Modeling and Simulation in Science,
Engineering and Technology

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Large-Scale Networks in Engineering and Life Sciences

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ISSN 2164-3679 ISSN 2164-3725 (electronic)
Modeling and Simulation in Science, Engineering and Technology
ISBN 978-3-319-08436-7 ISBN 978-3-319-08437-4 (eBook)
DOI 10.1007/978-3-319-08437-4
Springer Heidelberg New York Dordrecht London

Library of Congress Control Number: 2014953776

Mathematics Subject Classification (2010): 34A26, 92C42, 94C05, 90B10, 90C27

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

Modeling, analysis, and control of complex large-scale systems are becoming increasingly important. Large-scale systems are often the result of networked interactions among an ample number of subsystems. Examples of large-scale networked systems include biochemical reaction networks, communication networks such as mobile phone networks and the Internet, complex chemical production processes, neural networks, fish and bird swarms, and circuit networks in microprocessors. The objective of the 2011 summer school *Large-Scale Networks in Engineering and Life Sciences* of the International Max Planck Research School Magdeburg was to provide insights and tools for modeling, analysis, optimization, and control of large-scale networks in life sciences and engineering. The chapters provided in this book are based on the lectures given during this summer school. They cover a wide range of applications and focus on mathematical modeling of the different network structures in these areas. Thus, this book complements recent monographs on the theory of networks such as "Networks: An Introduction" by Newman (Cambridge University Press, 2010) and "The Structure of Complex Networks" by Estrada (Oxford University Press, 2011) or the edited volume "Network Science. Complexity in Nature and Technology" by Estrada, Fox, and Higham (Springer, 2010).

The chapters in this book are mostly self-contained introductions to network modeling in various areas. They can be read independently and may serve as the basis for a seminar series or, in combination with the introductory texts mentioned above, as course supplements for a course on Network Theory and Applications. We hope the book will be useful for graduate students or beginners in the respective fields with a solid mathematical background, but also as a compendium for network researchers. Since different fields employ different techniques as outlined below, we expect that fruitful ideas can result from studying how other disciplines approach network structures.

Basically, the book can be partitioned into four parts. The first part, consisting only of Chap. 1, treats the mathematical theory of (bio)-chemical reaction networks. It can also serve as a self-contained introduction into the geometric theory of ordinary differential equations. Two different applications of network theory in electrical engineering areas are the topic of Chaps. 2 and 3; these can be considered as

the second part. Optimization of and on networks is a fundamental issue in discrete mathematics and is treated in the fourth chapter, which can be considered again as a part on its own. The last three chapters discuss biological networks from different view points and together form a fourth part of the book.

In the following, we provide a brief introduction to the individual chapters of this book. Chapter 1 by Flockerzi gives an "Introduction to the Geometric Theory of Ordinary Differential Equations with Applications to Chemical Processes". Though providing the fundamentals of the geometric theory of differential equations in a general setting, it is tailored to applications to (bio-)chemical reaction networks and chemical separation processes. Thus, quite often, the ordinary differential equations under investigation are derived from underlying partial differential equations as in the search for solutions of quasi-linear partial differential equations by the method of characteristics. The *geometric theory* addresses invariant and integral manifolds, e.g., center manifolds for bifurcation problems and slow invariant manifolds for networks with slow and fast variables and/or processes. In applications, the associated reduction methods are based on suitable quasi-stationary approximations of such (slow) invariant manifolds. Several model problems illustrate applications of the derived methods to different instances of chemical reaction networks.

In the second chapter, Reis introduces "Circuit Modelling with Differential–Algebraic Equations". Electrical circuits underlie most electronic devices in everyday life, ranging from computers to tablets and cell phones to car electronics. Mathematical models of these circuits are based on graph and network theory and are the core of circuit and device simulation in industrial design processes. The chapter provides a basic and self-contained introduction to the mathematical description of electrical circuits consisting of resistances, capacitances, inductances, as well as voltage and current sources. The standard methods for the modeling of circuits by differential–algebraic equations—"modified nodal analysis" and "modified loop analysis"—are presented, and a detailed analysis of the mathematical properties of these equations is included.

The third chapter by Egerstedt, de la Croix, and Kingston on "Interacting with Networks of Mobile Agents" discusses the design of control, communication, and coordination strategies for multi-agent networks, a central issue in current research in systems and control theory. Applications of distributed, mobile agent systems or "swarms" include, but are by no means limited to, multi-agent robotics, distributed sensor networks, interconnected manufacturing chains, and data networks. The question discussed is how humans can control or influence the behavior of the swarm. Lagrangian and Eulerian models are proposed to model the movements of the agents. Both of them are amenable to human manipulation. Interaction of the agents are modeled by graphs/networks, and controllability and manipulability notions for the human-swarm interaction are introduced, based on which control strategies are developed.

Chapter 4 "Combinatorial Optimization: The Interplay of Graph Theory, Linear and Integer Programming Illustrated on Network Flow" by Wagler deals with combinatorial optimization which is the main mathematical discipline dealing with optimizing networks. It uses basic elements from graph theory, geometry, linear and

integer programming. The network flow problem is used as a running example to illustrate the concepts and methods introduced. It does not require prior knowledge in advanced optimization techniques. Basic introductions into linear programming, including the simplex method, and integer programming are provided.

The 5th chapter, by Klamt, Hädicke, and von Kamp, is dedicated to the "Stoichiometric and Constraint-Based Analysis of Biochemical Reaction Networks". Although the methods presented therein rely solely on the stoichiometry of metabolic networks, they provide essential information on key functional properties and deliver various testable predictions. The chapter presents the relevant mathematical foundations of different approaches of this kind and discusses various applications in biology and biotechnology.

The contribution of Blätke, Rohr, Heiner, and Marwan in Chap. 6 is focused on "A Petri Net Based Framework for Biomodel Engineering". Petri nets provide a versatile framework for the computation of biochemical reaction networks and gene regulatory networks, particularly useful in the context of systems biology. Starting with basic definitions, the authors provide an introduction to different classes of Petri nets, static and dynamic modeling applications, database-assisted automatic composition and modification of Petri nets as well as automatic reconstruction of networks based on time series data sets.

In Chap. 7, "Hybrid Modeling for Systems Biology", von Stosch, Carinhas and Oliveira deal with the theoretical fundamentals of hybrid semi-parametric modeling to integrate extensive experimental data sets obtained by "omics" technologies developed over recent years into global quantitative models. Their approach combines available knowledge about mechanisms in the form of parametric mathematical models (bottom-up) with nonparametric models that are determined from experimental data (top-down). Examples are given for small metabolic networks of insect cells (*Spodoptera frugiperda*, Sf9) used for production of baculoviruses, dynamic models of metabolism of animal cells (baby hamster kidney, BHK) in fed-batch cultures with unknown reaction kinetics, and a signal transduction network involving transcription factor A (TFA) with intrinsic time delays.

Finally, we would like to express our gratitude to all authors of the chapters in this book for their dedicated effort to provide useful tutorials, a task often much more time consuming than writing about latest research results to an informed community. Numerous experts in network theory and applications served as reviewers for the chapters. We are very grateful for their help in improving readability and tutorial value of the individual manuscripts. Last but not least, our thanks go to Barbara Hellriegel and Katherina Steinmetz from Springer Basel AG for their never ending endurance in waiting for the final manuscript as well as their support throughout the development of this project.

