APPROXIMATIONS OF KOOPMAN OPERATOR SEMIGROUPS

A Dissertation

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Mathematics

by
Ibrahem M. AL Jabea
B.S., Al al-Bayt University, 2005
M.S., Louisiana State University, 2022
May 2025

Acknowledgments

I sincerely thank my advisors, Dr. Frank Neubrander and Dr. Mustafa Hajij, for their patience, guidance, and support throughout my graduate studies. Their knowledge and experience have been invaluable to my research and growth.

I also appreciate Dr. James Oxley for his mentorship in teaching, as well as Dr. Oliver Dasbach, Dr. Bijaya Karki, and Dr. Harris Wong for serving on my committees and providing valuable feedback.

I am grateful to the Department of Mathematics for its support and resources.

Most of all, I thank my wife, Noujoud, for her endless love and encouragement.

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Abstract

The main purpose of this dissertation is to study approximation methods for nonlinear systems using Bernhard Koopman's Global Linearization Method or Sophus Lie's method of continuous transformation groups. This approach enables the application of linear semigroup methods to a nonlinear system by focusing on the dynamics of the observables of the states, rather than directly studying the dynamics of the states. In this dissertation, we studied the pointwise semigroup and introduce the modified space $C_m(\Omega)$ and the modified Koopman-Lie semigroups. We use a splitting operator and outline a systematic approach for approximating the pointwise Koopman-Lie semigroup flows

$$t \to T(t)g(x) := g(\sigma(t,x)) = e^{t\mathcal{K}}g(x),$$

where $t \to \sigma(t,x) \in \Omega$ is the underlying flow describing the dynamical system, where

$$\mathcal{F}(\Omega,\mathbb{C}) := \{g : \Omega \to \mathbb{C}\}$$

denotes the vector space of all functionals (observations) g from the set Ω into $\mathbb{C}$.

Also, we used a particular simple way of computing $e^{t\mathcal{K}}g(x)$ for measurements g that are eigenfunctions of $\mathcal{K}$ to eigenvalues λ; that is, functions g_λ that satisfy $\mathcal{K}g_\lambda(x) = \lambda g_\lambda(x)$ for all $x \in \Omega$. In this case,

$$T(t)g_\lambda(x) = e^{t\mathcal{K}}g_\lambda(x) = g_\lambda(\sigma(t,x)) = e^{t\lambda}g_\lambda(x).$$

In particular, we investigated the extent to which eigenvalues and eigenfunctions of the linear Koopman-Lie operator, which generates the observations of the underlying nonlinear system, can serve as useful tools for approximating and/or studying the qualitative properties of the underlying nonlinear flow (see [38]).

Chapter 1. Introduction

> "Among all of the mathematical disciplines the theory of differential equations is the most important... It furnishes the explanation of all those elementary manifestations of nature which involve time." —*Sophus Lie*

A dynamical system is a system whose state is determined by a set of variables (state and time variables) and rules (functions). In other words, dynamical systems are described by their trajectories evolving in state space over time. They are generally nonlinear, and this nonlinearity is often a central challenge in analyzing and describing the systems mathematically. However, in contrast to nonlinear systems, the tools used to analyze linear systems are now part of the mathematics curriculum worldwide (e.g., linear algebra, complex analysis, functional analysis, spectral theory, etc.).

Towards the end of the 19th century, several scientists highlighted the impossibility of precisely determining the state of every particle (position, momentum, etc.) within a gas or fluid. Notable figures in this development include Ludwig Boltzmann (1844–1906), Josiah Gibbs (1839–1903), and Henri Poincaré (1854–1912). This insight made it clear that understanding the evolution of macroscopic quantities, such as temperature and pressure, over time was essential. This shift in focus contributed to the development of an alternative framework for dynamical systems, based on the concept of the dynamics of observables — a framework later formalized in quantum mechanics by Heisenberg, Dirac, and von Neumann.

A key element within this framework is the Koopman-Lie operator — a linear operator that effectively captures the dynamics of observations within a dynamical system. By encoding the evolution of observable functions along the trajectories of dynamical systems, the Koopman-Lie operator provides a global linearization of nonlinear systems. This approach enables the study of nonlinear dynamical systems using the tools of linear mathematics, offering a powerful framework for analyzing complex dynamics (see [22] and [23]).

While preparing this dissertation, we came across Gerhard Kowalewski's 1931 book *Introduction to the Theory of Continuous Groups*; see [24]. Kowalewski, a doctoral student of Sophus Lie in the 1890s at the University of Leipzig in Germany, demonstrates that Lie had already employed the concept of flow semigroups and their generators—referred to as Lagrange operators—in his study of ordinary differential equations

$$x'(t) = F(x(t)),$$

where $F = (F_1, \ldots, F_N)$ and $F_i : \mathbb{R}^N \supset \Omega \to \mathbb{R}$. To further emphasize Lie's foundational contributions to the framework later developed by Bernhard Koopman, we will henceforth name key elements of the resulting theory—flows and their generators—after both Bernhard Koopman and Sophus Lie, [27].

In Chapter 3, we will outline a program to approximate pointwise linear Koopman-Lie semigroup flows

$$t \to T(t)g(x) := g(\sigma(t,x)), \tag{1.0.1}$$

where $t \to \sigma(t,x) \in \Omega$ is the underlying flow describing the dynamical system, where

$$\mathcal{F}(\Omega, \mathbb{C}) := \{g : \Omega \to \mathbb{C}\}$$

denotes the vector space of all functionals (observations) g from the set Ω into $\mathbb{C}$. The map $t \to \sigma(t,x) \in \Omega$ is defined for all $0 \leq t < m(x)$, where

$$m(x) = \sup\{T : \sigma(t,x) \in \Omega \text{ for all } 0 \leq t < T\}$$

is the blow-up or escape time of a flow σ in Ω with initial value $\sigma(0,x) = x \in \Omega$ and $\sigma(t,\sigma(s,x)) = \sigma(t+s,x)$ for all $0 \leq t, s, t+s < m(x)$. Throughout this work, if Ω is a topological space, we always assume that $m : x \to m(x)$ is a continuous function from Ω to $(0,\infty]$ or, equivalently, that $1/m$ is continuous from Ω to $[0,\infty)$. For $g \in \mathcal{F}(\Omega,\mathbb{C})$, the flow properties imply that

$$T(0)g(x) = g(x)$$

for all $x \in \Omega$ and

$$T(t)T(s)g(x) = T(t+s)g(x)$$

for all $x \in \Omega_{t+s}$, where

$$\Omega_t := \{x \in \Omega : t < m(x)\}.$$

Moreover, for $x \in \Omega_t$, the map $x \to T(t)g(x)$ is pointwise linear in the sense that

$$T(t)(ag_1 + g_2)(x) = aT(t)g_1(x) + T(t)g_2(x)$$

for all $g_1, g_2 \in \mathcal{F}(\Omega,\mathbb{C})$ and $a \in \mathbb{C}$. Clearly, if the flow is global (i.e., if $m(x) = \infty$ for all $x \in \Omega$), then $T(t)g(x) = g(\sigma(t,x))$ defines a linear operator $T(t)$ with domain and range in $\mathcal{F}(\Omega,\mathbb{C})$, see Section (2.4). However, if the flow is local (i.e., if $m(x) < \infty$ for some $x \in \Omega$), then a pointwise linear Koopman-Lie semigroup flow $t \to T(t)g(x) = g(\sigma(t,x))$ does not fit into any of the classical semigroup theories because $T(t)$ does not define a linear operator with domain and range in a vector space of functions. However, and this is somewhat surprising, the infinitesimal generator

$$\mathcal{K}g : x \to \lim_{t\to 0^+} \frac{T(t)g(x) - g(x)}{t} = \lim_{t\to 0^+} \frac{g(\sigma(t,x)) - g(x)}{t} \tag{1.0.2}$$

is always a well defined linear operator with domain

$$D(\mathcal{K}) := \{g \in \mathcal{F}(\Omega, \mathbb{C}) : \text{limit in (1.0.2) exists for all } x \in \Omega\}$$

and range in $\mathcal{F}(\Omega, \mathbb{C})$. Formally, $\mathcal{K}$ is given by

$$\mathcal{K}g(x) = T'(0)g(x) = g'(x) \cdot \sigma'(0, x). \tag{1.0.3}$$

and

$$T(t)g(x) = e^{t\mathcal{K}}g(x) = g(\sigma(x, t))$$

for all $x \in \Omega$ and $0 \leq t < m(x)$.

Since the semigroup flow is generated by the Koopman-Lie operator $\mathcal{K}$, and as we will see below, since $\mathcal{K}$ can often be decomposed into a sum of operators $\mathcal{K} = \mathcal{K}_1 + \cdots + \mathcal{K}_n$, we suggest using operator splitting methods to approximate $e^{t\mathcal{K}}g(x) = g(\sigma(x, t)) = e^{t(\mathcal{K}_1 + \cdots + \mathcal{K}_n)}g(x)$; e.g., exponential splitting based on standard product formulas such as the Lie-Trotter and Strang product formulas or via composition methods by F. Castella, P. Chartier, S. Descombes, G. Vilmart as well as E. Hansen and A. Ostermann (see [18] and [44]), which allow us to approximate $e^{t\mathcal{K}}g(x)$ in terms of the explicitly computable semigroups $e^{t\mathcal{K}_i}g(x)$. Furthermore, we will indicate a particular simple way of computing $e^{t\mathcal{K}}g(x)$ for measurements g that are eigenfunctions of $\mathcal{K}$ to eigenvalues λ; that is, functions g_λ that satisfy $\mathcal{K}g_\lambda(x) = \lambda g_\lambda(x)$ for all $x \in \Omega$. In this case,

$$e^{t\mathcal{K}}g_\lambda(x) = g_\lambda(\sigma(t, x)) = e^{t\lambda}g_\lambda(x).$$

We will provide several examples that show how $\sigma(t, x)$ can be determined by the knowledge of $g_\lambda(\sigma(t, x)) = e^{t\lambda}g_\lambda(x)$ for sufficiently many eigenfunctions g_λ. Also, as shown in [38], the eigenvalues of the Koopman-Lie operator $\mathcal{K}$ provide information that is useful for the stability analysis of the underlying dynamical system. For example, in certain spaces $\mathcal{M}$ of observations, finite-time blow-up occurs if and only of $\mathcal{K}$ has a positive eigenvalue. Information about an underlying dynamical system can be captured by selecting an appropriate functional space $\mathcal{F}(\Omega, \mathbb{R})$. As shown in [3], for a subset $\Omega \subset \mathbb{R}^N$, a sequence $\{x_n\}$ converges to x as $n \to \infty$ if and only if

$$g(x_n) \to g(x) \quad \text{for all } g \in C_b(\Omega, \mathbb{R}).$$

This result provides a characterization of convergence in terms of functionals (generalized observables), allowing the analysis of the underlying system through the behavior of bounded, continuous functionals.

In Chapter 4, we propose, among others, to study the eigenvalues and eigenvectors of Koopman-Lie operators in detail. In this setting, it is important to notice that we have the freedom to appropriately choose a $T(t)-$invariant subspace $\mathcal{M} \subset \mathcal{F}(\Omega, \mathbb{C})$ of observations. For example, if one can find a finite-dimensional space $\mathcal{M} = \text{span}\{g_1, g_2, \ldots, g_n\}$ that is invariant under $\mathcal{K}$, then the associated finite dimensional representation $\mathcal{K}|_{\mathcal{M}} := \mathbf{K}$ of the Koopman-Lie operator $\mathcal{K}$ will have an eigenvalue with an eigenfunction in $\mathcal{M}$, and the matrix exponential $e^{t\mathbf{K}}g$ can be computed explicitly for all $g \in \mathcal{M}$.

Some of our research focuses on the existence and Koopman-Lie eigenfunctions, specifically identifying and investigating the existence of finite-dimensional invariant subspaces $\mathcal{M} \subset \mathcal{F}(\Omega, \mathbb{C})$ of observations, and, in particular, identifying such subspaces as "Koopman-Lie eigenfunctions" for nonlinear systems of ODEs. We propose to analyze an algorithm we constructed for computing finite-dimensional invariant subspaces $\mathcal{M}$ of observations and explicit Koopman-Lie eigenfunctions for a variety of nonlinear systems of ODEs, particularly in two dimensions, with the potential for generalization to higher dimensions. This algorithm requires a well-chosen initial library of observables $g \in \mathcal{F}(\Omega, \mathbb{C})$, and it is the focus of our investigations to determine under which conditions our algorithm will be able to explicitly compute a sufficient number of Koopman-Lie eigenfunctions in finite time.

Chapter 2. Koopman-Lie Semigroups

> " The purpose of mathematics is not to find the truth, but to find the best possible description of the truth."
> —*Bernard Koopman*

Let X be a real or complex vector space. A *semigroup* is a family of linear maps $T(t) : X \to X$ $(t \geq 0)$ that satisfy

(1) $T(0) = I$,

(2) $T(t + r) = T(t)T(r)$ for all $t, r \geq 0$.

If the property (2) holds only for $0 \leq t, r, t + r \leq T$ for some $T > 0$, then the semigroup is called *local*, For example, let $g \in C[0, 1]$ and define

$$T(t)g(x) = g\left(\frac{x}{1 - xt}\right), \quad \text{for } 0 \leq x \leq 1 \text{ and } 0 \leq t < 1.$$

Then, $T(t)$ defines a local semigroup for $0 \leq t < 1$.

As we will see below, such semigroups appear, for example, in the context of Koopman's global linearization of nonlinear evolutionary processes. To explain this in more detail, we will introduce in the following sections the notions of a flow, the associated semigroups (semigroup flows), and their Koopman-Lie generators.

2.1. Flows

Let Ω be a nonempty set, $\phi \neq I \subseteq \mathbb{R}$ a time interval, and $\Omega_I = I \times \Omega$. We assume that for each $(s, x) \in \Omega_I$ there exists a stopping time $m(s, x) \in (0, \infty]$ such that $[s, s + m(s, x)) \subset I$ and a function

$$\gamma(\cdot) = \gamma_{(s,x)}(\cdot) = \gamma(\cdot + s\ , s, x) : [0, m(s, x)) \to \Omega \tag{2.1.1}$$

that satisfies

(1) $\gamma(s, s, x) = x$, and

(2) $\gamma(t+r+s, r+s, \gamma(r+s, s, x)) = \gamma(t+r+s, s, x)$

for all $0 \leq t, r, t+r < m(s,x)$. The function $\gamma(\cdot)$ is called a *flow map* in Ω and the point $(s,x) \in \Omega_I$ is called the initial space-time state. For $0 \leq t < m(s,x)$, $\gamma(t+s,s,x) \in \Omega$ represents the state of a system and

$$(t+s, \gamma(t+s,s,x) \in \Omega_I$$

represents the space-time state after time t has passed. A *flow*

$$\Psi := \{\gamma(\cdot + s, s, x) : [0, m(s,x)) \to \Omega \mid \ (s,x) \in \Omega_I\} \tag{2.1.2}$$

is the family of all flow maps γ in Ω and the ordered pair (Ω_I, Ψ) is called a *deterministic system*.

A flow map $\gamma(\cdot)$ is said to be time-autonomous if there exists $s_0 \in I$ such that $m(s_0, x) = m(s,x)$ and

$$\gamma(t+s, s, x) = \gamma(t+s_0, s_0, x)$$

for all $(s,x) \in \Omega_I$ and $0 \leq t \leq m(s,x) = m(s_0,x) := m(x)$.

For a time-autonomous flow, define

$$\sigma(t,x) := \gamma(t+s_0, s_0, x)$$

for $x \in \Omega$ and $0 \leq t < m(x)$. Then $\sigma(0,x) = x$ for all $x \in \Omega$. Also, if $x \in \Omega$ and $0 \leq t, r, t+r < m(x)$, then it follows from (2) that

$$\begin{aligned}\sigma(t, \sigma(s,x)) &= \gamma(t+s_0, s_0, \sigma(s,x)) = \gamma(t+s_0, s_0, \gamma(s+s_0, s_0, x)) \\ &= \gamma(t+s+s_0, s+s_0, \gamma(s+s_0, s_0, x)) \\ &= \gamma(t+s+s_0, s_0, x) = \sigma(t+s, x).\end{aligned}$$

This leads to the following definition. Let Ω be a non-empty set. Assume that for each $x \in \Omega$ there exists a $m(x) \in (0, \infty]$ and a function

$$\sigma(\cdot, x) : [0, m(x)) \to \Omega$$

such that, for all $x \in \Omega$ and $0 \leq t, r, t + r < m(x)$,

$$\sigma(0, x) = x \text{ and } \sigma(t, \sigma(r, x)) = \sigma(t + r, x). \tag{2.1.3}$$

Then $t \to \sigma(t, x)$ is called a *time-autonomous flow map* in Ω with initial state $x \in \Omega$. Moreover,

$$\Sigma := \{\sigma(\cdot, x) : [0, m(x)) \to \Omega \mid \sigma(0, x) = x;\ x \in \Omega\}$$

is called an autonomous flow in Ω and the ordered pair (Ω, Σ) is called an *autonomous deterministic system.*

Let $I := [a, \infty)$ be a time interval. Then every autonomous flow $\sigma(\cdot, x) : [0, m(x)) \to \Omega$ induces a flow

$$\gamma = \gamma(\cdot + s, s, x) : [0, m(s, x)) \to \Omega$$

by defining $m(s, x) := m(x)$ and $\gamma(\cdot + s, s, x) := \sigma(\cdot, x)$ for all $(s, x) \in \Omega_I$. Conversely, the next proposition shows that every flow Ψ can be represented as an autonomous flow in the "larger" space-time set $\Omega_I := \Omega \times I$.

Proposition 2.1.1. *Let Ω be a non-empty set, $\phi \neq I \subseteq \mathbb{R}$ an interval, $\Omega_I = I \times \Omega$, $(s, x) \in \Omega_I$ and let (Ω_I, Ψ) be a deterministic dynamical system with flow maps $t \to \gamma(t + s, s, x) \in \Omega$ for $(s, x) \in \Omega_I$ and $t \in [0, m(s, x))$. Then*

$$t \to \sigma(t, \bar{x_s}) = \sigma(t, (s, x)) := (t + s, \gamma(t + s, s, x)) \in \Omega_I \tag{2.1.4}$$

is a time-autonomous flow in Ω_I *with initial space-time state* $\bar{x_s} := (s,x) \in \Omega_I$ *and* $t \in [0, m(\bar{x_s}))$, *where* $m(\bar{x_s}) := m(s,x)$.

Proof. Obviously, $\sigma(0,\bar{x_s}) = (s, \gamma(s,s,x)) = (s,x) = \bar{x_s}$ for all $\bar{x_s} \in \Omega_I$. Moreover,

$$\begin{aligned}
\sigma(t, \sigma(r, \bar{x_s})) &= \sigma(t, (r+s, \gamma(r+s, s, x))) \\
&= (t+r+s, \gamma(t+r+s, r+s, \gamma(r+s, s, x))) \\
&= (t+r+s, \gamma(t+r+s, s, x)) \\
&= \sigma(t+r, (s,x)) = \sigma(t+r, \bar{x_s})
\end{aligned}$$

for $\bar{x_s} = (s,x) \in \Omega_I$ and $0 \le t, r, t+r < m(s,x)$. □

Because of Proposition 2.1.1, we will henceforth restrict our attention to autonomous dynamical systems. Nevertheless, we will highlight examples where the autonomous flow arises from an arbitrary flow via (2.1.4).

2.2. The Koopman-Lie Global Linearization Approach

Let (Ω, Σ) be an autonomous deterministic system, let Z be a complex vector space of observations, and let

$$\mathcal{F} = \mathcal{F}(\Omega, Z) := \{g : \Omega \to Z\}$$

be the complex vector space of Z-valued measurements (functionals) of the states in Ω (observables). For $x \in \Omega$, $g \in \mathcal{F}$, $\sigma \in \Sigma$, and $0 \le t < m(x)$ we define

$$T(t)g(x) := g(\sigma(t,x)). \tag{2.2.1}$$

Then, for $0 \le t < m(x)$, $t \to T(t)g(x) = g(\sigma(t,x)) \in Z$ is the observation under g of the flow map $t \to \sigma(t,x) \in \Omega$ with initial state $x \in \Omega$ at $t = 0$. The key of Koopman's and Lie's approach is that, for $g \in \mathcal{F}(\Omega, Z)$ the functions $t \to T(t)g(x)$ $(x \in \Omega, 0 \le t < m(x)$

define a *pointwise linear semigroup flow.* That is, if $x \in \Omega$, $0 \leq t, h, t+h < m(x)$, $f, g \in \mathcal{M}$, and $\lambda \in \mathbb{C}$, then the following " pointwise exponential properties " hold:

(1) $T(0)g(x) = g(x)$,

(2) $T(t+h)g(x) = T(t)T(h)g(x)$, and

(3) $T(t)[\lambda \cdot g + f](x) = \lambda \cdot T(t)g(x) + T(t)f(x)$.

The key property of the stopping time $m(x) = \sup\{T > 0 : \sigma(t,x) \in \Omega \text{ for all } 0 \leq t < T\}$ of a flow in the study of pointwise linear semigroup flows is as follows

Proposition 2.2.1. *Let* (Ω, Σ) *be an autonomous deterministic system with stopping time* $m(x) = \sup\{T > 0 : \sigma(t,x) \in \Omega\ , 0 \leq t < T\}$. *Then*

$$m(\sigma(t,x)) = m(x) - t$$

for all $x \in \Omega$ *and* $0 \leq t < m(x)$. *Moreover, if* $m_{inf} := \inf\{m(x) : x \in \Omega\}$, *then either* $m_{inf} = 0$ *or* $m_{inf} = \infty$.

Proof. Suppose that there exists $x \in \Omega$ such that $0 < m(x) < \infty$. Let $0 \leq t_0 < m(x)$ and define $\bar{x} := \sigma(t_0, x) \in \Omega$. Then $\sigma(t, \bar{x}) = \sigma(t, \sigma(t_0, x)) = \sigma(t + t_0, x)$, implies that $m(\bar{x}) = m(x) - t_0$. This shows that either $m_{inf} = 0$ or $m_{inf} = \infty$. □

Clearly, if $m_{inf} = \infty$, then (2.2.1) defines linear operators from the vector space $\mathcal{F}(\Omega, Z)$ into itself, satisfying $T(0) = I$ and $T(t+r) = T(t)T(r)$ for all $t, r \geq 0$. The situation is more elaborate if $m_{inf} = 0$. In this case, for all $g \in \mathcal{F}(\Omega, Z)$ and all $t > 0$, the function $h : x \to T(t)g(x) = g(\sigma(t,x))$ is not in $\mathcal{F}(\Omega, Z)$ since h is not defined for $x \in \Omega$ for which $m(x) < t$. That is, if $m_{inf} = 0$, then $T(t)g \notin \mathcal{F}$, for all $g \in \mathcal{F}$. To overcome this obstacle, there are two ways to proceed. The first way is to use time-dependent domains $\Omega_t := \{x \in \Omega : t < m(x)\}$ and investigate $T(t)g(x) := g(\sigma(t,x))$ in terms of linear operators from $\mathcal{F}(\Omega, Z)$ to $\mathcal{F}(\Omega_t, Z)$ where $\Omega_t \subset \Omega_s \subset \Omega_0 = \Omega$ if $t \geq s \geq 0$. The second way is to consider the modified Koopman-Lie semigroup

$$T(t)g(x) = \begin{cases} g(\sigma(t,x)) & 0 \leq t < m(x), \\ \\ 0 & t \geq m(x). \end{cases} \tag{2.2.2}$$

on the modified space $\mathcal{F}_m(\Omega, Z)$, which will be defined in Section 2.4.

In either way, the exponential properties, (i) and (ii) suggest that $t \to T(t)g(x) = e^{t\mathcal{K}}g(x)$, where $\mathcal{K}g(x) = T'(0)g(x)$. Since Z is a Banach space, one can define the linear operator $\mathcal{K}$ with domain and range in $\mathcal{F}(\Omega, Z)$ by

$$\mathcal{K}g : x \to \lim_{t \to 0^+} \frac{T(t)g(x) - g(x)}{t} = \lim_{t \to 0^+} \frac{g(\sigma(t,x)) - g(x)}{t} \tag{2.2.3}$$

for $g \in D(\mathcal{K}) := \{g \in \mathcal{F} : \text{limit in (2.2.3) exists for all}\, x \in \Omega\}$.

The linear operator $\mathcal{K} : D(\mathcal{K}) \subset \mathcal{F} \to \mathcal{F}$ is called the *generator* of the pointwise linear semigroup flow $t \to T(t)g(x) = g(\sigma(t,x))$ or the *Koopman-Lie generator* of the flow $t \to \sigma(t,x)$. It is important to note that the Koopman-Lie generator $\mathcal{K}$ is a well defined linear operator on $\mathcal{F}$ (possibly with trivial domain) even if $m_{inf} = \inf\{m(x) : \ x \in \Omega\} = 0$.

