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Nonlinearities and Alternative States of Biogeochemical Cycling in Terrestrial Ecosystems

Compartmental systems as Markov chains: age, transit time, and entropy

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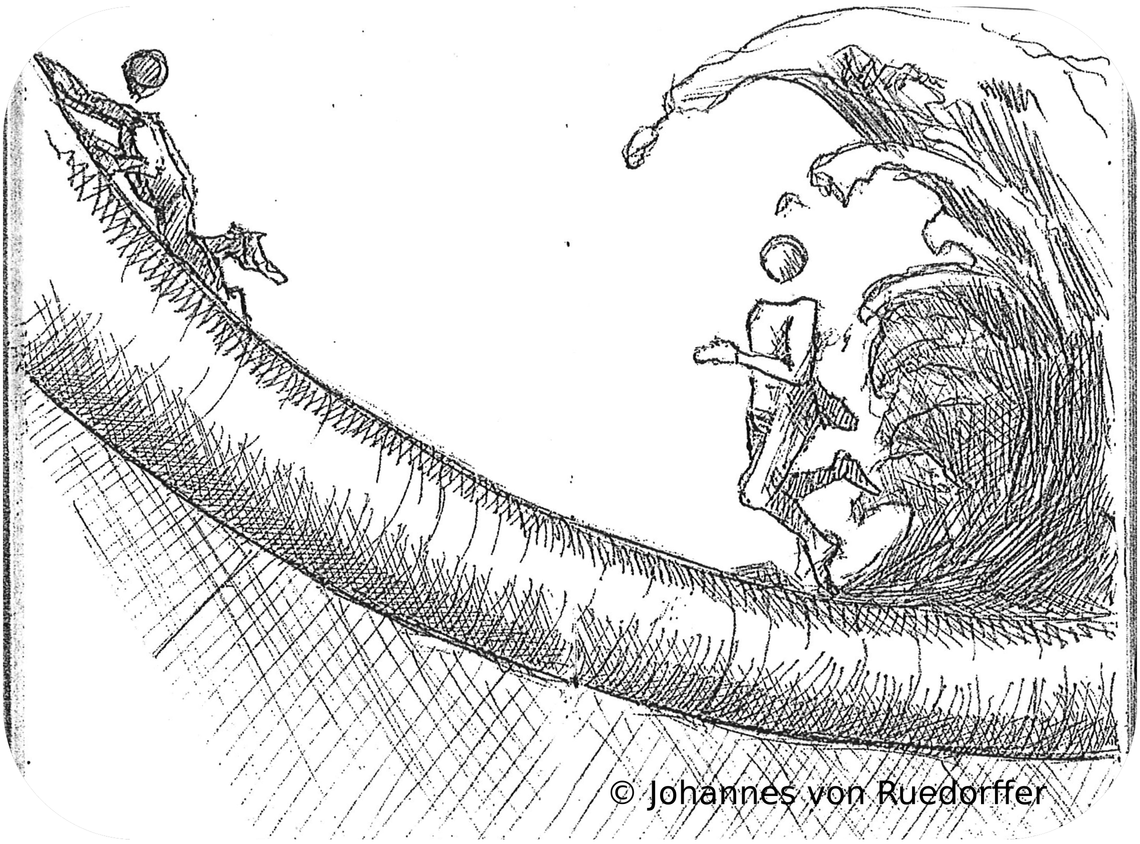
Dein vor Freude und Zuneigung strahlendes Gesicht
ist eine meiner ersten und liebsten Erinnerungen.
Hoffentlich hast Du mich auch noch
irgendwie erkannt.
Zu meinem Geburtstag.

Mach's gut, mein Freund!

Beste Grüße von besten Freunden.



The fossil-fuel transit-time density.

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Acronyms and symbols

Acronyms

Acronym	Description
BTT	backward transit time
FTT	forward transit time
cf.	compare (abbreviation of Latin *confer*)
e.g.	for example (abbreviation of Latin *exempli gratia*)
i.e.	that is (abbreviation of Latin *id est*)
MIC	microbial biomass carbon
ODE	ordinary differential equation
SOC	soil organic carbon

Number systems

Symbol	Description	Page
$\mathbb{C}$	complex numbers	xxvii
$\mathbb{N}$	natural numbers starting from 1	xxvii
$\mathbb{R}$	real numbers	xxvii
$\mathbb{R}_+$	nonnegative real numbers	xxvii
$\mathbb{R}^d_+$	nonnegative orthant of $\mathbb{R}^d$	xxvii

Norms

Symbol	Description	Page
$\lvert y\rvert$	absolute value of a real or complex number y	xxvii
$\lVert\mathbf{v}\rVert$	vector norm of the absolute coordinates sum of a vector $\mathbf{v}$	xxvii
$\lVert\mathrm{M}\rVert$	matrix norm of maximum absolute column sums of a matrix M	xxvii

Units

Symbol	Description
g C	grams of carbon
m	meter
P	peta (10^{15})
yr	year
bits	entropy unit with respect to logarithmic base 2
nats	entropy unit with respect to logarithmic base e

Entropy symbols

Symbol	Description	Page
$\mathbb{H}[Y]$	Shannon- or differential entropy of the random variable Y	66
$\mathbb{H}_0(M)$	path entropy of the initial values of an open compartmental system M	96
$\mathbb{H}[Y_1 \mid Y_2]$	conditional Shannon- or differential entropy of the random variable Y_1 given the random variable Y_2	68
$\mathbb{H}[Y_1, Y_2]$	joint Shannon- or differential entropy of the two random variables Y_1 and Y_2	67
$\mathbb{H}_{\mathcal{P}}(M)$	path entropy of an open compartmental system M	79
$\mathbb{H}_T(X)$	finite-time entropy of the stochastic process X until time T	69
$\mathbb{H}_{T,\tau}(X)$	τ-entropy of the stochastic process X until time T	91
$\wp$	path space of a particle that travels through an open compartmental system	76
$\mathcal{P}_\infty$	infinite particle path $\mathcal{P}_\infty = ((\zeta_n, T_n)_{n\in\mathbb{N}}$	70
θ	entropy rate	68
$\theta_0(M)$	instantaneous entropy rate of the initial values of an open compartmental system M	97
$\theta_{\mathbf{inst}}(M)$	instantaneous entropy rate of an open compartmental system M	96
$\theta_{\mathcal{P}_\infty}(M)$	entropy rate per jump of an open compartmental system M	79
$\theta_Z(M)$	entropy rate per unit time of an open compartmental system M	79

Other symbols

Symbol	Description	Page
$\mathbf{0}$	column vector comprising zeros	2
$\mathbf{1}$	column vector comprising ones	3
$\mathbb{1}$	indicator function	2
$V \sim D$	random variable V distributed according to probability distribution D	18
$\approx$	depending on the context either "up to $o(\tau)$" or "approximately, rounded"	34
$\emptyset$	empty set	17
∞	(plus) infinity	xxviii
$n!$	factorial of $n \in \mathbb{N}$, $n! = n\,(n-1)\cdots 1$, $0! := 1$	18
$f * g$	convolution of two functions f and g: $(f*g)(t) = \int_{-\infty}^{t} f(t)\,g(t-\tau)\,\mathrm{d}\tau$	84
$m_1 \otimes m_2$	product measure of two measures m_1 and m_2	76
D_k	partial derivative with respect to the kth coordinate	2
$\mathrm{diag}\,(\mathbf{v})$	diagonal matrix comprising the components of vector $\mathbf{v}$	23
$\mathrm{Exp}(\lambda)$	exponential distribution with rate parameter $\lambda > 0$ and expected value λ^{-1}	67
$\mathbb{E}\,[Y]$	expected/mean value of the random variable Y	18
$\mathbb{E}[V \mid E]$	conditional expectation of the random variable V given the event E	19

Symbol	**Description**	**Page**
e	Euler's number, base of natural logarithm, $e = \sum_{k=0}^{\infty} 1/k!$	6
e^{M}	matrix exponential, (Appendix A)	6
I	identity matrix	6
$\mathcal{N}$	mean first hitting time of the absorbing state by the embedded jump chain	71
$o(\tau)$	little-o notation: $\lim_{\tau \to 0} o(\tau)/\tau = 0$	91
$\mathbb{P}(E)$	probability of the event E	xxviii
$\mathbb{P}(E_2 \mid E_1)$	conditional probability of event E_2 given event E_1	17
$\mathrm{PH}(\boldsymbol{\beta}, \mathrm{B})$	phase-type distribution with initial distribution $\boldsymbol{\beta}$ and transition rate matrix B	18
Φ	state-transition matrix (B)	43
$\sigma[Y]$	standard deviation of the random variable Y	34
$\mathcal{T}$	transit time / absorption time	17
$\mathbf{v}^\top$, $\mathrm{M}^\top$	transpose of a vector $\mathbf{v}$ or a matrix M	1
t_0	starting time of all considered systems	xxvii
X^*	diagonal matrix of steady-state system contents	23
$\mathbf{x}^*$	steady-state vector of system contents	6

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Zusammenfassung

Wir untersuchen Verbindungen zwischen deterministischen Kompartimentsystemen und stochastischen Markow-Ketten.

Kompartimentsysteme sind spezielle nichtnegative dynamische Systeme, die den Fluss von beispielsweise Masse oder Energie in ein System hinein, durch das System hindurch und aus dem System heraus beschreiben, wobei ein solches System aus mehreren sogenannten Kompartimenten besteht. Wie allgemein üblich nehmen wir dabei an, dass das System gut gemischt ist: Material, welches in ein ein neues Kompartiment gelangt, ist sofort perfekt mit dem bereits vorhanden Material vermischt. Gemeinhin werden Kompartimentsysteme mathematisch durch ein System von gewöhnlichen Differentialgleichungen der Form

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x} = \mathrm{B}\,\mathbf{x} + \mathbf{u}$$

beschrieben. Hierbei ist $\mathbf{x}$ der Vektor des Systeminhaltes, also der Größe von Interesse, die wir im Weiteren Material nennen wollen. Der nichtnegative Eingangsvektor $\mathbf{u}$ beschreibt Menge und Verteilung neu hinzukommenden Materials. Von der quadratischen Matrix B fordern wir drei Eigenschaften: 1) alle Diagonalelemente sind nichtpositiv, 2) alle Nichtdiagonalelemente sind nichtnegativ, und 3) alle Spaltensummen sind nichtpositiv. Unter diesen Bedingungen werden sowohl die Matrix B als auch das System selbst als *kompartimental* bezeichnet und das System ist massenbilanziert. Wir nehmen weiterhin an, dass das System sich im Gleichgewicht befindet. Das bedeutet $\mathbf{x}(t) = \mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$. Bezüglich Kompartimentsystemen im Gleichgewicht sind wir an den folgenden Größen interessiert:

- Das *Systemalter* beschreibt die seit dem Eintritt verstrichene Zeit von sich im System befindlichem Material.
- Das *Kompartimentalter* beschreibt das Systemalter des Materials eines bestimmten Kompartiments.
- Die *Transitzeit* beschreibt die Zeitspanne, die zwischen dem Eintritt von Material in das System und seinem Austritt aus dem System verstreicht.
- Die *Verbleibende Systemlebenszeit* beschreibt, wie lange es dauert, bis Material, welches sich im System befindet, das System verlässt.
- Die *Verbleibende Kompartimentlebenszeit* beschreibt die Verbleibende Systemlebenszeit des Materials eines bestimmten Kompartiments.

Wir betrachten außerdem eine absorbierende zeitstetige Markow-Kette X. Ihre Anfangsverteilung ist durch den normierten Systemeingangsvektor $\mathbf{u}$ gegeben; ihre quadratische Übergangsmatrix wird aus der Kompartimentmatrix B konstruiert, indem wir sie um eine Dimension vergrößern, welche ein Umweltkompartiment darstellt, das alles das System verlassende Material aufsammelt. Jetzt konstruieren wir einen regenerativen Prozess Z, indem wir X unendlich oft an sich selbst aneinander heften. Den in Z eingebetteten Erneuerungsprozess bezeichnen wir mit J. Wir können X als die zufällige Reise eines

einzelnen Partikels durch das System interpretieren, bis es das System verlässt, während Z die unendliche zufällige Reise eines Partikels beschreibt, der unmittelbar nach seinem Systemaustritt wieder in das System eintritt. Der Erneuerungsprozess J beschreibt die Wiedereintrittszeiten des Partikels zurück ins System. Wie sich herausstellt, hat jede der fünf deterministischen Systemgrößen von Interesse ein stochastisches Gegenstück:

- Systemalter $\longleftrightarrow$ Rückwärtsrekurrenzzeit von J,
- Kompartimentalter $\longleftrightarrow$ bedingte Rückwärtsrekurrenzzeit von Z,
- Transitzeit $\longleftrightarrow$ Absorptionszeit von X,
- Verbleibende Systemlebenszeit $\longleftrightarrow$ Vorwärtsrekurrenzzeit von J,
- Verbleibende Kompartimentlebenszeit $\longleftrightarrow$ bedingte Vorwärtsrekurrenzzeit von Z; und zusätzlich
- Gleichgewichtsvektor $\longleftrightarrow$ Vektor der mittleren Aufenthaltszeiten von X, und
- Austrittsvektor $\longleftrightarrow$ Verteilung des letzten Zustandes von X vor Absorption.

Des Weiteren gilt, dass sich die Rollen von Alter und Verbleibender Lebenszeit vertauschen, falls wir das zeitinvertierte System betrachten.

Jetzt lassen wir die Gleichgewichtsannahme fallen, aber gehen davon aus, dass wir eine eindeutige Lösungstrajektorie des Systems gegeben haben. Für diese spezielle Trajektorie berechnen wir explizite Formeln sowohl der Verteilungen von System- und Kompartimentalter als auch der Verteilungen von System- und Kompartimentlebenszeit. Wie sich weiter herausstellt, müssen wir hier zwischen zwei Arten von Transitzeiten unterscheiden. Die *Vorwärtstransitzeit* beschreibt die Zeitspanne, die Material für seine Reise durch das System benötigen wird, zum Zeitpunkt seines Eintritts. Die *Rückwärtstransitzeit* beschreibt die Zeit, die Material für seine Reise durch das System benötigt hat, zum Zeitpunkt seines Austritts. Es wird dann deutlich, dass die beiden nur zeitverschobene Versionen von einander sind. Außerdem leiten wir ein gewöhnliches Differentialgleichungssystem her, um die zeitliche Entwicklung von Momenten der Kompartimentalter des Systems zu berechnen, und wir finden gewöhnliche Differentialgleichungen für die zeitliche Entwicklung von Altersquantilen.

Anschließend versuchen wir, ein Komplexitätsmaß für Kompartimentsysteme auf Basis der Shannon-Informationsentropie des zufälligen Pfades eines einzelnen durch das System reisenden Teilchens zu entwerfen. Wir zeigen verschiedene Interpretationsmöglichkeiten dieser sogenannten *Pfadentropie* auf und analysieren ihre Tauglichkeit, als Komplexitätsmaß zu dienen. Wir setzen sie in Relation zu existierenden Komplexitätsmaßen für dynamische Systeme und zu verschiedenen Entropiekonzepten stochastischer Prozesse. Da sowohl die Systemstabilität als auch seine Komplexität eng mit der mittleren Transitzeit des Systems verbunden sind, lässt sich eine tiefe Verbindung zwischen Stabilität und Komplexität zumindest erahnen.

Abstract

We investigate connections between deterministic compartmental systems and stochastic Markov chains.

Compartmental systems are particular nonnegative dynamical systems that describe the flow of, for instance, mass or energy into, through, and out of a system that consists of different so-called compartments. We make the common well-mixed assumption which states that material that enters a compartment immediately mixes with the already present material. Usually, compartmental systems are mathematically described by a system of ordinary differential equations (ODEs) of the shape

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x} = \mathrm{B}\,\mathbf{x} + \mathbf{u}.$$

Here, $\mathbf{x}$ is the state vector containing the system content of the quantity of interest, which we call material, and $\mathbf{u}$ is a nonnegative vector of newly incoming material. We require the square matrix B to exhibit three properties: 1) all diagonal entries are nonpositive, 2) all off-diagonal entries are nonnegative, and 3) all column sums are nonpositive. Under these circumstances, both the matrix B and the system itself are called *compartmental* and the system is mass balanced. Let us further assume that the system is in equilibrium, i.e., $\mathbf{x}(t) = \mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$. Regarding compartmental systems in equilibrium, we are interested in the following quantities that describe the system dynamics:

- The *system age* describes the time that has passed since material that is in the system had entered it.
- The *compartment age* describes the system age of material in a particular compartment.
- The *transit time* describes the time span between material entering the system and leaving it.
- The *remaining system lifetime* describes how long material that is in the system will still be in the system before leaving it.
- The *remaining compartment lifetime* describes the remaining system lifetime of material in a particular compartment.

We also consider an absorbing continuous-time Markov chain X. Its initial distribution is given by the normalized input vector $\mathbf{u}$ of the system, and its square transition-rate matrix is constructed out of the system's compartmental matrix B by adding one dimension for an environmental compartment that collects all the material that leaves the system. Now, we construct a regenerative process Z by concatenating X indefinitely with itself and denote the embedded renewal process of Z by J. While we can interpret X as the stochastic travel of a single particle through the system until its exit, Z describes the indefinite stochastic travel of a particle that enters the system again immediately after each exit. The renewal process J represents the reentry times of the particle back into the system. As it turns out, each of the five deterministic system quantities of interest has a stochastic counterpart:

- system age $\longleftrightarrow$ backward recurrence time of J,
- compartment age $\longleftrightarrow$ conditional backward recurrence time of Z,
- transit time $\longleftrightarrow$ absorption time of X,
- remaining system lifetime $\longleftrightarrow$ forward recurrence time of J,
- remaining compartment lifetime $\longleftrightarrow$ conditional forward recurrence time of Z; and additionally,
- steady-state vector $\longleftrightarrow$ mean occupation time vector of X, and
- release vector $\longleftrightarrow$ distribution of last state of X before absorption.

Furthermore, we see that the roles of age and remaining lifetime interchange if we consider the time-reversed system.

Now, we drop the equilibrium assumption but we assume to be given a unique solution trajectory of the system. For this particular trajectory, we compute explicit formulas for the distributions of system/compartment age and remaining system/compartment lifetimes. As it also turns out, we have to distinguish between two types of transit time here. The *forward transit time* describes the time span material will need to travel through the system at the moment of entry. The *backward transit time* describes the time material has needed to travel through the system at the moment of exit. It becomes then clear that the two are simply time-shifted versions of one another. Furthermore, we derive an ODE system to compute the evolution of moments of the compartment-age distribution through time and ODEs for the time evolution of age quantiles.

Then, we try to establish a complexity measure for compartmental systems based on the Shannon information entropy of the stochastic path created by a single particle while it travels through the system. We show different interpretations of this so-called *path entropy* and analyze its capability of serving as a complexity measure. We put it in relation to existing complexity measures of dynamical systems and to different entropy concepts of stochastic processes. Since both the system's stability and its complexity are closely related to the system's mean transit time, a deep connection between stability and complexity can at least be conjectured.

Introduction

The aim of this thesis is to interconnect the two mathematical fields *dynamical systems* and *probability theory* by means of compartmental systems theory and Markov chain theory. To great extent, compartmental systems and Markov chains are studied independently of each other, even though these two mathematical objects share a wide range of properties. Their similarity is based on two underlying principles: 1) While compartmental systems preserve mass or energy of some type, Markov chains preserve probability mass. 2) While compartmental systems are usually considered to be well-mixed, Markov chains have the property that the future is independent of the past. These two principles define the structure and properties of both compartmental systems and Markov chains.

1. A historical retrospect

The first theoretical treatise of compartmental system reaches back to Sheppard et al. (1962). Ten years later, Jacquez et al. (1972) published a seminal book in which they not only presented the then state-of-the-art compartmental systems theory, but also pointed in many directions of future research. Anderson (1983) then wrote a complete essay on the topic addressing aspects such as general theory, structure, stability, model identification, controllability, and tracer kinetics. The qualitative theory of compartmental systems in terms of classification and stability properties was later addressed by Jacquez & Simon (1993). A modern text on the topic is the monograph by Haddad et al. (2010).

The theory of Markov chains began in 1906 when Markov doubted the necessity of independence for the Weak Law Of Large Numbers (Seneta, 1996). Kolmogorov (1931) then extended the theory to continuous-time Markov chains and introduced many of the main concepts such as transition functions or the Kolmogorov-Chapman equations. Based on transition functions, Feller (e.g., 1954), Dynkin (e.g., 1965), and many others studied evolution equations and ergodic behavior. There is a huge amount of standard literature on Markov chains, we might only mention Anderson (1991) and Kallenberg (2002) here.

While there have been tentative approaches to connect Markov chains with ecosystem models (Walter, 1979; Anderson, 1983), the idea does not seem to have fallen on fertile ground at that time and has widely fallen into oblivion shortly after.

2. Some introductory technical notes

In mathematical modeling of natural systems it is often required that the trajectory remains always in the positive orthant. Dynamical systems with this property are called nonnegative dynamical systems. A particular subclass of these are the compartmental systems as they additionally obey conservation laws regarding for instance mass, energy, or money. Compartmental systems describe flow models in which material is exchanged with the outside world and among different entities, called compartments. It is hereby usually assumed that material entering a compartment immediately mixes with the already present material. This property, called well-mixedness, is the reason why the future behavior of material in the system depends only on its current position and is independent of the past. Even though there are plenty of ways to describe well-mixed compartmental systems, the most common way is by means of system of ordinary differential equations (ODEs):

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x} = \mathrm{B}\,\mathbf{x} + \mathbf{u}.$$

Here, $\mathbf{x}$ is the state vector containing the system content of the quantity of interest, from now on called material, and $\mathbf{u}$ is a nonnegative vector of newly incoming material. The key property of compartmental systems is, in order for the system to balance mass, that the square matrix $\mathrm{B} = (B_{ij})$ exhibits the three properties

(i) $B_{ii} \leq 0$ for all i,

(ii) $B_{ij} \geq 0$ for all $i \neq j$, and

(iii) $\sum\limits_i B_{ij} \leq 0$ for all j.

Then, B is called *compartmental* and governs all internal cycling of material as well as the exit of material from the system.

A Markov process is a particular stochastic process in which the future of the process is independent of the past. We call Markov processes that are continuous in time and have a finite state space $\widetilde{S}$ *continuous-time Markov chains*, even though in the literature there are different names for them. The infinitesimal future of a probability distribution on $\widetilde{S}$ is governed by a so-called *infinitesimal generator* or *transition-rate matrix* $\mathrm{Q} = (Q_{ij})$. In order for the Markov chain to preserve probability mass, this square transition-rate matrix has the properties

(I) $Q_{ii} \leq 0$ for all i,

(II) $Q_{ij} \geq 0$ for all $i \neq j$, and

(III) $\sum\limits_i Q_{ij} = 0$ for all j.

It is important to note here that in standard probability literature the indices i and j are interchanged.

We immediately notice that the only difference between the properties of B and Q can be found in the difference between (iii) and (III). Suppose we are given a d-dimensional compartmental system. We increase the system by one dimension by adding a column and a row to B such that all columns sum to zero. This results in a transition-rate matrix of a continuous-time Markov chain on the state space $\widetilde{S} = \{1, 2, \ldots, d, d+1\}$. This simple observation is the basis of the thesis at hand and most of the results that follow are derived from it.

3. Relevance of compartmental systems and Markov chains

In a large variety of scientific fields such as systems biology, toxicology, pharmacokinetics (Anderson, 1983), ecology (Eriksson, 1971; Rodhe & Björkström, 1979; Matis et al., 1979; Manzoni & Porporato, 2009), hydrology (Nash, 1957; Botter et al., 2011; Harman & Kim, 2014), biogeochemistry (Manzoni & Porporato, 2009; Sierra & Müller, 2015), or epidemiology (Jacquez & Simon, 1993), models are based on the principle of mass conservation. In many cases such models are nonnegative dynamical systems that can be described by first-order systems of ODEs with strong structural constraints. Such systems are called compartmental systems (Anderson, 1983; Walter & Contreras, 1999; Haddad et al., 2010). We can classify such systems as combinations of linear/nonlinear and autonomous/nonautonomous (time-independent/time-dependent). For the sake of simplicity, most classical examples model natural processes by linear autonomous compartmental systems (e.g., tracer kinetics, carbon cycle, leaky fluid tanks). On the one hand, the simple structure of such systems allows a good understanding of undergoing processes in the modeled system. On the other hand, natural systems usually show highly complex interactions and depend on a constantly changing environment. Consequently, most of the time nonlinear nonautonomous compartmental models (Kloeden & Pötzsche, 2013) are more appropriate to model natural systems.

The theory of Markov processes is the most extensively developed part of probability theory. It covers, in particular, Poisson processes, Brownian motions, and all other Lévy processes (Çinlar, 2011). They can be classified into time-homogeneous/time-inhomogeneous, discrete/continuous state space, and finite/infinite state space. Consequently, they are very flexible and find important applications in fields such as telecommunication networks, queuing theory, insurance theory (Asmussen, 2003), and almost infinitely many more. In Chapter 2, absorbing continuous-time Markov chains are the basis to construct renewal- and regenerative processes that appropriately link Markov chains with compartmental systems. The main advantage of this link is that when we solve a problem in either Markov chain theory or compartmental systems theory, we automatically solve an according problem in the other field.

4. Age, transit time, remaining lifetime, and entropy

Ages, transit times, and remaining lifetimes are key quantities of compartmental systems that can be considered to better understand underlying system dynamics and to compare models with different sizes or structures. While age describes how old material in the system is, transit time describes how long material needs to travel through the entire system from entry to exit. Remaining lifetime, on the other hand, describes how long particles that are currently in the system still need until they leave the system (Bolin & Rodhe, 1973). These quantities provide us with information about the time scales on which systems operate. Also the concepts of residence time or turnover times can be useful for that purpose. However, the latter two concepts have to be clearly separated from what is presented in the present thesis. For more information about this issue and also about the historical confusion regarding all the different age- and time concepts, see Sierra et al. (2016). The results of Chapters 2 and 3 generalize classical approaches of computing ages and transit times (Bolin & Rodhe, 1973; Thompson & Randerson, 1999; Manzoni et al., 2009; Rasmussen et al., 2016). Furthermore, the concept of remaining lifetime is introduced to compartmental systems theory.

The Shannon information entropy as a complexity measure is only one new approach to the already confusing field of complexity of dynamical systems (Ebeling et al., 1998). It can be used to describe the uncertainty of a particle's path through the system, as a tool for honest modeling by means of the maximum entropy principle (Jaynes, 1957a,b), and as a means for comparing path properties of models with different sizes and structures.

5. Organization of the thesis

In Chapter 1, we introduce the basic theory of compartmental systems along the lines of Jacquez et al. (1972), Jacquez & Simon (1993), and Anderson (1983). From the principle of mass conservation, we derive the general structure of ODE systems that describe compartmental systems. Afterwards, we introduce compartmental matrices, classify compartmental systems, and present a short excursion on stability properties. At the end, we introduce the concepts of age, transit time, and remaining lifetime.

Chapter 2 is loosely based on Metzler & Sierra (2018). Here, we concentrate on the links between open compartmental systems in equilibrium and absorbing continuous-time Markov chains. We compute explicit formulas of the distributions of ages, transit times, and remaining lifetimes of compartmental systems and show how they find their probabilistic counterparts in backward recurrence times, absorption times, and forward recurrence times of renewal- and regenerative processes, respectively. These processes are constructed by repeatedly concatenating an absorbing Markov chain with itself. Subsequently, we apply the derived formulas to two well-known carbon cycle systems.

Chapter 3, which is free of probability theory and based on Metzler et al. (2018), extends the results on the distributions of ages, transit times, and remaining lifetimes to nonautonomous and possibly even nonlinear systems. Furthermore, we derive ODEs to compute the evolution of the mean age, higher-order moments, and age quantiles through time in a very convenient way. Then, we apply the derived theoretical results to a simple global carbon cycle model to answer two questions of high societal interest: *How old is atmospheric carbon? How long will a significant fraction of a pulse of fossil fuel carbon, emitted to the atmosphere today, remain in the system?* Finally, we show how existing nonlinearities noticeably affect not only the total stocks but also the distributions of ages and transit times in the employed model.

In Chapter 4, we focus on developing a complexity measure for compartmental systems based on Shannon information entropy. To that end, we first give a short overview of Shannon information entropy for random variables and stochastic processes along the lines of Cover & Thomas (2006). Then, we introduce three entropy concepts for compartmental systems in equilibrium: entropy rate per jump, entropy rate per unit time, and path entropy. These concepts are then analyzed in terms of their capability of serving as complexity measures. Furthermore, they are used as tools for model identification by means of the maximum entropy principle (Jaynes, 1957a,b). For some historical remarks on this principle, see Cover & Thomas (2006, Chapter 12). At the end, we extend the concepts of path entropy and entropy rate to systems out of equilibrium.

Chapter 5 summarizes the results of the thesis and puts them in relation to each other. Furthermore, we put the results in a broader context and give an outlook on possible future research in the field.

The main text is followed by four appendices. Appendices A and B provide basic properties of the matrix exponential and the state-transition matrix, respectively. Usually, these properties are used tacitly throughout the main text, because we assume the reader to be familiar with them.

A number of stochastic processes are central to the thesis. Appendix C presents them along with their most important properties with respect to the main text.

In Appendix D, we present some small compartmental systems in equilibrium with simple structure along with the densities of their age- and transit-time distributions as well as the according mean values. The formulas shown are derived from the general theory on age- and transit-time distributions in Chapter 2. They coincide with the formulas that were derived by Manzoni et al. (2009) on a tedious case-by-case basis via Laplace transforms.

6. General notes on setup and notation

We work with the following number systems:

- the natural numbers $\mathbb{N} := \{1, 2, 3, \ldots\}$,
- the real numbers $\mathbb{R}$,
- the complex numbers $\mathbb{C}$,
- for $d \in \mathbb{N}$, the d-dimensional vector space $\mathbb{R}^d$ over $\mathbb{R}$,
- for $d_1, d_2 \in \mathbb{N}$, the space $\mathbb{R}^{d_1 \times d_2}$ of real $d_1 \times d_2$-matrices,
- the nonnegative real numbers $\mathbb{R}_+ := \{r \in \mathbb{R} : r \geq 0\}$,
- for $d \in \mathbb{N}$, the nonnegative orthant $\mathbb{R}^d_+ := \{\mathbf{v} = (v_i)_{i=1,2,\ldots,d} \in \mathbb{R}^d : v_i \geq 0 \text{ for } i = 1, 2, \ldots, d\}$, and
- all obvious variants of them.

Throughout the entire thesis, vectors $\mathbf{v} = (v_i)_i$ are written in bold face and matrices $\mathrm{M} = (M_{ij})_{i,j}$ in upright face. The same holds true for vector- and matrix-valued functions, respectively. A vector or matrix is considered nonnegative or positive if all their elements are nonnegative or positive, respectively. The only vector norm used is the l_1-norm given by

$$\|\mathbf{v}\| := \sum_i |v_i|,$$

where $|v_i|$ denotes the absolute value of v_i. The only matrix norm used is the one induced by the l_1-norm, i.e., the norm of maximum absolute column sums

$$\|\mathrm{M}\| := \max_j \sum_i |M_{ij}|.$$

We omit subscripts of vectors and matrices if it does not lead to confusion.

The number n is usually natural. The number $d \in \mathbb{N}$ usually denotes the dimension of the ODE system that describes the compartmental system at hand. Equivalently, d denotes the number of compartments of the considered system. Consequently, $S := \{1, 2, \ldots, d\}$ is the state space of the absorbing continuous-time Markov chain X that describes the travel of a single particle through the system, and $\widetilde{S} := \{1, 2, \ldots, d, d+1\}$ is the state space of X extended by an absorbing state $d+1$, also called *environmental state*. The regenerative process Z describes the travel of a particle that immediately reenters the system after its exit, while its counterpart $\widetilde{Z}$ describes the travel of a particle that remains for some time in the environmental state before it reenters the system. To guarantee that all particles eventually leave the system, we consider only systems in which the compartmental matrix B is invertible. This invertibility is also required for all $\mathrm{B}(\mathbf{x}, t)$, where $\mathbf{x} \in \mathbb{R}^d_+$ and $t \geq t_0$. Here, $t_0 \in \mathbb{R}$ is some fixed initial time of the compartmental system. We suppose that elements involved in stated ODE systems are such that the systems are uniquely solvable, and that the solution is sufficiently smooth. Furthermore, we consider well-mixed compartmental systems only.

All involved random variables and stochastic processes are supposed to be supported by a sufficiently rich probability space $(\Omega, \mathcal{F}, \mathbb{P})$. In Chapter 2, we deal with random variables $Y : \Omega \to \mathbb{R}$. Consequently,

$$F_Y(y) := \mathbb{P}(Y \leq y) \to 1 \text{ as } y \to \infty.$$

We call F_Y the *cumulative probability distribution* of Y. Hence, for a given function $f_Y : \mathbb{R} \to \mathbb{R}_+$ such that

$$F_Y(y) = \int_{-\infty}^{y} f_Y(\sigma)\,\mathrm{d}\sigma, \quad y \in \mathbb{R},$$

we have

$$\int_{-\infty}^{\infty} f_Y(y)\,\mathrm{d}y = 1.$$

We call f_Y the *probability density function* of Y. Note that we do not mention explicitly that $f_Y(y) = 0$ for $y < 0$ when it is obvious (e.g., when Y describes an age or a transit time). We use the nonstandard term *cumulative probability distribution* to veer away from the terms used in Chapter 3 where we do not deal with probability masses but with masses in general. In Chapter 3, the counterpart of the cumulative probability distribution is called *cumulative distribution* and is denoted by P or, if it describes ages, *cumulative age distribution.* The counterpart of the probability density function is simply called *density function* and denoted by p.

Often in the literature, Markov chains are assumed to be supported on a discrete time set and Markov processes on continuous time intervals. Since most of the time in this thesis we deal with continuous-time objects, we do not make this distinction and always speak of *Markov chains.* If necessary, we put *discrete-time* or *continuous-time* in front. This way, we stick to the notation of Anderson (1991). In the following, all involved Markov chains are equipped with a finite discrete state space called S or $\tilde{S}$. Such processes are also known as Markov jump processes in the literature. Note that all our stochastic processes are assumed to be right-continuous and we use the terms *steady state* and *equilibrium* interchangeably. Furthermore, we omit the terms *almost surely (a.s.)* and *almost everywhere (a.e.)*, because the additional technical notation would not serve any practical purpose in this thesis.

Another important remark is that renewal processes are often defined to be counting processes that count the number of occurrences of events. However, throughout this thesis, we follow the definition of Asmussen (2003) which specifies renewal processes as the sequence of moments in time at which evens occur.

CHAPTER 1

Introduction to compartmental systems

Our goal in this chapter is to derive the general structure of ODE systems that describe compartmental systems from the principle of mass conservation, to introduce compartmental matrices, to classify compartmental systems, and to introduce important system diagnostics.

1.1. From mass conservation to a first-order ordinary differential equation system

Following Jacquez & Simon (1993), a compartment is an amount of kinetically homogeneous material. Kinetically homogeneous means that any material entering the system is immediately mixed with the material of the compartment. Compartmental systems describe the flow of material into different compartments, the subsequent distribution of the material among the different compartments, and eventually the exit of the material from the system of compartments.

Suppose we are given a fixed real-valued starting time t_0 and a set $S = \{1, 2, \dots, d\}$ of compartments, with d being a natural number. Throughout this chapter, i and j are assumed to be elements of S. For all j, the amount of material in compartment j at time $t \geq t_0$ is denoted by $x_j(t)$. We collect the $x_j(t)$ in a vector $\mathbf{x}(t) := (x_1(t), \dots, x_d(t))^\top$, where the superscript $\top$ stands for the transpose. Furthermore, let $I_j(t)$ and $O_j(t)$ describe the flux of material entering and leaving compartment j at time t, respectively. For any compartment j, the law of mass conservation implies

(i) $\frac{\mathrm{d}}{\mathrm{d}t}\, x_j(t) = I_j(t) - O_j(t)$, and

(ii) if a compartment is empty, nothing can flow out.

From condition (ii), we can derive the following lemma which is a variation of a result of Jacquez & Simon (1993, Appendix 1), but with a more elaborate (multi-dimensional) proof. The original proof is only given for the one-dimensional case.

Lemma 1.1 *Let $n \in \mathbb{N}$, $i \neq j$, and $F_{ij} : (\mathbf{x}, t) \mapsto F_{ij}(\mathbf{x}, t) \in \mathbb{R}_+$ a nonnegative flux from compartment j to compartment i, which is n times continuously differentiable in $\mathbf{x}$ with $F_{ij}(\mathbf{x}, t) = 0$ if $x_j = 0$. Then, there is a function $B_{ij} : (\mathbf{x}, t) \mapsto B_{ij}(\mathbf{x}, t) \in \mathbb{R}_+$ such that $F_{ij}(\mathbf{x}, t) = B_{ij}(\mathbf{x}, t)\, x_j$. Furthermore, B_{ij} is $n-1$ times continuously differentiable in $\mathbf{x}$.*

Proof. We fix $\mathbf{x} \geq 0$ and $t \geq t_0$. For the sake of simplicity of notation omit t as the second variable in functions. Moreover, for $s \in [0, 1]$ we define a vector $\mathbf{y}(s) \in \mathbb{R}^d_+$ by $y_k(s) := x_k$

for $k \neq j$ and $y_j(s) := s\,x_j$, and we define a function $G : [0,1] \to \mathbb{R}_+$ by $G(s) := F_{ij}(\mathbf{y}(s))$. Taking the derivative of G with respect to $s \in (0,1)$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}s}\,G(s) = \sum_{k\in S} \mathrm{D}_k F_{ij}(\mathbf{y}(s))\,\frac{\mathrm{d}}{\mathrm{d}s}\,y_k(s),$$

where D_k denotes the partial derivative with respect to the kth coordinate, and $\frac{\mathrm{d}}{\mathrm{d}s}\,y_k(s) = \mathbb{1}_{\{k=j\}}\,x_j$. Here, $\mathbb{1}_{\{k=j\}}$ is the indicator function, defined to be 1 if $k = j$ and 0 otherwise. Denoting by $\mathbf{0}$ the vector comprising zeros and using (ii), we can compute

$$\begin{aligned} F_{ij}(\mathbf{x}) &= F_{ij}(\mathbf{x}) - 0 = F_{ij}(\mathbf{x}) - F_{ij}(\mathbf{0}) \\ &= G(1) - G(0) = \int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}\,G(s)\,\mathrm{d}s \\ &= \int_0^1 \sum_{k\in S} \mathrm{D}_k\,F_{ij}(\mathbf{y}(s))\,\frac{\mathrm{d}}{\mathrm{d}s}\,y_k(s)\,\mathrm{d}s \\ &= \int_0^1 \mathrm{D}_j\,F_{ij}(\mathbf{y}(s))\,x_j\,\mathrm{d}s \\ &= x_j\,B_{ij}(\mathbf{x}), \end{aligned}$$

where $B_{ij}(\mathbf{x}) := \int_0^1 \mathrm{D}_j\,F_{ij}(\mathbf{y}(s))\,\mathrm{d}s$ is $n-1$ times differentiable in $\mathbf{x}$. Note that B_{ij} depends on $\mathbf{x}$ through the definition of $\mathbf{y}$. □

We now aim at applying this lemma so as to derive a system of ODEs that describes the flow of material in a compartmental system. To this end, we need to split the inputs to compartments into external and internal inputs. External inputs enter the compartment from outside the system and internal inputs enter the compartment by coming in from other compartments. For compartment i, we denote them by u_i and $I_{\mathrm{int},i}$, respectively. The same needs to be done for outputs from the compartments, where we write r_i for fluxes leaving the system from compartment i, and $O_{\mathrm{int},i}$ denotes internal outputs from compartment i that move to another compartment. From (i), for $i \in S$, we then obtain

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,x_i(t) &= I_i(t) - O_i(t) \\ &= u_i(t) + I_{\mathrm{int},i}(t) - (r_i(t) + O_{\mathrm{int},i}(t)) \\ &= u_i(t) + \sum_{j\neq i} F_{ij}(\mathbf{x}(t),t) - \left[r_i(\mathbf{x}(t),t) + \sum_{j\neq i} F_{ji}(\mathbf{x}(t),t) \right]. \end{aligned} \tag{1.1}$$

For $i \neq j$, we can now use Lemma 1.1 to infer the existence of functions $B_{ij}, z_i : \mathbb{R}_+^d \times [t_0,\infty) \to \mathbb{R}_+$ such that

$$\begin{aligned} F_{ij}(\mathbf{x}(t),t) &= B_{ij}(\mathbf{x}(t),t)\,x_j(t), \\ F_{ji}(\mathbf{x}(t),t) &= B_{ji}(\mathbf{x}(t),t)\,x_i(t), \text{ and} \\ r_i(\mathbf{x}(t),t) &= z_i(\mathbf{x}(t),t)\,x_i(t). \end{aligned}$$

We plug the newly obtained functions B_{ij} and z_i into Eq. (1.1) and see

$$\frac{\mathrm{d}}{\mathrm{d}t}\,x_i(t) = u_i(t) + \sum_{j\neq i} B_{ij}(\mathbf{x}(t),t)\,x_j(t) - \left[z_i(\mathbf{x}(t),t) + \sum_{j\neq i} B_{ji}(\mathbf{x}(t),t \right] x_i(t). \tag{1.2}$$

By defining

$$B_{ii}(\mathbf{x}(t), t) := -\left[z_i(\mathbf{x}(t), t) + \sum_{j \neq i} B_{ji}(\mathbf{x}(t), t)\right], \tag{1.3}$$

we see

$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_i(t) = u_i(t) + \sum_{j \in S} B_{ij}(\mathbf{x}(t), t)\, x_j(t).$$

In matrix notation we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \mathbf{x}(t) = \mathrm{B}(\mathbf{x}(t), t)\, \mathbf{x}(t) + \mathbf{u}(\mathbf{x}(t), t), \tag{1.4}$$

where $\mathrm{B} = (B_{ij}) : \mathbb{R}^d_+ \times [t_0, \infty) \to \mathbb{R}^{d \times d}$ is a square matrix-valued function and $\mathbf{u} = (u_i) : \mathbb{R}^d_+ \times [t_0, \infty) \to \mathbb{R}^d_+$ is a nonnegative vector-valued function.

For the sake of simplicity of notation, from now on we occasionally omit the arguments of the functions.

Remark 1.2 Let $i \neq j$. From Eq. (1.2), we can identify $z_i\, x_i$ and $\left(\sum_{j \neq i} B_{ji}\right) x_i$ as the external and internal outputs from compartment i, respectively. Eq. (1.3) makes us then interpret $-B_{ii}\, x_i$ as the total output from compartment i. Furthermore, the same equation shows $z_i = -(B_{ii} + \sum_{j \neq i} B_{ji}) = -\sum_{j \in S} B_{ji}$, or in vector notation

$$\mathbf{z}^\top = -\mathbf{1}^\top\, \mathrm{B}, \tag{1.5}$$

where $\mathbf{1}$ is the column vector filled with ones.

This observation motivates the following definition.

Definition 1.3 Let $i \neq j$. Then, the B_{ij}'s are called *fractional transfer coefficients* or simply *transfer rates*. They describe the rates of how fast material moves from compartment j to compartment i. The $-B_{ii}$'s are called *decay rates*. They describe the rate of how fast material leaves compartment i. Finally, the z_i's are called *output rates* or *release rates*. They describe how fast material leaves the system from compartment i.

1.2. Definition of compartmental matrices and compartmental systems

Matrix B in Eq. (1.4) has particular properties which we investigate more closely in this section. Always bear in mind that by the law of mass conservation all fluxes are required to be nonnegative as well as all components of the vector $\mathbf{x}$. Since for all i,

$$0 \leq O_i = \left(z_i + \sum_{j \neq i} B_{ji}\right) x_i = -B_{ii}\, x_i,$$

we have $B_{ii} \leq 0$. For all $j \neq i$, additionally $0 \leq F_{ij} = B_{ij}\, x_j$. Consequently, $B_{ij} \geq 0$. Furthermore, for all j,

$$0 \leq r_j = z_j\, x_j = -\left(B_{jj} + \sum_{i \neq j} B_{ij}\right) x_j = \left(-\sum_{i \in S} B_{ij}\right) x_j.$$

Hence, $\sum_{i \in S} B_{ij} \leq 0$. These results motivate the following definitions.

Definition 1.4 A square matrix $\mathrm{B} = (B_{ij})$ is called a *compartmental matrix* if

(i) $B_{ii} \leq 0$ for all i,

(ii) $B_{ij} \geq 0$ for all $i \neq j$, and

(iii) $\sum\limits_{i \in S} B_{ij} \leq 0$ for all j.

Definition 1.5 Let $f : \mathbb{R}^d_+ \times [t_0, \infty) \to \mathbb{R}^d_+$ be such that the initial value problem

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) &= f(\mathbf{x}(t), t), \quad t > t_0, \\ \mathbf{x}(t_0) &= \mathbf{x}^0 \in \mathbb{R}^d_+, \end{aligned} \tag{1.6}$$

has a unique solution on $[t_0, \infty)$. Furthermore, let $\mathrm{B} = (B_{ij}) : \mathbb{R}^d_+ \times [t_0, \infty) \to \mathbb{R}^{d \times d}$ and $\mathbf{u} = (u_i) : \mathbb{R}^d_+ \times [t_0, \infty) \to \mathbb{R}^d_+$ be bounded continuous functions. If we can write f as

$$f(\mathbf{x}(t), t) = \mathrm{B}(\mathbf{x}(t), t)\,\mathbf{x}(t) + \mathbf{u}(\mathbf{x}(t), t), \quad t \geq t_0,$$

with the matrix $\mathrm{B}(\mathbf{x}, t)$ being compartmental for all $\mathbf{x} \in \mathbb{R}^d_+$ and $t \geq t_0$, then we call the first-oder system (1.6) of ODEs a *compartmental system*. We can state it more explicitly as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) &= \mathrm{B}(\mathbf{x}(t), t)\,\mathbf{x}(t) + \mathbf{u}(\mathbf{x}(t), t), \quad t > t_0, \\ \mathbf{x}(t_0) &= \mathbf{x}^{\mathbf{0}} \in \mathbb{R}^d_+. \end{aligned} \tag{1.7}$$

The function $\mathbf{x} : [t_0, \infty) \to \mathbb{R}^d_+$ is called *system state trajectory* or the system's *solution trajectory*, and $\mathbf{u} : \mathbb{R}^d_+ \times [t_0, \infty) \in \mathbb{R}^d_+$ is the system's *external input function*.

If $\mathrm{B}(\mathbf{x}, t) = \mathrm{B}(t)$ and $\mathbf{u}(\mathbf{x}, t) = \mathbf{u}(t)$ for all $\mathbf{x} \in \mathbb{R}^d_+$ and all $t \geq t_0$, i.e., B and $\mathbf{u}$ are independent of the system state $\mathbf{x}(t)$, then the system is called *linear*, otherwise it is called *nonlinear*.

If $\mathrm{B}(\mathbf{x}, t) = \mathrm{B}(\mathbf{x})$ and $\mathbf{u}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x})$ for all $\mathbf{x} \in \mathbb{R}^d_+$ and all $t \geq t_0$, i.e., B and $\mathbf{u}$ do not explicitly depend on the time t, then the system is called *autonomous*, otherwise it is called *nonautonomous*.

A linear autonomous compartmental system takes the particular shape

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) &= \mathrm{B}\,\mathbf{x}(t) + \mathbf{u}, \quad t > t_0, \\ \mathbf{x}(t_0) &= \mathbf{x}^0 \in \mathbb{R}^d_+, \end{aligned} \tag{1.8}$$

where B is a compartmental matrix and $\mathbf{u}$ is a nonnegative external input vector.

Remark 1.6 Many models of vegetation processes include a state-dependent input function $\mathbf{u}$. For instance, the amount of carbon coming into a vegetation system through photosynthesis may depend on the available leaf carbon.

A compartmental system guarantees that no material gets lost or is produced out of nowhere. Consequently, all components of the state vector are nonnegative at all times provided that the initial state vector is nonnegative. However, three potential issues may arise. We examine them for the case of a linear autonomous system:

(1) There exists a compartment j with $B_{jj} = 0$, which means that this compartment does not lose any material. On the contrary, the compartment accumulates material indefinitely if it receives inputs.

(2) All column sums of B vanish. Since the negative column sums coincide with the release rates, the system does not lose any material and might accumulate material indefinitely.

(3) There exists a subsystem of compartments that does not lose any material, meaning that some material remains stuck in a subcycle. If this subsystem receives external inputs, it will accumulate material indefinitely.

To avoid all three of these undesired effects, we require the compartmental matrix B to be invertible. This requirement is motivated by the following lemma.

Lemma 1.7 *If a compartmental matrix* $\mathrm{B} = (B_{ij}) \in \mathbb{R}^{d\times d}$ *is invertible, then*

(i) $B_{jj} < 0$ *for all* j*,*

(ii) there is a compartment j *with external outputs, i.e.,* $z_j > 0$*, and*

(iii) there is no subsystem of compartments that does not lose any material.

Proof. We begin with proving (i). To this end, we assume that there is a compartment j with $B_{jj} = 0$, and we fix this j. By Definition 1.4 of compartmental matrices, we know $B_{ij} \geq 0$ for $i \neq j$. Furthermore, the release rate $z_j = -\sum_{i\in S} B_{ij} \geq 0$ by the same definition. Multiplying Eq. (1.3) by -1, we obtain

$$0 = -B_{jj} = z_j + \sum_{i\neq j} B_{ij},$$

and it is immediately obvious that $B_{ij} = 0$ for all i. Consequently, the jth column of B vanishes, which prevents B from being invertible. Since B is invertible by assumption, there cannot exist a j such that $B_{jj} = 0$ and (i) is proven.

Now, we prove (ii). To this end, we assume all column sums of B to be 0, which means $z_j = 0$ for all j. By Eq. (1.5), $\mathrm{B}^\top \mathbf{1} = -\mathbf{z} = \mathbf{0}$. Consequently, the kernel of $\mathrm{B}^\top$ contains a nonzero vector, which proves that $\mathrm{B}^\top$ and also B are not invertible. This again violates the assumption of the lemma and Eq. (1.5) is proven.

To prove (iii), we assume that there is a $\widehat{d}$-dimensional subsystem that does not lose any material. We collect the compartments of this subsystem in the set $\widehat{S}$ and denote the corresponding compartmental matrix by $\widehat{\mathrm{B}}$. The release rates $\widehat{z}_j$ of the subsystem vanish. Consequently, the $\widehat{d}$-dimensional vector $\mathbf{1}^\top$ is in the kernel of $\widehat{\mathrm{B}}$, and the nonnegative vector $\mathbf{y} = (y_j)_{j=1,2,\ldots,d}$ defined by

$$y_j = \begin{cases} 1, & j \in \widehat{S}, \\ 0, & \text{otherwise}, \end{cases}$$

is in the kernel of B, which again contradicts the lemma's assumption that B be invertible, and the proof is complete. □

The invertibility of the compartmental matrix thus guarantees that all material that enters the system will eventually leave it. For a linear autonomous system this motivates the definition of an open system. This definition naturally carries over to general compartmental systems.