Magdeburg
June 23, 2014

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Chapter 1
Introduction to the Geometric Theory of ODEs with Applications to Chemical Processes

Dietrich Flockerzi

Abstract We give an introduction to the geometric theory of ordinary differential equations (ODEs) tailored to applications to biochemical reaction networks and chemical separation processes. Quite often, the ordinary differential equations under investigation are "reduced" partial differential equations (PDEs) as in the search of traveling wave solutions. So, we also address ODE topics that have their origin in the PDE context.

We present the mathematical theory of invariant and integral manifolds, in particular, of center and slow manifolds, which reflect the splitting of variables and/or processes into slow and fast ones. The invariance of a smooth manifold is characterized by a quasilinear partial differential equation, and the widely used approximations of invariant manifolds are derived from such PDEs. So we also offer, to some extent, an introduction to quasilinear PDEs. The basic ideas and crucial tools are illustrated with numerous examples and exercises. Concerning the proofs, we confine ourselves to outline the crucial steps and refer, especially in the first three sections, to the literature.

The final Sects. 1.4 and 1.5 on reaction–separation processes and on chromatographic separation present new results, including their proofs. They are the outcome of many fruitful discussions with my colleagues Malte Kaspereit and Achim Kienle.

Keywords Stability · Integral manifolds and method of characteristics · Center manifolds and asymptotic phases · Reduction methods and bifurcations · Quasi-stationary approximations and singular perturbations · Slow invariant manifolds · Reactive and chromatographic separation networks

Outline This contribution is not written as an introduction to the *basic theory* of ODEs. We assume the reader to have some experience with linear algebra (spectral theory, Schur normal form), analysis (multidimensional integration, contraction

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P. Benner et al. (eds.), *Large-Scale Networks in Engineering and Life Sciences*, Modeling and Simulation in Science, Engineering and Technology,
DOI 10.1007/978-3-319-08437-4_1

principle), and ODEs (explicit solution methods, linear systems, stability, simple bifurcations).

We recapitulate certain properties of ODEs in Sect. 1.1 in order to prepare the stage and to open up new perspectives for the *geometric theory* of ODEs. Section 1.2, dedicated to two-dimensional systems, introduces invariant manifolds in the familiar form of invariant orbits and addresses computational aspects for the associated partial differential equations (e.g., method of characteristics). Moreover, Sect. 1.2 presents the necessary tools for discussing more complicated bifurcation phenomena (normal forms, blow-up transformations). The concluding Sect. 1.2.5 sheds some new light on eigenspaces of linear systems and provides the key idea for the general nonlinear geometric theory by characterizing the eigenspaces as the sets of initial values leading to solutions of restricted exponential growth as $t \to \pm\infty$.

Section 1.3 deals with the classical local stable, unstable and center manifolds for n-dimensional systems and introduces the fundamental reduction principle: Questions about the asymptotic behavior in an n-dimensional state space can often be answered by reduced systems in a state space of dimension m with $m < n$. Ideally, one has $m = 1$ or $m = 2$ as for the standard scenarios of stationary bifurcations or Hopf bifurcations. For systems with two time scales t and $\tau = t/\varepsilon$, we discuss extensively the validity of quasi-stationary approximations and of quasi-steady-state approximations in Sects. 1.3.5 and 1.3.6. Considering reaction–separation networks, Sect. 1.4 continues this study of two-time-scale systems and offers the reduction to a separation model without a reactive part. Finally, Sect. 1.5 extends the method of characteristics (Sect. 1.2.2) to systems of first-order quasilinear PDEs and addresses chromatographic separation processes using equilibrium theory. We obtain innovative spectral results for adsorption equilibria, described by Langmuir-type isotherms, in particular, by bi-Langmuir isotherms (see [36]).

All sections start with a short outline and are divided in various subsections. Their titles and the headings of all the results and remarks may serve as a grasshopper's guide through this contribution. For readers who are especially interested in applications from systems biology and chemical engineering, we refer to the topics of

- activator–inhibitor models in Exercise 1.26, in Sect. 1.1.4.3, and in Sect. 1.3.6,
- volume transport and traveling waves in Sect. 1.1.2.3, Sect. 1.2.2 (see Exercises 2.6 and 2.7), in Exercise 3.7(3) and Remark 3.16, and, finally, in Sect. 1.5,
- reaction networks in Sect. 1.1.4.3 and in Sects. 1.4.2 and 1.4.3 with the introductory Example 1.28,
- chromatographic separation in Sect. 1.5 with the introductory Exercise 2.7.

Over the years, I was inspired and influenced by the work of many authors: I would like to refer to the ODE books [2, 16, 17, 63, 67, 77], the PDE books [11] and [25], and the monographs [10, 23, 26, 68, 69, 83] and [22, 75, 76] from the more applied side. I apologize for not mentioning all the other valuable sources. Finally, I thank Hector Rubiera Landa for his assistance with the figures.

1.1 Basic Theory of Ordinary Differential Equations

This introductory section discusses the basic questions and concepts in the theory of ordinary differential equations. The presentation is tailored to the geometric theory of systems of ordinary differential equations: It emphasizes the concepts and tools in simple settings and introduces illustrating academic examples and "real-world" processes from chemical engineering in their simplest versions.

Section 1.1.1 is dedicated to scalar differential equations, including their bifurcation diagrams, and to n-dimensional linear systems. By introducing scalar differential inequalities, we arrive at comparison theorems and the crucial Gronwall lemma. First consequences of the fundamental theorem on existence and uniqueness of solutions are discussed in Sect. 1.1.2: We comment on sensitivity analysis, on volume transport, and on bounded system response and establish Lyapunov's theorem on first approximations. The following Sects. 1.1.3 and 1.1.4 present the basic results from stability theory, in particular LaSalle's invariance principle, as they can be found in any textbook on ODEs. Illustrations include activator–inhibitor systems and reversible reaction networks from systems biology and chemical engineering (see Sect. 1.1.4.3).

1.1.1 Questions of Existence and Uniqueness

We first pose the standing hypothesis and the formulation of initial value problems and then address the basic questions of existence and uniqueness, of approximations and reductions.

Standing Hypothesis *Let $f : D \to \mathbb{R}^n$ be a continuous function on a nonempty, open, and connected set $D \subset \mathbb{R} \times \mathbb{R}^n$, and let (τ, ξ) be an element of D.*

Problem Formulation *Does there exist an open interval $I \ni \tau$ and does there exist a continuously differentiable function $\varphi : I \to \mathbb{R}^n$ (symbolically, $\varphi \in C^1(I, \mathbb{R}^n)$) with $\varphi(\tau) = \xi$ and*

$$\big(t, \varphi(t)\big) \in D, \quad \frac{d\varphi}{dt}(t) = f\big(t, \varphi(t)\big) \quad \forall t \in I?$$

In case a function $\varphi(\cdot)$ has these properties, it is called a *solution of the initial value problem (IVP)*

$$\frac{dx}{dt} = f(t, x), \quad x(\tau) = \xi, \tag{1.1}$$

on I with respect to D or, in short terms, a *solution of the differential equation* $\frac{dx}{dt} = f(t, x)$ for given initial data $(\tau, \xi) \in D$. With $\dot{x} := \frac{dx}{dt}$, a more precise notation of a solution of (1.1) (on I with respect to D) is given by $\varphi(\cdot\,; \tau, \xi)$:

$$\dot{\varphi}(t; \tau, \xi) = f\big(t, \varphi(t; \tau, \xi)\big) \quad \text{for all } t \in I \text{ with } \varphi(\tau; \tau, \xi) = \xi. \tag{1.2}$$

In case (τ, ξ) determines the solution uniquely, we will discuss $\varphi(t; \tau, \xi)$ as a function of all arguments (cf. Theorem 1.18). The variable t is often interpreted as *time*, and the variable x as *state*, so that τ and ξ refer to the *initial time* and to the *initial state*, respectively. We call D a *region* in $\mathbb{R} \times \mathbb{R}^n$. Typically, D is taken in the form $D = J \times G$ with an open interval J and a nonempty, open, and connected set $G \subset \mathbb{R}^n$.