In the literature, semigroups and Koopman-Lie semigroups for which $m_{inf} = \infty$ are well studied on $T(t)$-invariant subspaces of $\mathcal{M} \subset \mathcal{F}(\Omega, Z)$; see, for example, [9], [10], [12], [25], [36]. This is less true for Koopman-Lie semigroups for which $m_{inf} = 0$. To our knowledge, aside from [37], [38], [39], pointwise linear semigroup flows with $m_{inf} := \inf\{m(x) : x \in \Omega\} = 0$ have not yet been systematically studied as operators from $\mathcal{F}(\Omega, Z)$ into $\mathcal{F}(\Omega_t, Z)$. The same is true for local semigroups $\{T(t) : 0 \leq t < T\}$, pointwise linear semigroup flows $t \to T(t)g(x) = g(\sigma(t,x))$, and modified Koopman-Lie semigroups (2.2.2).

As mentioned earlier, instead of considering the operators $T(t)$ acting on $\mathcal{F}(\Omega, Z)$ with range in $\mathcal{F}(\Omega, Z)$ (if $m_{inf} = \infty$) or $\mathcal{F}(\Omega_t, Z)$ (if $m_{inf} = 0$), one could as well take a subspace $\mathcal{M} \subset \mathcal{F}(\Omega, Z)$ or $\mathcal{M}_t \subset \mathcal{F}(\Omega_t, Z)$ that is measurement-invariant (or equivalently, $T(t)$-invariant). That is, for $t \geq 0$, and $g \in \mathcal{M}$. The measurement $x \to T(t)g(x) = g(\sigma(t, x)) \in \mathcal{M}$. It should be observed that by introducing the concept of $T(t)$-invariant function spaces $\mathcal{M}$ of $\mathcal{F}(\Omega, \mathbb{C})$, we can consider classical function spaces like $C_b(\Omega)$ if Ω is a topological space or even a finite-dimensional vector space $\mathcal{M} = \{g_1, g_2, \cdots, g_n\}$ for some $g_i \in \mathcal{F}(\Omega, Z)$.

As noted above, the exponential properties (1), (2) and (3) suggest that a pointwise linear semigroup flow $t \to T(t)g(x) = g(\sigma(t, x))$ may be represented as

$$T(t)g(x) = e^{t\mathcal{K}}g(x), \tag{2.2.4}$$

where $e^{t\mathcal{K}}g(x)$ is computable via one of the many representations of the exponential function. For example, if $\mathcal{K}$ would be a bounded linear operator, then possible representations of the exponential function $t \to e^{t\mathcal{K}}$ are given by the Taylor expansion

$$e^{t\mathcal{K}}g(x) = \sum_{n=0}^{\infty} \frac{t^n}{n!}\mathcal{K}^n g(x),$$

(this approach was taken by Sophus Lie in the development of the theory of Lie series) or by the Chernoff product formula

$$e^{t\mathcal{K}}g(x) = \lim_{n\to\infty} r\left(\frac{t\mathcal{K}}{n}\right)^n g(x),$$

where r is a smooth function with $r(0) = r'(0) = 1$, or by

$$e^{t\mathcal{K}}g(x) = \frac{1}{2\pi i}\int_{\Gamma} e^{t\lambda}(\lambda I - \mathcal{K})^{-1}g(x)\, d\lambda,$$

where Γ is a closed path around the spectrum of $\mathcal{K}$.

As mentioned above, the literature covers many classes of linear operators $\mathcal{K}$ for which $e^{t\mathcal{K}}g(x)$ can be defined in a mathematically rigorous way (e.g., generators of semigroups that are uniformly continuous, strongly continuous, bi-continuous, equi-continuous on locally convex spaces, integrated semigroups, distribution semigroups, etc.). However, for many Koopman-Lie generators $\mathcal{K}$ it remains an open problem in what sense the identify (2.2.4) is valid. One of the goals of my dissertation research to investigate how the pointwise linear semigroup flow $t \to T(t)g(x) = e^{t\mathcal{K}}g(x) = g(\sigma(t,x))$ can be approximated in terms of the Koopman-Lie generator $\mathcal{K}$.

Example 2.2.2. [Sophus Lie]. Let $F : \mathbb{R}^N \to \mathbb{R}^N$ be given by $F = (F_1, ..., F_N)$ where $F_i : \mathbb{R}^N \to \mathbb{R}$ and assume that $x'(t) = F(x(t))$, $x(0) = x \in \Omega \subset \mathbb{R}^N$ has a unique classical solution $\sigma(t,x) := x(t)$ for all $x \in \Omega$ and $0 \le t < m(x)$. Then it is easy to see that $t \to \sigma(t,x) := x(t)$ defines an autonomous flow and that the corresponding Koopman-Lie generator, see (2.2.3), of the pointwise linear semigroup flow $T(t)g(x) := g(\sigma(t,x))$ is formally given by

$$\begin{aligned}\mathcal{K}g(x) :=& \lim_{t\to 0} \frac{g(\sigma(t,x)) - g(x)}{t} = \frac{dg(\sigma(t,x))}{dt}\bigg|_{t=0} \\ =& \dot{g}(\sigma(t,x)) \cdot \dot{\sigma}(t,x)\bigg|_{t=0} = \dot{g}(x(0)) \cdot F(x(0)) = \dot{g}(x) \cdot F(x) \\ =& \sum_{i=1}^{N} \frac{\partial g}{\partial x_i}(x) \cdot F_i(x) = \sum_{i=1}^{N} \mathcal{K}_i g(x),\end{aligned} \tag{2.2.5}$$

where $\mathcal{K}_i g(x) = \frac{\partial g}{\partial x_i}(x) \cdot F_i(x)$ generates the semigroup

$$e^{t\mathcal{K}_i}g(x) = g(x_1, ..., x_{i-1}, \sigma_i(t, x_i), x_{i+1}, ..., x_N), \tag{2.2.6}$$

and where $\sigma_i(t, x_i)$ solves the one-dimensional, separable equation

$$\dot{u}(t) = F_i(x_1, x_2, ..., x_{i-1}, u(t), x_{i+1}, ..., x_N) \text{ with } u(0) = x_i. \tag{2.2.7}$$

As Example 2.2.2 shows, for flows $t \to \sigma(t, x)$ induced by solutions of ordinary differential equation $x'(t) = F(x(t))$, $x(0) = x \in \Omega$, the induced pointwise linear semigroup flow $t \to T(t)g(x) = g(\sigma(t, x))$ has a formal Koopman-Lie generator $\mathcal{K}$ that splits into a sum of one-dimensional Koopman-Lie generators $\mathcal{K}_i$, i.e,

$$\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2 + ... + \mathcal{K}_N.$$

Since formally,

$$T(t)g(x) = e^{t\mathcal{K}}g(x) = e^{t(\mathcal{K}_1+\mathcal{K}_2+...+\mathcal{K}_N)}g(x),$$

it is a natural approach to try to compute $T(t)g(x) = g(\sigma(t, x)) = e^{t\mathcal{K}}g(x)$ by using operator splitting formulas like the Lie-Trotter product formula

$$e^{t(\mathcal{K}_1+\mathcal{K}_2+...+\mathcal{K}_N)} = \lim_{n\to\infty}(e^{\frac{t}{n}\mathcal{K}_1}e^{\frac{t}{n}\mathcal{K}_2}...e^{\frac{t}{n}\mathcal{K}_N})^n.$$

In the remainder of this chapter, we will refine this approach to make precise in what sense the pointwise linear semigroup flow

$$t \to T(t)g(x) = e^{t\mathcal{K}}g(x) = g(\sigma(t, x))$$

can be approximated in terms of the Koopman-Lie generator $\mathcal{K}$. To analyze the convergence of such operator splitting methods, we will review some basic facts from the theories of strongly continuous and bi-continuous semigroups and apply them to both global and local pointwise linear semigroup flows.

In Chapter 4, we propose an alternative way to compute $e^{t\mathcal{K}}g(x) = g(\sigma(t,x))$ via finite-dimensional invariant Koopman-Lie subspaces. Instead of working on $\mathcal{F}(\Omega,\mathbb{C})$ or a "large" $T(t)$-invariant subspace thereof, we aim to construct a "small," finite-dimensional subspace $\mathcal{M} \subset D(\mathcal{K}) \subset \mathcal{F}(\Omega,\mathbb{C})$, spanned by linearly independent measurements $\{g_1, g_2, ..., g_n\} \in \mathcal{F}(\Omega,\mathbb{C})$, such that $\mathcal{K}\mathcal{M} \subset \mathcal{M}$.

Example 2.2.3. In cases where the autonomous flow

$$\sigma(t,\bar{x}_s) := (t+s, \gamma(t+s,s,x))$$

is induced by a non-autonomous flow $t \to \gamma(t+s,s,x)$, the pointwise linear operator semigroup flow is given by

$$t \to T(t)g(s,x) = g(t+s,\gamma(t+s,s,x)) \tag{2.2.8}$$

where $0 \le t \le m(s,x)$, $(s,x) \in \Omega_I$, and $g \in \mathcal{M} \subset \mathcal{F}(\Omega_I, Z)$. For such semigroup flows, the Koopman-Lie generator of (2.2.8) is formally given by

$$\begin{aligned}\mathcal{K}g(s,x) &:= \lim_{t\to 0} \frac{T(t)g(s,x) - g(s,x)}{t} \\ &= \lim_{t\to 0} \frac{g(t+s,\gamma(t+s,s,x)) - g(s,x)}{t}\end{aligned} \tag{2.2.9}$$

with domain $D(\mathcal{K}) = \{g \in \mathcal{M} : \mathcal{K}g(s,x) \text{ exists for all } (s,x) \in \Omega_I \text{ and } \mathcal{K}g \in \mathcal{M}\}$. Formally, for $g \in D(\mathcal{K})$,

$$\mathcal{K}g(s,x) = g_s(s,x) + g_x(s,x)\gamma'(s,s,x) = \mathcal{K}_1 g(s,x) + \mathcal{K}_2 g(s,x). \tag{2.2.10}$$

□

In cases where a non-autonomous flow $\gamma(\cdot,s,x) := x(\cdot)$ is induced by the unique solution of the non-autonomous system

$$x'(t) = F(t,x(t)),\ x(s) = x \in \mathbb{R}^{\mathbb{N}}\ (t \ge s) \tag{2.2.11}$$

for some $F : \mathbb{R}^{N+1} \to \mathbb{R}^N$, one can define $u(t) := x(t+s)$, $y(t) := t+s$, $w(t) := (y(t), u(t))$ and rewrite (2.2.11) as an autonomous system

$$\begin{aligned} u'(t) &= F(y(t), u(t)),\ u(0) = x \\ y'(t) &= 1, y(0) = s. \end{aligned} \tag{2.2.12}$$

Therefore, $w(t) = (y(t), u(t)) = (t+s, \gamma(t+s, s, x) = \sigma(t, \bar{x}_s)$ is a solution of (2.2.12) $w'(t) = \tilde{F}(w(t))$, $w(0) = \bar{x}_s = (s, x)$, where $\tilde{F}(t, x(t)) = (1, F(t, x(t))$ is a function from $\mathbb{R}^{N+1}$ to $\mathbb{R}^{N+1}$. It follows that the non-autonomous problem (2.2.11) for $F : \mathbb{R}^{N+1} \to \mathbb{R}^N$ can be rewritten as an autonomous problem (2.2.12) for $\tilde{F} : \mathbb{R}^{N+1} \to \mathbb{R}^{N+1}$, and can therefore be solved as outlined in Example 2.2.2.

2.3. Strongly Continuous and Bi-continuous Semigroups

Let X be a complex vector space and $\mathcal{L}(X)$ be the set of bounded linear operators from X into X. A family $\{T(t), t \geq 0\} \subseteq \mathcal{L}(X)$ is called a *strongly continuous semigroup* if

(1) $T(0) = I$,

(2) $T(t+r) = T(t)T(r)$ for all $t, r \geq 0$,

(3) $t \to T(t)x$ is continuous from $[0, \infty)$ into X for each $x \in X$.

If $\{T(t), t \geq 0\} \subset \mathcal{L}(X)$ is a semigroup of linear operators, then the linear operator $\mathcal{A}$ defined by

$$D(\mathcal{A}) = \{x \in X : \lim_{t \to 0^+} \frac{T(t)x - x}{t} := y \text{ exists in } X\},\ \mathcal{A}x := y \text{ for } x \in D(\mathcal{A})$$

is called the generator of the semigroup $\{T(t), t \geq 0\}$.

If the semigroup is strongly continuous, then the domain $D(\mathcal{A})$ is dense in X, $\mathcal{A}$ is a closed linear operator, and there exists $w \in \mathbb{R}$ such that $\lambda I - \mathcal{A}$ is invertible for all $\lambda \in \mathbb{C}$ with $Re(\lambda) > w$ (see [11]). Also, it is well known that all strongly continuous semigroups are *exponentially bounded*; i.e., if (1)-(3) hold, then there exist $M \geq 1$ and $\omega \in \mathbb{R}$ such that $\|T(t)\| \leq Me^{\omega t}$ for all $t \geq 0$, (see, e.g [11], page 39).

The following result presents the fundamental properties of strongly continuous semigroups; for more details, refer to [11] and [15].

Proposition 2.3.1. *Let $(\mathcal{A}, D(\mathcal{A}))$ be the generator of a strongly contiuous semigroup T. Then the following are valid.*

(1) The semigroup T commutes with $\mathcal{A}$ on $D(\mathcal{A})$ and, for all $t \geq 0$,

$$T(t)x - x = \begin{cases} \mathcal{A}\int_0^t T(s)xds & \text{if } x \in X \\ \int_0^t T(s)\mathcal{A}xds & \text{if } x \in D(\mathcal{A}). \end{cases} \tag{2.3.1}$$

(2) $(\mathcal{A}, D(\mathcal{A}))$ is a closed linear operator and $D(\mathcal{A})$ is dense in X.

The following example shows that qualitative properties of a pointwise linear semigroup flow rely heavily on the choice of the space $\mathcal{M} \subseteq \mathcal{F}(\Omega, Z)$.

Example 2.3.2. Let $\Omega = \mathbb{R}_+$ and let $t \to \sigma(t, x) = t + x$ be the unique solution of $x'(t) = 1$ with initial $x(0) = x \in \Omega$. Then, $m_{inf} = \inf\{m(x); x \in \Omega\} = \infty$, and the induced Koopman-Lie semigroup is given by

$$t \to T(t)g(x) = g(\sigma(t, x)) = g(t + x). \tag{2.3.2}$$

This defines a semigroup on $\mathcal{F} = \mathcal{F}(\Omega, \mathbb{C})$ and on all $T(t)$-invariant function spaces $\mathcal{M} \subset \mathcal{F}$. However, while the algebraic semigroup properties, $T(0) = I$, and $T(t + r) = T(t)T(r)$ for all $t, r \geq 0$ hold on all $T(t)$-invariant $\mathcal{M} \subset \mathcal{F}$, the regularity property (3) depends heavily on $\mathcal{M}$. For example,

(1) if $\mathcal{M} := C_0([0, \infty), \mathbb{C}) = \{g \in C_b([0, \infty), \mathbb{C}) : \lim_{x\to\infty} g(x) = 0\}$, then it can be easily seen that the semigroup (2.3.2) is strongly continuous since g vanishes at infinity and is

uniformly continuous on compact intervals.

(2) if $\mathcal{M} := C_b([0,\infty),\mathbb{C})$, then the shift semigroup (2.3.2) is not strongly continuous. This can be seen by taking $g(x) = e^{ix^2}$. Then,

$$\begin{aligned}\|T(t+r)g - T(t)g\| &= \sup_{x\geq 0} |e^{i(t+r+x)^2} - e^{i(t+x)^2}| \\ &= \sup_{x\geq 0} |e^{i(t^2+2tx+2tr+2xr+r^2+x^2)} - e^{i(t^2+2xt+x^2)}| \\ &= \sup_{x\geq 0} |e^{i(2tr+2xr+r^2)} - 1| = 2\end{aligned}$$

for all $t, r \geq 0$. So, $t \to T(t)g$ is nowhere continuous and, therefore, not measurable on $[0,\infty)$ since it is not almost separably valued (see, for example Pettis' Theorem in [1]).

□

The shift semigroup (2.3.2) on $\mathcal{M} := C_b([0,\infty),\mathbb{C})$ is an example of semigroup that is not strongly continuous but "*bi-continuous*". The bi-continuous semigroup framework, introduced by F. Kühnemund in her dissertation [25] at the University of Tübingen, provides an efficient approach to the work of Dorroh, Lovelady, Neuberger, and Sentilles, see [25], [12], and [13]. One of the key features of the bi-continuous semigroup framework is that many important results from the theory of strongly continuous semigroups can be lifted to bi-continuous semigroups.

The shift semigroup (2.3.2) on $\mathcal{M} := C_b([0,\infty),\mathbb{C})$ is bi-continuous in the following sense: for each $t \geq 0$, $T(t)$ is a continuous (bounded) linear operator from the Banach space $\mathcal{M}$ into itself with respect to norm topology on $\mathcal{M}$, while for each $f \in \mathcal{M}$ the map $t \to T(t)f$ from $[0,\infty) \to C_b([0,\infty),\mathbb{C})$ is continuous with respect to the compact-open topology, or equivalently, the topology of uniform convergence on compact sets. This leads to the concept of bi-admissible Banach spaces $(\mathcal{M}, ||\cdot||, \tau)$.

Definition 2.3.3. Let $(X, ||\cdot||)$ be a Banach space and let τ be a topology on X. Then $(X, ||\cdot||, \tau)$ is a bi-admissible Banach space if the following conditions are met:

(i) The topology τ is locally convex and is determined by a directed family of seminorms $\mathcal{P}$ for which $p(x) \leq \|x\|$ for all $x \in X$ and $p \in \mathcal{P}$.

(ii) Any sequence in X that is bounded with respect to the norm $||\cdot||$ and is Cauchy under the topology τ will converge within the space (X, τ).

(iii) The topology τ is Hausdorff and coarser than the $||\cdot||$-topology.

(iv) The space $(X, \tau)^*$ is norming for $(X, ||\cdot||)$; i.e., $||x|| = \sup\{|\mu(x)|\}$, where the supremum is taken over all $\mu \in (X, \tau)' \subset (X, \|\cdot\|)'$ with $\|\mu\| \leq 1$.

Let Ω be a complete, separable, metric space (Polish space) and let $C_b(\Omega)$ denote the Banach space of bounded complex-valued function on Ω equipped with the sup norm $||f||_\infty := \sup_{x\in\Omega} |f(x)|$. Then $C_b(\Omega)$ has an additional locally convex topology β defined as the finest locally convex topology on $C_b(\Omega)$ agreeing with the compact-open topology τ_c on $\|\cdot\|_\infty$-bounded sets, where τ_c is defined by the family of seminorms $\mathbb{P} = \{p_K : K \subseteq \Omega, K \text{ compact }\}$, where $p_K(f) := \sup\{|f(x)| : x \in K\}$.

F. D. Sentilles [47] obtained the following fundamental result in 1972 (see also [25]).

Theorem 2.3.4. *Let Ω be a complete, separable, metric space (Polish space). Then $f_n \in C_b(\Omega)$ converges with respect to β if and only if $\|f_n\|_\infty$ is bounded and f_n converges with respect to τ_c. Moreover, $C_b(\Omega)$ is bi-admissible with respect to $\|\cdot\|_\infty$ and β.*

Locally convex topologies and families of seminorms are closely related. In particular, every locally convex space possesses a separating family of continuous seminorms. Conversely, a separating family of seminorms on a vector space can be used to define a locally convex topology, ensuring that each seminorm is continuous, see Theorems 1.36 and

1.37, [45]. This relationship can be described as follows: Let $\{p_\alpha\}_{\alpha\in I}$ be a family of seminorms on a vector space X, where α is in some index set I. Then $\{p_\alpha\}_{\alpha\in I}$ is called separating if for every $x \in X$ with $x \neq 0$, there exists an $\alpha \in I$ such that $p_\alpha(x) > 0$. Every separating family of seminorms $\{p_\alpha\}_{\alpha\in I}$ defines a locally convex Hausdorff topology σ on X by taking as a base finite intersections of the sets

$$B_{\alpha,n} := \{x \in X \mid p_\alpha(x) < \frac{1}{n}\},$$

where $\alpha \in I$ and $n \in \mathbb{N}$.

For a given separating family of seminorms $\{p_\alpha\}_{\alpha\in I}$, define $X_p := (X, \tau)$ to be X equipped with the locally convex Hausdorff topology τ generated by $\{p_\alpha\}_{\alpha\in I}$. Conversely, for every locally convex Hausdorff topology τ with base B on X, we can construct a separating family of continuous seminorms $\{\mu_V\}_{V\in B}$ by considering the Minkowski functional

$$\mu_V(x) = \inf\{\lambda > 0 \mid x \in \lambda V\},$$

for every $V \in B$. The topology generated by $\{\mu_V\}_{V\in B}$ and τ coincide. Thus, the concept of a bi-admissible Banach space can be reformulated in terms of the seminorms that generate its topology τ.

Definition 2.3.5. Let $(X, \|\cdot\|)$ be a Banach space and let τ be the topology generated by a family of seminorms $\{p_\alpha\}_{\alpha\in I}$ on X. Then $X = (X, \|\cdot\|, \tau)$ is a bi-admissible Banach space if p_α satisfies the following conditions:

(i) $\|x\| = \sup_{\alpha\in I} p_\alpha(x)$ for all $x \in X$.

(ii) Every norm-bounded, p-Cauchy sequence is p-convergent in X.

(iii) $x = 0$ if and only if $p_\alpha(x) = 0$ for all $\alpha \in I$ (separating).

(iv) $(X, \tau)^*$ is norming for $(X, \|\cdot\|)$.

Example 2.3.6. Let X be Banach space. Then$(C_b([0,\infty),X),\|\cdot\|_\infty,\tau_c)$ is bi-admissable Banach space.

Proof. It is well known that $(C_b([0,\infty),X),\|\cdot\|_\infty)$ is Banach space. The seminorms $p_n(f) := \sup_{0\le s\le n}\|f(s)\|$ meet the conditions (i) - (iii) of Definition 2.3.5. Now we show that $(C_b([0,\infty),X),\tau_c)^*$ is norming for $(C_b([0,\infty),X),\|\cdot\|)$. Observe that for all $s \ge 0$ and $x^* \in X^*$ with $\|x^*\| \le 1$, the point evaluations φ_{s,x^*} defined by $\langle f,\varphi_{s,x^*}\rangle := \langle f(s),x^*\rangle$ are contained in $(C_b([0,\infty),X),\tau_c)^*$ and $\|\varphi_{s,x^*}\| \le 1$. The Hahn-Banach Theorem implies that for all $x \in X$, there is an $x^* \in X^*$ with $\|x^*\| = 1$ and $\|x\| = |\langle x,x^*\rangle|$. Now, for all $f \in C_b([0,\infty),X)$, there is a sequence $s_n \ge 0$ and $x_n^* \in X^*$ with $\|x_n^*\| = 1$ such that

$$\|f\| = \sup_n \|f(s_n)\| = \sup_n |\langle f(s_n),x_n^*\rangle| = \sup_n |\langle f,\varphi_{s_n,x_n^*}\rangle|$$

$$\le \sup_{\varphi\in(C_b([0,\infty),X),\tau_c)^*,\|\varphi\|\le 1} |\langle f,\varphi\rangle| \le \sup_{\varphi\in(C_b([0,\infty),X),\|\cdot\|_\infty)^*,\|\varphi\|\le 1} |\langle f,\varphi\rangle| \le \|f\|.$$

Therefore, $(C_b([0,\infty),X),\|\cdot\|_\infty,\tau_c)$ is bi-admissible. □

Having introduced the concept of a bi-admissible Banach space, we can now proceed to introduce the concept of bi-continuous semigroups.

Definition 2.3.7. Let $(X,\|\cdot\|,\tau)$ be a bi-admissible Banach space. An operator family $\{T(t) : t \ge 0\} \subseteq \mathcal{L}(X)$ is a bi-continuous semigroup with respect to τ and of type ω if the following conditions hold:

(i) $T(0) = I$ and $T(t+s) = T(t)T(s)$ for all $s,t \ge 0$.

(ii) The operators are exponentially bounded, i.e.; $\|T(t)\| \le Me^{\omega t}$ for all $t \ge 0$ and some constants $M \ge 1$ and $\omega \in \mathbb{R}$.

(iii) The map $t \to T(t)f$ $(t \ge 0)$ is strongly τ-continuous for each $f \in X$.

(iv) $T(t)$ is locally bi-equicontinuous, where for every τ-convergent null sequence $f_n \subset X$, $\tau\text{-}\lim_{n\to\infty} T(t)f_n = 0$ uniformly for t in compact intervals of $\mathbb{R}_+$.