Definition 1.8 A compartmental system (1.7) is called *open*, if for all $\mathbf{x} \in \mathbb{R}^d_+$ and all $t \geq t_0$ the compartmental matrix $\mathrm{B}(\mathbf{x}, t)$ is invertible.

Remark 1.9 From the preceding discussion, we know that open compartmental systems have the following properties. For all $\mathbf{x} \in \mathbb{R}^d_+$ and all $t \geq t_0$,

(i) $B_{ii}(\mathbf{x}, t) < 0$ for all i,

(ii) $B_{ij}(\mathbf{x}, t) \geq 0$ for all $i \neq j$,

(iii) $\sum\limits_{i \in S} B_{ij}(\mathbf{x}, t) \leq 0$ for all j,

(iv) there exists a compartment j with external outputs, i.e., $z_j(\mathbf{x}, t) > 0$, and

(v) there is no subsystem that does not have any outputs.

Since we know that for open linear autonomous compartmental systems all material that enters the system will eventually leave the system, it is natural to ask the following two questions: *Can we infer some kind of stability properties of the system? How long does material need to travel through the system, from entering the system to leaving it?* Let us turn our attention to the question of stability first.

1.3. Stability of compartmental systems

Definition 1.10 Let $\mathbf{x}$ and $\mathbf{y}$ be two solution trajectories of a compartmental system with initial values $\mathbf{x}^0$ and $\mathbf{y}^0$, respectively. The compartmental system is called *exponentially stable* if there exist $K \geq 1$ and $\gamma > 0$ such that

$$\|\mathbf{x}(t) - \mathbf{y}(t)\| \leq K\, e^{-\gamma\,(t-t_0)}\, \|\mathbf{x}^0 - \mathbf{y}^0\| \text{ for all } t \geq t_0.$$

Lemma 1.11 *Let* B *be the compartmental matrix of an open linear autonomous compartmental system. Then all eigenvalues of* B *have negative real part.*

Proof. We apply the Gershgorin circle theorem (Varga, 2009, Theorem 1.11). It guarantees that all eigenvalues of B are located in the closed disc $\{\lambda \in \mathbb{C} : |B_{jj} - \lambda| \leq R_j\}$ with radius $R_j = \sum_{i \neq j} B_{ij}$ and centered at B_{jj} for at least one j. (Recall that B_{jj} is negative.) By Definition 1.4 of compartmental matrices, the radius $R_j \leq -B_{jj}$. Consequently, all eigenvalues are located in the left half of the complex plane with the rightmost possible eigenvalue being equal to zero. Since the system is supposed to be open, B is invertible and cannot have a zero eigenvalue. Hence, all eigenvalues of B have negative real part. □

Definition 1.12 Let Eq. (1.7) be a compartmental system with arbitrary initial value. If there exists $\mathbf{x}^* \in \mathbb{R}^d_+$ such that, for all $t \geq t_0$,

$$\mathrm{B}(\mathbf{x}^*, t)\, \mathbf{x}^* + \mathbf{u}(\mathbf{x}^*, t) = \mathbf{0},$$

then $\mathbf{x}^*$ is called a *steady state* or *equilibrium* of the compartmental system.

Proposition 1.13 *Every open linear autonomous compartmental system* (1.8) *is exponentially stable. Furthermore, the system has the unique steady state* $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ *to which all solutions converge as* $t \to \infty$*, independently of the initial value* $\mathbf{x}^0$.

Proof. We denote by e^{M} the matrix exponential (Appendix A) of a square matrix M and by I the identity matrix. The unique solution $\mathbf{x}$ of the linear system (1.8) is given by

(Brockett, 2015, Corollary of Theorem 1.6.1)

$$\mathbf{x}(t) = e^{(t-t_0)\,\mathrm{B}}\,\mathbf{x}^0 + \int\limits_{t_0}^{t} e^{(t-\tau)\,\mathrm{B}}\,\mathbf{u}\,\mathrm{d}\tau, \quad t \geq t_0, \tag{1.9}$$

which we can compute to

$$\mathbf{x}(t) = e^{(t-t_0)\,\mathrm{B}}\,\mathbf{x}^0 + \mathrm{B}^{-1}\left(e^{(t-t_0)\,\mathrm{B}} - \mathrm{I}\right)\mathbf{u}, \quad t \geq t_0.$$

Now let $\mathbf{x}$ and $\mathbf{y}$ denote two solutions of Eq. (1.8) with initial values $\mathbf{x}^0$ and $\mathbf{y}^0$, respectively. For $t \geq t_0$,

$$\begin{aligned}\|\mathbf{x}(t) - \mathbf{y}(t)\| &= \|e^{(t-t_0)\,\mathrm{B}}\,\mathbf{x}^0 - e^{(t-t_0)\,\mathrm{B}}\,\mathbf{y}^0\| \\ &= \|e^{(t-t_0)\,\mathrm{B}}\left[\mathbf{x}^0 - \mathbf{y}^0\right]\| \\ &\leq \|e^{(t-t_0)\,\mathrm{B}}\| \cdot \|\mathbf{x}^0 - \mathbf{y}^0\|.\end{aligned}$$

From Lemma 1.11 we already know that all eigenvalues of B are negative. By Engel & Nagel (2000, Theorem I.3.14) there exist $K \geq 1$ and $\gamma > 0$ such that

$$\|e^{(t-t_0)\,\mathrm{B}}\| \leq K\,e^{-(t-t_0)\,\gamma}. \tag{1.10}$$

Note that the matrix norm here is supposed to be the operator norm. In our case, the matrix norm of maximum absolute column sums coincides with the operator norm based on the vector norm of the absolute coordinate sum. Consequently,

$$\|\mathbf{x}(t) - \mathbf{y}(t)\| \leq K\,e^{-\gamma\,(t-t_0)} \cdot \|\mathbf{x}^0 - \mathbf{y}^0\|$$

for all $t \geq t_0$, and the compartmental system is exponentially stable.

Obviously, since $\mathrm{B}\,\mathbf{x}^* + \mathbf{u} = -\mathrm{B}\,\mathrm{B}^{-1}\,\mathbf{u} + \mathbf{u} = \mathbf{0}$, the vector $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ is a steady state of the given compartmental system. The existence of another steady state $\mathbf{y}^* \neq \mathbf{x}^*$ would violate the exponential stability of the system. Also because of the exponential stability, all solutions with an arbitrary initial value $\mathbf{x}^0 \in \mathbb{R}^d_+$ must necessarily converge toward $\mathbf{x}^*$ as $t \to \infty$. □

Corollary 1.14 *As long as the compartmental matrix* B *is invertible, we see directly from Eq.* (1.10) *that for any* $\mathbf{v} \in \mathbb{R}^d_+$ *the term* $e^{(t-t_0)\,\mathrm{B}}\,\mathbf{v}$ *vanishes as* $t \to \infty$.

For linear nonautonomous systems, the concept of steady states is not very useful since the system input as well as the transfer rates might permanently change. Nevertheless, the concept of exponential stability from Definition 1.10 is still appropriate. In the autonomous case, it describes how all trajectories approach one single point $\mathbf{x}(t) = \mathbf{x}^*$ in space. In the nonautonomous case, exponential stability means that any pair of trajectories will exponentially fast come arbitrarily close to each other as $t \to \infty$, even though neither of them might ever become constant (Figure 1.1). Very general conditions for an open linear autonomous system to be exponentially stable are given in Rasmussen et al. (2016, Theorem 1).

So far, we have only dealt with stability of linear compartmental systems, and we do not engage in the topic of stability of nonlinear compartmental systems. This topic is beyond the scope of this thesis. In nonlinear stability analysis, to quote Jacquez & Simon (1993), "anything can happen." Nevertheless, Jacquez & Simon (1993) categorize nonlinear compartmental systems in terms of their stability properties. In addition to this paper, also Anderson & Roller (1991) is a valuable resource for this opaque topic.

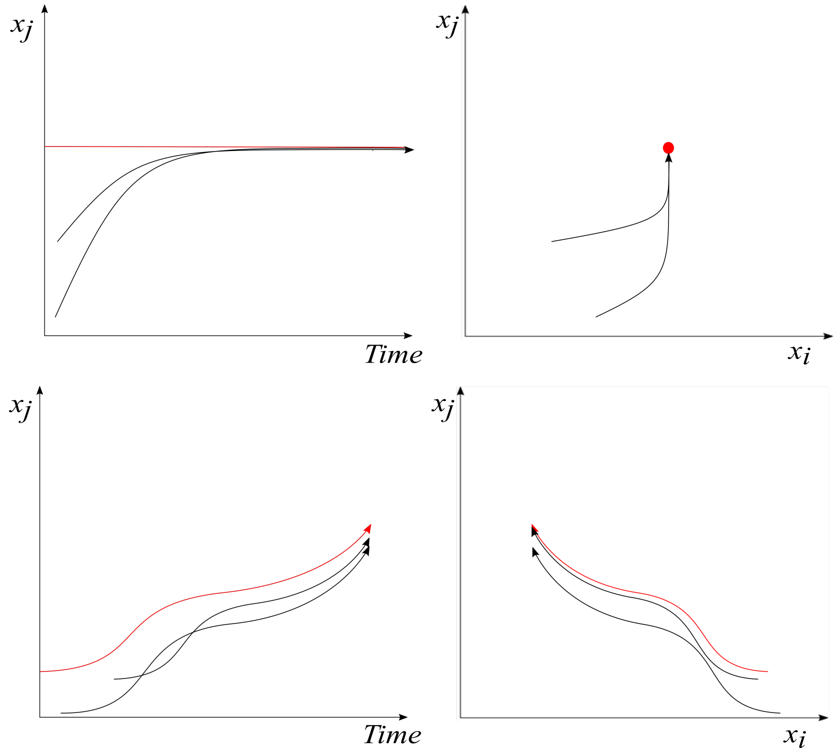


Figure 1.1. Trajectories of exponentially stable autonomous (upper plots) and exponentially stable nonautonomous (lower plots) linear compartmental systems with respect to time (left) and in a two-dimensional state space (right). In the autonomous case, all trajectories converge to a fixed point in the state space (red dot) independently of their initial conditions, while in the nonautonomous case all trajectories are forward attracting. In case of an infinite history of the system, there exists a unique pullback attracting trajectory (red curve). (Figure and caption modified from Sierra et al. (2018).)

1.4. Ages, transit times, and remaining lifetimes of compartmental systems

Now we turn our attention to the second question: *How long does material need to travel through the system, from entering the system to leaving it?*

All exponentially stable open compartmental systems share the property that material enters the system at its arrival time t_a and exits from the system at a later point t_e in time. The duration $t_e - t_a$ is the time that the material needs to travel through the system and we call it transit time. Since a general compartmental system's inner dynamics might be subject to permanent change, we discriminate two types of transit time. The underlying concept of this discrimination is the concept of age. We also split the concept of age into two different quantities: the age of all particles in the system and the age of particles that belong to a particular compartment. Both quantities play an important role not only for their close relation to the idea of transit time but also in their own right. A third important concept is, how long particles that are already in the system will still remain there before they exit. We call this concept remaining lifetime and, again, we discriminate between all particles in the system and particles that belong to a particular compartment.

Concept 1.15 The *system age* $A(t)$ of a compartmental system at time t is the time span $t - t_a$ that the system's current material has already spent in the system under the constraint that the material has entered the system at time t_a.

The *compartment age* $a_j(t)$ with respect to compartment j of a compartmental system is the system age of the material contained in compartment j at time t.

We will define *age* more precisely in Section 2.2.6. For now, we assume to have a precise definition of age. Based on this precise definition, we can now focus on the transit time.

Definition 1.16 The *forward transit time* $\mathrm{FTT}(t_a)$ of a compartmental system is the age that the material will have at time t_e of its exit from the system under the constraint that the material enters the system at time t_a.

The *backward transit time* $\mathrm{BTT}(t_e)$ of a compartmental system is the age of the material in the output from the system at exit time t_e.

Definition 1.17 The *remaining system lifetime* $L(t)$ of a compartmental system at time t is the time span $t_e - t$ that the system's current material will still spend in the system before its exit at time t_e.

The *remaining compartment lifetime* $l_j(t)$ with respect to compartment j of a compartmental system is the remaining system lifetime of the material contained in compartment j at time t.

The concepts of age, transit time, and remaining lifetime are central to major parts of this thesis in that we not only derive formulas to compute their distributions, moments, and quantiles, but also connect them to appropriate probabilistic quantities. Afterwards, we apply the derived formulas to relevant examples from soil organic matter decomposition and the global carbon cycle.

CHAPTER 2

Compartmental systems in equilibrium and continuous-time Markov chains

For open compartmental systems, it is natural to ask for ages, transit times, and remaining lifetimes. They give insight into the inner structure of the system and into internal dynamics, and provide us with additional information to make us better understand the system. Furthermore, they are important metrics if we want to compare different models that describe similar or different systems. Moreover, we can better constrain model parameters when we compare tracer measurements with theoretical results on ages and transit times. For example, we can improve our knowledge about the global carbon cycle if we find out how old carbon is in the soils, in the vegetation, or in the atmosphere. If we aim at constructing large-scale models by conflating many small-scale models, be it spatially or temporally, even knowledge on ages and transit times on microbial scale turns out to be useful.

In this chapter, which is loosely based on Metzler & Sierra (2018), we consider two ecological models represented by compartmental systems in equilibrium and ask the questions for their respective age structures, transit times, and remaining lifetimes. As it turns out, these questions can be answered from two perspectives. The first perspective is the the dynamical systems point of view, whereas the second one is of probabilistic nature. We show that many deterministic concepts have a stochastic counterpart. This link between two different mathematical fields is based on 1) the restrictions of keeping mass balanced in compartmental systems and conserving probability mass in the theory of stochastic processes, and 2) the well-mixedness of compartments and the future's independence of the past in Markov chains.

Throughout this chapter, several stochastic processes play a major role. They are introduced in Appendix C along with some of their most important properties. Some examples of compartmental systems in equilibrium with very simple structure along with applications of the formulas derived in this chapter to these systems are presented in Appendix D.

2.1. Introduction of two ecological examples

We consider two examples of carbon cycle models. Even though the first system is linear and the second one is nonlinear, both systems' properties can be investigated by the same approach because the two systems find themselves in equilibrium. For each of the systems, we ask for the internal carbon's age structure and for how long carbon needs to transit the system.

2.1.1. A linear autonomous global carbon cycle model, I

We consider the global carbon cycle model introduced by Emanuel et al. (1981) (Figure 2.1). Since Thompson & Randerson (1999) numerically calculated age- and transit-time distributions using an impulse response function approach, this model is a very good test case once we have developed a general theory for ages and transit times. The model comprises five compartments: non-woody tree parts x_1, woody tree parts x_2, ground vegetation x_3, detritus/decomposers x_4, and active soil carbon x_5. Since the model is considered to be in equilibrium, the initial state is negligible and, the model is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathrm{B}\,\mathbf{x}(t) + \mathbf{u}, \quad t > 0,$$

where the input vector is given by $\mathbf{u} = (77.00;\, 0.00;\, 36.00;\, 0.00;\, 0.00)^\top\,\mathrm{Pg\,C\,yr^{-1}}$ and the compartmental matrix by

$$\mathrm{B} = \begin{pmatrix} -77/37 & 0 & 0 & 0 & 0 \\ 31/37 & -31/452 & 0 & 0 & 0 \\ 0 & 0 & -36/69 & 0 & 0 \\ 21/37 & 15/452 & 12/69 & -48/81 & 0 \\ 0 & 2/452 & 6/69 & 3/81 & -11/1121 \end{pmatrix} \mathrm{yr}^{-1}.$$

The numbers are chosen exactly as in Thompson & Randerson (1999). The input vector is expressed in units of petagrams of carbon per year ($\mathrm{Pg\,C\,yr^{-1}}$) and the fractional transfer coefficients in units of per year (yr^{-1}). Because B is a lower triangular matrix with nonzero diagonal entries, it is invertible. Furthermore, B is compartmental and hence we deal with an open system, wherefore it is reasonable to ask for age and transit time of this model. We are not yet in the position to answer these questions, but there are some interesting quantities we can already compute. So is the steady-state vector of carbon contents given by

$$\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u} = (37.00;\, 452.00;\, 69.00;\, 81.00;\, 1,121.00)^\top\,\mathrm{Pg\,C}$$

and the respiration vector (external output vector, release vector) in steady state by

$$\mathbf{r} = (z_j\, x_j^*)_{j=1,2,\ldots,5} = (25.00;\, 14.00;\, 18.00;\, 45.00;\, 11.00)^\top\,\mathrm{Pg\,C\,yr^{-1}}.$$

2.1.2. A nonlinear autonomous soil organic matter decomposition model, I

Consider the nonlinear autonomous compartmental system

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathrm{B}(\mathbf{x}(t))\,\mathbf{x}(t) + \mathbf{u}, \quad t > 0, \tag{2.1}$$

where $\mathrm{B} : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is a matrix-valued mapping. In this setup, the fractional transfer coefficients are not constant but depend on the system's content.

Assume now that system (2.1) is in a steady state $\mathbf{x}^*$. From $\mathrm{d}\,\mathbf{x}^*/\mathrm{d}\,t = 0$ follows that the compartment contents x_j^* do not change in time, and the mapping B turns into a matrix with constant coefficients. Hence, if we assume the nonlinear autonomous compartmental system (2.1) to be in a steady state, we can treat it as a linear autonomous compartmental system.

As an example, consider the nonlinear two-compartment carbon cycle model described by Wang et al. (2014) (Figure 2.2). We denote by C_s and C_b soil organic carbon and soil microbial biomass ($\mathrm{g\,C\,m^{-2}}$), respectively, by ε the carbon use efficiency or fraction of assimilated carbon that is converted into microbial biomass (unit-less), by μ_b the turnover rate

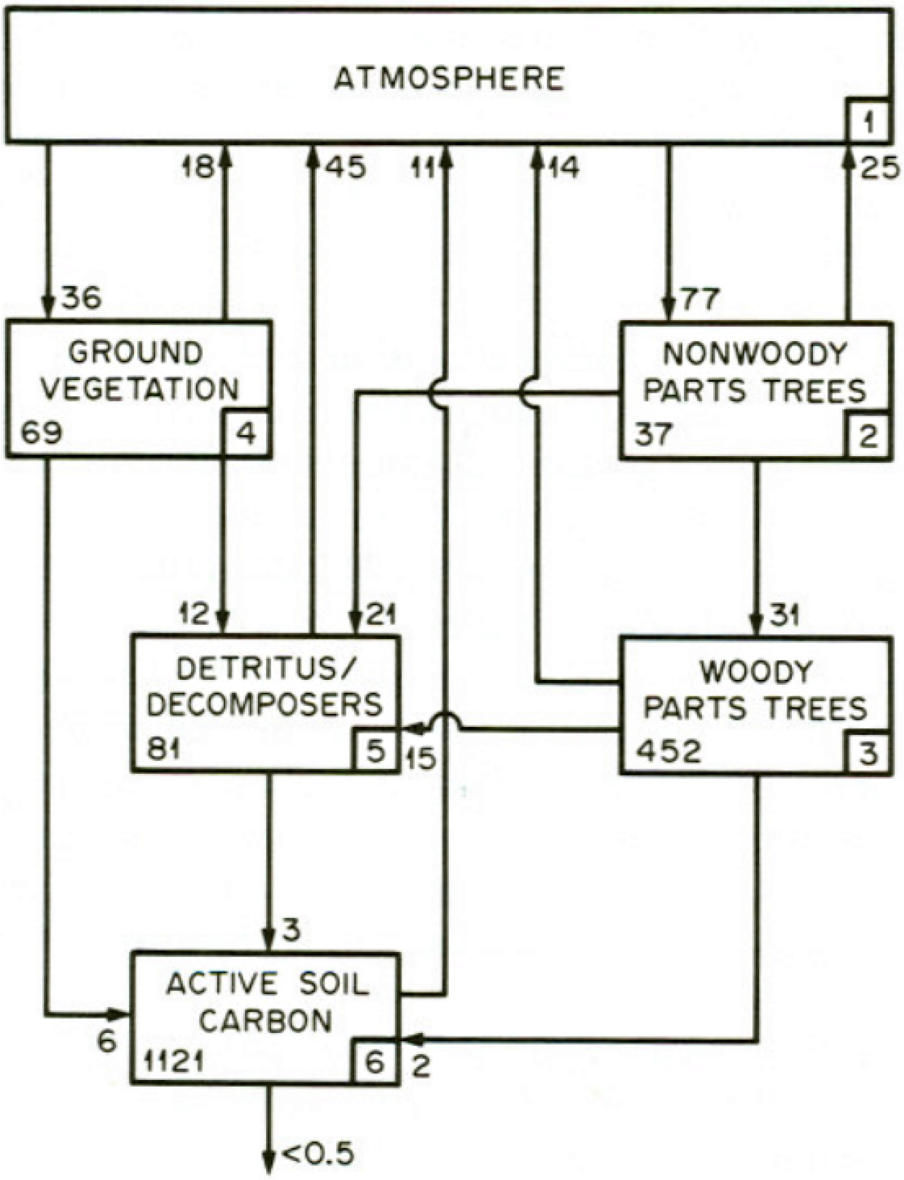


Figure 2.1. Schematic of the linear autonomous global carbon cycle model in steady state introduced by Emanuel et al. (1981). The model comprises five compartments: non-woody tree parts x_1 (2; 37 Pg C), woody tree parts x_2 (3; 452 Pg C), ground vegetation x_3 (4; 69 Pg C), detritus/decomposers x_4 (5; 81 Pg C), and active soil carbon x_5 (6; 1, 121 Pg C). The atmosphere (1) is considered to be outside of the modeled system but provides the system with external inputs and receives external outputs from it. Numbers next to arrows indicate fluxes between compartments in Pg C yr^{-1}. (Figure extracted from Emanuel et al. (1981))

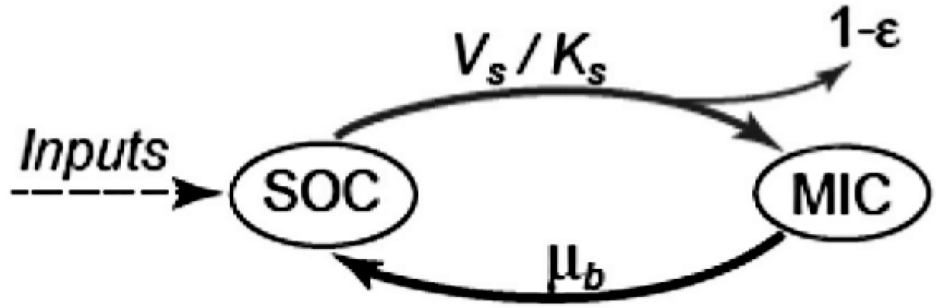


Figure 2.2. Scheme of the nonlinear autonomous carbon cycle model introduced by Wang et al. (2014). The two compartments C_s and C_b are here denoted by soil organic carbon (SOC) and microbial biomass carbon (MIC), the external input flux F_{npp} is denoted by *Inputs*, the maximum rate of soil carbon assimilation by V_s, the half saturation constant by K_s, the carbon use efficiency by ε, and the turnover rate of microbial biomass by μ_b, respectively. (Figure extracted from Wang et al. (2014))

of microbial biomass per year (yr^{-1}), by F_{npp} the carbon influx into soil ($\mathrm{g\,C\,m^{-2}\,yr^{-1}}$), and by V_s and K_s the maximum rate of soil carbon assimilation per unit microbial biomass per year (yr^{-1}) and the half-saturation constant for soil carbon assimilation by microbial biomass ($\mathrm{g\,C\,m^{-2}}$), respectively. Then, we can describe the model by

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} C_s \\ C_b \end{pmatrix} = \begin{pmatrix} -\lambda(\mathbf{x}) & \mu_b \\ \varepsilon\lambda(\mathbf{x}) & -\mu_b \end{pmatrix}\begin{pmatrix} C_s \\ C_b \end{pmatrix} + \begin{pmatrix} F_{npp} \\ 0 \end{pmatrix}.$$

The matrix B depends on $\mathbf{x} = (C_s, C_b)^\top$ through λ's dependence on $\mathbf{x}$, which is given by

$$\lambda(\mathbf{x}) = \frac{C_b V_s}{C_s + K_s}. \tag{2.2}$$

Steady-state formulas for the compartment contents can be computed as

$$C_s^* = \frac{K_s}{\frac{V_s\varepsilon}{\mu_b} - 1} \quad \text{and} \quad C_b^* = \frac{F_{npp}}{\mu_b\left(-1 + \frac{1}{\varepsilon}\right)}.$$

From Wang et al. (2014), we take the parameter values $F_{npp} = 345.00\,\mathrm{g\,C\,m^{-2}\,yr^{-1}}$, $\mu_b = 4.38\,\mathrm{yr}^{-1}$, $\varepsilon = 0.39$, and $K_s = 53{,}954.83\,\mathrm{g\,C\,m^{-2}}$. Since the description of V_s is missing in the original publication, we let it be equal to $59.13\,\mathrm{yr}^{-1}$ to approximately meet the given steady-state compartment contents $C_s^* = 12{,}650.00\,\mathrm{g\,C\,m^{-2}}$ and $C_b^* = 50.36\,\mathrm{g\,C\,m^{-2}}$.

With the given parameters, the steady-state transfer matrix $\mathrm{B} = \mathrm{B}(\mathbf{x}^*)$ and the input vector $\mathbf{u}$ are given by

$$\mathrm{B} = \begin{pmatrix} -0.0447 & 4.38 \\ 0.0174 & -4.38 \end{pmatrix}\mathrm{yr}^{-1} \quad \text{and} \quad \mathbf{u} = \begin{pmatrix} 345.00 \\ 0.00 \end{pmatrix}\mathrm{g\,C\,m^{-2}\,yr^{-1}},$$

respectively. Obviously, the given parameter values lead to an open linear compartmental system in equilibrium. Consequently, again we can ask for the age structure and the transit time of the system.

In contrast to the system from the first example, this system exhibits a feedback. This feedback results from dead soil microbial biomass being considered as new soil organic matter. The feedback can also be recognized by noting that B is not triangular.

2.2. Age, transit time, and remaining lifetime

Even if a compartmental system is in equilibrium, material permanently enters and leaves the system. Consequently, the material in the system is a mix of material with different ages as is the material that leaves the system at some fixed point in time. We aim at finding explicit formulas for the age-, transit-time, and remaining lifetime distributions of compartmental systems in equilibrium.

The advantages of considering systems in equilibrium are twofold. On the one hand, the system's internal dynamics remain unchanged. On the other hand, initial values do not distort the age structure. Consequently, the point in time when we observe the system is negligible. The well-mixedness of the compartments resembles the fact that the history of particles has no influence on their future, while the linearity of the systems reflects that particles behave independently from each other. Consequently, we can look at the typical journey of a single particle and afterwards collect the indefinite amount of single particles with infinitesimal weight and size.

2.2.1. The one-particle perspective

Consider a single particle that enters the system at a compartment according to $\mathbf{u}$ and then, at each time step, whether it stays or moves on is decided on basis of its current position and its schedule. If the decision is to move on, then it can move to another compartment or leave the system, depending only on the connections of the current compartment. The particle follows a schedule and a map given by the compartmental matrix B. The diagonal entries of B govern how long the particle stays in a certain compartment, and the off-diagonal entries provide the connections to other compartments. By leaving the system, the particle finishes a cycle and immediately starts a new one by reentering the system.

During each cycle, the sequence of compartments to which the particle belongs at successive time steps constitutes a stochastic process called *discrete-time Markov chain*. If we let the size of the time steps tend to zero, the particle's future becomes continuously uncertain. We can then represent the particle's path during a single cycle through the system by a *continuous-time Markov chain* (Norris, 1997), which we call X throughout the chapter. When the Markov chain changes its state from j to i, the particle is considered to move from compartment j to compartment i. When the Markov chain is absorbed, the particle leaves the system.

The act of sending the particle back into the system right after leaving has its stochastic counterpart in a regenerative process Z with embedded renewal process $J = (J_n)_{n\geq 0}$. The renewals J_n, $n > 1$, coincide with the regeneration times of Z and represent the reentries of the particle.

It is important to note that, with respect to standard notation in probability theory, we use reversed index order in the following. For instance, in classical probability theory notation we would use $\mathrm{B}^\top$ instead of B and also $\mathrm{Q}^\top$ instead of Q (defined in Eq. (2.4) below). We deviate from the standard notation since the reversed index order is natural for compartmental systems and this way the connections between the deterministic and the stochastic mathematical structures involved become more obvious and notation less confusing.

2.2.2. Compartmental systems and Markov chains

As nonlinear autonomous compartmental systems in equilibrium behave like linear autonomous compartmental systems in equilibrium, for the remainder of this chapter we consider the linear system of ODEs as given by Eq. (1.8), but already starting in equilibrium, i.e.,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) &= \mathrm{B}\,\mathbf{x}(t) + \mathbf{u}, \quad t > 0,\\ \mathbf{x}(0) &= \mathbf{x}^*.\end{aligned} \tag{2.3}$$

Here $\mathbf{u} \in \mathbb{R}^d_+$ and we assume the compartmental matrix B to be invertible to ensure that the system is open. Furthermore, $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ such that the system is in steady state from the very beginning. Without loss of generality, we can then assume $t_0 = 0$.

Compartmental systems and Markov chains are very similar even though the former are deterministic- and the latter are probabilistic objects. We now show that open linear autonomous compartmental systems correspond to absorbing homogeneous continuous-time Markov chains.

Material permanently leaves from the open system (2.3). We close the system by collecting all leaving material in an additional *environmental compartment* $d+1$. To do so, we add another row to the compartmental matrix B to make all column sums equal to zero and we add another column that does not allow material to leave compartment $d+1$ once it has arrived there. The resulting (non-invertible) compartmental matrix is

$$\mathrm{Q} = \begin{pmatrix} \mathrm{B} & \mathbf{0} \\ \mathbf{z}^\top & 0 \end{pmatrix}. \tag{2.4}$$

We recall from Eq. (1.5) that $\mathbf{z}^\top = -\mathbf{1}^\top\,\mathrm{B}$ and see that Q is the transition-rate matrix of an absorbing homogeneous continuous-time Markov chain $X = (X_t)_{t\geq 0}$ on the state space $\{1, 2, \dots, d, d+1\}$. Its absorbing state is state $d+1$. Let

$$\boldsymbol{\beta} := \|\mathbf{u}\|^{-1}\,(u_1, u_2, \dots, u_d)^\top. \tag{2.5}$$

The probability of the continuous-time Markov chain X with initial distribution $\boldsymbol{\beta}$ being in state $j \in S = \{1, 2, \dots, d\}$ at time $t \geq 0$ is

$$\mathbb{P}(X_t = j) = \left(e^{t\,\mathrm{B}}\,\boldsymbol{\beta}\right)_j. \tag{2.6}$$

Assume now that material $\mathbf{u} \in \mathbb{R}^d_+$ comes into system (2.3) at time $\tau > 0$. Since the system is linear, the way how this material will be distributed can be modeled by the homogeneous linear ODE system

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\,\widetilde{\mathbf{x}}(t) &= \mathrm{B}\,\widetilde{\mathbf{x}}(t), \quad t > \tau,\\ \widetilde{\mathbf{x}}(\tau) &= \mathbf{u}.\end{aligned} \tag{2.7}$$

Furthermore, the fractional transfer coefficients of this system are time-independent, so we can shift the entire system to the left and consider it to have started at time $\tau = 0$. From Eq. (1.9), we know that the content of compartment j at time $t \geq 0$ is then given by

$$\widetilde{x}_j(t) = \left(e^{t\,\mathrm{B}}\,\mathbf{u}\right)_j. \tag{2.8}$$

This implies together with definition (2.5) of $\boldsymbol{\beta}$ and Eq. (2.6) that

$$\mathbb{P}(X_t = j) = \frac{\widetilde{x}_j(t)}{\|\mathbf{u}\|}.$$

Consequently, $\mathbb{P}(X_t = j)$ is the proportion of the initially present amount of material in system (2.7) that is in compartment j at time t. Hence, the continuous-time Markov chain X describes the stochastic travel of a single particle through the compartmental system (2.3). When the traveling particle leaves the compartmental system, the process X jumps to the absorbing state $d+1$.

2.2.3. Transit time and absorption time

For compartmental systems, two types of transit time can be considered (Nir & Lewis, 1975) from the one-particle point of view. Recall from Definition 1.16 that the forward transit time $\mathrm{FTT}(t_a)$ is the time that a particle needs to travel through the system after it arrives at time t_a. The backward transit time $\mathrm{BTT}(t_e)$ specifies the age that a particle has at the moment it is leaving the system, i.e., the time it needs to travel through the system given that it exits at time t_e. For an autonomous system in steady state, one would expect the two types of transit time to coincide and to be independent of t_a and t_e, respectively. For now, we will concentrate on the derivation of explicit formulas for the forward transit-time distribution. We turn to the backward transit-time distribution later because it requires results on age distributions of the system.

Recall that the absorbing continuous-time Markov chain $X = (X_t)_{t\geq 0}$ describes the travel of a particle through the compartmental system (2.3). When the particle leaves the system, X jumps to its absorbing state $d+1$.

Definition 2.1 The *absorption time* of a continuous-time Markov chain X is a random variable that tells the moment in time, when X reaches its absorbing state. It is defined by

$$\mathcal{T} := \inf\{\, t \geq 0 : \, X_t = d+1\} \quad (\inf \emptyset := \infty).$$

Lemma 2.2.1 in Neuts (1981) guarantees that $\mathcal{T}$ is finite with probability one if the compartmental matrix B is invertible. Consequently,

$$\lim_{t\to\infty} \mathbb{P}(X_t = i \,|\, X_0 = j) = \lim_{t\to\infty} \left(e^{t\,\mathrm{B}}\right)_{ij} = 0, \quad i, j \in S.$$

This corresponds well with Corollary 1.14 and the idea that every particle will eventually leave the open system (2.3).

Proposition 2.2 *Let $\mathcal{T}$ denote the absorption time of X. Then*

(i) the cumulative probability distribution of $\mathcal{T}$ is given by

$$F_{\mathcal{T}}(t) = 1 - \mathbf{1}^\top e^{t\,\mathrm{B}}\,\boldsymbol{\beta}, \quad t \geq 0, \quad \textit{and}$$

(ii) its probability density function by

$$f_{\mathcal{T}}(t) = \mathbf{z}^\top e^{t\,\mathrm{B}}\,\boldsymbol{\beta}, \quad t \geq 0.$$

Proof. (1) At time $t \geq 0$, the cumulative probability distribution $F_{\mathcal{T}}(t) = \mathbb{P}(\mathcal{T} \leq t)$ of the absorption time $\mathcal{T}$ is equal to the probability of X_t not being in any of the states $j \in S$. Consequently, Eq. (2.6) leads to

$$F_{\mathcal{T}}(t) = 1 - \sum_{j\in S} \mathbb{P}(X_t = j) = 1 - \mathbf{1}^\top e^{t\,\mathrm{B}}\,\boldsymbol{\beta}, \quad t \geq 0.$$

(2) Using $\mathbf{z}^\top = -\mathbf{1}^\top\,\mathrm{B}$ from Eq. (1.5), the probability density function of $\mathcal{T}$ is

$$f_{\mathcal{T}}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\, F_{\mathcal{T}}(t) = \mathbf{z}^\top e^{t\,\mathrm{B}}\,\boldsymbol{\beta}, \quad t \geq 0. \tag{2.9}$$

□

Definition 2.3 A probability distribution according to the probability density function $f_{\mathcal{T}}$ in Eq. (2.9) is called *phase-type distribution* with initial distribution $\boldsymbol{\beta}$ and transition-rate matrix B. We denote it by $\mathrm{PH}(\boldsymbol{\beta}, \mathrm{B})$.

The notation $\mathrm{PH}(\boldsymbol{\beta}, \mathrm{B})$ and the unifying matrix formalism we use here were introduced by Neuts (1981). Phase-type distributions constitute a highly versatile class of probability distributions and are closely related to the solutions of systems of linear differential equations with constant coefficients. As mixtures of exponential distributions they generalize, among others, the Erlang-, the hypoexponential, and the hyperexponential distributions. We have proved the following theorem.

Theorem 2.4 *The forward transit time* FTT *of an open compartmental system in equilibrium with compartmental matrix* B *and input vector* $\mathbf{u}$ *and the absorption time* $\mathcal{T}$ *of an absorbing continuous-time Markov chain with transition-rate matrix* Q *as defined in Eq.* (2.4) *and initial distribution* $\boldsymbol{\beta}$ (2.5) *are identically and phase-type distributed. More precisely,* $\mathrm{FTT}, \mathcal{T} \sim \mathrm{PH}(\boldsymbol{\beta}, \mathrm{B})$.

We collect some properties of the forward transit time that follow immediately from $\mathrm{FTT} \sim \mathrm{PH}(\mathbf{u}/\|\mathbf{u}\|, \mathrm{B})$.

Corollary 2.5 *For* $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ *being the equilibrium of the system,*

(i) the cumulative probability distribution of the forward transit time is given by

$$F_{\mathrm{FTT}}(t) = 1 - \mathbf{1}^\top\, e^{t\,\mathrm{B}}\, \frac{\mathbf{u}}{\|\mathbf{u}\|}, \quad t \geq 0,$$

(ii) its probability density function by

$$f_{\mathrm{FTT}}(t) = \mathbf{z}^\top\, e^{t\,\mathrm{B}}\, \frac{\mathbf{u}}{\|\mathbf{u}\|}, \quad t \geq 0,$$

(iii) its expected value by

$$\mathbb{E}\,[\mathrm{FTT}] = -\mathbf{1}^\top\, \mathrm{B}^{-1}\, \frac{\mathbf{u}}{\|\mathbf{u}\|} = \frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}, \quad \textit{and}$$

(iv) its nth moment by

$$\mathbb{E}\,[(\mathrm{FTT})^n] = (-1)^n\, n!\, \mathbf{1}^\top\, \mathrm{B}^{-n}\, \frac{\mathbf{u}}{\|\mathbf{u}\|}, \quad n \in \mathbb{N}.$$

Here, $n! = n\,(n-1)\cdots 2\cdot 1$ *denotes the factorial of* n *with the convention* $0! := 1$.

Remark 2.6 (1) Since for the forward transit time only the future after the particle's arrival is considered and not the past, Theorem 2.4 and Corollary 2.5 hold still true even if the linear autonomous compartmental system is not in equilibrium.

(2) The relation $\mathbb{E}\,[\mathcal{T}] = \mathbb{E}\,[\mathrm{FTT}] = \|\mathbf{x}^*\|/\|\mathbf{u}\|$ (mean forward transit time equals total stocks over total inputs) will be used frequently throughout this thesis without mentioning it each single time. It is helpful to always keep it in mind.

2.2.4. Steady state and occupation time

The Markov chain $X = (X)_{t\geq 0}$ takes on different states $i \in S$ before it is absorbed. We are now interested in the connection of the steady state of the compartmental system (2.3) and occupation times of X.

Definition 2.7 The *occupation time* of state $i \in S$ by the absorbing continuous-time Markov chain X is the time that X spends in state i before absorption. It is defined by $O_i := \int_0^\infty \mathbb{1}_{\{X_t=i\}}\,\mathrm{d}t$, and we denote by $\mathbf{O} := (O_i)_{i\in S}$ the corresponding *occupation time vector*.

Furthermore, we define the *partial occupation time* of state $i \in S$ by X as the time that X spends in i before a fixed time $y \geq 0$. It is given by $O_i(y) := \int_0^y \mathbb{1}_{\{X_t=i\}}\,\mathrm{d}t$. We denote the corresponding vector by $\mathbf{O}(y) := (O_i(y))_{i\in S}$.

Lemma 2.8 *(1) The steady-state compartment content x_i^* for $i \in S$ is proportional to the expected occupation time of state i by the absorbing continuous-time Markov chain X. More precisely,*

$$x_i^* = \|\mathbf{u}\|\,\mathbb{E}\,[O_i]\,.$$

(2) The sum of the mean occupation times of all states results in the mean forward transit time of the compartmental system, i.e.,

$$\sum_{i\in S} \mathbb{E}\,[O_i] = \mathbb{E}\,[\mathcal{T}] = \mathbb{E}\,[\mathrm{FTT}]\,.$$

Proof. (1) Using $\mathbb{E}\left[\mathbb{1}_{\{X_t=i\}}\right] = \mathbb{P}(X_t = i)$, the stead-state content of compartment $i \in S$ can be computed to

$$\|\mathbf{u}\|\,\mathbb{E}\,[O_i] = \|\mathbf{u}\| \int_0^\infty \mathbb{P}(X_t = i)\,\mathrm{d}t = \int_0^\infty \left(e^{t\,\mathrm{B}}\,\mathbf{u}\right)_i\,\mathrm{d}t = \left(-\mathrm{B}^{-1}\,\mathbf{u}\right)_i = x_i^*. \tag{2.10}$$

(2) We sum the occupation times over all states $i \in S$ and obtain

$$\sum_{i\in S} \mathbb{E}\,[O_i] = \sum_{i\in S} \frac{x_i^*}{\|\mathbf{u}\|} = \frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|} = \mathbb{E}\,[\mathcal{T}]\,.$$

□

The following result is already well known (Anderson, 1983, Section 14A) and it helps understand the meaning of $-\mathrm{B}^{-1}$.

Proposition 2.9 *The matrix entry $(-\mathrm{B}^{-1})_{ij}$ is the mean time the Markov chain X stays in state $i \in S$ before absorption, given it starts in state $j \in S$ at time t_0.*

Proof. We can compute the conditional occupation time of state i by X given $X_0 = j$ by

$$\begin{aligned}
\mathbb{E}\,[O_i \,|\, X_0 = j] &= \frac{\mathbb{E}\left[O_i \cdot \mathbb{1}_{\{X_0=j\}}\right]}{\mathbb{P}(X_0 = j)} = \frac{\mathbb{E}\left[\int_0^\infty \mathbb{1}_{\{X_t=i,\,X_0=j\}}\,\mathrm{d}t\right]}{\mathbb{P}(X_0 = j)} \\
&= \int_0^\infty \mathbb{P}(X_t = i \,|\, X_0 = j)\,\mathrm{d}t = \int_0^\infty \left(e^{t\,\mathrm{B}}\right)_{ij}\,\mathrm{d}t \\
&= \left(-\mathrm{B}^{-1}\right)_{ij}\,.
\end{aligned}$$

□

2.2.5. Release and last state before absorption

For $j \in S$, the release of material from compartment j at time $t \geq 0$ to the environment is denoted by $r_j(t)$. It can be computed as the product of the rate $z_j(t)$ of material leaving compartment j toward the environment and the amount of material $x_j(t)$ contained in compartment j. For a system in steady state, $z_j(t) = z_j$ and $x_j(t) = x_j^*$ remain constant, and consequently $r_j = z_j\, x_j^*$ remains constant as well. Probabilistically, we expect r_j to be connected to the probability of the absorbing continuous-time Markov chain X to be absorbed through state j, i.e., that j is the last state of X before X jumps to its absorbing state $d+1$.

Lemma 2.10 *Let $E \in S$ denote the last state that X visits before it is absorbed by state $d+1$. Then*

$$\mathbb{P}(E = j) = z_j\, \left(-\mathrm{B}^{-1}\,\boldsymbol{\beta}\right)_j = \frac{r_j}{\|\mathbf{u}\|}, \quad j \in S,$$

i.e., the probability of a state j being the last one before absorption is proportional to the release from j to the environment.

Proof. Let $f_{\mathcal{T}}(t \,|\, X_t = j)$ be the conditional probability density function of the absorption time $\mathcal{T}$ of X at time t, given that $X_t = j$. Then,

$$\mathbb{P}(E = j) = \int\limits_0^\infty f_{\mathcal{T}}(t \,|\, X_t = j)\, \mathbb{P}(X_t = j)\, \mathrm{d}t. \tag{2.11}$$

From Eq. (2.6), we know $\mathbb{P}(X_t = j) = \left(e^{t\,\mathrm{B}}\,\boldsymbol{\beta}\right)_j$. We are left with computing the conditional probability density function. Because X is homogeneous,

$$f_{\mathcal{T}}(t \,|\, X_t = j) = f_{\mathcal{T}}(0 \,|\, X_0 = j).$$

As this is a probability density function, we can compute it by

$$f_{\mathcal{T}}(t \,|\, X_t = j) = \frac{\mathrm{d}}{\mathrm{d}t}\, \mathbb{P}(\mathcal{T} \leq t \,|\, X_t = j)$$

if the derivative exists, and evaluate it at $t = 0$. With $\mathbf{z}^\top = -\mathbf{1}^\top\,\mathrm{B}$ from Eq. (1.5) we obtain

$$\begin{aligned} f_{\mathcal{T}}(0 \,|\, X_0 = j) &= \frac{\mathrm{d}}{\mathrm{d}t}\left[1 - \sum_{i \in S} \left(e^{t\,\mathrm{B}}\right)_{ij}\right]_{t=0} \\ &= -\sum_{i \in S} \left(\mathrm{B}\, e^{t\,\mathrm{B}}\right)_{ij}\Big|_{t=0} \\ &= -\sum_{i \in S} B_{ij} \\ &= z_j. \end{aligned}$$

We plug $f_{\mathcal{T}}(t \,|\, X_t = j) = z_j$ in Eq. (2.11) and get

$$\mathbb{P}(E = j) = \int\limits_0^\infty z_j\, \mathbb{P}(X_t = j)\, \mathrm{d}t = z_j \int\limits_0^\infty \left(e^{t\,\mathrm{B}}\,\boldsymbol{\beta}\right)_j\, \mathrm{d}t = z_j\, \left(-\mathrm{B}^{-1}\,\boldsymbol{\beta}\right)_j, \tag{2.12}$$

which by Eq. (2.10) and $\boldsymbol{\beta} = \mathbf{u}/\|\mathbf{u}\|$ turns into

$$\mathbb{P}(E = j) = z_j \, \mathbb{E}\,[O_j] = z_j \, \frac{x_j^*}{\|\mathbf{u}\|} = \frac{r_j}{\|\mathbf{u}\|}.$$

□

Corollary 2.11 *Summing $\mathbb{P}(E = j)$ over all $j \in S$, we get*

$$\|\mathbf{r}\| = \|\mathbf{u}\|, \tag{2.13}$$

since absorption of X is certain. Hence, in steady state the total release equals the total input.

2.2.6. Age, occupation time, and backward recurrence time

Recall from Concept 1.15 that the age of material in the system or in a particular compartment is the time span between its entry into the system and the current time. The steady-state content $\mathbf{x}^*$ of system (2.3) has an age structure such that

$$x_j^* = \lim_{y \to \infty} P_j(y), \quad y \geq 0,$$

where $P_j(y)$ is the amount of material in compartment $j \in S$ that is not older than y. We call P_j the *cumulative compartment-age distribution* of compartment j. Furthermore, each compartment has a nonnegative *compartment-age density function* p_j such that

$$P_j(y) = \int_0^y p_j(\sigma) \, \mathrm{d}\sigma, \quad y \geq 0.$$

We collect the cumulative compartment-age distributions P_j and the compartment-age density functions p_j in the *cumulative age distribution vector* $\mathbf{P} := (P_j)_{j \in S}$ and in the *age density function vector* $\mathbf{p} := (p_j)_{j \in S}$, respectively, such that

$$\mathbf{x}^* = \lim_{y \to \infty} \mathbf{P}(y) = \int_0^\infty \mathbf{p}(\sigma) \, \mathrm{d}\sigma.$$

Our next goal is to find a reasonable explicit definition for $\mathbf{P}$ and $\mathbf{p}$. In population dynamics, it is well known that the McKendrick-von Foerster equation governs the evolution of a population's size and its age structure (McKendrick, 1926; von Foerster, 1959). In resemblance of our notation, the one-dimensional McKendrick-von Foerster equation is given by

$$\frac{\partial}{\partial y} p(y,t) + \frac{\partial}{\partial t} p(y,t) = -\kappa(y,t) \, p(y,t),$$

where $p(y,t)$ denotes the age density of the size of the population with age y at time t, and κ is an age- and time-dependent death-rate function. In the spirit of this equation, an age density function vector of the compartmental system (2.3) should satisfy some sort of multi-dimensional McKendrick-von Foerster equation, where the according death-rate function κ is independent of the age y since all compartments are well mixed, and κ is also independent of time t because the system is in equilibrium.

We look at the general solution equation (1.9) of the linear autonomous compartmental system (2.3) and conjecture tentatively, for $y \geq 0$,

$$\begin{aligned} \mathbf{P}(y) &= \lim_{t\to\infty} \int\limits_{t-y}^{t} e^{(t-\tau)\,\mathrm{B}}\,\mathbf{u}\,\mathrm{d}\tau = \int\limits_{0}^{y} e^{\sigma\,\mathrm{B}}\,\mathbf{u}\,\mathrm{d}\sigma \\ &= \left(e^{y\,\mathrm{B}} - \mathrm{I}\right)\mathrm{B}^{-1}\,\mathbf{u} = \left(\mathrm{I} - e^{y\,\mathrm{B}}\right)\,\mathbf{x}^*, \end{aligned} \tag{2.14}$$

because the material $\mathbf{u}$ coming into the system at time $\tau \in [t-y, t]$ has age $\sigma = t - \tau \leq y$ at time t, and only the amount $e^{(t-\tau)\,\mathrm{B}}\,\mathbf{u}$ of it is still present at time t. From Eq. (2.14), we immediately derive the tentative age density function vector

$$\mathbf{p}(y) = e^{y\,\mathrm{B}}\,\mathbf{u}, \quad y \geq 0. \tag{2.15}$$

Proposition 2.12 *The tentative age density function vector as given by Eq.* (2.15) *satisfies the multi-dimensional McKendrick-von Foerster equation*

$$\left(\frac{\partial}{\partial y} + \frac{\partial}{\partial t}\right)\mathbf{p}(y) = \mathrm{B}\,\mathbf{p}(y), \quad y \geq 0, \tag{2.16}$$

where the compartmental matrix B *plays the role of an age- and time-independent death rate.*

Proof. We consider the left hand side of Eq. (2.16) and see

$$\left(\frac{\partial}{\partial y} + \frac{\partial}{\partial t}\right)\mathbf{p}(y) = \frac{\mathrm{d}}{\mathrm{d}y}\,\mathbf{p}(y) = \frac{\mathrm{d}}{\mathrm{d}y}\,e^{y\,\mathrm{B}}\,\mathbf{u} = \mathrm{B}\,e^{y\,\mathrm{B}},$$

which obviously coincides with the right hand side. □

This result motivates the following definition.

Definition 2.13 The *cumulative age distribution vector* of system (2.3) is given by

$$\mathbf{P}(y) = \left(\mathrm{I} - e^{y\,\mathrm{B}}\right)\mathbf{x}^*, \quad y \geq 0,$$

and the corresponding *age density function vector* by

$$\mathbf{p}(y) = e^{y\,\mathrm{B}}\,\mathbf{u}, \quad y \geq 0.$$

In this chapter, we aim at drawing links between properties of deterministic compartmental systems and probabilistic Markov chains. In order to do so for the age structure of the system, we introduce the random age vector $\mathbf{a} = (a_j)_{j\in S}$ such that the random variable a_j describes the age of a randomly picked particle from compartment j. The cumulative probability distribution of a_j and the corresponding probability density function can be obtained by normalizing, i.e., by dividing the cumulative compartment-age distribution P_j and the associated compartment-age density function p_j by the corresponding compartment content x_j^*.