In case f in (1.1) is independent of t, the initial value problem is called *autonomous* or *time-invariant*. Of course, the right-hand side f of the differential equation provides the slope of any solution $x = \varphi(\cdot)$. The first Taylor polynomial at τ is given by $\xi + f(\tau, \xi)(t - \tau)$.

Basic Questions

(1) When does a solution $\varphi(\cdot; \tau, \xi)$ of the IVP (1.1) exist? When is it unique? What is the maximal interval $[\tau, t^+)$ of existence in forward time? What causes a finite t^+? When does one have $t^+ = \infty$? How does a solution "behave" for $t \to t^+$?

(2) Are there special initial values ξ leading to simple solutions like constant or periodic solutions? Given a particular solution, for example, a steady-state solution ξ^*, how do solutions "behave" that start near ξ^* at time τ?

(3) Can the asymptotic behavior of a solution $\varphi(\cdot)$ of (1.1) on $[\tau, \infty)$ be determined by some reduced system?

For example, by a scalar test function $V = V(x)$, for instance, $V(x) = x^{\mathrm{T}}x$, so that properties of $v(t) := V(\varphi(t))$ and $\dot{v}(t) = V_x(\varphi(t))f(t, \varphi(t))$ allow one to draw conclusions on the asymptotic behavior of $\varphi(\cdot)$ (comparison theorems, Lyapunov functions). Or, for example, by a simpler reduced initial value problem $\dot{y} = g(t, y)$, $y(\tau) = \eta$, where the asymptotic behavior of y-solutions determines the asymptotic behavior of x-solutions? In more precise terms:

- Do there exist transformations $S(t, \cdot)$ from the y-domain into the x-domain and $R(t, \cdot)$ from the x-domain into the y-domain such that the difference of the solutions $x(\cdot) = \varphi(\cdot; \tau, \xi)$ and $y(\cdot) = \psi(\cdot; \tau, \eta)$ with $\eta := R(\tau, \xi)$ satisfies

$$\lim_{t \to \infty} \left| \varphi(t; \tau, \xi) - S\big(t, \psi\big(t; \tau, R(\tau, \xi)\big)\big) \right| = 0, \tag{1.3}$$

so that $\eta = R(\tau, \xi)$ is the initial value in the y-space that synchronizes the two solutions $x(\cdot)$ and $y(\cdot)$ asymptotically?

(4) Under what circumstances does a "good" approximation $\tilde{f}(t, x)$ of $f(t, x)$ imply that the corresponding solution $\tilde{\varphi}(t; \tau, \xi)$ is a "good" approximation of the solution $\varphi(t; \tau, \xi)$?

(5) When can solutions of (1.1) be computed analytically? What are sufficient conditions for having robustness in numerical solvers? When is it a priori known that a given IVP is a "delicate" one for numerical solvers?

All these questions can be stated for the past, that is, for backward time on $(t^-, \tau]$ or $(-\infty, \tau]$. This can be done by reversing the time via the substitution $s := -t$ and

$\psi(s) := \varphi(t; \tau, \xi)$. For a (1.1)-solution $\varphi(\cdot\,; \tau, \xi)$, the chain rule leads to

$$\frac{d\psi(s)}{ds} = \frac{d\varphi(t; \tau, \xi)}{dt}(-1) = -f\big(t, \varphi(t; \tau, \xi)\big) = -f\big(-s, \psi(s)\big)$$

and $\psi(-\tau) = \xi$, so that $\psi(\cdot)$ is the solution of the IVP

$$\frac{dy}{ds} = f(-s, y), \quad y\big(\tau^*\big) = \xi, \tag{1.4}$$

with $\tau^* := -\tau$, now in "forward time" s.

We illustrate some phenomena and methods for initial value problems of the form (1.1) in low space dimension n. The examples are chosen such that solutions can be computed explicitly. In general, necessary conditions are exploited to derive candidate solutions. Such candidate solutions have to be verified in the end.

Remark 1.1 (Separation of variables for $\dot{x} = a(t)b(x)$) We consider scalar initial value problems with continuous $f : D \to \mathbb{R}$ for $D = \mathbb{R} \times \mathbb{R}$. If $f(t, x)$ in (1.1) is independent of x and given by a continuous function $t \mapsto a(t)$, then the function $\varphi(t; \tau, \xi) = \xi + \int_\tau^t a(s)ds$ is a unique solution of the initial value problem (1.1).

Now, let the right-hand side $f = f(t, x)$ in (1.1) be the product of a continuous function $t \mapsto a(t)$ and a continuous function $x \mapsto b(x)$, and let $\varphi(\cdot)$ be a solution of

$$\dot{x} = f(t, x) = a(t)b(x), \quad x(\tau) = \xi, \tag{1.5a}$$

on an open interval I containing τ. Then we have

$$\frac{\dot{x}(t)}{b(\varphi(t))} = a(t) \tag{1.5b}$$

as long as the division by $b(\varphi(t))$ is allowed. For $b(\xi) \neq 0$, the function $b(\varphi(\cdot))$ does not vanish on an open interval $J \subset I$ containing τ. In case of $b(\xi) = 0$, we have the t-independent solution $x^*(t) := \xi$ of (1.5a). Such a t-independent solution is called an *equilibrium*, a *stationary*, or a *steady-state* solution. For initial value problems (1.5a) with unique solutions, the equation $b(\xi) = 0$ entails $\varphi(t) = \xi$ for all $t \in \mathbb{R}$.