The following definition is required to outline the main properties of bi-continuous semigroups and their generators.

Definition 2.3.8. Let $(X, \|\cdot\|, \tau)$ be a bi-admissible Banach space.

(a) A subset $D \subset X$ is called bi–dense if for every $g \in X$ there exists a $\|\cdot\|$-bounded sequence $g_n \in D$ which is τ–convergent to g.

(b) An operator $(\mathcal{K}, D(\mathcal{K}))$ is called bi-closed, if for all sequences $g_n \in D$ with $\sup_{n\in\mathbb{N}}\{\|g_n\|, \|\mathcal{K}g_n\|\} < \infty$, $\tau - \lim g_n = g$, and $\tau - \lim \mathcal{K}g_n = f$, we have $g \in D(\mathcal{K})$ and $\mathcal{K}g = f$.

(c) The generator $(\mathcal{K}, D(\mathcal{K}))$ of a bi-continuous semigroup $T(t)$ on X is given by

$$\mathcal{K}g := \tau - \lim_{t\to 0^+} \frac{T(t)g - g}{t}$$

for all $g \in D(\mathcal{K}) := \{g \in X : \tau - \lim_{t\to 0^+} \frac{T(t)g-g}{t} \text{ exists}, \sup_{0<t\leq 1}\{\frac{\|T(t)g-g\|}{t}\} < \infty\}$.

In the following, we review some key results from the theory of bi-continuous semigroups. The bi-continuous semigroup framework, introduced by F. Kühnemund in her dissertation [25] at the University of Tübingen, provides an efficient approach to the work of Dorroh, Lovelady, Neuberger, and Sentilles, see [25], [12], and [13].

Theorem 2.3.9. *Let $(\mathcal{K}, D(\mathcal{K}))$ be the generator of a bi–continuous semigroup $T(t)$ of type ω on a bi-admissible Banach space $(X, \|\cdot\|, \tau)$. Then the following properties hold.*

(i) The generator $(\mathcal{K}, D(\mathcal{K}))$ is bi-closed and the domain $D(\mathcal{K})$ is bi-dense.

(ii) All $\lambda \in \mathbb{C}$ with $\Re(\lambda) > \omega$ are in the resolvent set of $\mathcal{K}$ (therefore $\mathcal{K}$ is closed) and,

for all $g \in X$,

$$R(\lambda, A)g = \tau - \int_0^\infty e^{-\lambda t} T(t)g\, dt.$$

(iii) Let X_0 *be the norm-closure of* $D(\mathcal{K})$. *Then* X_0 *is* $T(t)$*–invariant and the restriction of* $T(t)$ *to* X_0 *is a strongly continuous semigroup generated by the part of* $\mathcal{K}$ *in* X_0.

Proof. For a proof, see [25]. □

Theorem 2.3.4 immediately yields the following corollary (see also [12]).

Corollary 2.3.10. *Let* Ω *be a complete, separable, metric space (Polish space). An operator family* $\{T(t) : t \geq 0\} \subseteq \mathcal{L}(C_b(\Omega))$ *is a bi-continuous semigroup with respect to* β *and of type* ω *if and only if the following conditions hold:*

(i) $T(0) = I$ *and* $T(t+s) = T(t)T(s)$ *for all* $s, t \geq 0$.

(ii) The operators are exponentially bounded, i.e.; $\|T(t)\| \leq Me^{\omega t}$ *for all* $t \geq 0$ *and some constants* $M \geq 1$ *and* $\omega \in \mathbb{R}$.

(iii) The map $t \to T(t)f$ $(t \geq 0)$ *is strongly* τ_c*-continuous for each* $f \in C_b(\Omega)$).

(iv) $T(t)$ *is locally bi-equicontinuous, where for every norm-bounded,* τ_c*-convergent null sequence* $f_n \in C_b(\Omega)$, *it follows that* $\tau_c\text{-}\lim_{n\to\infty} T(t)f_n = 0$ *uniformly for* t *in compact intervals of* $\mathbb{R}_+$.

Proof. See, [12]. □

In the following example, we will use Corollary 2.3.10 to show that the shift semigroup is bi-continuous.

Example 2.3.11. The shift semigroup $T(t)f := f(t+\cdot)$, $f \in C_b([0,\infty),\mathbb{C})$ is a bi-continuous semigroup. To see this, observe that $C_b([0,\infty),\mathbb{C})$ is bi-admissible and that the properties (i) and (ii) of Definition 2.3.7 are satisfied. Let $f \in C_b([0,\infty),\mathbb{C})$, $\epsilon > 0$, and $M > 0$. Since f is uniformly continuous on $[0, M]$, if follows from

$$\sup_{0\leq x<M} |T(t)f(x) - f(x)| = \sup_{0\leq x<M} |f(x+t) - f(x)|$$

that there is a $\delta > 0$ such that, for all $0 \leq t < \delta$, $\sup\limits_{0\leq x<M} |T(t)f(x) - f(x)| < \epsilon$. Thus, the map $t \to T(t)f$ is strongly τ_c-continuous from $[0,\infty)$ into $C_b([0,\infty),\mathbb{C})$, where τ_c is topology of uniform convergence in a compact subset of $[0,\infty)$. Now, we prove item (iv) of Corollary 2.3.10. Let f_n be a norm-bounded sequence in $C_b([0,\infty),\mathbb{C})$ that converges to zero in the τ_c topology (i.e., $||f_n||_\infty \leq C$ for all n, and for every $M > 0$, $\sup_{x\in[0,M]} |f_n(x)| \to 0$ as $n \to \infty$). We need to show that for all $M, T > 0$, we have $\sup\limits_{x\in[0,M]} |T(t)f_n(x)| \to 0$ uniformly in $t \in [0,T]$. This follows directly from the fact that $\sup\limits_{x\in[0,M]} |T(t)f_n(x)| = \sup\limits_{x\in[0,M]} |f_n(t+x)| \leq \sup\limits_{x\in[0,T+M]} |f_n(x)| \to 0$ as $n \to \infty$. □

The Koopman-Lie semigroup $T(t)g(x) := g(\sigma(t,x)$ induced by a jointly continuous and global flow $\sigma : \mathbb{R}_+ \times \Omega \to \Omega$ in a Polish Space Ω may not always be strongly continuous for $g \in C_b(\Omega)$ with respect to the sup-norm. In joint work done by J.R. Dorroh and J.W. Neuberger, Koopman-Lie generators $(\mathcal{K}, D(\mathcal{K}))$ of jointly continuous and global flows on Ω were completely defined, where the graph (g, f) consists of $g, f \in C_b(\Omega)$ for which

$$\mathcal{K}g(x) = f(x) = \lim_{t\to 0^+} \frac{g(\sigma(t,x)) - g(x)}{t} \text{ for all } x \in \Omega.$$

The main result of the joint work of Dorroh and Neuberger [12, 25] concerning jointly continuous, global flows, as follows.

Theorem 2.3.12. [Dorroh-Neuberger]. *Let Ω be a complete, separable, metric space (Polish space) and let $(\mathcal{K}, D(\mathcal{K}))$ be a linear operator on $C_b(\Omega)$. The following are equivalent:*

a) $(\mathcal{K}, D(\mathcal{K}))$ *is the Koopman-Lie generator of a jointly continuous, global flow in* Ω.

b) $(\mathcal{K}, D(\mathcal{K}))$ *is a derivation (i.e.,* $\mathcal{K}(fg) = (\mathcal{K}f)g + f(\mathcal{K}g)$ *for all* $f, g \in D(\mathcal{K})$ *and generates a bi-continuous semigroup with respect to* τ_c *induced by a jointly continuous flow.*

In particular, Koopman-Lie semigroups induced by jointly continuous, global flows in a Polish space Ω *are bi-continuous contractions in* $(C_b(\Omega), \|\cdot\|_\infty, \tau_c)$.

Proof. See [25] and [12]. □

In the following example, we will demonstrate how to prove the bi-continuous semigroup property using Definition 2.3.7 and Theorem 2.3.12.

Example 2.3.13. Consider

$$x'(t) = -x(t)^2, \quad t \geq 0, \quad x(0) = x \in \Omega = [0, \infty),$$

with unique, jointly continuous, global solution $\sigma(t, x) = \frac{x}{1+tx} \in \Omega$. The Koopman-Lie semigroup is given by

$$T(t)g(x) = g(\sigma(t, x)) = g\left(\frac{x}{1 + tx}\right) \tag{2.3.3}$$

with generator $\mathcal{K}g(x) = -x^2 g'(x)$. It follows from the Dorroh-Neuberger Theorem 2.3.12 that the Koopman-Lie semigroup is bi-continuous in $(C_b([0, \infty), \|\cdot\|_\infty, \tau_c)$.

The map $t \to T(t)g$ is continuous as a map from $[0, \infty)$ into $C_b([0, \infty), \mathbb{C})$ endowed with the topology of uniform convergence on compact subsets of $[0, \infty)$. For any compact subset $[0, M] \subset [0, \infty)$, the condition $\sup_{x \in [0,M]} |T(t)g(x) - g(x)| \to 0$ as $t \to 0^+$ is satisfied. Since $g \in C_b([0, \infty), \mathbb{C})$ is uniformly continuous on compact subset $[0, M]$, for all $\epsilon > 0$, there exists $\delta > 0$ such that $|g(y) - g(x)| \leq \epsilon$ whenever $|y - x| < \delta$ for all $x, y \in [0, M]$. We have

$$|\sigma(t, x) - x| = \left| \frac{x}{1 + tx} - x \right| = \frac{tx^2}{1 + tx} \leq tx^2 \leq tM^2.$$

For sufficiently small $t < \frac{\delta}{M^2}$, we have $tM^2 < \delta$. By the uniform continuity of g on $[0, M]$, we get

$$|T(t)g(x) - g(x)| = \left| g\left(\frac{x}{1 + tx} \right) - g(x) \right| < \epsilon$$

for all $x \in [0, M]$ and $t < \frac{\delta}{M^2}$. Thus, we have shown that $t \to T(t)g$ is a continuous map from $[0, \infty)$ into $C_b([0, \infty), \mathbb{C})$ endowed with the topology of uniform convergence on compact subset of $[0, \infty)$. It is obvious that the operators $T(t)$ constitute a semigroup of bounded linear operators with $\|T(t)\| \leq 1$ for $t \geq 0$ on $C_b([0, \infty), \mathbb{C})$. To complete the proof that the semigroup is bi-continuous on $C_b([0, \infty), \mathbb{C})$, we need to prove item (iv) of Definition 2.3.7. That is, we show that $T(t)$ is locally bi-equicontinuous, meaning that for every τ_c-convergent null sequence $g_n \in C_b([0, \infty), \mathbb{C})$, it follows that $\tau_c\text{-}\lim_{n \to \infty} T(t)g_n = 0$ uniformly for t in compact intervals of $\mathbb{R}_+$. For this, let g_n be a τ_c-convergent null sequence in $C_b([0, \infty)], \mathbb{C})$; i.e., for all $M > 0$, $\sup_{z \in [0,M]} |g_n(z)| \to 0$. Since $\frac{x}{1+tx} \in [0, M]$ for all $x \in [0, M]$ and all $t \geq 0$, it follows that

$$\sup_{x \in [0,M], t \geq 0} |T(t)g_n(x)| = \sup_{x \in [0,M], t \geq 0} |g_n(\frac{x}{1 + tx})| \leq \sup_{z \in [0,M]} |g_n(z)| \to 0$$

as $n \to \infty$. Thus, $\tau_c\text{-}\lim_{n \to \infty} T(t)g_n = 0$ uniformly for $t \geq 0$. $\square$

2.4. Modified Koopman-Lie Semigroups

To simplify the notation, let m be a continuous function from Ω to $(0,\infty]$. Alternatively, $m : \Omega \to (0,\infty]$ is such that $\frac{1}{m} : \Omega \to [0,\infty)$ is a continuous function.

Let $x \in \Omega \subset \mathbb{R}^N$ and let $t \to \sigma(t,x)$ be a global flow; $m(x) = \infty$ for all $x \in \Omega$. Then $T(t)g(x) = g(\sigma(t,x))$ defines a linear operator $T(t)$ with a domain and range in $\mathcal{F}(\Omega,\mathbb{C})$ or in a $T(t)$-invariant subspace of $\mathcal{F}(\Omega,\mathbb{C})$. However, if the flow σ is local (i.e., if $m(x) < \infty$ for some $x \in \Omega$), then the pointwise linear Koopman-Lie semigroup flow $t \to T(t)g(x) = g(\sigma(t,x))$ does not fit any of the classical semigroup theories because $m_{inf} = \inf\{m(x), x \in \Omega\} = 0$ (see Proposition 2.2.1) and $g(\sigma(t,x))$ is defined only if $t < m(x)$. For example, consider the IVP

$$x'(t) = 1, \quad x(0) = x \in \Omega := [0,1),$$

with the solution $t \to \sigma(t,x) := x(t) = t + x$ for $0 \leq t < m(x) = 1 - x$. For $g \in C_b[0,1)$,

$$t \to T(t)g(x) := g(t+x), \quad t \in [0, 1-x)$$

is a pointwise linear semigroup flow with Koopman-Lie generator $\mathcal{K}g(x) := T'(0)g(x) = g'(x)$, $D(\mathcal{K}) := \{g \in C_b[0,1) : g' \in C_b[0,1)\}$. Observe that for fixed $t \in [0,1)$ and $g \in C_b[0,1)$, the function

$$h_t : x \to T(t)g(x) = g(x+t)$$

is only defined for $x \in [0, 1-t)$. This implies that the operator $T(t)$ is a bounded linear operator from $C_b[0,1)$ to $C_b[0,1-t)$ but not from $C_b[0,1)$ into itself. To address this situation, we consider the modified space $C_0[0,1) := \{g \in C_b[0,1) \quad | \lim_{x\to 1} g(x) = 0\}$, and the “modified Koopman-Lie semigroup” on $C_0[0,1)$ defined as:

$$T(t)g(x) = \begin{cases} g(x+t) & \text{if } 0 \leq t < m(x) = 1-x, \\ 0 & \text{if } t \geq m(x) = 1-x. \end{cases}$$

Observe that $x \to T(t)g(x)$ is continuous at $x = 1-t$, that $T(t)$ defines a bounded linear semigroup, and

$$\lim_{x\to 1} T(t)g(x) = 0.$$

Thus, for all $t \geq 0$, $T(t)$ is a well-defined bounded linear operator from $C_0[0,1)$ into itself (see also Example 2.4.7).

As a second example, we consider the IVP

$$x'(t) = x(t)^2, \quad t \geq 0, \quad x(0) = x \in \mathbb{R},$$

with the solution $t \to \sigma(t,x) := \frac{x}{1-tx}$ for $t \geq 0$ and stopping time

$$m(x) = \begin{cases} \frac{1}{x} & \text{if } x > 0, \\ \infty & \text{if } x \leq 0. \end{cases}$$

In this situation, if we consider $\Omega := [0,1]$ and take $g \in C[0,1]$, then $T(t)g \in C[0,1]$ for $0 \leq t < 1$, where

$$T(t)g(x) = g\left(\frac{x}{1-xt}\right) \quad \text{for } 0 \leq x \leq 1.$$

Thus, $T(t)$ defines a local semigroup for $0 \leq t < 1$. Let $t \geq 0$ be fixed.

However, if $\Omega := [0,\infty)$, the function

$$T(t)g(x) = g(\sigma(t,x)) = g\left(\frac{x}{1-tx}\right) \tag{2.4.1}$$

is not well-defined on Ω. For example, if $t = \frac{1}{4}$, then 2.4.1 is not defined for $x > 4$. This shows that $T(t)$ as defined in 2.4.1 is not a semigroup of operators on any function space from $\Omega := [0, \infty)$ into $\mathbb{R}$. But, as before, we consider the modified space

$$C_0[0, \infty) := \{g \in C_b[0, \infty) \quad | \lim_{x \to \infty} g(x) = 0\},$$

and the "modified Koopman-Lie semigroup" on $C_0[0, 1)$ defined as:

$$T(t)g(x) = \begin{cases} g(\frac{x}{1-xt}) & \text{if } 0 \leq t < m(x) = \frac{1}{x}, \\ \\ 0 & \text{if } t \geq m(x) = \frac{1}{x}. \end{cases}$$

For fixed $t > 0$, it is clear that $x \to T(t)g(x)$ is continuous at $x = \frac{1}{t}$. Moreover, we have

$$\lim_{x \to \infty} T(t)g(x) = 0.$$

Consequently, $T(t)g \in C_0[0, \infty)$ and $T(t)$ is a well-defined linear operator from $C_0[0, \infty)$ into itself (see also Example 2.4.4).

As a final example, consider the IVP

$$x'(t) = \frac{-1}{2x(t)}, \quad x(0) = x \in \Omega := (0, \infty) \tag{2.4.2}$$

with solution $t \to \sigma(t, x) := \sqrt{x^2 - t} \in (0, \infty)$ for $0 \leq t < m(x) = x^2$. Again, for fixed $t > 0$, the function $x \to T(t)g(x) = g(\sqrt{x^2 - t})$ is not well-defined if $x^2 < t$, and therefore, $T(t)$ is not a semigroup of operators on any function space from $(0, \infty)$ into $\mathbb{R}$. However, as above, on the modified space

$$\widetilde{C_0}(0, \infty) := \{g \in C_b(0, \infty) \quad | \lim_{x \to 0} g(x) = 0\},$$

the corresponding modified Koopman-Lie semigroup can be defined as

$$T(t)g(x) = \begin{cases} g(\sqrt{x^2 - t}) & \text{if } \ 0 \leq t < m(x) = x^2, \\ \\ 0 & \text{if } \ t \geq m(x) = x^2. \end{cases}$$

Then $T(t)g \ \in \ \widetilde{C_0}(0, \infty)$ and it follows that $T(t)$ is a bounded linear operator from $\widetilde{C_0}(0, \infty)$ into itself (see also Example 2.4.9).

For flows with $m_{inf} = \inf\{m(x), x \in \Omega\} = 0$ (i.e., local flows), the Koopman-Lie semigroup $T(t)g : x \to g(\sigma(t, x))$ is defined only for $x \in \Omega_t := \{x \in \Omega : m(x) > t\}$, not for all $x \in \Omega$. However, as the examples above suggest, for local flows it may still be possible to define a modified Koopman-Lie semigroup on appropriately adjusted function spaces $C_m(\Omega)$ that depend on the properties of the flow $\sigma(t, x)$ and its stopping times $m(x)$.

In the rest of this section, we explore whether the proposed modified space $C_m(\Omega)$ is well-defined and functional in different scenarios.

To construct the space $C_m(\Omega)$, we begin with a locally compact $\Omega \subseteq \mathbb{R}^N$; see Appendix A. Define

$$\overline{\Omega}^{\infty} := \begin{cases} \overline{\Omega} & \text{if } \Omega \text{ is bounded,} \\ \\ \overline{\Omega} \cup \{\infty\} & \text{if } \Omega \text{ is unbounded.} \end{cases}$$

A neighborhood of $''\infty''$ is given by $\mathcal{U}_\infty := \{\Omega - K\} \cup \{\infty\}$, where $K \subset \Omega$ is a compact subset of Ω. Let $m : \Omega \to (0, \infty]$ be a continuous function and let the boundary $\partial\Omega$ be defined as

$$\partial(\Omega) := \overline{\Omega}^{\infty} \setminus \text{int}(\Omega).$$

Then the "modified boundary" is defined as

$$\partial_m(\Omega) := \{\tilde{x} \in \partial(\Omega) \mid \exists x_n \in \Omega, \text{ such that } x_n \to \tilde{x} \text{ and } m(x_n) \to 0\} \,. \tag{2.4.3}$$

The modified space $C_m(\Omega)$ can be defined as

$$C_m(\Omega) := \{g \in C_b(\Omega) \mid \lim_{x \to \partial_m(\Omega)} g(x) = 0\}. \tag{2.4.4}$$

It is easy to see that the space $C_m(\Omega)$ is a Banach space when equipped with the supremum norm $\|g\|_\infty := \sup_{x \in \Omega} |g(x)|$, see Appendix A.

2.4.1. Modified Koopman-Lie semigroups on $C_m(\Omega)$

To discuss modified Koopman-Lie semigroups, we need to define joint continuity for a local flow σ with $m_{inf} = 0$.

Definition 2.4.1. Let $\Omega \subseteq \mathbb{R}^N$ be locally compact. A local flow $\sigma : [0, m(x)) \times \Omega \to \Omega$ is said to be jointly continuous if

(1) its stopping time function $m : x \to m(x)$ is continuous from Ω into $(0, \infty]$,

(2) $t \to \sigma(t, x)$ is continuous for $t \in [0, m(x))$ for all $x \in \Omega$, and

(3) $x \to \sigma(t, x)$ is continuous on $\Omega_t = \{x \in \Omega : m(x) > t\}$ for all $t \geq 0$. That is, if $x \in \Omega$, $t > m(x)$, and $x_n \to x$ such that $m(x_n) > t$, then $\sigma(t, x_n) \to \sigma(t, x)$.

Remark 2.4.2. Recall from Proposition 2.2.1 that if $m(x) > t$, then

$$m(\sigma(t, x)) = m(x) - t.$$

Given a local flow $t \to \sigma(t, x)$ with stopping times $m(x)$, the modified pointwise linear semigroup flow is defined as

$$T(t)g(x) := \begin{cases} g(\sigma(t, x)) & 0 \leq t < m(x), \\ 0 & t \geq m(x). \end{cases} \tag{2.4.5}$$

When considering (2.4.5), the first key issue is whether the operators $T(t)$ defined by (2.4.5) map $C_m(\Omega)$ into itself. The following assumption provides a condition on the local flow σ that ensures the modified Koopman-Lie semigroup (2.4.5) maps $C_m(\Omega)$ into itself.

Assumption A : Let $x_n \in \Omega$. Then $|x_n| \to \infty$ if and only if $m(x_n) \to 0$.

Since $m(\sigma(t, x) = m(x) - t$, Assumption A implies the following weaker assumption.

Assumption A* : Let $x_n \in \Omega$. If $m(x_n) > t$ and $m(x_n) \to t$, then $|\sigma(t, x_n)| \to \infty$.

Let $\Omega \subset \mathbb{R}^N$ be locally compact. For local flows in Ω satisfying Assumption A* we will consider, among others, the modified space

$$C_0(\Omega) := \{g \in C_b(\Omega) : \text{ if } x_n \in \Omega \text{ and } |x_n| \to \infty, \text{ then } g(x_n) \to 0\}.$$

Proposition 2.4.3. *Let $\Omega \subseteq \mathbb{R}^N$ be closed and consider a local, jointly continuous flow σ that meets Assumption A*. Then, the modified Koopman-Lie semigroup $\{T(t), t \geq 0\}$ defined by (2.4.5) is a bounded linear operator from $C_0(\Omega)$ into itself.*

Proof. For a fixed $t \geq 0$ and $g \in C_0(\Omega)$, we show that the function $h_t(x) := T(t)g(x) \in C_0(\Omega)$. Let $x_0 \in \Omega$, for $0 \leq t < m(x_0)$, and $r > 0$ there exists a neighborhood

$$U_r(x_0) := \{x \in \Omega \mid d(x, x_0) < r \text{ and } m(x) > t\},$$

where d is the metric defined on Ω. Since the flow σ is jointly continuous and $g \in C_0(\Omega)$, it follows that for all $x \in U_r$, we have

$$\lim_{x \to x_0} T(t)g(x) = \lim_{x \to x_0} g(\sigma(t, x)) = g(\sigma(t, x_0)) = T(t)g(x_0).$$

In the case where $m(x_0) < t$, because of the continuity of m, there exists a neighborhood U_r of x_0 such that $m(x) < t$ for all $x \in U_r(x_0)$. Thus,

$$\lim_{x \to x_0} T(t)g(x) = 0 = T(t)g(x_0).$$

Now, we show that the modified Koopman-Lie semigroup is continuous at $m(x_0) = t$. Let $x_n \in \Omega$, with $x_n \to x_0$ and $m(x_n) > t$. By the continuity of m, we have $m(x_n) \to m(x_0) = t$. Define $x_n^+ := \{x_n \mid m(x_n) \leq t\}, \quad x_n^- := \{x_n \mid m(x_n) > t\}$. Then, $T(t)g(x_n^+) = 0 = T(t)g(x_0)$. Moreover, by Assumption A* , $|\sigma(t, x_n^-)| \to \infty$, which implies $T(t)g(x_n^-) = g(\sigma(t, x_n^-)) \to g(\infty) = 0 = T(t)g(x_0)$. Thus, we conclude that $T(t)g(x) \in C_0(\Omega)$.