Definition 2.14 For $j \in S$, the random variable a_j with probability density function

$$f_{a_j}(y) = \frac{1}{x_j^*}\,p_j(y), \quad y \geq 0,$$

is called *compartment age* of compartment j, while the random variable A with probability density function

$$f_A(y) = \frac{1}{\|\mathbf{x}^*\|}\,\|\mathbf{p}(y)\|,\quad y \geq 0,$$

is called *system age*. The random vector $\mathbf{a} = (a_j)_{j\in S}$ is called *compartment age vector.*

Corollary 2.15 *Let* $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ *be the steady-state vector,* $\mathrm{X}^* := \mathrm{diag}(x_1^*, x_2^*, \ldots, x_d^*)$, *and* $\mathbf{a}$ *the compartment-age vector of the compartmental system* (2.3)*. Then,*

(i) the cumulative probability distribution vector of $\mathbf{a}$ *is given by*

$$F_{\mathbf{a}}(y) = \mathbf{1} - (\mathrm{X}^*)^{-1}\,e^{y\,\mathrm{B}}\,\mathbf{x}^*,\quad y \geq 0,$$

(ii) its probability density function vector by

$$f_{\mathbf{a}}(y) = (\mathrm{X}^*)^{-1}\,e^{y\,\mathrm{B}}\,\mathbf{u},\quad y \geq 0,$$

(iii) its vector of expected values by

$$\mathbb{E}\,[\mathbf{a}] = -(\mathrm{X}^*)^{-1}\,\mathrm{B}^{-1}\,\mathbf{x}^*,\quad \textit{and}$$

(iv) its vector of nth moments by

$$\mathbb{E}\,[\mathbf{a}^n] = (-1)^n\,n!\,(\mathrm{X}^*)^{-1}\,\mathrm{B}^{-n}\,\mathbf{x}^*,\quad n \in \mathbb{N}.$$

As each compartment has one, also the entire system has an unknown age probability density function f_A, where A can be interpreted as the age of a randomly picked particle from the system. We denote the cumulative probability distribution of A by F_A.

Corollary 2.16 *Let* $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ *be the steady-state vector,* $\mathrm{X}^* = \mathrm{diag}(x_1^*, x_2^*, \ldots, x_d^*)$, *and* A *the system age of the compartmental system* (2.3)*. Then*

(i) the cumulative probability distribution of the system age A *is given by*

$$F_A(y) = 1 - \mathbf{1}^\top\,e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|},\quad y \geq 0,$$

(ii) its probability density function by

$$f_A(y) = \mathbf{z}^\top\,e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|},\quad y \geq 0.$$

(iii) its expected value by

$$\mathbb{E}\,[A] = -\mathbf{1}^\top\,\mathrm{B}^{-1}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|},\quad \textit{and}$$

(iv) its nth moment by

$$\mathbb{E}\,[A^n] = (-1)^n\,n!\,\mathbf{1}^\top\,\mathrm{B}^{-n}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|},\quad n \in \mathbb{N}.$$

Proof. We sum P_j over all compartments $j \in S$, normalize by dividing by the total system content $\|\mathbf{x}^*\|$, and use $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ to see, for $y \geq 0$,

$$F_A(y) = \frac{1}{\|\mathbf{x}^*\|} \sum_{j\in S} P_j(y) = \frac{1}{\|\mathbf{x}^*\|} \sum_{j\in S} \left(\mathbf{x}^* - e^{y\,\mathrm{B}}\,\mathbf{x}^*\right)_j = 1 - \mathbf{1}^\top e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|}.$$

To obtain $f_A(y)$, we take the derivative of $F_A(y)$ with respect to y and use $\mathbf{z}^\top = -\mathbf{1}^\top\,\mathrm{B}$ from Eq. (1.5). The rest is done by straightforward calculation. □

Remark 2.17 We immediately notice that the system age is phase-type distributed. In contrast to the forward transit time with initial distribution $\boldsymbol{\beta} = \mathbf{u}/\|\mathbf{u}\|$, the initial distribution for the system age is $\boldsymbol{\eta} := \mathbf{x}^*/\|\mathbf{x}^*\|$. Consequently, the system age A can also be interpreted as the forward transit time $\widetilde{\mathcal{T}}$ of a linear autonomous compartmental system with constant external input vector $\widetilde{\mathbf{u}} := \mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$.

Since we are interested in a connection between the age of material in the compartmental system (2.3) and the absorbing continuous-time Markov chain X, we use Lemma 2.8 to see

$$\mathbf{P}(y) = \left(\mathrm{I} - e^{y\,\mathrm{B}}\right)\mathbf{x}^* = \left(\mathrm{I} - e^{y\,\mathrm{B}}\right)\,\|\mathbf{u}\|\,\mathbb{E}\left[\mathbf{O}\right].$$

Immediately, we recognize a link between the cumulative age distribution vector and the vector $\mathbb{E}\left[\mathbf{O}\right]$ of mean occupation times of the absorbing continuous-time Markov chain X.

Lemma 2.18 *The cumulative age distribution vector of the compartmental system* (2.3) *and the partial occupation times of the absorbing continuous-time Markov chain X are connected through*

$$\mathbf{P}(y) = \|\mathbf{u}\|\,\mathbb{E}\left[\mathbf{O}(y)\right], \quad y \geq 0.$$

Proof. For $i \in S$ and $y \geq 0$, we compute

$$\|\mathbf{u}\|\,\mathbb{E}\left[O_i(y)\right] = \|\mathbf{u}\|\,\mathbb{E}\left[\int_0^y \mathbb{1}_{\{X_t=i\}}\,\mathrm{d}t\right] = \|\mathbf{u}\| \int_0^y \mathbb{P}(X_t = i)\,\mathrm{d}t = \int_0^y \left(e^{t\,\mathrm{B}}\,\mathbf{u}\right)_i\,\mathrm{d}t,$$

which by Eq. (2.14) finishes the proof. □

To this point, we have drawn a connection between age distributions of the compartmental system (2.3) and occupation times of the absorbing continuous-time Markov chain X defined in Section 2.2.2. There is another interesting relation, namely between occupation times of X and renewal/regenerative processes, which in turn links the latter also to compartment- and system ages.

We take up again the continuous-time Markov chain $X = (X_t)_{t\geq 0}$ which describes the travel of a single particle through the compartmental system. In contrast to earlier situations, we now let the particle reenter the system immediately after it has left, and we do so over and over again. We obtain a sequence $(Z^n)_{n\geq 1}$ with $Z_1 := X$, of independent cycles, all behaving like X, and a sequence of reentry times $J := (J_n)_{n\geq 0}$ with $J_0 := 0$. The sequence $J = (J_n)_{n\geq 0}$ of the particle's reentry times constitutes a renewal process with interarrival times $T_n = J_n - J_{n-1}\,(n \in \mathbb{N})$, $T_0 := 0$, and $T_1 = \mathcal{T}$. The reentry times of the particle are the renewals of J. The interarrival-time distribution is the phase-type distribution describing the absorption time $\mathcal{T}$of X. Hence $F_{\mathcal{T}}$ is the interarrival-time cumulative probability distribution. The number of renewals/reentries up to time $t \geq 0$ is defined by

$$N_t := \max\{\, n \geq 0 :\; J_n \leq t\}.$$

Now, we define a continuous-time process on the state space S by glueing the Z^n's together. For $t \geq 0$,

$$Z_t := \begin{cases} Z^n_{t-J_{n-1}}, & J_{n-1} \leq t < J_n \text{ and } n \in \mathbb{N}, \\ 0, & \text{else.} \end{cases} \tag{2.17}$$

The process $Z = (Z_t)_{t\geq 0}$ is a regenerative process, because after each renewal a new cycle begins, which is independent of the previous cycles and governed by the same probability law as them. The cycle lengths of Z coincide with the interarrival times of J, the embedded renewal process of Z.

Definition 2.19 Let $t \geq 0$. The time span $A_t := t - J_{N_t}$ is called *backward recurrence time* and the time span $L_t := J_{N_t+1} - t$ is called *forward recurrence time* of J at time t.

Let additionally $Z_t = j \in S$. Then $A^j_t := t - J_{N_t}$ is called *j-conditional backward recurrence time* and the time span $L^j_t := J_{N_t+1} - t$ is called *j-conditional forward recurrence time* of Z at time t.

In other words, A_t describes the time that has elapsed since the last renewal and L_t the time span until the next renewal. The conditional recurrence times consider A_t and L_t under the condition of Z_t being in a predefined, fixed state.

For fixed $t \geq 0$, $y \geq 0$, and $j \in S$, the corresponding cumulative probability distributions are given by

$$\begin{aligned} F_{A_t}(y) &= \mathbb{P}(A_t \leq y), \\ F_{A^j_t}(y) &= \mathbb{P}(A_t \leq y \,|\, Z_t = j), \\ F_{L_t}(y) &= \mathbb{P}(L_t \leq y), \quad \text{and} \\ F_{L^j_t}(y) &= \mathbb{P}(L_t \leq y \,|\, Z_t = j). \end{aligned}$$

The following lemma is the cornerstone to connect occupation times of X with the regenerative process Z. It results from a straightforward application of Theorem VI.1.2 in Asmussen (2003) to the indicator function. The limiting probability (as $t \to \infty$) of a regenerative process, with the same cycle lengths as Z, of being in a certain state equals the fraction of time of the process being in this state during the first cycle.

Lemma 2.20 *Let $Y = (Y_t)_{t\geq 0}$ be a regenerative process with the same embedded renewal process as Z and state space $S_Y := \{0, 1, \ldots, m\}$ for some $m \in \mathbb{N}$. Then, for $j \in S_Y$,*

$$\lim_{t\to\infty} \mathbb{P}(Y_t = j) = \frac{1}{\mathbb{E}[\mathcal{T}]}\, \mathbb{E}\left[\int_0^{\mathcal{T}} \mathbb{1}_{\{Y_t = j\}} \, \mathrm{d}t\right].$$

Lemma 2.21 *The limiting distribution of Z as defined in Eq.* (2.17) *satisfies*

$$\lim_{t\to\infty} \mathbb{P}(Z_t = j) = \frac{\mathbb{E}[O_j]}{\mathbb{E}[\mathcal{T}]} = \frac{x^*_j}{\|\mathbf{x}^*\|} = \eta_j.$$

Proof. We apply Lemma 2.20 to Z and then use Lemma 2.8 and $\mathbb{E}[\mathcal{T}] = \|\mathbf{x}^*\|/\|\mathbf{u}\|$. □

Now we are left with bringing the partial occupation times $O_j(y)$ come into the game.

Lemma 2.22 *Let Z denote the process defined in Eq.* (2.17), *and fix $y \geq 0$. Then*

$$\lim_{t\to\infty} \mathbb{P}(A_t \leq y, Z_t = j) = \frac{\mathbb{E}[O_j(y)]}{\mathbb{E}[\mathcal{T}]}, \quad j \in S.$$

Proof. We fix $j \in S$ and $y \geq 0$. Now we define a two-valued regenerative process $Y^j(y) = (Y_t^j(y))_{t\geq 0}$ with embedded renewal process J by

$$Y_t^j(y) := \begin{cases} 1, & A_t \leq y \text{ and } Z_t = j, \\ 0, & \text{else.} \end{cases}$$

We apply Lemma 2.20 to $Y^j(y)$ and obtain

$$\begin{aligned} \lim_{t\to\infty} \mathbb{P}(Y_t^j(y) = 1) &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\,\mathbb{E}\left[\int_0^{\mathcal{T}} \mathbb{1}_{\{Y_\tau^j(y)=1\}}\,\mathrm{d}\tau\right] = \frac{1}{\mathbb{E}\,[\mathcal{T}]}\,\mathbb{E}\left[\int_0^{\mathcal{T}} \mathbb{1}_{\{A_\tau\leq y,\,X_\tau=j\}}\,\mathrm{d}\tau\right] \\ &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\,\mathbb{E}\left[\int_0^{y} \mathbb{1}_{\{X_\tau=j\}}\,\mathrm{d}\tau\right] = \frac{\mathbb{E}\,[O_j(y)]}{\mathbb{E}\,[\mathcal{T}]}. \end{aligned}$$

□

Theorem 2.23 *(1) Let $j \in S$. The cumulative probability distribution of the j-conditional backward recurrence time A_t^j of the regenerative process Z converges with $t \to \infty$ to the cumulative probability distribution of the compartment age a_j of the compartmental system* (2.3)*.*

(2) The cumulative probability distribution of the backward recurrence time A_t of the regenerative process Z converges with $t \to \infty$ to the cumulative probability distribution of the system age A of the compartmental system (2.3)*.*

Proof. We fix $y \geq 0$.

(1) From Lemma 2.18 we know $P_j(y) = \|\mathbf{u}\|\,\mathbb{E}\,[O_j(y)]$. Together with Lemma 2.22 this yields

$$\begin{aligned} P_j(y) &= \|\mathbf{u}\|\,\mathbb{E}\,[\mathcal{T}]\,\lim_{t\to\infty} \mathbb{P}(A_t \leq y, Z_t = j) \\ &= \|\mathbf{u}\|\,\mathbb{E}\,[\mathcal{T}]\,\lim_{t\to\infty} \mathbb{P}(A_t \leq y \,|\, Z_t = j)\,\mathbb{P}(Z_t = j), \end{aligned}$$

and hence by Lemma 2.21

$$\begin{aligned} P_j(y) &= \|\mathbf{u}\|\,\frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}\,\lim_{t\to\infty} \mathbb{P}(A_t \leq y \,|\, Z_t = j)\,\frac{x_j^*}{\|\mathbf{x}^*\|} \\ &= x_j^*\,\lim_{t\to\infty} \mathbb{P}(A_t \leq y \,|\, Z_t = j). \end{aligned}$$

We normalize by dividing by x_j^* and obtain

$$F_{a_j}(y) = \lim_{t\to\infty} \mathbb{P}(A_t \leq y \,|\, Z_t = j) = \lim_{t\to\infty} F_{A_t^j}(y),$$

which finishes the proof of (1).

(2) As in the first part of the proof, we know

$$P_j(y) = \|\mathbf{u}\|\,\mathbb{E}\,[\mathcal{T}]\,\lim_{t\to\infty} \mathbb{P}(A_t \leq y, Z_t = j)$$

and hence

$$\sum_{j\in S} P_j(y) = \|\mathbf{u}\|\,\frac{\|\mathbf{x}^*\|}{\|\mathbf{u}\|}\,\lim_{t\to\infty} \mathbb{P}(A_t \leq y).$$

We normalize by dividing by $\|\mathbf{x}^*\|$ and obtain

$$F_A(y) = \lim_{t\to\infty} \mathbb{P}(A_t \leq y) = \lim_{t\to\infty} F_{A_t}(y),$$

and the proof is finished. □

Remark 2.24 By Theorem 2.23 and Lemma 2.22,

$$\begin{aligned} F_A(y) &= \lim_{t\to\infty} \mathbb{P}(A_t \le y) = \lim_{t\to\infty} \sum_{j\in S} \mathbb{P}(A_t \le y, Z_t = j) \\ &= \frac{1}{\mathbb{E}[\mathcal{T}]} \sum_{j\in S} \mathbb{E}[O_j(y)] = \frac{1}{\mathbb{E}[\mathcal{T}]} \int_0^y \sum_{j\in S} \mathbb{P}(X_t = j)\,\mathrm{d}t \\ &= \frac{1}{\mathbb{E}[\mathcal{T}]} \int_0^y [1 - F_{\mathcal{T}}(t)]\,\mathrm{d}t. \end{aligned}$$

Consequently, F_A is the cumulative probability distribution of the stationary distribution of Z's embedded renewal process J. Hence, F_A reflects the relation of the steady state of the compartmental system (2.3) and an infinite history of the regenerative process Z.

2.2.7. Remaining lifetime and forward recurrence time

Recall from Definition 1.17 that the remaining lifetime of material in the system is the length of the time period until its exit from the system. The remaining compartment lifetime vector $\mathbf{l} := (l_j)_{j\in S}$ has an unknown probability density function vector $f_{\mathbf{l}}$ and we denote its cumulative probability distribution vector by $F_{\mathbf{l}}$.

Proposition 2.25 *We consider the compartmental system* (2.3)*. For $j \in S$,*

(i) the cumulative probability distribution of compartment j's remaining lifetime l_j is given by

$$F_{l_j}(y) = 1 - \sum_{i\in S} \left(e^{y\,\mathrm{B}}\right)_{ij}, \quad y \ge 0,$$

(ii) its probability density function by

$$f_{l_j}(y) = -\sum_{i\in S} \left(\mathrm{B}\, e^{y\,\mathrm{B}}\right)_{ij} = \sum_{i\in S} z_i \left(e^{y\,\mathrm{B}}\right)_{ij}, \quad y \ge 0,$$

(iii) its expected value by

$$\mathbb{E}[l_j] = -\sum_{i\in S} \left(\mathrm{B}^{-1}\right)_{ij}, \quad \textit{and}$$

(iv) its nth moment by

$$\mathbb{E}[(l_j)^n] = (-1)^n\, n! \sum_{i\in S} \left(\mathrm{B}^{-n}\right)_{ij}, \quad n \in \mathbb{N}.$$

Proof. In steady state, compartment j contains an amount x_j^* of material. Following Eq. (2.8), $y \ge 0$ units of time later the amount $\sum_{i\in S}(e^{y\,\mathrm{B}})_{ij}\, x_j^*$ of that is remaining in the system. Consequently, the proportion of material in compartment j at an arbitrary point in time that is still the system at y time units later is then $\sum_{i\in S}(e^{y\,\mathrm{B}})_{ij}$, and

$$F_{l_j}(y) = 1 - \sum_{i\in S}(e^{y\,\mathrm{B}})_{ij}, \quad y \ge 0.$$

The remaining statements follow from straightforward computations. □

The time L that the material in the system is going to remain is called remaining system lifetime. We denote its probability density function by f_L and its cumulative probability distribution by F_L.

Proposition 2.26 *The cumulative probability distribution of the remaining system lifetime L of the compartmental system* (2.3) *is given by*

$$F_L(y) = 1 - \mathbf{1}^\top e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|}, \quad y \geq 0.$$

Proof. The system contains an amount x_j^* of material in compartment j. Following (2.8), $y \geq 0$ units of time later the amount $\sum_{i\in S}(e^{y\,\mathrm{B}})_{ij}\,x_j^*$ of that is remaining in the system. Consequently, the proportion of material in the system at an arbitrary point in time that is still the system y time units later, is then

$$\sum_{j\in S}\sum_{i\in S}\left(e^{y\,\mathrm{B}}\right)_{ij}\,\frac{x_j^*}{\|\mathbf{x}^*\|}.$$

Hence,

$$\begin{aligned} F_L(y) &= 1 - \sum_{i\in S}\sum_{j\in S}(e^{y\,\mathrm{B}})_{ij}\,\frac{x_j^*}{\|\mathbf{x}^*\|} = 1 - \sum_{i\in S}\left(e^{y\,\mathrm{B}}\,\mathbf{x}^*\right)_i\,\frac{1}{\|\mathbf{x}^*\|} \\ &= 1 - \mathbf{1}^\top e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|}. \end{aligned}$$

□

Theorem 2.27 *(1) Let $j \in S$. The cumulative probability distribution of the j-conditional forward recurrence time L_t^j of the regenerative process Z converges with $t \to \infty$ to the cumulative probability distribution of the remaining compartment lifetime l_j j of the compartmental system* (2.3)*.*

(2) The cumulative probability distribution of the forward recurrence time L_t of the regenerative process Z converges with $t \to \infty$ to the cumulative probability distribution of the remaining system lifetime L of the compartmental system (2.3)*.*

Proof. (1) For $j \in S$ and $y \geq 0$,

$$\lim_{t\to\infty} F_{L_t^j}(y) = \lim_{t\to\infty} \mathbb{P}(L_t \leq y \,|\, Z_t = j) = \lim_{t\to\infty} \frac{\mathbb{P}(L_t \leq y, Z_t = j)}{\mathbb{P}(Z_t = j)}.$$

We start with the numerator and define a two-valued regenerative process

$$Y^j(y) = (Y_t^j(y))_{t\geq 0}$$

with embedded renewal process J by

$$Y_t^j(y) := \begin{cases} 1, & L_t \leq y \text{ and } Z_t = j, \\ 0, & \text{else.} \end{cases}$$

We apply Lemma 2.20 to $Y^j(y)$ and obtain

$$\begin{aligned}\lim_{t\to\infty} \mathbb{P}(L_t \le y,\, Z_t = j) &= \lim_{t\to\infty} \mathbb{P}(Y_t^j(y) = 1)\\ &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\,\mathbb{E}\left[\int_0^{\mathcal{T}} \mathbb{1}_{\{Y_\tau^j(y)=1\}}\,\mathrm{d}\tau\right]\\ &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\,\mathbb{E}\left[\int_0^{\mathcal{T}} \mathbb{1}_{\{L_\tau\le y,\,X_\tau=j\}}\,\mathrm{d}\tau\right].\end{aligned}$$

For $\tau \le \mathcal{T}$, obviously $\{L_\tau \le y\} = \{\mathcal{T} \le \tau + y\}$. Furthermore, $X_\tau = j$ guarantees $\tau \le \mathcal{T}$. Hence,

$$\begin{aligned}\lim_{t\to\infty} \mathbb{P}(L_t \le y,\, Z_t = j) &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\,\mathbb{E}\left[\int_0^{\infty} \mathbb{1}_{\{\mathcal{T}\le\tau+y,\,X_\tau=j\}}\,\mathrm{d}\tau\right]\\ &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\int_0^{\infty} \mathbb{P}(\mathcal{T} \le \tau + y, X_\tau = j)\,\mathrm{d}\tau\\ &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\int_0^{\infty} \mathbb{P}(\mathcal{T} \le \tau + y \,|\, X_\tau = j)\,\mathbb{P}(X_\tau = j)\,\mathrm{d}\tau\\ &= \frac{1}{\mathbb{E}\,[\mathcal{T}]}\left[1 - \sum_{i\in S}\left(e^{y\,\mathrm{B}}\right)_{ij}\right]\int_0^{\infty} \mathbb{P}(X_\tau = j)\,\mathrm{d}\tau\\ &= \frac{\mathbb{E}\,[O_j]}{\mathbb{E}\,[\mathcal{T}]}\left[1 - \sum_{i\in S}\left(e^{y\,\mathrm{B}}\right)_{ij}\right].\end{aligned}$$

We turn to the denominator, and from Lemma 2.21 we know that

$$\lim_{t\to\infty} \mathbb{P}(Z_t = j) = \frac{\mathbb{E}\,[O_j]}{\mathbb{E}\,[\mathcal{T}]}.$$

We divide the numerator by the denominator, the result coincides with $F_{l_j}(y)$ from Proposition 2.25, and the proof of (1) is complete.

(2) We invoke the result for the numerator from (1) to obtain

$$\begin{aligned}\lim_{t\to\infty} F_{L_t}(y) = \lim_{t\to\infty} \mathbb{P}(L_t \le y) &= \lim_{t\to\infty} \sum_{j\in S} \mathbb{P}(L_t \le y, Z_t = j)\\ &= \sum_{j\in S} \frac{\mathbb{E}\,[O_j]}{\mathbb{E}\,[\mathcal{T}]}\left[1 - \sum_{i\in S}\left(e^{y\,\mathrm{B}}\right)_{ij}\right].\end{aligned}$$

We use $\|\mathbf{u}\|\,\mathbb{E}\,[O_j] = x_j^*$ from Lemma 2.8, $\mathbb{E}\,[\mathcal{T}] = \|\mathbf{x}^*\|/\|\mathbf{u}\|$, and get

$$\begin{aligned}\lim_{t\to\infty} F_{L_t}(y) = \sum_{j\in S} \frac{x_j^*}{\|\mathbf{x}^*\|}\left[1 - \sum_{i\in S}\left(e^{y\,\mathrm{B}}\right)_{ij}\right] &= 1 - \sum_{i\in S}\sum_{j\in S}\left(e^{y\,\mathrm{B}}\right)_{ij}\frac{x_j^*}{\|\mathbf{x}^*\|}\\ &= 1 - \mathbf{1}^\top e^{y\,\mathrm{B}}\,\frac{x_j^*}{\|\mathbf{x}^*\|},\end{aligned}$$

which coincides with $F_L(y)$ from Proposition 2.26, and the proof of (2) is finished. □

2.2.8. The time-reversed system

Recall $\boldsymbol{\eta} = \mathbf{x}^*/\|\mathbf{x}^*\|$. We assume $x_j^* > 0$ for all $j \in S$ and consider the system

$$\begin{aligned} \dot{\widehat{\mathbf{x}}}(t) &= \widehat{\mathrm{B}}\,\widehat{\mathbf{x}}(t) + \widehat{\mathbf{u}}, \quad t > 0, \\ \widehat{\mathbf{x}}(0) &= \mathbf{x}^*. \end{aligned} \tag{2.18}$$

with $\widehat{\mathrm{B}} = (\mathrm{diag}\,\boldsymbol{\eta})\,\mathrm{B}^\top\,(\mathrm{diag}\,\boldsymbol{\eta})^{-1}$ and $\widehat{u}_j = z_j\,x_j^*$.

Lemma 2.28 *System* (2.18) *is open, linear, autonomous, and compartmental.*

Proof. Linearity is inherited from system (2.3) and autonomy is obvious. Furthermore, $\widehat{\mathbf{u}}$ is nonnegative since $\mathbf{z}$ and $\mathbf{x}^*$ are. We show that $\widehat{\mathrm{B}}$ is a compartmental matrix by proving that it satisfies the conditions of Definition 1.4:

(i) Let $j \in S$. Since B is compartmental and $\boldsymbol{\eta} > 0$, $\widehat{B}_{jj} = \eta_j\,B_{jj}\,\eta_j^{-1} = B_{jj} \le 0$.

(ii) Let $i, j \in S$ with $i \neq j$. Since B is compartmental and $\boldsymbol{\eta} > 0$, $\widehat{B}_{ij} = \eta_i\,B_{ji}\,\eta_j^{-1} \ge 0$.

(iii) Let $j \in S$. Since $u_j \ge 0$ and $\eta_j > 0$,

$$\sum_{i\in S} \widehat{B}_{ij} = \sum_{i\in S} \eta_i\,B_{ji}\,\eta_j^{-1} = \frac{1}{\eta_j}\sum_{i\in S} B_{ji}\,\eta_i = \frac{1}{\eta_j}\,(B\,\eta)_j.$$

We use $\boldsymbol{\eta} = \mathbf{x}^*/\|\mathbf{x}^*\|$ and $\mathrm{B}\,\mathbf{x}^* = -\mathbf{u}$ to see

$$\sum_{i\in S} \widehat{B}_{ij} = -\frac{\|\mathbf{x}^*\|}{x_j^*}\,\frac{u_j}{\|\mathbf{x}^*\|} = -\frac{u_j}{x_j^*} \le 0.$$

The openness of the system follows from

$$\widehat{z}_j = -\sum_{i\in S} \widehat{B}_{ij} = \frac{u_j}{x_j^*} \ge 0 \tag{2.19}$$

and the fact that here is at least one $j \in S$ for which strict inequality holds. Otherwise system (2.3) has no input and the steady state $\mathbf{x}^*$ vanishes. This contradicts our assumption $x_j^* > 0$ for all j. □

Analogously to compartmental system (2.3), we denote by $\widehat{X}$ and $\widehat{Z}$ the absorbing continuous-time Markov chain and the regenerative process associated to system (2.18), respectively. Other symbols are translated in the same manner.

Lemma 2.29 *System* (2.18) *can be interpreted as the time-reversed system of system* (2.3) *in the sense that, for* $h \ge 0$,

$$\lim_{t\to\infty} \mathbb{P}(Z_{t-h} = i \,|\, Z_t = j) = \lim_{t\to\infty} \mathbb{P}(\widehat{Z}_{t+h} = i \,|\, \widehat{Z}_t = j), \quad i, j \in S.$$

Proof. On the one hand, $\lim_{t\to\infty} \mathbb{P}(\widehat{Z}_{t+h} = i \,|\, \widehat{Z}_t = j) = (e^{h\,\widehat{\mathrm{B}}})_{ij}$. On the other hand, using Bayes' theorem, Lemma 2.21, as well as the properties (v) and (vi) of the matrix exponential (Appendix A), we see

$$\begin{aligned}\lim_{t\to\infty} \mathbb{P}(Z_{t-h} = i \,|\, Z_t = j) &= \lim_{t\to\infty} \mathbb{P}(Z_t = j \,|\, Z_{t-h} = i)\, \frac{\mathbb{P}(Z_{t-h} = i)}{\mathbb{P}(Z_t = j)} \\ &= (e^{h\,\mathrm{B}})_{ji}\, \frac{\eta_i}{\eta_j} \\ &= \eta_i\, (e^{h\,\mathrm{B}})^\top_{ij}\, \eta_j^{-1} \\ &= (e^{h\,\widehat{\mathrm{B}}})_{ij} \\ &= \lim_{t\to\infty} \mathbb{P}(\widehat{Z}_{t+h} = i \,|\, \widehat{Z}_t = j).\end{aligned}$$

□

Definition 2.30 We call the compartmental system (2.18) the *time-reversed system* of the *original* compartmental system (2.3).

The time-reversed and the original system share several important properties.

Proposition 2.31 *The time-reversed system* (2.18) *and the original system* (2.3) *have the same total amounts of inputs, the same steady state, and their respective distributions of forward transit time and system age coincide.*

Proof. First, we notice from Eq. (2.13) that $\|\widehat{\mathbf{u}}\| = \|\mathbf{u}\|$. Furthermore,

$$e^{t\,\widehat{\mathrm{B}}} = (\operatorname{diag}\boldsymbol{\eta})\, \left(e^{t\,\mathrm{B}}\right)^\top\, (\operatorname{diag}\boldsymbol{\eta})^{-1}.$$

Then, for $t \geq 0$, the cumulative probability distribution of the reversed forward transit time $\widehat{\mathrm{FTT}}$ is given by Corollary 2.5 as

$$\begin{aligned}F_{\widehat{\mathrm{FTT}}}(t) &= 1 - \mathbf{1}^\top \left(e^{t\widehat{\mathrm{B}}}\right) \frac{\widehat{\mathbf{u}}}{\|\widehat{\mathbf{u}}\|} \\ &= 1 - \mathbf{1}^\top\, (\operatorname{diag}\boldsymbol{\eta})\, \left(e^{t\,\mathrm{B}}\right)^\top\, (\operatorname{diag}\boldsymbol{\eta})^{-1}\, \frac{\widehat{\mathbf{u}}}{\|\mathbf{u}\|} \\ &= 1 - \sum_{i\in S}\sum_{j\in S} \eta_i\, \left(e^{t\,\mathrm{B}}\right)_{ji}\, \eta_j^{-1}\, \frac{\widehat{u}_j}{\|\mathbf{u}\|},\end{aligned}$$

which turns with $\widehat{u}_j = z_j\, x_j^*$ and $\eta_i\, \eta_j^{-1}\, x_j^* = x_i^*$ into

$$\begin{aligned}F_{\widehat{\mathrm{FTT}}}(t) &= 1 - \sum_{j\in S} z_j \sum_{i\in S} \left(e^{t\,\mathrm{B}}\right)_{ji}\, \frac{x_i^*}{\|\mathbf{u}\|} \\ &= 1 - \mathbf{z}^\top\, e^{t\,\mathrm{B}}\, \frac{\mathbf{x}^*}{\|\mathbf{u}\|}.\end{aligned}$$

With $\mathbf{z}^\top = -\mathbf{1}^\top\, \mathrm{B}$ and $\mathrm{B}\,\mathbf{x}^* = -\mathbf{u}$, we see

$$F_{\widehat{\mathrm{FTT}}}(t) = 1 - \mathbf{1}^\top\, \left(e^{t\,\mathrm{B}}\right)\, \frac{\mathbf{u}}{\|\mathbf{u}\|},$$

which equals $F_{\mathrm{FTT}}(t)$ from Corollary 2.5.

We turn to the steady state. For $i \in S$,

$$\widehat{x}_i^* = -(\widehat{\mathrm{B}}^{-1}\, \widehat{\mathbf{u}})_i = -\sum_{j\in S} \left(\widehat{\mathrm{B}}^{-1}\right)_{ij}\, \widehat{u}_j,$$

which turns with $\widehat{\mathrm{B}}^{-1} = (\operatorname{diag}\boldsymbol{\eta})\,\left(\mathrm{B}^{-1}\right)^{\top}\,(\operatorname{diag}\boldsymbol{\eta})^{-1}$ and $\widehat{u}_j = z_j\,x_j^*$ into

$$\widehat{x}_i^* = -\sum_{j\in S} \eta_i\,(\mathrm{B}^{-1})_{ji}\,\eta_j^{-1}\,z_j\,x_j^*.$$

We use $z_j = -\sum_{k\in S} B_{kj}$ and obtain

$$\widehat{x}_i^* = \sum_{j\in S} \eta_i\,(\mathrm{B}^{-1})_{ji}\,\eta_j^{-1}\sum_{k\in S} B_{kj}\,x_j^* = \eta_i\,\|\mathbf{x}^*\|\sum_{k\in S}\sum_{j\in S} B_{kj}\,(\mathrm{B}^{-1})_{ji}.$$

Since $\sum_{k\in S}\sum_{j\in S} B_{kj}\left(\mathrm{B}^{-1}\right)_{ji} = \mathrm{I}_{ki}$, we get

$$\widehat{x}_i^* = \eta_i\,\|\mathbf{x}^*\| = x_i^*.$$

In the remaining step, we show the equality of the system-age distributions. For $y \geq 0$, we know from Corollary 2.16 that

$$f_{\widehat{A}}(y) = \widehat{\mathbf{z}}^{\top}\,e^{y\,\widehat{\mathrm{B}}}\,\frac{\widehat{\mathbf{x}}^*}{\|\widehat{\mathbf{x}}^*\|}.$$

Consequently, using $\widehat{\mathbf{z}}^{\top} = -\mathbf{1}^{\top}\,\widehat{\mathrm{B}}$ and $\widehat{\mathrm{B}} = (\operatorname{diag}\boldsymbol{\eta})\,\mathrm{B}^{\top}\,(\operatorname{diag}\boldsymbol{\eta})^{-1}$

$$\begin{aligned} f_{\widehat{A}}(y) &= -\mathbf{1}^{\top}\,\widehat{\mathrm{B}}\,(\operatorname{diag}\,\boldsymbol{\eta})\,\left(e^{y\,\mathrm{B}}\right)^{\top}\,(\operatorname{diag}\boldsymbol{\eta})^{-1}\,\boldsymbol{\eta} \\ &= -\mathbf{1}^{\top}\,(\operatorname{diag}\boldsymbol{\eta})\,\mathrm{B}^{\top}\,\left(e^{y\,\mathrm{B}}\right)^{\top}\,\mathbf{1} \\ &= -\mathbf{1}^{\top}\,(\operatorname{diag}\boldsymbol{\eta})\,\left(e^{y\,\mathrm{B}}\right)^{\top}\,\mathrm{B}^{\top}\,\mathbf{1}. \end{aligned}$$

This real number equals its transpose and hence

$$f_{\widehat{A}}(y) = -\mathbf{1}^{\top}\,\mathrm{B}\,\left(e^{y\,\mathrm{B}}\right)(\operatorname{diag}\boldsymbol{\eta})\,\mathbf{1} = \mathbf{z}^{\top}\,e^{y\,\mathrm{B}}\,\boldsymbol{\eta} = \mathbf{z}^{\top}\,e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\|\mathbf{x}^*\|},$$

which equals $f_A(y)$ from Corollary 2.16. □

However, these symmetries do not carry over to compartment age and remaining compartment lifetime. They show a different relationship.

Proposition 2.32 *The compartment-age vector* $\widehat{\mathbf{a}}$ *of the time-reversed system* (2.18) *and the vector* $\mathbf{l}$ *of remaining compartment lifetimes of the original system* (2.3) *are identically distributed. Likewise, the vector* $\mathbf{a}$ *of compartment ages of the original system and the remaining lifetime vector* $\widehat{\mathbf{l}}$ *of the time-reversed system are identically distributed.*

Proof. Because of Corollary 2.15 we can write the time-reversed compartment-age probability density function for $j \in S$ and $y \geq 0$ as

$$f_{\widehat{a}_j}(y) = \frac{1}{\widehat{x}_j^*}\left(e^{y\,\widehat{\mathrm{B}}}\,\widehat{\mathbf{u}}\right)_j,$$

which by $\widehat{u}_i = z_i\,x_i^*$ becomes

$$f_{\widehat{a}_j}(y) = \frac{1}{x_j^*}\sum_{i\in S}\eta_j\,\left(e^{y\,\mathrm{B}}\right)_{ij}\,\eta_i^{-1}\,z_i\,x_i^*.$$

We use $(x_j^*)^{-1}\,\eta_j\,\eta_i^{-1}\,x_i^* = 1$ to see

$$f_{\widehat{a}_j}(y) = \sum_{i\in S} z_i\,\left(e^{y\,\mathrm{B}}\right)_{ij},$$

which coincides by Proposition 2.25 with the probability density function $f_{l_j}(y)$ of the remaining compartment lifetime of the original system.

We continue with the proof of the second statement. Again by Corollary 2.15, we write the compartment-age probability density function of the original system for $j \in S$ and $y \geq 0$ as

$$f_{a_j}(y) = \frac{1}{x_j^*}\left(e^{y\,\mathrm{B}}\,\mathbf{u}\right)_j = \frac{1}{x_j^*}\sum_{i\in S}\left(e^{y\,\mathrm{B}}\right)_{ji}\,u_i,$$

which by $u_i = \widehat{z}_i\,x_i^*$ from Eq. (2.19) becomes

$$f_{a_j}(y) = \frac{1}{x_j^*}\sum_{i\in S}\eta_j\left(e^{y\,\widehat{\mathrm{B}}}\right)_{ij}\eta_i^{-1}\,\widehat{z}_i\,x_i^* = \sum_{i\in S}\widehat{z}_i\,(e^{y\,\widehat{\mathrm{B}}})_{ij} = \sum_{i\in S}\widehat{z}_i\,(e^{y\,\widehat{\mathrm{B}}})_{ij},$$

which coincides by Corollary 2.25 with the probability density function $f_{\widehat{l}_j}(y)$ of the remaining compartment lifetime of the time-reversed system. □

Proposition 2.33 *System* (2.3) *and its time-reversed version* (2.18) *are dual in the sense that the time-reversed system of the time-reversed system is again the original system.*

Proof. Obviously,

$$\begin{aligned}\widehat{\widehat{\mathrm{B}}} &= (\operatorname{diag}\boldsymbol{\eta})\,\widehat{\mathrm{B}}^\top\,(\operatorname{diag}\boldsymbol{\eta})^{-1}\\ &= (\operatorname{diag}\boldsymbol{\eta})\,[(\operatorname{diag}\boldsymbol{\eta})\,\mathrm{B}^\top\,(\operatorname{diag}\boldsymbol{\eta})^{-1}]^\top\,(\operatorname{diag}\boldsymbol{\eta})^{-1}\\ &= \mathrm{B}.\end{aligned}$$

Furthermore, by $\widehat{z}_j = u_j/x_j^*$ from Eq. (2.19) and $\widehat{x}_j^* = x_j^*$,

$$\widehat{\widehat{u}}_j = \widehat{z}_j\,\widehat{x}_j^* = \frac{u_j}{x_j^*}\,x_j^* = u_j, \quad j \in S.$$

□

2.2.9. Backward transit time equals forward transit time

Recall from Definition 1.16 that the backward transit time BTT is the age of material as it exits the system.

Proposition 2.34 *The backward transit time and the forward transit time of the open linear compartmental system* (2.3) *are identically distributed.*

Proof. The backward transit time is a weighted average of compartment releases and compartment ages. More precisely, for $y \geq 0$,

$$f_{\mathrm{BTT}}(y) = \frac{1}{\|\mathbf{r}\|}\sum_{j\in S} r_j\,f_{a_j}(y).$$

Corollary 2.15 tells us now, together with $\|\mathbf{r}\| = \|\mathbf{u}\|$ from Eq. (2.13), that

$$\begin{aligned} f_{\mathrm{BTT}}(y) &= \frac{1}{\|\mathbf{u}\|} \sum_{j\in S} z_j\, x_j^*\, \frac{1}{x_j^*}\, \left(e^{y\,\mathrm{B}}\,\mathbf{u}\right)_j \\ &= \mathbf{z}^\top\, e^{y\,\mathrm{B}}\, \frac{\mathbf{u}}{\|\mathbf{u}\|}, \end{aligned}$$

which by Corollary 2.5 coincides with the probability density function $f_{\mathrm{FTT}}(y)$ of the forward transit time. □

Since the absorption time $\mathcal{T}$ of the continuous-time Markov chain X, the forward transit time FTT, and the backward transit time BTT are all identically distributed in the sense that their probability density functions coincide, we use the symbol $\mathcal{T}$ for either of them in the remainder of this chapter.

2.3. Application to the two ecological examples

We return to the two ecological examples from Section 2.1 and apply the now established theory about ages and transit times to them.

2.3.1. A linear autonomous global carbon cycle model, II

Recall the example introduced in Section 2.1.1. The transit time $\mathcal{T}$ is phase-type distributed with probability density function (Figure 2.3)

$$\begin{aligned} f_{\mathcal{T}}(t) \approx\ & 0.31\, e^{-77/37\,t} + 0.018\, e^{-31/452\,t} + 0.52\, e^{-36/69\,t} \\ & - 0.3\, e^{-48/81\,t} + 0.001\, e^{-11/1121\,t}, \quad t \geq 0. \end{aligned}$$

Its expected value $\mathbb{E}\,[\mathcal{T}] \approx 15.58\,\mathrm{yr}$ is identical to the value found by Thompson & Randerson (1999), and the standard deviation of the transit time is $\sigma\,[\mathcal{T}] \approx 45.01\,\mathrm{yr}$.

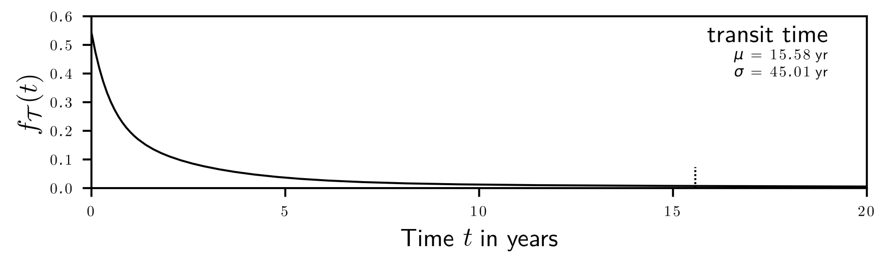


Figure 2.3. Graph of the probability density function of the transit time $\mathcal{T}$ of the model by Emanuel et al. (1981). Its shape and the low value of $f_{\mathcal{T}}$ at the mean value $\mu = 15.58\,\mathrm{yr}$ of $\mathcal{T}$ are evidence of a long tail of this distribution. This long tail results from the relatively large amount of carbon stored in the active soil compartment with its mean age of 107.62 yr. The standard deviation of $\mathcal{T}$ is denoted by σ.

Furthermore, the probability density function of the system age is given by

$$\begin{aligned} f_A(y) \approx\ & 0.096\, e^{-77/37\,y} + 0.017\, e^{-31/452\,y} + 0.064\, e^{-36/69\,y} \\ & - 0.033\, e^{-48/81\,y} + 0.0066\, e^{-11/1121\,y}, \quad y \geq 0. \end{aligned}$$

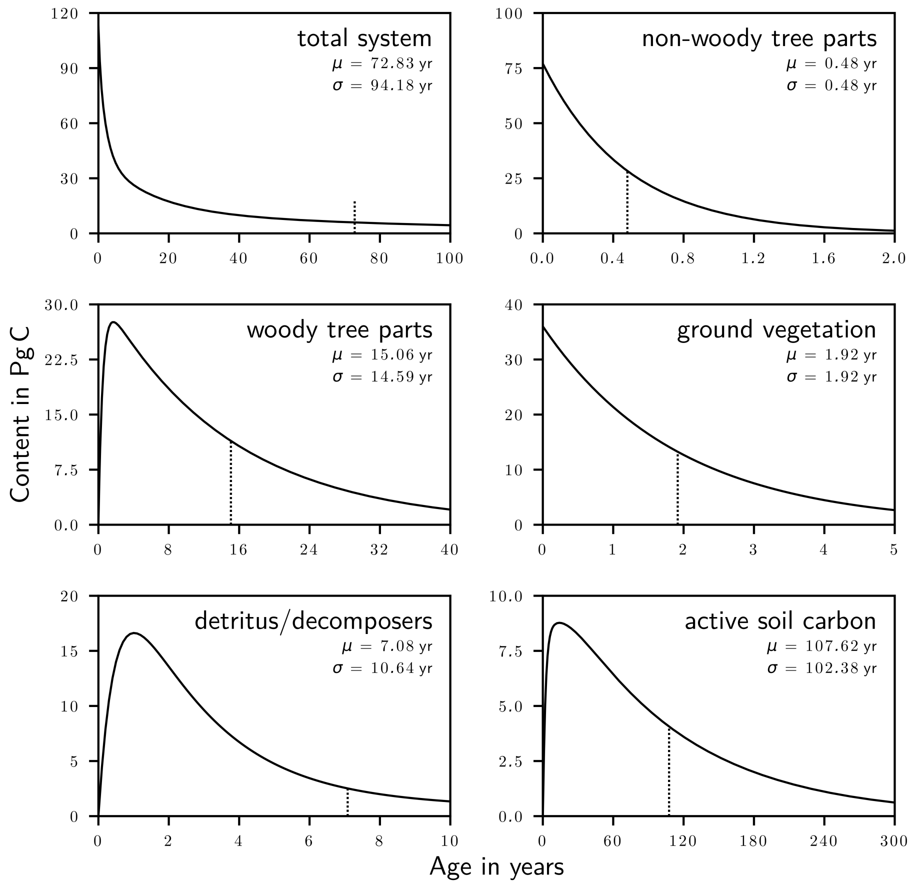


Figure 2.4. Carbon content with respect to age in the model by Emanuel et al. (1981). Dotted lines indicate the mean age denoted by μ, the standard deviation is denoted by σ. The top left panel is for the entire system, whereas the other five panels correspond to the different compartments.

Its expected value $\mathbb{E}[A] = 72.83\,\mathrm{yr}$ is very similar to the value $72.82\,\mathrm{yr}$ reported by Thompson & Randerson (1999). Its standard deviation is given by $\sigma[A] = 94.18\,\mathrm{yr}$.

Additionally, we can calculate the vector that contains the age probability density functions for the compartments as

$$f_{\mathbf{a}}(y) = \begin{pmatrix} 2.1 & 0 & 0 & 0 & 0 \\ -0.071 & 0.071 & 0 & 0 & 0 \\ 0 & 0 & 0.52 & 0 & 0 \\ -0.35 & 0.025 & 1.1 & -0.76 & 0 \\ 0.00052 & -0.0033 & -0.011 & 0.0035 & 0.01 \end{pmatrix} \begin{pmatrix} e^{-77/37\,y} \\ e^{-31/452\,y} \\ e^{-36/69\,y} \\ e^{-48/81\,y} \\ e^{-11/1121\,y} \end{pmatrix}, \quad y \geq 0,$$

from which we obtain the mean-age vector, which is given by

$$\mathbb{E}[\mathbf{a}] = (0.48;\ 15.06;\ 1.92;\ 7.08;\ 107.62)^\top\ \mathrm{yr}.$$

Then the standard deviation vector is

$$\sigma[\mathbf{a}] = (0.48;\ 14.59;\ 1.92;\ 10.64;\ 102.38)^\top\ \mathrm{yr}.$$

From these probability density functions, the system's and the compartments' contents can be plotted with respect to their age (Figure 2.4). This gives useful information about the range of ages for each compartment and how they contribute to the system-age distribution. In comparison to the results of Thompson & Randerson (1999), our approach not only provides mean values for ages and transit times, but also exact formulas for their respective probability distributions. In their approach, these authors obtained results that depended on the simulation time and therefore include numerical errors, something that can be easily avoided by using our derived explicit formulas.

2.3.2. A nonlinear autonomous soil organic matter decomposition model, II

We consider the example introduced in Section 2.1.2. The derived formulas allow us to calculate the mean transit time and mean ages together with the according probability density functions for different values of the model's parameters (Figure 2.5). In particular, we can explore the effects of different values of the parameter ε on the ages and transit times. This parameter controls the proportion of carbon that is transferred from the substrate C_s to the microbial biomass compartment C_b, and it is commonly referred to as the *carbon use efficiency*. Interestingly, if the carbon use efficiency ε increases, the mean transit time and the mean ages of the model decrease (Figure 2.6), a behavior that at first glance appears counterintuitive. It can be explained by two opposing effects. On the one hand, an increase of carbon use efficiency keeps a higher fraction of carbon in the system due to lower respiration. This has an increasing effect on the transit time. On the other hand, a higher carbon use efficiency ε implies a lower steady-state content of compartment C_s and a higher one of compartment C_b. Consequently, from Eq. (2.2) we obtain an increasing value of $\lambda(\mathbf{x}^*)$. This value is the process rate of the compartment C_s. The higher it is, the faster the particles travel through the system. The latter effect prevails here and a decrease in the transit time can be observed.

The graph of the mean transit time for this model with $\varepsilon = 0.39$ (Figure 2.6) lies directly on the one of the mean system age. The huge difference in the compartments' steady-state contents causes very little difference in the initial probability vectors $\boldsymbol{\beta}$ and $\boldsymbol{\eta}$ of the respective phase-type distributions. This results in very similar distributions of transit time and system age.