For initial values ξ with $b(\xi) \neq 0$, (1.5b) implies

$$\int_\tau^t \frac{\dot{\varphi}(s)}{b(\varphi(s))}\, ds = \int_\xi^{\varphi(t)} \frac{dx}{b(x)}$$

whenever the integration and the subsequent substitution are admissible. With antiderivatives $A(t)$ of $a(\cdot)$ and $B(x)$ of $\frac{1}{b(\cdot)}$ and with

$$M(t, x) := B(x) - A(t) = \int^x \frac{ds}{b(s)} - \int^t a(s)\, ds, \tag{1.5c}$$

we arrive at the implicit representation

$$M(t,x) - M(\tau,\xi) = B(x) - B(\xi) - \big[A(t) - A(\tau)\big] = 0$$

of the solution $x = \varphi(t)$. Because of $\frac{d}{dt}M(t,\varphi(t)) = 0$, the expression $M(t,x)$ is equal to the constant $M(\tau,\varphi(\tau)) = M(\tau,\xi)$ along the solution $x = \varphi(t)$; later on, M will be called a *first integral* or a *conservation law*. Finally, if B is invertible in a neighborhood of ξ with inverse function B^{-1}, we are led to the explicit necessary condition

$$x = \varphi(t) = B^{-1}\big(B(\xi) + A(t) - A(t)\big) \tag{1.5d}$$

wherever the preceding steps have been admissible. In a final step, we have to prove the sufficiency, that is, we have to verify that (1.5d) defines indeed a solution of (1.5a) on a suitable t-interval. The presented method for solving (1.5a) is called *separation of variables*. Since it relies on the computation of antiderivatives and inverse functions, it does not necessarily lead to explicit formulae for the solutions of (1.5a).

1.1.1.1 Variation of Constants

Remark 1.2 (Variation of constants for scalar $\dot{x} = a(t)x + u(t)$) We first consider scalar initial value problems of the form

$$\dot{x} = f(t,x) = a(t)x + u(t), \quad x(\tau) = \xi, \tag{1.6a}$$

with continuous $a : \mathbb{R} \to \mathbb{R}$ and $u : \mathbb{R} \to \mathbb{R}$, so that the right-hand side $f : \mathbb{R} \times R \to \mathbb{R}$ is continuous in (t,x) and affine in x. For $u(\cdot) \equiv 0$, we have the uniquely determined solution

$$x(t) = \Phi(t,\tau)\xi, \quad \Phi(t,\tau) := \exp\left(\int_\tau^t a(s)\,ds\right) \tag{1.6b}$$

on the whole $\mathbb{R}$ (by separation of variables). For an *inhomogeneity* $u(\cdot) \not\equiv 0$, we use the transformation $x \mapsto y = \Phi(\tau,t)x$ of the state variable x, which leads to the "trivial IVP"

$$\dot{y}(t) = \big[\Phi(t,\tau)\big]^{-1}u(t) = \Phi(\tau,t)u(t), \quad y(\tau) = \xi,$$

with the solution

$$y(t) = \xi + \int_\tau^t \Phi(\tau,s)u(s)\,ds.$$

Hence, we arrive at the explicit representation

$$\varphi(t;\tau,\xi) = \Phi(t,\tau)\xi + \int_\tau^t \Phi(t,s)u(s)\,ds, \quad t \in \mathbb{R}, \tag{1.7}$$

of the uniquely determined solution of (1.6a). Here, the claimed uniqueness is easily shown (see also Remark 1.12(c)). For a constant $a(t) \equiv \alpha$, we have $\Phi(t,\tau) = e^{\alpha(t-\tau)}$.

This method of solving affine initial value problems is called *variation of constants* because of $x(t) = \Phi(t,\tau)\xi$ in (1.6b) is replaced by $x(t) = \Phi(t,\tau)y(t)$ with a time-varying y.

By a recursive application of Remark 1.2 we deduce the solution of n-dimensional affine systems

$$\dot{x} = f(t,x) = A(t)x + u(t), \quad x(\tau) = \xi \in \mathbb{R}^n, \tag{1.8}$$

with a continuous upper triangular $(n \times n)$-matrix $A(\cdot)$ and a continuous n-vector $u(\cdot)$. With the solution $x_n(t)$ of the last equation, we solve for $x_{n-1}(t)$, and so on. The solution $x(t)$ of (1.8) is then still given by an expression as in (1.7), where $\Phi(t,\tau)$ now stands for a certain $(n \times n)$-matrix that is continuously differentiable in t.

In case of an n-dimensional system

$$\dot{x} = Ax + b(t), \quad x(\tau) = \xi, \tag{1.9a}$$

with a constant $(n \times n)$-matrix A and a continuous n-vector $b(\cdot)$, we first compute the upper triangular Schur normal form $R = Q^* A Q \in \mathbb{C}^{n\times n}$ with unitary $Q \in \mathbb{C}^{n\times n}$, for example, (1.15) for $n = 2$. The subsequent coordinate transformation $x(t) = Qy(t)$ along solutions of (1.9a) leads to the affine differential equation

$$\dot{y}(t) = Ry(t) + u(t), \quad y(\tau) = \eta := Q^*\xi,\ u(t) := Q^* b(t) \tag{1.9b}$$

for the vector-valued function y ($y(t) \in \mathbb{C}^n$, $t \in \mathbb{R}$). The complex-valued solution $y(t)$ of (1.9b), still of the form (1.7), then defines the real-valued solution $x(t)$ of (1.9a) via $x(t) = Qy(t)$. With the matrix exponential

$$\exp(Rt) := \sum_{j=0}^{\infty} \frac{1}{j!} R^j t^j \ \in \mathbb{R}^{n\times n}, \quad t \in \mathbb{R}, \tag{1.9c}$$

satisfying $Q\exp(Rt)Q^* = \exp(QRQ^*t) = \exp(At)$, we have

$$x(t) = Qy(t) = \exp\big(A(t-\tau)\big)\xi + \int_\tau^t \exp\big(A(t-s)\big)b(s)\,ds. \tag{1.9d}$$

We observe that the transformation $x(t) = Qy(t)$ has led to a cascade of one-dimensional affine differential equations. In the special case of a diagonal matrix R, the transformation offers a reduction from an n-dimensional linear system to n one-dimensional linear systems that are completely decoupled. We summarize these results in the following proposition.

Proposition 1.3 (Fundamental matrix/Variation of constants)

(a) *The n-dimensional linear initial value problem*

$$\dot{x} = Ax, \quad x(\tau) = \xi, \tag{1.10}$$

with $A \in \mathbb{R}^{n\times n}$ possesses a unique solution $x(t) = \varphi(t;\tau,\xi) = \Phi(t-\tau)\xi$, which is linear in ξ. The so-called "fundamental matrix"

$$\Phi(t) \equiv \exp(At) := \sum_{j=0}^{\infty} \frac{1}{j!} A^j t^j \ \in \mathbb{R}^{n\times n}, \quad t \in \mathbb{R}, \tag{1.11a}$$

satisfies

$$\dot{\Phi}(t) = A\Phi(t), \quad \Phi(0) = I_{n\times n}, \quad \text{and} \quad \det\big(\Phi(t)\big) = e^{\operatorname{trace}(A)t} \neq 0. \tag{1.11b}$$

(b) *If all eigenvalues λ_j of A satisfy the estimate*

$$\operatorname{Re}(\lambda_j) < \rho \quad \text{for some } \rho \in \mathbb{R}, \tag{1.12a}$$

then there exists a constant $M \geq 1$ such that

$$\big|\varphi(t;\xi)\big| \leq M|\xi|e^{\rho t} \quad \text{for } t \geq 0. \tag{1.12b}$$

In case A is diagonalizable (over $\mathbb{C}$), the estimate $\operatorname{Re}(\lambda_j) \leq \rho$ is sufficient for (1.12b).