□

Example 2.4.4. Consider

$$x'(t) = x^2(t), \;\; x(0) = x \in \Omega := [0, \infty).$$

with the solution $t \to \sigma(t, x) := \frac{x}{1-tx} \in \Omega$ for $0 \leq t < m(x) = \frac{1}{x}$. Observe that the function $T(t)g(x) = g(\frac{x}{1-xt})$ is only defined on time-dependent domains $\Omega_t := [0, \frac{1}{t})$, but not on $\Omega = [0, \infty)$. Thus, $T(t)g(x) = g(\frac{x}{1-xt})$ is not a semigroup of operators on any function space. To define $T(t)g(x)$ on Ω, we consider the modified space

$$C_m[0, \infty) := \{g \in C_b([0, \infty)| \lim_{x \to \infty} g(x) = 0\},$$

and the modified Koopman-Lie semigroup on

$$T(t)g(x) = \begin{cases} g(\frac{x}{1-xt}) & 0 \leq x < \frac{1}{t} \\ \\ 0 & x \geq \frac{1}{t} \end{cases}$$

For fixed $t > 0$, the map $x \to T(t)g(x)$ is continuous at $x = \frac{1}{t}$, and $\lim_{x\to\infty} T(t)g(x) = 0$. Thus, $T(t)g \in C_m[0,\infty)$ and $T(t)$ is well-defined operator from $C_m[0,\infty)$ into itself.

Now, we show that $\{T(t), t \geq 0\}$ is strongly continuous, i.e., the map $t \to T(t)g$ is continuous for all $t \geq 0$. However, it is sufficient to show that it is continuous at $t = 0$. Let $g \in C_m[0,\infty)$, and choose $\delta_g > 0$ such that $|g(x)| < \frac{\epsilon}{3}$ for all $x \geq \delta_g$. For any compact subset $[0,\delta_g] \subset [0,\infty)$, the condition $\sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| \to 0$ as $t \to 0^+$ is satisfied. Since $g \in C_m(\Omega)$ is uniformly continuous on compact subset $[0,\delta_g]$, for all $\epsilon > 0$, there exists $\delta > 0$ such that $|g(y) - g(x)| \leq \epsilon$ whenever $|y - x| < \delta$ for all $x, y \in [0,\delta_g]$. We have

$$|\sigma(t,x) - x| = \left|\frac{x}{1-tx} - x\right| = \left|\frac{tx^2}{1-tx}\right| \leq \frac{t\delta_g^2}{1-t\delta_g},$$

as long as $x < \frac{1}{t}$. For sufficiently small $t < \frac{1}{2\delta_g}$, we have $\frac{t\delta_g^2}{1-t\delta_g} < \delta_g$. By the uniform continuity of g on $[0,\delta_g]$, we obtain

$$|T(t)g(x) - g(x)| = \left|g\left(\frac{x}{1-tx}\right) - g(x)\right| < \frac{\epsilon}{3}$$

for all $x \in [0,\delta_g]$ and $t < \frac{1}{2\delta_g}$. Therefore,

$$\sup_{0\leq x\leq\delta_g} |g(\frac{x}{1-xt}) - g(x)| \to 0 \text{ as } t \to 0^+.$$

If $x \geq \delta_g$, then $x > \frac{\delta_g}{1+t\delta_g}$, that is, $\frac{x}{1-tx} > \delta_g$. This implies that

$$\sup_{x\in[\delta_g,\frac{1}{t}]} |T(t)g(x)| \to 0.$$

Consequently,

$$\begin{aligned}\|T(t)g - T(0)g\|_\infty &= \sup_{x\in[0,\infty)} |T(t)g(x) - g(x)| \\ &\leq \sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| + \sup_{x\in[\delta_g,\infty)} |T(t)g(x) - g(x)| \\ &\leq \sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| + \sup_{x\in[\delta_g,\frac{1}{t})} |T(t)g(x)| \\ &\quad + \sup_{x\geq\frac{1}{t}} |T(t)g(x)| + \sup_{x\geq\delta_g} |g(x)| \to 0 \quad \text{as long as} \quad t < \frac{1}{\delta_g}.\end{aligned} \tag{2.4.6}$$

Thus, $T(t) : C_m(\Omega) \to C_m(\Omega)$ is strongly continuous $C_m(\Omega)$-semigroup.

Remark 2.4.5. Observe that the modified space $C_m[0,\infty)$ coincides with $C_0[0,\infty)$.

Example 2.4.6. Consider the initial value problem:

$$x'(t) = x^3(t), \;\; x(0) = x, \quad x \in \Omega := [0,\infty).$$

The flow map $t \to \sigma(t,x)$ is given by

$$\sigma(t,x) = \frac{x}{\sqrt{1-2tx^2}}, \quad \text{for } 0 \leq t < m(x) = \frac{1}{2x^2}.$$

The modified space is given by

$$C_m(\Omega) := \{g \in C_b([0,\infty) | \lim_{x\to\infty} g(x) = 0\}.$$

Let $g \in C_m(\Omega)$, and define the operator

$$T(t)g(x) := g(\sigma(t,x)), \quad 0 \leq t < \frac{1}{2x^2}.$$

Then, the map $t \to T(t)g$ is defined on $\Omega_t := [0, \frac{1}{\sqrt{2t}})$. Thus, $T(t) : C_m(\Omega) \to C_m(\Omega_t)$. We extend $T(t)$ to $C_m(\Omega)$ by applying 2.4.5,

$$T(t)g(x) = \begin{cases} g\left(\frac{x}{\sqrt{1-2tx^2}}\right), & 0 \leq t < \frac{1}{2x^2}, \\ 0, & t \geq \frac{1}{2x^2}. \end{cases}$$

Clearly, the map $x \to T(t)g(x) = g\left(\frac{x}{\sqrt{1-2tx^2}}\right)$ is continuous at $x = \frac{1}{\sqrt{2t}}$ since $\lim_{x\to\frac{1}{\sqrt{2t}}} g\left(\frac{x}{\sqrt{1-2tx^2}}\right) = 0$. Therefore, $T(t)g \in C_m([0,\infty))$ and $T(t)$ is well-defined operator from $C_m[0,\infty)$ into itself.

Similar to Example (2.4.4), we show that the map $t \to T(t)g$ is continuous at $t = 0$. In the same manner, we choose $\delta_g > 0$ such that $|g(x)| < \frac{\epsilon}{3}$ for all $x \geq \delta_g$. Since g is uniformly continuous on compact subsets, for all $\epsilon > 0$, there exists $\delta > 0$ such that

$$|g(y) - g(x)| \leq \epsilon \quad \text{whenever } |y - x| < \delta, \quad \text{for all } x, y \in [0, \delta_g].$$

We have the bound

$$|\sigma(t,x) - x| = \left|\frac{x}{\sqrt{1-2tx^2}} - x\right| = \left|\frac{2tx^3}{\sqrt{1-2tx^2}(1-2tx^2)}\right| \leq \frac{2t\delta_g^3}{(1-2t{\delta_g}^2)^{3/2}}.$$

For sufficiently small $t < \frac{1}{4{\delta_g}^2}$, we have

$$\frac{2t\delta_g^3}{(1-2t{\delta_g}^2)^{3/2}} < \delta_g.$$

By the uniform continuity of g on $[0, \delta_g]$, we get

$$|T(t)g(x) - g(x)| = \left|g\left(\frac{x}{\sqrt{1-2tx^2}}\right) - g(x)\right| < \frac{\epsilon}{3}, \quad \text{for all } x \in [0, \delta_g] \text{ and } t < \frac{1}{4{\delta_g}^2}.$$

Therefore,

$$\sup_{0\leq x\leq\delta_g} |T(t)g(x) - g(x)| \to 0 \quad \text{as } t \to 0^+.$$

If $x \geq \delta_g$, then $x > \frac{\delta_g}{\sqrt{1+2t{\delta_g}^2}}$ for all $t \geq 0$, which implies that $\frac{x}{\sqrt{1-2tx^2}} > \delta_g$ whenever

$2tx^2 < 1$. Therefore, $\sup_{x\in[\delta_g,\frac{1}{\sqrt{2t}})} |T(t)g(x)| \to 0$. Consequently,

$$\begin{aligned} \|T(t)g - T(0)g\|_\infty &= \sup_{x\in[0,\infty)} |T(t)g(x) - g(x)| \\ &\le \sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| + \sup_{x\in[\delta_g,\infty)} |T(t)g(x) - g(x)| \\ &\le \sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| + \sup_{x\in[\delta_g,\frac{1}{\sqrt{2t}})} |T(t)g(x)| \\ &\quad + \sup_{x\ge\frac{1}{\sqrt{2t}}} |T(t)g(x)| + \sup_{x\ge\delta_g} |g(x)| \to 0 \quad \text{as long as} \quad t < \frac{1}{2{\delta_g}^2}. \end{aligned} \tag{2.4.7}$$

Thus, $T(t)$ is a strongly continuous semigroup on $C_m[0,\infty)$. □

If Ω is not closed but only a locally compact, we need to verify whether Proposition 2.4.3 still holds. In the next example, we show that the modified Koopman-Lie semigroup 2.4.5 is still well-defined and strongly continuous on $C_m(\Omega)$, even when Ω is not closed.

Example 2.4.7. Consider the IVP

$$x'(t) = 1,\ x(0) = x \in \Omega := [0,1).$$

The flow $\sigma(t,x) = x + t$ is defined as long as $0 \le x + t < 1$, i.e., $m(x) = 1 - x$. Again, the function $T(t)g(x) = g(x+t)$ is not well-defined on $\Omega = [0,1)$, i.e, $T(t)g(x) = g(x+t)$ is not a semigroup of operators on any function space on $[0,1)$. However, everything works if we consider the modified space

$$C_m(\Omega) := \{g \in C_b([0,1) |\ \lim_{x\to 1} g(x) = 0\}$$

and define the modified Koopman-Lie semigroup on $C_m[0,1)$ as

$$T(t)g(x) = \begin{cases} g(x+t) & 0 \le t < 1 - x, \\ 0 & t \ge 1 - x. \end{cases}$$

For fixed $t > 0$, it is clear that the map $x \to T(t)g(x)$ is continuous at $x = 1-t$, and $\lim_{x\to 1} T(t)g(x) = 0$. Thus, $T(t)g \in C_m[0,1)$ and $T(t)$ is a well-defined operator from $C_m[0,1)$ into itself. Moreover, $T(t)$ is bounded and $\|T(t)\| \leq 1$. Observe that $\sup_{0\leq x<1} |T(t)g(x)| = \sup_{0\leq x<1} g(x+t) \leq \sup_{0\leq x<1-t} g(x+t) + \sup_{1-t\leq x<1} g(x+t) = \sup_{0\leq y<1} |g(y)| = \|g\|$. Therefore, $\|T(t)\| = \sup_{\|g\|\leq 1} \|T(t)g\| \leq \sup_{\|g\|\leq 1} \|g\| = 1$.

Now, we show that $\{T(t), t \geq 0\}$ is strongly continuous; that is, the map $t \to T(t)g$ is continuous at $t = 0$.

Let $g \in C_m(\Omega)$, then

$$\begin{aligned}
\|T(t)g - T(0)g\|_\infty &= \sup_{x\in[0,1)} |T(t)g(x) - g(x)| \\
&\leq \sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| + \sup_{x\in[\delta_g,1)} |T(t)g(x) - g(x)| \\
&\leq \sup_{x\in[0,\delta_g]} |T(t)g(x) - g(x)| + \sup_{x\in[\delta_g,1-t)} |T(t)g(x)| \\
&\quad + \sup_{x\geq 1-t} |T(t)g(x)| + \sup_{x\geq\delta_g} |g(x)| \to 0 \quad \text{as long as} \quad t < 1-\delta_g.
\end{aligned}$$

By the uniform continuity on the compact subset $[0,\delta_g] \subset [0,1)$, and $g \in C_m(\Omega)$, for every $\epsilon > 0$, $\exists \delta_g$, such that $|g(x)| < \epsilon$ for all $x \geq \delta_g$. Thus, $t \to T(t)g$ is a strongly continuous $C_m(\Omega)$-semigroup.

Remark 2.4.8. Observe that the space $C_0[0,1)$ coincides with the modified space $C_m[0,1)$. However, if $\Omega = (0,1)$, then the modified space is given by

$$C_m(\Omega) := \{g \in C_b(\Omega) \mid \lim_{x\to 1} g(x) = 0\},$$

and

$$C_0(\Omega) := \{g \in C_b(\Omega) \mid \lim_{x\to 0} g(x) = \lim_{x\to 1} g(x) = 0\}.$$

Hence, we have $C_0(\Omega) \subseteq C_m(\Omega)$. Moreover, if $\Omega = [0, \infty)$, then the modified space satisfies $C_m(\Omega) = C_b(\Omega)$.

Example 2.4.9. Consider

$$x'(t) = \frac{-1}{2x(t)}, \quad t \geq 0, \quad x(0) = x \in \Omega = (0, \infty),$$

the flow $\sigma(t, x) = \sqrt{x^2 - t} \in \Omega$, $0 \leq t < m(x) := x^2$.

The function $T(t)g(x) = g(\sqrt{x^2 - t})$ is not well-defined if $x^2 < t$, and therefore $T(\cdot)$ is not a semigroup of operators on any function space from $(0, \infty)$ into $\mathbb{R}$. However, as above, we can define the modified space as

$$C_m(0, \infty) := \{g \in C_b(0, \infty) \quad | \lim_{x \to 0} g(x) = 0\}, \tag{2.4.8}$$

and the modified Koopman-Lie semigroup,

$$T(t)g(x) = \begin{cases} g(\sqrt{x^2 - t}) & \text{if } \ 0 \leq t < m(x) = x^2, \\ \\ 0 & \text{if } \ t \geq m(x) = x^2. \end{cases} \tag{2.4.9}$$

is bounded linear operator from the modified space C_m to itself. Similar to the previous examples, we can show that $T(t) : C_m(0, \infty) \to C_m(0, \infty)$ is a strongly continuous semigroup.

Next, we will consider a two-dimensional example.

Example 2.4.10. Consider the initial set $\Omega_0 := (-1, \infty) \times (-\infty, 1)$, and the system

$$\begin{aligned} &x'(t) = x^2(t), \quad x(0) = x \in (-1, \infty) \\ &y'(t) = 1, \quad y(0) = y \in (-\infty, 1). \end{aligned} \tag{2.4.10}$$

The flow $\sigma(t,(x,y)) = (\frac{x}{1-xt}, y+t)$ exists if $0 \leq t < m(x,y)$, where

$$m(x,y) = \begin{cases} \min\{\frac{1}{x}, y+t\} & x > 0 \\ \\ 1-y & x \leq 0. \end{cases}$$

The modified space $C_m(\Omega)$ can be obtained from 2.4.4 as follows:

$$C_m(\Omega) := \{g \in C_b(\Omega) \mid \lim_{(x,y)\to(\infty,y)} g(x,y) = 0 \text{ and } \lim_{(x,y)\to(x,1)} g(x,y) = 0\}.$$

The map $t \to T(t)g$ is only defined on time-dependent domains $\Omega_t := \{(x,y) \in \Omega \quad | t < m(x,y)\}$. Thus, $T(t) : C_m(\Omega) \to C_m(\Omega_t)$, and can be extended to $C_m(\Omega) \to C_m(\Omega)$ by the modified Koopman-Lie semigroup

$$T(t)g(x,y) = \begin{cases} g(\frac{x}{1-xt}, y+t) & 0 \leq t < m(x,y) \\ \\ 0 & t \geq m(x,y). \end{cases}$$

For $t > 0$, if $m(x,y) = \min\left\{\frac{1}{x}, 1-y\}\right\}$, then the map $x \to T(t)g(x)$ is continuous at $x = \frac{1}{t}$ or $y = 1-t$, and

$$\lim_{(x,y)\to(\infty,y)} g(x,y) = 0 \quad \text{and} \quad \lim_{(x,y)\to(x,1)} g(x,y) = 0.$$

Thus, $T(t)g \in C_m(\Omega)$ and $T(t)$ is a well-defined operator from $C_m(\Omega)$ into itself. $\square$

Chapter 3. Exponential Splitting of the Koopman-Lie Operator.

> "There's a way to do it better – find it."
>
> —*John von Neumann*

3.1. Introduction

To approximate solutions of initial value problems such as

$$x'(t) = F(x(t)), x(0) = x_0, \tag{3.1.1}$$

where $F = (F_1, \cdots, F_N)$, and $F_i : \mathbb{R}^N \supset \Omega \mapsto \mathbb{R}^N$, the Koopman-Lie global linearization approach provides a significant advantage by analyzing the nonlinear problem (3.1.1) in terms of the linear Koopman-Lie semigroup $e^{t\mathcal{K}}g(x_0) = g(x(t))$. Moreover, the Koopman operator can be decomposed into N operators $\mathcal{K}_1, \mathcal{K}_2, \ldots, \mathcal{K}_N$, where each $\mathcal{K}_i$ captures a one-dimensional aspect of the dynamics – and, most importantly, where the semigroups $e^{t\mathcal{K}_i}$ are computable via separation of variables.

Suppose that, for each $x \in \Omega$, there exists $m(x) > 0$ such that the IVP (3.1.1) has a unique solution $u : [0, m(x)) \to \Omega$. If so, for $x \in \Omega$ and $t \in [0, m(x))$, define $\sigma(t, x) := x(t)$. By Proposition 2.1.1, $t \to \sigma(t, x)$ defines a flow in Ω with induced pointwise linear Koopman semigroup flow $T(t)g(x) := g(\sigma(t, x))$, where the measurement g is chosen from a $T(t)$-invariant subspace $\mathcal{M} \subset \mathcal{F}(\Omega, \mathbb{C})$. By Example 2.2.2, the Koopman generator is given by

$$\mathcal{K}g(x) = \sum_{i=1}^{N} \frac{\partial g}{\partial x_i}(x) \cdot F_i(x) = \sum_{i=1}^{N} \mathcal{K}_i g(x),$$

with $\mathcal{K}_i g(x) := F_i(x) g_{x_i}(x)$ for $1 \le i \le N$. Approximating

$$g(\sigma(t, x)) = T(t)g(x) = e^{t\mathcal{K}}g(x) = e^{t(\mathcal{K}_1 + \cdots \mathcal{K}_N)}g(x)$$

is challenging and computationally expensive. However, by splitting the problem into one-dimensional subproblems $T_i(t)g(x) = e^{t\mathcal{K}_i}g(x)$, where each sub-problem can be computed explicitly via separation of variables for all $1 \leq i \leq N$, the computation becomes more manageable. Each $\mathcal{K}_i$ captures a one-dimensional aspects of the dynamics, and generates the semigroup

$$T_i(t)g(x) = e^{t\mathcal{K}_i}g(x) = g(x_1, \cdots, x_{i-1}, \sigma_i(t, x_i), x_{i+1}, \cdots, x_N),$$

where $\sigma_i(t, x_i)$ is the solution of the separable, first-order problem

$$u'(t) = F_i(x_1, \cdots, x_{i-1}, u(t), x_{i+1}, \cdots, x_N), u(0) = x_i.$$

As we shall see in the following section on "Chernoff's Product Formula", one can approximate

$$e^{t\mathcal{K}}g(x) = e^{t(\mathcal{K}_1 + \cdots \mathcal{K}_N)}g(x) = g(\sigma(t, x))$$

in terms of operators like

$$V(t)g(x) := e^{t\mathcal{K}_1} \circ \cdots \circ e^{t\mathcal{K}_N}g(x)$$

for which $V(0) = I$ and $V'(0) = \mathcal{K}$.

3.2. Chernoff's Product Formula

Standard references for Chernoff's Product Formula, a key result of semigroup theory, include [11], [42], [15], [44], and – for our purposes most importantly – the work of Franziska Kühnemund [25] in which she extends the result to the bi-continuous case.

For Chernoff's product formula to hold in a Banach space X, let

$$V(\cdot) : [0, \infty) \to \mathcal{L}(X)$$

satisfy $V(0) = I$, $\|V(t)^m\| \leq M$ for all $t \geq 0$, $m \in \mathbb{N}$, and some $M \geq 1$ and assume that

$$\mathcal{K}x := \lim_{h \to 0^+} \frac{V(h)x - x}{h}$$

exists for all $x \in D \subset X$, where D and $(\lambda_0 - \mathcal{K})D$ are dense subspaces in X for some $\lambda_0 > 0$. Then the closure $\bar{\mathcal{K}}$ of $\mathcal{K}$ generates a strongly continuous semigroup $(T(t))_{t \geq 0}$ with $\|T(t)\| \leq M (t \geq 0)$ which is given by

$$T(t)x = \lim_{n \to \infty} V(\frac{t}{n})^n x. \tag{3.2.1}$$

for all $x \in X$ and where the limit exists uniformly for t in compact intervals.

In order to estimate the speed of convergence, one can employ the non-commutative binomial theorem as follows. Let $h = \frac{t}{n}$. Then

$$\begin{aligned}
\|(V(h)^n - T(t)\| = \|(V(h)^n - T(h)^n\| &\leq \| \sum_{k=0}^{n-1} V(h)^{n-1-k} \Big[V(h) - T(h) \Big] T(h)^k \| \\
&\leq \sum_{k=0}^{n-1} \|V(h)^{n-1-k}\| \| \Big[V(h) - T(h) \Big] T(h)^k \| \qquad (3.2.2) \\
&\leq M \sum_{k=0}^{n-1} \| \Big[V(h) - T(h) \Big] T(kh) \| \leq nM^2 \|V(h) - T(h)\|.
\end{aligned}$$

The inequality above indicates that the error estimates for $\|(V(h)^n x - T(t)x\|$ can be derived from an estimate of $\|V(h) - T(h)\|$ for small values of h. To do so, one considers approximations $V(t)$ that are *"of order p"*; that is $V(t)$ for which, in the case of matrices, the first p Taylor coefficients coincide with the first p Taylor coefficients of

$$T(t)x = e^{t\mathcal{K}}x = x + t\mathcal{K}x + \frac{t^2}{2!}\mathcal{K}^2 x + \cdots + \frac{t^p}{p!}\mathcal{K}^p x + \cdots .$$

Then, formally, for small values of h, one would then expect to obtain an estimate like

$$\begin{aligned} &\|V(h)x - T(h)x\| \\ &\quad \leq \|\frac{h^{p+1}}{(p+1)!}(V(0)^{p+1}x - \mathcal{K}^{p+1}x) + \frac{h^{p+2}}{(p+2)!}(V(0)^{p+2}x - \mathcal{K}^{p+2}x) + \cdots \| \\ &\quad \leq \frac{h^{p+1}}{(p+1)!}\tilde{M}_x \end{aligned} \tag{3.2.3}$$

for some $\tilde{M}_x \geq 0$. Together with estimate (3.2.2), and setting $h = \frac{t}{n}$, we would then have

$$\|(V(\frac{t}{n})^n x - T(t)x\| \leq \frac{1}{n^p}\frac{t^{p+1}}{(p+1)!}M^2\tilde{M}_x. \tag{3.2.4}$$

In 2009, E. Hansen and A. Ostermann showed in [17] and [18] that the estimates (3.2.3) and (3.2.4) hold for splitting methods of the form

$$V(t) := \prod_{j=1}^{s} e^{\alpha_{j,1}t\mathcal{K}_1} \cdots e^{\alpha_{j,N}t\mathcal{K}_N}, \tag{3.2.5}$$

where $T(t) = e^{t\mathcal{K}}$ and $\mathcal{K} = \mathcal{K} + \ldots\mathcal{K}$, and where the real or complex coefficients α_j's and β_j's are chosen in such a way that the method $V(t)$ has algebraic order p. For more details, see Section 3.4.

Many of the central results of the theory of strongly continuous semigroups, especially those based on Laplace transform methods, can be lifted to the bi-continuous case, [25]. One of the significant results is that Chernoff's product formula extends to bi-continuous semigroups.