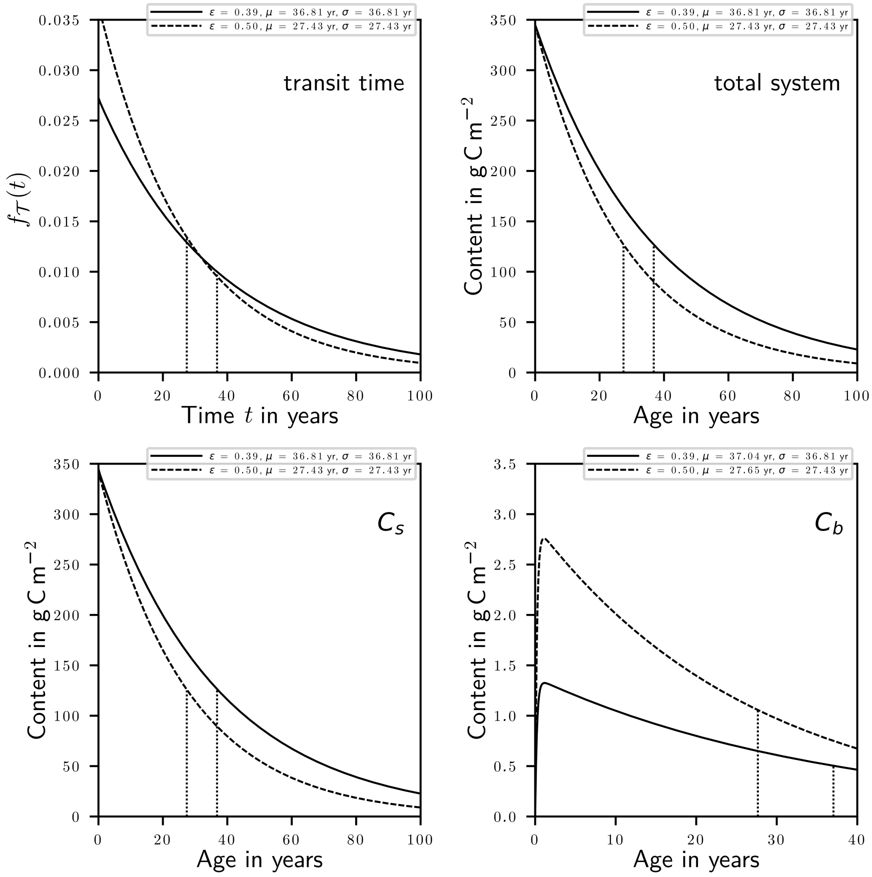


Figure 2.5. Transit-time and age distributions of the model by Wang et al. (2014). Vertical dashed lines represent the mean μ, the standard deviation is denoted by σ. All panels show graphs for two different values of carbon use efficiency ε.

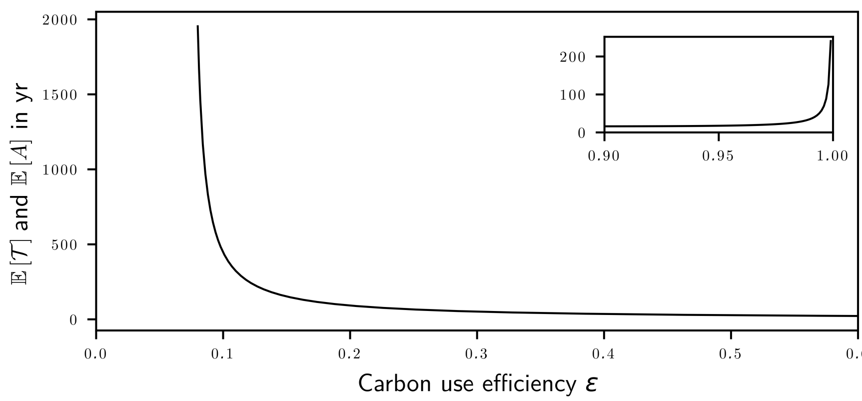


Figure 2.6. Mean transit time $\mathbb{E}[\mathcal{T}]$ and mean system age $\mathbb{E}[A]$ in dependence on the carbon use efficiency ε of the two-compartment nonlinear model proposed by Wang et al. (2014). The small figure shows the explosion of the mean transit time if the carbon use efficiency tends to 1.

2.4. Discussion

We derived simple, explicit, and general formulas for the cumulative probability distributions, probability density functions, expected values, and higher order moments of transit time, ages, and remaining lifetimes of open compartmental systems in steady state. These formulas can be found in different places in this chapter. For convenience, Table 2.1 provides a quick overview.

Table 2.1. Overview of derived formulas for open compartmental systems in equilibrium.

Metric	Density	nth moment	First moment
Transit time	$\mathbf{z}^\top e^{t\,\mathrm{B}}\,\frac{\mathbf{u}}{\lVert\mathbf{u}\rVert}$	$(-1)^n\,n!\,\mathbf{1}^\top\,\mathrm{B}^{-n}\,\frac{\mathbf{u}}{\lVert\mathbf{u}\rVert}$	$-\mathbf{1}^\top\,\mathrm{B}^{-1}\,\frac{\mathbf{u}}{\lVert\mathbf{u}\rVert}$, $\frac{\lVert\mathbf{x}^*\rVert}{\lVert\mathbf{u}\rVert}$
Age vector	$(\mathrm{X}^*)^{-1}\,e^{y\,\mathrm{B}}\,\mathbf{u}$	$(-1)^n\,n!\,(\mathrm{X}^*)^{-1}\,\mathrm{B}^{-n}\,\mathbf{x}^*$	$-(\mathrm{X}^*)^{-1}\,\mathrm{B}^{-1}\,\mathbf{x}^*$
Remaining lifetime vector ($j \in S$)	$\sum_{i\in S} z_i\,(e^{y\,\mathrm{B}})_{ij}$	$(-1)^n\,n!\,\sum_{i\in S}(\mathrm{B}^{-n})_{ij}$	$-\sum_{i\in S}(\mathrm{B}^{-1})_{ij}$
System age, remaining system lifetime	$\mathbf{z}^\top e^{y\,\mathrm{B}}\,\frac{\mathbf{x}^*}{\lVert\mathbf{x}^*\rVert}$	$(-1)^n\,n!\,\mathbf{1}^\top\,\mathrm{B}^{-n}\,\frac{\mathbf{x}^*}{\lVert\mathbf{x}^*\rVert}$	$-\mathbf{1}^\top\,\mathrm{B}^{-1}\,\frac{\mathbf{x}^*}{\lVert\mathbf{x}^*\rVert}$

$\mathbf{z}^\top = -\mathbf{1}^\top\,\mathrm{B}$ is the row vector of release rates.
$\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ is the steady-state vector.
$\mathrm{X}^* = \mathrm{diag}(x_1^*, x_2^*, \ldots, x_d^*)$ is the diagonal matrix comprising the components of the steady-state vector.

Afterwards, we used these formulas and applied them to two examples of ecologically motivated open compartmental systems in equilibrium. We obtained the associated numerical results by using a Python package called LAPM, which we had released earlier. It can be found at `https://github.com/MPIBGC-TEE/LAPM`, and it treats linear autonomous compartmental models both symbolically and numerically.

In ecological systems, the problems of defining transit times in the first place (Sierra et al., 2016) and then finding solutions have a long history. The traditional approach via the impulse response function (Thompson & Randerson, 1999) depends on the availability of computational resources, and the explicit formulas of Manzoni et al. (2009) hold only for models with a very simple structure and were obtained by a tedious procedure using Laplace transforms.

We not only obtained explicit formulas, we also drew links between the deterministic setup of open compartmental systems in equilibrium and the stochastic setup of absorbing continuous-time Markov chains and regenerative processes. As it turned out, all deterministic system diagnostics we considered have a probabilistic counterpart. So corresponds the transit time of an open compartmental system in equilibrium to the absorption time of a continuous-time Markov chain, whereas the ages and remaining lifetimes correspond to backward- and forward recurrence times of a regenerative process, respectively (Figure 2.7). Analogous relations hold for compartment ages and conditional backward recurrence times as well as for remaining compartment lifetimes and conditional forward recurrence times. By connecting two fields of mathematics, namely dynamical systems theory and probability theory, we showed that they can profit from each other and that

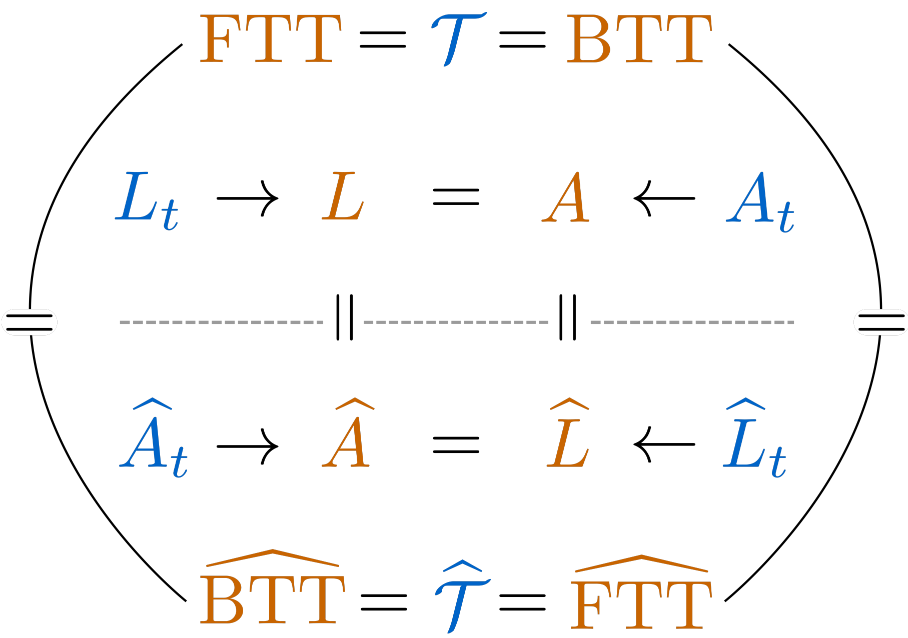


Figure 2.7. Relations between deterministic (orange) and stochastic (blue) quantities. Horizontal and vertical equal signs denote equality in distribution (i.e., equality of the cumulative probability distributions), arrows denote convergence in distribution as $t \to \infty$ (i.e., convergence of the cumulative probability distribution). The upper half considers the linear autonomous compartmental system (2.3) in equilibrium, the lower half its time-reversed system (2.18). Deterministic quantities are – with or without hat – forward transit time (FTT), backward transit time (BTT), remaining system lifetime (L), and system age (A). Stochastic quantities are absorption time ($\mathcal{T}$), forward recurrence time (L_t), and backward recurrence time (A_t).

it is possible to gain insight by considering both at the same time.

We dealt exclusively with well-mixed systems here and linked them to Markov chain theory. However, in real-world systems fluxes might depend on the time the particle has already spent in its current compartment. Such systems find its probabilistic counterpart in the theory of Markov renewal processes, where the future state not only depends on the process' current state, but also on the elapsed time since the system has entered this state. Since there is not much deterministic theory available on that topic while Markov renewal processes have already been extensively studied (Çinlar, 1969; Çinlar, 1975; Janssen & Manca, 2006), it might be fruitful to further investigate the link between these two research areas.

CHAPTER 3

Ages, transit times, and remaining lifetimes of compartmental systems out of equilibrium

In the previous chapter, we derived the distributions of ages, transit times, and remaining lifetimes of well-mixed compartmental systems in equilibrium. However, the equilibrium restriction is often very unrealistic since most systems in nature are intrinsically nonlinear and influenced by time-dependent factors (e.g., a fluctuating external environment). Hence, very often it is more reasonable to consider a well-mixed compartmental system that is nonlinear and nonautonomous. Such a system can be described by

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) &= \mathrm{B}(\mathbf{x}(t),t)\,\mathbf{x}(t) + \mathbf{u}(\mathbf{x}(t),t), \quad t \in (t_0, T) \\ \mathbf{x}(t_0) &= \mathbf{x}^0. \end{aligned} \tag{3.1}$$

Here, $t_0 \in \mathbb{R}$ is a fixed initial time and we denote by $S := \{1, 2, \ldots, d\}$ the set of the system's compartments. Furthermore, $\mathbf{x}(t) \in \mathbb{R}^d_+$ is the vector of compartment contents at time $t \in [t_0, T]$, $\mathrm{B} = (B_{ij})_{i,j\in S} : \mathbb{R}^d_+ \times [t_0, T] \to \mathbb{R}^{d\times d}$ is a matrix-valued function depending on the current system content and time, $\mathbf{u} : \mathbb{R}^d_+ \times [t_0, T] \to \mathbb{R}^d_+$ is a nonnegative vector-valued function depending on the current system content and time, and $\mathbf{x}^0 \in \mathbb{R}^d_+$ is the initial vector of compartment contents at time t_0. Furthermore, $\mathrm{B}(\mathbf{x}, t)$ is required to be invertible for all $(\mathbf{x}, t) \in \mathbb{R}^d_+ \times (t, T)$, such that the system is open by Definition 1.8. We fix a terminal time $T > t_0$ because data for B or $\mathbf{u}$ might be available on a bounded time interval only.

For such systems out of steady state, formulas for age- and transit-time distributions have been developed for one-compartment hydrological systems, without expanding the theory to networks of multiple interconnected compartments (Botter et al., 2011; Calabrese & Porporato, 2015; Harman, 2015). A first milestone in this direction was the introduction of the mean age system (Rasmussen et al., 2016), a system of ODEs describing the time evolution of mean compartment ages of linear systems with time-dependent coefficients.

In this chapter, along the lines of Metzler et al. (2018), we derive formulas not only for means, but for entire distributions of ages, transit times, and remaining lifetimes of nonautonomous models. Our approach even works for nonlinear models. We further extend the mean age system to higher order moments. This allows a simple computation also of the variance and the standard deviation. Additionally, we provide ODEs to describe the time evolution of quantiles such as the median of age distributions. This new framework results in fast computations of entire age distributions and their moments than what it was possible before. These results generalize many earlier results from different scientific fields such as atmospheric sciences, ecology, and hydrology.

As an example application of our theoretical results, we apply them to a simple global carbon cycle model and address two questions: *How old is atmospheric carbon? How long will a significant fraction of a pulse of fossil-fuel carbon, emitted to the atmosphere today, remain in the system?* We compare transit times and ages of a nonlinear and a linear version of the considered model and highlight significant differences in their age structure, which are impossible to characterize by the mean ages alone.

In contrast to Chapter 2, here we do not deal with probabilities. The entire theory of this chapter is deterministic. Instead of considering probability density functions f_{a_j} and cumulative probability distributions F_{a_j} of compartment ages, we now exclusively consider nonnegative compartment-age density functions p_j and cumulative compartment-age distributions P_j such that, for $t \in [t_0, T]$,

$$x_j(t) = \int\limits_0^\infty p_j(a,t)\,\mathrm{d}a = \lim_{\xi\to\infty} P_j(\xi,t)$$

and

$$P_j(\xi,t) = \int\limits_0^\xi p_j(a,t)\,\mathrm{d}a, \quad \xi \geq 0.$$

Here, $P_j(\xi,t)$ denotes the amount of material in compartment $j \in S$ at time t with age $a \leq \xi$. We collect the compartment-age density functions p_j and the cumulative compartment-age distributions P_j in the age density function vector $\mathbf{p} = (p_j)_{j\in S}$ and the cumulative age distribution vector $\mathbf{P} = (P_j)_{j\in S}$, respectively. Analogies to the results from Chapter 2 become obvious as soon as we normalize the p_j's and the P_j's by the respective compartment contents such that they turn into probability density functions and cumulative probability distributions, respectively.

3.1. Linear interpretation of the nonlinear solution

Only in special cases can we find an analytical solution to the initial value problem (3.1). Nevertheless, we assume to know the unique solution at least numerically and denote it by $\mathbf{x}$. We define a time-dependent and matrix-valued function $\widetilde{\mathrm{B}}$ by plugging the solution $\mathbf{x}$ into B, i.e., $\widetilde{\mathrm{B}}(t) := \mathrm{B}(\mathbf{x}(t),t)$. Likewise, we proceed with $\mathbf{u}$ and obtain $\widetilde{\mathbf{u}}(t) := \mathbf{u}(\mathbf{x}(t),t)$. The linear nonautonomous compartmental system

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{y}(t) &= \widetilde{\mathrm{B}}(t)\,\mathbf{y}(t) + \widetilde{\mathbf{u}}(t), \quad t \in (t_0, T), \\ \mathbf{y}(t_0) &= \mathbf{x}^0, \end{aligned} \tag{3.2}$$

has a unique solution that we denote by $\mathbf{y}$. Since $\mathbf{x}$ is the unique solution to system (3.1) and both systems are equivalent, $\mathbf{y} = \mathbf{x}$. Below, we consider linear systems only, because we can always think of the solution of a nonlinear system (3.1) as being the solution of the equivalent linear system (3.2). This linear interpretation of $\mathbf{x}$ allows us to derive semi-analytical formulas for many properties of nonlinear systems. The prefix "semi" reflects here the fact that all the theory works only under the assumption that $\mathbf{x}$ is already known. Moreover, derived distributions of ages, transit times, and remaining lifetimes relate to this particular trajectory $\mathbf{x}$ only.

3.2. General solution of the linear system

We consider the linear nonautonomous compartmental system

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) &= \mathrm{B}(t)\,\mathbf{x}(t) + \mathbf{u}(t), \quad t \in (t_0, T), \\ \mathbf{x}(t_0) &= \mathbf{x}^0. \end{aligned} \tag{3.3}$$

The unique solution $\mathbf{x}$ to this system on $[t_0, T]$ is given by (Brockett, 2015, Theorem 1.6.1)

$$\mathbf{x}(t) = \Phi(t, t_0)\,\mathbf{x}^0 + \int_{t_0}^{t} \Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau, \quad t \in [t_0, T], \tag{3.4}$$

where Φ denotes the state-transition matrix of the system (Appendix B). This state-transition matrix describes the transport of material through the system. Since the system is nonautonomous, Φ depends on two time variables, and since Φ is matrix-valued, it maps an input vector to an output vector. In particular, if $\mathbf{v} := \Phi(t, \tau)\,\mathbf{u}$, then $\mathbf{v}$ is the vector that describes the time-t-distribution of the material that was distributed according to $\mathbf{u}$ at time $\tau \leq t$.

From Eq. (3.4), we see that the vector $\mathbf{x}(t)$ of compartment contents at time t is given as the sum of two terms. The term $\Phi(t, t_0)\,\mathbf{x}^0$ describes the material that has remained from the initial contents, whereas the term $\int_{t_0}^{t} \Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau$ describes the material that has remained until time t out of inputs that came later than t_0. In particular, $\Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau$ describes the material that has entered the system infinitesimally close to time τ and is still in the system at time t. Consequently, at time t the amount $\Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau$ of material in the system has age $t - \tau$.

3.3. Age distributions

As mentioned in Section 2.2.6, in population dynamics the McKendrick-von Foerster equation governs the populations' age structure and its size. In our notation, it is given by

$$\frac{\partial}{\partial a}\,p(a, t) + \frac{\partial}{\partial t}\,p(a, t) = -\kappa(a, t)\,p(a, t),$$

where κ is an age- and time-depending death-rate function. As before in Chapter 2, in the compartmental system (3.3) all compartments are well-mixed. Hence, the according death-rate function is independent of the age a. However, it might depend on time because exit rates from the system might do so. We now try to use the recent observations on the age of $\Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau$ to identify the age density function vector $\mathbf{p}$ and to show that it indeed satisfies a certain kind of McKendrick-von Foerster equation.

Recall from Concept 1.15 that the age $A(t)$ of material in the system at time $t \in [t_0, T]$ is the time span $t - t_a$ between its arrival in the system at time t_a and the current time t. We assume that the initial content $\mathbf{x}^0$ has a given age density function $\mathbf{p}^0$ such that $\mathbf{x}^0 = \int_0^\infty \mathbf{p}^0(a)\,\mathrm{d}a$, where $\mathbf{p}^0(a)\,\mathrm{d}a \in \mathbb{R}^d_+$ is the vector of material with age infinitesimally close to a at time t_0. The recent observation that the amount $\Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau$ has age $t - \tau$ motivates the following theorem.

Theorem 3.1 *The age density function vector of the linear nonautonomous compartmental system* (3.3) *at time* $t \in [t_0, T]$ *and age* $a \geq 0$ *is given by*

$$\mathbf{p}(a, t) = \mathbf{g}(a, t) + \mathbf{h}(a, t), \tag{3.5}$$

where

$$\mathbf{g}(a,t) = \mathbb{1}_{[t-t_0,\infty)}(a)\,\Phi(t,t_0)\,\mathbf{p}^0(a-(t-t_0))$$

is the age density vector of the material that has been in the system from the beginning, and

$$\mathbf{h}(a,t) = \mathbb{1}_{[0,t-t_0)}(a)\,\Phi(t,t-a)\,\mathbf{u}(t-a)$$

is the age density vector of the material that has entered the system after t_0*.*

To prove this result, we show that $\mathbf{p}$ as given by Eq. (3.5) satisfies a multi-dimensional version of the McKendrick-von Foerster equation for the compartmental system (3.3).

Proposition 3.2 *For* $a > 0$ *and* $t \in (t_0, T)$*, the vector* $\mathbf{p}$ *of age density functions as defined in Eq.* (3.5) *satisfies the multi-dimensional McKendrick-von Foerster equation*

$$\left(\frac{\partial}{\partial a} + \frac{\partial}{\partial t}\right)\mathbf{p}(a,t) = \mathrm{B}(t)\,\mathbf{p}(a,t), \tag{3.6}$$

with boundary condition

$$\mathbf{p}(0,t) = \mathbf{u}(t), \quad t \in (t_0, T], \tag{3.7}$$

and initial condition

$$\mathbf{p}(a,t_0) = \mathbf{p}^0(a), \quad a \geq 0. \tag{3.8}$$

Remark 3.3 Eq. (3.6) can be interpreted as a multi-dimensional McKendrick-von Foerster equation because, for the ith compartment,

$$\left(\frac{\partial}{\partial a} + \frac{\partial}{\partial t}\right) p_i(a,t) = \kappa_i(t)\,p_i(a,t),$$

where $\kappa_i(t) = \sum_{j\neq i} B_{ij}(t) + B_{ii}(t)$ is the combination of the incoming and outgoing rates of material with age a at time t.

Proof of Proposition 3.2. We prove now that the age density function vector $\mathbf{p}$ satisfies the multi-dimensional McKendrick-von Foerster equation (3.6). To that end, we compute its total differential along the characteristics $a(t) = a^0 + (t-t_0)$ by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{p}(a,t) &= \frac{\partial}{\partial a}\,\mathbf{p}(a,t)\,\frac{\mathrm{d}}{\mathrm{d}t}\,a(t) + \frac{\partial}{\partial t}\,\mathbf{p}(a,t)\,\frac{\mathrm{d}}{\mathrm{d}t}\,t \\ &= \left(\frac{\partial}{\partial a} + \frac{\partial}{\partial t}\right)\mathbf{p}(a,t),\end{aligned}$$

where $a^0 \geq 0$ is some initial age. We continue in two steps. In the first step, we show that Eq. (3.6) holds on $C_1 := \{(a,t) : t \in (t_0,T),\ a \geq t-t_0\}$ with initial condition (3.8). In the second step, we show that Eq. (3.6) holds on $C_2 := \{(a,t) : t \in (t_0,T),\ 0 \leq a < t-t_0\}$ with boundary condition (3.7).

Step 1. On C_1 we have $\mathbf{p}(a,t) = \mathbf{g}(a,t)$. Consequently, we prove the initial condition (3.8) by

$$\mathbf{p}(a,t_0) = \Phi(t_0,t_0)\,\mathbf{p}^0(a-(t_0-t_0)) = \mathbf{p}^0(a).$$

Furthermore,

$$\mathbf{p}(a,t) = \Phi(t,t_0)\,\mathbf{p}^0(a^0),$$

where $a^0 = a(t) - (t - t_0)$ does not change with time on the characteristics. Consequently,

$$\begin{aligned}\left(\frac{\partial}{\partial a} + \frac{\partial}{\partial t}\right) \mathbf{p}(a,t) &= \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{p}(a,t)\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\,\Phi(t,t_0)\,\mathbf{p}^0(a^0)\\ &= \mathrm{B}(t)\,\Phi(t,t_0)\,\mathbf{p}^0(a^0)\\ &= \mathrm{B}(t)\,\mathbf{p}(a,t),\end{aligned}$$

which proves Eq. (3.6) on C_1.

Step 2. On C_2 we have $\mathbf{p}(a,t) = \mathbf{h}(a,t)$. Consequently, we prove the boundary condition (3.7) by

$$\mathbf{p}(0,t) = \Phi(t, t-0)\,\mathbf{u}(t-0) = \mathbf{u}(t).$$

Furthermore,

$$\mathbf{p}(a,t) = \Phi(t,\tau)\,\mathbf{u}(\tau),$$

where $\tau = t - a(t)$ does not change with time on the characteristics because $a(t) = t - \tau$. Consequently,

$$\begin{aligned}\left(\frac{\partial}{\partial a} + \frac{\partial}{\partial t}\right) \mathbf{p}(a,t) &= \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{p}(a,t)\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\,\Phi(t,\tau)\,\mathbf{u}(\tau)\\ &= \mathrm{B}(t)\,\Phi(t,\tau)\,\mathbf{u}(\tau)\\ &= \mathrm{B}(t)\,\mathbf{p}(a,t),\end{aligned}$$

which proves Eq. (3.6) on C_2. □

We denote by capital letters the cumulative age distributions corresponding to age density functions. This means for the initial age density function vector $\mathbf{p}^0 = (p_j^0)_{j\in S}$ and $\xi \geq 0$ that $\mathbf{P}^0(\xi) = (P_j^0(\xi))_{j\in S} = \int_0^\xi \mathbf{p}^0(a)\,\mathrm{d}a$ is the vector of initial compartment contents with age $a \leq \xi$. Then, the next result follows immediately from Eq. (3.5).

Corollary 3.4 *The vector of cumulative distributions of the compartment ages of system* (3.3) *is given by*

$$\mathbf{P}(\xi,t) = \mathbf{G}(\xi,t) + \mathbf{H}(\xi,t), \tag{3.9}$$

where

$$\mathbf{G}(\xi,t) = \mathbb{1}_{\{\xi \geq t-t_0\}}\,\Phi(t,t_0)\,\mathbf{P}^0(\xi - (t-t_0)) \tag{3.10}$$

is the vector of compartment contents with age $a \leq \xi$ at time t that have been in the system from the beginning, and

$$\mathbf{H}(\xi,t) = \int\limits_{\max\{t-\xi,\,t_0\}}^{t} \Phi(t,\tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau \tag{3.11}$$

is the vector of compartment contents with age $a \leq \xi$ at time t that came into the system after t_0. As long as $\xi \leq t - t_0$, the latter can also be expressed as the compartment contents at time t minus all the material that was already in the system at time $t - \xi$ and survived until time t, i.e.,

$$\mathbf{H}(\xi,t) = \mathbf{x}(t) - \Phi(t, t-\xi)\,\mathbf{x}(t-\xi).$$

Corollary 3.5 *The age density function of the entire system is the sum of the compartment-age density functions. It is given by*

$$\|\mathbf{p}(a,t)\| = \sum_{i\in S} p_i(a,t), \quad a \geq 0, \quad t \in [t_0, T]. \tag{3.12}$$

The material in the system with age $a \leq \xi$ at time $t \in [t_0, T]$ is given by the cumulative distribution of the system age, i.e., by $\|\mathbf{P}(\xi, t)\|$.

3.4. Moments of the age distributions

For any nonnegative integer k and any (not necessarily normalized) density vector $\mathbf{p}$ of a d-dimensional nonnegative vector $\mathbf{x} = \int_0^\infty \mathbf{p}(a)\,\mathrm{d}a$,

$$\bar{\mathbf{a}}^{\mathbf{x},k} := \mathrm{X}^{-1} \int\limits_0^\infty a^k\, \mathbf{p}(a)\,\mathrm{d}a, \tag{3.13}$$

denotes the kth moment of the density vector $\mathbf{p}$, where $\mathrm{X} = \mathrm{diag}(x_1, x_2, \ldots, x_d)$ is the diagonal matrix comprising the components of $\mathbf{x} = (x_j)_{j\in S}$. Note that $\bar{\mathbf{a}}^{\mathbf{x},0} = \mathbf{1}$, the vector comprising ones. For $k = 1$ we obtain the mean-age vector. The unboundedness of the upper limit of the integral causes issues in the numerical computation of an age moment directly from Eq. (3.13). To circumvent this problem, we can use the McKendrick-von Foerster equation (3.6).

From now on, we assume that the initial age density function vector $\mathbf{p}^0$ admits finite moments up to a fixed order $n \in \mathbb{N}$ and denote them by $\bar{\mathbf{a}}^{0,k}$, $k = 1, 2, \ldots, n$. We derive two ways of computing moments of the age distributions of system (3.3). The first one is using a semi-explicit formula.

Proposition 3.6 *The nth moment $\bar{\mathbf{a}}^n(t) := \bar{\mathbf{a}}^{\mathbf{x}(t),n}$ of the age distribution of the compartmental system* (3.3) *at time $t \in [t_0, T]$ is given by*

$$\begin{aligned}\bar{\mathbf{a}}^n(t) = \mathrm{X}(t)^{-1} \Bigg[&\sum_{k=0}^{n} \binom{n}{k} (t-t_0)^{n-k}\, \Phi(t, t_0)\, \mathrm{X}^0\, \bar{\mathbf{a}}^{0,k} \\ &+ \int\limits_0^{t-t_0} a^n\, \Phi(t, t-a)\, \mathbf{u}(t-a)\,\mathrm{d}a \Bigg].\end{aligned} \tag{3.14}$$

Here, $\mathrm{X}(t) = \mathrm{diag}(x_1, x_2, \ldots, x_d)(t)$ is the diagonal matrix containing the compartment contents at time t, $\mathrm{X}^0 = \mathrm{X}(t_0)$, and $\bar{\mathbf{a}}^{0,k}$ ($k = 0, 1, \ldots, n$) denote the moments of the initial age distribution $\mathbf{p}^0$.

Proof. We define

$$\mathbf{y}(t) := \Phi(t, t_0)\, \mathbf{x}^0, \quad t \in [t_0, T], \tag{3.15}$$

and

$$\mathbf{z}(t) := \int\limits_{t_0}^{t} \Phi(t, \tau)\, \mathbf{u}(\tau)\,\mathrm{d}\tau, \quad t \in [t_0, T]. \tag{3.16}$$

Consequently, $\mathbf{x} = \mathbf{y} + \mathbf{z}$, where $\mathbf{y}$ describes the evolution of the initial material and $\mathbf{z}$ the evolution of material that comes later into the system. We use the shorthand $\bar{\mathbf{a}}^n$ for

$\bar{\mathbf{a}}^n(t) = \bar{\mathbf{a}}^{\mathbf{x}(t),n}$ and note that we can compute the nth moment of the age density function vector of $\mathbf{x}$ by the corresponding moments of the age density function vectors of $\mathbf{y}$ and $\mathbf{z}$ by

$$\bar{a}_i^n = \frac{y_i\,\bar{a}_i^{\mathbf{y},n} + z_i\,\bar{a}_i^{\mathbf{z},n}}{x_i}, \quad i \in S, \tag{3.17}$$

or, in vector notation,

$$\bar{\mathbf{a}}^n(t) = \mathrm{X}(t)^{-1}\,\left[\mathrm{Y}(t)\,\bar{\mathbf{a}}^{\mathbf{y},n}(t) + \mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},n}(t)\right]. \tag{3.18}$$

We see from Eq. (3.13) that

$$\mathrm{Y}(t)\,\bar{\mathbf{a}}^{\mathbf{y},n}(t) = \int_0^\infty a^n\,\mathbf{g}(a,t)\,\mathrm{d}a,$$

which by

$$\mathbf{g}(a,t) = \mathbb{1}_{[t-t_0,\infty)}(a)\,\Phi(t,t_0)\,\mathbf{p}^0(a-(t-t_0))$$

and a change of variables from a to $\tau = a-(t-t_0)$ can be transformed into

$$\mathrm{Y}(t)\,\bar{\mathbf{a}}^{\mathbf{y},n}(t) = \Phi(t,t_0)\int_0^\infty [\tau+(t-t_0)]^n\,\mathbf{p}^0(\tau)\,\mathrm{d}\tau.$$

An application of the binomial theorem and Eq. (3.13) leads to

$$\mathrm{Y}(t)\,\bar{\mathbf{a}}^{\mathbf{y},n}(t) = \sum_{k=0}^n \binom{n}{k}\,(t-t_0)^{n-k}\,\Phi(t,t_0)\,\mathrm{X}^0\,\bar{\mathbf{a}}^{0,k}. \tag{3.19}$$

Furthermore, again by Eq. (3.13),

$$\mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},n}(t) = \int_0^\infty a^n\,\mathbf{h}(a,t)\,\mathrm{d}a = \int_0^{t-t_0} a^n\,\mathbf{h}(a,t)\,\mathrm{d}a. \tag{3.20}$$

We plug the sum of Eq. (3.19) and Eq. (3.20) into Eq. (3.18) to complete the proof. □

Note that the integral involved in Eq. (3.14) is now over the half-open but finite interval $[0, t-t_0)$. Hence, a numerical computation of the nth age moment of the compartmental system (3.3) does not have to deal with an indefinite integral such as that involved in Eq. (3.13).

Another way to compute the age moments is to set up and solve an appropriate system of first-order ODEs, which we call the *compartment-age moment system*. This system is a straightforward $d\cdot(n+1)$-dimensional generalization of the mean age system derived in Rasmussen et al. (2016). To derive the compartment-age moment system, we try to represent the time derivative of the kth moment of the age of compartment $i \in S$ by known quantities. For that purpose, we need some auxiliary results based on $\mathbf{y}$ and $\mathbf{z}$ as defined in Eq. (3.15) and Eq. (3.16), respectively.

Lemma 3.7 *For $k = 1, 2, \ldots, n$, and $t \in [t_0, T]$,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,g_i(a,t)\,\mathrm{d}a = \sum_{j\in S} B_{ij}(t)\,y_j(t)\,\bar{a}_j^{\mathbf{y},k}(t) + k\,y_i(t)\,\bar{a}_i^{\mathbf{y},k-1}(t), \quad i \in S.$$

Proof. For simplicity of notation, we do not consider a single component g_i, but the entire vector $\mathbf{g}$. We begin with the left hand side

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_0^\infty a^k\,\mathbf{g}(a,t)\,\mathrm{d}a$$

and use

$$\mathbf{g}(a,t)=\mathbb{1}_{[t-t_0,\infty)}\,\Phi(t,t_0)\,\mathbf{p}^0(a-(t-t_0))$$

to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\Phi(t,t_0)\int\limits_{t-t_0}^\infty a^k\,\mathbf{p}^0(a-(t-t_0))\,\mathrm{d}a,$$

which by the product rule turns into

$$\mathrm{B}(t)\,\Phi(t,t_0)\int\limits_{t-t_0}^\infty a^k\,\mathbf{p}^0(a-(t-t_0))\,\mathrm{d}a+\Phi(t,t_0)\,\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_{t-t_0}^\infty a^k\,\mathbf{p}^0(a-(t-t_0))\,\mathrm{d}a.$$

We transform the first term back, and together with a change of variables in the second term from a to $\tau := a-(t-t_0)$, this brings

$$\mathrm{B}(t)\int\limits_0^\infty a^k\,\mathbf{g}(a,t)\,\mathrm{d}a+\Phi(t,t_0)\,\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_0^\infty(\tau+(t-t_0))^k\,\mathbf{p}^0(\tau)\,\mathrm{d}\tau.$$

We use Eq. (3.13) in the first term, and in the second term we bring the derivative under the integral by means of the dominated convergence theorem to get

$$\mathrm{B}(t)\,\mathrm{Y}(t)\,\bar{\mathbf{a}}^{\mathbf{y},k}(t)+\Phi(t,t_0)\int\limits_0^\infty k\,(\tau+(t-t_0))^{k-1}\,\mathbf{p}^0(\tau)\,\mathrm{d}\tau.$$

We undo the change of variables in the second term and transform it back to obtain

$$\mathrm{B}(t)\,\mathrm{Y}(t)\bar{\mathbf{a}}^{\mathbf{y},k}(t)+k\int\limits_{t-t_0}^\infty a^{k-1}\,\mathbf{g}(a,t)\,\mathrm{d}a,$$

which equals

$$\mathrm{B}(t)\,\mathrm{Y}(t)\bar{\mathbf{a}}^{\mathbf{y},k}(t)+k\,\mathrm{Y}(t)\,\bar{\mathbf{a}}^{\mathbf{y},k-1}(t).$$

Computing the ith component, we get

$$\sum_{j\in S}B_{ij}(t)\,y_j(t)\,\bar{a}_j^{\mathbf{y},k}(t)+k\,y_i(t)\,\bar{a}_i^{\mathbf{y},k-1}(t),$$

and we are finished with the proof. □

Lemma 3.8 *For $k=1,2,\dots,n$, and $t\in[t_0,T]$,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,h_i(a,t)\,\mathrm{d}a=\sum_{j\in S}B_{ij}(t)\,z_j(t)\,\bar{a}_j^{\mathbf{z},k}(t)+k\,z_i(t)\,\bar{a}_i^{\mathbf{z},k-1}(t),\quad i\in S.$$

Proof. Again for simplicity of notation, we do not consider a single component h_i, but the entire vector $\mathbf{h}$. From

$$\mathbf{h}(a,t) = \mathbb{1}_{[0,t-t_0)}(a)\,\Phi(t,t-a)\,\mathbf{u}(t-a),$$

we get

$$\int_0^\infty a^k\,\mathbf{h}(a,t)\,\mathrm{d}a = \lim_{\varepsilon\searrow 0} \int_0^{t-t_0-\varepsilon} a^k\,\mathbf{h}(a,t)\,\mathrm{d}a.$$

We can interchange the limit and the derivative to see

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,\mathbf{h}(a,t)\,\mathrm{d}a = \lim_{\varepsilon\searrow 0} \frac{\mathrm{d}}{\mathrm{d}t}\int_0^{t-t_0-\varepsilon} a^k\,\mathbf{h}(a,t)\,\mathrm{d}a.$$

By an application of the Leibniz rule to the right hand side, we obtain

$$\lim_{\varepsilon\searrow 0}\int_0^{t-t_0-\varepsilon} a^k\,\frac{\partial}{\partial t}\,\mathbf{h}(a,t)\,\mathrm{d}a + (t-t_0-\varepsilon)^k\,\mathbf{h}(t-t_0-\varepsilon,t). \tag{3.21}$$

In Step 2 of the proof of Proposition 3.2, we derived that, for $a \in [0, t-t_0-\varepsilon]$,

$$\frac{\partial}{\partial t}\,\mathbf{h}(a,t) = \mathrm{B}(t)\,\mathbf{h}(a,t) - \frac{\partial}{\partial a}\,\mathbf{h}(a,t),$$

which we plug into the first term of expression (3.21) and turn it into

$$\lim_{\varepsilon\searrow 0}\int_0^{t-t_0-\varepsilon} a^k\,\left[\mathrm{B}(t)\,\mathbf{h}(a,t) - \frac{\partial}{\partial a}\,\mathbf{h}(a,t)\right]\,\mathrm{d}a,$$

which in turn equals by Eq. (3.13)

$$\mathrm{B}(t)\,\mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},k}(t) - \lim_{\varepsilon\searrow 0}\int_0^{t-t_0-\varepsilon} a^k\,\frac{\partial}{\partial a}\,\mathbf{h}(a,t)\,\mathrm{d}a.$$

We integrate by parts and use again Eq. (3.13) to get

$$\mathrm{B}(t)\,\mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},k}(t) - \lim_{\varepsilon\searrow 0}\,(t-t_0-\varepsilon)^k\,\mathbf{h}(t-t_0-\varepsilon,t) + k\,\mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},k-1}(t).$$

Together with expression (3.21), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,\mathbf{h}(a,t)\,\mathrm{d}a = \mathrm{B}(t)\,\mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},k}(t) + k\,\mathrm{Z}(t)\,\bar{\mathbf{a}}^{\mathbf{z},k-1}(t),$$

which completes the proof by considering the ith component. □

Lemma 3.9 *For $k = 1, 2, \dots, n$, and $t \in [t_0, T]$,*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\left[x_i(t)\,\bar{a}_i^k(t)\right] = \sum_{j\in S} B_{ij}(t)\,x_j(t)\,\bar{a}_j^k(t) + k\,x_i(t)\,\bar{a}_i^{k-1}(t), \quad i \in S.$$

Proof. For simplicity of notation, we will eventually omit the time-dependencies of functions. From Eq. (3.13) and $\mathbf{p}(a,t) = \mathbf{g}(a,t) + \mathbf{h}(a,t)$, we know

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[x_i(t)\,\bar{a}_i^k(t)\right] = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,p_i(a,t)\,\mathrm{d}a = \frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,g_i(a,t)\,\mathrm{d}a + \frac{\mathrm{d}}{\mathrm{d}t}\int_0^\infty a^k\,h_i(a,t)\,\mathrm{d}a.$$

Consequently, we can apply Lemmas 3.7 and 3.8 and use

$$x_j\,\bar{a}_j{}^k = y_j\,\bar{a}_j^{\mathbf{y},k} + z_j\,\bar{a}_j^{\mathbf{z},k}$$

from Eq. (3.17) to obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(x_i\,\bar{a}_i^k\right) &= \sum_{j\in S} B_{ij}\,y_j\,\bar{a}_j^{\mathbf{y},k} + k\,y_i\,\bar{a}_i^{\mathbf{y},k-1} + \sum_{j\in S} B_{ij}\,z_j\,\bar{a}_j^{\mathbf{z},k} + k\,z_i\,\bar{a}_i^{\mathbf{z},k-1}\\ &= \sum_{j\in S} B_{ij}\left(y_j\,\bar{a}_j^{\mathbf{y},k} + z_j\,\bar{a}_j^{\mathbf{z},k}\right) + k\left(y_i\,\bar{a}_i^{\mathbf{y},k-1} + z_i\,\bar{a}_i^{\mathbf{z},k-1}\right)\\ &= \sum_{j\in S} B_{ij}\,x_j\,\bar{a}_j^k + k\,x_i\,\bar{a}_i^{k-1}.\end{aligned}$$

□

We are now in the position to prove the following theorem.

Theorem 3.10 *The compartment-age moments of order $k \le n$ of the compartmental system* (3.3) *on the time interval* $[t_0,T]$ *can be obtained by solving the $d\cdot(n+1)$-dimensional first-order ODE system*

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mathbf{x}\\ \bar{\mathbf{a}}^1\\ \vdots\\ \bar{\mathbf{a}}^n\end{pmatrix}(t) &= \begin{pmatrix}\mathrm{B}(t)\,\mathbf{x}(t)+\mathbf{u}(t)\\ \boldsymbol{\gamma}^1(t,\mathbf{x},\mathbf{1},\bar{\mathbf{a}}^1)\\ \vdots\\ \boldsymbol{\gamma}^n(t,\mathbf{x},\bar{\mathbf{a}}^{n-1},\bar{\mathbf{a}}^n)\end{pmatrix}, \quad t\in(t_0,T),\\ (\mathbf{x},\bar{\mathbf{a}}^1,\dots,\bar{\mathbf{a}}^n)(t_0) &= (\mathbf{x}^0,\bar{\mathbf{a}}^{0,1},\bar{\mathbf{a}}^{0,2},\dots,\bar{\mathbf{a}}^{0,n}),\end{aligned} \tag{3.22}$$

where, for $k=1,2,\dots,n$, $\boldsymbol{\gamma}^k := (\gamma_1^k,\gamma_2^k,\dots,\gamma_d^k)^\top$, and for $i=1,2,\dots,d$,

$$\gamma_i^k(t,\mathbf{x},\bar{\mathbf{a}}^{k-1},\bar{\mathbf{a}}^k) := k\,\bar{a}_i^{k-1} + \frac{1}{x_i}\left[\sum_{j\in S} B_{ij}\,x_j\left(\bar{a}_j^k - \bar{a}_i^k\right) - \bar{a}_i^k\,u_i\right].$$

Notice that we occasionally omitted the time-dependencies to simplify notation.

Proof. Let $k\in\{1,2,\dots,n\}$. We compute the time derivative of $\bar{a}_i^k$ in $t\in(t_0,T)$ by

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\bar{a}_i^k(t) = \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{x_i(t)\,\bar{a}_i^k(t)}{x_i(t)}\right]$$

and apply the quotient rule and Lemma 3.9 to get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\,\bar{a}_i^k &= \frac{1}{x_i^2}\left[\left(\sum_{j\in S} B_{ij}\,x_j\,\bar{a}_j^k + k\,x_i\,\bar{a}_i^{k-1}\right)\,x_i - x_i\,\bar{a}_i^k\,\frac{\mathrm{d}}{\mathrm{d}t}\,x_i\right]\\ &= k\,\bar{a}_i^{k-1} + \frac{1}{x_i}\left[\sum_{j\in S} B_{ij}\,x_j\,\bar{a}_j^k - \bar{a}_i^k\,\left(\sum_{j\in S} B_{ij}\,x_j + u_i\right)\right]\\ &= k\,\bar{a}_i^{k-1} + \frac{1}{x_i}\left[\sum_{j\in S} B_{ij}\,x_j\,\left(\bar{a}_j^k - \bar{a}_i^k\right) - \bar{a}_i^k\,u_i\right].\end{aligned}$$

Now, we can bring all components $i \in S$ into one vector and the proof is complete. □

We call Eq. (3.22) the *compartment-age moment system* of the linear nonautonomous compartmental system (3.3). Because of its particular structure, it has the advantage of solving the compartments' age moments through time alongside the compartments' contents. This procedure is both fast and numerically robust.

So far, we have derived formulas to compute distributions of the compartment ages. Now we turn to the system age. Following Eq. (3.13), the nth moment of the system age at time $t \in [t_0, T]$ is defined by

$$\bar{A}^n(t) = \frac{1}{\|\mathbf{x}(t)\|}\int_0^\infty a^n\,\|\mathbf{p}(a,t)\|\,\mathrm{d}a. \tag{3.23}$$

Corollary 3.11 *The nth moment of the system age of the compartmental system* (3.3) *is given by*

$$\bar{A}^n(t) = \frac{\mathbf{x}^\top(t)\,\bar{\mathbf{a}}^n(t)}{\|\mathbf{x}(t)\|}, \quad t \in [t_0, T].$$

Proof. By definition of the system-age moment and by Eq. (3.13) applied to the compartment-age moments $\bar{a}_j^n$,

$$\begin{aligned}\bar{A}^n(t) &= \frac{1}{\|\mathbf{x}(t)\|}\int_0^\infty a^n\,\|\mathbf{p}(a,t)\|\,\mathrm{d}a &&= \frac{1}{\|\mathbf{x}(t)\|}\sum_{j\in S}\int_0^\infty a^n\,p_j(a,t)\,\mathrm{d}a\\ &= \frac{1}{\|\mathbf{x}(t)\|}\sum_{j\in S} x_j(t)\,\bar{a}_j^n(t) &&= \frac{\mathbf{x}^\top(t)\,\bar{\mathbf{a}}^n(t)}{\|\mathbf{x}(t)\|}.\end{aligned}$$

□

3.5. Quantiles of the age distributions

In addition to moments, quantiles are important statistics of age distributions.

Definition 3.12 Fix $q \in (0, 1)$. The *q-quantile of the age of compartment $i \in S$* of the compartmental system (3.3) at time $t \in [t_0, T]$ is defined as $\xi_i(t)$ such that

$$P_i(\xi_i(t), t) = q\,x_i(t). \tag{3.24}$$

Analogously, the *q-quantile of the system age* at time $t \in [t_0, T]$ is defined as $\xi(t)$ such that

$$\|\mathbf{P}(\xi(t), t)\| = q\,\|\mathbf{x}(t)\|. \tag{3.25}$$

For the special case $q = 1/2$, the q-quantile is called *median.*

In general, the computation of quantiles relies on the computationally expensive inverse of the cumulative age distribution. The following theorem allows us to compute a particular age quantile of a single compartment on the entire interval $[t_0, T]$ by solving an ODE, provided that we know the associated quantile of the initial age distribution.

Theorem 3.13 *For $q \in (0, 1)$, the q-quantile of the age of compartment $i \in S$ of the compartmental system* (3.3) *can be obtained by solving*

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\xi_i(t) &= 1 + \frac{u_i(t)\,(q-1) + [\mathrm{B}(t)\ (q\,\mathbf{x}(t) - \mathbf{P}(\xi_i, t))]_i}{p_i(\xi_i, t)}, \quad t \in (t_0, T), \\ \xi_i(t_0) &= \xi_i^0, \end{aligned} \tag{3.26}$$

where ξ_i^0 is given such that $P_i^0(\xi_i^0) = q\,x_i^0$.

Proof. Starting at time $t = t_0$ with given $\xi_i(t_0) = \xi_i^0$, the time evolution of the q-quantile $\xi_i(t)$ of the age of compartment i can be described by taking the time derivative in both sides of Eq. (3.24), which gives

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^{\xi_i(t)} p_i(a, t)\,\mathrm{d}a = q\ [\mathrm{B}(t)\,\mathbf{x}(t)]_i + q\,u_i(t). \tag{3.27}$$

Using the Leibniz rule, we can rewrite the left hand side to

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^{\xi_i(t)} p_i(a, t)\,\mathrm{d}a = \int_0^{\xi_i(t)} \frac{\partial}{\partial t}\,p_i(a, t)\,\mathrm{d}a + p_i(\xi_i(t), t)\,\frac{\mathrm{d}}{\mathrm{d}t}\,\xi_i(t). \tag{3.28}$$

Outside the Lebesgue-null set $\{a \geq 0 : a = t - t_0\}$, the McKendrick-von Foerster equation (3.6) holds. Consequently,

$$\int_0^{\xi_i(t)} \frac{\partial}{\partial t}\,p_i(a, t)\,\mathrm{d}a = \int_0^{\xi_i(t)} \left([\mathrm{B}(t)\,\mathbf{p}(a, t)]_i - \frac{\partial}{\partial a}\,p_i(a, t)\right)\,\mathrm{d}a.$$

On the right hand side, we see

$$\int_0^{\xi_i(t)} [\mathrm{B}(t)\,\mathbf{p}(a, t)]_i\ \mathrm{d}a = [\mathrm{B}(t)\,\mathbf{P}(\xi_i(t), t)]_i\,.$$

Furthermore, $\int_0^{\xi_i(t)} \frac{\partial}{\partial a}\,p_i(a, t)\,\mathrm{d}a = p_i(\xi_i(t), t) - p_i(0, t)$, and we use the boundary condition $p_i(0, t) = u_i(t)$ to obtain

$$\int_0^{\xi_i(t)} \frac{\partial}{\partial t}\,p_i(a, t)\,\mathrm{d}a = [\mathrm{B}(t)\,\mathbf{P}(\xi_i(t), t)]_i - p_i(\xi_i(t), t) + u_i(t).$$

Now, we plug it into Eq. (3.28), get

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^{\xi_i(t)} p_i(a,t)\,\mathrm{d}a = [\mathrm{B}(t)\,\mathbf{P}(\xi_i(t),t)]_i - p_i(\xi_i(t),t) + u_i(t) + p_i(\xi_i(t),t)\,\frac{\mathrm{d}}{\mathrm{d}t}\,\xi_i(t),$$

replace the left hand side by the right hand side of Eq. (3.27), and solve for $\frac{\mathrm{d}}{\mathrm{d}t}\,\xi_i(t)$ to finish the proof. □

Analogously, we can prove the following result.

Corollary 3.14 *For $q \in (0,1)$, the q-quantile of the system age of the compartmental system* (3.3) *can be obtained by solving*

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\xi(t) &= 1 + \frac{\|\mathbf{u}(t)\|\,(q-1) + \sum\limits_{i\in S} [\mathrm{B}(t)\ (q\,\mathbf{x}(t) - \mathbf{P}(\xi,t))]_i}{\|\mathbf{p}(\xi,t)\|}, \quad t \in (t_0, T) \\ \xi(t_0) &= \xi^0, \end{aligned} \tag{3.29}$$

where ξ^0 is given such that $\|\mathbf{P}^0(\xi^0)\| = q\,\|\mathbf{x}^0\|$.