(c) *The affine initial value problem*

$$\dot{x} = Ax + b(t), \quad x(\tau) = \xi, \tag{1.13a}$$

with continuous inhomogeneity $b : \mathbb{R} \to \mathbb{R}^n$ has a unique solution, given by the variation-of-constants formula

$$x(t) = \varphi(t;\tau,\xi) = \exp\big(A(t-\tau)\big)\xi + \int_0^t \exp\big(A(t-s)\big)b(s)\,ds \tag{1.13b}$$

as the sum of a particular solution of the inhomogeneous system (1.13a) and the general solution of the associated homogeneous system (1.10).

The formula for $\det(\Phi(t))$ in (1.11b) proves $\Phi(t)$ to be regular for all $t \in \mathbb{R}$ and describes the volume transport. At the initial time $t = 0$, the expression $\det(\Phi(0))$ gives the volume $\det(Q) = 1$ of the unit cube $Q = [0,1]^n$, at time $t > 0$ it gives the volume of the set $\varphi(t;0,Q) := \{\Phi(t)\xi : \xi \in Q\}$, that is, the volume of the evolution of Q under the solution mapping $\varphi(t;0,\cdot) : Q \to \mathbb{R}^n$. See Liouville's formula in Sect. 1.1.2.3.

Example 1.4 (Time-varying matrices and growth rates) Part (b) of the above proposition does not apply to general time-varying matrices $A(t)$ as the following example shows:

The eigenvalues $\lambda_j(t)$ of the matrix $A(t) = \Omega(t)A_0\Omega^{-1}(t)$, defined via

$$A_0 = \begin{pmatrix} -1 & -4 \\ 0 & -2 \end{pmatrix}, \qquad \Omega(t) = e^{Jt} = \begin{pmatrix} \cos\omega t & -\sin\omega t \\ \sin\omega t & \cos\omega t \end{pmatrix} \quad \text{for } J = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix},$$

are given by $\lambda_1(t) = -1$ and $\lambda_2(t) = -2$ ($\omega \neq 0$). Nevertheless, there exist ωs and ξs such that the IVP

$$\dot{x} = A(t)x, \quad x(0) = \xi, \tag{1.14}$$

allows unbounded solutions on $[0, \infty)$. This can be easily seen with the help of the transformation $x = \Omega(t)y$ along solutions $x(t)$ of (1.14) since it leads to $\dot{y} = [A_0 - J]y$.

Example 1.5 (Resonance) Given a two-dimensional linear system $\dot{x} = Ax$ with real (2×2)-matrix A and initial condition $x(0) = \xi$, we first establish its Schur normal form: We choose a unitary transformation

$$x \in \mathbb{R}^2 \mapsto y := S^*x \in \mathbb{C}^2 \quad \text{with } S = (u_1, u_2) \in \mathbb{C}^{2\times 2},\ S^*S = I = SS^*,$$

leading to the equivalent initial value problem

$$\dot{y} = S^*ASy = \begin{pmatrix} \lambda_1 & \mu \\ 0 & \lambda_2 \end{pmatrix} y =: Ry, \quad y(0) = \eta := S^*\xi \tag{1.15}$$

with $\lambda_j = u_j^*Au_j$, $j = 1, 2$, and $\mu = u_1^*Au_2$. This system is in cascade form, so variation of constants leads to

$$y = \Psi(t)\eta = \begin{pmatrix} e^{\lambda_1 t} & \mu m(t) \\ 0 & e^{\lambda_2 t} \end{pmatrix} \eta, \quad m(t) = \begin{cases} e^{\lambda_1 t}t, & \lambda_1 = \lambda_2, \\ [e^{\lambda_2 t} - e^{\lambda_1 t}]/[\lambda_2 - \lambda_1], & \lambda_1 \neq \lambda_2. \end{cases}$$

Hence, we have $\Psi(t) = \sum_{j=0}^{\infty} \frac{1}{j!} R^j t^j = \exp(Rt)$ and

$$x = \varphi(t; 0, \xi) = S\Psi(t)S^*\xi = \sum_{j=0}^{\infty} \frac{1}{j!} \big[SRS^*\big]^j t^j \xi = \exp(At)\xi =: \Phi(t)\xi \tag{1.16}$$

for the solution of the above IVP in $\mathbb{R}^2$. The exceptional case where the eigenvalues satisfy $\lambda_1 = \lambda_2 =: \lambda$ and where $\Psi(t)$ is given by $e^{\lambda t}\left(\begin{smallmatrix} 1 & t \\ 0 & 1 \end{smallmatrix}\right)$ is called a case of resonance. Here, $\chi(t) := e^{-\lambda t}\|\varphi(t, \xi)\|$ is **not** bounded on $[0, \infty)$.

Remark 1.6 (Saddle, node, focus, center) Given a two-dimensional linear system $\dot{x} = Ax$ with real (2×2)-matrix A, we choose a real similarity transformation $x \in \mathbb{R}^2 \mapsto y := T^{-1}x \in \mathbb{R}^2$ to arrive at a real system

$$\dot{y} = Ry \tag{1.17}$$

with R being equal to one of the following matrices R_j:

$$R_1 = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \qquad R_2 = \begin{pmatrix} \lambda & \mu \\ 0 & \lambda \end{pmatrix}, \quad \text{or} \quad R_3 = \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} \tag{1.18}$$

for $\mu \neq 0$ and $\beta \neq 0$. The solutions of $\dot{y} = Ry$ as functions of time can easily be determined (see Example 1.5).

(i) In case of $R = R_1$ and negative λ_1, λ_2, the origin is called an (exponentially) *stable node* of (1.17) and hence of $\dot{x} = Ax$. For $\lambda_2 < \lambda_1 < 0$, the axis $Y_1 := \{(y_1, 0) \in \mathbb{R}^2\}$ is *invariant* in the sense that, for an initial value $\eta \in Y_1$, the corresponding solution remains in Y_1 for all t. The axis Y_1 represents the *slow stable eigenspace* corresponding to the exponential decay $e^{\lambda_1 t}$, and the invariant axis $Y_2 := \{(0, y_2) \in \mathbb{R}^2\}$ represents the *fast stable or strongly stable eigenspace* corresponding to the (faster) exponential decay $e^{\lambda_2 t}$. All initial values outside of Y_2 lead to solutions that decay exponentially toward the origin along the slow stable eigenspace with the rate $e^{\lambda_1 t}$.

In case of $R = R_1$ and $\lambda_1 > 0 > \lambda_2$, the two invariant axes Y_1 and Y_2 represent the *unstable and stable eigenspaces* with associated exponential decay rate $e^{\lambda_1 t}$ as $t \to -\infty$ and $e^{\lambda_2 t}$ as $t \to +\infty$, respectively. The origin is then called a *saddle point* of (1.17) and hence of $\dot{x} = Ax$.

By separation of variables (for $\lambda_1 \neq 0 \neq \lambda_2$), we obtain the "invariant curves" in the y-space

$$y_2 = \Gamma_1(y_1) = \eta_2 \left(\frac{y_1}{\eta_1}\right)^{\lambda_2/\lambda_1} \quad \text{or} \quad y_1 = \Gamma_2(y_2) = \eta_1 \left(\frac{y_2}{\eta_2}\right)^{\lambda_1/\lambda_2} \tag{1.19}$$

whenever the right-hand sides are well defined. For example, any (1.17)-solution $y(t) = \varphi(t; 0, \eta)$ with $\eta_2 = \Gamma_1(\eta_1)$ satisfies $y_2(t) = \Gamma_1(y_1(t))$ on its interval of existence. Of course, the shape and the smoothness of the function $y_2 = \Gamma_1(y_1)$ depends heavily on the quotient λ_2/λ_1. For example, in the case of $\lambda_2 < \lambda_1 < 0$, Γ_1 is in class C^m if and only if $\lambda_2 \leq m\lambda_1$.

