\mathcal{L}$ on the linear space of continuously differentiable functions given by

$$\mathcal{L} = \rho(Z) - k\mathcal{D}\sigma(Z), \tag{8.56}$$

where $\mathcal{D}\mathbf{u}(t_n) = \mathbf{u}_t(t_n) := \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}(t_n)$, Z the time shift operator, and ρ, σ are the characteristic polynomials for the LMM.

Lemma 8.78. The one-step error of the LMM (8.45) is

$$\mathcal{L}\mathbf{u}(t_n) = C_0\mathbf{u}(t_n) + C_1 k\mathbf{u}_t(t_n) + C_2 k^2 \mathbf{u}_{tt}(t_n) + \cdots, \tag{8.57}$$

where

$$\begin{array}{l} C_0 = \sum_{j=0}^{s} \alpha_j \\ C_1 = \sum_{j=0}^{s} (j\alpha_j - \beta_j) \\ C_2 = \sum_{j=0}^{s} \left(\frac{1}{2} j^2 \alpha_j - j\beta_j\right) \\ \vdots \\ C_q = \sum_{j=0}^{s} \left(\frac{1}{q!} j^q \alpha_j - \frac{1}{(q-1)!} j^{q-1} \beta_j\right). \end{array} \tag{8.58}$$

Notation 10. We write $f(x) = \Theta(g(x))$ as $x \to 0$ if there exist constants $C, C' > 0$ and $x_0 > 0$ such that $Cg(x) \leq f(x) \leq C'g(x)$ for all $x \leq x_0$.

Definition 8.79. An LMM has *order of accuracy* p if

$$\mathcal{L}\mathbf{u}(t_n) = \Theta(k^{p+1}) \text{ as } k \to 0, \tag{8.59}$$

i.e., if in (8.58) we have $C_0 = C_1 = \cdots = C_p = 0$ and $C_{p+1} \neq 0$. Then C_{p+1} is called the *error constant.* The LMM is *consistent* if it has order of accuracy $p \geq 1$.

Example 8.80. For Euler's method, the coefficients C_j's in (8.58) can be computed directly from Example 8.68 as $C_0 = C_1 = 0, C_2 = \frac{1}{2}, C_3 = \frac{1}{6}$.

Exercise 8.81. Compute the first five coefficients C_j's of the trapezoidal rule and the midpoint rule from Examples 8.69 and 8.71.

Example 8.82. A necessary condition for $\|\mathbf{E}^n\| = O(k)$ is $\|\mathcal{L}\mathbf{u}(t_n)\| = O(k^2)$ since there are $\frac{T}{k}$ time steps, and hence the first two terms in (8.57) should be zero, i.e.,

$$\sum_{j=0}^{s} \alpha_j = 0, \qquad \sum_{j=0}^{s} j\alpha_j = \sum_{j=0}^{s} \beta_j, \tag{8.60}$$

which is equivalent to

$$\rho(1) = 0 \quad \text{and} \quad \rho'(1) = \sigma(1). \tag{8.61}$$

Second-order accuracy further requires

$$\frac{1}{2}\sum_{j=0}^{s} j^2\alpha_j = \sum_{j=0}^{s} j\beta_j.$$

In general, pth-order accuracy requires (8.60) and

$$\forall q = 2, \ldots, p, \quad \sum_{j=0}^{s} \frac{1}{q!} j^q \alpha_j = \sum_{j=0}^{r} \frac{1}{(q-1)!} j^{q-1}\beta_j. \tag{8.62}$$

Exercise 8.83. Express conditions of $\mathcal{L} = O(k^3)$ using characteristic polynomials.

Exercise 8.84. Derive coefficients of LMMs shown below by the method of undetermined coefficients and a programming language with symbolic computation such as `Matlab`.