Proof. Starting at time $t = t_0$ with given $\xi(t_0) = \xi^0$, the time evolution of the q-quantile $\xi(t)$ of the system age can be described by taking the time derivative in both sides of Eq. (3.25), which gives

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^{\xi(t)} \|\mathbf{p}(a,t)\|\,\mathrm{d}a = q \sum_{i\in S} [\mathrm{B}(t)\,\mathbf{x}(t)]_i + q\,\|\mathbf{u}(t)\|. \tag{3.30}$$

Using the Leibniz rule, we can rewrite the left hand side to

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^{\xi(t)} \|\mathbf{p}(a,t)\|\,\mathrm{d}a = \int_0^{\xi(t)} \frac{\partial}{\partial t}\,\|\mathbf{p}(a,t)\|\,\mathrm{d}a + \|\mathbf{p}(\xi(t),t)\|\,\frac{\mathrm{d}}{\mathrm{d}t}\,\xi(t). \tag{3.31}$$

Outside the Lebesgue-null set $\{a \geq 0 : a = t - t_0\}$, the McKendrick-von Foerster equation (3.6) holds. Consequently,

$$\int_0^{\xi(t)} \frac{\partial}{\partial t}\,\|\mathbf{p}(a,t)\|\,\mathrm{d}a = \int_0^{\xi(t)} \left(\sum_{i\in S} [\mathrm{B}(t)\,\mathbf{p}(a,t)]_i - \frac{\partial}{\partial a}\,\|\mathbf{p}(a,t)\| \right) \mathrm{d}a.$$

On the right hand side, we see

$$\int_0^{\xi(t)} \sum_{i\in S} [\mathrm{B}(t)\,\mathbf{p}(a,t)]_i\ \mathrm{d}a = \sum_{i\in S} [\mathrm{B}(t)\,\mathbf{P}(\xi_i(t),t)]_i\,.$$

Furthermore, $\int_0^{\xi(t)} \frac{\partial}{\partial a}\,\|\mathbf{p}(a,t)\|\,\mathrm{d}a = \|\mathbf{p}(\xi(t),t)\| - \|\mathbf{p}(0,t)\|$, and we use the boundary condition $\mathbf{p}(0,t) = \mathbf{u}(t)$ to obtain

$$\int_0^{\xi(t)} \frac{\partial}{\partial t}\,\|\mathbf{p}(a,t)\|\,\mathrm{d}a = \sum_{i\in S} [\mathrm{B}(t)\,\mathbf{P}(\xi(t),t)]_i - \|\mathbf{p}(\xi(t),t)\| + \|\mathbf{u}(t)\|.$$

Now, we plug it into Eq. (3.31), get

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\limits_0^{\xi(t)} \|\mathbf{p}(a,t)\|\,\mathrm{d}a = \sum_{i\in S}[\mathrm{B}(t)\,\mathbf{P}(\xi(t),t)]_i - \|\mathbf{p}(\xi(t),t)\| + \|\mathbf{u}(t)\| + \|\mathbf{p}(\xi(t),t)\|\,\frac{\mathrm{d}}{\mathrm{d}t}\,\xi(t),$$

replace the left hand side by the right hand side of Eq. (3.30), and solve for $\frac{\mathrm{d}}{\mathrm{d}t}\,\xi(t)$ to finish the proof. □

3.6. Transit-time distributions

Recall from Definition 1.16 that the backward transit time $\mathrm{BTT}(t_e)$ is the age of material in the output from the system at exit time $t_e \in [t_0, T]$, and that we further assume that for fixed $n \in \mathbb{N}$ the nth moment of the initial age density function vector $\mathbf{p}^0$ exists. We furthermore denote by $\mathbf{z}(t_e)$ the vector of outflow rates from the system at time t_e. It is given by

$$z_j(t_e) = -\sum_{i\in S} B_{ij}(t_e), \quad j \in S,$$

where z_j is the outflow-rate function from compartment j. We can write the age density function of the outflow at time t_e as

$$p_{\mathrm{BTT}}(a,t_e) = \mathbf{z}^\top(t_e)\,\mathbf{p}(a,t_e), \quad a \geq 0, \quad t_e \in [t_0,T]. \tag{3.32}$$

Owing to the well-mixed assumption, the outflow from compartment j at time t_e is given by $r_j(t_e) = z_j(t_e)\,x_j(t_e)$. Consequently, $\mathbf{r}(t_e)$ denotes the vector of outflows from the system at time t_e.

Proposition 3.15 *The nth moment of the backward transit time at time $t_e \in [t_0,T]$ of the compartmental system 3.3 is given by*

$$\overline{\mathrm{BTT}}^n(t_e) = \frac{\mathbf{r}^\top(t_e)\,\bar{\mathbf{a}}^n(t_e)}{\|\mathbf{r}(t_e)\|}.$$

Proof. By Eq. (3.13),

$$\overline{\mathrm{BTT}}^n(t_e) = \frac{1}{\|\mathbf{r}(t_e)\|}\int\limits_0^\infty a^n\,p_{\mathrm{BTT}}(a,t_e)\,\mathrm{d}a = \frac{1}{\|\mathbf{r}(t_e)\|}\,\mathbf{z}^\top(t_e)\int\limits_0^\infty a^n\,\mathbf{p}(a,t_e)\,\mathrm{d}a.$$

We use $\mathbf{r}^\top(t_e) = \mathbf{z}^\top(t_e)\,\mathrm{X}(t_e)$ and again Eq. (3.13) to complete the proof. □

Recall, again from Definition 1.16, that for material entering the system at its arrival time $t_a \in (t_0, T]$, we consider its forward transit time $\mathrm{FTT}(t_a)$ as the age $a \geq 0$ that the material will have when it exits the system at time $t_e = t_a + a$. The exit time t_e might be later than the finite time horizon T, consequently the distribution of $\mathrm{FTT}(t_a)$ is cut off at the age $a = T - t_a$ A proper mean forward transit time cannot be computed, and proper quantiles might not possible to compute. The density function

$$p_{\mathrm{FTT}}(a,t_a) = \mathbf{z}^\top(t_a+a)\,\mathbf{p}(a,t_a+a), \quad t_a \in (t_0,T], \tag{3.33}$$

describes the part from the input at time t_a that leaves the system at time $t_a + a \leq T$. We can now easily prove a generalized version of Niemi's theorem (Niemi, 1977).

Proposition 3.16 *The forward- and backward transit time of the compartmental system* (3.3) *are time-shifted versions of each other. More precisely, for* $t_0 < t_a \leq t_e = t_a + a \leq T$,

$$p_{\mathrm{FTT}}(a, t_a) = p_{\mathrm{BTT}}(a, t_e). \tag{3.34}$$

Proof. The relation $t_e = t_a + a$ yields by Eq. (3.32) that $p_{\mathrm{BTT}}(a, t_e) = \mathbf{z}^\top(t_a+a)\,\mathbf{p}(a, t_a+a)$, which coincides with the right hand side of Eq. (3.33). □

Remark 3.17 If we want to compute the moments of $\mathrm{FTT}(t_a)$, we must rely on Eq. (3.13) and deal with the indefinite integral. Unfortunately, we cannot profit from the close link between FTT and BTT provided by Eq. (3.34), since the exit time $t_e = t_a + a$ depends on a.

3.7. Remaining lifetime distributions

Let $t \in [t_0, T]$. Recall from Definition 1.17 that the remaining lifetime $L(t)$ of material in the system at time t is the length of the time period from time t until the material's exit from the system. Furthermore, the remaining compartment lifetime $l_j(t)$ of a compartment $j \in S$ at time t is the remaining system lifetime of material in compartment j at time t. Just as it is the case with the forward transit time, the exit time of the material might be beyond the finite time horizon T, and the remaining lifetime distributions are cut off at $y = T - t$.

A fixed compartment $j \in S$ contains an amount $x_j(t)$ of material at time t. After a period of $y \geq 0$ units of time, the amount $\sum_{i\in S} \Phi_{ij}(t+y, t)\, x_j(t)$ of the original amount $x_j(t)$ is still in the system, distributed over different compartments.

Corollary 3.18 *We consider the compartmental system* (3.3)*. For* $t \in [t_0, T]$ *and* $j \in S$,

(i) the cumulative distribution of compartment j*'s remaining lifetime* $l_j(t)$ *at time* t *and* $y \in [0, T-t]$ *is given by*

$$P_{l_j}(y, t) = x_j(t) \left[1 - \sum_{i\in S} \Phi_{ij}(t+y, t)\right] \quad \textit{and}$$

(ii) its density function by

$$p_{l_j}(y, t) = -\sum_{i\in S} \left[\mathrm{B}(t+y)\,\Phi(t+y, t)\right]_{ij}\, x_j(t) = \sum_{i\in S} z_i(t+y)\,\Phi_{ij}(t+y, t)\, x_j(t).$$

The corresponding remaining system lifetime $L(t)$ *has*

(iii) its cumulative distribution given by

$$P_L(y, t) = \|\mathbf{x}(t)\| - \mathbf{1}^\top\,\Phi(t+y, t)\,\mathbf{x}(t) \quad \textit{and}$$

(iv) its density function given by

$$p_L(y, t) = \mathbf{z}^\top(t+y)\,\Phi(t+y, t)\,\mathbf{x}(t).$$

3.8. Consistency with systems in equilibrium

As a special case of the open linear nonautonomous compartmental system (3.3), we consider now the autonomous system (1.8). Hence, we have the special situation that $\mathrm{B}(t) = \mathrm{B}$ and $\mathbf{u}(t) = \mathbf{u}$ are both time-independent. Note that also $\mathbf{z}(t) = \mathbf{z}$ does not depend on time anymore. We denote the unique solution of this system by $\mathbf{x}$ and know from Proposition 1.13 that $\mathbf{x}(t) \to \mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$ as $t \to \infty$. Our goal is to show that, as $t \to \infty$, the distributions of ages, transit times, and remaining lifetimes of the nonautonomous interpretation coincide with those of the equilibrium interpretation of Chapter 2.

In the autonomous case, the state-transition matrix becomes a matrix exponential (Appendices B and A). More precisely,

$$\Phi(t+y,t) = e^{y\,\mathrm{B}}, \quad y \geq 0, \quad t \geq t_0.$$

The age density function vector from Eq. (3.5) has now the shape

$$\mathbf{p}(a,t) = \mathbf{g}(a,t) + \mathbf{h}(a,t), \quad a \geq 0, \quad t \geq t_0,$$

where

$$\mathbf{g}(a,t) = \mathbb{1}_{[t-t_0,\infty)}(a)\, e^{(t-t_0)\,\mathrm{B}}\, \mathbf{p}^0(a-(t-t_0))$$

and

$$\mathbf{h}(a,t) = \mathbb{1}_{[0,t-t_0)}(a)\, e^{a\,\mathrm{B}}\, \mathbf{u}.$$

By Corollary 1.14, $\lim_{t\to\infty} \mathbf{g}(a,t) = \mathbf{0}$ for all $a \geq 0$. Consequently,

$$\lim_{t\to\infty} \mathbf{p}(a,t) = e^{a\,\mathrm{B}}\,\mathbf{u}, \quad a \geq 0,$$

is the vector that contains the age density functions of the different compartments for $t \to \infty$.

Recall that the density functions in this chapter are not normalized. In order to link them to the normalized probability density functions of Chapter 2, we must normalize them. To that end, we multiply $\mathbf{p}$ by $(\mathbf{X}^*)^{-1} = \mathrm{diag}(x_1^*, \ldots, x_d^*)$. We further divide p_{BTT} and p_{FTT} by the total system input $\|\mathbf{u}\|$, and p_{l_j} by x_j^* for all $j \in S$. Then it becomes immediately obvious that the results in the nonautonomous case are generalizations of the respective results in the autonomous case.

3.9. Application to a simple global carbon cycle model

We consider the simple global carbon cycle model introduced by Rodhe & Björkström (1979) and depicted in Figure 3.1.

3.9.1. Detailed model description

The model consists of three compartments: atmosphere (A), terrestrial biosphere (T), and surface ocean (S). The letter D stands for the external compartment deep ocean with infinite content. We denote by $C_A = C_A(t)$, $C_T = C_T(t)$, and $C_S = C_S(t)$ the respective carbon contents in Pg C at time t in years (yr). Two external fluxes add carbon to the system. The first one, u_S, is constant and goes from the deep ocean to the surface ocean, whereas the second one, $u_A = u_A(t)$, is time-dependent and represents carbon added to the atmosphere by the burning of fossil fuels. Carbon can leave the system only if it moves

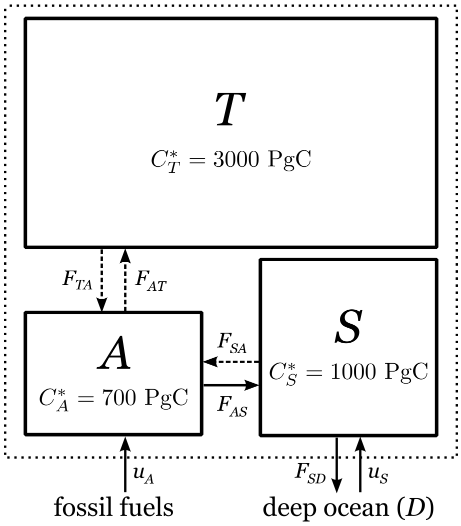


Figure 3.1 Simple global carbon cycle model with three compartments (solid boxes within dashed square): atmosphere (A), terrestrial biosphere (T), and surface ocean (S). The indicated carbon contents are the respective equilibrium values. External to the modeled system are fossil-fuel sources and the deep ocean (D). The model compartments and the external sources are connected by linear (solid arrows) and possibly nonlinear (dashed arrows) fluxes of carbon. (Figure extracted from Metzler et al. (2018))

from the surface ocean to the deep ocean. A flux from compartment X to compartment Y is denoted by F_{XY} and the following fluxes exist in the model, all given in $\mathrm{Pg\,C\,yr^{-1}}$:

$$\begin{aligned} F_{AT} &= 60\,(C_A/700)^{\alpha}, & F_{AS} &= 100\,C_A/700, \\ F_{TA} &= 60\,C_T/3000 + f_{TA}, & F_{SA} &= 100\,(C_S/1000)^{\beta}, \\ F_{SD} &= 45\,C_S/1000, & u_S &= 45. \end{aligned} \tag{3.35}$$

Here, $f_{TA} = f_{TA}(t)$ represents an internal flux from the terrestrial biosphere to the atmosphere caused by land-use change (e.g., deforestation). Its values and also the values of the external inputs through fossil-fuel emissions $u_A(t)$ are taken as time series data from the RCP/ECP8.5 scenario (Fujino et al., 2006; Meinshausen et al., 2011). These time series data cover the period from the year $t_0 = 1765$ until the year $T = 2500$. The two parameters α and β control the fluxes from the atmosphere to the terrestrial biosphere and from the surface ocean to the atmosphere, respectively. If both parameters are equal to 1 and f_{TA} vanishes, then the model is linear, otherwise it is nonlinear.

The model can now be described by the three ODEs, for $t \in (t_0, T)$,

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\, C_A(t) &= F_{TA}(t) + F_{SA} - F_{AT} - F_{AS} + u_A(t), \\ \frac{\mathrm{d}}{\mathrm{d}t}\, C_T(t) &= F_{AT} - F_{TA}(t), \\ \frac{\mathrm{d}}{\mathrm{d}t}\, C_S(t) &= F_{AS} - F_{SA} - F_{SD} + u_S. \end{aligned} \tag{3.36}$$

Note that the right hand side of Eq. (3.36) depends through Eq. (3.35) not only on t, but also on the state vector $\mathbf{x}(t) = (C_A(t), C_T(t), C_S(t))^\top$. If we now define the state- and time-dependent compartmental matrix $\mathrm{B} = \mathrm{B}(\mathbf{x}(t), t)$ by

$$\mathrm{B} = \begin{pmatrix} -C_A^{-1}\,(F_{AT} + F_{AS}) & C_T^{-1}\,F_{TA} & C_S^{-1}\,F_{SA} \\ C_A^{-1}\,F_{AT} & -C_T^{-1}\,F_{TA} & 0 \\ C_A^{-1}\,F_{AS} & 0 & -C_S^{-1}\,(F_{SA} + F_{SD}) \end{pmatrix} \tag{3.37}$$

and $\mathbf{u}(t) = (u_A(t), 0, u_S)^\top$, then the model fits in the framework of Eq. (3.1) describing the nonlinear nonautonomous compartmental system

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) &= \mathrm{B}(\mathbf{x}(t), t)\,\mathbf{x}(t) + \mathbf{u}(t), \quad t \in (t_0, T), \\ \mathbf{x}(t_0) &= \mathbf{x}^0. \end{aligned} \tag{3.38}$$

We consider the system at time $t_0 = 1765$ to be in equilibrium, hence

$$\mathbf{x}^0 = (700, 3000, 1000)^\top. \tag{3.39}$$

3.9.2. Simulation and results

We consider two different parameter sets: (1) $(\alpha, \beta) = (0.2, 10)$ and (2) $(\alpha, \beta) = (1, 1)$. Parameter set (1) is from the original publication (Rodhe & Björkström, 1979) and describes a nonlinear scenario. Parameter set (2) makes together with $f_{TA} = 0$ the model become linear and we use this scenario as a reference measure for the nonlinear version (1). In the year 1765, the system is in equilibrium and exhibits different age density functions in different compartments (Figure 3.2). After the year 1765, we perturb the system by an

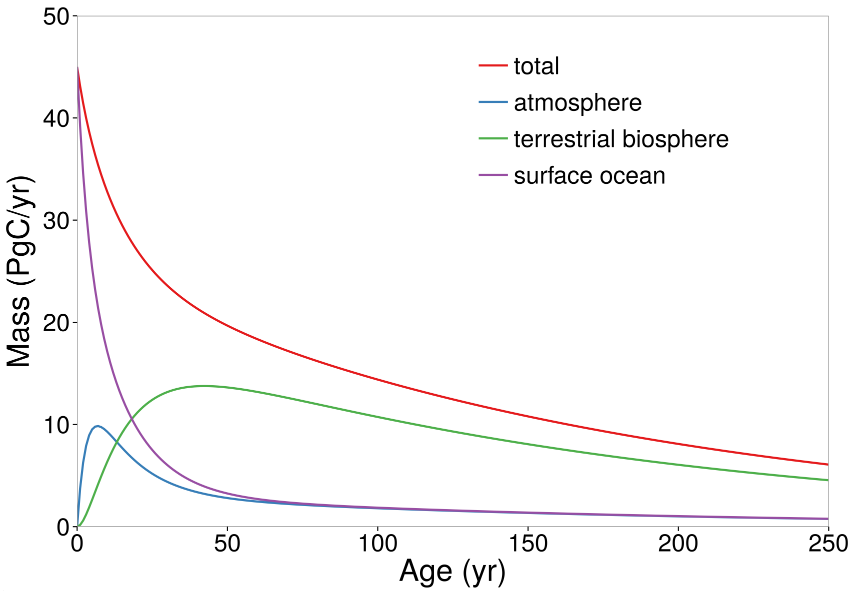


Figure 3.2. Pre-industrial carbon age density functions of the three compartments atmosphere (blue), terrestrial biosphere (green), and surface ocean (purple). The red curve shows the age density function of the entire system. (Figure extracted from Metzler et al. (2018))

additional external input flux u_A of carbon to the atmosphere caused by fossil-fuel combustion, and by an additional internal flux f_{TA} caused by land-use change (Figure 3.3). For the interval 1765–2100, the data correspond to the Representative Concentration Pathways 8.5 Scenario (RCP8.5), whereas the data for the interval 2100–2500 stem from the Extended Concentration Pathways Scenario 8.5 (ECP8.5). We assume constant emissions after 2100, followed by a smooth transition to stabilized atmospheric CO_2 concentrations after the year 2250 achieved by linear adjustment of emissions after the year 2150. The perturbations make the age density functions change with time such that they can be depicted by two-dimensional surfaces in a three-dimensional space (Figure 3.4).

To obtain useful information from these density functions, we address two climate-relevant questions inspired by O'Neill et al. (1997).

How old is atmospheric carbon?

The entire time evolutions of the atmospheric carbon's age density functions derived from the two versions of the model are depicted in Figure 3.4 (left panel: nonlinear, middle panel: linear), and so we can answer the question of atmospheric carbon age for all times

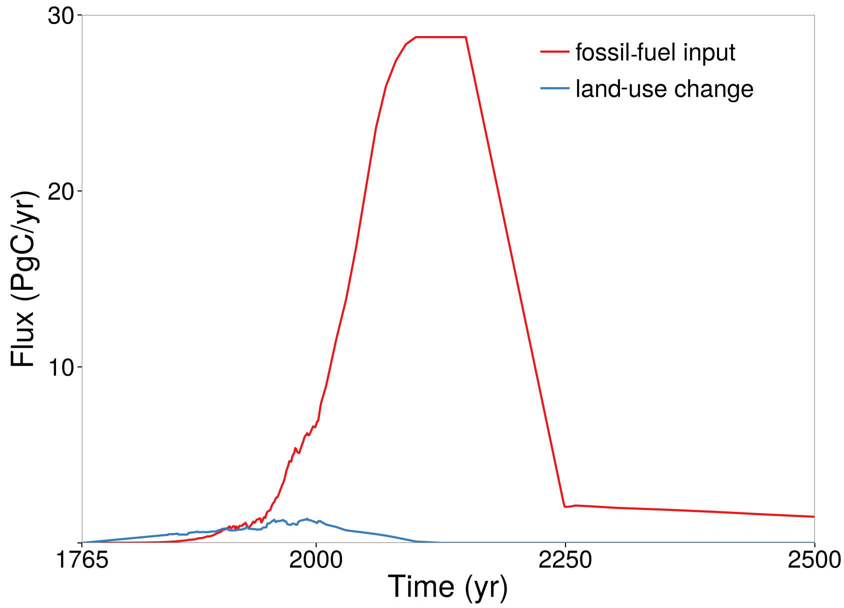


Figure 3.3. Anthropogenic perturbations of the global carbon cycle by carbon inputs to the atmosphere caused by fossil-fuel emissions (u_A, red) and land-use change (f_{TA}, blue) according to RCP/ECP8.5. (Figure extracted from Metzler et al. (2018))

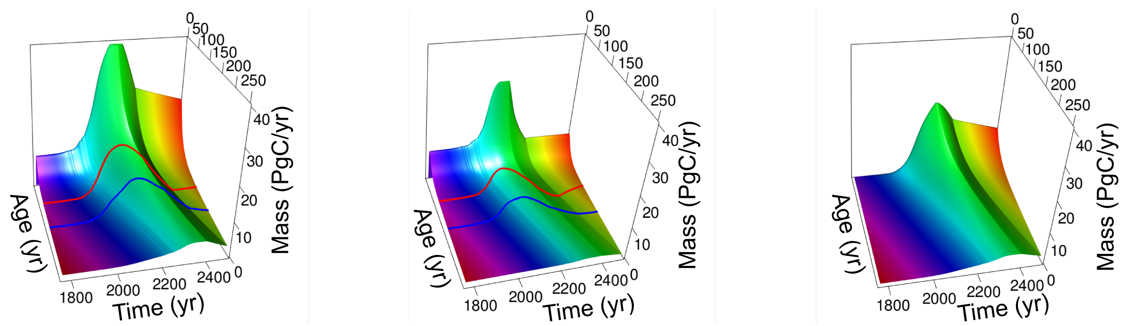


Figure 3.4. Time evolution of the atmospheric carbon's age density function. The left panel is for the nonlinear version of the model, the middle panel for the linear version, and the right panel shows the difference between the two (panel 1 minus panel 2). Red curves show the median age and blue curves the mean age. The surface color is constant along the time-age diagonal, it reflects the moment of entry into the system. At the very left edges of the first two panels (time = 1765 yr) we can identify the equilibrium age density function of the atmospheric carbon (cf. Figure 3.2), whereas the front edges (age = 250 yr) show how much carbon is in the system with age equal to 250 yr from the year 1765 through the year 2500. (Figure extracted from Metzler et al. (2018))

between 1765 and 2500. In the year 2017, its mean age in the nonlinear model version is 126.35 yr (linear: 128.32 yr) and the median age is equal to 61.76 yr (62.69 yr). The standard deviation equals 161.72 yr (162.92 yr) indicating that the age distribution has a long tail, a feature which cannot be revealed from the mean alone.

In these numbers, we recognize only very little differences between the nonlinear and the linear model versions. Nevertheless, we can observe important differences in the entire evolution of the age distributions depicted in the left and the middle panel of Figure 3.4. The differences are twofold. First, the pure amount of atmospheric carbon is much higher in the nonlinear model version. Second, the age distributions of atmospheric carbon show also different shapes for the two scenarios. This results in the non-flat surface to be seen in the right panel depicting the difference between the density functions of atmospheric carbon in the nonlinear and the linear version of the model.

How long will a significant fraction of a pulse of fossil-fuel carbon, emitted to the atmosphere today, remain in the system?

We consider carbon entering directly into the atmosphere at specific times t_a and want to know how long it will take to remove it from the system. The forward transit time at time t_a describes how old material entering the system at time t_a will be at the time of its exit. As indicated by the left panel of Figure 3.5, for the nonlinear model version the forward transit-time distribution of material injected between 1800 and 2170 constantly shifts to older ages, while it shifts back to younger ages after 2170. The medians of the forward transit time of material injected in the years 1800, 1990, 2015 (Paris Agreement), 2170, and 2300 are given by 79.85 yr, 82.91 yr, 86.12 yr, 108.91 yr, and 102.61 yr, respectively. As the right panel of Figure 3.5 shows, the situation is very different in the linear scenario. Here, the forward transit-time distribution does not depend at all on the injection time and remains the same as in the steady state in the year 1765 because the coefficients of B remain constant over time. Obviously, taking into account nonlinear processes leads to a significant increase of the lifetime of fossil-fuel derived carbon in the system according to this model.

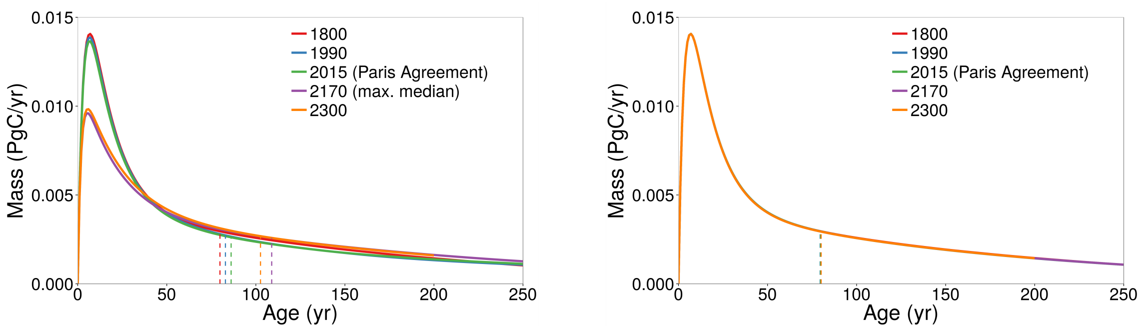


Figure 3.5. Forward transit-time density functions of fossil-fuel carbon entering the atmosphere in the years 1800 (red), 1990 (blue), 2015 (green), 2170 (purple), and 2300 (orange). The left panel shows the nonlinear version and the right panel the linear one. Orange curves end at the age of 200 yr, because our simulation only lasts until the year 2500. The medians (dashed vertical lines) in the nonlinear version increase until the year 2170, and then start decreasing. In the linear version, the distributions and medians remain constant. (Figure extracted from Metzler et al. (2018))

3.9.3. Derivation of the results from the example application

First of all, we solve the system (3.38) numerically on the time interval $[1765, 2500]$ and obtain a solution trajectory $\mathbf{x} = \mathbf{x}(t)$. With this solution in hand, we can at all times $t \in (1765, 2500)$ compute the compartmental matrix $\mathrm{B} = \mathrm{B}(\mathbf{x}(t), t)$.

Equilibrium age densities

At time $t_0 = 1765$, the system is supposed to be in equilibrium and the land-use change flux $f_{TA}(t_0)$ vanishes. We plug Eq. (3.35) and Eq. (3.39) in matrix (3.37) and get

$$\mathrm{B}(\mathbf{x}^0, t_0) = \begin{pmatrix} -160/700 & 60/3000 & 100/1000 \\ 60/700 & -60/3000 & 0 \\ 100/700 & 0 & -145/1000 \end{pmatrix}.$$

If we set $\mathrm{B}^0 := \mathrm{B}(\mathbf{x}^0, t_0)$ and $\mathbf{u}^0 := \mathbf{u}(t_0) = (0, 0, 45)^\top$, then $\mathrm{B}^0\,\mathbf{x}^0 + \mathbf{u}^0 = \mathbf{0}$. We further define $\mathrm{X}^0 := \mathrm{diag}(x_1^0, x_2^0, x_3^0)$. The steady-state formula from Corollary 2.15 gives

$$f_{\mathbf{a}}(a) = \left(\mathrm{X}^0\right)^{-1}\, e^{a\,\mathrm{B}^0}\, \mathbf{u}^0, \quad a \geq 0.$$

Furthermore, $\mathbf{p}^0 = \mathrm{X}^0\, f_{\mathbf{a}}$. Consequently, the initial age density function vector is given by

$$\mathbf{p}^0(a) = e^{a\,\mathrm{B}^0}\, \mathbf{u}^0, \quad a \geq 0. \tag{3.40}$$

Atmospheric age

The two leftmost panels of Figure 3.4 depict the two-dimensional surfaces (nonlinear and linear model version) corresponding to $\mathbf{p} = \mathbf{p}(a, t)$ in the time interval 1765–2500 yr and the age interval 0–250 yr. The scalar field $\mathbf{p}$ can be obtained by Eq. (3.5). By Eq. (3.40), we have already computed the initial age density function vector $\mathbf{p}^0$, and the vector-valued input function $\mathbf{u}$ is given by the RCP/ECP8.5 scenario. Consequently, we are only missing the state-transition matrix Φ. We compute Φ by numerically solving the matrix ODE system (B.1) on $\{(t_2, t_1) \in [1765, 2500] \times [1765, 2500] :\, t_2 \geq t_1\}$ and can then proceed to compute $\mathbf{p}$ on $[0, 250] \times [1765, 2500]$.

To obtain a time trajectory of the mean age and the second moment of the atmospheric carbon, we follow Eq. (3.22) and solve the 9-dimensional ODE system, for $t_0 = 1765$ and $T = 2500$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \mathbf{x} \\ \bar{\mathbf{a}}^1 \\ \bar{\mathbf{a}}^2 \end{pmatrix}(t) = \begin{pmatrix} \mathrm{B}(\mathbf{x}(t), t)\,\mathbf{x}(t) + \mathbf{u}(t) \\ \boldsymbol{\gamma}^1(t, \mathbf{x}(t), \mathbf{1}, \bar{\mathbf{a}}^1(t)) \\ \boldsymbol{\gamma}^2(t, \mathbf{x}(t), \bar{\mathbf{a}}^1(t), \bar{\mathbf{a}}^2(t)) \end{pmatrix}, \quad t \in (t_0, T)$$
$$(\mathbf{x}, \bar{\mathbf{a}}^1, \bar{\mathbf{a}}^2)(t_0) = (\mathbf{x}^0, \bar{\mathbf{a}}^{0,1}, \bar{\mathbf{a}}^{0,2}),$$

where, for $k = 1, 2$, $\boldsymbol{\gamma}^k = (\gamma_1^k, \gamma_2^k, \gamma_3^k)^\top$ and for $i = 1, 2, 3$,

$$\gamma_i^k(t, \mathbf{x}, \bar{\mathbf{a}}^{k-1}, \bar{\mathbf{a}}^k) = k\,\bar{a}_i^{k-1} + \frac{1}{x_i}\left[\sum_{j=1}^{3} B_{ij}\, x_j\, \left(\bar{a}_j^k - \bar{a}_i^k\right) - \bar{a}_i^k\, u_i\right].$$

The initial age moments $\bar{\mathbf{a}}^{0,1}$ and $\bar{\mathbf{a}}^{0,2}$ can be obtained using the equilibrium formula from Corollary 2.15, i.e.,

$$\bar{\mathbf{a}}^{0,n} = (-1)^n\, n!\, \left(\mathrm{X}^0\right)^{-1}\, \left(\mathrm{B}^0\right)^{-n}\, \mathbf{x}^0, \quad n = 1, 2.$$

Then $\mu_1(t) := \bar{a}_1^1(t)$ is the mean age of the atmospheric carbon at time t and $\mu_2(t) := \bar{a}_1^2(t)$ its second moment. The standard deviation at time t can be computed as the square root of $\mu_2(t) - \mu_1^2(t)$.

The trajectory of the age median of atmospheric carbon can be computed by solving Eq. (3.26) for $q = 0.5$ and $i = 1$. To that end, the cumulative compartment-age distribution $\mathbf{P}$ needs to be obtained by Eq. (3.9) together with

$$\mathbf{P}^0(a) = \left(\mathrm{B}^0\right)^{-1} \left(e^{a\,\mathrm{B}^0} - \mathrm{I}\right) \mathbf{u}(t_0), \quad a \geq 0. \tag{3.41}$$

To obtain Eq. (3.41), we only need to integrate Eq. (3.40). The initial age median ξ_1^0 of the atmospheric carbon at time t_0 needs to be approximated by a nonlinear optimization algorithm such that $P_1^0(\xi_1^0) = 0.5\, x_1^0$.

Forward transit time of fossil-fuel derived carbon

To compute the density function of the forward transit time of fossil-fuel derived carbon, we simply change the input vector to $\mathbf{u}(t) := (u_A(t), 0, 0)^\top$ and apply Eq. (3.33). By using the new input vector, we consider the subsystem of only fossil-fuel derived carbon. We can treat this subsystem separately by means of the linear system that we derived by plugging the numerical solution into the nonlinear system.

Quantiles q, such as the median ($q = 0.5$), for the forward transit time at arrival time t_a need to be computed by nonlinear optimization algorithms. To that end, $P_{\mathrm{FTT}}(\xi, t_a) = q\,\|\mathbf{u}(t_a)\|$ must be solved for ξ, where

$$P_{\mathrm{FTT}}(a, t_a) = \|\mathbf{u}(t_a)\| - \|\Phi(t_a + a, t_a)\,\mathbf{u}(t_a)\|$$

describes the difference between the total input at time t_a and what remained of it at time $t_a + a$. Then, $t_a + \xi$ is the time at which the proportion q of the total input $\|\mathbf{u}(t_a)\|$ from time t_a will have left the system.

3.10. Discussion

We obtained age-, transit-time, and remaining lifetime distributions for well-mixed compartmental systems. Our results are not restricted to linear models or systems in steady state, but hold even for nonlinear nonautonomous models. This fundamental advance allows us to drop the assumption that the system is in equilibrium – an assumption which is unreasonable for most natural systems.

The derivation of the formulas for the age density functions only relies on the general solution formula (3.4) for linear nonautonomous systems. In nonlinear systems, a known solution trajectory is interpreted linearly and then the system can be treated as if it were linear – as long as we consider only one particular trajectory. This approach also allows us to consider age density functions of subsystems such as all material that entered the system through a specific compartment.

Additionally, we obtained ODEs to compute means, higher order moments, and quantiles (e.g., the median) of ages. We can use these ODEs to obtain, by very fast computations, much more precise characterizations of age distributions than it was possible before by only looking at the means.

The power of these results is shown in an application to a simple global carbon cycle model. We demonstrated how much age- and transit-time distributions differ between a nonlinear and a linear version of the model. First of all, nonlinearities lead to a tremendously higher amount of carbon in the atmosphere. Secondly, these two versions of a simple model already suggest that the lifetime of fossil-fuel derived atmospheric carbon before being absorbed by the deep ocean is substantially increased by nonlinear processes (Archer & Brovkin, 2008). Such sizable differences in age- and transit-time distributions of two models might be a criterion to select one model or the other.

We want to stress that the we model used here is very simple and used mainly to demonstrate the power and versatile applications of our mathematical framework in a comprehensible manner. However, it is important to emphasize that for any global carbon cycle model represented as well-mixed compartmental system, no matter how many compartments it comprises, we could answer questions of high scientific and societal interest (e.g., the age of the current atmospheric carbon, the future exit age of carbon that now enters the system).

Our results are not restricted to carbon cycle models, of course, but can be readily applied to all kinds of well-mixed compartmental systems. To that end, we provide a Python package that implements all theoretical results and makes them usable by a few simple commands (`https://github.com/MPIBGC-TEE/CompartmentalSystems`). This package also includes a demonstration (Jupyter) notebook and an HTML file with code to reproduce the figures and to show more characteristics of the presented model.

A different approach than ours is needed when the well-mixed assumption of the compartments is dropped. The fluxes could be age-dependent, a very common case in hydrology, where the focus mostly lies on the annual water balance of catchments (McDonnell, 2017). Such catchments are usually modeled as one compartment with one influx (precipitation) and two age-dependent outfluxes (evaporation, runoff) (Botter et al., 2011; Harman, 2015; Porporato & Calabrese, 2015). Even though this case does not fit directly in our framework, it is possible to approximate the one-compartment system with age-dependent outflows by a multiple-compartment well-mixed system. For time-independent systems, this approximation bases on the fact that every nonnegative probability distribution can be approximated arbitrarily well by a phase-type distribution (Asmussen, 2003). Doing a similar kind of approximation for a nonautonomous single-catchment model allows the full application of the theory presented here. A recent commentary emphasizes the restrictions of single-catchment models and highlights the need for splitting the single catchment into several compartments (McDonnell, 2017). Our results deliver the demanded "theoretical framework that includes both flow and the age distribution of these flowing and stored waters".

In Chapter 2, we used stochastic objects to infer deterministic results and vice versa. We showed that many objects in the deterministic world have a counterpart in the stochastic world. However, in the present chapter we used a purely deterministic setup in the framework of linear nonautonomous compartmental systems. Since mass conservation in the deterministic setup finds its counterpart as probability mass conservation in the stochastic setup, there are good chances to transfer the present theory to inhomogeneous Markov chains as well as to inhomogeneous renewal- (Daley & Vere-Jones, 2008) and regenerative processes (Thorisson, 1986, 1988), and to discover new relationships between the two fields.

CHAPTER 4

Entropy and complexity of compartmental systems

4.1. Motivation

Ages, transit times, and remaining lifetimes are diagnostic tools of open compartmental systems. They also help compare behavior and quality of different models. Nevertheless, structurally very different models might show very similar ages, transit times, and remaining lifetimes. If we are in the position to choose among such models, which is the one to select? By common sense, the answer is to select the least complex model and we can ask the question:

Can a model with fewer compartments reach the same complexity as a model with more compartments?

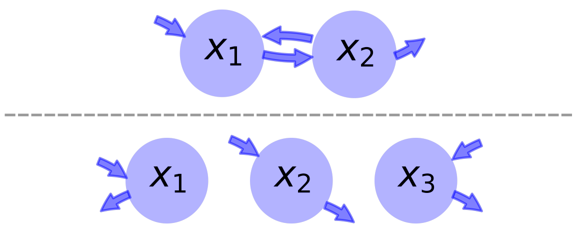


Figure 4.1. Which model is more complex, the two-compartment model with feedback or the three-compartment model without feedback?

This leads to the problem of how to define complexity for compartmental systems in the first place (Figure 4.1). Walter & Contreras (1999, Chapter 23) ask a complexity measure/index to have at least the following natural properties:

(1) For a given structure, the index should have its greatest value when the flow rates are even (all the same).

(2) Given two structures with the same number of compartments and even flow rates, the index should have a larger value for the one with more nonzero flow rates.

Many common complexity measures of dynamical systems are closely related to the information content of the system and hence to some kind of entropy. Two examples are the topological entropy and the Kolmogorov-Sinai/metric entropy. However, linear autonomous compartmental systems are asymptotically stable. By Pesin's theorem (Pesin, 1977), both the metric- and the topological entropy vanish and cannot serve as a complexity measure here; we need a different concept.

Alternatively, we can interpret compartmental systems as weighted directed graphs. There are numerous different complexity measures for graphs. Dehmer & Mowshowitz (2011) provide a comprehensive overview of the history of graph entropy measures. Unfortunately, most of such entropy measures are based on the number of vertices, vertex degree, edges, or degree sequence (Trucco, 1956). Thus, they concentrate on only the structural information of the graph. There are also graph theoretical measures that take edges and weights into account by using probability schemes. Their drawback is that the underlying meaning of complexity becomes difficult to interpret because the assigned probabilities seem somewhat arbitrary (Bonchev & Buck, 2005).

Since in the previous chapters we, amongst others, addressed the transit times of particles that travel through the system, we are naturally guided to a different approach. In terms of a single particle that moves through the system governed by a stochastic process, we can ask how difficult it is for us to guess the particle's current compartment, the particle's next compartment, and the particle's previous compartment. The more difficult it is to answer these three questions, the higher the complexity of the model should be. Consequently, a model's complexity should increase with the number of compartments, the number of fluxes leaving compartments, and the number of fluxes entering compartments. A weighted average of these numbers seems desirable. But how to choose the correct weights?

Since in open systems all material that enters the system also exits it later on, in this chapter we try to define a reasonable complexity measure for open compartmental systems based on the Shannon entropy (Shannon & Weaver, 1949) of the stochastic path covered by a particle from the moment of entering the system until the moment of leaving it. We further define a model's information content and touch the above mentioned problem of model selection, based on the concept of maximum entropy.

4.2. Introduction to information entropy

We introduce basic concepts of information entropy along the lines of Cover & Thomas (2006). There are two concepts of entropy of a random variable, depending on whether the random variable has a discrete or a continuous distribution.

Definition 4.1 (1) Let Y_d be a discrete real-valued random variable with range R_d and probability mass function p. The *Shannon information entropy* or *Shannon entropy* or *information entropy*, or simply *entropy* of Y_d is defined by

$$\mathbb{H}(Y_d) = -\sum_{y\in R_d} p(y)\,\log p(y) = -\mathbb{E}\left[\log p(Y_d)\right].$$

By convention, $0\,\log 0 := 0$.

(2) Let Y_c be a continuous real-valued random variable with range R_c and probability density function f. Then the *differential entropy* or simply *entropy* of Y_c is defined by

$$\mathbb{H}(Y_c) = -\int_{R_c} f(y)\,\log f(y)\,\mathrm{d}y = -\mathbb{E}\left[\log f(Y_c)\right].$$

Remark 4.2 Depending on the base of the logarithm, the unit of the entropy changes. For base 2, the unit is called bits and for base e, the unit is called nats. If not stated differently, we use the value e as logarithmic base, i.e., we use the natural logarithm.

The entropy $\mathbb{H}(Y)$ of a random variable Y has two intertwined interpretations. On the one hand, $\mathbb{H}(Y)$ is a measure of uncertainty, i.e., a measure of how difficult it is to predict the outcome of a realization of Y. On the other hand, $\mathbb{H}(Y)$ is also a measure of the information content of Y, i.e., a measure of how much information we gain once we learn about the outcome of a realization of Y. It is important to note that, even though their definitions and information theoretical interpretations are quite similar, the Shannon- and the differential entropy have one main difference. The Shannon entropy is always nonnegative, whereas the differential entropy can have negative values. Consequently, the Shannon entropy is an absolute measure of information and makes sense in its own right. The differential entropy, however, is not an absolute information measure. Hence, the differential entropy of a random variable makes sense only in comparison with the differential entropy of another random variable.

The left panel of Figure 4.2 depicts the Shannon entropy of a Bernoulli random variable Y_d with $\mathbb{P}(Y_d = 1) = 1 - \mathbb{P}(Y_d = 0) = p$ with $p \in [0, 1]$. This random variable could represent the outcome of a coin toss. We can see that the entropy is low when p is close to 0 or 1. In these cases, we have some information that the coin is biased, and hence we have a preference if we guess the outcome. The entropy is maximum if the coin is fair ($p = 1/2$), since we have no additional information about the outcome of the coin toss. The Shannon entropy of Y_d is

$$\mathbb{H}(Y_d) = -p \, \log p - (1 - p) \, \log(1 - p).$$

The right panel of Figure 4.2 shows the differential entropy of an exponentially distributed random variable $Y_c \sim \mathrm{Exp}(\lambda)$ with rate parameter $\lambda > 0$, probability density function $f(y) = \lambda \, e^{-\lambda \, y}$ for $y \geq 0$, and $\mathbb{E}\,[Y_c] = \lambda^{-1}$.

We can imagine it to represent the duration of stay of a particle in a well-mixed compartment in a linear autonomous compartmental system, where λ is the total outflow rate from the compartment. The higher the outflow rate is, the likelier is an early exit of the particle, and the easier it is to predict the moment of exit. Hence, the differential entropy decreases with increasing λ. It is given by

$$\mathbb{H}(Y_c) = 1 - \log \lambda.$$

Definition 4.3 Let Y_1, Y_2 be two discrete random variables with joint probability mass function p and ranges R_1 and R_2, respectively. The *joint entropy* of Y_1 and Y_2 is defined by

$$\mathbb{H}(Y_1, Y_2) = -\sum_{y_1 \in R_1} \sum_{y_2 \in R_2} p(y_1, y_2) \, \log p(y_1, y_2) = -\mathbb{E}\left[\log p(Y_1, Y_2)\right].$$

Note that the joint entropy is symmetric, i.e., $\mathbb{H}(Y_1, Y_2) = H(Y_2, Y_1)$.

Definition 4.4 Let Y_1 and Y_2 be two discrete random variables with joint probability mass function p. Furthermore, let p_2 denote the probability mass function of Y_2 and denote by $p(y_1 \,|\, y_2)$ the conditional probability $\mathbb{P}(Y_1 = y_1 \,|\, Y_2 = y_2)$.

Then the *conditional entropy* of Y_1 given Y_2 is defined by

$$\begin{aligned}\mathbb{H}(Y_1 \,|\, Y_2) &= \sum_{y_2 \in R_2} \mathbb{H}(Y_1 \,|\, Y_2 = y_2)\, p_2(y_2) \\ &= -\sum_{y_2 \in R_2} p_2(y_2) \sum_{y_1 \in R_1} p(y_1 \,|\, y_2)\, \log p(y_1 \,|\, y_2) \\ &= -\sum_{y_2 \in R_2} \sum_{y_1 \in R_1} p(y_1, y_2)\, \log p(y_1 \,|\, y_2) \\ &= -\mathbb{E}\left[\log p(Y_1 \,|\, Y_2)\right].\end{aligned}$$

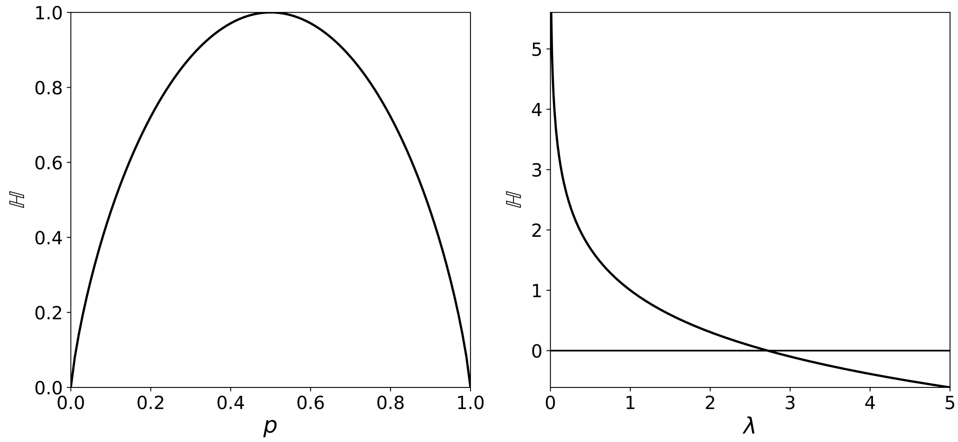


Figure 4.2. Entropy of Bernoulli- and exponentially distributed random variables. The left panel shows the Shannon entropy (logarithmic base 2) of a Bernoulli random variable depending on its success probability p. The right panel shows the differential entropy with logarithmic base e of an exponentially distributed random variable depending on its rate parameter λ.

The joint entropy of two random variables is the entropy of one variable plus the conditional entropy of the other. This is expressed in

$$\mathbb{H}(Y_1, Y_2) = \mathbb{H}(Y_2) + \mathbb{H}(Y_1 \,|\, Y_2). \tag{4.1}$$

Let Y_3 be a third discrete random variable. Then

$$\mathbb{H}(Y_1, Y_2 \,|\, Y_3) = \mathbb{H}(Y_1 \,|\, Y_3) + \mathbb{H}(Y_2 \,|\, Y_1, Y_3). \tag{4.2}$$

Let $Y_1, Y_2, \ldots, Y_n$ be discrete random variables. By repeated application of Eq. (4.1) and Eq. (4.2), we obtain the *chain rule*

$$\mathbb{H}(Y_1, Y_2, \ldots, Y_n) = \sum_{k=1}^{n} \mathbb{H}(Y_k \,|\, Y_{k-1}, \ldots, Y_1). \tag{4.3}$$

Remark 4.5 We defined the joint- and conditional entropy for discrete random variables only. Analogous definitions can be made for continuous random variables. Also the chain rule holds for differential entropy.

Definition 4.6 The *entropy rate* of a discrete-time stochastic process $Y = (Y_n)_{n \in \mathbb{N}}$ is defined by

$$\theta(Y) = \lim_{n \to \infty} \frac{1}{n}\, \mathbb{H}(Y_1, Y_2, \ldots, Y_n) = -\frac{1}{n}\, \mathbb{E}\left[\log p_n(Y_1, Y_2, \ldots, Y_n)\right]$$

if the limit exists. Here, p_n denotes the joint probability mass function of $Y_1, Y_2, \ldots, Y_n$.

The discrete-time entropy rate describes the long-term average increase of the processes' entropy per time step. The statements of the following lemma are proven in Cover & Thomas (2006, Theorem 4.2.1).

Lemma 4.7 *For a stationary discrete-time stochastic process $Y = (Y_n)_{n\in\mathbb{N}}$, the entropy rate is*

$$\theta(Y) = \lim_{n\to\infty} \mathbb{H}(Y_n \,|\, Y_{n-1}, \ldots, Y_1).$$

Consequently, if Y is a stationary discrete-time Markov chain, its entropy rate is

$$\theta(Y) = \mathbb{H}(Y_2 \,|\, Y_1).$$

According to Bad Dumitrescu (1988) and Girardin & Limnios (2003), we can also define the entropy rate for continuous-time processes. To that end, we first define the entropy on a finite time interval.

Definition 4.8 The *finite-time entropy* of the continuous-time stochastic process $Z = (Z_t)_{t\geq 0}$ until $T \geq 0$ is defined as

$$\mathbb{H}_T(Z) = -\int f_T(z)\, \log f_T(z)\, \mathrm{d}\mu_T(z),$$

where f_T is the likelihood of $(Z_t)_{0\leq t\leq T}$ with respect to some reference measure μ_T, if it exists.

Definition 4.9 The *entropy rate* of a continuous-time stochastic process $Z = (Z_t)_{t\geq 0}$ is defined by

$$\theta(Z) = \lim_{T\to\infty} \frac{1}{T}\, \mathbb{H}_T(Z)$$

if the limit exists.