(ii) In case of $R = R_2$ and negative λ, the origin is still called an (exponentially) *stable node* of (1.17) and hence of $\dot{x} = Ax$. Here, there is just one invariant linear subspace, namely Y_1. In case of $R = R_3$, the origin is called an (exponentially) *stable focus* for negative α and a *center* for $\alpha = 0$.

(iii) The origin $y = 0$ of (1.17) or, equivalently, the origin $x = 0$ of $\dot{x} = Ax$ is called *hyperbolic* if each eigenvalue has a nonzero real part. Otherwise it is called *nonhyperbolic* or *critical*.

In Examples 1.27, 2.5, and 2.10 and in Sect. 1.2.5, we present alternative ways to discuss such linear systems. These alternatives prepare the stage for the discussion of nonlinear systems.

1.1.1.2 Uniqueness and Comparison Theorems

We address questions on the maximal interval of existence and on the uniqueness of solutions.

Exercise 1.7 (Maximal interval of existence for $\dot{x} = ax^\gamma$) Consider initial value problems of the form $\dot{x} = ax^\gamma$, $x(\tau) = \xi$, for constant $a \neq 0$ and various positive γ and show:

(a) The IVP $\dot{x} = ax^2$, $x(\tau) = \xi \geq 0$, on $D = \mathbb{R} \times \mathbb{R}$ with positive a possesses for each ξ a uniquely determined solution on an interval $(-\infty, t^+)$. The maximal $t^+ = t^+(\xi)$ is finite, and the solution becomes unbounded as $t \to t^+$.
(b) The IVP $\dot{x} = -\frac{1}{2x}$, $x(1) = \xi > 0$, on $D = \mathbb{R} \times (0, \infty)$ possesses for each $\xi > 0$ a uniquely determined solution on an interval $(-\infty, t^+)$. The maximal $t^+ = t^+(\xi)$ is finite, and the solution approaches the boundary of D.
(c) The IVP $\dot{x} = ax^{1/3}$, $x(\tau) = \xi \geq 0$, on $D = \mathbb{R} \times \mathbb{R}$ with negative a provides an example where solutions of initial value problems are not uniquely determined. Compare Example 1.8.

Example 1.8 (Fluid level in a tank (Torricelli's law)) We consider the autonomous scalar IVP (1.1) on $\mathbb{R} \times \mathbb{R}$ with $f(x) = 0$ for $x < 0$ and $f(x) = -\sqrt{x}$ for $x \geq 0$. We take the initial value $x(0) = \xi$ to be nonnegative. One might interpret the state x as the fluid level in a tank. Then, the chosen right-hand side f reflects Torricelli's law.

We always have the trivial solution $\varphi_0(t) \equiv 0$ in case of $\xi = 0$. If $\varphi(t)$ is a solution with a positive initial value ξ, then we arrive, by separation of variables, at

$$\varphi(t) = \left(\sqrt{\xi} - \frac{t}{2}\right)^2 \quad \text{for } 0 \leq t < 2\sqrt{\xi}$$

satisfying $\varphi(t) \to 0$ as $t \to 2\sqrt{\xi}$. It is easily verified that the function

$$\varphi^*(t) = \begin{cases} \varphi(t) & \text{on } [0, 2\sqrt{\xi}), \\ 0 & \text{on } [2\sqrt{\xi}, \infty) \end{cases}$$

is a continuously differentiable solution of (1.1). The tank runs empty in *finite* time $T = 2\sqrt{\xi}$ and remains empty afterwards. In backward time, we do not have the uniqueness: If the tank is empty at some time $T_* > 0$, that is, $x(T_*) = 0$, we cannot derive the initial fluid level ξ. We note that, given two solutions $x_1(t)$ and $x_2(t)$ of the present IVP, the function $\delta(t) := |x_2(t) - x_1(t)|^2 \geq 0$ satisfies $\dot{\delta}(t) \leq 0$, implying the uniqueness in forward time.

Example 1.8 shows that the continuity of $f(t, x)$ is not sufficient for the unique solvability of the initial value problem (1.1). We introduce a slightly stronger hypothesis by asking f to satisfy local Lipschitz conditions with respect to x, that is,

by asking f to be continuous in (t,x) and to be Lipschitz-continuous in x. We formulate this more restrictive hypothesis as

Hypothesis 1.9 (H_{Lip}) *The function $f : D \to \mathbb{R}^n$, defined on a region $D \subset \mathbb{R} \times \mathbb{R}^n$, is Lipschitz-continuous, that is, for any $(\tau,\xi) \in D$, there exist a box*

$$Q_{\alpha,\beta} = \big\{(t,x) : |t-\tau| \le \alpha, |x-\xi| \le \beta\big\} \subset D$$

and a (Lipschitz) constant $L \ge 0$ such that

$$\big|f(t,x_2) - f(t,x_1)\big| \le L|x_2 - x_1| \quad \text{on } Q_{\alpha,\beta}. \tag{1.20}$$

Remark 1.10 (Lipschitz continuity) The Lipschitz constant L provides a (locally uniform) bound for the difference quotient $|f(t,x_2) - f(t,x_1)|/|x_2 - x_1|$, $x_1 \ne x_2$, of f. In case f is continuous in (t,x) and continuously differentiable with respect to x in a neighborhood U of ξ, it satisfies such a local Lipschitz condition because of

$$\big|f(t,x_2) - f(t,x_1)\big| \le \int_0^1 \big|f_x\big(t, x_1 + s(x_2 - x_1)\big)\big|\, ds\, |x_2 - x_1| \le L|x_2 - x_1|, \tag{1.21}$$

where L stands for an upper bound of $|f_x(t, x_1 + s(x_2 - x_1))|$ for $s \in [0,1]$ and $(t,x_1), (t,x_2) \in Q_{\alpha,\beta} \subset U$.

Theorem 1.11 (Scalar comparison theorem/Differential inequalities) *We suppose that f is a scalar continuous function on a neighborhood of*

$$Q = \big\{(t,x) \in \mathbb{R}^2 : \tau \le t \le \tau + \alpha, |x - \xi| \le \beta\big\}$$

with the Lipschitz property

$$\big|f(t,x_2) - f(t,x_1)\big| \le L|x_2 - x_1| \quad \text{on } Q. \tag{1.22a}$$

If continuously differentiable functions $\varphi(t)$ and $\psi(t)$ satisfy on $[\tau, \tau+\alpha]$

$$\begin{aligned} &\big(t,\varphi(t)\big) \in Q, \qquad \big(t,\psi(t)\big) \in Q, \\ &\dot\varphi(t) \ge f\big(t,\varphi(t)\big), \qquad \dot\psi(t) \le f\big(t,\psi(t)\big), \quad \varphi(\tau) \ge \psi(\tau), \end{aligned} \tag{1.22b}$$

then $\varphi(t) \ge \psi(t)$ on $[\tau, \tau+\alpha]$.