Theorem 3.2.1. *(Chernoff's Bi-Continuous Product Formula) Let $(\mathcal{K}, D(\mathcal{K}))$ be a linear operator on a bi-admissible Banach space $(X, \|\cdot\|, \tau)$, where $D(\mathcal{K})$ and $(\lambda_0 I - \mathcal{K})D(\mathcal{K})$ are bi-dense in X for some $\lambda_0 > \omega \geq 0$. Moreover, let $V(t) \in \mathcal{L}(X)$ be such that $||V(t)^n|| \leq Me^{\omega nt}$ for all $n \in \mathbb{N}_0$ and $t \in [0, \delta)$. If*

$$V'(0+)g = \|\cdot\| - \lim_{t\to 0^+} \frac{V(t)g - g}{t} = \mathcal{K}g$$

for all $g \in D(\mathcal{K})$ *and if* $\{V(t)^m : t \geq 0\}$ *is locally bi–equicontinuous uniformly for* $m \in \mathbb{N}$, *then the bi-closure of* $(\mathcal{K}, D(\mathcal{K}))$ *generates a bi-continuous semigroup* $T(t)$ *and*

$$T(t)g = \tau - \lim_{n\to\infty} \left(V(\frac{t}{n})\right)^n g \tag{3.2.6}$$

for all $g \in X$ *and* $t \geq 0$ *uniformly in* t *on compact intervals.*

Proof. See [25]. □

If one applies (3.2.6 to bi-continuous Koopman-Lie semigroups on $C_b(\Omega)$, then one obtains that

$$T(t)g(\cdot) = g(\sigma(t,\cdot)) = \tau - \lim_{n\to\infty} \left(V(\frac{t}{n})\right)^n g(\cdot) = \tau - \lim_{n\to\infty} g(\sigma_n(t,\cdot)) \tag{3.2.7}$$

uniformly in compact time intervals for all $g \in C_b(\Omega)$. The following proposition, due to Arun Banjara [3], shows that (3.2.7) implies that, for all $x \in \Omega$,

$$\sigma(t,x) = \lim_{n\to\infty} \sigma_n(t,x). \tag{3.2.8}$$

Definition 3.2.2. Let Ω be a metric space. Then, for $x_n, x \in \Omega$, we say that x_n is weak-$C_b(\Omega)$ convergent to x and write $x_n \xrightarrow{C_b(\Omega)} x$ if $g(x_n) \to g(x)$ for all $g \in C_b(\Omega)$.

Proposition 3.2.3. *Let* $\Omega \subset \mathbb{R}^N$. *Then the following statements are equivalent.*

a) $x_n \to x$ *as* $n \to \infty$,

b) $g(x_n) \to g(x)$ *as* $n \to \infty$ *for all* $g \in C_b(\Omega, \mathbb{R})$.

Proof. See [3]. □

Many approximation formulas can be derived from Chernoff's Product Formula. For example,

(1) $V(t) := T_1(t)T_2(t)$, where $T_1(t)$ and $T_2(t)$ are strongly continuous contraction semigroups on a Banach space X with generators $(\mathcal{K}_1 D(\mathcal{K}_1))$ and $(\mathcal{K}_2, D(\mathcal{K}_2))$, respectively. Then $V(0) = I$ and $\|V(t)^m\| \leq 1$ for all $t \geq 0$, $m \in \mathbb{N}$ and

$$\begin{aligned}\mathcal{K}x = \lim_{h\to 0^+} \frac{V(h)x - x}{h} &= \lim_{h\to 0^+} \frac{T_1(h)T_2(h)x - x}{h} \\ &= \lim_{h\to 0^+} T_1(h)\frac{T_2(h)x - x}{h} + \lim_{h\to 0^+} \frac{T_1(h)x - x}{h} \\ &= \mathcal{K}_2 x + \mathcal{K}_1 x.\end{aligned} \tag{3.2.9}$$

So, consider $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ on $D := D(\mathcal{K}_1) \cap D(\mathcal{K}_2)$ and assume that D and $(\lambda_0 - \mathcal{K}_1 - \mathcal{K}_2)D$ are dense in X. Then, by Chernoff's theorem,

$$\mathcal{K} := \overline{\mathcal{K}_1 + \mathcal{K}_2}$$

generates a strongly continuous semigroup $(T(t))_{(t\geq 0)}$ given by the *Lie-Trotter product formula*

$$T(t)x = \lim_{n\to\infty} \left(T_1(\frac{t}{n})T_2(\frac{t}{n}) \right)^n x \tag{3.2.10}$$

for all $x \in X$ and the limit is uniform for t in compact intervals. The Lie-Trotter product formula has approximation order 1; that is, in general there exists a constant $M_{g,t}$ such that

$$\|T(t)g - \left(V_{LT}(\frac{t}{n}) \right)^n g\| \leq \frac{M_{g,t}}{n}.$$

(2) If $V(t) := T_2(\frac{t}{2})T_1(t)T_2(\frac{t}{2})$. Then, by Chernoff's theorem,

$$\mathcal{K} := \overline{\mathcal{K}_1 + \mathcal{K}_2}$$

generates a strongly continuous semigroup $(T(t))_{(t\geq 0)}$ given by the *Strang product formula*

$$T(t)x = \lim_{n\to\infty} \left(T_2(\frac{t}{2n})T_1(\frac{t}{n})T_2(\frac{t}{2n})) \right)^n x \tag{3.2.11}$$

for all $x \in X$ and the limit is uniform for t in compact intervals. In general, the Strang product formula has approximation order 2; that is, in general there exists a constant $M_{g,t}$ such that

$$\|T(t)g - \left(V_S(\frac{t}{n})\right)^n g\| \leq \frac{M_{g,t}}{n^2}.$$

Remark 3.2.4. The Lie-Trotter and Strang product formulas can also be employed in cases where the Koopman-Lie generator $\mathcal{K}$ can be split into N simpler parts $\mathcal{K} = \mathcal{K}_1 + \cdots + \mathcal{K}_N$. Then we can rewrite the Lie-Trotter and Strang product formulas, as follows:

(3) If $V(t) := T_1(t)T_2(t)\cdots T_N(t)$. Then, the higher dimensional Lie-Trotter product formula is given by

$$T(t)x = \lim_{n\to\infty}\left(T_1(\frac{t}{n})T_2(\frac{t}{n})\cdots T_N(\frac{t}{n})\right)^n x. \tag{3.2.12}$$

(4) If $V(t) := T_N(\frac{t}{2})\cdots T_1(t)\cdots T_N(\frac{t}{2})$. Then, the higher dimensional Strang product formula is given by

$$T(t)x = \lim_{n\to\infty}\left(T_N(\frac{t}{2n})\cdots T_2(\frac{t}{2n})T_1(\frac{t}{n})T_2(\frac{t}{2n})\cdots T_N(\frac{t}{2n})\right)^n x. \tag{3.2.13}$$

3.3. Nonlinear Versions of Standard Product Formulas

In this section, we apply Koopman-Lie's global linearization method to exponential splitting schemes for nonlinear ordinary differential equations (ODEs) of the form

$$x'(t) = F(t, x(t)), x(s) = x,$$

where $F : \mathbb{R}^2 \to \mathbb{R}$. More generally, later in this section, we consider systems of N-dimensional ODEs. To gain further insight into the splitting method, we examine two-dimensional nonlinear ODEs of the form:

$$\begin{aligned} x'(t) &= F(x(t), y(t)), x(0) = x \\ y'(t) &= G(x(t), y(t)), y(0) = y \end{aligned} \tag{3.3.1}$$

where F, G are smooth functions from $\mathbb{R}^2 \to \mathbb{R}$. As we will see below, the splitting approach leads to numerically efficient versions of the Lie-Trotter and other product formulas for nonlinear ODEs.

To see this, let $(s, x) \in \Omega_I \subset [0, \infty) \times \mathbb{R}$ be such that

$$x'(t) = F(t, x(t)), x(s) = x \tag{3.3.2}$$

has a unique, continuously differentiable solution $t \to x(t)$ for which $t \to x(t+s) = \gamma(s+t, s, x)$ exists for $0 \leq t < m(s, x)$. Let $\tilde{x}(t) := x(s+t)$. Then it is clear that solving (3.3.2) is equivalent to solving

$$\tilde{x}'(t) = F(s+t, x(s+t)) = F(s+t, \tilde{x}(t)), \;\; \tilde{x}(0) = x. \tag{3.3.3}$$

The associated pointwise linear Koopman-Lie flow semigroup is given by

$$T(t)g(s, x) = e^{t\mathcal{K}}g(s, x) = g(s+t, \gamma(t+s, s, x)) \tag{3.3.4}$$

for $0 \leq t < m(s, x)$ with formal generator

$$\begin{aligned} \mathcal{K}g(s, x) &= g_s(s, x) + \gamma'(s, s, x)g_x(s, x) \\ &= g_s(s, x) + F(s, x)g_x(s, x) \\ &= \mathcal{K}_1 g(s, x) + \mathcal{K}_2 g(s, x). \end{aligned} \tag{3.3.5}$$

Now, we will approximate the solution of (3.3.3) by using the Lie-Trotter product formula. The procedure is as follows:

$$\begin{aligned} T(t)g(s,x) &= g(s+t,\gamma(t+s,s,x)) \\ &= e^{t\mathcal{K}}g(s,x) = e^{t(\mathcal{K}_1+\mathcal{K}_2)}g(s,x) \\ &= \lim_{n\to\infty}(e^{\frac{t}{n}\mathcal{K}_1}e^{\frac{t}{n}\mathcal{K}_2})^n g(s,x) \\ &= \lim_{n\to\infty}(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(s,x), \end{aligned} \tag{3.3.6}$$

where we assume that the operators $\mathcal{K}$, $\mathcal{K}_1$, and $\mathcal{K}_2$ generate strongly continuous contraction semigroups $T(t)$, $T_1(t)$, and $T_2(t)$ on an appropriate Koopman-Lie Banach space $\mathcal{M} \subseteq \mathcal{F}(\Omega_I, Z)$ such that

$$\begin{aligned} T_1(t)g(s,x) &= e^{t\mathcal{K}_1}g(s,x) = g(s+t,x) \\ T_2(t)g(s,x) &= e^{t\mathcal{K}_2}g(s,x) = g(s,\sigma_s(t,x)), \end{aligned} \tag{3.3.7}$$

and $r \to \sigma_s(r,x)$ solves the autonomous, separable frozen-time problem

$$x'(r) = F(s,x(r)), \quad x(0) = x. \tag{3.3.8}$$

Now, we will compute

$$(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(s,x) = g(s+t,x_{n,n}).$$

Step 1:

$$\begin{aligned} T_1(\frac{t}{n})T_2(\frac{t}{n})g(s,x) &= T_1(\frac{t}{n})g(s,\sigma_s(\frac{t}{n},x)) \\ &= T_1(\frac{t}{n})g(s,x_{1,n}) = g(s+\frac{t}{n},x_{1,n}), \end{aligned}$$

where $x_{1,n} = \sigma_s(\frac{t}{n},x)$ and $r \to \sigma_s(r,x_{0,n})$ solves

$$x'(r) = F(s,x(r)), \;\; x(0) = x_{0,n} = x.$$

Step 2:

$$
\begin{aligned}
(T_1(\frac{t}{n})T_2(\frac{t}{n}))^2 g(s,x) &= T_1(\frac{t}{n})T_2(\frac{t}{n})g(s+\frac{t}{n},x_{1,n}) \\
&= T_1(\frac{t}{n})g(s+\frac{t}{n},\sigma_{s+\frac{t}{n}}(\frac{t}{n},x_{1,n})) = g(s+\frac{2t}{n},x_{2,n}),
\end{aligned}
$$

where $x_{2,n} = \sigma_{s+\frac{t}{n}}(\frac{t}{n}, x_{1,n})$ and $r \to \sigma_{s+\frac{t}{n}}(r, x_{1,n})$ solves $x'(r) = F(s+\frac{t}{n}, x(r)),\ \ x(0) = x_{1,n}$.

This implies the following algorithm. For $0 \le k \le n$ define $x_{k,n}$ by

$$
\begin{aligned}
x_{0,n} &:= x, \\
x_{1,n} &:= \sigma_s(\frac{t}{n}, x_{0,n}), \\
x_{2,n} &:= \sigma_{s+\frac{t}{n}}(\frac{t}{n}, x_{1,n}), \\
&\ \vdots \\
x_{n,n} &:= \sigma_{s+\frac{(n-1)t}{n}}(\frac{t}{n}, x_{n-1,n}),
\end{aligned}
\tag{3.3.9}
$$

where $r \to \sigma_{s+\frac{(k-1)t}{n}}(r, x_{k-1,n})$ solves

$$
x'(r) = F(s+\frac{(k-1)t}{n}, x(r)),\ \ x(0) = x_{k-1,n}.
$$

Step n: After n steps, this yields

$$
(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(s,x) = g(s+t, x_{n,n}).
$$

Then, under "suitable" conditions on the function $F(t,x)$, g and $\mathcal{M}$

$$
\lim_{n\to\infty}(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(s,x) = \lim_{n\to\infty} g(s+t, x_{n,n}) = g(s+t, \gamma(t+s,s,x)).
$$

Thus, we suggest that

$$
\lim_{n\to\infty} x_{n,n} = \gamma(s+t,s,x),
$$

Algorithm 3.1. Lie-Trotter product of nonlinear one-dimensional ODEs of the form (3.3.2)

Require: $\sigma_s(r, x)$, T: time interval, n: number of iterations

procedure $(x)_{n,n} := NL_x$
  for $t \leftarrow T$ **do**
    $x \leftarrow x_0$
    $L_x \leftarrow x$
    for $i \leftarrow n$ **do**
      $L_x \leftarrow \sigma_{s+\frac{(i-1)t}{n}}(\frac{t}{n}, L_x)$
      $NL_x \leftarrow L_x$
    end for
    return $x_{n,n} := NL_x$
  end for

solves the non-autonomous problem (3.3.2). The "formal" order of convergence is $\frac{1}{n}$ (see also Section 3.4 and the numerical examples below).

Based on Theorem 3.4.1, we can use other linear operator splitting methods that lead to nonlinear approximations that converge faster. One example is the *Strang Product Formula* given by

$$\begin{aligned} T(t)g(s,x) &= g(s+t, \gamma(t+s,s,x)) \\ &= e^{t\mathcal{K}}g(s,x) = e^{t(\mathcal{K}_1+\mathcal{K}_2)}g(s,x) \\ &= \lim_{n\to\infty}(e^{\frac{t}{2n}\mathcal{K}_1}e^{\frac{t}{n}\mathcal{K}_2}e^{\frac{t}{2n}\mathcal{K}_1})^n g(s,x) \\ &= \lim_{n\to\infty}(T_1(\frac{t}{2n})T_2(\frac{t}{n})T_1(\frac{t}{2n}))^n g(s,x). \end{aligned} \tag{3.3.10}$$

The algorithm for the nonlinear Strang Product Formula for (3.3.2) is as follows. For $s \geq 0$ and $0 \leq r < m(s,x)$, let $r \to \sigma_s(r,x)$ solve the autonomous, separable frozen-time problem

$$x'(r) = F(s, x(r)), \quad x(0) = x. \tag{3.3.11}$$

Now, we will compute $(T_1(\frac{t}{2n})T_2(\frac{t}{n})T_1(\frac{t}{2n}))^n g(s,x)$.

Step 1:

$$T_1(\frac{t}{2n})T_2(\frac{t}{n})T_1(\frac{t}{2n})g(s,x) = T_1(\frac{t}{2n})T_2(\frac{t}{n})g(s+\frac{t}{2n},x))$$
$$= T_1(\frac{t}{2n})g(s+\frac{t}{2n},\sigma_{s+\frac{t}{2n}}(\frac{t}{n},x))$$
$$= g(s+\frac{t}{n},\sigma_{s+\frac{t}{2n}}(\frac{t}{n},x)) = g(s+\frac{t}{n},x_{1,n}),$$

where $x_{1,n} = \sigma_{s+\frac{t}{2n}}(\frac{t}{n},x)$ and $r \to \sigma_{s+\frac{t}{2n}}(r,x_{0,n})$ solves $x'(r) = F(s+\frac{t}{2n},x(r)),\ x(0) = x_{0,n} = x$.

Step 2:

$$(T_1(\frac{t}{2n})T_2(\frac{t}{n})T_1(\frac{t}{2n}))^2 g(s,x) = T_1(\frac{t}{2n})T_2(\frac{t}{n})T_1(\frac{t}{2n})g(s+\frac{t}{n},x_{1,n})$$
$$= T_1(\frac{t}{2n})T_2(\frac{t}{n})g(s+\frac{3t}{2n},x_{1,n})$$
$$= T_1(\frac{t}{2n})g(s+\frac{3t}{2n},\sigma_{s+\frac{3t}{2n}}(\frac{t}{n},x_{1,n}))$$
$$= g(s+\frac{2t}{n},\sigma_{s+\frac{3t}{2n}}(\frac{t}{n},x_{1,n})) = g(s+\frac{2t}{n},x_{2,n}),$$

where $x_{2,n} = \sigma_{s+\frac{3t}{2n}}(\frac{t}{n},x_{1,n})$ and $r \to \sigma_{s+\frac{3t}{2n}}(r,x_{1,n})$ solves

$$x'(r) = F(s+\frac{3t}{2n},x(r)),\ x(0) = x_{1,n}.$$

This implies the following algorithm. For $0 \le k \le n$ define $x_{k,n}$ by

$$\begin{aligned} x_{0,n} &:= x, \\ x_{1,n} &:= \sigma_{s+\frac{t}{2n}}(\frac{t}{n},x_{0,n}), \\ x_{2,n} &:= \sigma_{s+\frac{3t}{2n}}(\frac{t}{n},x_{1,n}), \\ &\vdots \\ x_{n,n} &:= \sigma_{s+\frac{(2n-1)t}{2n}}(\frac{t}{n},x_{n-1,n}), \end{aligned} \tag{3.3.12}$$

where $r \to \sigma_{s+\frac{(2k-1)t}{2n}}(r,x_{k-1,n})$ solves

$$x'(r) = F(s+\frac{(2k-1)t}{2n},x(r)),\ \ x(0) = x_{k-1,n}.$$

Step n: After n steps, this yields

$$(T_1(\frac{t}{2n})T_2(\frac{t}{n})T_1(\frac{t}{2n}))^n g(s,x) = g(s+t, x_{n,n}).$$

Algorithm 3.2. Strang product of nonlinear one-dimensional ODEs of the form (3.3.2)

Require: $\sigma_s(r,x)$, T: time interval, n: number of iterations

procedure $(x_{n,n} := NS_x)$
    for $t \leftarrow T$ **do**
        $S_x \leftarrow x_0$
        for $i \leftarrow n$ **do**
            $S_x \leftarrow \sigma_{s+\frac{(2i-1)t}{n}}(\frac{t}{n}, S_x)$
            $NS_x \leftarrow S_x$
        end for
        return $x_{n,n} := NS_x$
    end for

Then, under "suitable" conditions on F, g and $\mathcal{M}$,

$$\lim_{n\to\infty} x_{n,n} = \gamma(s+t, s, x),$$

solves the non-autonomous problem (3.3.2). The "formal" order of convergence is $\frac{1}{n^2}$ (see also Section 3.4 and the numerical examples below).

Now, we will consider a two-dimensional system of nonlinear ODEs of the form

$$\begin{aligned} x'(t) &= F(x(t), y(t)), x(0) = x \\ y'(t) &= G(x(t), y(t)), y(0) = y, \end{aligned} \tag{3.3.13}$$

where F, G are smooth functions from $\mathbb{R}^2 \to \mathbb{R}$. We assume that for $(x,y) \in \Omega \subseteq \mathbb{R}^2$ there is a unique solution $\sigma(t,x,y) := (x(t), y(t)) \in \Omega \subseteq \mathbb{R}^2$ for small values of t; that is, $0 \le t < m(x,y)$.

The associated pointwise linear semigroup flow is given by

$$T(t)g(x,y) = e^{t\mathcal{K}} g(x,y) = g(\sigma(t,x,y)) \tag{3.3.14}$$

for $0 \leq t < m(x,y)$ with formal Koopman-Lie generator

$$\begin{aligned}\mathcal{K}g(x,y) &= g_x(x,y)F(x,y) + g_y(x,y)G(x,y) \\ &= \mathcal{K}_1 g(x,y) + \mathcal{K}_2 g(x,y).\end{aligned} \tag{3.3.15}$$

The solution of (3.3.13) can be approximated by the Lie-Trotter product formula

$$\begin{aligned}T(t)g(x,y) &= g(\sigma(t,x,y)) = e^{t\mathcal{K}}g(x,y) \\ &= e^{t(\mathcal{K}_1+\mathcal{K}_2)}g(x,y) = \lim_{n\to\infty}(e^{\frac{t}{n}\mathcal{K}_1}e^{\frac{t}{n}\mathcal{K}_2})^n g(s,x) \\ &= \lim_{n\to\infty}(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(x,y) = \lim_{n\to\infty} g(x_n,y_n) := \lim_{n\to\infty} g(x_{n,n}),\end{aligned} \tag{3.3.16}$$

where the operators $\mathcal{K}_1$, and $\mathcal{K}_2$ generate semigroups on an appropriate Koopman-Lie Banach space $\mathcal{M} \subseteq \mathcal{F}(\Omega, Z)$, and where

$$\begin{aligned}T_1(t)g(x,y) &= e^{t\mathcal{K}_1}g(x,y) = g(\sigma_y(t,x),y) \\ T_2(t)g(x,y) &= e^{t\mathcal{K}_2}g(x,y) = g(x,\sigma_x(t,y)),\end{aligned} \tag{3.3.17}$$

where $t \to \sigma_y(t,x)$ solves the separable equation

$$x'(t) = F(x(t),y), x(0) = x \tag{3.3.18}$$

and $t \to \sigma_x(t,y)$ solves the separable equation

$$y'(t) = G(x,y(t)), y(0) = y. \tag{3.3.19}$$

Now, we will derive an explicit formula of $x_{n,n} := (x_n, y_n)$. By using equations (3.3.17), (3.3.18), (3.3.19), and the Lie-Trotter product formula (3.3.16) we deduce the procedure as follows.

Step 1: Let $(x_0,y_0) := (x,y)$ be the initial state, then

$$\begin{aligned}T_1(\frac{t}{n})T_2(\frac{t}{n})g(x_0,y_0) &= T_1(\frac{t}{n})g(x_0,\sigma_{x_0}(\frac{t}{n},y_0)) \\ &= T_1(\frac{t}{n})g(x_0,y_1) = g(\sigma_{y_1}(\frac{t}{n},x_0),y_1) = g(x_1,y_1),\end{aligned}$$

where $\sigma_{x_0}(\frac{t}{n}, y_0) = y_1$, $\sigma_{y_1}(\frac{t}{n}, x_0) = x_1$, $r \to \sigma_{y_0}(r, x_0)$ solves the separable equation

$$x'(t) = F(x(t), y_0), x(0) = x_0$$

and $r \to \sigma_{x_0}(r, y_0)$ solves the separable equation $y^{'}(t) = G(x_0, y(t)), y(0) = y_0$.

$$\begin{aligned}\textbf{Step 2}:\ (T_1(\frac{t}{n})T_2(\frac{t}{n}))^2 g(x_0, y_0) =& T_1(\frac{t}{n})T_2(\frac{t}{n})g(x_1, y_1)\\ = T_1(\frac{t}{n})g(x_1, \sigma_{x_1}(\frac{t}{n}, y_1)) =& T_1(\frac{t}{n})g(x_1, y_2)\\ = g(\sigma_{y_2}(\frac{t}{n}, x_1), y_2) =& g(x_2, y_2),\end{aligned}$$

where $\sigma_{x_1}(\frac{t}{n}, y_1) = y_2$, $\sigma_{y_2}(\frac{t}{n}, x_1) = x_2$, $r \to \sigma_{y_2}(r, x_1)$ solves the separable equation

$$x'(t) = F(x(t), y_0), x(0) = x_1$$

and $r \to \sigma_{x_1}(r, y_2)$ solves the separable equation

$$y'(t) = G(x_1, y(t)), y(0) = y_2.$$

This yields the following algorithm. For $0 \le k \le n$, define $x_{k,n} = (x_k, y_y)$ by

$$\begin{aligned} x_{0,n} &:= (x_0, y_0),\\ x_{1,n} &:= (\sigma_{y_1}(\frac{t}{n}, x_0), \sigma_{x_0}(\frac{t}{n}, y_0)) = (x_1, y_1),\\ x_{2,n} &:= (\sigma_{y_2}(\frac{t}{n}, x_1), \sigma_{x_1}(\frac{t}{n}, y_1)) = (x_2, y_2),\\ &\vdots\\ x_{n,n} &:= (\sigma_{y_n}(\frac{t}{n}, x_{n-1}), \sigma_{x_{n-1}}(\frac{t}{n}, y_{n-1})) = (x_n, y_n),\end{aligned} \tag{3.3.20}$$

where $r \to \sigma_{y_k}(r, x_{k-1})$ solves

$$x'(r) = F(x(r), y_k), \quad x(0) = x_{k-1},$$

and $r \to \sigma_{x_k}(r, y_k)$ solves

$$y'(r) = G(x_k, y(r)), \quad y(0) = y_k.$$

Step n: After n steps, this yields

$$(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(x,y) = g(x_n, y_n).$$

This implies the following algorithm.