4.3. Compartmental systems in equilibrium

We come back to the d-dimensional open linear autonomous system (2.3) in equilibrium from Chapter 2 and denote it by M. Let X denote the associated absorbing continuous-time Markov chain and Z the infinite continuous-time process from Eq. (2.17). The system is given by

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) &= \mathrm{B}\,\mathbf{x}(t) + \mathbf{u}, \quad t > 0, \\ \mathbf{x}(0) &= \mathbf{x}^*. \end{aligned} \tag{4.4}$$

This system might have been linear from the beginning or it might result from an autonomous nonlinear system that has reached an equilibrium. Since B is invertible, by Proposition 1.13 this system has a globally attracting fixed point $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$, so it has no positive Lyapunov exponents. Consequently, its metric- and topological entropy are zero by Pesin's theorem and cannot serve as complexity measures. We need a different approach to define a complexity measure for such systems.

To that end, we look at the path that a single particle covers while it travels through the system. This path is a finite sequence of pairs (ζ_n, T_n), where ζ_n stands for the nth compartment visited by the particle and T_n for the sojourn time in the nth compartment. A particle leaving the system is modeled as entering the so-called *environmental compartment* $d+1$. The particle is then supposed to stay there for an infinitesimal amount of time before it reenters the system. The particle's then infinite path $\mathcal{P}_\infty := ((\zeta_n, T_n))_{n\in\mathbb{N}}$ consists of two Markov processes. The first one, $\zeta = (\zeta_n)_{n\in\mathbb{N}}$ with values in

$$\widetilde{S} = \{1, 2, \dots, d, d+1\}$$

describes the sequence of visited compartments and is a discrete-time Markov chain. The second one, the sojourn-time process $(T_n)_{n\in\mathbb{N}}$, with values in $\mathbb{R}_+$ describes the sequence of sojourn times. If at time step $n \in \mathbb{N}$ the particle is in compartment $j \in S = \{1, 2, \dots, d\}$, then $T_n \sim \operatorname{Exp}(\lambda_j)$, where $\lambda_j := -B_{jj}$. Since we cannot model an infinitesimal sojourn time for the environmental compartment $d+1$, we define its sojourn-time distribution to be $\operatorname{Exp}(\lambda_{d+1})$ for $\lambda_{d+1} := 1$ and correct for it later.

Based on these basic structures of a path, we compute three different types of entropy. For a better understanding, we provide a summary of the desirable relations among the three different types:

(1) As a particle travels through the system, it jumps a certain number of times to the next compartment until it finally jumps out of the system to the environmental compartment $d+1$. Between two jumps, the particle resides in some compartment. Each jump comes with the uncertainties about which compartment will be next and how long will the particle stay there. The *entropy rate per jump* measures the average of these uncertainties with respect to the mean number of jumps.

(2) The travel of the particle takes a certain time. In each unit time interval before the particle leaves, uncertainties exist whether the particle jumps, where it jumps, and even how often it jumps. The mean of these uncertainties over the mean length of the travel interval is measured by the *entropy rate per unit time*.

(3) The *path entropy* measures the entire uncertainty about the particles travel through the system. We should be able to compute it if we multiply the mean entropy rate per jump by the mean number of jumps, and also if we multiply the entropy rate per unit time by the mean transit time.

4.3.1. Entropy rate per jump

The noninvertible matrix

$$\mathrm{Q} = \begin{pmatrix} \mathrm{B} & \boldsymbol{\beta} \\ \mathbf{z}^\top & -1 \end{pmatrix} \tag{4.5}$$

with $\mathbf{z}^\top = -\mathbf{1}^\top \mathrm{B}$ and $\boldsymbol{\beta} = \mathbf{u}/\|\mathbf{u}\|$ is the transition-rate matrix of the continuous-time Markov chain that represents the particle's infinite journey. With aid from the diagonal matrix

$$\begin{aligned} \mathrm{D}_\mathrm{Q} :&= -\operatorname{diag}(Q_{11}, Q_{22}, \dots, Q_{dd}, Q_{d+1,d+1}) \\ &= -\operatorname{diag}(B_{11}, B_{22}, \dots, B_{dd}, -1) \\ &= \quad \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_d, \lambda_{d+1}), \end{aligned}$$

we define $\mathrm{P} := \mathrm{Q}\,\mathrm{D}_\mathrm{Q}^{-1} + \mathrm{I}$. Then, with $\lambda_j = -B_{jj}$ for $j \in S = \{1, 2, \dots, d\}$, the

$$P_{ij} = \begin{cases} 0, & i = j, \\ \lambda_j^{-1} B_{ij} & i \neq j, \qquad i, j \leq d, \\ \beta_i, & i \leq d, \qquad j = d+1, \\ \lambda_j^{-1} z_j, & i = d+1, \qquad j \leq d, \end{cases} \tag{4.6}$$

constitute the transition matrix P of the discrete-time Markov chain ζ. Note the index order: $P_{ij} = \mathbb{P}(\zeta_{n+1} = i \,|\, \zeta_n = j)$ is the conditional probability of ζ jumping to state i in the next step given that it is in state j at time step n.

We define a $(d+1)$-dimensional column vector $\mathbf{y} := (x_1^*, x_2^*, \ldots, x_d^*, \|\mathbf{u}\|)^\top = (\mathbf{x}^*, \|\mathbf{u}\|)^\top$ and compute

$$(\mathrm{Q}\,\mathbf{y})_i = \sum_{j=1}^{d+1} Q_{ij}\, y_j = \sum_{j=1}^{d} B_{ij}\, x_j^* + \beta_i\, \|\mathbf{u}\| = -u_i + u_i = 0, \quad i \in \widetilde{S}, \tag{4.7}$$

because the system is in equilibrium. Then, $\boldsymbol{\pi} := \|\mathrm{D_Q}\,\mathbf{y}\|^{-1}\,\mathrm{D_Q}\,\mathbf{y}$ is a stationary distribution of ζ, because

$$\begin{aligned}\mathrm{P}\,\boldsymbol{\pi} &= \|\mathrm{D_Q}\,\mathbf{y}\|^{-1}\left[\mathrm{Q}\,\mathrm{D_Q^{-1}} + \mathrm{I}\right]\mathrm{D_Q}\,\mathbf{y} \\ &= \|\mathrm{D_Q}\,\mathbf{y}\|^{-1}\,(\mathrm{Q}\,\mathbf{y} + \mathrm{D_Q}\,\mathbf{y}) \\ &= \|\mathrm{D_Q}\,\mathbf{y}\|^{-1}\,\mathrm{D_Q}\,\mathbf{y} \\ &= \boldsymbol{\pi}.\end{aligned}$$

Since B is invertible, by Lemma 1.7 and definition (4.6) of P, the discrete-time Markov chain ζ is irreducible. Lemma C.9 implies that

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} \mathbb{P}(\zeta_k = j) = \pi_j, \quad j \in \widetilde{S}.$$

Our subsequent interest is in long-term averages of the type

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} \mathbb{P}(\zeta_k = j)\, f(i,j)$$

for functions $f : \widetilde{S} \times \widetilde{S} \to \mathbb{R}$. Consequently, we can simply equip ζ with the stationary initial distribution $\boldsymbol{\pi}$, making ζ a stationary discrete-time Markov chain from now on.

Let $\mathrm{P_B} := (P_{ij})_{i,j\in S}$ denote the matrix P restricted to the first d coordinates, and define

$$\mathrm{D_B} := -\operatorname{diag}(B_{11}, B_{22}, \ldots, B_{dd}) = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_d).$$

Furthermore, from now on we denote by

$$\mathcal{N} := \mathbb{E}\left[\inf\{n \in \mathbb{N} \,:\, \zeta_n = d+1\}\right]$$

the mean of the first hitting time of state $d+1$ by ζ. It is given by

$$\mathcal{N} = \sum_{i=1}^{d} (\mathrm{M}\,\boldsymbol{\beta})_i,$$

where $\mathrm{M} = (\mathrm{I} - \mathrm{P_B})^{-1}$ is the fundamental matrix of the absorbing continuous-time Markov chain X. Moreover, we denote by N_i the mean number of visits of ζ to compartment $i \in S$ per cycle, which is given by

$$N_i = (\mathrm{M}\,\boldsymbol{\beta})_i.$$

Lemma 4.10 *With the definitions from above,*

$$\|\mathrm{D_Q}\,\mathbf{y}\| = \|\mathbf{u}\|\,(1 + \mathcal{N}).$$

Proof. Recall that X denotes the absorbing continuous-time Markov chain that represents one run of a particle through the system, and $\boldsymbol{\beta} = \mathbf{u}/\|\mathbf{u}\|$. The fundamental matrix of X is given by

$$\mathrm{M} = (\mathrm{I} - \mathrm{P}_\mathrm{B})^{-1} = \left[\mathrm{I} - (\mathrm{B}\,\mathrm{D}_\mathrm{B}^{-1} + \mathrm{I})\right]^{-1} = -\mathrm{D}_\mathrm{B}\,\mathrm{B}^{-1}.$$

Now, the total number of jumps of X before absorption is given by

$$\mathcal{N} = \sum_{i=1}^{d} (\mathrm{M}\,\boldsymbol{\beta})_i = \|\mathbf{u}\|^{-1} \sum_{i=1}^{d} \left(-\mathrm{D}_\mathrm{B}\,\mathrm{B}^{-1}\,\mathbf{u}\right)_i = \|\mathbf{u}\|^{-1} \sum_{i=1}^{d} \lambda_i\, x_i^*.$$

We finish the proof with

$$\|\mathrm{D}_\mathrm{Q}\,\mathbf{y}\| = \sum_{i=1}^{d} \lambda_i\, x_i^* + \|\mathbf{u}\| = \|\mathbf{u}\|\,(\mathcal{N} + 1).$$

□

Remark 4.11 Since $\mathcal{N}$ denotes the mean of the first hitting time of the environmental compartment,

$$1 + \mathcal{N} = \frac{\|\mathrm{D}_\mathrm{Q}\,\mathbf{y}\|}{\|\mathbf{u}\|}$$

is the mean number of jumps per cycle. The 1 stands for the jump into the system.

Corollary 4.12 *The* i*th component* π_i *of the stationary distribution* $\boldsymbol{\pi}$ *of* ζ *represents the fraction of the mean number of visits to compartment* i *per cycle. The environmental compartment* $d+1$ *experiences exactly one visit per cycle.*

Proof. For $i \in S$, the mean number of visits of state i per cycle is given by

$$\begin{aligned} N_i &= (\mathrm{M}\,\boldsymbol{\beta})_i = \left(-\mathrm{D}_\mathrm{B}\,\mathrm{B}^{-1}\,\boldsymbol{\beta}\right)_i = \|\mathbf{u}\|^{-1}\,\left(-\mathrm{D}_\mathrm{B}\,\mathrm{B}^{-1}\,\mathbf{u}\right)_i \\ &= \frac{\lambda_i\,x_i^*}{\|\mathbf{u}\|} = \frac{(\mathrm{D}_\mathrm{Q}\,\mathbf{y})_i}{\|\mathbf{u}\|} = \frac{\pi_i\,\|\mathrm{D}_\mathrm{Q}\,\mathbf{y}\|}{\|\mathbf{u}\|} \\ &= \pi_i\,(1 + \mathcal{N}). \end{aligned} \tag{4.8}$$

For $i = d+1$,

$$\pi_{d+1} = \frac{\|\mathbf{u}\|}{\|\mathrm{D}_\mathrm{Q}\,\mathbf{y}\|} = \frac{\|\mathbf{u}\|}{\|\mathbf{u}\|\,(1+\mathcal{N})} = \frac{1}{1+\mathcal{N}}. \tag{4.9}$$

□

Lemma 4.13 *The entropy rate of the compartment chain* ζ *is given by*

$$\theta(\zeta) = \sum_{j=1}^{d} \pi_j \left[\sum_{i=1, i\neq j}^{d} -\frac{B_{ij}}{\lambda_j}\,\log\left(\frac{B_{ij}}{\lambda_j}\right) - \frac{z_j}{\lambda_j}\,\log\left(\frac{z_j}{\lambda_j}\right)\right] - \pi_{d+1} \sum_{i=1}^{d} \beta_i\,\log\beta_i. \tag{4.10}$$

Proof. With the initial distribution $\boldsymbol{\pi}$, the compartment chain ζ becomes stationary. We invoke Lemma 4.7 and obtain

$$\begin{aligned} \theta(\zeta) = \mathbb{H}(\zeta_2 \,|\, \zeta_1) &= \sum_{j=1}^{d+1} \mathbb{P}(\zeta_1 = j)\,\mathbb{H}(\zeta_2 \,|\, \zeta_1 = j) = \sum_{j=1}^{d+1} \pi_j \sum_{i=1}^{d+1} -P_{ij}\,\log P_{ij} \\ &= \sum_{j=1}^{d} \pi_j \left[\sum_{i=1, i\neq j}^{d} -\frac{B_{ij}}{\lambda_j}\,\log\left(\frac{B_{ij}}{\lambda_j}\right) - \frac{z_j}{\lambda_j}\,\log\left(\frac{z_j}{\lambda_j}\right)\right] - \pi_{d+1} \sum_{i=1}^{d} \beta_i\,\log\beta_i. \end{aligned}$$

□

Now that the entropy rate of the compartment chain ζ is determined, we seek the entropy rate of the path $\mathcal{P}_\infty$. To that end, we first consider a path of finite length.

Lemma 4.14 *For $n \in \mathbb{N}$,*

$$\mathbb{H}((\zeta_1, T_1), \ldots, (\zeta_n, T_n)) = \sum_{k=1}^{n} \mathbb{H}(T_k \,|\, \zeta_k) + n\,\theta(\zeta).$$

Proof. For notational compactness, we write $\mathbb{H}_n$ for $\mathbb{H}((\zeta_1, T_1), \ldots, (\zeta_n, T_n))$. By the chain rule Eq. (4.3) and Eqs. (4.2) and (4.1),

$$\begin{aligned}
\mathbb{H}_n &= \sum_{k=1}^{n} \mathbb{H}((\zeta_k, T_k) \,|\, (\zeta_{k-1}, T_{k-1}), \ldots, (\zeta_1, T_1)) \\
&= \sum_{k=1}^{n} \mathbb{H}(T_k \,|\, \zeta_k, (\zeta_{k-1}, T_{k-1}), \ldots, (\zeta_1, T_1)) \\
&\quad + \sum_{k=1}^{n} \mathbb{H}(\zeta_k \,|\, (\zeta_{k-1}, T_{k-1}), \ldots, (\zeta_1, T_1)) \\
&= \sum_{k=1}^{n} \mathbb{H}(T_k \,|\, \zeta_k) + \sum_{k=1}^{n} \mathbb{H}(\zeta_k \,|\, \zeta_{k-1}).
\end{aligned}$$

The compartment chain ζ is stationary, consequently $\mathbb{H}(\zeta_k \,|\, \zeta_{k-1}) = \theta(\zeta)$ and the proof is complete. □

Proposition 4.15 *The entropy rate of the infinite path $\mathcal{P}_\infty = ((\zeta_n, T_n))_{n\in\mathbb{N}}$ is given by*

$$\theta(\mathcal{P}_\infty) = \sum_{j=1}^{d} \pi_j \,(1 - \log \lambda_j) + \theta(\zeta).$$

Proof. By Definition 4.6, and Lemma 4.14,

$$\theta(\mathcal{P}_\infty) = \lim_{n\to\infty} \frac{1}{n}\, \mathbb{H}((\zeta_1, T_1), \ldots, (\zeta_n, T_n)) = \lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} \mathbb{H}(T_k \,|\, \zeta_k) + n\,\theta(\zeta).$$

Furthermore, for $k \in \mathbb{N}$,

$$\mathbb{H}(T_k \,|\zeta_k) = \sum_{j=1}^{d+1} \mathbb{P}(\zeta_k = j)\, \mathbb{H}(T_k \,|\, \zeta_k = j) = \sum_{j=1}^{d+1} \pi_j\, \mathbb{H}(T_k \,|\, \zeta_k = j).$$

For $j \in S$, we have $T_k \sim \mathrm{Exp}(\lambda_j)$ if $\zeta_k = j$. However, for the environmental compartment $j = d + 1$ we assume an infinitesimal sojourn time, i.e., an immediate exit. Hence, we truncate the sum at $j = d$ and do not consider any entropy for the sojourn time of the environmental pool. This leads to

$$\mathbb{H}(T_k \,|\zeta_k) = \sum_{j=1}^{d} \pi_j \,(1 - \log \lambda_j),$$

which is independent of k. We get

$$\theta(\mathcal{P}_\infty) = \lim_{n\to\infty} \frac{1}{n} \left[n \sum_{j=1}^{d} \pi_j \,(1 - \log \lambda_j) + n\,\theta(\zeta) \right],$$

and the proof is finished. □

Remark 4.16 Proposition 4.15 states, after a rearrangement of terms,

$$\theta(\mathcal{P}_\infty) = \sum_{j=1}^{d} \pi_j \left[(1 - \log \lambda_j) + \sum_{i=1, i\neq j}^{d} -\frac{B_{ij}}{\lambda_j} \log\left(\frac{B_{ij}}{\lambda_j}\right) - \frac{z_j}{\lambda_j} \log\left(\frac{z_j}{\lambda_j}\right) \right]$$
$$- \pi_{d+1} \sum_{i=1}^{d} \beta_i \log \beta_i.$$

We plug in π_j and π_{d+1} from Eqs. (4.8) and (4.9), respectively, and see

$$\theta(\mathcal{P}_\infty) = \frac{1}{1+\mathcal{N}} \sum_{j=1}^{d} N_i \left[(1 - \log \lambda_j) + \sum_{i=1, i\neq j}^{d} -\frac{B_{ij}}{\lambda_j} \log\left(\frac{B_{ij}}{\lambda_j}\right) - \frac{z_j}{\lambda_j} \log\left(\frac{z_j}{\lambda_j}\right) \right]$$
$$- \frac{1}{\mathcal{N}+1} \sum_{i=1}^{d} \beta_i \log \beta_i.$$

Consequently, $\theta(\mathcal{P}_\infty)$ is an entropy rate measured per jump and we can interpret it as

$$\theta(\mathcal{P}_\infty) = \frac{1}{\mathcal{N}+1} \left(\mathbb{H}(\text{entry}) + \sum_{j\in S} N_j \left[\mathbb{H}(\text{sojourn time in j}) + \mathbb{H}(\text{next jump}) \right] \right).$$

4.3.2. Entropy rate per unit time

Recall the continuous-time process Z defined in Eq. (2.17). It describes the continuous-time path of a particle through the system and being sent back in immediately after its exit. So, Z is the continuous-time version of the discrete-time path $\mathcal{P}_\infty$. However, we define $\widetilde{Z}$ to describe the continuous-time path of the permanently reentering particle with an Exp(1)-distributed sojourn time in the environmental compartment $d+1$. Note that Z and $\widetilde{Z}$ describe two similar yet different particle paths. While Z is a regenerative process with state space S, $\widetilde{Z}$ is a continuous-time Markov chain with state space $\widetilde{S}$ and transition-rate matrix Q from Eq. (4.5). Because its jump chain ζ is irreducible, $\widetilde{Z}$ is irreducible too. Furthermore, from Eq. (4.7) we know that $\boldsymbol{\nu} = (\nu_j)_{j\in\widetilde{S}} := \|\mathrm{Q}\,\mathbf{y}\|^{-1}\,\mathrm{Q}\,\mathbf{y}$ is its stationary distribution.

Following Girardin & Limnios (2003),

$$\theta(\widetilde{Z}) = \sum_{j=1}^{d+1} \nu_j \sum_{i=1, i\neq j}^{d+1} P_{ij}\,(1 - \log P_{ij}). \tag{4.11}$$

Proposition 4.17 *The entropy rate per unit time of the continuous-time path Z is given by*

$$\begin{aligned}\theta(Z) = &-\frac{1}{\mathbb{E}\left[\mathcal{T}\right]}\sum_{i=1}^{d}\beta_i\,\log\beta_i\\ &+\frac{1}{\mathbb{E}\left[\mathcal{T}\right]}\sum_{j=1}^{d}\frac{x_j^*}{\|\mathbf{u}\|}\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right]\\ &-\frac{1}{\mathbb{E}\left[\mathcal{T}\right]}\sum_{i=1}^{d}\beta_i\,\log\beta_i\\ &+\sum_{j=1}^{d}\frac{x_j^*}{\|\mathbf{x}^*\|}\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right].\end{aligned}$$

Proof. Recall $\mathrm{Q}\,\mathbf{y}=\mathbf{0}$ with $\mathbf{y}=(\mathbf{x}^*,\|\mathbf{u}\|)^\top$, $\boldsymbol{\eta}=\mathbf{x}^*/\|\mathbf{x}^*\|$, and $\mathbb{E}\left[\mathcal{T}\right]=\|\mathbf{x}^*\|/\|\mathbf{u}\|$. We divide $\mathbf{y}$ by $\|\mathbf{x}^*\|$, obtain $(\boldsymbol{\eta},1/\mathbb{E}\left[\mathcal{T}\right])^\top$, and normalize this to

$$\boldsymbol{\nu}=\frac{\mathbb{E}\left[\mathcal{T}\right]}{\mathbb{E}\left[\mathcal{T}\right]+1}\left(\boldsymbol{\eta},\frac{1}{\mathbb{E}\left[\mathcal{T}\right]}\right)^\top=\frac{1}{\mathbb{E}\left[\mathcal{T}\right]+1}\left(\frac{\mathbf{x}^*}{\|\mathbf{u}\|},1\right)^\top. \tag{4.12}$$

We see $\mathrm{Q}\,\boldsymbol{\nu}=\mathbf{0}$ and $\|\boldsymbol{\nu}\|=1$. Consequently, the stationary distribution $\boldsymbol{\nu}$ of $\widetilde{Z}$ is given by Eq. (4.12), and we obtain from Eq. (4.11)

$$\begin{aligned}\theta(\widetilde{Z}) &= \frac{1}{\mathbb{E}\left[\mathcal{T}\right]+1}\sum_{j=1}^{d}\frac{x_j^*}{\|\mathbf{u}\|}\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right]\\ &\quad+\frac{1}{\mathbb{E}\left[\mathcal{T}\right]+1}\sum_{i=1}^{d}\beta_i(1-\log\beta_i)\\ &= -\frac{1}{\mathbb{E}\left[\mathcal{T}\right]+1}\left(\sum_{i=1}^{d}\beta_i\,\log\beta_i+1\right)\\ &\quad+\frac{1}{\mathbb{E}\left[\mathcal{T}\right]+1}\sum_{j=1}^{d}\frac{x_j^*}{\|\mathbf{u}\|}\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right].\end{aligned}$$

To get to the entropy rate of Z, we need to do two corrections here. First, the 1 inside the first parenthesis comes from $1=1-\log 1$ and represents the entropy of the sojourn time in the environmental compartment $d+1$. Second, $\theta(\widetilde{Z})$ indicates a cycle length of $\mathbb{E}\left[\mathcal{T}\right]+1$, where again the 1 stands for the mean sojourn time in the environmental compartment. Since Z jumps immediately out of this compartment, there is no uncertainty in the sojourn time here, because no time is spent in this compartment. Hence, the cycle length of Z is $\mathbb{E}\left[\mathcal{T}\right]$. We omit the 1's in question and use $\mathbb{E}\left[\mathcal{T}\right]=\|\mathbf{x}^*\|/\|\mathbf{u}\|$ to finish the proof. □

Remark 4.18 For a one-dimensional compartmental system M_λ with rate $\lambda>0$, positive external input, and associated regenerative process Z_λ,

$$\theta(Z_\lambda)=\frac{1}{\lambda^{-1}}\,(1-\log\lambda),$$

which equals the differential entropy $1-\log\lambda$ of $\mathcal{T}\sim\mathrm{Exp}(\lambda)$ divided by $\mathbb{E}\left[\mathcal{T}\right]=\lambda^{-1}$. The exponential distribution $\mathrm{Exp}(\lambda)$ is the interarrival-time distribution of a Poisson process with intensity rate λ. The renewals of this Poisson process determine the moments of exit of the particle from the system. Consequently, $\theta(Z_\lambda)$ is is the entropy rate per unit time of the Poisson process.

Migrating to a d-dimensional system, for $i \neq j$, $B_{ij}\,(1-\log B_{ij})$ is the entropy rate of a Poisson process that determines whether the particle jumps to compartment i, as long as it resides in compartment j. With $x_j^*/\|\mathbf{u}\| = \mathbb{E}\,[O_j]$ being the mean occupation time of compartment j during a single run through the system,

$$\theta(Z) = \frac{1}{\mathbb{E}\,[\mathcal{T}]}\left[\mathbb{H}(\text{entry}) + \sum_{j=1}^{d} \mathbb{E}\,[O_j]\left(\sum_{i=1, i\neq j}^{d} \mathbb{H}(\text{Poisson}(i\,|\,j)) + \mathbb{H}(\text{Poisson}(\text{exit}\,|\,j))\right)\right].$$

4.3.3. Path entropy

We shift our interest away from a average uncertainties such as entropy rates toward the uncertainty of one entire particle run through the system. Consequently, our object of study is now the absorbing continuous-time Markov chain X from Chapter 2, which describes one single particle run through the system. We consider X on the state space $\widetilde{S} = \{1, 2, \ldots, d, d+1\}$ with initial distribution $\boldsymbol{\beta} = \mathbf{u}/\|\mathbf{u}\|$ on $S = \{1, 2, \ldots, d\}$ and with state-transition matrix Q as defined by Eq. (2.4), i.e.,

$$\mathrm{Q} = \begin{pmatrix} \mathrm{B} & \mathbf{0} \\ \mathbf{z}^\top & 0 \end{pmatrix}.$$

Along the lines of Albert (1962), we construct a space $\wp$ that contains all possible paths that can be taken by a particle that runs through the system until it leaves. Let $\wp_n := (S\times\mathbb{R}_+)^n \times \{d+1\}$ denote the space of paths that visit n compartments/states before ending up in the environmental compartment/absorbing state $d+1$. By $\wp := \bigcup_{n=1}^{\infty} \wp_n$ denote the space of all eventually absorbed paths. Note that, since B is invertible, a path through the system is finite with probability 1. Let l denote the Lebesgue measure on $\mathbb{R}_+$ and c the counting measure on S. Furthermore, let σ_n be the sigma-finite product measure on $\wp_n$. It is defined by $\sigma_n := (c \otimes l)^n \otimes c$. Almost all sample functions of $(X_t)_{t\geq 0}$ can be represented as a point $p \in \wp$ (Doob, 1953, Chapter VI). Consequently, we can represent X by a finite-length path $\mathcal{P}(X) = ((\xi_1, T_1), (\xi_2, T_2), \ldots, (\xi_n, T_n), \xi_{n+1})$ for some $n \in \mathbb{N}$, where $\xi_{n+1} = d+1$.

For each set $W \subseteq \wp$ for which $W \cap \wp_n$ is σ_n-measurable for each $n \in \mathbb{N}$, we define $\sigma^*(W) := \sum_{n=1}^{\infty} \sigma_n(W \cap \wp_n)$. It is defined on the σ-field $\mathcal{F}^*$ which is the smallest σ-field containing all sets $W \subseteq \wp$ whose projection on $\mathbb{R}_+^n$ is a Borel set for each $n \in \mathbb{N}$. Let σ be a measure on *all* sample functions, defined for all subsets W whose intersection with $\wp$ is in $\mathcal{F}^*$. We define it by $\sigma(W) := \sigma^*(W \cap \wp)$.

Let $p = ((x_1, t_1), (x_2, t_2,), \ldots, (x_n, t_n), d+1) \in \wp$ for some $n \in \mathbb{N}$. For $i \neq j$, we denote by $N_{ij}(p)$ the total number of path p's transitions from j to i and by $R_j(p)$ the total amount of time spent in j.

Lemma 4.19 *The probability density function of $\mathcal{P} = \mathcal{P}(X)$ with respect to σ is given by*

$$f_{\mathcal{P}}(p) = \beta_{x_1}\left(\prod_{j=1}^{d}\prod_{i=1, i\neq j}^{d+1} (Q_{ij})^{N_{ij}(p)}\right)\prod_{j=1}^{d} e^{-\lambda_j\, R_j(p)},$$

$$p = ((x_1, t_1), (x_2, t_2), \ldots, (x_n, t_n), d+1) \in \wp.$$

Proof. Let $x_1, x_2, \ldots, x_n \in S$, $x_{n+1} = d+1$, and $t_1, t_2, \ldots, t_n \in \mathbb{R}_+$. Since

$$\begin{aligned}
&\mathbb{P}((\xi_1 = x_1, T_1 \le t_1), (\xi_2 = x_2, T_2 \le t_2), \ldots, (\xi_n = x_n, T_n \le t_n), \xi_{n+1} = d+1) \\
&\qquad = \mathbb{P}(\xi_{n+1} = d+1 \,|\, \xi_n = x_n) \prod_{k=1}^{n} \mathbb{P}(\xi_k = x_k, T_k \le t_k \,|\, \xi_{k-1} = x_{k-1}) \\
&\qquad = P_{d+1,x_n} \left[\prod_{k=2}^{n} P_{x_k x_{k-1}} \left(1 - e^{-\lambda_{x_k} t_k}\right) \right] \beta_{x_1} \left(1 - e^{-\lambda_{x_1} t_1}\right) \\
&\qquad = \int\limits_{\mathbb{T}_n} \beta_{x_1} \prod_{k=1}^{n} Q_{x_{k+1} x_k} \, e^{-\lambda_{x_k} \tau_k} \, \mathrm{d}\tau_1 \mathrm{d}\tau_2 \cdots \mathrm{d}\tau_n
\end{aligned}$$

with $\mathbb{T}_n = \{(\tau_1, \tau_2, \ldots, \tau_n) \in \mathbb{R}_+^n : 0 \le \tau_1 \le t_1, 0 \le \tau_2 \le t_2, \ldots, 0 \le \tau_n \le t_n\}$, the probability density function of $\mathcal{P} = \mathcal{P}(x)$ with respect to σ is given by

$$f_{\mathcal{P}}(p) = \beta_{x_1} \prod_{k=1}^{n} Q_{x_{k+1} x_k} \, e^{-\lambda_{x_k} t_k}, \qquad p = ((x_1, t_1), (x_2, t_2), \ldots, (x_n, t_n), d+1) \in \wp.$$

The term $Q_{x_{k+1} x_k} = Q_{ij}$ enters exactly $N_{ij}(p)$ times. Furthermore,

$$\prod_{k=1}^{n} e^{-\lambda_{x_k} t_k} = \prod_{k=1}^{n} \prod_{j=1}^{d} \mathbb{1}_{\{x_k = j\}} \, e^{-\lambda_j t_k} = \prod_{j=1}^{d} e^{-\lambda_j \sum\limits_{k=1}^{n} \mathbb{1}_{\{x_k = j\}} t_k} = \prod_{j=1}^{d} e^{-\lambda_j R_j(p)}.$$

We make the according substitutions and the proof is finished. □

Theorem 4.20 *The entropy of the absorbing continuous-time Markov chain X is given by*

$$\mathbb{H}(X) = -\sum_{i=1}^{d} \beta_i \log \beta_i + \sum_{j=1}^{d} \frac{x_j^*}{\|u\|} \left[\sum_{i=1, i \ne j}^{d} B_{ij} \,(1 - \log B_{ij}) + z_j \,(1 - \log z_j) \right].$$

Proof. Let X have the finite path representation

$$\mathcal{P} = \mathcal{P}(X) = ((\xi_1, T_1), (\xi_2, T_2), \ldots, (\xi_n, T_n), d+1)$$

for some $n \in \mathbb{N}$, and denote by $f_{\mathcal{P}}$ its probability density function. Then, by Lemma 4.19,

$$-\log f_{\mathcal{P}}(\mathcal{P}) = -\log \beta_{\xi_1} - \sum_{j=1}^{d} \sum_{i=1, i \ne j}^{d+1} N_{ij}(\mathcal{P}) \log Q_{ij} + \sum_{j=1}^{d} \lambda_j \, R_j(\mathcal{P}).$$

We compute the expectation and get

$$\begin{aligned}
\mathbb{H}(X) = \mathbb{H}(\mathcal{P}) &= -\mathbb{E}\left[\log f_{\mathcal{P}}(\mathcal{P})\right] \\
&= -\mathbb{E}\left[\log \beta_{\xi_1}\right] - \sum_{j=1}^{d} \sum_{i=1, i \ne j}^{d+1} \mathbb{E}\left[N_{ij}(\mathcal{P})\right] \log Q_{ij} + \sum_{j=1}^{d} \lambda_j \, \mathbb{E}\left[R_j(\mathcal{P})\right] \\
&= \mathbb{H}(\xi_1) + \sum_{j=1}^{d} \lambda_j \, \mathbb{E}\left[R_j(\mathcal{P})\right] - \sum_{j=1}^{d} \sum_{i=1, i \ne j}^{d+1} \mathbb{E}\left[N_{ij}(\mathcal{P})\right] \log Q_{ij}.
\end{aligned}$$

Obviously, $\mathbb{E}[R_j(\mathcal{P})] = \mathbb{E}[O_j] = x_j^*/\|\mathbf{u}\|$ is the mean occupation time of compartment $j \in S$ by X. Furthermore, for $i \in \widetilde{S}$ and $j \in S$ such that $i \neq j$, by Eqs. (4.8) and (4.6),

$$\mathbb{E}[N_{ij}(\mathcal{P})] = \mathbb{E}[N_j(\mathcal{P})]\; P_{ij} = \begin{cases} \frac{x_j^*}{\|\mathbf{u}\|} B_{ij}, & i \leq d, \\ \frac{x_j^*}{\|\mathbf{u}\|} z_j, & i = d+1. \end{cases}$$

Together with $\lambda_j = \sum_{i=1, i\neq j}^{d} B_{ij} + z_j$, we obtain

$$\begin{aligned} \mathbb{H}(X) &= \mathbb{H}(\xi_1) + \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left[\left(\sum_{i=1, i\neq j}^{d} B_{ij} + z_j \right) - \sum_{i=1, i\neq j}^{d} B_{ij} \log B_{ij} - z_j \log z_j \right] \\ &= -\sum_{i=1}^{d} \beta_i \log \beta_i + \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left[\sum_{i=1, i\neq j}^{d} B_{ij}\,(1 - \log B_{ij}) + z_j\,(1 - \log z_j) \right]. \end{aligned}$$

□

Proposition 4.21 *The entropy $\mathbb{H}(X)$ is consistent with the entropy rate per jump $\theta(\mathcal{P}_\infty)$ and the entropy rate per unit time $\theta(Z)$. More precisely,*

$$\mathbb{H}(X) = (1 + \mathcal{N})\,\theta(\mathcal{P}_\infty) = \mathbb{E}[\mathcal{T}]\;\theta(Z).$$

Proof. The relation $\mathbb{H}(X) = \mathbb{E}[\mathcal{T}]\;\theta(Z)$ is immediately obvious from Proposition 4.17. From Proposition 4.15 and Lemma 4.13, we have

$$\begin{aligned} \theta(\mathcal{P}_\infty) &= \sum_{j=1}^{d} \pi_j\,(1 - \log \lambda_j) + \sum_{j=1}^{d} \pi_j \left[\sum_{i=1, i\neq j}^{d} -\frac{B_{ij}}{\lambda_j} \log\left(\frac{B_{ij}}{\lambda_j}\right) - \frac{z_j}{\lambda_j} \log\left(\frac{z_j}{\lambda_j}\right) \right] \\ &\quad - \pi_{d+1} \sum_{i=1}^{d} \beta_i \log \beta_i \end{aligned}$$

With Eqs. (4.8) and (4.9), we obtain

$$\begin{aligned} (1 + \mathcal{N})\,\theta(\mathcal{P}_\infty) &= \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \lambda_j\,(1 - \log \lambda_j) \\ &\quad + \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left[\sum_{i=1, i\neq j}^{d} -B_{ij} \log\left(\frac{B_{ij}}{\lambda_j}\right) - z_j \log\left(\frac{z_j}{\lambda_j}\right) \right] \\ &\quad - \sum_{i=1}^{d} \beta_i \log \beta_i \\ &= \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left(\sum_{i=1, i\neq j}^{d} B_{ij} + z_j \right) (1 - \log \lambda_j) \\ &\quad + \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left[\sum_{i=1, i\neq j}^{d} B_{ij}(\log \lambda_j - \log B_{ij}) + z_j\,(\log \lambda_j - \log z_j) \right] \\ &\quad - \sum_{i=1}^{d} \beta_i \log \beta_i \end{aligned}$$

$$= -\sum_{i=1}^{d} \beta_i \log \beta_i + \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left[\sum_{i=1, i \neq j}^{d} B_{ij} \left(1 - \log B_{ij}\right) + z_j \left(1 - \log z_j\right) \right]$$
$$= \mathbb{H}(X).$$

□

Remark 4.22 Analogously to the interpretation of $\theta(Z)$ in Remark 4.18, we can interpret the entropy of X as

$$\mathbb{H}(X) = \mathbb{H}(\text{entry}) + \sum_{j=1}^{d} \mathbb{E}\left[O_j\right] \left[\sum_{i=1, i \neq j}^{d} \mathbb{H}(\text{Poisson}(i \,|\, j)) + \mathbb{H}(\text{Poisson}(\text{exit} \,|\, j)) \right].$$

Definition 4.23 If $\mathbf{u} \in \mathbb{R}_+^d$, and $\mathrm{B} \in \mathbb{R}^{d \times d}$ is compartmental and invertible, then we denote by $(\mathbf{u}, \mathrm{B})$ the linear autonomous compartmental system (4.4) and by X, $\mathcal{P}_\infty$, and Z the associated absorbing continuous-time Markov chain, infinite path, and infinite continuous-time path, respectively.

Furthermore, the *path entropy* of $M = (\mathbf{u}, \mathrm{B})$ is defined as $\mathbb{H}_{\mathcal{P}}(M) := \mathbb{H}(X)$, its *entropy rate per jump* by $\theta_{\mathcal{P}_\infty}(M) := \theta(\mathcal{P}_\infty)$, and its *entropy rate per unit time* by $\theta_Z(M) := \theta(Z)$.

4.3.4. The maximum entropy principle

Let us again consider a Bernoulli random variable Y with $\mathbb{P}(Y = 1) = 1 - \mathbb{P}(Y = 0) = p$ with $p \in [0, 1]$. As shown in the left panel of Figure 4.2, the entropy of this class of distributions is maximum if $p = 1/2$, when heads and tails are equally likely. Consequently, it is most difficult to predict the outcome of a coin toss in case of a fair coin. The farther away p is from $1/2$, the more information we have about the future outcome. In the extreme cases of $p = 0$ or $p = 1$ we know the outcome perfectly.

Assume we know that a coin is being tossed for 100 times, but we have no information about the value p that belongs to the probability of a heads outcome in one coin toss. If we were to bet on the number of heads that will have occurred after 100 trials, how would we decide? We are looking for the expected value (and multiply it by 100) of a probability distribution in the class of Bernoulli distributions with $p \in [0, 1]$ that represents our state of knowledge best. As already mentioned, we have no information about p whatsoever. Consequently, we have to assume $p = 1/2$ and bet on 50 heads after 100 trials. Any $p \neq 1/2$ lowers the entropy of the according Bernoulli distribution. The entropy difference between the distributions with $p = 1/2$ and $p \neq 1/2$ represents a positive amount of additional information that we have about p. Since we have no additional information about p, the probability distribution that represents our knowledge best is the maximum entropy distribution with $p = 1/2$. Any other choice of $p = 1/2$ implies that we use knowledge about p that we do not have.

This so-called *maximum entropy principle* arose in statistical mechanics. Its relationships to information theory and stochastics were established in Jaynes (1957a,b). The goal of this section is to transfer the maximum entropy principle to compartmental systems in order to identify the compartmental system that represents our state of knowledge best in different situations.

Examples of maximum entropy models

Recall that the path entropy of a linear autonomous compartmental system $M = (\mathbf{u}, \mathrm{B})$ is given by

$$\mathbb{H}_{\mathcal{P}}(M) = \mathbb{H}(X) = -\sum_{i=1}^{d} \beta_i \, \log \beta_i + \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \left[\sum_{i=1, i\neq j}^{d} B_{ij} \, (1 - \log B_{ij}) + z_j \, (1 - \log z_j) \right].$$

In order to obtain maximum entropy models under simple constraints, we now adapt ideas of Girardin (2004).

Proposition 4.24 *Consider the set $\mathcal{M}$ of open compartmental systems* (4.4) *with a predefined nonzero input vector* $\mathbf{u}$*, a predefined mean transit time* $\mathbb{E}\,[\mathcal{T}]$*, and an unknown steady-state vector comprising nonzero components. The compartmental system* $M = (\mathbf{u}, \mathrm{B})$ *with*

$$\mathrm{B} = \begin{pmatrix} -\lambda & 1 & \cdots & 1 \\ 1 & -\lambda & 1 \cdots & 1 \\ \vdots & & \ddots & \vdots \\ 1 & \cdots & 1 & -\lambda \end{pmatrix},$$

where $\lambda = d - 1 + 1/\mathbb{E}\,[\mathcal{T}]$*, is the maximum entropy model in* $\mathcal{M}$*.*

Remark 4.25 Intuitively, this result is obvious. The system has a high symmetry, the particle is equally likely to jump among different pools, and the Poisson process with intensity rate 1 is the one with maximum entropy rate. Furthermore, the resulting rates $z_j = 1/\mathbb{E}\,[\mathcal{T}]$ of leaving the system are chosen such that the mean transit time constraint is fulfilled.

Proof of Proposition 4.24. We can express the constraint $\mathbb{E}\,[\mathcal{T}] = \|\mathbf{x}^*\|/\|\mathbf{u}\|$ by

$$C_1 = \frac{1}{\|\mathbf{u}\|} \sum_{j=1}^{d} x_j^* - \mathbb{E}\,[\mathcal{T}] = 0.$$

From the steady-state formula $\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u}$, we obtain another set of d constraints, which we can describe by

$$\frac{1}{\|\mathbf{u}\|} \, (\mathrm{B}\,\mathbf{x}^*)_i = -\beta_i, \quad i = 1, 2, \ldots, d.$$

We rewrite the left hand side as

$$\begin{aligned} \frac{1}{\|\mathbf{u}\|} \, (\mathrm{B}\,\mathbf{x}^*)_i &= \frac{1}{\|\mathbf{u}\|} \sum_{j=1}^{d} B_{ij} \, x_j^* = \frac{1}{\|\mathbf{u}\|} \left(\sum_{j=1, j\neq i}^{d} B_{ij} \, x_j^* + B_{ii} \, x_i^* \right) \\ &= \frac{1}{\|\mathbf{u}\|} \sum_{j=1, j\neq i}^{d} B_{ij} \, x_j^* - \frac{1}{\|\mathbf{u}\|} \, x_i^* \left(\sum_{k=1, k\neq i}^{d} B_{ki} + z_i \right), \end{aligned}$$

which leads to the constraints

$$C_{2,i} = \frac{1}{\|\mathbf{u}\|} \sum_{j=1, j\neq i}^{d} B_{ij} \, x_j^* - \frac{1}{\|\mathbf{u}\|} \, x_i^* \left(\sum_{k=1, k\neq i}^{d} B_{ki} + z_i \right) + \beta_i = 0, \quad i \in S. \tag{4.13}$$

The Lagrangian is now given by

$$L = \mathbb{H}(X) + \gamma_0\, C_1 + \sum_{i=1}^{d} \gamma_i\, C_{2,i} \tag{4.14}$$

and its partial derivatives with respect to B_{ij} $(i \neq j)$, z_j, and x_j^* by

$$\|\mathbf{u}\| \frac{\partial}{\partial B_{ij}} L = -x_j^* \log B_{ij} + \gamma_i\, x_j^* - \gamma_j\, x_j^*,$$
$$\|\mathbf{u}\| \frac{\partial}{\partial z_j} L = -x_j^* \log z_j - \gamma_j\, x_j^*,$$

and

$$\begin{aligned}\|\mathbf{u}\| \frac{\partial}{\partial x_j^*} L = &\sum_{i=1,i\neq j}^{d} B_{ij}\,(1-\log B_{ij}) + z_j\,(1-\log z_j)\\ &+ \gamma_0 + \sum_{i=1,i\neq j}^{d} \gamma_i\, B_{ij} - \gamma_j \left(\sum_{k=1,k\neq j}^{d} B_{kj} + z_j\right),\end{aligned}$$

respectively. Setting $\frac{\partial}{\partial B_{ij}} L = 0$ gives $B_{ij} = e^{\gamma_i-\gamma_j}$, and setting $\frac{\partial}{\partial z_j} L = 0$ gives $z_j = e^{-\gamma_j}$. We plug this into $\frac{\partial}{\partial x_j^*} L = 0$ and get

$$\begin{aligned}0 = &\sum_{i=1,i\neq j}^{d} e^{\gamma_i-\gamma_j}\,[1-(\gamma_i-\gamma_j)] + e^{-\gamma_j}\,[1-(-\gamma_j)]\\ &+ \gamma_0 + \sum_{i=1,i\neq j}^{d} \gamma_i\, e^{\gamma_i-\gamma_j} - \gamma_j \left(\sum_{k=1,k\neq j}^{d} e^{\gamma_k-\gamma_j} + e^{-\gamma_j}\right)\\ = &\sum_{i\neq j,i\neq j} e^{\gamma_i-\gamma_j} + e^{-\gamma_j} + \gamma_0.\end{aligned}$$

Subtracting $e^{-\gamma_j}$ from both sides and multiplying with e^{γ_j} leads to

$$\gamma_0\, e^{\gamma_j} + \sum_{i=1,i\neq j}^{d} e^{\gamma_i} = -1, \quad j = 1,2,\dots,d.$$

This is equivalent to the linear system $\mathrm{Y}\,\mathbf{v} = \mathbf{-1}$ with

$$\mathrm{Y} = \begin{pmatrix} \gamma_0 & 1 & \cdots & 1\\ 1 & \gamma_0 & 1\cdots & 1\\ \vdots & & \ddots & \vdots\\ 1 & \cdots & 1 & \gamma_0 \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} e^{\gamma_1}\\ e^{\gamma_2}\\ \vdots\\ e^{\gamma_d} \end{pmatrix}, \quad \mathbf{-1} = \begin{pmatrix} -1\\ -1\\ \vdots\\ -1 \end{pmatrix}.$$

The case $\gamma_0 = 1$ has no solution $\mathbf{v}$ since $e^{\gamma_i} > 0 > -1$. For $\gamma_0 \neq 1$ the matrix Y has a nonzero determinant which makes the system uniquely solvable. For symmetry reasons, $\gamma_i = \gamma_j =: \gamma$ for all $i,j = 1,2,\dots,d$. Consequently, for $i \neq j$, we get $B_{ij} = 1$, and by summing Eq. (4.13) over $i \in S$,

$$\begin{aligned}0 = \|\mathbf{u}\| \sum_{i=1}^{d} C_{2,i} &= \sum_{i=1}^{d} \sum_{j=1,j\neq i}^{d} B_{ij}\, x_j^* - \sum_{i=1}^{d} x_i^* \left(\sum_{k=1,k\neq i}^{d} B_{ki} + z_i\right) - \|\mathbf{u}\|\\ &= -\sum_{i=1}^{d} x_i^*\, z_i - \|\mathbf{u}\|,\end{aligned}$$

which can also be expressed by $\mathbf{z}^T\,\mathbf{x}^* = \|\mathbf{u}\|$. We simply plug in $z_i = e^{-\gamma}$ and get $e^{-\gamma}\,\|\mathbf{x}^*\| = \|\mathbf{u}\|$, which means $z_i = 1/\mathbb{E}\,[\mathcal{T}]$. Consequently,

$$\mathrm{B} = \begin{pmatrix} -\lambda & 1 & \cdots & 1 \\ 1 & -\lambda & 1\cdots & 1 \\ \vdots & & \ddots & \vdots \\ 1 & \cdots & 1 & -\lambda \end{pmatrix}.$$

Uniqueness of this solution follows from its construction, we remain with showing maximality. To this end, we split the entropy into to three parts, i.e., $\mathbb{H}(X) = H_1 + H_2 + H_3$ with

$$\begin{aligned} H_1 &= -\sum_{i=1}^{d} \beta_i\,\log\beta_i, \\ H_2 &= \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|}\,z_j\,(1-\log z_j),\ \text{ and} \\ H_3 &= \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \sum_{i=1, i\neq j}^{d} B_{ij}\,(1-\log B_{ij}). \end{aligned}$$

The term H_1 is independent of B_{ij} and z_j for all $i, j \in S$ and $i \neq j$, and can thus be ignored. By Lemma 2.10, we can rewrite the second term as

$$H_2 = \sum_{j=1}^{d} \mathbb{P}(E=j)\,(1-\log z_j) = \sum_{j=1}^{d} \mathbb{H}(T_E \,|\, E=j)\,\mathbb{P}(E=j) = \mathbb{H}(T_E \,|\, E),$$

where E denotes X's last state before absorption and T_E the exponentially distributed sojourn time in E right before absorption. We see that H_2 becomes maximal if the knowledge of E contains no information about T_E. Hence, $z_j = z_i$ for $i, j \in S$. Since we need to ensure the systems' constraint on $\mathbb{E}\,[\mathcal{T}]$, we get $z_j = 1/\mathbb{E}\,[\mathcal{T}]$ for all $j \in S$.

In order to see that $B_{ij} = 1$ $(i \neq j)$ leads to maximal entropy, we first note that

$$H_3 = \sum_{j=1}^{d} \frac{x_j^*}{\|\mathbf{u}\|} \sum_{i=1, i\neq j}^{d} 1\cdot(1-\log 1) = (d-1)\sum_{j=1}^{d} \mathbb{E}\,[O_j] = (d-1)\,\mathbb{E}\,[\mathcal{T}]$$

by Lemma 2.8. We now disturb B_{kl} for fixed $k, l \in S$ with $k \neq l$ by a sufficiently tiny ε, which may be positive or negative. We define $B_{kl}(\varepsilon) := B_{kl} + \varepsilon$, and a change from λ_j to $\lambda_j(\varepsilon) := \lambda_j + \varepsilon > 0$ ensures $z_j(\varepsilon) = z_j$, implying that the system's mean transit time remains unchanged, i.e., $\mathbb{E}\,[\mathcal{T}(\varepsilon)] = \mathbb{E}\,[\mathcal{T}]$. The ε-disturbed H_3 is given by

$$\begin{aligned} H_3(\varepsilon) &= \sum_{j=1}^{d} \frac{x_j^*(\varepsilon)}{\|\mathbf{u}\|} \sum_{i=1, i\neq j}^{d} 1\cdot(1-\log 1)\,\left(1-\mathbb{1}_{\{i=k,\, j=l\}}\right) + \frac{x_l^*(\varepsilon)}{\|\mathbf{u}\|}\,(1+\varepsilon)\,[1-\log(1+\varepsilon)] \\ &= \sum_{j=1}^{d} \frac{x_j^*(\varepsilon)}{\|\mathbf{u}\|} \sum_{i=1, i\neq j}^{d} \left(1-\mathbb{1}_{\{i=k,\, j=l\}}\right) + \frac{x_l^*(\varepsilon)}{\|\mathbf{u}\|}\,(1-\delta) \end{aligned}$$

for some $\delta > 0$ since the map $x \mapsto x\,(1-\log x)$ has its global maximum at $x = 1$.