Proof The assumption that $\Delta(t) = \varphi(t) - \psi(t)$ satisfies (i) $\Delta(s) = 0$ for $s \in [\tau, \tau + \alpha]$ and (ii) $\Delta(t) < 0$ on an interval of the form $(s, s + \varepsilon)$, $\varepsilon > 0$, leads by (1.22b) to a contradiction: We have $\dot{\Delta}(t) \geq -L|\Delta(t)| = L\Delta(t)$ on $[s, s + \varepsilon]$ with $\Delta(s) = 0$, implying $\frac{d}{dt}[e^{-Lt}\Delta(t)] \geq 0$ and $\Delta(t) \geq 0$ on $(s, s + \varepsilon)$. □

This proof reveals the key feature of the Lipschitz continuity of f: Locally, the derivative $\dot{\Delta}(t) = f(t, \psi(t) + \Delta(t)) - f(t, \psi(t))$ is bounded below by the *linear* expression $L\Delta(t)$.

Remark 1.12 (Comparison theorem and uniqueness)

(A) The special case $\dot{\psi}(t) = f(t, \psi(t))$, $\varphi(\tau) = \psi(\tau)$, in (1.22b) tells us that $\varphi(t)$ is above $\psi(t)$ for $t \geq \tau$. Hence, $\varphi(t)$ is called a *supersolution*. Similarly, the special case $\dot{\varphi}(t) = f(t, \varphi(t))$, $\varphi(\tau) = \psi(\tau)$, in (1.22b) leads to a *subsolution* $\psi(t)$.

(B) In case $\dot{\psi}(t) = f(t, \psi(t))$, $\dot{\varphi}(t) = f(t, \varphi(t))$, and $\varphi(\tau) = \psi(\tau)$, we deduce the uniqueness: $\varphi(t) \equiv \psi(t)$ on $[\tau, \tau + \alpha]$. So we have the following corollary in the scalar case:

- Given an IVP $\dot{x} = f(t, x)$, $x(\tau) = \xi$, on a neighborhood of the set $Q_{\alpha\beta}$ with continuous f satisfying (1.21), any two solutions $\varphi_1(t; \tau, \xi)$ and $\varphi_2(t; \tau, \xi)$ with $(t, \varphi_1(t))$ and $(t, \varphi_1(t))$ in Q on $[\tau - \alpha, \tau + \alpha]$ are identical on $[\tau - \alpha, \tau + \alpha]$.

(C) We now derive the *uniqueness* result for the n-dimensional system (1.1) in the setup of (H_{Lip}). Let $\Delta(t) = \varphi_2(t; \tau, \xi) - \varphi_1(t; \tau, \xi)$ be the difference of two solutions on $[\tau - \alpha, \tau + \alpha]$ with respect to $Q_{\alpha,\beta}$. We have

$$\dot{\Delta}(t) = f\big(t, \varphi_2(t; \tau, \xi)\big) - f\big(t, \varphi_1(t; \tau, \xi)\big), \quad \Delta(\tau) = 0.$$

Together with the Lipschitz condition (1.20), an integration with respect to t, $t \geq \tau$, leads to a linear differential inequality for $V(t) := \int_\tau^t |\Delta(s)|\, ds \geq 0$, namely

$$\dot{V}(t) = \big|\Delta(t)\big| \leq L \int_\tau^t \big|\Delta(s)\big|\, ds =: LV(t), \quad V(\tau) = 0. \tag{1.23a}$$

This implies $\frac{d}{dt}[e^{-Lt}V(t)] \leq 0$ with $e^{-L\tau}V(\tau) = 0$. To the right of τ, we deduce $e^{-Lt}V(t) \leq 0$, and hence $V(t) \equiv 0$. In an analogous manner we argue for $t \leq \tau$.

In the preceding argument, the implicit estimate (1.23a) for $|\Delta(t)|$ has led to an explicit estimate for $V(t)$. The following result, often called the *Gronwall lemma*, deals with a more general case. We would like to point out that, besides the variation-of-constants formula, the Gronwall lemma is one of the crucial tools in the theory of differential equations.

Lemma 1.13 (Gronwall lemma) *Let u, μ, ρ be nonnegative continuous functions on the interval $I = [\tau, T]$ with values in $\mathbb{R}$. Then the implicit estimate*

$$u(t) \le \mu(t) + v(t), \quad v(t) := \int_\tau^t \rho(s)u(s)\,ds \text{ on } I \tag{1.24}$$

entails the explicit estimate

$$u(t) \le \mu(t) + \int_\tau^t \mu(s)\rho(s)\exp\left[\int_s^t \rho(\sigma)\,d\sigma\right] ds \quad \text{on } I. \tag{1.25}$$

In case $\mu(t)$ satisfies $\mu(\tau) \le \mu(s) \le \mu(t)$ for all $\tau \le s \le t \le T$, (1.25) implies

$$u(t) \le \mu(t)\exp\left[\int_\tau^t \rho(\sigma)\,d\sigma\right] \quad \text{on } I. \tag{1.26}$$

Proof Estimate (1.24) yields $\dot v(t) = \rho u(t) \le \rho(t)\mu(t) + \rho v(t)$. A multiplication with the positive

$$m(t,\tau) = \exp\left[-\int_\tau^t \rho(\sigma)\,d\sigma\right]$$

leads to $(mv)^{\cdot} \le m\rho\mu$, then, by integrating over $[\tau, t]$, to

$$u(t) \le \mu(t) + \frac{1}{m(t,\tau)}\int_\tau^t m(s,\tau)\rho(s)\mu(s)\,ds = \mu(t) + \int_\tau^t \mu(s)\rho(s)m(s,t)\,ds,$$

and hence to (1.25). In case of a monotone μ, we use the estimate $\mu(s) \le \mu(t)$ in the integrand of (1.25) to arrive at (1.26). □

1.1.1.3 Scalar Bifurcations

Example 1.14 introduces an argument that can be applied to any autonomous scalar initial value problem $\dot x = f(x)$, $x(\tau) = \xi$, with a continuously differentiable right-hand side $f : \mathbb{R} \to \mathbb{R}$ when "uniqueness" and "existence on $\mathbb{R}$" are guaranteed:

- Let x_- and x_+ be zeros of f, and let f be positive on (x_-, x_+). For $\xi \in (x_-, x_+)$, the solution $\varphi(t; \tau, \xi)$ is strictly increasing in t with $\lim_{t\to\pm\infty}\varphi(t;\tau,\xi) = x_\pm$.

Example 1.14 (Logistic growth model—Outlook on Lyapunov functions) We consider the scalar model of logistic growth

$$\dot x = f(x) := ax\left(1 - \frac{x}{K}\right), \quad x(0) = \xi \ge 0, \tag{1.27a}$$

with a quadratic polynomial $f : \mathbb{R} \to \mathbb{R}$ and positive parameters a and K. Stationary solutions are given by $\varphi_0(t) = \varphi(t; 0, 0) \equiv 0$ and $\varphi_K(t) = \varphi(t; 0, K) \equiv K$.