Algorithm 3.3. Lie-Trotter product of nonlinear two-dimensional ODEs of the form (3.3.13)

Require: $\sigma_x(t,y)$, $\sigma_y(x,t)$, T: time interval, n: number of iterations

procedure $(x_n, y_n) := (NL_x, NL_y)$
  for $t \leftarrow T$ **do**
    $L_x \leftarrow x_0$
    $L_y \leftarrow y_0$
    for $i \leftarrow n$ **do**
      $L_x \leftarrow \sigma_{L_y}(\frac{t}{n}, L_x)$
      $L_y \leftarrow \sigma_{L_x}(\frac{t}{n}, L_y)$
      $NL_x \leftarrow L_x$
      $NL_y \leftarrow L_y$
    end for
    return $(x_n, y_n) := (NL_x,\ NL_y)$
  end for

If we assume some suitable conditions on the functions F, G, g and $\mathcal{M}$, then

$$\lim_{n\to\infty}(T_1(\frac{t}{n})T_2(\frac{t}{n}))^n g(x,y) = \lim_{n\to\infty} g(x_n, y_n) = g(\sigma(t,x,y)) = g((x(t), y(t))$$

and

$$\lim_{n\to\infty} x_{n,n} := \lim_{n\to\infty}(x_n, y_n) = (x(t), y(t)) := \sigma(t, x, y).$$

Similarly, we can derive the following algorithm for the Strang product formula.

3.4. Higher-order Exponential Splitting Schemes

In [17] and [18], E. Hansen and A. Ostermann consider exponential splitting schemes

$$V_p(t) := \prod_{j=1}^{s} e^{\alpha_j t \mathcal{K}_1} e^{\beta_j t \mathcal{K}_2}, \tag{3.4.1}$$

Algorithm 3.4. Strang product of nonlinear two-dimensional ODEs of the form (3.3.13)

Require: $\sigma_x(t, y)$, $\sigma_y(x, t)$, T: time interval, n: number of iterations

procedure $(x_n, y_n) := (NS_x, NS_y)$
  for $t \leftarrow T$ **do**
    $S_x \leftarrow x_0$
    $S_y \leftarrow y_0$
    for $i \leftarrow n$ **do**
      $S_x \leftarrow \sigma_{S_y}(\frac{t}{2n}, S_x)$
      $S_y \leftarrow \sigma_{S_x}(\frac{t}{n}, S_y)$
      $S_x \leftarrow \sigma_{S_y}(\frac{t}{2n}, S_x)$
      $NS_x \leftarrow S_x$
      $NS_y \leftarrow S_y$
    end for
    return $(x_n, y_n) := (NS_x,\ NS_y)$
  end for

where the real or complex coefficients α_j's and β_j's are chosen in such a way that the method is algebraically of order p, meaning that whenever the operators $\mathcal{K}, \mathcal{K}_i$ are replaced by finite matrices $\mathcal{M}, \mathcal{M}_i$, we have

$$\|V(t) - e^{t\mathcal{M}}\| = O(t^{p+1}).$$

For such s-stage schemes, they provide a general error-estimate framework for the approximations of solutions of linear problems of the form

$$x'(t) = \mathcal{K}x(t) = (\mathcal{K}_1 + \mathcal{K}_2)x(t), \quad x(0) = x \tag{3.4.2}$$

where $\mathcal{K}_1$, $\mathcal{K}_1$, and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ are generators of strongly continuous contraction semigroups (or analytic contraction semigroups if the coefficients α_j's and β_j's are complex). Their analysis is based on the consideration of the operators E_{p+1} that can be obtained as the product of exactly $p + 1$ factors chosen among $\mathcal{K}_1$ or $\mathcal{K}_2$.

Theorem 3.4.1. *[17], [18]. Let $\mathcal{K}_1$, $\mathcal{K}_2$, and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ be generators of strongly continuous contraction semigroups on a Banach space X (or analytic contraction semi-*

groups if the coefficients α_j*'s and* β_j*'s are complex). Assume that there exists a subspace* $U \subset D(\mathcal{K}^{p+1})$ *such that all* $E_{p+1}e^{t\mathcal{K}} : U \to X$ *are well defined and all* $E_{p+1}e^{t\mathcal{K}}u$ *are uniformly bounded in* $t \in [0,T]$ *for any* $u \in U$*. Then, for all* $u \in U$ *and* $T > 0$*, there exists a constant* $M_{u,T}$ *such that*

$$\|V_p(\frac{t}{n})^n u - e^{t\mathcal{K}}u\| \leq M_{u,T}\frac{t^{p+1}}{n^p(p+1)!}, \quad 0 \leq t \leq T. \tag{3.4.3}$$

Outline of proof: The proof is based on estimate of the form (3.2.2); i.e,

$$\begin{aligned}\|V_p(\frac{t}{n})^n x - (e^{\frac{t\mathcal{K}}{n}})^n x\| &= \|\sum_{j=0}^{n-1} V_p(\frac{t}{n})^{n-j-1}(V_p(\frac{t}{n}) - e^{\frac{t\mathcal{K}}{n}})e^{j\frac{t\mathcal{K}}{n}}x\| \\ &\leq \sum_{j=0}^{n-1} \|(V_p(\frac{t}{n}) - e^{\frac{t\mathcal{K}}{n}})e^{j\frac{t\mathcal{K}}{n}}x\|\end{aligned} \tag{3.4.4}$$

and a sophisticated and elaborate estimate of the term $\|(V_p(\frac{t}{n}) - e^{\frac{t\mathcal{K}}{n}})e^{j\frac{t\mathcal{K}}{n}}x\|$. □

Remark 3.4.2. Since the proof of Theorem 3.4.1 given in [17] is of an algebraic nature, it can be extended to bi-continuous contraction semigroups without changing any of arguments.

For more details on higher-order splitting methods and consistency bounds, see [19], [29], and [48].

Remark 3.4.3. It is a well-known fact, that splitting schemes of the form (3.4.1) with real coefficients $\gamma_{j,i}$ must include at least one negative coefficient $\gamma_{j,i}$ whenever the algebraic order p is larger than 2. Consequently, such higher-order schemes can only be applied if the operator $\mathcal{K}_i$ generates a group rather than a semigroup or if complex coefficients $\gamma_{j,i}$ are allowed. The latter approach was adopted in [18], where E. Hansen and A. Ostermann extended Theorem 3.4.1 to support splitting methods of algebraic order $p \geq 3$ with complex coefficients $\gamma_{j,i} \in \Sigma_\alpha := \{z \in \mathbb{C} : |\arg(z)| < \alpha\}$ for $1 \leq j \leq m$ and $1 \leq i \leq N$ and assuming that the operators $\mathcal{K}, \mathcal{K}_i$ $(1 \leq i \leq N)$ generate analytic contraction semigroups on Σ_α. This allowed the use of algebraically higher-order schemes for analytic semigroups; for details, see [18] and [3].

To obtain a 3-stage splitting of the form (3.4.1), consider

$$\mathcal{K} = \alpha_1\mathcal{K}_1 + \beta_1\mathcal{K}_2 + \alpha_2\mathcal{K}_1 + \beta_2\mathcal{K}_2 + \alpha_3\mathcal{K}_1 + \beta_3\mathcal{K}_2$$

with $\alpha_1 + \alpha_2 + \alpha_3 = 1$, $\beta_1 + \beta_2 + \beta_3 = 1$ for which the associated product formula

$$V(t) = e^{\alpha_1 t\mathcal{K}_1} e^{\beta_1 t\mathcal{K}_2} e^{\alpha_2 t\mathcal{K}_1} e^{\beta_2 t\mathcal{K}_2} e^{\alpha_3 t\mathcal{K}_1} e^{\beta_3 t\mathcal{K}_2}$$

is algebraically of order $p = 3$.

The coefficients α_i and β_i are chosen such that the first 4 terms of the Taylor expansions of $e^{t(\mathcal{K}_1+\mathcal{K}_2)}$ and $V(t)$ coincide to obtain classical order 3 (see the Hansen-Ostermann Theorem 3.4.1). As shown in [4], for all s-stage splitting schemes with classical order $p \geq 3$ for which all coefficients α_i, β_i are real numbers, at least one of them must be negative. Since, in general, not all semigroups $e^{t\mathcal{K}}$ and $e^{t\mathcal{K}_i}$ are well-defined for negative times t, such schemes would not work for higher-order approximations unless the corresponding semigroup(s) are (local) groups. By comparing the coefficients α_i, β_i, one can derive the following proposition.

Proposition 3.4.4. *Let* $\alpha = \frac{1}{2} + \frac{i\sqrt{3}}{6}$ *and*

$$V_3(t) = e^{\alpha\frac{t}{2}\mathcal{K}_2} e^{\alpha t\mathcal{K}_1} e^{\frac{t}{2}\mathcal{K}_2} e^{\bar{\alpha} t\mathcal{K}_1} e^{\bar{\alpha}\frac{t}{2}\mathcal{K}_2}. \tag{3.4.5}$$

Then the formula of the complex product $V_3(t)$ *is algebraically of order* $p = 3$.

Remark 3.4.5. Deriving higher-order methods by comparing coefficients becomes increasingly challenging as the number of coefficients grows rapidly. To overcome these algebraic complexities, the following statements explore how higher-order splitting schemes can be constructed by composing lower-order schemes.

These statements give higher-order product formulas for splittings $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2$ and $\mathcal{K} = \mathcal{K}_1 + \mathcal{K}_2 + \cdots + \mathcal{K}_N$ that were obtained via composition methods by F. Castella, P. Chartier, S. Descombes, G. Vilmart as well as E. Hansen and A. Ostermann in 2009 (see [18] and [44]). We follow the exposition given in [18]. Examples of composition methods that can be found in these articles are as follows, where

$$V_2(t) = e^{\frac{t}{2}\mathcal{K}_2} e^{t\mathcal{K}_1} e^{\frac{t}{2}\mathcal{K}_2} := S(0,t) = S_t$$

denotes the Strang product.

(1) For $1 \leq k \leq 4$, $V_p(t) = S(k,t) := S(k-1, \bar{\alpha}_k t) S(k-1, \alpha_k t)$ with the complex coefficients $\alpha_k := \frac{1}{2} + i\frac{\sin(\pi/(k+2))}{2+2\cos(\pi/(k+2))}$. Then the splitting schemes $V_p(t)$ are of order $p = k+2$ and have $2^{k+1}+1$ exponential terms. Moreover, if $k = 1$, then we get a splitting method of order 3

$$V_3(t) = S(1,t) = S(0, \bar{\alpha}_t) S(0, \alpha_t).$$

where, the coefficients $\alpha = 0.5 - 0.288675i$. Therefore, $V_3(t) = e^{\frac{\alpha t}{2}\mathcal{K}_1} e^{\alpha t \mathcal{K}_2} e^{\frac{t}{2}\mathcal{K}_1} e^{\bar{\alpha} t \mathcal{K}_2} e^{\frac{\bar{\alpha} t}{2}\mathcal{K}_1}$.

(2) For $1 \leq k \leq 3$ define $V_p(t) = S(k,t) := S(k-1, \alpha_k t) S(k-1, 1-2\alpha_k t) S(k-1, \alpha_k t)$ with, $\alpha_k := \frac{e^{\pi i/(2k+1)}}{2^{1/(2k+1)} + e^{\pi i/(2k+1)}}$. Then the splitting schemes $V_p(t)$ are of order $p = 2k+2$ and have $2(3^k)+1$ exponential terms.

(3) For $1 \leq k \leq 6$, $V_p(t) = S(k,t) := S(k-1, \alpha_k t) S(k-1, \bar{\alpha}_k t) S(k-1, \bar{\alpha}_k t) S(k-1, \alpha_k t)$ with $\alpha_k := \frac{1}{4} + i\frac{\sin(\pi/(2k+1))}{4+4\cos(\pi/(2k+1))}$. Then the splitting schemes $V_p(t)$ are of order $p = 2k+2$ and have $2(4^k)+1$ exponential terms.

3.5. Numerical Experiments

In this section, we present numerical examples to validate the product splitting formulas by approximating solutions to the Van der Pol equation, the two-dimensional and three-dimensional Lotka-Volterra systems, and a non-autonomous equation exhibiting finite blow-up.

Example 3.5.1. Consider the initial value problem

$$x'(t) = \frac{1}{10-t}x(t), \;\; x(s) = x \in \Omega := \mathbb{R}, \;\; (0 \leq s \leq t < 10). \tag{3.5.1}$$

The unique solution is given by

$$x(t) = \frac{10-s}{10-t}x \tag{3.5.2}$$

with the stopping time $m(s,x) = 10 - s$.

Let $r \to \sigma_s(r,x)$ be the solution of $x'(r) = \frac{1}{10-s}x(r)$, $x(0) = x$. So,

$$\sigma_s(r,x) = x(r) = e^{\frac{1}{10-s}r}x.$$

Applying the Lie-Trotter algorithm (3.3.9), yields

$$\begin{aligned}
x_{0,n} &= x, \\
x_{1,n} &= \sigma_s(\frac{t}{n}, x_{0,n}) = e^{\frac{1}{10-s}\frac{t}{n}}x_{0,n} = e^{\frac{1}{10-s}\frac{t}{n}}x, \\
x_{2,n} &= \sigma_{s+\frac{t}{n}}(\frac{t}{n}, x_{1,n}) = e^{\frac{1}{10-(s+\frac{t}{n})}\frac{t}{n}}x_{1,n} = e^{\frac{1}{10-(s+\frac{t}{n})}\frac{t}{n}}e^{\frac{1}{10-s}\frac{t}{n}}x, \\
&\vdots \\
x_{n,n} &= \sigma_{s+\frac{(n-1)t}{n}}(\frac{t}{n}, x_{n-1,n}) = e^{\frac{1}{10-(s+\frac{(n-1)t}{n})}\frac{t}{n}}x_{n-1,n} = \prod_{i=1}^{n-1} e^{\frac{1}{10-(s+\frac{it}{n})}\frac{t}{n}}x.
\end{aligned} \tag{3.5.3}$$

The algorithm for Strang product formula (3.3.12) yields

$$
\begin{aligned}
x_{0,n} &:= x, \\
x_{1,n} &:= \sigma_{s+\frac{t}{2n}}(\frac{t}{n}, x_{0,n}) = e^{\frac{1}{10-(s+\frac{t}{2n})}\frac{t}{n}} x, \\
x_{2,n} &:= \sigma_{s+\frac{3t}{2n}}(\frac{t}{n}, x_{1,n}) = e^{\frac{1}{10-(s+\frac{3t}{2n})}\frac{t}{n}} e^{\frac{1}{10-(s+\frac{t}{2n})}\frac{t}{n}} x, \\
&\vdots \\
x_{n,n} &:= \sigma_{s+\frac{(2n-1)t}{2n}}(\frac{t}{n}, x_{n-1,n}) = \prod_{i=1}^{n} e^{\frac{1}{10-(s+\frac{(2i-1)t}{2n})}\frac{t}{n}} x.
\end{aligned}
\tag{3.5.4}
$$

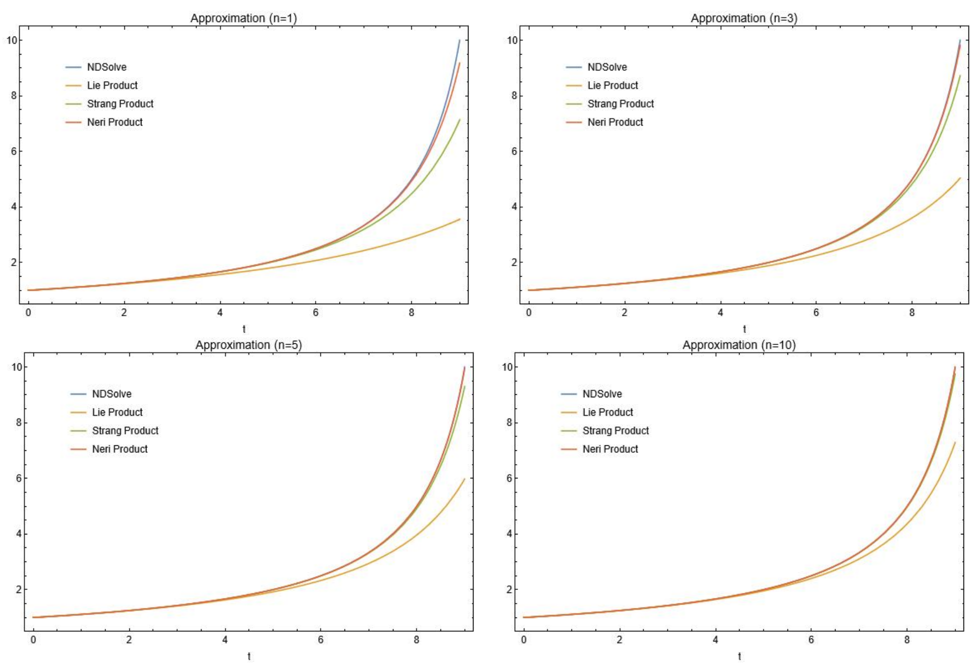


Figure 3.1. Plot of (3.5.1) and of the approximations $x_{n,n}$ for Lie-Trotter and Strang with $n = 1, 3, 5$ and 10.

The tables show the absolute error of the Lie-Trotter approximation (E_{Lie}) and Strang product (E_{Strang}) with $n = 1, 3, 5$ and 10.

Table 3.1. Absolute error of Lie-Trotter product (E_{Lie}).

t	$n = 1$	$n = 3$	$n = 5$	$n = 10$
1.0	0.0059	0.0020	0.0012	0.0006
2.0	0.0286	0.0101	0.0061	0.0031
3.0	0.0787	0.0291	0.0178	0.0090
4.0	0.1748	0.0683	0.0423	0.0217
5.0	0.3513	0.1473	0.0928	0.0482
6.0	0.6779	0.3112	0.2009	0.1062
7.0	1.3196	0.6817	0.4562	0.2488
8.0	2.7745	1.6741	1.1889	0.6853
9.0	7.5404	5.6133	4.4438	2.8992

Table 3.2. Absolute error of Strang product (E_{Strang}).

t	$n = 1$	$n = 3$	$n = 5$	$n = 10$
1.0	0.000108194	0.0000120851	4.36732×10^{-6}	1.11008×10^{-6}
2.0	0.00115114	0.000129952	0.0000468494	0.0000117255
3.0	0.00532392	0.000616061	0.000222506	0.0000556469
4.0	0.0179452	0.00216812	0.000786471	0.000197153
5.0	0.0522659	0.00677339	0.00247696	0.000623447
6.0	0.143582	0.0207988	0.00772582	0.00195936
7.0	0.397701	0.0687725	0.0263858	0.00680487
8.0	1.20633	0.278452	0.114992	0.0310401
9.0	4.86355	1.84692	0.925169	0.294043

Now, we investigate the constant $M_{x,T,P}$ for each of the Lie-Trotter, Strang product formulas. To do so, we need to compute $E_{Lie}\frac{2!n}{t^2}$ and $E_{Strang}\frac{3!n^2}{t^3}$.

Table 3.3. The values of $E_{Lie}\frac{2!n}{t^2}$.

t	$n=1$	$n=3$	$n=5$	$n=10$
1.0	0.0119	0.0122	0.01225	0.0123
2.0	0.0143	0.0152	0.01535	0.0155
3.0	0.0175	0.0194	0.0198	0.0201
4.0	0.0219	0.0256	0.0265	0.0271
5.0	0.0281	0.0353	0.0371	0.0385
6.0	0.0377	0.0519	0.0558	0.059
7.0	0.0539	0.0835	0.09310102041	0.1015
8.0	0.0867	0.1569	0.1858	0.2141
9.0	0.1862	0.4158	0.5486	0.7158

Table 3.4. The values of $E_{Strang}\frac{3!n^2}{t^3}$.

t	$n=1$	$n=3$	$n=5$	$n=10$
1.0	0.0006	0.00065	0.00066	0.00066
2.0	0.00086	0.00088	0.000878	0.000879
3.0	0.00118	0.0012	0.00124	0.00124
4.0	0.0017	0.0018	0.0018	0.00185
5.0	0.00251	0.00293	0.00297	0.00299
6.0	0.00399	0.0052	0.0054	0.0054
7.0	0.00695	0.01083	0.01154	0.0119
8.0	0.01414	0.0294	0.03369	0.0364
9.0	0.04003	0.13681	0.19036	0.242

Based on the tables above and since $M_{x,T,p} \geq E_{Lie}\frac{(2!)n}{t^2}$, and $M_{x,T,p} \geq E_{Strang}\frac{(3!)n^2}{t^3}$ for all $t \in [0,8]$. Then candidates for the constants $M_{x,T,p}$ are 1 and 0.1.

Example 3.5.2. The **Lotka-Volterra model**, also known as the predator-prey model, consists of a system of differential equations that describe the dynamics of two interacting species: a predator and its prey. The model is given by

$$\begin{aligned} x'(t) &= \alpha x(t) - \beta x(t)y(t) = F_1(x(t), y(t)) \text{ with } F_1(x,y) = \alpha x - \beta xy, \text{ and} \\ y'(t) &= \delta x(t)y(t) - \gamma y(t) = F_2(x(t), y(t)) \text{ with } F_2(x,y) = \delta xy - \gamma y, \end{aligned} \tag{3.5.5}$$

where $x(t), y(t)$ represent the prey and predator populations, respectively and $(x(0), y(0)) = (x, y) \in \Omega := \mathbb{R}^2_+$. The parameters $\alpha, \beta, \delta, \gamma$ denote the prey's growth rate, the predation rate, the predator's growth rate, and the predator's natural death rate, respectively.

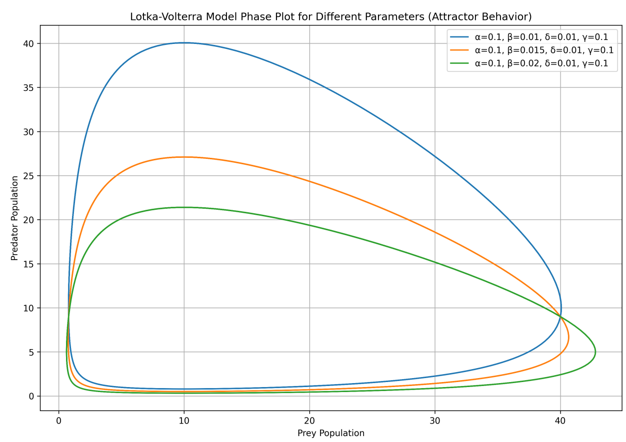


Figure 3.2. Lotka-Volterra model

If $u'(t) := (x'(t), y'(t)) = (F_1(u(t)), F_2(u(t)))$, $u(0) = (x, y) := u$, has unique, global, jointly continuous solutions $\sigma(t, u) \in \Omega$ then

$$T(t)g(x,y) = T(t)g(u) := g(\sigma(t,u)) = e^{t\mathcal{K}}g(u) = e^{t(\mathcal{K}_1 + \mathcal{K}_2)}g(u)$$

is bi-continuous on $C_b(\Omega)$, where the associated Koopman-Lie flow semigroup operator is given by

$$\begin{aligned} \mathcal{K}g(x,y) &= F_1(x,y)g_x(x,y) + F_2(x,y)g_y(x,y) \\ &= (\alpha x - \beta xy)g_x(x,y) + (\delta xy - \gamma y)g_y(x,y) \\ &= \mathcal{K}_1 g(x,y) + \mathcal{K}_2 g(x,y), \end{aligned} \tag{3.5.6}$$

and the Koopman-Lie semigroups generated by $\mathcal{K}_1$ and $\mathcal{K}_2$ are given by

$$e^{t\mathcal{K}_1}g(x,y) = g(\sigma_y(t,x),y) = g(xe^{t(\alpha-\beta y)},y) \tag{3.5.7}$$

and

$$e^{t\mathcal{K}_2}g(x,y) = g(x,\sigma_x(t,y)) = g(x,ye^{t(\delta x-\gamma)}) \tag{3.5.8}$$

where, $\sigma_y(t,x)$ solves the frozen problem $x'(t) = F_1(x(t),y), x(0) = x$, and $\sigma_x(t,y)$ solves the frozen problem $y'(t) = F_2(x,y(t)), y(0) = y$. Thus,

$$g(\sigma(t,x)) = T(t)g(x) = \lim_{n\to\infty}\left(V(\frac{t}{n})\right)^n g(x) = \lim_{n\to\infty} g(x_n(t,x)).$$

By Proposition 3.2.3, $\sigma(t,x) = \lim_{n\to\infty} x_n(t,x)$. This is equivalent to solving

$$(x'(t),y'(t)) = (F_1(x(t),y(t)),F_2(x(t),y(t))),(x(0),y(0)) = (x,y)$$

via separation of variables after splitting into first-order sub-problems.

The Lie-Trotter product formula 3.2.10 can be computed using the following algorithm with starting values $x_0 := x$, $y_0 := y$. Then, for $0 \le k \le n-1$, we use the iterative process

$$\begin{aligned} x_{k+1} &= \sigma_{y_k}(\frac{t}{n}, x_k), \\ y_{k+1} &= \gamma_{x_{k+1}}(\frac{t}{n}, y_k). \end{aligned}$$

Then, $x_n = x_n(t) \approx x(t)$ $y_n = y_n(t) \approx y(t)$ with approximation order $C\frac{t^2}{n}$.