Consequently,

$$\begin{aligned} H_3(\varepsilon) &= \left[\sum_{j=1}^{d} \frac{x_j^*(\varepsilon)}{\|\mathbf{u}\|} \sum_{i=1, i\neq j}^{d} 1\right] - \delta\, \frac{x_l^*(\varepsilon)}{\|\mathbf{u}\|} &&= (d-1) \sum_{j=1}^{d} \mathbb{E}\left[O_j(\varepsilon)\right] - \delta\, \frac{x_l^*(\varepsilon)}{\|\mathbf{u}\|} \\ &= (d-1)\,\mathbb{E}\left[\mathcal{T}(\varepsilon)\right] - \delta\, \frac{x_l^*(\varepsilon)}{\|\mathbf{u}\|} &&= (d-1)\,\mathbb{E}\left[\mathcal{T}\right] - \delta\, \frac{x_l^*(\varepsilon)}{\|\mathbf{u}\|} \\ &< H_3. \end{aligned}$$

Hence, disturbing B_{ij} away from 1 reduces the entropy of the system, and the proof is complete. □

Remark 4.26 In the special case $d = 1$ for a one-dimensional compartmental system, we obtain $B = -1/\mathbb{E}\left[\mathcal{T}\right]$. Since in this case $\mathcal{T} \sim \mathrm{Exp}(-B_{11})$, we see that the exponential distribution is the maximum entropy distribution in the class of all nonnegative continuous probability distributions with fixed expected value. This special case is very well known (Cover & Thomas, 2006, Example 12.2.5).

Proposition 4.27 *Consider the set* $\mathcal{M}$ *of open compartmental systems* (4.4) *with a predefined nonzero input vector* $\mathbf{u}$ *and a predefined positive steady-state vector* $\mathbf{x}^*$. *The compartmental system* $M = (\mathbf{u}, \mathrm{B})$ *with* $\mathrm{B} = (B_{ij})_{i,j\in S}$ *given by*

$$B_{ij} = \begin{cases} \sqrt{\frac{x_i^*}{x_j^*}}, & i \neq j, \\ -\sum\limits_{k=1, k\neq j}^{d} \sqrt{\frac{x_k^*}{x_j^*}} - \frac{1}{\sqrt{x_j^*}}, & i = j, \end{cases}$$

is the maximum entropy model in $\mathcal{M}$.

Proof. The mean transit time $\mathbb{E}\left[\mathcal{T}\right] = \|\mathbf{x}^*\|/\|\mathbf{u}\|$ of the system is fixed. Hence, the Lagrangian L is the same as in Eq. (4.14), and setting $\frac{\partial}{\partial B_{ij}}\, L = 0$ leads to

$$-\log B_{ij} + \gamma_i - \gamma_j = 0, \quad i \neq j.$$

An interchange of the indices and summing the two equations gives

$$\log B_{ij} + \log B_{ji} = 0.$$

Hence, $B_{ij}\, B_{ji} = 1$. A good guess gives $B_{ij}^2 = x_i^*/x_j^*$ and $\gamma_j = \frac{1}{2}\, \log x_j^*$. From $\frac{\partial}{\partial z_j}\, L = 0$, we get

$$-\log z_j - \gamma_j = 0, \quad j \in S,$$

and in turn $z_j = (x_j^*)^{-1/2}$. Maximality and uniqueness of this solution follow from the strict concavity of $\mathbb{H}(X)$ as a function of B_{ij} and z_j for fixed $\mathbf{x}^*$. We can see this strict concavity by

$$\frac{\partial^2}{\partial B_{ij}^2}\, \mathbb{H}(X) = \frac{\partial}{\partial B_{ij}}\, \frac{-x_j^*}{\|\mathbf{u}\|}\, \log B_{ij} = -\frac{x_j^*}{\|\mathbf{u}\|\, B_{ij}} < 0$$

and

$$\frac{\partial^2}{\partial z_j^2}\, \mathbb{H}(X) = \frac{\partial}{\partial z_j}\, \frac{-x_j^*}{\|\mathbf{u}\|}\, \log z_j = -\frac{x_j^*}{\|\mathbf{u}\|\, z_i} < 0.$$

□

Structural model identification via the maximum entropy principle

Suppose we observe a natural system and conduct measurements from which we try to construct a linear autonomous compartmental model in equilibrium that represents the observed natural system as well as possible. The first question that arises is the one for the number of compartments the model should ideally have. The maximum entropy principle cannot be helpful here because by adding more and more compartments we can theoretically increase the entropy of the model indefinitely. Consequently, the problem of finding the right dimension of system (4.4) has to be solved by other means. One way to do it is to analyze an impulse response function of the system and its Laplace transform, the transfer function of the system, which might be possible to obtain by tracer experiments (Anderson, 1983; Walter, 1986).

In Anderson (1983, Chapter 16) the *structural identification problem* of linear autonomous systems is described as follows. Suppose we are interested in determining a d-dimensional system of form (4.4). We are interested in sending an impulse into the system at time $t = 0$ and analyzing its further behavior. To that end, we rewrite the system to

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathbf{x}(t) &= \mathrm{B}\,\mathbf{x}(t) + \mathrm{A}\,\mathbf{u}, \quad t \geq 0, \\ \mathbf{x}(0) &= \mathbf{0}, \\ \mathbf{y}(t) &= \mathrm{C}\,\mathbf{x}(t), \quad t \geq 0. \end{aligned} \tag{4.15}$$

Note that the roles of A and B are interchanged here with respect to Anderson (1983). In a typical tracer experiment, we choose an input vector $\mathbf{u}$ and the *input distribution matrix* A, which defines how the input vector enters the system. Then, we decide which compartments we can observe to determine the *output connection matrix C*. The experiment is now to inject an impulse into the system and to record the output function $\mathbf{y}(t) = \mathrm{C}\,\mathbf{x}(t)$. Bellman & Åström (1970) pointed out that the input-output relation is given by

$$\begin{aligned} \mathbf{y}(t) = \mathrm{C}\,\mathbf{x}(t) &= \mathrm{C} \int_0^t e^{(t-\tau)\,\mathrm{B}}\,\mathrm{A}\,\mathbf{u}(\tau)\,\mathrm{d}\tau \\ &= \left[\mathrm{C}\,e^{t\,\mathrm{B}}\,\mathrm{A}\right] * \mathbf{u}(t), \end{aligned}$$

where $*$ is the convolution operator. The model parameters enter the input-output relation only in the matrix-valued *impulse response function*

$$\Psi(t) := \mathrm{C}\,e^{t\,\mathrm{B}}\,\mathrm{A}, \quad t \geq 0,$$

or in the *transfer function*

$$\widehat{\Psi}(s) := \mathrm{C}\,(s\,\mathrm{I} - \mathrm{B})^{-1}\,\mathrm{A},$$

the Laplace transform matrix of Ψ. Consequently, all identifiable parameters of A, B, and C must be identified through Ψ or $\widehat{\Psi}$. Difficulties arise because the entries of the matrices Ψ and $\widehat{\Psi}$ are usually nonlinear expressions of the elements of A, B, and C.

Definition 4.28 System (4.15) is called *identifiable* if this nonlinear system of equations has a unique solution $(\mathrm{A}, \mathrm{B}, \mathrm{C})$ for given Ψ or $\widehat{\Psi}$. Otherwise the system is called *nonidentifiable.*

Usually, the matrices A and C are already know from the experiment's setup. What remains is to identify the compartmental matrix B. The following example is inspired by

Anderson (1983, Example 16 C). It shows how the maximum entropy principle can help take a decision which model to use if not all parameters can be uniquely determined from the transfer function $\widehat{\Psi}$.

Example 4.29 We are interested in determining the entries of the compartmental matrix B belonging to the 2-dimensional linear autonomous compartmental system

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}(t) = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}(t) + \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad t > 0. \tag{4.16}$$

We immediately notice $\mathbf{u} = (1, 0)^\top$ and $\mathrm{A} = \mathrm{I}$. Further, we decide to measure the contents of compartment 1 such that $\mathrm{C} = (1, 0)$. We recall $\mathbf{z}^\top = -\mathbf{1}^\top\,\mathrm{B}$ and obtain $z_1 = -B_{11} - B_{21}$ and $z_2 = -B_{22} - B_{12}$. The real-valued transfer function is then given by

$$\widehat{\Psi}(s) = \frac{s + \gamma_1}{s^2 + \gamma_2\, s + \gamma_3},$$

where

$$\begin{aligned} \gamma_1 &= B_{12} + z_2, \\ \gamma_2 &= B_{21} + z_1 + B_{12} + z_2, \\ \gamma_3 &= z_1\, B_{12} + z_1\, z_2 + B_{21}\, z_2. \end{aligned} \tag{4.17}$$

We assume that $\widehat{\Psi}$ is known from measurements, i.e., γ_1, γ_2, and γ_3 are known impulse response parameters. We have the four unknown parameters B_{11}, B_{12}, B_{21}, and B_{22}, or equivalently, B_{12}, B_{21}, z_1, and z_2, but only three equations to determine them. Consequently, the system is nonidentifiable and it remains a class $\mathcal{M}$ of models which all satisfy Eq. (4.17). Which model out of $\mathcal{M}$ are we going to select now?

Here, the maximum entropy principle comes into play. We intend to select the model that best represents the information given by our measurement data. We have to find $M^* = (\mathbf{u}, \mathrm{B}^*)$ such that

$$M^* = \underset{M \in \mathcal{M}}{\arg\max}\; \theta_Z(M).$$

We maximize the entropy rate per unit time here instead of the path entropy, because by slowing down the model, we could potentially increase its mean transit time and with it its path entropy indefinitely.

Let us turn to a numerical example in which we suppose to be given $\gamma_1 = 3$, $\gamma_2 = 5$, and $\gamma_3 = 4$. A nonlinear optimization algorithm with the arbitrarily chosen initial values $B_{12} = 3$, $B_{21} = 0$, $z_1 = 1$, and $z_2 = 1$ ends approximately with the terminal compartmental matrix

$$\mathrm{B}^* \approx \begin{pmatrix} -2.00 & 1.90 \\ 1.05 & -3.00 \end{pmatrix}$$

and the terminal entropy rate per unit time $\theta_Z(M^*) \approx 1.92$. Unfortunately, it is not guaranteed that this solution is a global maximum entropy model in $\mathcal{M}$.

The nonidentifiability of the model from $\widehat{\Psi}$ alone is underlined by the fact that another system $\widetilde{M} = (\mathbf{u}, \widetilde{\mathrm{B}}) \in \mathcal{M}$ with

$$\widetilde{\mathrm{B}} = \begin{pmatrix} -2.00 & 2.00 \\ 1.00 & -3.00 \end{pmatrix}$$

results in the same transfer function, but a different entropy rate per unit time, i.e., $\theta_Z(\widetilde{M}) \approx 1.90$ (Figure 4.3).

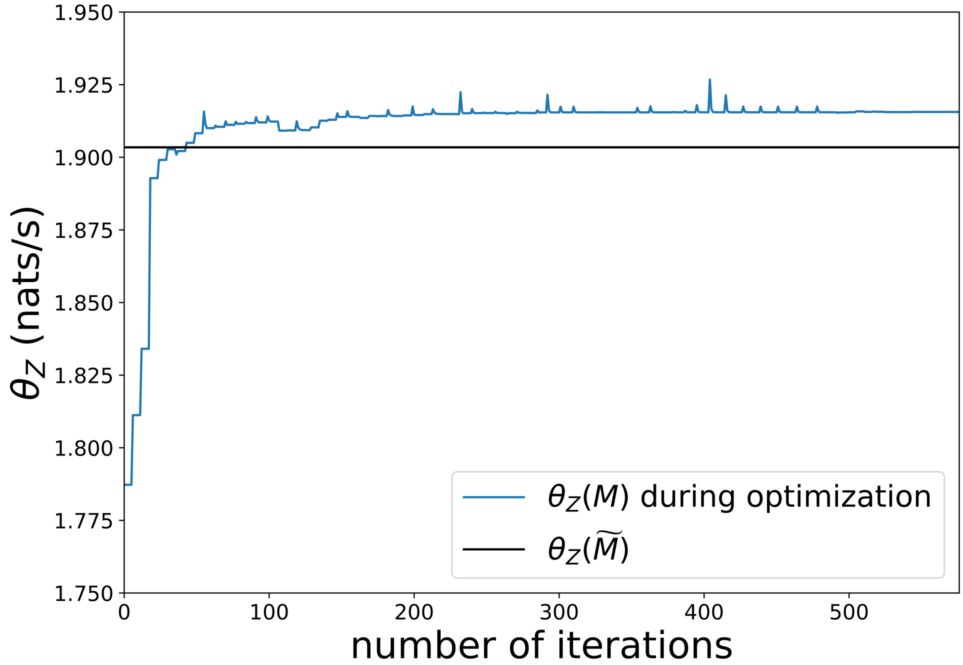


Figure 4.3. Entropy rate per unit time of system (4.16). The blue curve shows the evolution of the entropy rate per unit time during the nonlinear optimization process. Peaks higher than the terminal value show attempts of the optimization algorithm that do not perfectly satisfy all constraints. The black line shows the entropy rate per unit time of model $\widetilde{M}$.

This example is only supposed to give a first impression of how the maximum entropy principle can be used in combination with entropy rates or path entropy in similar situations. Practical examples usually have a high level of complexity such that existence and uniqueness of a maximum entropy model have to be studied on a case-by-case basis.

4.3.5. Entropy as a measure of complexity

We come back to the two desired properties that a complexity measure for compartmental systems should have, as stated in Section 4.1:

(1) For a given structure, the index should have its greatest value when the flow rates are even (all the same).

(2) Given two structures with the same number of compartments and even flow rates, the index should have a larger value for the one with more nonzero flow rates.

Do the path entropy or the entropy rates of compartmental systems satisfy these properties?

Consider the three compartmental systems $M_0 = (\mathbf{u}, \mathrm{B})$, $M_1 = (\mathbf{u}, \mathrm{B}^1_R)$, and $M_2 = (\mathbf{u}, \mathrm{B}^2_R)$ as depicted in Figure 4.4 with compartmental matrices

$$\mathrm{B} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathrm{B}^1_R = \begin{pmatrix} -1 & R \\ 0 & -(1+R) \end{pmatrix}, \quad \mathrm{B}^2_R = \begin{pmatrix} -(1+R) & R \\ R & -(1+R) \end{pmatrix},$$

respectively. The three systems are supposed to have the input vector $\mathbf{u} = (1,1)^\top$ in common, and the parameter R is a nonnegative real.

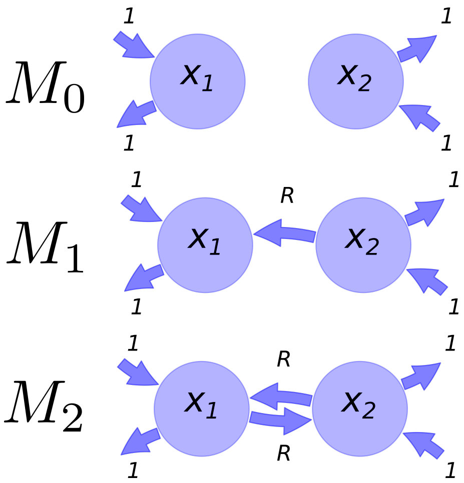


Figure 4.4 Schematics of the compartmental systems M_0, M_1, and M_2 associated to the different compartmental matrices B, B_R^1, and B_R^2, respectively. The different compartmental matrices lead to different connections between the pools. The 1's represent the external input- and output rates, while $R \geq 0$ is a parameter that defines the rates between the two compartments. In the upper model M_0, the parameter R is equal to 0.

For $R = 0$, we see $\mathrm{B} = \mathrm{B}_R^1 = \mathrm{B}_R^2$ and the systems M_0, M_1, and M_2 have no internal connections. If we change R to an arbitrary positive number, we introduce one internal connection to M_1 and two internal connections to M_2. In both cases, the entropy (path entropy and entropy rate per unit time) should increase in order to have the desired property (2) of complexity measures. But as shown in Figure 4.5, depending on the value of R also a decrease can happen. Consequently, the entropy does not have property (2). The maximum entropy of the system M_1 clearly occurs for $R < 1$, when not all rates of the system are equal. So the entropy also lacks property (1). However, this property is satisfied if the system does not lack any connections as shown by system M_2. Here, the maximum entropy occurs at $R = 1$, which reflects the statement of Proposition 4.24.

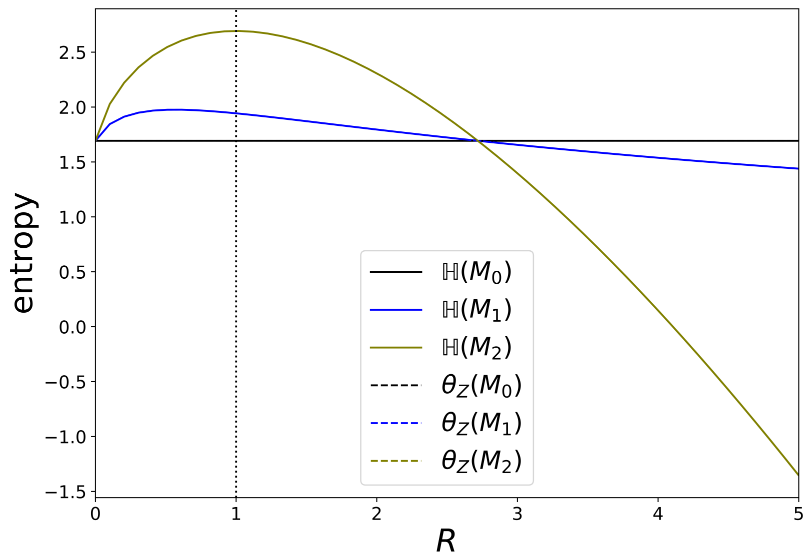


Figure 4.5. Path entropy (solid lines) and entropy rate per unit time (dashed lines) of the systems M_0 (black), M_1 (blue), and M_2 (olive), respectively. Path entropy and entropy rate coincide for all models and for all $R \geq 0$ because the mean transit remains constant ($\mathbb{E}[\mathcal{T}] = 1$). The vertical dotted line at $R = 1$ indicates the situation in which all existing fluxes have the same rate.

Path entropy and entropy rate are measures for the complex behavior of particles while they travel through the system. They are additional concepts to classical complexity measures such as number of compartments, number of connections, Kolmogorov complexity, effective measure complexity, logical depth, ZIV-Lempel coding, or total information (Ebeling et al., 1998). All of these can be applied to compartmental systems and each one is a measure for a different system property. Hence, the choice of the complexity concept is highly subjective and context-dependent. The book by Ebeling et al. (1998) treats this delicate topic in a very comprehensive way.

For instance, the question which of the two models in Figure 4.1 is more complex cannot be answered definitely the way it is posed. A definite answer requires the formulation of a more precise question. The answer depends on the property of interest as Table 4.1 shows. Depending on whether we consider the entropy rate per jump, the entropy rate per unit time, or the path entropy, we get different results - even with different model orders.

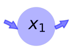
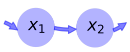
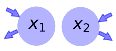
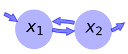
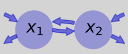
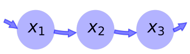
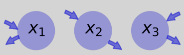
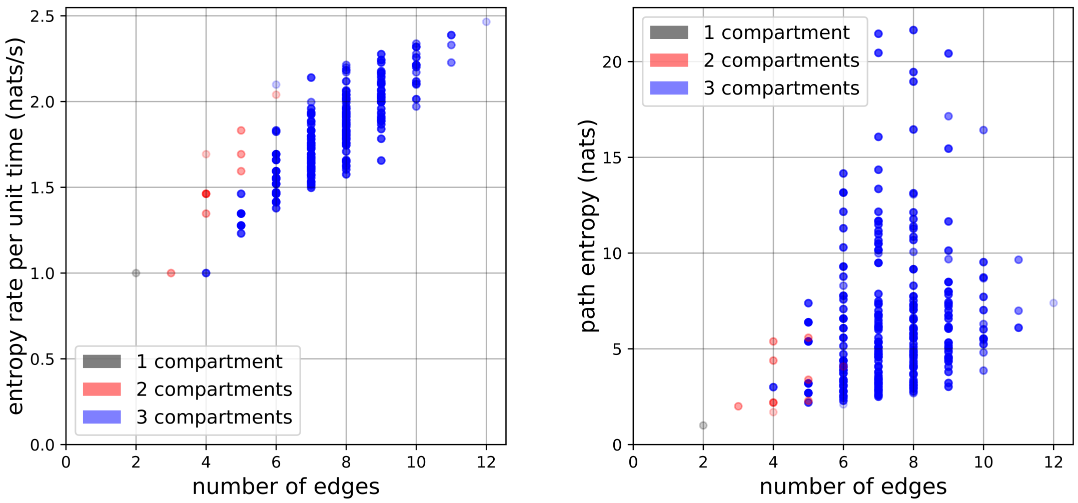
	Structure	$\theta_{\mathcal{P}_\infty}$	θ_Z	$\mathbb{E}[\mathcal{T}]$	$\mathrm{H}_{\mathcal{P}}$
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = -\lambda\,x + 1$	$0.5\,(1-\log\lambda)$	$\lambda\,(1-\log\lambda)$	$1/\lambda$	$1-\log\lambda$
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = \begin{pmatrix}-1 & 0\\ 1 & -1\end{pmatrix}\,x + \begin{pmatrix}1\\0\end{pmatrix}$	0.67	1.00	2.00	2.00
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = \begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix}\,x + \begin{pmatrix}1\\1\end{pmatrix}$	0.85	1.69	1.00	1.69
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = \begin{pmatrix}-1 & 0.5\\ 1 & -1\end{pmatrix}\,x + \begin{pmatrix}1\\0\end{pmatrix}$	1.08	1.35	<u>4.00</u>	<u>5.39</u>
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = \begin{pmatrix}-1 & 0.5\\ 0.5 & -1\end{pmatrix}\,x + \begin{pmatrix}1\\1\end{pmatrix}$	<u>1.36</u>	2.04	2.00	4.08
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = \begin{pmatrix}-1 & 0 & 0\\ 1 & -1 & 0\\ 0 & 1 & -1\end{pmatrix}\,x + \begin{pmatrix}1\\0\\0\end{pmatrix}$	0.75	1.00	3.00	3.00
	$\frac{\mathrm{d}}{\mathrm{d}t}\,x = \begin{pmatrix}-1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}\,x + \begin{pmatrix}1\\1\\1\end{pmatrix}$	1.05	<u>2.10</u>	1.00	2.10

Table 4.1. Overview of different entropies of simple models with different structures. The columns from left to right represent a schematic of the model, its mathematical representation, its entropy rate per jump, its entropy rate per unit time, its mean transit time, and its path entropy. Underlined numbers are the highest values per column. The two gray rows emphasize the examples of the model structures considered at the beginning of the chapter in Figure 4.1.

Even though the entropy of compartmental systems as introduced here does not satisfy classical properties of complexity measures with respect to single models, it exhibits complexity properties with respect to model classes. Consider the model class

$$\begin{aligned}\mathcal{M} := \{M = (\mathbf{u}, \mathrm{B}) \text{ compartmental} : \mathrm{B} \text{ is invertible},&\\ B_{jj} = -1,&\\ B_{ij} = 0 \text{ or } B_{ij} = 1/n_j,\ z_j = 0 \text{ or } z_j = 1/n_j,&\\ u_j = 0 \text{ or } u_j = 1\}.&\end{aligned}$$

Here, $n_j = \sum_{i\neq j} \mathbb{1}_{\{B_{ij}>0\}} + \mathbb{1}_{\{z_j>0\}}$ is the number of fluxes leaving compartment j, and in the third line we assume $i \neq j$. Since B is required to be invertible, $n_j > 0$ for all j. Furthermore, the dimension of models $M \in \mathcal{M}$ is arbitrary. In other words, $\mathcal{M}$ consists of models in which all compartments have the same velocity -1, and for each compartment all possible outgoing jumps are equally likely, having probability $1/n_j$. Not all jumps are possible, because the corresponding connection does not necessarily exist. All existing input connections have rate 1. All models in this class are maximum entropy rate models with respect to their connective structure. Note that this connective structure includes both external and internal fluxes.



(a) entropy rate per unit time **(b)** path entropy

Figure 4.6. Distribution of models with up to three compartments in the space spanned by entropy and number of connections/edges. Each dot in the plane represents a compartmental system. On the x-axis we see the number of internal and external connections or edges of the model. The y-axis represents the entropy rate per unit time in panel (a) and the path entropy in panel (b). The color of the dots represents the number of compartments (1: black, 2: red, 3: blue). The darker the color of the dots in terms of transparency, the more models have the same number of edges and entropy.

We can now identify classical complexity-measure properties of the entropy rate per unit time on $\mathcal{M}$. We denote by $\mathcal{M}(d, n) \subseteq \mathcal{M}$ the subclass of models with d compartments and n connections or edges, and we denote by $M_{\max}(d, n)$ an arbitrary model with maximal entropy rate per unit time in this subclass. In panel (a) of Figure 4.6 we see that $\theta_Z(M_{\max}(d, n)) \leq \theta_Z(M_{\max}(d + 1, n))$ and $\theta_Z(M_{\max}(d, n)) \leq \theta_Z(M_{\max}(d, n + 1))$. This means that adding compartments or edges increases the maximum entropy rate per unit time in $\mathcal{M}$, even though it does not necessarily increase the entropy per unit time of a particular model. This property does not hold for the path entropy, because adding compartments or connections might shorten the path and the maximum path entropy decreases. Additionally, we see from Proposition 4.24 that the entropy rate becomes maximum for equal rates if the model is totally connected. Consequently, the entropy rate per unit time is a complexity measure on specific model classes rather than one for single models.

Furthermore, we can answer the initial question of this chapter. In both panels of Figure 4.6, we can identify two-dimensional systems (red dots) with equally many or fewer edges in the realm of the three-dimensional systems (blue dots). Depending on the model structure, it is possible to find lower-dimensional systems being more complex than higher dimensional ones.

4.4. Compartmental systems out of equilibrium

So far, we considered entropy only for systems in equilibrium. The goal of this section is to extend the concept of entropy to systems out of equilibrium. We abstain from using a fixed finite time horizon for the sake of simplicity of the presentation, even though in practical applications data might be available only for a limited amount of time. In this case, the according integrals have to be cut off at the appropriate points.

We consider the d-dimensional linear nonautonomous compartmental system (3.3), given by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) &= \mathrm{B}(t)\,\mathbf{x}(t) + \mathbf{u}(t), \quad t > t_0,\\ \mathbf{x}(t_0) &= \mathbf{x}^0.\end{aligned} \tag{4.18}$$

Recall from Definition 1.5 that $\mathrm{B}(t)$ is required to be bounded for all $t \geq t_0$. We denote this system by $M = (\mathbf{u}, \mathrm{B}, t_0, \mathbf{x}^0)$. As in Section 3.1, the system might have been linear from the beginning or result from a linear interpretation of a solution trajectory of a nonlinear system. The unique solution $\mathbf{x}$ to this system is given by

$$\mathbf{x}(t) = \Phi(t, t_0)\,\mathbf{x}^0 + \int\limits_{t_0}^{t} \Phi(t, \tau)\,\mathbf{u}(\tau)\,\mathrm{d}\tau, \quad t \geq t_0, \tag{4.19}$$

where Φ denotes the state-transition matrix of the system (Appendix B).

Analogously to Section 2.2.2, we first establish a link between this system and an inhomogeneous continuous-time Markov chain. To that end, assume that material $\mathbf{u}(s_0) \in \mathbb{R}^d_+$ comes into system (4.18) at time $s_0 > t_0$. Since the system is linear, the way how this material will be distributed can be modeled by the homogeneous linear ODE system

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\,\widetilde{\mathbf{x}}(t) &= \mathrm{B}(t)\,\widetilde{\mathbf{x}}(t), \quad t > s_0,\\ \widetilde{\mathbf{x}}(s_0) &= \mathbf{u}(s_0).\end{aligned}$$

From Eq. (4.19), we know that the proportion of the material $u_j(s_0)$, entering the system through compartment j, that is in compartment i at time $t > s_0$ equals

$$\widetilde{x}_i(t) = \Phi_{ij}(t, s_0).$$

Consequently, an inhomogeneous continuous-time Markov chain $X^{s_0} = (X^{s_0}_t)_{t \geq s_0}$ with state space $S = \{1, 2, \ldots, d\}$, initial distribution $\boldsymbol{\beta}(s_0) = \mathbf{u}(s_0)/\|\mathbf{u}(s_0)\|$, and transition probabilities

$$\mathbb{P}(X^{s_0}_t = i \,|\, X^{s_0}_s = j) = \Phi_{ij}(t, s), \quad s_0 \leq s \leq t, \quad i, j \in S,$$

describes the stochastic travel of a single particle through system (4.18) if the particle arrives at time $s_0 > t_0$. When the particle leaves the system, X^{s_0} jumps to its absorbing state $d + 1$.

Corollary 4.30 *For $t \geq s_0$,*

$$\mathbb{P}(X^{s_0}_t = j) = \begin{cases} [\Phi(t, s_0)\,\boldsymbol{\beta}(s_0)]_j\,, & j \leq d,\\ 1 - \|\Phi(t, s_0)\,\boldsymbol{\beta}(s_0)\|, & j = d + 1.\end{cases}$$

4.4.1. Path entropy and instantaneous entropy

We fix $s_0 > t_0$ and are interested in the path entropy and the entropy rate per unit time of a particle that enters the system at time s_0. Hence, we need to identify the entropy of X^{s_0}. The jump-chain approach from Section 4.3.1 and the entropy-rate approach from

Section 4.3.2 rely heavily on the existence of a stationary distribution. To find a stationary distribution of an inhomogeneous Markov chain with potentially permanently changing transition probabilities is possible only in very special cases. Furthermore, the construction of the measure σ^* along the lines of Albert (1962) in Section 4.3.3 holds for homogeneous Markov chains only.

Consequently, we use a different and more direct approach that coincides with the idea of τ-entropy per unit time as defined in Gaspard & Wang (1993). For $T > s_0$ and $N \in \mathbb{N}$, let $\tau := (T - s_0)/N$ be a grid size, and consider the interval partitioning $s_0 < s_1 = s_0 + \tau < \cdots < s_N = s_0 + N\,\tau = T$ on $[s_0, T]$. First, we are interested in the joint entropy

$$\mathbb{H}_{T,\tau}(X^{s_0}) := \mathbb{H}(X^{s_0}_{s_0}, X^{s_0}_{s_1}, \ldots, X^{s_0}_{s_N}), \tag{4.20}$$

which we call τ-*entropy* of X on $[s_0, T]$. Second, we decrease the grid size to obtain the finite-time entropy

$$\mathbb{H}_T(X^{s_0}) := \lim_{\tau\to 0} \mathbb{H}_{T,\tau}(X^{s_0}) = \lim_{N\to\infty} \mathbb{H}_{T,\tau}(X^{s_0}).$$

Then, we increase the time horizon to determine the entropy

$$\mathbb{H}(X^{s_0}) = \lim_{T\to\infty} \mathbb{H}_T(X^{s_0}).$$

Furthermore, we define

$$P_{ij}(s_k) := \mathbb{P}(X_{s_{k+1}} = i \,|\, X_{s_k} = j)$$

for $k = 0, 1, \ldots, N-1$, $j \in S = \{1, 2, \ldots, d\}$, and $i \in \widetilde{S} = \{1, 2, \ldots, d, d+1\}$.

Lemma 4.31 *By the above definitions,*

$$P_{ij}(s_k) = \begin{cases} B_{ij}(s_k)\,\tau + o(\tau), & i \neq j,\ i \leq d, \\ z_j(s_k)\,\tau + o(\tau), & i = d+1, \\ 1 - [\lambda_j(s_k)\,\tau + o(\tau)], & i = j, \end{cases}$$

where $o(\tau)$ is little-o notation for $o(\tau)/\tau \to 0$ as $\tau \to 0$.

Proof. Let $X_{s_k} = j \in S$. As mentioned in Remark 4.18, in the autonomous case the time until the next jump to $i \neq j$ is exponentially distributed with rate B_{ij}. Consequently, the probability of a jump to i in the time interval $I_k = [s_k, s_k + \tau)$ is associated to a Poisson process with intensity rate B_{ij}.

In the nonautonomous case, the rates B_{ij} depend on time and the jump probabilities are associated to an inhomogeneous Poisson process with intensity functions $B_{ij}(t)$ ($i \neq j, i \leq d$) for internal jumps and $z_j(t)$ ($i = d+1$) for jumps to the absorbing state $d+1$. The probability of not jumping at all in I_k ($i = j$) is expressed by the complementary event to having a jump. The probability of more than one jump in the small interval is $o(\tau)$ by the very nature of Poisson processes. □

Lemma 4.32 *The τ-entropy of X on $[s_0, T]$ is given by*

$$\mathbb{H}_{T,\tau}(X) = \mathbb{H}(X_{s_0}) + \sum_{j=1}^{d} \sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j) \Bigg[\sum_{i=1, i\neq j}^{d} -B_{ij}(s_k)\, \log B_{ij}(s_k) - z_j(s_k)\, \log z_j(s_k)$$

$$- \frac{1}{T-s_0} \log\left(1 - \frac{\lambda_j(s_k)\,(T-s_0)}{N}\right)^N \Bigg]$$

$$+ \sum_{j=1}^{d} \sum_{k=0}^{N-1} \tau\,\mathbb{P}(X_{s_k} = j)\,\lambda_j(s_k)\,\log\left[1 - \lambda_j(s_k)\,\tau\right]$$

$$- \log(\tau) \left[\sum_{j=1}^{d} \sum_{k=0}^{N-1} \tau\,\mathbb{P}(X_{s_k} = j)\,\lambda_j(s_k) \right].$$

Proof. Recall from Eq. (4.20) that

$$\mathbb{H}_{T,\tau}(X) = \mathbb{H}(X_{s_0}, X_{s_1}, \ldots, X_{s_N}),$$

which by an application of the chain rule Eq. (4.3) turns into

$$\mathbb{H}_{T,\tau}(X) = \mathbb{H}(X_{s_0}) + \sum_{k=0}^{N-1} \mathbb{H}(X_{s_{k+1}} \mid X_{s_k}).$$

Definition 4.4 of conditional entropy leads to

$$\mathbb{H}_{T,\tau}(X) = \mathbb{H}(X_{s_0}) + \sum_{k=0}^{N-1} \sum_{j=1}^{d+1} \mathbb{P}(X_{s_k} = j)\,\mathbb{H}(X_{s_{k+1}} \mid X_{s_k} = j).$$

From the moment on in which the particle leaves the system, there will be no additional uncertainty anymore. Consequently, it suffices to consider $j \leq d$. By Lemma 4.31, we obtain

$$\begin{aligned}
\mathbb{H}_{T,\tau}(X) &= \mathbb{H}(X_{s_0}) + \sum_{k=0}^{N-1} \sum_{j=1}^{d} \mathbb{P}(X_{s_k} = j)\,\mathbb{H}(X_{s_{k+1}} \mid X_{s_k} = j) \\
&= \mathbb{H}(X_{s_0}) - \sum_{k=0}^{N-1} \sum_{j=1}^{d} \mathbb{P}(X_{s_k} = j) \sum_{i=1}^{d+1} P_{ij}(s_k)\,\log P_{ij}(s_k) \qquad (4.21) \\
&= \mathbb{H}(X_{s_0}) - \sum_{j=1}^{d} \sum_{i=1}^{d+1} \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\,P_{ij}(s_k)\,\log P_{ij}(s_k).
\end{aligned}$$

From now on, we concentrate on the term

$$- \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\,P_{ij}(s_k)\,\log P_{ij}(s_k).$$

According to Lemma 4.31, we distinguish three cases. In all cases, we omit the $o(\tau)$'s from Lemma 4.31, because when we take the limit $N \to \infty$ later on, the result is the same, and this way we can keep the structure of the proof clean. To keep that in mind, we replace the equal sign "=" by "≈" until we finally take the limit $N \to \infty$.

1) Let $i \neq j, i \leq d$. We have

$$\begin{aligned}
- \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\,P_{ij}(s_k)\,\log P_{ij}(s_k) &\approx - \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\,B_{ij}(s_k)\,\tau\,\log\left[B_{ij}(s_k)\,\tau\right] \\
&\approx - \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\,B_{ij}(s_k)\,\tau\,\log B_{ij}(s_k)
\end{aligned}$$

$$
\begin{aligned}
&- \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, B_{ij}(s_k)\, \tau\, \log \tau \\
&\approx - \sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, B_{ij}(s_k)\, \log B_{ij}(s_k) \\
&\quad - \log(\tau) \left[\sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, B_{ij}(s_k) \right].
\end{aligned}
$$

2) Let $i = d+1$. Analogously to 1),

$$
\begin{aligned}
- \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, P_{ij}(s_k)\, \log P_{ij}(s_k) &\approx - \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, z_j(s_k)\, \tau\, \log [z_j(s_k)\, \tau] \\
&\approx - \sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, z_j(s_k)\, \log z_j(s_k) \\
&\quad - \log(\tau) \left[\sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, z_j(s_k) \right].
\end{aligned}
$$

3) Let $i = j$. In this case, the particle does not move to another compartment in the interval $[s_k, s_{k+1})$, hence

$$
\begin{aligned}
&- \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, P_{ij}(s_k)\, \log P_{ij}(s_k) \\
&\qquad \approx - \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, [1 - \lambda_j(s_k)\, \tau]\, \log [1 - \lambda_j(s_k)\, \tau] \\
&\qquad \approx - \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, \tau\, \frac{N}{T - s_0}\, \log [1 - \lambda_j(s_k)\, \tau] \\
&\qquad \quad + \sum_{k=0}^{N-1} \mathbb{P}(X_{s_k} = j)\, \lambda_j(s_k)\, \tau\, \log [1 - \lambda_j(s_k)\, \tau] \\
&\qquad \approx - \sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, \frac{1}{T - s_0}\, \log \left(1 - \frac{\lambda_j(s_k)\, (T - s_0)}{N}\right)^N \\
&\qquad \quad + \sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, \lambda_j(s_k)\, \log [1 - \lambda_j(s_k)\, \tau].
\end{aligned}
$$

We plug the results from 1), 2), and 3) into Eq. (4.21) and use

$$
\begin{aligned}
&- \log(\tau) \left[\sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j) \left(\sum_{i=1, i \neq j}^{d} B_{ij}(s_k) + z_j(s_k) \right) \right] \\
&\qquad = - \log(\tau) \left[\sum_{k=0}^{N-1} \tau\, \mathbb{P}(X_{s_k} = j)\, \lambda_j(s_k) \right]
\end{aligned}
$$

to complete the proof. □

Remark 4.33 The term

$$-\log(\tau)\left[\sum_{j=1}^{d}\sum_{k=0}^{N-1}\tau\,\mathbb{P}(X_{s_k}=j)\,\lambda_j(s_k)\right]$$

represents an offset, which is a direct result of the discretization process. The smaller the grid size τ, the larger this offset, which tends to infinity with a rate proportional to $-\log\tau$ as $\tau\to 0$.

The effect is the same as in computing the differential entropy of a continuous random variable by discretizing its range, computing the discrete entropy based on the discretization, and then letting the grid size tend to zero. The reason behind this effect is that a realization of a continuous random variable, if transmitted, requires an infinite amount of bits if it is to be recovered with perfect precision (Cover & Thomas, 2006, Theorem 8.3.1).

Theorem 4.34 *The path entropy of particles entering system* (4.18) *at time* $s_0 > t_0$ *is given by*

$$\begin{aligned}\mathbb{H}(X^{s_0}) &= -\sum_{j=1}^{d}\beta_j(s_0)\,\log\beta_j(s_0)\\ &\quad+\sum_{j=1}^{d}\int_{s_0}^{\infty}[\Phi(t,s_0)\,\boldsymbol{\beta}(s_0)]_j\\ &\quad\times\left(\sum_{i=1,i\neq j}^{d}B_{ij}(t)\,[1-\log B_{ij}(t)]+z_j(t)\,[1-\log z_j(t)]\right)\mathrm{d}t.\end{aligned}$$

Proof. We look at the τ-entropy $\mathbb{H}_{T,\tau}(X)$ of X on $[s_0,T]$ as given by Lemma 4.32. As mentioned in Remark 4.33, the offset of $\mathbb{H}_{T,\tau}(X)$ explodes as $\tau\to 0$. We drop it for now. While we elaborate on the reasoning in Section 4.5, we concentrate now on the remaining terms. The first term, $\mathbb{H}(X_{s_0})$ describes the uncertainty of through which compartment the particle enters the system at time s_0. It is obviously given by

$$\mathbb{H}(X_{s_0}) = -\sum_{j=1}^{d}\beta_j(s_0)\,\log\beta_j(s_0).$$

The term

$$\sum_{k=0}^{N-1}\tau\,\mathbb{P}(X_{s_k}=j)\left[-\sum_{i=1,i\neq j}^{d}B_{ij}(s_k)\,\log B_{ij}(s_k)-z_j(s_k)\,\log z_j(s_k)\right]$$

is a Riemann sum and converges to

$$\int_{s_0}^{T}\mathbb{P}(X_t=j)\left[-\sum_{i=1,i\neq j}^{d}B_{ij}(t)\,\log B_{ij}(t)-z_j(t)\,\log z_j(t)\right]\mathrm{d}t$$

as $N\to\infty$. Since $\mathrm{B}(t)$ is required to be bounded for all $t>t_0$, also $\lambda_j(s_k)$ is bounded and even uniformly bounded on $[s_0,T]$. For $t\in[s_0,T]$, choose a sequence $(k_N(t))_{N\in\mathbb{N}}$ such that $t\in[s_{k_N(t)},s_{k_N(t)+1}]$ for all $N\in\mathbb{N}$. Then,

$$\left(1-\frac{\lambda_j(s_k)\,(T-s_0)}{N}\right)^N$$

converges to $e^{-\lambda_j(t)\,(T-s_0)}$ as $N\to\infty$. The convergence is even uniform on $[s_0,T]$. Then,

$$\log\left(1-\frac{\lambda_j(s_k)\,(T-s_0)}{N}\right)^N$$

converges uniformly to $-\lambda_j(t)\,(T-s_0)$ on $[s_0,T]$. Thanks to this uniform convergence,

$$\lim_{N\to\infty} -\sum_{k=0}^{N-1}\tau\,\mathbb{P}(X_{s_k}=j)\frac{1}{(T-s_0)}\,\log\left(1-\frac{\lambda_j(s_k)\,(T-s_0)}{N}\right)^N = \int\limits_{s_0}^{T}\mathbb{P}(X_t=j)\,\lambda_j(t)\,\mathrm{d}t.$$

Furthermore, from Corollary 4.30 we know

$$\mathbb{P}(X_t=j)=\left[\Phi(t,s_0)\,\boldsymbol{\beta}(s_0)\right]_j,\quad j\in S.$$

The remaining term

$$\sum_{j=1}^{d}\sum_{k=0}^{N-1}\tau\,\mathbb{P}(X_{s_k}=j)\,\lambda_j(s_k)\,\log\left[1-\lambda_j(s_k)\,\tau\right]$$

vanishes as $N\to\infty$ since, owing to the uniform boundedness of $\lambda_j(s_k)$ on $[s_0,T]$, the term $\log\left[1-\lambda_j(s_)\,\tau\right]$ converges uniformly to 0.

We combine these partial results, substitute $\lambda_j(t)$ by $\sum_{i=1,i\neq j}^{d}B_{ij}(t)+z_j(t)$, and obtain

$$\begin{aligned}\mathbb{H}_T(X^{s_0}) &= -\sum_{j=1}^{d}\beta_j(s_0)\,\log\beta_j(s_0)\\ &\quad+\sum_{j=1}^{d}\int\limits_{s_0}^{T}\left[\Phi(t,s_0)\,\boldsymbol{\beta}(s_0)\right]_j\\ &\quad\times\left[\sum_{i=1,i\neq j}^{d}B_{ij}(t)\left[1-\log B_{ij}(t)\right]+z_j(t)\left[1-\log z_j(t)\right]\right]\mathrm{d}t.\end{aligned}$$

Letting $T\to\infty$ completes the proof. □

Corollary 4.35 *The entropy $\mathbb{H}(X^{s_0})$ is consistent with the autonomous case.*

Proof. We consider system (4.4) as nonautonomous and compute

$$\begin{aligned}\mathbb{H}(X^{s_0}) &= -\sum_{j=1}^{d}\beta_j(s_0)\,\log\beta_j(s_0)\\ &\quad+\sum_{j=1}^{d}\int\limits_{s_0}^{\infty}\left[\Phi(t,s_0)\,\boldsymbol{\beta}(s_0)\right]_j\\ &\quad\times\left[\sum_{i=1,i\neq j}^{d}B_{ij}(t)\left[1-\log B_{ij}(t)\right]+z_j(t)\left[1-\log z_j(t)\right]\right]\mathrm{d}t\\ &= -\sum_{j=1}^{d}\beta_j\,\log\beta_j\end{aligned}$$

$$
\begin{aligned}
&+\sum_{j=1}^{d}\int\limits_{s_0}^{\infty}\Big[e^{(t-s_0)\,\mathrm{B}}\,\boldsymbol{\beta}\Big]_j\,\mathrm{d}t\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right]\\
&=-\sum_{j=1}^{d}\beta_j\,\log\beta_j\\
&+\sum_{j=1}^{d}\left(-\mathrm{B}^{-1}\,\boldsymbol{\beta}\right)_j\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right]\\
&+\sum_{j=1}^{d}\frac{x_j^*}{\|\mathbf{u}\|}\left[\sum_{i=1,i\neq j}^{d}B_{ij}\,(1-\log B_{ij})+z_j\,(1-\log z_j)\right].
\end{aligned}
$$

□

Definition 4.36 We call

$$
\begin{aligned}
\theta_{\mathrm{inst}}(X^{s_0},t)=&\sum_{j=1}^{d}\left[\Phi(t,s_0)\,\boldsymbol{\beta}(s_0)\right]_j\\
&\times\left[\sum_{i=1,i\neq j}^{d}B_{ij}(t)\,[1-\log B_{ij}(t)]+z_j(t)\,[1-\log z_j(t)]\right]
\end{aligned}
$$

the *instantaneous entropy rate* of X^{s_0} at time $t\geq s_0$.

We intend to extend the path entropy and the instantaneous entropy rate of a single particle entering the system at time $s_0>t_0$ to the entire system. To that end, we compute a weighted average of the path entropy of all particles that ever enter the system. The weights are based on the amount of input at a particular time. Furthermore, we have to consider the initial value $\mathbf{x}^0$. We denote the path entropy of a particle in the system at time t_0 by $\mathbb{H}_0$. Accordingly to $\mathbb{H}(X^{s_0})$, it is given by

$$
\begin{aligned}
\mathbb{H}_0:=&-\sum_{j=1}^{d}\eta_j^0\,\log\eta_j^0\\
&+\sum_{j=1}^{d}\int\limits_{t_0}^{\infty}\left[\Phi(t,t_0)\,\boldsymbol{\eta}^0\right]_j\left[\sum_{i=1,i\neq j}^{d}B_{ij}(t)\,[1-\log B_{ij}(t)]+z_j(t)\,[1-\log z_j(t)]\right]\,\mathrm{d}t,
\end{aligned}
$$

where $\boldsymbol{\eta}^0=\mathbf{x}^0/\|\mathbf{x}^0\|$. Analogously, the instantaneous entropy rate at time $t\geq t_0$ of a particle that has been in the system at time t_0 is given by

$$
\theta_0(t):=\sum_{j=1}^{d}\left[\Phi(t,t_0)\,\boldsymbol{\eta}^0\right]_j\left[\sum_{i=1,i\neq j}^{d}B_{ij}(t)\,[1-\log B_{ij}(t)]+z_j(t)\,[1-\log z_j(t)]\right].
$$

Definition 4.37 Denote by $M=(\mathbf{u},\mathrm{B},t_0,\mathbf{x}^0)$ the linear nonautonomous compartmental system (4.18). The *path entropy* of M is defined as

$$
\mathbb{H}_{\mathcal{P}}(M)=\lim_{T\to\infty}\frac{1}{U(t_0,T)\,(T-t_0)}\left[\|\mathbf{x}^0\|\,\mathbb{H}_0+\int\limits_{t_0}^{T}\|\mathbf{u}(s_0)\|\,\mathbb{H}(X^{s_0})\,\mathrm{d}s_0\right],
$$

where $U(t_0,T) = \|\mathbf{x}^0\| + \int_{t_0}^T \|\mathbf{u}(s_0)\|\,\mathrm{d}s_0$ denotes the total initial system content plus the total amount of system input in the interval $(t_0,T]$.

The *instantaneous entropy rate* of system M at time $t \geq t_0$ is defined as

$$\theta_{\mathrm{inst}}(M,t) = \sum_{j=1}^{d} \frac{x_j(t)}{\|\mathbf{x}(t)\|} \left[\sum_{i=1, i\neq j}^{d} B_{ij}(t)\,[1-\log B_{ij}(t)] + z_j(t)\,[1-\log z_j(t)] \right].$$

Note the similarity of the nonautonomous system's instantaneous entropy rate and the entropy rate per unit time of systems in equilibrium.

4.5. Discussion

In the two previous chapters, we focused on diagnostics of compartmental systems such as transit time, age, and remaining lifetime. These diagnostics were then computed for different models and also used to compare them. The main motivation of the present chapter was to compare models also in terms of complexity and to find out whether a model with fewer compartments can be at least as complex as a model with more compartments. As it turned out, the answer highly depends on the choice of the complexity measure. There is not one single complexity measure that is the correct choice for all purposes. One has to asses carefully which is the particular model property of interest.

This leads automatically to the problem of either using an already existing complexity measure for compartmental systems or introducing a new one. Some examples for existing and well-studied complexity measures for dynamical systems are topological entropy, Kolmogorov-Sinai/metric entropy, effective measure complexity, forecasting complexity, total information, and Shannon-Kolmogorov entropy. For detailed overviews over different kinds of entropy-related complexity measures, see Gaspard & Wang (1993), Ebeling et al. (1998), and Cover & Thomas (2006).

Since two of the most popular complexity measures for dynamical systems, namely topological and metric entropy, vanish and cannot measure complexity of compartmental systems, we introduced another concept. In the style of Chapter 2, we interpreted the system from a one-particle point of view and analyzed it in terms of information entropy. When a particle moves through the system, it creates a path from the time of its entry until the time of its exit. We can describe this path in three ways: (1) as a discrete sequence of pairs consisting of visited compartments and associated sojourn times; (2) as a continuous-time stochastic process representing the visited compartments; (3) as a random variable in the path space. Based on these three ways, we introduced for systems in equilibrium (1) the entropy rate per jump, (2) the entropy rate per unit time, and (3) the entropy of the entire path. Then, we showed that these three interpretations lead to the same path entropy, which is a measure of how difficult the path of the particle is to predict at the moment of entry.

We then identified the maximum entropy models in two situations in which different kinds of information about the system are given. Furthermore, we showed with the help of an example how the maximum entropy principle can help pick a particular model out of a remaining set of models, when a unique model identification based on available (measurement) information fails. The idea behind this procedure was that we wanted to select the model that reflects best the state of our given knowledge and in this sense is the most honest model. Here, the maximum entropy principle cannot only help identify parameter values of the model but also the model's connectivity structure.