In the discussion to follow, we use the fact that IVPs of the form (1.27a) have unique solutions. Initial values $\xi \in (0, K)$ will lead to strictly increasing solutions in $(0, K)$, whereas initial values $\xi > K$ will entail strictly decreasing solutions in (K, ∞). In case such solutions exist for all $t \geq 0$, they will be convergent as $t \to \infty$. By an indirect argument, the limiting value of such solutions $\varphi(t; 0, \xi)$ with $\xi > 0$ is necessarily given by K: The stationary solution K acts as a supersolution for solutions $\varphi(t; \tau, \xi)$ with $\xi \in (0, K)$ and as a subsolution for $\varphi(t; \tau, \xi)$ with $\xi > K$.

On the other hand, solutions $\varphi(t; 0, \xi)$ with $\xi > 0$ and $\xi \neq K$ can be easily found by separation of variables. With the help of partial fractions we arrive, formally, at

$$e^{at} = \big|x(K - \xi)\big| / \big|\xi(K - x)\big|.$$

Because of the above a priori bounds, we can drop the absolute values to obtain

$$x(t) = \frac{K\xi}{Ke^{-at} + \xi(1 - e^{-at})}, \quad t \geq 0. \tag{1.27b}$$

It is easily verified that $x(t)$ is indeed the solution $\varphi(t; 0, \xi)$ of the IVP (1.27a) on the time interval $[0, \infty)$ with the asymptotic value $K = \lim_{t \to \infty} \varphi(t; 0, \xi)$.

It is worth noting that the two assumptions on "uniqueness" and on "existence on $\mathbb{R}^+$" have already led to the asymptotic value K (without the explicit formula (1.27b)).

For an alternative argument, we may consider the scalar nonnegative function

$$V(x) = -\int_K^x \left(1 - \frac{s}{K}\right) ds = \frac{1}{2K}(x - K)^2, \quad x \in \mathbb{R},$$

vanishing only at $x = K$. Along a solution $x(t) = \varphi(t; 0, \xi)$ of (1.27a) with $\xi > 0$, existing on $[0, \infty)$, we have

$$\frac{d}{dt} V\big(x(t)\big) = V_x\big(x(t)\big) f\big(x(t)\big) = -ax\left(1 - \frac{x(t)}{K}\right)^2 \leq 0.$$

Therefore, $V(x(t))$ is convergent as $t \to \infty$, necessarily toward 0. This implies the convergence of $x(t)$ toward K. Test functions of this type will later be called Lyapunov functions.

Remark 1.15 (Bifurcation diagrams) In analogy to the logistic growth model (1.27a), we may discuss the following parameter-dependent initial value problems:

$$\dot{x} = f_1(x, \alpha) = \alpha - x^2, \quad x(0) = \xi, \tag{1.28a}$$

$$\dot{x} = f_2(x, \alpha) = x(\alpha - x), \quad x(0) = \xi, \tag{1.28b}$$

$$\dot{x} = f_3(x, \alpha) = x\big(\alpha - x^2\big), \quad x(0) = \xi, \tag{1.28c}$$

for $(x, \alpha) \in \mathbb{R}^2$ and all $t \in \mathbb{R}$. We note that α can be considered as the state variable by adjoining the trivial equation $\dot{\alpha} = 0$. Each of the three IVPs in (1.28a)–(1.28c)

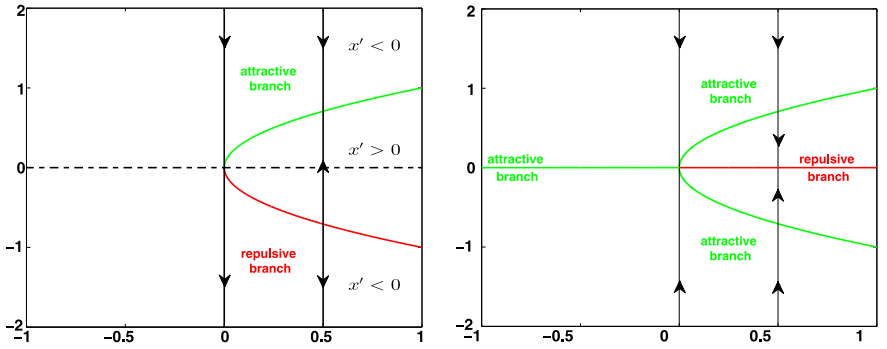

Fig. 1 Bifurcation diagrams in the (α, x)-plane: *To the left*, saddle-node bifurcation for (1.28a) showing an attractive branch of equilibria in the first and a repulsive branch in the fourth quadrant. *To the right*: Pitchfork bifurcation for (1.28c) showing two attractive branches for $\alpha > 0$ separated by the branch $(\alpha, 0)$ of trivial equilibria $x = 0$. Theses are attractive for $\alpha \leq 0$ and repulsive for $\alpha > 0$

reveals for $\alpha < 0$, $\alpha = 0$, and $\alpha > 0$ a drastically different behavior for its solutions and their asymptotic limiting sets. A sketch in the (α, x)-plane of these limiting sets as $t \to \pm\infty$, that is, of the zero-set of $f(x, \alpha)$, is called a *bifurcation diagram* offering a *saddle-node bifurcation* in (1.28a), a *transcritical bifurcation* in (1.28b), and a *pitchfork bifurcation* in (1.28c) (see Fig. 1).

In each of the three cases, the trivial steady state $x \equiv 0$ is *critical* for the parameter value $\alpha_0 = 0$ in the sense that the derivative $(f_j)_x$ vanishes at $(x, \alpha) = (0, 0)$. Hence, the sufficient conditions of the implicit function theorem for the unique solvability of $f(x, \alpha) = 0$, in terms of $x = x(\alpha)$ near $(x, \alpha) = (0, 0)$, are not satisfied. In general, Descartes's rule and Newton's diagram are helpful tools to discuss the zeros of polynomial right-hand sides $f(x, \alpha)$.

A trivial extension of (1.28c) into a two-dimensional state space is provided by

$$\dot{r} = r\big(\alpha - r^2\big), \qquad \dot{\theta} = \omega > 0 \tag{1.29a}$$

in polar coordinates (r, θ) with $x = (r\cos(\theta), r\sin(\theta))^{\mathrm{T}}$, $r \geq 0$, $\theta \in [0, 2\pi)$. The corresponding x-system reads

$$\dot{x} = F(x, \alpha) := \begin{pmatrix} \alpha - r^2 & -\omega \\ \omega & \alpha - r^2 \end{pmatrix} x. \tag{1.29b}$$

If α passes from negative to positive values, the trivial solution $r = 0$ changes from being attractive to being repulsive. For $\alpha > 0$, all nontrivial solutions approach the circle $C(\alpha) := \{(r, \theta) : r = \sqrt{\alpha}\}$ in the x-space, called "limit cycle"; see Fig. 2. One solution generating this limit cycle is given by

$$x^*(t) = \sqrt{\alpha}\big(\cos(\omega t + \theta_*), \sin(\omega t + \theta_*)\big)^{\mathrm{T}}$$

for a fixed $\theta_* \in [0, 2\pi)$. A solution $x(t) = r(t)(\cos(\theta(t)), \sin(\theta(t)))^{\mathrm{T}}$ is asymptotically in phase with $x^*(t)$ if and only if $\theta(t) = \omega t + \theta_0 = \omega t + \theta_*$, that is, $\theta_0 = \theta_*$.