Also, the Strang product formula 3.2.11 can be computed using the following algorithm with starting values $x_0 := x$, $y_0 := y$. Then, for $0 \le k \le n-1$, we use the iterative process

$$\begin{aligned} x_{k+\frac{1}{2}} &= \sigma_{y_k}(\frac{t}{2n}, x_k), \\ y_{k+1} &= \gamma_{x_{k+\frac{1}{2}}}(\frac{t}{n}, y_k), \\ x_{k+1} &= \sigma_{y_{k+1}}(\frac{t}{2n}, x_{k+\frac{1}{2}}). \end{aligned}$$

Then, $x_n = x_n(t) \approx x(t)$ $y_n = y_n(t) \approx y(t)$ with approximation order $C\frac{t^3}{n^2}$. In the following numerical experiments, we consider $\alpha = 0.5$, $\beta = 0.02$, $\delta = 0.01$, and $\gamma = 0.1$ with the initial condition $(x(0), y(0)) = (100, 10)$. The following results compare the Lie-Trotter product and Strang splitting with the solutions $(\widetilde{x}(t), \widetilde{y}(t))$ obtained via the Runge-Kutta method (RK45).

Table 3.5. Lie-Trotter Product of Lotka-Volterra model, $n = 10000$.

t	$x(t)$	$y(t)$	$\widetilde{x}(t)$	$\widetilde{y}(t)$
1	117.160670620	27.604837164	117.143820465	27.600467195
2	75.643384472	69.143994558	75.615237258	69.129778453
3	21.942726609	98.691442365	21.934236637	98.679538925
4	4.825482261	100.000531711	4.824448573	99.993309504
5	1.151414702	92.805048116	1.151392438	92.799722713
6	0.322330576	84.514382737	0.322382332	84.5099123
7	0.106184183	76.618782889	0.10621877	76.614846323
8	0.040702636	69.374318295	0.040721713	69.37079497
9	0.017915321	62.78971665	0.0179260502	62.786544021
10	0.008939381	56.821746577	0.008945989	56.818882625

Table 3.6. Absolute error of Lie-Trotter of Lotka-Volterra model, $n = 10000$.

t	$E_r x(t)$	$E_r y(t)$
1	0.004369969	0.004369969
2	0.028147214	0.014216105
3	0.008489972	0.01190344
4	0.001033688	0.007222207
5	2.2264E-05	0.005325403
6	5.1756E-05	0.004470437
7	3.4587E-05	0.003936566
8	1.9077E-05	0.003523325
9	1.07292E-05	0.003172629
10	6.608E-06	0.002863952

Table 3.7. Strang Product of Lotka-Volterra model, $n = 10000$.

t	$x(t)$	$y(t)$	$\widetilde{x}(t)$	$\widetilde{y}(t)$
1	117.143751536	27.600501854	117.143820465	27.600467195
2	75.615382104	69.129762398	75.615237258	69.129778453
3	21.934292173	98.679585668	21.934236637	98.679538925
4	4.8244526642	99.993382872	4.824448573	99.993309504
5	1.151391314	92.79979168	1.151392438	92.799722713
6	0.322381629	84.50997424	0.322382332	84.5099123
7	0.10621816	76.614902263	0.10621877	76.614846323
8	0.040721599	69.370845206	0.040721713	69.37079497
9	0.017926029	62.786589394	0.0179260502	62.786544021
10	0.00894579	56.818923838	0.008945989	56.818882625

Table 3.8. Absolute error of Strang of Lotka-Volterra model, $n = 10000$.

t	$E_r x(t)$	$E_r y(t)$
1	3.4659E-05	3.4659E-05
2	0.000144846	1.6055E-05
3	5.5536E-05	4.6743E-05
4	4.0912E-06	7.3368E-05
5	1.124E-06	6.8967E-05
6	7.03E-07	6.194E-05
7	6.1E-07	5.594E-05
8	1.14E-07	5.0236E-05
9	2.12E-08	4.5373E-05
10	1.99E-07	4.1213E-05

Example 3.5.3. In Section 3.3, we already two-dimensional systems of nonlinear ODEs of the form (3.3.13) and the associated Koopman-Lie flow semigroups (see, 3.3.15), (3.3.17), and (3.3.18). This framework can be readily applied to generalized Van der Pol equation of the form

$$x''(t) - a(x(t))x'(t) - b(x(t)) = 0 \tag{3.5.9}$$

with initial values $(x(0), x'(0)) = (x, y) \in \Omega = \mathbb{R}^2$ and where $a(\cdot)$ and $b(\cdot)$ are sufficiently smooth real-valued functions such that the following first order problem has unique, global, jointly continuous solutions for all $x_1, x_2 \in \Omega := \mathbb{R}^2$.

First, we rewrite (3.5.9) as a first order system

$$\begin{aligned} x'(t) &= y(t), \\ y'(t) &= a(x(t))x'(t) + b(x(t)) \end{aligned} \tag{3.5.10}$$

and solve

$$\begin{aligned} x'(t) &= F(x(t), y(t)) \text{ with } F(x, y) = y, \text{ and} \\ y'(t) &= G(x(t), y(t)) \text{ with } G(x, y) = a(x)y + b(x). \end{aligned} \tag{3.5.11}$$

Let $\sigma(t, x) := (x(t), y(t))$ be the global, jointly continuous flow defined by the unique solution $x(\cdot)$ and $y(\cdot)$ of the above system. The associated Koopman-Lie flow semigroup operator $T(t)g(x) := g(\sigma(t, x))$ is bi-continuous on $C_b(\mathbb{R}^2)$ with generator $\mathcal{K}$, which is given by:

$$\begin{aligned} \mathcal{K}g(x, y) &= F(x, y)g_x(x, y) + G(x, y)g_y(x, y) \\ &= yg_x(x, y) + (a(x)y + b(x))g_y(x, y) \\ &= \mathcal{K}_1 g(x, y) + \mathcal{K}_2 g(x, y), \end{aligned} \tag{3.5.12}$$

and the Koopman-Lie semigroups generated by $\mathcal{K}_1$ and $\mathcal{K}_2$ are given by

$$e^{t\mathcal{K}_1} g(x, y) = g(ty + x, y) \tag{3.5.13}$$

and

$$e^{t\mathcal{K}_2} g(x, y) = \begin{cases} g(x, \frac{b(x)(e^{a(x)t}-1)}{a(x)} + ye^{a(x)t}) & \text{if } a(x) \neq 0 \\ \\ g(x, b(x)t + y) & \text{if } a(x) = 0. \end{cases} \tag{3.5.14}$$

If $a(x(t)) = 1 - x^2(t)$ and $b(x(t)) = -x(t)$, then (3.5.9) becomes the classical Van der Pol equation

$$x^{''}(t) - (1 - x^2(t))x'(t) + x(t) = 0, \tag{3.5.15}$$

for the initial values $(x(0), x'(0)) = (0, 1)$. Applying the splitting methods described in Section 3.3, yields

$$\sigma_y(t, x) = ty + x$$

as well as

$$\sigma_x(t, y) = \begin{cases} \frac{x(1-e^{(1-x^2)t})}{1-x^2} + ye^{(1-x^2)t} & 1 - x^2 \neq 0 \\ \\ -xt + y & 1 - x^2 = 0 \end{cases}$$

Now, we investigate the approximation on the time interval $[0, 2.5]$ and $n > 1$.

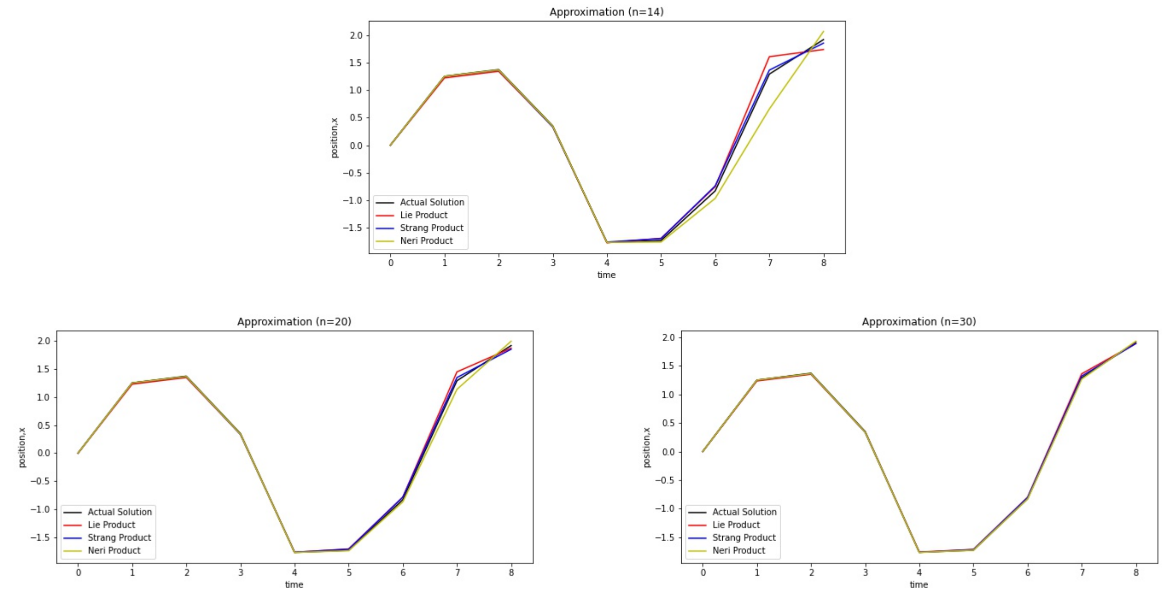


Figure 3.3. Plot of (3.5.15) and the approximations of $x_{n,n}$, for Lie-Trotter, and Strang with $n = 14$, $n = 20$, and $n = 30$.

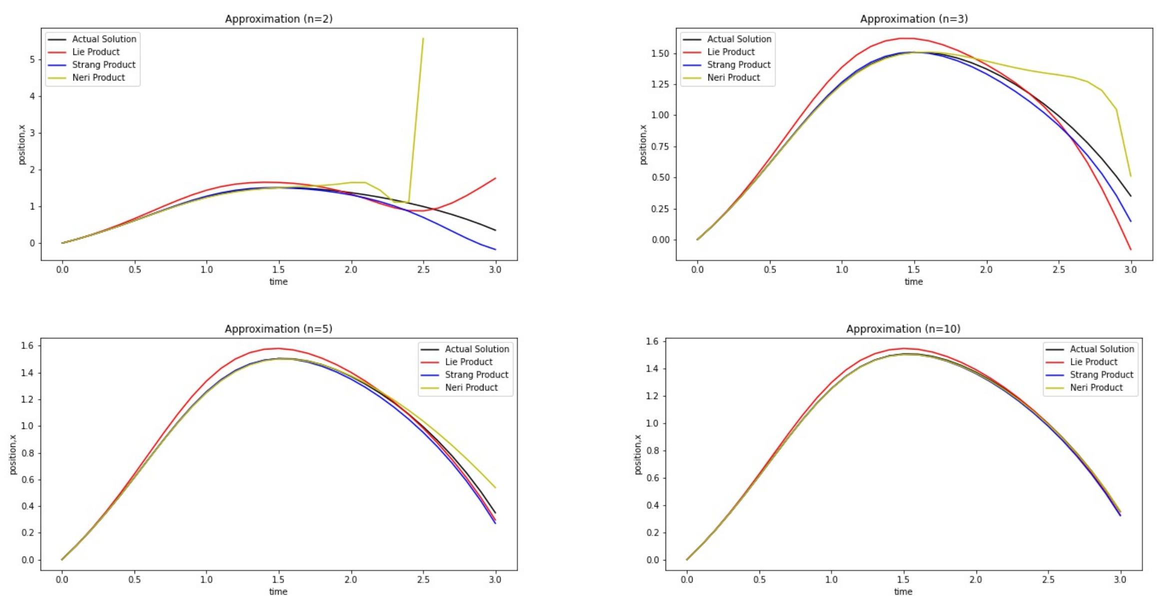


Figure 3.4. Plot of (3.5.15) and the approximations of $x_{n,n}$, for Lie-Trotter and Strang with $n = 2$, 3, 5 and 10.

Table 3.9. Absolute error of Lie-Trotter product (E_{Lie}).

t	$n=2$	$n=3$	$n=5$	$n=10$
0.25	0.016343	0.011142	0.006809	0.003454
0.5	0.064243	0.044899	0.028023	0.014463
0.75	0.127475	0.091454	0.058273	0.030532
1.0	0.174688	0.129131	0.083553	0.044084
1.25	0.194779	0.148395	0.096594	0.051689
1.5	0.21287	0.155385	0.097941	0.051993
1.75	0.268507	0.158893	0.094213	0.048427
2.0	0.3712	0.160081	0.090271	0.04429
2.25	0.482078	0.16204	0.087201	0.04027
2.5	0.528574	0.177817	0.084583	0.035773

Table 3.10. Absolute error of Strang product (E_{Strang}).

t	$n=2$	$n=3$	$n=5$	$n=10$
0.25	0.000069	0.000035	0.000016	0.000008
0.5	0.001526	0.000753	0.000315	0.000123
0.75	0.009833	0.004469	0.001654	0.000459
1.0	0.033582	0.013521	0.004627	0.00101
1.25	0.065834	0.027059	0.010973	0.004195
1.5	0.052395	0.039886	0.017389	0.007453
1.75	0.051609	0.062623	0.023786	0.010148
2.0	0.214013	0.099904	0.031798	0.013071
2.25	0.357868	0.121313	0.041921	0.016384
2.5	0.416515	0.074116	0.055516	0.02024

Example 3.5.4. Consider the Lotka-Volterra model in three dimensions:

$$\begin{aligned} x'(t) &= x(t)(1-y(t)), \\ y'(t) &= y(t)(x(t)-z(t)), \\ z'(t) &= z(t)(y(t)-1), \end{aligned} \tag{3.5.16}$$

where $(x(0), y(0), z(0)) = (x, y, z) \in \Omega := \mathbb{R}^3_+$and rewrite the system 3.5.16 as

$$\begin{aligned} x'(t) &= F_1(x(t), y(t), z(t)) \text{ with } F_1(x, y, z) = x(1-y), \\ y'(t) &= F_2(x(t), y(t), z(t)) \text{ with } F_2(x, y, z) = y(x-z), \text{ and} \\ z'(t) &= F_3(x(t), y(t), z(t)) \text{ with } F_3(x, y, z) = z(y-1). \end{aligned} \tag{3.5.17}$$

Since $u'(t) := (x'(t), y'(t), z'(t)) = (F_1(u(t)), F_2(u(t)), F_3(u(t)))$, $u(0) = (x, y, z) := u$, has unique, global, jointly continuous solutions $\sigma(t, u) \in \Omega$, it follows that

$$T(t)g(x, y, z) = T(t)g(u) := g(\sigma(t, u)) = e^{t\mathcal{K}}g(u) = e^{t(\mathcal{K}_1+\mathcal{K}_2+\mathcal{K}_3)}g(u)$$

is bi-continuous on $C_b(\Omega)$, where the associated Koopman-Lie flow semigroup operator is given by

$$\begin{aligned} \mathcal{K}g(x, y, z) &= F_1(x, y, z)g_x(x, y, z) + F_2(x, y, z)g_y(x, y, z) + F_3(x, y, z)g_z(x, y, z) \\ &= x(1-y)g_x(x, y, z) + y(x-z)g_y(x, y, z) + z(y-1)g_z(x, y, z) \\ &= \mathcal{K}_1 g(x, y, z) + \mathcal{K}_2 g(x, y, z) + \mathcal{K}_3 g(x, y, z), \end{aligned} \tag{3.5.18}$$

and the Koopman-Lie semigroups generated by $\mathcal{K}_1$, $\mathcal{K}_2$, and $\mathcal{K}_3$ are given by

$$\begin{aligned} T_1(t)g(x, y, z) &= e^{t\mathcal{K}_1}g(x, y, z) = g(\sigma_{y,z}(x, y, z)) = g(xe^{t(1-y)}, y, z) \\ T_2(t)g(x, y, z) &= e^{t\mathcal{K}_2}g(x, y, z) = g(\sigma_{x,z}(x, y, z)) = g(x, ye^{(x-z)t}, z) \\ T_3(t)g(x, y, z) &= e^{t\mathcal{K}_3}g(x, y, z) = g(\sigma_{x,y}(x, y, z)) = (x, y, ze^{t(y-1)}) \end{aligned}$$

where $\sigma_{y,z}(t,x)$ solves the frozen problem $x'(t) = F_1(x(t), y, z), x(0) = x$, $\sigma_{x,z}(t, y, z)$ solves the frozen problem $y'(t) = F_2(x, y(t), z), y(0) = y$, and $\sigma_{x,z}(t, y, z)$ solves the frozen problem $z'(t) = F_2(x, y, z(t)), z(0) = z$. Thus,

$$g(\sigma(t,x)) = T(t)g(x) = \lim_{n\to\infty} \left(V(\frac{t}{n})\right)^n g(x) = \lim_{n\to\infty} g(x_n(t,x)),$$

where $V(t)$ be chosen from the list 3.2. By Proposition 3.2.3, $\sigma(t,x) = \lim_{n\to\infty} x_n(t,x)$.

The Lie-Trotter product formula (3.2.12), can be computed as

$$T_1(t)T_2(t)T_3(t)g(x,y,z) = T_1(t)T_2(t)g(x,y,z_{1,t}) = T_1(t)g(x,y_{1,t},z_{1,t}) = g(x_{1,t},y_{1,t},z_{1,t}),$$

where $z_{1,t} = ze^{t(y-1)}$, $\quad y_{1,t} = ye^{t(x-z_1)}$ $\quad$ and $\quad x_{1,t} = xe^{t(1-y_1)}$. Then

$$T_1(t)T_2(t)T_3(t)g(x,y,z) = T_1(t)T_2(t)g(x,y,z_{1,t}) = T_1(t)g(x,y_{1,t},z_{1,t}) = g(x_{1,t},y_{1,t},z_{1,t}),$$

where $z_{2,t} = z_{1,t}e^{t(y_{1,t}-1)}$, $\quad y_{2,t} = y_{1,t}e^{t(x_{1,t}-z_{2,t})}$ $\quad$ and $\quad x_{2,t} = x_{1,t}e^{t(1-y_{2,t})}$. Thus, by induction,

$$(T_1(t)T_2(t)T_3(t))^n g(x,y,z) = T_1(t)T_2(t)T_3(t)g(x_{n-1,t},y_{n-1,t},z_{n-1,t}) = g(x_{n,t},y_{n,t},z_{n,t}),$$

where $z_{n,t} = z_{n-1,t}e^{t(y_{n-1,t}-1)}$, $\quad y_{n,t} = y_{n-1,t}e^{t(x_{n-1,t}-z_{n,t})}$ $\quad$, and $\quad x_{n,t} = x_{n-1,t}e^{t(1-y_{n,t})}$. Therefore, by replacing t by t/n we obtain

$$(T_1(\frac{t}{n})T_2(\frac{t}{n})T_3(\frac{t}{n}))^n g(x,y,z) = g(x_{n,\frac{t}{n}}, y_{n,\frac{t}{n}}, z_{n,\frac{t}{n}})$$

where $(x_{n,\frac{t}{n}}, y_{n,\frac{t}{n}}, z_{n,\frac{t}{n}})$ approximates the solution $(x(t), y(t), z(t))$.

The Lie-Trotter product formula can be computed using the following algorithm with starting values $x_0 := x$, $y_0 := y$. Then, for $0 \le k \le n-1$, we use the iterative process

$$z_{k+1} = \sigma_{y_k, x_k}(\frac{t}{n}, z_k),$$

$$y_{k+1} = \sigma x_k, z_{k+1}(\frac{t}{n}, y_k),$$

$$x_{k+1} = \sigma_{y_{k+1}, z_{k+1}}(\frac{t}{n}, x_k).$$

Then $x_n = x_n(t) \approx x(t)$ and $y_n = y_n(t) \approx y(t)$ with approximation order $C\frac{t^2}{n}$.

In order to use the Strang product formula (3.2.13), we need to compute

$$\begin{aligned}
&T_3(t/2)T_2(t/2)T_1(t)T_2(t/2)T_3(t/2)g(x,y,z) \\
&= T_3(t/2)T_2(t/2)T_1(t)T_2(t/2)g\big(x, y, ze^{\frac{t}{2}(y-1)}\big) \\
&= T_3(t/2)T_2(t/2)T_1(t)g\big(x, ye^{\frac{t}{2}(x-z_{1,\frac{t}{2}})}, z_{1,\frac{t}{2}}\big) \\
&= T_3(t/2)T_2(t/2)g\big(xe^{t(1-y_{1,\frac{t}{2}})}, y_{1,\frac{t}{2}}, z_{1,\frac{t}{2}}\big) \\
&= T_3(t/2)g\big(x_{1,t}, y_{1,\frac{t}{2}}e^{\frac{t}{2}(x_{1,t}-z_{1,\frac{t}{2}})}, z_{1,t/2}\big) = g\big(x_{1,t}, y_{2,\frac{t}{2}}, z_{2,\frac{t}{2}}\big),
\end{aligned}$$

where $z_{1,\frac{t}{2}} = ze^{\frac{t}{2}(y-1)}$, $y_{1,\frac{t}{2}} = ye^{\frac{t}{2}(x-z_{1,\frac{t}{2}})}$, $x_{1,t} = xe^{t(1-y_{1,\frac{t}{2}})}$, $y_{2,\frac{t}{2}} = y_{1,\frac{t}{2}}e^{\frac{t}{2}(x_{1,t}-z_{1,\frac{t}{2}})}$, and $z_{2,\frac{t}{2}} = ze^{\frac{t}{2}(y_{2,\frac{t}{2}}-1)}$. By induction,

$$(T_3(t/2)T_2(t/2)T_1(t)T_2(t/2)T_3(t/2))^n g(x,y,z) = g(x_{n,t}, y_{n,\frac{t}{2}}, z_{n,\frac{t}{2}}).$$

Therefore, by replacing t by t/n we obtain

$$(T_3(\frac{t}{2n})T_2(\frac{t}{2n})T_1(\frac{t}{n})T_2(\frac{2t}{n})T_3(\frac{t}{2n}))^n g(x,y,z) = g(x_{n,\frac{t}{n}}, y_{n,\frac{t}{n}}, z_{n,\frac{t}{n}})$$

where $(x_{n,\frac{t}{n}}, y_{n,\frac{t}{n}}, z_{n,\frac{t}{n}})$ approximates the solution $(x(t), y(t), z(t))$ of (3.5.16). In the following numerical experiments, we consider the initial condition $(x(0), y(0), z(0)) = (10, 5, 2)$. The results compare the solutions obtained via the Lie-Trotter product and Strang splitting with the approximations $(\widetilde{x}(t), \widetilde{y}(t), \widetilde{z}(t))$ obtained with the Runge-Kutta method (RK45).

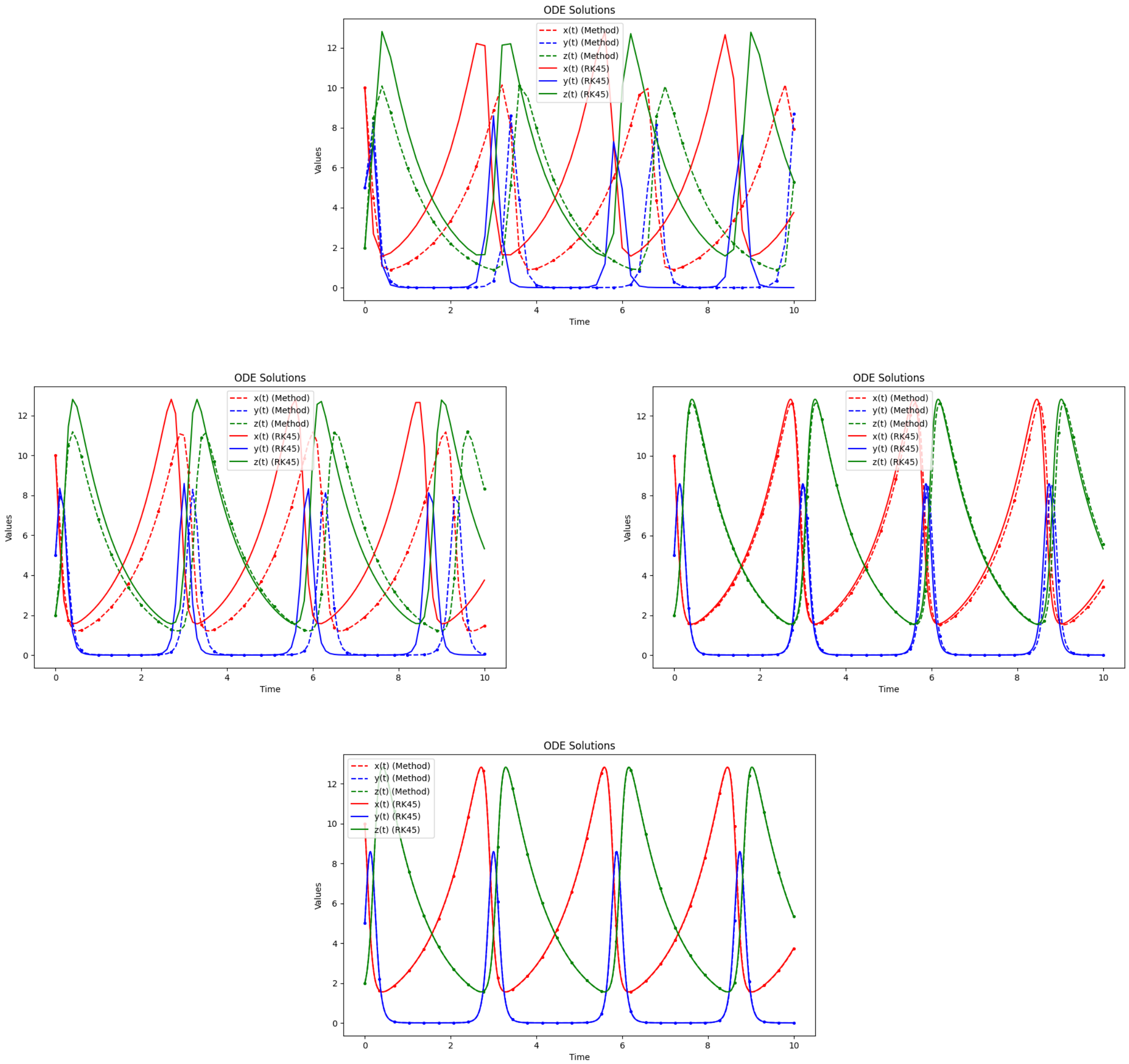


Figure 3.5. Lie-Trotter with $n = 50$, 100, 1000 and 100000.