We then examined whether the entropy rate per unit time and the path entropy satisfy two classical properties of complexity measures. We found out that they do not; adding compartments and/or edges to a given model does not necessarily increase the entropy, at least not on a single-model basis. However, if we consider certain model classes, then we see that the maximum entropy rate per unit time in such classes fulfills this property.

There is also another way of looking at compartmental systems. We can interpret the compartmental system as a weighted directed graph, and there are plenty of complexity measures on graphs (Dehmer & Mowshowitz, 2011). But in contrast to most of the existing complexity measures on graphs, the weights of the path entropy do not seem to be arbitrarily chosen just to guarantee typical properties of complexity measures. Instead, they naturally emerge from the question of what happens to a particle in the system. However, from the viewpoint of how complicated the compartmental matrix looks, the interpretation of the path entropy is counterintuitive. Usually, the more symmetrically and simple the matrix looks, the more complex becomes the system in terms of path entropy (e.g., Proposition 4.24).

If we can find the maximum entropy model in a class $\mathcal{M}$ of models, then the difference between the maximum entropy and the entropy of another model $M \in \mathcal{M}$ could serve as a complexity measure for M, even though Shannon called this difference *information* (Bonchev & Buck, 2005). Such an alternative complexity measure works in the opposite direction of the path entropy. In fact, it measures the additional information a modeler put into M with respect to the most uninformed model, and this additional information is then called complexity. The path entropy, however, values the most stupid model as highly complex. As with all other complexity measures, it is important to have clearly in mind, what the system property of interest exactly is. This is already true for purely structural complexity aspects that ignore transfer rates (Dehmer & Mowshowitz, 2011).

As mentioned in Sections 4.1 and 4.3, Pesin's theorem implies that the metric entropy of all open compartmental system vanishes. Furthermore, the metric entropy of continuous-time stochastic processes is infinite which is caused by the discretization in time, on which the metric entropy relies. When we introduced the entropy rate per jump in Section 4.3.1, from the very beginning we used discrete (states) and continuous (sojourn times) random variables. This way, by the definition of differential entropy, we avoided a discretization in time. However, for the path entropy of nonautonomous systems we used a time-discretization approach and obtained an infinite offset as mentioned in Remark 4.33. This infinite offset is the very reason why the metric entropy for continuous-time stochastic processes is infinite (Gaspard & Wang, 1993, Eq. (3.30)). If we ignore it justified by the alternative derivation of the path entropy by means of differentiable entropy, we obtain an entropy measure that allows us to evaluate the complexity of open compartmental systems.

Probabilistically, the path entropy is the entropy of an absorbing continuous-time Markov chain. Just as in Chapter 3, where we extended the theory of ages, transit times, and remaining lifetimes from systems in equilibrium to systems out of equilibrium, in Section 4.4 we extended the concept of path entropy to nonautonomous systems, now by discretizing in time – the fourth way to obtain the path entropy. In nonautonomous systems, the path entropy of a particle is no longer constant but depends on the particle's entry time into the system. It might be interesting to investigate seasonal entropy cycles and long-term entropy trends for natural systems such as carbon cycle systems and to figure out what certain entropy patterns can tell us about the real world and vice versa. Nevertheless, the introduction of entropy for nonautonomous compartmental systems in this chapter is to be conceived as a first step in this direction only. Transferring autonomous entropy concepts such as maximum entropy and model identification to nonautonomous systems might be a profound field of research in the future. In particular, measurement data are usually time-dependent, and it is an intriguing question how complex a model needs to be to be capable of reproducing a data set with a certain information content.

CHAPTER 5

Conclusions and outlook

Compartmental systems are particular deterministic dynamical systems that describe the flow of material, energy, or other quantities such as money through a system that comprises a number of well-mixed compartments (Jacquez et al., 1972; Anderson, 1983; Jacquez & Simon, 1993; Walter & Contreras, 1999; Haddad et al., 2010). Continuous-time Markov chains are stochastic processes on a state space, in which the future state is independent of the past (Kallenberg, 2002).

In this thesis, we mainly investigated the relation between compartmental systems and continuous-time Markov chains based on the properties mass balance and well-mixedness of compartmental systems as well as on the probability mass balance and the Markov property of continuous-time Markov chains. This way, we built a bridge between a deterministic and a stochastic theory.

First, we derived compartmental systems as systems of ODEs from the two principles of conservation of mass and well-mixedness of compartments. This lead to the main objects of study: compartmental matrices. As it turned out, compartmental matrices have the same properties as transition-rate matrices of absorbing continuous-time Markov chains. Thereby, we found that for open compartmental systems in equilibrium the deterministic quantities system age, transit time, and remaining system lifetime follow phase-type distributions with respective parameters. We also derived explicit formulas for the distributions of compartment ages and remaining compartment lifetimes. Furthermore, we showed that if we consider the time-reversed system, the roles of age and remaining lifetime interchange.

Manzoni et al. (2009) had also identified the compartment-age and transit-time distributions, but only for compartmental systems with a very simple structure. Even earlier, Thompson & Randerson (1999) had already derived age- and transit-time distributions for the global ecosystem model introduced by Emanuel et al. (1981). However, their method was purely numerical and computationally intensive. With the explicit formulas we derived, we can easily address systems of arbitrary size with immediate and precise results.

We also found that system age and remaining system lifetime of open compartmental systems in equilibrium find their stochastic counterparts in the backward and forward recurrence times of a particular renewal process, respectively. Furthermore, compartment ages and remaining compartment lifetimes are related to conditional backward- and forward recurrence times of a particular regenerative process, respectively. The construction of this regenerative process relies on an absorbing continuous-time Markov chain whose absorption time is the stochastic counterpart of the deterministic transit time of the compartmental system. It is this back and forth between determinism and stochasticism, which shows how deterministic and stochastic theory can profit from each other. Each time one solves a problem in one of the two fields, automatically a second problem is solved in the other field. If the second problem has not existed so far, it might be worth to investigate where it can be found. This way, one might gain a deeper knowledge of the entire structure of the particular field or subfield of interest. We implemented the stochastically motivated formulas for the deterministic concepts of age, transit time, remaining lifetime in the Python package `https://github.com/MPIBGC-TEE/LAPM`. The derivation of the mainly stochastically motivated formulas for the distributions of age, transit time, and remaining lifetime for compartmental systems in equilibrium solved a deterministic problem that had been around for decades, at least in ecology (Rodhe & Björkström, 1979).

Once the structures of these formulas were clear, it was straightforward to extend them to systems out of equilibrium. Consequently, we obtained formulas for the distributions of age, transit time, and remaining lifetime for nonautonomous compartmental systems. These systems can even be nonlinear as long as we are given a unique solution trajectory. The results are then valid for this particular trajectory only because we need to construct a linear system with the same unique solution. This is a step forward with respect to the classical approach of linearizing the system in the neighborhood of a single point, usually an equilibrium. Yet there is still a long way to go to find a consistent age- and transit-time theory for nonlinear systems themselves, not only for single solution trajectories of them.

Furthermore, we developed an ODE system to efficiently compute the evolution of moments of the age distributions through time. This ODE system, called compartment-age system, generalizes the mean age system introduced by Rasmussen et al. (2016). Another set of ODEs allows an efficient computation of quantiles of the age distributions through time. Moreover, we showed that forward and backward transit time are simply time-shifted versions of one another, which is a multi-dimensional generalization of Niemi's theorem (Niemi, 1977). The Python package `https://github.com/MPIBGC-TEE/CompartmentalSystems` which we developed allows us to easily apply these results to nonautonomous compartmental systems.

For open compartmental systems in equilibrium, a finite mean transit time, or mean absorption time, $\mathbb{E}[\mathcal{T}] = \|\mathbf{x}^*\|/\|\mathbf{u}\| = \|-\mathrm{B}^{-1}\,\mathbf{u}\|/\|\mathbf{u}\|$ implies the invertibility of B, and in turn Proposition 1.13 implies the system's exponential stability. However, for nonautonomous systems exponential stability seems to be a much stronger property than finiteness of the mean transit time. Rasmussen et al. (2016, Theorem 1) provide sufficient conditions for a linear nonautonomous compartmental system to be exponentially stable. However, the compartmental matrix

$$\mathrm{B} = \begin{pmatrix} -1 & 1 \\ 0 & -2 \end{pmatrix},$$

which clearly leads to an exponentially stable autonomous system, does not satisfy the provided sufficient conditions if considered nonautonomous. Consequently, one could possibly define a stability concept for nonautonomous compartmental systems based on the mean transit time that is more appropriate than exponential stability. Such a more relaxed stability concept might then also be used to find out how fast a system is allowed to slow down and still retain stability. Stability here in the sense that the system avoids congestion by still turning over the input fast enough, even though the turnover decelerates.

While in Chapter 2 we drew links between deterministic and probabilistic theory and transferred knowledge in both directions, in Chapter 3 the entire theory for nonautonomous compartmental systems was purely deterministic. The field of nonautonomous dynamical systems has been prospering in the last decades (e.g., Kloeden & Rasmussen 2011 and references therein). Transferring important results over to probability theory could also help push forward the theory of inhomogeneous Markov chains.

In Chapter 4, we focused on the construction of a complexity measure of open compartmental systems in equilibrium. We considered the path of a single particle that travels through the system and introduced three measures of uncertainty regarding this path. (1) The entropy rate per jump is the mean uncertainty of the particle's travel per the mean number of jumps. A jump occurs each time the particle leaves its compartment of residence. We obtained it by considering the path as a pair of a discrete-time and a continuous-time Markov chain, one describing the sequence of visited compartments and the other one describing the respective sojourn times. (2) The mean entropy rate per unit time is the mean uncertainty of the particle's travel averaged over the mean length of the travel. We obtained it by considering a regenerative process that describes the infinite journey of a particle through the system that develops if the particle enters the system again immediately after its exit from the system. (3) The path entropy corresponds to the total uncertainty of one travel of a particle through the system. We obtained it by considering the path as a random variable in an appropriately constructed path space and identifying the path's probability density function. As it turned out, the three entropy concepts are consistent, and each one has its advantages depending on the purpose of study.

Furthermore, we found that the mean transit time is not only tightly connected with the stability of the system but also with the system's entropy. By transitivity, also stability and entropy are related, and it might well be worth to investigate this relation more closely. For instance, Haddad et al. (2010) examine the relation between stability and entropy of compartmental systems by considering compartmental systems as directed graphs. Looking at the relation between mean transit time and path entropy as stated in Theorem 4.20 (note that $\mathbb{E}[\mathcal{T}] = \sum_{j=1}^{d} x_j^*/\|\mathbf{u}\|$), it can be speculated that the system's stability increases with decreasing path entropy. This idea is inspired by the fact, that in the one-dimensional compartmental system M_λ from Remark 4.18, a low value of the path entropy $1 - \log \lambda$ is achieved for large values of λ. Furthermore, in terms of Definition 1.10, a high value of $\gamma = \lambda$ leads to a high convergence rate of trajectories and a high degree of exponential stability of the system. The concept of community complexity in ecology, however, goes exactly in the opposite direction. MacArthur (1955) states that "[t]he amount of choice which the energy has in following the paths up through the food web is a measure of the stability of the community." In this light, we can interpret the entropy rate $\theta(\zeta)$ given by Eq. (4.10) of the pure jump process ζ describing the sequence of visited compartments as a stability measure of the community. Consequently, a higher path entropy implies a higher stability of an ecological community. These two counteracting interpretations of the link between path entropy and stability certainly deserve a closer investigation in the future. The latter approach considers compartmental systems as systems of flow. How entropy can serve as a measure for complexity of systems of flow is discussed by Ulanowicz (2001). From his discussion, we can also infer that since path entropy and entropy rates incorporate stocks, connections, and rates, they are well-suited for describing system dynamics and hence complement age, transit time, and remaining lifetime in this regard.

The fact that the path entropy tends to increase along with the mean transit time has another interesting implication. Paths of particles through slow systems are more difficult to predict than paths through fast systems. If it is true that slow compartments are the ones that contain the highest amount of carbon in soils, then the entropy of soil carbon systems is intrinsically high. Consequently, carbon cycle in soil systems is very difficult to model because it is challenging to make accurate predictions for them. This might be the reason for the high variety of predicted soil carbon by different models (Friedlingstein et al., 2006, 2014), which has been stimulating the studies of scientists for more than a decade.

As mentioned before, in the course of deriving the path entropy in Section 4.3.3, we constructed the path space of the particle. With the path space and the path's probability density function in hand, we can evaluate any kind of functionals on paths, only one of which is the path entropy. Others encompass diverse cost functionals or efficiency functionals of different nature.

The idea of using an entropy-based approach for the determination of complexity of a system has widespread applications to social networks, mathematical psychology, traffic planning, machine learning, software development processes, linguistics, ecological systems, and systems biology (Ulanowicz, 2001). There are many scientific fields in which we can investigate the idea further. The presentation here is just one first step.

Usually, compartmental systems are described by systems of ODEs. This approach works well as long as the compartments are considered well-mixed. In natural systems (e.g., water flow through rivers, spilled oil in the sea), the well-mixed assumption is not bearable, and simple ODE systems are not capable of representing such situations adequately. For instance, one way of representing systems with age-dependencies is to model them by Markov renewal processes. In Markov renewal processes, the future of the system is not anymore independent of the past, but might additionally depend on how long the system has already been in the current state. Such processes have been extensively examined (Çinlar, 1969; Çinlar, 1975; Janssen & Manca, 2006), and a translation to dynamical systems might open an interesting way of dealing with age-dependencies in a deterministic setup. Another way of looking at compartmental systems is from the perspective of stochastic point processes. Just as a single Poisson process represents a one-dimensional compartmental system, a point process on the product space $[t_0, \infty) \times S$ can represent a multi-dimensional system. An element (t, j) of this product space bears the information that at time $t \in [t_0, \infty)$ the process changes its state to $j \in S$. In this setup, restrictions such as continuous time or well-mixedness are unnecessary because the point process can be defined in a very general manner (Daley & Vere-Jones, 2003, 2008). However, this is still not the most general way to represent compartmental systems because in nonlinear systems particles also interact with each other. These interactions could be reflected by interacting Markov chains (Spitzer, 1970).

If we imagine a particular scientific discipline to be a single snowflake in a snowstorm, then we should spread our arms and catch as many of them as we can. Afterwards we put them together into one pot and let them melt.

APPENDIX A

The matrix exponential

Definition A.1 For $t \in \mathbb{R}$ and B being be a real square matrix, the series

$$e^{t\,\mathrm{B}} := \mathrm{I} + t\,\mathrm{B} + \frac{1}{2!}\,t^2\,\mathrm{B}^2 + \cdots = \sum_{k=0}^{\infty} \frac{(t\,\mathrm{B})^k}{k!},$$

where I is the identity matrix, is called the *matrix exponential* of $t\,\mathrm{B}$.

Since $e^{t\,\mathrm{B}}$ has an infinite radius of convergence as a function of t (Norris, 1997, Section 2.10), it is straightforward to prove the following lemma which provides us with with all the properties of the matrix exponential that are used in the main text. The proofs can also be found in Horn & Johnson (1994) and Kwak & Hong (2004).

Lemma A.2 *Let $s, t \in \mathbb{R}$. The matrix exponential has the following properties:*

(i)

$$e^{(s+t)\,\mathrm{B}} = e^{s\,\mathrm{B}}\,e^{t\,\mathrm{B}};$$

(ii) the matrices B *and* $e^{t\,\mathrm{B}}$ *commute, i.e.,*

$$\mathrm{B}\,e^{t\,\mathrm{B}} = e^{t\,\mathrm{B}}\,\mathrm{B};$$

(iii) if B *is invertible, then the matrices* B^{-1} *and* $e^{t\,\mathrm{B}}$ *commute, i.e.,*

$$\mathrm{B}^{-1}\,e^{t\,\mathrm{B}} = e^{t\,\mathrm{B}}\,\mathrm{B}^{-1};$$

(iv) if B *is invertible, then*

$$e^{(t\,\mathrm{B})^{-1}} = \left(e^{t\,\mathrm{B}}\right)^{-1};$$

(v)

$$e^{t\,\mathrm{B}^\top} = \left(e^{t\,\mathrm{B}}\right)^\top;$$

(vi) if P *is any invertible square matrix with the same dimensions as* B*, then*

$$e^{t\,\mathrm{P}\,\mathrm{B}\,\mathrm{P}^{-1}} = \mathrm{P}\,e^{t\,\mathrm{B}}\,\mathrm{P}^{-1};$$

(vii) $e^{t\,\mathrm{B}}$ *is differentiable in all* $t \in \mathbb{R}$ *and*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,e^{t\,\mathrm{B}} = \mathrm{B}\,e^{t\,\mathrm{B}} = e^{t\,\mathrm{B}}\,\mathrm{B};$$

(viii) for $t \geq 0$*, the identity*

$$\mathrm{B} \int_0^t e^{\tau\,\mathrm{B}}\,\mathrm{d}\tau = -\mathrm{I} + e^{t\,\mathrm{B}}$$

holds;

(ix) if B *is invertible, then*

$$\int_0^\infty e^{\tau\,\mathrm{B}}\,\mathrm{d}\tau = -\mathrm{B}^{-1}.$$

APPENDIX B

The state-transition matrix

In contrast to the one-dimensional or the time-independent case, the state-transition matrix of a time-dependent multi-dimensional system can in general not be computed analytically. It has nevertheless some useful properties some of which we collect here. They can be found in Brockett (2015) and Desoer & Vidyasagar (2009).

Definition B.1 The *state-transition matrix* of the linear nonautonomous system described by Eq. (3.3) is the solution of the matrix equation

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\Phi(t,s) &= \mathrm{B}(t)\,\Phi(t,s), \quad t_0 < s \le t < T \\ \Phi(s,s) &= \mathrm{I}, \end{aligned} \tag{B.1}$$

where I is the identity matrix.

In general, the state-transition matrix is given by the *Peano-Baker series*

$$\begin{aligned} \Phi(t,s) = \mathrm{I} &+ \int_s^t \mathrm{B}(\tau_1)\,\mathrm{d}\tau_1 + \int_s^t \mathrm{B}(\tau_1) \int_s^{\tau_1} \mathrm{B}(\tau_2)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 \\ &+ \int_s^t \mathrm{B}(\tau_1) \int_s^{\tau_1} \mathrm{B}(\tau_2) \int_s^{\tau_2} \mathrm{B}(\tau_3)\,\mathrm{d}\tau_3\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 + \cdots . \end{aligned}$$

If $\mathrm{B}(t) = b(t)$ is a scalar, then the Peano-Baker series can be summed to

$$\Phi(t,s) = e^{\int_s^t b(\tau)\,\mathrm{d}\tau}.$$

If $\mathrm{B}(t) = \mathrm{B}$ is a real constant square matrix, then

$$\begin{aligned} \Phi(t,s) &= \mathrm{I} + \frac{1}{1!}\,(t-s)^1\,\mathrm{B}^1 + \frac{1}{2!}\,(t-s)^2\,\mathrm{B}^2 + \cdots \\ &= e^{(t-s)\,\mathrm{B}}, \end{aligned}$$

where $e^{(t-s)\,\mathrm{B}}$ denotes the matrix exponential (Appendix A).

If $\mathrm{B}(t) = b(t)\,\mathrm{B}$ is a scalar multiplied with a constant matrix, then

$$\Phi(t,s) = e^{\int_s^t b(\tau)\,\mathrm{d}\tau\,\mathrm{B}}.$$

APPENDIX C

Some stochastic processes

In the course of the main text, some stochastic processes occur over and over again and are central to this thesis. Here, we introduce them and some of their properties in a not too rigorous way, just to provide the basic ideas behind them.

C.1. Poisson processes

We intend to follow Ross (2010) to have a look at the Poisson process, one of the most important counting processes. Consequently, we introduce counting processes first.

Definition C.1 A *counting process* is a stochastic process $N = (N_t)_{t\geq 0}$ with nonnegative and nondecreasing integer values.

A counting process counts events. If $s < t$, then $N_t - N_s$ is the number of events occurred in the time interval $(s, t]$. A counting process is said to possess *independent increments* if the numbers of events that occur in disjoint time intervals are independent. A counting process is said to possess *stationary increments* if the distribution of the number of events that occur in any time interval depends only on the length of the interval. In order to introduce the Poisson process, we need to introduce the *little-o notation*.

Definition C.2 A function $f : \mathbb{R} \to \mathbb{R}$ is said to be $o(h)$ if $\lim_{h\to 0} f(h)/h = 0$. We then also write $f \in o(h)$.

Definition C.3 The counting process $N = (N_t)_{t\geq 0}$ is called a *(homogeneous) Poisson process* with *intensity rate* $\lambda > 0$ if

(i) $N_0 = 0$,

(ii) N has stationary and independent increments,

(iii) $\mathbb{P}(N_h = 1) = \lambda\, h + o(h)$, and

(iv) $\mathbb{P}(N_h \geq 2) = o(h)$.

Consider a Poisson process and denote the moment of the first event's occurrence by T_1. For $n > 1$, denote by T_n the elapsed time between the $(n-1)$st and the nth event. Then, the sequence $(T_n)_{n\in\mathbb{N}}$ is called the sequence of *interarrival times*. It is an important property of the Poisson process that for any $n \in \mathbb{N}$ the interarrival time T_n is exponentially distributed with rate λ and mean $1/\lambda$, i.e., $T_n \sim \mathrm{Exp}(\lambda)$.

Since the minimum $T := \min\{T_1, T_2\}$ of two independent exponentially distributed random variables $T_1 \sim \mathrm{Exp}(\lambda_1)$ and $T_2 \sim \mathrm{Exp}(\lambda_2)$ is again exponentially distributed, i.e., $T \sim \mathrm{Exp}(\lambda_1 + \lambda_2)$, it is not surprising that the superposition of two independent Poisson processes with intensity rates λ_1 and λ_2 is a Poisson process with intensity rate $\lambda = \lambda_1 + \lambda_2$ (Norris, 1997, Theorem 2.4.4).

If we omit the claim for stationary increments in Definition C.3, N becomes an *inhomogeneous Poisson process*. The constant intensity rate λ turns then into an intensity function $\lambda(t)$. Note that the superposition of two inhomogeneous Poisson processes with intensity rates $\lambda_1(t)$ and $\lambda_2(t)$ is again an (inhomogeneous) Poisson process with intensity function $\lambda(t) = \lambda_1(t) + \lambda_2(t)$ (Daley & Vere-Jones, 2003).

C.2. Renewal processes

Poisson processes are generalized by renewal processes in the sense that the interarrival times are not necessarily exponentially distributed anymore. In the literature, we can find two different ways of defining renewal processes. One way is to define a renewal process as a particular counting process N, the other way is to define a renewal process as the sequence of times at which events of N occur. Throughout the entire thesis, we stick to the latter definition, which is also used by Asmussen (2003).

Definition C.4 Let N be a counting process with $(T_n)_{n\in\mathbb{N}}$ being its sequence of interarrival times. The process $J = (J_0, J_1, J_2, \ldots)$ with $J_0 = 0$, and $J_n = T_1 + T_2 + \cdots + T_n$ for $n \in \mathbb{N}$ is called a *renewal process* if the sequence $(T_1, T_2, \ldots)$ is independent and identically distributed.

Definition C.5 Let J be a renewal process, let F denote the cumulative probability distribution of its interarrival times, and let μ be its mean interarrival time. Then the probability distribution whose cumulative probability distribution is given by

$$G(t) = \frac{1}{\mu} \int_0^t [1 - F(\tau)]\, \mathrm{d}\tau, \quad t > 0,$$

is called the *stationary distribution* of J.

Freely adapted from Janssen & Manca (2006, Section 2.9), when we start observing a renewal process that has already been running, the moment in time of the first observed event occurrence does not correspond to the current interarrival time but in fact to the current forward recurrence time. A (so-called delayed) renewal process, in which the first interarrival time is defined to be distributed according to the process' stationary distribution, takes that into account in the sense that now T_1 is the forward recurrence time of a renewal process that has already been running for an infinite amount of time.

C.3. Markov chains

Following Norris (1997, Chapter 1), we now introduce discrete-time Markov chains.

Definition C.6 Let S be a finite set. A nonnegative vector $\boldsymbol{\lambda} = (\lambda_j)_{j\in S}$ with $\sum_{j\in S} \nu_j = 1$ is called a *distribution* on S. A matrix $\mathrm{P} = (P_{ij})_{i,j\in S}$ is called *stochastic* on S if every column sum is a distribution on S.

Note that in contrast to standard notation in probability theory, we are interested in column sums instead of row sums. The reversed index order is more convenient when working with Markov chains and compartmental system contemporaneously.

Definition C.7 Let $\boldsymbol{\lambda} = (\lambda_j)_{j\in S}$ be a distribution on a finite set S, let P be a stochastic matrix on S, and let $Y = (Y_n)_{n=0,1,2,\dots}$ be a sequence of S-valued random variables. Furthermore, for all $n = 0, 1, 2, \dots$ and $j_0, j_1, \dots, j_n, j_{n+1} \in S$,

(i) $\mathbb{P}(Y_0 = j_0) = \lambda_{i_0}$ and

(ii) $\mathbb{P}(Y_{n+1} = j_{n+1} \,|\, Y_n = j_n, Y_{n-1} = j_{n-1}, \dots, Y_0 = j_0) = P_{j_{n+1}j_n}$.

Then we call Y a *(homogeneous) discrete-time Markov chain* on the *state space* S with *transition matrix* P and *initial distribution* $\boldsymbol{\lambda}$.

Definition C.8 Let Y be a discrete-time Markov chain on a finite state space S with transition matrix P. A positive distribution $\boldsymbol{\pi}$ on S is called a *stationary distribution* of Y if $\mathrm{P}\,\boldsymbol{\pi} = \boldsymbol{\pi}$. If the initial distribution of Y is stationary, then Y itself is also called *stationary*. Furthermore, Y is said to be *irreducible* if there is a path from state j to state i for all $i, j \in S$.

The following ergodic lemma is a combination of Theorem 1.7.7 and the *Ergodic theorem* 1.10.2 in Norris (1997) applied to the function $f(i) = \mathbb{1}_{\{i=j\}}$, $i, j \in S$.

Lemma C.9 *Let Y be an irreducible discrete-time Markov chain on a finite state space S with a stationary distribution $\boldsymbol{\pi} = (\pi_j)_{j\in S}$, and fix $j \in S$. Then,*

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \mathbb{P}(Y_k = j) = \pi_j.$$

Consequently, $\boldsymbol{\pi}$ is the unique stationary distribution of Y.

In Chapter 2 of Norris (1997), continuous-time Markov chains are introduced. To that end, first the concept of Q-matrices is presented.

Definition C.10 Let S be a finite set. A *Q-matrix* on S is a matrix $\mathrm{Q} = (Q_{ij})_{i,j\in S}$ satisfying the conditions

(i) $Q_{jj} \le 0$ for all j,

(ii) $Q_{ij} \ge 0$ for all $i \ne j$, and

(iii) $\sum_{i\in S} Q_{ij} = 0$ for all j.

Definition C.11 Let Q be a Q-matrix and $\boldsymbol{\lambda}$ a distribution on a finite set S. We say that a stochastic process $X = (X_t)_{t\ge 0}$ is a *continuous-time Markov chain* on the *state space* S with *transition-rate matrix* Q and *initial distribution* $\boldsymbol{\lambda}$ if the following conditions hold:

(i) $\mathbb{P}(X_0 = j) = \lambda_j$ for all $j \in S$;

(ii) for all $n = 0, 1, 2, \dots$, all times $0 \le t_0 \le t_1 \le \dots \le t_{n+1}$, and all $j_0, j_1, \dots, j_{n+1} \in S$,

$$\mathbb{P}(X_{t_{n+1}} = j_{n+1} \,|\, X_{t_n} = j_n, X_{t_{n-1}} = j_{n-1}, \dots, X_{t_0} = j_0) = \left(e^{(t_{n+1}-t_n)\,\mathrm{Q}}\right)_{j_{n+1}j_n}.$$

Let $i, j \in S$ and $0 \le s \le t$. Then

$$\mathbb{P}(X_t = i \,|\, X_s = j) = \mathbb{P}(X_{t-s} = i \,|\, X_0 = j)$$

does not explicitly depend on s and t but only on their distance $t - s$. Hence, X is called *homogeneous*. More generally, Q can be a function depending on time, then

$$\mathbb{P}(X_t = i \,|\, X_s = j)$$

depends explicitly on s and t and not only on the distance $t - s$. Then X is called *inhomogeneous*.

Let X be a (homogeneous) continuous-time Markov chain on a finite state space S with transition-rate matrix Q and initial distribution $\boldsymbol{\lambda}$. Then, for $i, j \in S$, the probability of X being in state i at time t having started in state j is equal to

$$\mathbb{P}(X_t = i \,|\, X_0 = j) = \left(e^{t\,\mathrm{Q}}\right)_{ij}.$$

By the law of total probability, the unconditional probability of being in state $i \in S$ at time t is

$$\sum_{j \in S} \mathbb{P}(X_t = i \,|\, X_0 = j)\, \mathbb{P}(X_0 = j) = \sum_{j \in S} \left(e^{t\,\mathrm{Q}}\right)_{ij} \lambda_j,$$

which gives

$$\mathbb{P}(X_t = i) = \left(e^{t\,\mathrm{Q}}\,\boldsymbol{\lambda}\right)_i.$$

Property (ii) of Definition C.11 states that the future evolution of a Markov process depends only on its current state and not on its history. This is called *Markov property*.

Definition C.12 Let X be a continuous-time Markov chain on a finite state space S with transition-rate matrix Q. A positive distribution $\boldsymbol{\nu}$ on S is called a *stationary distribution* of X if $\mathrm{Q}\,\boldsymbol{\nu} = \mathbf{0}$, where $\mathbf{0}$ is the appropriate column vector comprising zeros. If the initial distribution of X is stationary, then X itself is also called *stationary*. Furthermore, X is said to be *irreducible* if $\mathbb{P}(X_t = i \,|\, X_0 = j) > 0$ for all $i, j \in S$ and $t \ge 0$.

The following ergodic lemma is a combination of Theorem 3.5.3 and the *Ergodic theorem* 3.8.1 in Norris (1997) applied to the function $f(i) = \mathbb{1}_{\{i=j\}}$, $i, j \in S$.

Lemma C.13 *Let X be an irreducible continuous-time Markov chain on a finite state space S with a stationary distribution $\boldsymbol{\nu} = (\nu_j)_{j \in S}$, and fix $j \in S$. Then,*

$$\lim_{t \to \infty} \frac{1}{t} \int_0^t \mathbb{P}(X_t = j)\, \mathrm{d}t = \nu_j.$$

Consequently, $\boldsymbol{\nu}$ is the unique stationary distribution of X.

Closely connected to a continuous-time Markov chain X is the discrete-time Markov chain $Y = (Y_n)_{n=0,1,2,\ldots}$ that keeps track of the jumps of X. This process is defined such that $Y_0 := X_0$ and every time $t > 0$ the process X jumps into another state, the process Y takes on the new value of X_t. Hence, Y_n represents the state of the process X after the nth jump. Clearly, the state-space of Y is also S.

Definition C.14 Let X be a continuous-time Markov chain on a finite state space S with transition-rate matrix Q and initial distribution $\boldsymbol{\lambda}$. The discrete-time Markov chain Y with state space S, initial distribution $\boldsymbol{\lambda}$, and transition matrix $\mathrm{P} = (P_{ij})_{i,j \in S}$ given by

$$P_{ij} = \begin{cases} -Q_{ij}/Q_{jj}, & j \neq i \text{ and } Q_{jj} \neq 0, \\ 0, & j \neq i \text{ and } Q_{jj} = 0, \end{cases}$$
$$P_{jj} = \begin{cases} 0, & Q_{jj} \neq 0, \\ 1, & Q_{jj} = 0. \end{cases}$$

is called *embedded chain* or *jump chain* of X.

Let us now consider a continuous-time Markov chain $X = (X_t)_{t \geq 0}$ with a special structure. Its finite state-space $\widetilde{S}$ is supposed to be equal to $\{1, 2, \ldots, d, d+1\}$ for some natural number $d \geq 1$, and its transition-rate matrix has the shape

$$\mathrm{Q} = \begin{pmatrix} \mathrm{B} & \mathbf{0} \\ \mathbf{z}^\top & 0 \end{pmatrix} \in \mathbb{R}^{(d+1)\times(d+1)}.$$

Let $S = \{1, 2, \ldots, d\} \subseteq \widetilde{S}$. The $d \times d$-matrix $\mathrm{B} = (B_{ij})_{i,j \in S}$ is supposed to meet the requirements (i) and (ii) of a Q-matrix, but instead of property (iii) of Definition C.10, it fulfills only the weaker condition

$$\sum_{i \in S} B_{ij} \leq 0 \text{ for all } j \in S.$$

Additionally, we ask B to be invertible. Since Q is required to be a Q-matrix, the vector $\mathbf{z} \in \mathbb{R}^d$ must contain the missing parts to make the columns sum to zero. Consequently, $z_j = -\sum_{i \in S} B_{ij}$ or, in matrix notation,

$$\mathbf{z}^\top = -\mathbf{1}^\top \mathrm{B},$$

where $\mathbf{1}^\top$ denotes the d-dimensional row vector comprising ones. This means that the z_j's are nonnegative and denote the transition rates from j to $d+1$. The $(d+1)$st column of Q comprises zeros. Hence, the process X cannot change its state anymore once it has reached state $d+1$. For that reason, $d+1$ is called the *absorbing state* of X. We exclude the trivial case in which the process starts in its absorbing state by considering only initial distributions $\boldsymbol{\lambda} = (\lambda_j)_{j \in \widetilde{S}}$ with $\lambda_{d+1} = 0$ and define

$$\boldsymbol{\beta} := (\lambda_1, \lambda_2, \ldots, \lambda_d)^\top \in \mathbb{R}^d$$

to be the new initial distribution of X.

Definition C.15 We call X an *absorbing continuous-time Markov chain* on the finite state space $S = \{1, 2, \ldots, d\}$ with *transition-rate matrix* B, *initial distribution* $\boldsymbol{\beta}$, and *absorbing state* $d+1$.

A standard linear algebra argument shows that

$$e^{t\,\mathrm{Q}} = \begin{pmatrix} e^{t\,\mathrm{B}} & \mathbf{0} \\ * & 1 \end{pmatrix}, \quad t \geq 0,$$

where the asterisk $*$ is a place holder for a d-dimensional row vector. This means that, for $i, j \in S$,

$$\mathbb{P}(X_t = i \mid X_0 = j) = \left(e^{t\,\mathrm{B}}\right)_{ij}, \quad t \geq 0,$$

and

$$\mathbb{P}(X_t = i) = \left(e^{t\,\mathrm{B}}\,\boldsymbol{\beta}\right)_i, \quad t \geq 0.$$

Definition C.16 Let X be an absorbing continuous-time Markov chain on a finite state space S, and denote by P the transition matrix of the jump chain Y of X. Then

$$\mathrm{M} := \sum_{k=0}^{\infty} \mathrm{P}^k = (\mathrm{I} - \mathrm{P})^{-1}$$

is called the *fundamental matrix* of X and Y.

The element M_{ij} is the mean number of visits to state i before absorption, given that the chain started in state j.

C.4. Regenerative processes

A certain combination of continuous-time Markov chains and renewal processes leads to *regenerative processes*. Ross (2010) gives an understandable definition without being too technical.

Definition C.17 A process $Z = (Z_t)_{t \geq 0}$ on a finite state space S with the property that there exist time points $J_1, J_2, \ldots$ at which the process probabilistically restarts itself, is called a *regenerative process*. The time points $J_1, J_2, \ldots$ are called the *regeneration times* of Z.

In other words, with probability 1 there exists a time J_1, such that the continuation of the process beyond J_1 is a probabilistic replica of the whole process starting at 0. Then, automatically, there exist further times $J_2, J_3, \ldots$ with the same property as J_1. Using the definition given by Asmussen (2003), with $J_0 := 0$ the process $J = (J_n)_{n=0,1,2,\ldots}$ is a renewal process with interarrival times $T_1 = J_1 - J_0$, $T_2 = J_2 - J_1$, ...We call J the *embedded renewal process* of Z.

APPENDIX D

Examples of simple compartmental systems in equilibrium

D.1. One single compartment

Consider the one-compartment system represented by the linear ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}\,x(t) = -\lambda\,x(t) + u, \quad t > 0,$$

for $\lambda > 0$. In this simplest possible framework, $\mathrm{B} = -\lambda$, $\mathbf{z} = \lambda$, $\mathrm{B}^{-1} = -1/\lambda$, and $\boldsymbol{\beta} = 1$. The according phase-type distribution is just the exponential distribution. The cumulative probability distribution of the transit time $\mathcal{T}$ is

$$F_{\mathcal{T}}(t) = 1 - e^{-\lambda\,t}, \quad t \geq 0,$$

its probability density function is

$$f_{\mathcal{T}}(t) = \lambda\,e^{-\lambda\,t}, \quad t \geq 0,$$

and the expected absorption time or mean transit time is $\mathbb{E}\left[\mathcal{T}\right] = 1/\lambda$. The mean-age vector $\mathbf{a}$ coincides with the system age A and its probability density function is

$$f_A(y) = \lambda\,e^{-\lambda\,y}, \quad y \geq 0,$$

which leads to the mean age of $\mathbb{E}\left[A\right] = 1/\lambda$. The fact that transit time and age have the same distribution reflects the memorylessness of the exponential distribution.

D.2. Two compartments without feedback

A more interesting example is a two-compartment system given by

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\,x_1(t) &= -\lambda_1\,x_1(t) + u_1, \\
\frac{\mathrm{d}}{\mathrm{d}t}\,x_2(t) &= \alpha\,\lambda_1\,x_1(t) - \lambda_2\,x_2(t) + u_2,
\end{aligned}$$

with $\lambda_1 > 0$, $\lambda_2 > 0$, and $0 \leq \alpha \leq 1$. We furthermore assume $\lambda_1 \neq \lambda_2$. Then

$$\mathrm{B} = \begin{pmatrix} -\lambda_1 & 0 \\ \alpha\lambda_1 & -\lambda_2 \end{pmatrix}, \quad \mathrm{B}^{-1} = \begin{pmatrix} -\frac{1}{\lambda_1} & 0 \\ -\frac{\alpha}{\lambda_2} & -\frac{1}{\lambda_2} \end{pmatrix},$$

$\mathbf{z} = (-\alpha\,\lambda_1 + \lambda_1, \lambda_2)^\top$, $\mathbf{u} = (u_1, u_2)^\top$, and $\boldsymbol{\beta} = \left(\frac{u_1}{u_1+u_2}, \frac{u_2}{u_1+u_2}\right)^\top$.

The matrix exponential is given by

$$e^{t\,\mathrm{B}} = \begin{pmatrix} e^{-\lambda_1 t} & 0 \\ \frac{\alpha\lambda_1}{\lambda_1-\lambda_2}\left(e^{-\lambda_2 t} - e^{-\lambda_1 t}\right) & e^{-\lambda_2 t} \end{pmatrix}$$

and the cumulative probability distribution of the transit time $\mathcal{T}$ is

$$F_{\mathcal{T}}(t) = -\frac{\alpha\lambda_1 u_1\left(e^{-\lambda_2 t} - e^{-\lambda_1 t}\right)}{(\lambda_1-\lambda_2)(u_1+u_2)} - \frac{u_1 e^{-\lambda_1 t}}{u_1+u_2} - \frac{u_2 e^{-\lambda_2 t}}{u_1+u_2} + 1.$$

Its probability density function is given by

$$f_{\mathcal{T}}(t) = \frac{\lambda_2 u_2 e^{-\lambda_2 t}}{u_1+u_2} + \frac{u_1}{u_1+u_2}\left(\frac{\alpha\lambda_1\lambda_2}{\lambda_1-\lambda_2}\left(e^{-\lambda_2 t} - e^{-\lambda_1 t}\right) + \left(-\alpha\lambda_1+\lambda_1\right)e^{-\lambda_1 t}\right)$$

and its mean absorption time by

$$\mathbb{E}\left[\mathcal{T}\right] = \frac{u_1\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)}{u_1+u_2} + \frac{u_2}{\lambda_2\left(u_1+u_2\right)}.$$

For the age distribution we first need to compute the steady-state solution and its normalized version. We obtain

$$\mathbf{x}^* = -\mathrm{B}^{-1}\,\mathbf{u} = \left(\frac{u_1}{\lambda_1}, \frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2}\right)^\top,$$

$$\boldsymbol{\eta} = \frac{\mathbf{x}^*}{\|\mathbf{x}^*\|} = \left(\frac{u_1}{\lambda_1\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}, \frac{\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2}}{\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}}\right)^\top.$$

Using $A \sim \mathrm{PH}(\boldsymbol{\eta}, \mathrm{B})$ leads for $y \geq 0$ to

$$\begin{aligned}
F_A(y) &= -\frac{\alpha u_1\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right)}{(\lambda_1-\lambda_2)\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} - \frac{\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2}\right)e^{-\lambda_2 y}}{\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}} \\
&\quad + 1 - \frac{u_1 e^{-\lambda_1 y}}{\lambda_1\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}, \\
f_A(y) &= \frac{\lambda_2\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2}\right)e^{-\lambda_2 y}}{\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}} \\
&\quad + \frac{u_1}{\lambda_1\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}\left(\frac{\alpha\lambda_1\lambda_2}{\lambda_1-\lambda_2}\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right) + \left(-\alpha\lambda_1+\lambda_1\right)e^{-\lambda_1 y}\right), \\
\mathbb{E}\left[A\right] &= \frac{\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2}}{\lambda_2\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} + \frac{u_1\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)}{\lambda_1\left(\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}.
\end{aligned}$$

The probability density function of the compartment-age vector $\mathbf{a}$ is given by

$$\mathbf{f_a}(y) = \left(\lambda_1 e^{-\lambda_1 y}, \frac{\alpha\lambda_1\lambda_2 u_1\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right)}{(\lambda_1-\lambda_2)(\alpha u_1+u_2)} + \frac{\lambda_2 u_2 e^{-\lambda_2 y}}{\alpha u_1+u_2}\right)^\top,$$

which leads to the mean-age vector

$$\mathbb{E}\left[\mathbf{a}\right] = \left(\frac{1}{\lambda_1}, \frac{\alpha u_1}{\lambda_1\left(\alpha u_1+u_2\right)} + \frac{\frac{\alpha u_1}{\lambda_2} + \frac{u_2}{\lambda_2}}{\alpha u_1+u_2}\right)^\top.$$

D.2.1. Serial compartments - hypoexponential distribution

If $u_2 = 0$ and $\alpha = 1$, the particle enters the system in compartment 1 and must travel through compartment 2 before absorption. This leads to the transit time $\mathcal{T}$ being hypoexponentially distributed. That is, $\mathcal{T}$ is distributed like the sum of two independent exponential distributions. Consequently, for $t \geq 0$,

$$\begin{aligned}
F_{\mathcal{T}}(t) &= -\frac{\lambda_1}{\lambda_1 - \lambda_2}\left(e^{-\lambda_2 t} - e^{-\lambda_1 t}\right) + 1 - e^{-\lambda_1 t}, \\
f_{\mathcal{T}}(t) &= \frac{\lambda_1 \lambda_2}{\lambda_1 - \lambda_2}\left(e^{-\lambda_2 t} - e^{-\lambda_1 t}\right), \\
\mathbb{E}\left[\mathcal{T}\right] &= \frac{1}{\lambda_2} + \frac{1}{\lambda_1}.
\end{aligned}$$

The steady-state solution and its normalized version are

$$\mathbf{x}^* = \left(\frac{u_1}{\lambda_1}, \frac{u_1}{\lambda_2}\right)^\top \quad \text{and} \quad \boldsymbol{\eta} = \left(\frac{u_1}{\lambda_1\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}, \frac{u_1}{\lambda_2\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}\right)^\top.$$

For the system age A and $y \geq 0$ follows

$$\begin{aligned}
F_A(y) &= -\frac{u_1\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right)}{(\lambda_1 - \lambda_2)\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} + 1 - \frac{u_1 e^{-\lambda_2 y}}{\lambda_2\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} - \frac{u_1 e^{-\lambda_1 y}}{\lambda_1\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}, \\
f_A(y) &= \frac{\lambda_2 u_1\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right)}{(\lambda_1 - \lambda_2)\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} + \frac{u_1 e^{-\lambda_2 y}}{\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}}, \\
\mathbb{E}\left[A\right] &= \frac{u_1}{\lambda_2^2\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} + \frac{u_1\left(\frac{1}{\lambda_2} + \frac{1}{\lambda_1}\right)}{\lambda_1\left(\frac{u_1}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}.
\end{aligned}$$

For $u_1 = 1$ this turns into

$$\begin{aligned}
F_A(y) &= -\frac{\alpha\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right)}{(\lambda_1 - \lambda_2)\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)} - \frac{\alpha e^{-\lambda_2 y}}{\lambda_2\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)} + 1 - \frac{e^{-\lambda_1 y}}{\lambda_1\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)}, \\
f_A(y) &= \frac{\alpha e^{-\lambda_2 y}}{\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}} + \frac{1}{\lambda_1\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)}\left(\frac{\alpha \lambda_1 \lambda_2}{\lambda_1 - \lambda_2}\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right) + \left(-\alpha\lambda_1 + \lambda_1\right) e^{-\lambda_1 y}\right), \\
\mathbb{E}\left[A\right] &= \frac{\alpha}{\lambda_2^2\left(\frac{\alpha}{\lambda_2} + \frac{1}{\lambda_1}\right)} + \frac{1}{\lambda_1}.
\end{aligned}$$

The probability density function of the compartment-age vector $\mathbf{a}$ is given by

$$f_{\mathbf{a}}(y) = \left(\lambda_1 e^{-\lambda_1 y}, \frac{\lambda_1 \lambda_2}{\lambda_1 - \lambda_2}\left(e^{-\lambda_2 y} - e^{-\lambda_1 y}\right)\right)^\top,$$

which leads to the mean-age vector $\mathbb{E}\left[\mathbf{a}\right] = \left(\frac{1}{\lambda_1}, \frac{1}{\lambda_2} + \frac{1}{\lambda_1}\right)^\top$.

If furthermore $\lambda_1 = \lambda_2$, then the hypoexponential distribution turns into an Erlang distribution, which is the convolution of two independent and identically distributed exponential distributions.

D.2.2. Parallel compartments - hyperexponential distribution

The case of $\alpha = 0$ represents a purely parallel system and the transit time $\mathcal{T}$ is hyperexponentially distributed. For $t \geq 0$ this means

$$F_{\mathcal{T}}(t) = -\frac{u_1 e^{-\lambda_1 t}}{u_1 + u_2} - \frac{u_2 e^{-\lambda_2 t}}{u_1 + u_2} + 1,$$
$$f_{\mathcal{T}}(t) = \frac{\lambda_1 u_1 e^{-\lambda_1 t}}{u_1 + u_2} + \frac{\lambda_2 u_2 e^{-\lambda_2 t}}{u_1 + u_2},$$
$$\mathbb{E}\left[\mathcal{T}\right] = \frac{u_2}{\lambda_2 \left(u_1 + u_2\right)} + \frac{u_1}{\lambda_1 \left(u_1 + u_2\right)}.$$

The steady-state solution and its normalized version are given by

$$\mathbf{x}^* = \left(\frac{u_1}{\lambda_1}, \frac{u_2}{\lambda_2}\right)^\top \quad \text{and} \quad \boldsymbol{\eta} = \left(\frac{u_1}{\lambda_1 \left(\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}, \frac{u_2}{\lambda_2 \left(\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}\right)^\top.$$

For the system age A and $y \geq 0$ follows

$$F_A(y) = 1 - \frac{u_2 e^{-\lambda_2 y}}{\lambda_2 \left(\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} - \frac{u_1 e^{-\lambda_1 y}}{\lambda_1 \left(\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)},$$
$$f_A(y) = \frac{u_1 e^{-\lambda_1 y}}{\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}} + \frac{u_2 e^{-\lambda_2 y}}{\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}},$$
$$\mathbb{E}\left[A\right] = \frac{u_2}{\lambda_2^2 \left(\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)} + \frac{u_1}{\lambda_1^2 \left(\frac{u_2}{\lambda_2} + \frac{u_1}{\lambda_1}\right)}.$$

The probability density function of the compartment-age vector $\mathbf{a}$ is given by $f_{\mathbf{a}}(y) = \left(\lambda_1 e^{-\lambda_1 y}, \lambda_2 e^{-\lambda_2 y}\right)^\top$. This leads to the mean-age vector $\mathbb{E}\left[\mathbf{a}\right] = \left(\frac{1}{\lambda_1}, \frac{1}{\lambda_2}\right)^\top$.

D.3. Two compartments with feedback

Manzoni et al. (2009) considered also the simple two-compartment system with feedback

$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_1(t) = -\lambda_1\, x_1(t) + \lambda_2\, x_2(t) + u_1,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\, x_2(t) = \alpha\, \lambda_1\, x_1(t) - \lambda_2\, x_2(t),$$

in which material enters and leaves the system only through the first compartment, but in between it might spend some time in the second compartment. The compartmental matrix and the input vector are

$$\mathrm{B} = \begin{pmatrix} -\lambda_1 & \lambda_2 \\ \alpha\lambda_1 & -\lambda_2 \end{pmatrix} \quad \text{and} \quad \mathbf{u} = \begin{pmatrix} u_1 \\ 0 \end{pmatrix},$$

where $0 < \alpha < 1$. Manzoni et al. (2009) provide the Laplacians of the probability density functions of the transit time and the system age. The Laplacian of the probability density function of a $\mathrm{PH}(\boldsymbol{\beta}, \mathrm{B})$-distribution is given by

$$\widehat{f}_{\mathrm{PH}(\boldsymbol{\beta},\mathrm{B})}(s) = \mathbf{z}^\top \left(s\,\mathrm{I} - \mathrm{B}\right)^{-1} \boldsymbol{\beta}.$$

Consequently, the Laplacian of the probability density function of the transit time is given by

$$\widehat{f}_{\mathcal{T}}(s) = \frac{\lambda_1 (\alpha - 1) (\lambda_2 + s)}{\alpha\lambda_1\lambda_2 - (\lambda_1 + s) (\lambda_2 + s)}$$

and the Laplacian of the probability density function of the system age by

$$\widehat{f}_A(s) = \frac{\lambda_1\lambda_2 (\alpha - 1) (\alpha\lambda_1 + \lambda_2 + s)}{(\alpha\lambda_1 + \lambda_2) (\alpha\lambda_1\lambda_2 - (\lambda_1 + s) (\lambda_2 + s))}.$$

The expected values are given by

$$\mathbb{E}[T] = -\frac{\alpha\lambda_1 + \lambda_2}{\lambda_1\lambda_2 (\alpha - 1)}$$

and

$$\mathbb{E}[A] = -\frac{\alpha\lambda_1 (\lambda_1 + \lambda_2) + \lambda_2 (\alpha\lambda_1 + \alpha\lambda_2 - \lambda_2 (\alpha - 1))}{\lambda_1\lambda_2 (\alpha - 1) (\alpha\lambda_1 + \lambda_2)},$$

respectively.

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Hiermit erkläre ich,

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Jena, den Holger Metzler