Adams-Bashforth formulas in Definition 8.67

number of steps s	order p	β_s	β_{s-1}	β_{s-2}	β_{s-3}	β_{s-4}
1	1	0	1		(EULER)	
2	2	0	$\frac{3}{2}$	$-\frac{1}{2}$		
3	3	0	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$	
4	4	0	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$

Adams-Moulton formulas in Definition 8.67

number of steps s	order p	β_s	β_{s-1}	β_{s-2}	β_{s-3}	β_{s-4}
1	1	1		(BACKWARD EULER)		
1	2	$\frac{1}{2}$	$\frac{1}{2}$		(TRAPEZOID)	
2	3	$\frac{5}{12}$	$\frac{8}{12}$	$-\frac{1}{12}$		
3	4	$\frac{9}{24}$	$\frac{19}{24}$	$-\frac{5}{24}$	$\frac{1}{24}$	
4	5	$\frac{251}{720}$	$\frac{646}{720}$	$-\frac{264}{720}$	$\frac{106}{720}$	$-\frac{19}{720}$

BDF formulas in Definition 8.72

number of steps s	order p	α_s	α_{s-1}	α_{s-2}	α_{s-3}	α_{s-4}	β_s
1	1	1	-1	(BACKWARD EULER)			1
2	2	1	$-\frac{4}{3}$	$\frac{1}{3}$			$\frac{2}{3}$
3	3	1	$-\frac{18}{11}$	$\frac{9}{11}$	$-\frac{2}{11}$		$\frac{6}{11}$
4	4	1	$-\frac{48}{25}$	$\frac{36}{25}$	$-\frac{16}{25}$	$\frac{3}{25}$	$\frac{12}{25}$

Lemma 8.85. An LMM with $\sigma(1) \neq 0$ has order of accuracy p if and only if

$$\frac{\rho(e^\kappa)}{\sigma(e^\kappa)} = \kappa + \Theta(\kappa^{p+1}) \text{ as } \kappa \to 0. \tag{8.63}$$

where $\kappa = k\mathcal{D}$.

Theorem 8.86. An LMM with $\sigma(1) \neq 0$ has order of accuracy p if and only if

$$\begin{aligned} \tfrac{\rho(z)}{\sigma(z)} &= \log z + \Theta\left((z-1)^{p+1}\right) \\ &= \left[(z-1) - \tfrac{1}{2}(z-1)^2 + \tfrac{1}{3}(z-1)^3 - \cdots\right] \\ &\quad +\Theta((z-1)^{p+1}). \end{aligned} \tag{8.64}$$

as $z \to 1$.

Example 8.87. The trapezoidal rule has $\rho(z) = z - 1$ and $\sigma(z) = \frac{1}{2}(z+1)$. A comparison of (8.64) with the expansion

$$\frac{\rho(z)}{\sigma(z)} = \frac{z-1}{\frac{1}{2}(z+1)} = (z-1)\left[1 - \frac{z-1}{2} + \frac{(z-1)^2}{4} - \cdots\right]$$

confirms that the trapezoidal rule has order 2 with error constant $-\frac{1}{12}$.

Exercise 8.88. For the third-order BDF formula in Definition 8.72 and Exercise 8.84, derive its characteristic polynomials and apply Theorem 8.86 to verify that the order of accuracy is indeed 3.

8.6.2 Stability

Example 8.89 (A consistent but unstable LMM)**.** The LMM

$$\mathbf{U}^{n+2} - 3\mathbf{U}^{n+1} + 2\mathbf{U}^n = -k\mathbf{f}(\mathbf{U}^n, t_n) \tag{8.65}$$

has a one-step error given by

$$\begin{aligned} \mathcal{L}\mathbf{u}(t_n) &= \mathbf{u}(t_{n+2}) - 3\mathbf{u}(t_{n+1}) + 2\mathbf{u}(t_n) + k\mathbf{u}'(t_n) \\ &= \frac{1}{2}k^2\mathbf{u}''(t_n) + O(k^3), \end{aligned}$$

so the method is consistent with first-order accuracy. But the solution error may not exhibit first order accuracy, or even convergence. Consider the trivial IVP

$$u'(t) = 0, \qquad u(0) = 0,$$

with solution $u(t) \equiv 0$. The LMM (8.65) reads in this case

$$U^{n+2} = 3U^{n+1} - 2U^n \Rightarrow U^{n+2} - U^{n+1} = 2(U^{n+1} - U^n),$$

and therefore

$$U^n = 2U^0 - U^1 + 2^n(U^1 - U^0).$$

If we take $U^0 = 0$ and $U^1 = k$, then

$$U^n = k(2^n - 1) = k(2^{T/k} - 1) \to +\infty \text{ as } k \to 0.$$