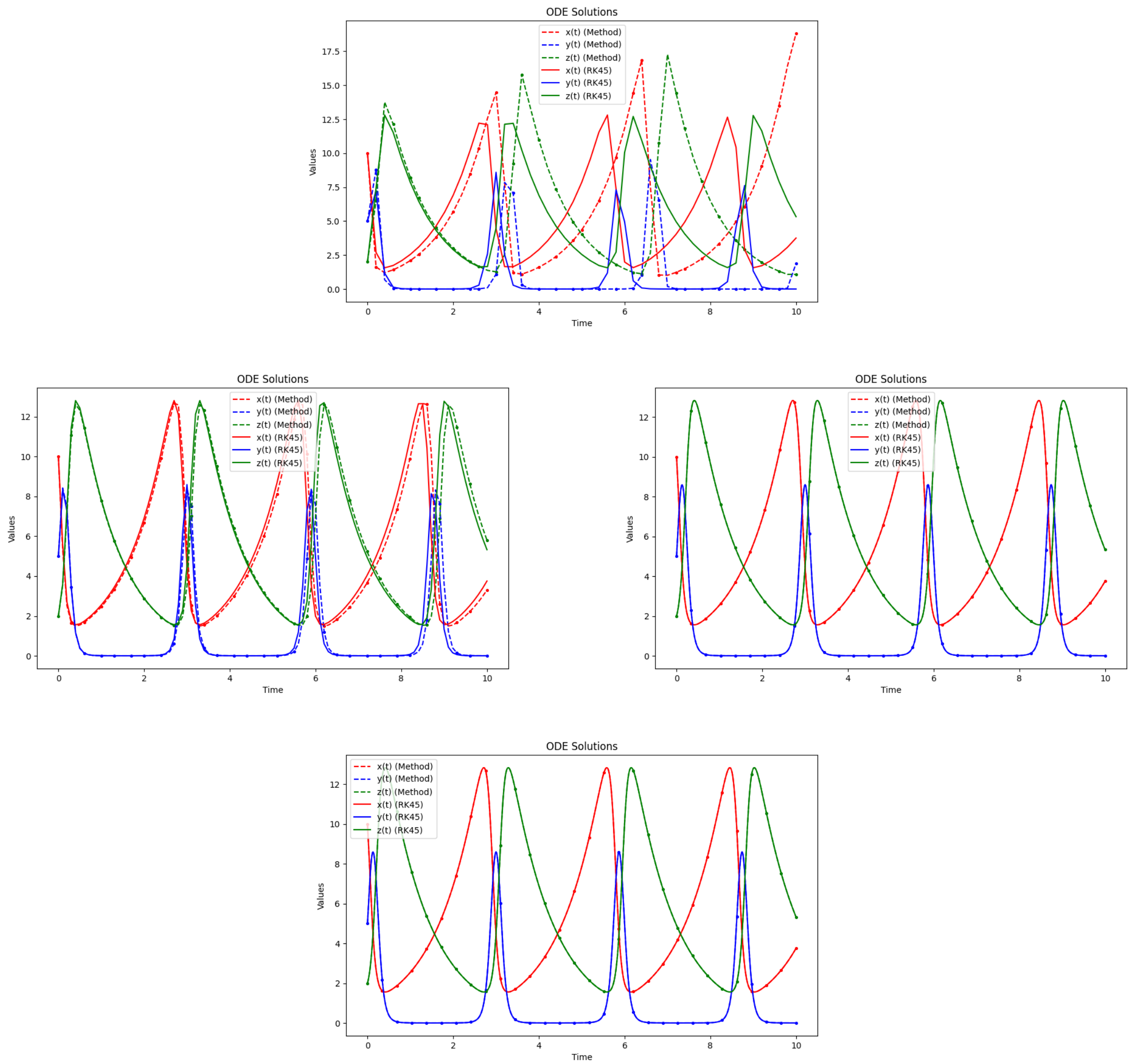


Figure 3.6. Strang with $n = 50$, 100, 1000 and 100000.

Table 3.11. Lie-Trotter of 3-dimentional Lotka-Volterra model, $n = 10000$.

t	$x(t)$	$y(t)$	z(t)	$\widetilde{x}(t)$	$\widetilde{y}(t)$	$\widetilde{z}(t)$
1	2.539358665	0.006884854	7.836776611	2.548201072	0.006827039	7.848676661
2	6.884939672	0.0037627	2.890413774	6.909033926	0.003761458	2.894762461
3	4.521697022	8.590502113	4.439027876	4.448045649	8.59724065	4.496354809
4	2.883422694	0.003799542	6.901632992	2.8988662695	0.003741118	6.899252441
5	7.81787936	0.006796928	2.545496538	7.859758915	0.006883753	2.544609303
6	2.019878504	5.097262772	9.90254875	1.988522903	4.941170514	10.057718329
7	3.274977274	0.002458917	6.076469194	3.298829967	0.002415725	6.062757995
8	8.871623684	0.014526079	2.243167583	8.935740307	0.014993352	2.238204683
9	1.564977245	1.423979608	12.734119539	1.565073422	1.330736849	12.778958848
10	3.720144306	0.001853373	5.349331862	3.754780839	0.001825631	5.326545535

Table 3.12. Absolute error of Lie-Trotter of 3-dimentional Lotka-Volterra model, $n = 10000$.

t	$E_r x(t)$	$E_r y(t)$	$E_r z(t)$
1	0.008842407	5.7815E-05	0.01190005
2	0.024094254	1.242E-06	0.004348687
3	0.073651373	0.006738537	0.057326933
4	0.015443576	5.8424E-05	0.002380551
5	0.041879555	8.6825E-05	0.000887235
6	0.031355601	0.156092258	0.155169579
7	0.023852693	4.3192E-05	0.013711199
8	0.064116623	0.000467273	0.0049629
9	9.6177E-05	0.093242759	0.044839309
10	0.034636533	2.7742E-05	0.022786327

Table 3.13. Strang product of 3-dimentional Lotka-Volterra model, $n = 10000$.

t	$x(t)$	$y(t)$	z(t)	$\widetilde{x}(t)$	$\widetilde{y}(t)$	$\widetilde{z}(t)$
1	2.548190914	0.006827073	7.848673569	2.548201072	0.006827039	7.848676661
2	6.909006575	0.003761182	2.894760423	6.909033926	0.003761458	2.894762461
3	4.448910663	8.597672769	4.495448067	4.448045649	8.59724065	4.496354809
4	2.8987129796	0.003740592	6.899585734	2.8988662695	0.003741118	6.899252441
5	7.859356954	0.0068768866	2.544727129	7.859758915	0.006883753	2.544609303
6	1.989137578	4.945311843	10.054508574	1.988522903	4.941170514	10.057718322
7	3.298336	0.002414746	6.063638979	3.298829967	0.002415725	6.062757995
8	8.934462624	0.014956381	2.2385139295	8.935740307	0.014993352	2.238204683
9	1.564970999	1.334121434	12.77971443	1.565073422	1.330736849	12.778958848
10	3.753494814	0.001823703	5.3283459125	3.754780839	0.001825631	5.326545535

Table 3.14. Absolute error of Strang of 3-dimentional Lotka-Volterra model, $n = 10000$.

t	$E_r x(t)$	$E_r y(t)$	$E_r z(t)$
1	1.0158E-05	3.4E-08	3.092E-06
2	2.7351E-05	2.76E-07	2.038E-06
3	0.000865014	0.000432119	0.000906742
4	0.00015329	5.26E-07	0.000333293
5	0.000401961	6.8664E-06	0.000117826
6	0.000614675	0.004141329	0.003209755
7	0.000493967	9.79E-07	0.000880984
8	0.001277683	3.6971E-05	0.000309246
9	0.000102423	0.003384585	0.000755582
10	0.001286025	0.000001928	0.001800377

Chapter 4. Koopman-Lie Invariant Subspace

"In mathematics the art of proposing
a question must be held of higher
value than solving it."

—*Georg Cantor*

4.1. Introduction

In Chapter 3, we discussed a program to approximate the pointwise linear Koopman-Lie semigroup flow $T(t)g(x) = e^{t\mathcal{K}}g(x) = g(\sigma(t,x))$, where $t \to \sigma(t,x)$ is the underlying flow describing the dynamical system, and where $g \in \mathcal{M} \subset \mathcal{F}(\Omega,\mathbb{R})$ is an observation. Since the semigroup flow is generated by the Koopman-Lie operator $\mathcal{K}$, and since $\mathcal{K}$ can often be decomposed into a sum of operators, we suggested using operator splitting methods; e.g., exponential splitting based on standard product formulas such as the Lie-Trotter and Strang product formulas.

The Koopman-Lie operator, in general, is an infinite-dimensional linear operator acting on a function space $\mathcal{F}(\Omega, Z)$. In this chapter, we suggest an alternative way to compute $e^{t\mathcal{K}}g(x) = g(\sigma(t,x))$ via finite-dimensional invariant Koopman-Lie subspaces. Instead of working on $\mathcal{F}(\Omega,\mathbb{C})$ or a "large" $e^{t\mathcal{K}}$-invariant subspace thereof, our aim is to construct a "small," finite-dimensional subspace $\mathcal{M} \subset D(\mathcal{K}) \subset \mathcal{F}(\Omega,\mathbb{C})$, spanned by linearly independent observables $\{g_1, g_2, ..., g_n\} \in \mathcal{F}(\Omega,\mathbb{C})$, such that $\mathcal{K}\mathcal{M} \subset \mathcal{M}$. This approach allows us to lift the nonlinear dynamical system to a linear one via the observables $\{g_i\}_{i=1}^n$ and obtain information on the underlying flow $\sigma(t,x)$ describing the dynamical system.

A particularly simple way to find an invariant subspace $\mathcal{M}$ and compute $g(\sigma(t,x)) = e^{t\mathcal{K}}g(x)$ is for an observable g that is an eigenfunction of $\mathcal{K}$ to an eigenvalue λ; i.e., a function g that satisfies $\mathcal{K}g(x) = \lambda g(x)$ for all $x \in \Omega$. In this case,

$$g(\sigma(t,x)) = T(t)g(x) = e^{t\mathcal{K}}g(x) = e^{t\lambda}g(x)$$

for all $x \in \Omega$.

Suppose that $\mathbf{g} = [g_1, g_2, \ldots, g_n]^T$ is a list of observables. Formally, $\sigma'(0,x)$ determines $\mathcal{K}\mathbf{g}(x) := \mathbf{g}'(x) \cdot \sigma'(0,x)$ in terms of generators

$$e^{t\mathcal{K}}\mathbf{g}(x) = T(t)\mathbf{g}(x) = \mathbf{g}(\sigma(t,x))$$

for a large class of observations $\mathbf{g}$. Now, if the class of observables $\mathbf{g}$ is chosen properly, one can expect to obtain a wealth of information on $\sigma(t,x)$ from $\sigma'(0,x)$ alone. Therefore, the Koopman-Lie eigenfunction method offers a promising way to describe and study the dynamical system. The difficulties associated with utilizing this method involve the existence of eigenfunctions and identifying them. To address these difficulties, we will present theorems related to the existence and algorithms for explicitly computing the Koopman-Lie eigenfunctions for some dynamical systems, [26], [38], and [39].

4.2. Motivating Examples and the Existence of Koopman-Lie Invariant Subspaces.

In this section, we examine the Koopman-Lie eigenfunctions by considering two simple dynamical systems.

Example 4.2.1. Consider

$$x'(t) = x^2(t), x(0) = x \in \Omega := [0,\infty).$$

Then the initial value problem has a unique local solution $x(t) = \sigma(t,x)$ for all $x \in \Omega$. Clearly, $t \to \sigma(t,x)$ is a flow and since $\sigma'(t,x) = \sigma^2(t,x)$ is positive, it follows that Ω is invariant under σ; i.e, $\sigma(t,x) \in \Omega$ for all $x \in \Omega$ and $t > 0$ for which $\sigma'(t,x)$ exists. The associated linear semigroup flow $T(t)g(x) = g(\sigma(t,x))$ has a Koopman-Lie generator

$$\mathcal{K}g(x) = g'(x) \cdot \sigma'(0,x) = x^2 g'(x) \tag{4.2.1}$$

for suitable observations $g : [0,\infty) \to \mathbb{R}$ (or $\mathbb{C}$). Clearly, the flow $\sigma(t,x)$ could be easily computed by a simple integration using separation of variables. However, since separation of variables works only in a one-dimensional setting, we use the eigenvalue/eigenfunction construction described above. A function g_λ is an eigenfunction for the eigenvalue λ of the Koopman-Lie generator $\mathcal{K}$ if

$$\mathcal{K}g_\lambda(x) = x^2 g_\lambda'(x) = \lambda g_\lambda(x) \tag{4.2.2}$$

or

$$g_\lambda(x) = \bar{c}e^{-\frac{\lambda}{x}}$$

for some constant c and for $\lambda \geq 0$. If we take $c > 0$, then

$$g_\lambda^{-1}(x) = \frac{-\lambda}{\ln x - \ln c}$$

for $0 < x < c$, and

$$g_\lambda(\sigma(t,x)) = T(t)g_\lambda(x) = e^{\lambda t} g_\lambda(x).$$

This implies

$$\begin{aligned}\sigma(t,x) = g_\lambda^{-1}(e^{\lambda t} g_\lambda(x)) = g_\lambda^{-1}(ce^{\lambda t - \frac{\lambda}{x}}) &= \frac{-\lambda}{\ln(ce^{\lambda t - \frac{\lambda}{x}}) - \ln c} \\ =\frac{-\lambda}{\lambda t - \frac{\lambda}{x}} = \frac{x}{1-xt}&\end{aligned} \tag{4.2.3}$$

for $0 \leq t \leq \frac{1}{x}$. Since $m(x) = \frac{1}{x}$ for all $x \in [0,\infty)$, we get $T(t)g \notin \mathcal{F}(\Omega,\mathbb{R})$ for all $g \in \mathcal{F}(\Omega,\mathbb{R})$. In fact, $T(t)g(x)$ is only defined for those $x \in \Omega_t := \{x \in \Omega : m(x) = \frac{1}{x} > t\} = [0, \frac{1}{t})$ and $T(t) : g \to T(t)g$ is well defined only from $\mathcal{F}(\Omega,\mathbb{R})$ into $\mathcal{F}(\Omega_t,\mathbb{R})$.

Example 4.2.2. Consider the dynamical system

$$\begin{aligned} x_1'(t) &= \alpha x_1(t), \\ x_2'(t) &= \beta(x_2(t) - x_1^2(t)), \end{aligned} \tag{4.2.4}$$

with initial value $(x_1(0), x_2(0)) = (x_1, x_2) \in \Omega := \mathbb{R}^2$. The unique, global solution of (4.2.4) can be easily computed directly and is given by

$$\begin{aligned} x_1(t) &= x_1 e^{\alpha t}, \\ x_2(t) &= x_2 e^{\beta t} + \int_0^t e^{\beta(t-s)} \beta x_1^2 e^{2\alpha s}\, ds = x_2 e^{\beta t} - \frac{\beta}{2\alpha - \beta} x_1^2 (e^{2\alpha t} - e^{\beta t}). \end{aligned}$$

We will show next how this solution can also be computed by finding a finite-dimensional, invariant subspace $\mathcal{M} \subset \mathcal{F}(\Omega, \mathbb{R})$ of observations for the linear Koopman-Lie operator $\mathcal{K} : g \to \nabla g \cdot f$ that is associated with (4.2.4); i.e.,

$$\mathcal{K} = \alpha x_1 \frac{\partial}{\partial x_1} + \beta(x_2 - x_1^2) \frac{\partial}{\partial x_2}.$$

If we choose $\mathcal{M}$ to be the linear span $< g_1, g_2, g_3 > \subset \mathcal{F}(\mathbb{R}^2, \mathbb{R})$, where $g_1(x_1, x_2) := x_1$, $g_2(x_1, x_2) := x_2$, and $g_3(x_1, x_2) := x_1^2$, then,

$$\begin{aligned} \mathcal{K} g_1(x_1, x_2) &= \alpha x_1 = \alpha g_1(x_1, x_2), \\ \mathcal{K} g_2(x_1, x_2) &= \beta(x_2 - x_1^2) = \beta(g_2(x_1, x_2) - g_3(x_1, x_2), \\ \mathcal{K} g_3(x_1, x_2) &= 2\alpha x_1^2 = 2\alpha g_3(x_1, x_2). \end{aligned} \tag{4.2.5}$$

Therefore,

$$\begin{aligned} \mathcal{K} g_1 &= \mathbf{K}(1, 0, 0)_{\mathcal{M}} = (\alpha, 0, 0)_{\mathcal{M}} = \alpha g_1, \\ \mathcal{K} g_2 &= \mathbf{K}(0, 1, 0)_{\mathcal{M}} = (0, \beta, -\beta)_{\mathcal{M}} = \beta g_2 - \beta g_3, \\ \mathcal{K} g_3 &= \mathbf{K}(0, 0, 1)_{\mathcal{M}} = (0, 0, 2\alpha)_{\mathcal{M}} = 2\alpha g_3, \end{aligned}$$

and $\mathbf{K} := \mathcal{K}|_{\mathcal{M}}$ is a linear map from $\mathcal{M}$ into $\mathcal{M}$ given by

$$\mathbf{K} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & -\beta & 2\alpha \end{pmatrix}, \tag{4.2.6}$$

and

$$e^{t\mathbf{K}} = \begin{pmatrix} e^{\alpha t} & 0 & 0 \\ 0 & e^{\beta t} & 0 \\ 0 & -\frac{\beta}{2\alpha-\beta}(e^{2\alpha t} - e^{\beta t}) & e^{2\alpha t} \end{pmatrix}. \tag{4.2.7}$$

This implies that

$$\begin{aligned}
\mathcal{T}(t)g_1 &= e^{t\mathbf{K}}(1,0,0)_{\mathcal{M}} = (e^{\alpha t},0,0)_{\mathcal{M}} = e^{\alpha t}g_1 \\
\mathcal{T}(t)g_2 &= e^{t\mathbf{K}}(0,1,0)_{\mathcal{M}} = (0, e^{\beta t}, -\frac{\beta}{2\alpha-\beta}(e^{2\alpha t} - e^{\beta t}))_{\mathcal{M}} \\
&= e^{\beta t}g_2 - \frac{\beta}{2\alpha-\beta}(e^{2\alpha t} - e^{\beta t})g_3 \\
\mathcal{T}(t)g_3 &= e^{t\mathbf{K}}(0,0,1)_{\mathcal{M}} = (0,0,e^{2\alpha t})_{\mathcal{M}} = e^{2\alpha t}g_3.
\end{aligned}$$

Since

$$\mathcal{T}(t)g(x) = g(\sigma(t,x)) = g(x_1(t), x_2(t)),$$

where $x_1(t)$ and $x_2(t)$ are the unique solutions of (4.2.4) with initial value $x = (x_1, x_2)$, it follows that

$$\begin{aligned}
x_1(t) &= g_1(x_1(t), x_2(t)) = g_1(\sigma(t,x)) = \mathcal{T}(t)g_1(x) = e^{\alpha t}g_1(x) \\
&= e^{\alpha t}g_1(x_1,x_2)) = e^{\alpha t}x_1, \text{and} \\
x_2(t) &= g_2(x_1(t), x_2(t)) = g_2(\sigma(t,x)) = \mathcal{T}(t)g_2(x) \\
&= e^{\beta t}g_2(x_1,x_2) - \frac{\beta}{2\alpha-\beta}(e^{2\alpha t} - e^{\beta t})g_3(x_1,x_2) \\
&= e^{\beta t}x_2 - \frac{\beta}{2\alpha-\beta}(e^{2\alpha t} - e^{\beta t})x_1^2.
\end{aligned}$$

It can be easily seen that β is an eigenvalue of the matrix $\mathbf{K} := \mathcal{K}|_{\mathcal{M}}$ with eigenvector $g_4 := (0, 1, \frac{\beta}{2\alpha-\beta})_{\mathcal{M}} = g_2 + \frac{\beta}{2\alpha-\beta} g_3$. Therefore, If we choose $\tilde{\mathcal{M}}$ to be the linear span $< g_1, g_4 > \subset \mathcal{F}(\mathbb{R}^2, \mathbb{R})$, where $g_1(x_1, x_2) := x_1$ and $g_4(x_1, x_2) = x_2 + \frac{\beta}{2\alpha-\beta} x_1^2$, then,

$$\begin{aligned} \mathcal{K} g_1 &= \alpha g_1, \\ \mathcal{K} g_4 &= \beta g_4. \end{aligned} \tag{4.2.8}$$

Therefore, with respect to $\tilde{\mathcal{M}}$, the restriction $\tilde{\mathbf{K}} := \mathcal{K}|_{\tilde{\mathcal{M}}}$ is a linear map from $\tilde{\mathcal{M}}$ into itself given by

$$\tilde{\mathbf{K}} = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}, \tag{4.2.9}$$

and

$$e^{t\tilde{\mathbf{K}}} = \begin{pmatrix} e^{\alpha t} & 0 \\ 0 & e^{\beta t} \end{pmatrix}.$$

This implies that

$$\mathcal{T}(t) g_1 = e^{t\tilde{\mathbf{K}}}(1, 0)_{\tilde{\mathcal{M}}} = (e^{\alpha t}, 0)_{\tilde{\mathcal{M}}} = e^{\alpha t} g_1,$$

$$\mathcal{T}(t) g_2 = e^{t\tilde{\mathbf{K}}}(0, 1)_{\tilde{\mathcal{M}}} = (0, e^{\beta t})_{\tilde{\mathcal{M}}} = e^{\beta t} g_4.$$

Since

$$\mathcal{T}(t) g(x) = g(\sigma(t, x)) = g(x_1(t), x_2(t)),$$

where $x_1(t)$ and $x_2(t)$ are the unique solutions of (4.2.4) with initial value $x = (x_1, x_2)$, it follows that

$$\begin{aligned}
x_1(t) &= g_1(x_1(t), x_2(t)) = g_1(\sigma(t,x)) = \mathcal{T}(t)g_1(x) = e^{\alpha t}g_1(x) = e^{\alpha t}x_1, \\
x_2(t) + \frac{\beta}{2\alpha-\beta}x_1(t)^2 &= g_4(x_1(t), x_2(t)) = g_4(\sigma(t,x)) = \mathcal{T}(t)g_4(x) \\
&= e^{\beta t}g_4(x_1, x_2) = e^{\beta t}x_2 + \frac{\beta}{2\alpha-\beta}e^{\beta t}x_1^2, \text{ or} \\
x_2(t) &= e^{\beta t}x_2 + \frac{\beta}{2\alpha-\beta}e^{\beta t}x_1^2 - \frac{\beta}{2\alpha-\beta}x_1(t)^2 \\
&= e^{\beta t}x_2 - \frac{\beta}{2\alpha-\beta}(e^{2\alpha t} - e^{\beta t})x_1^2.
\end{aligned}$$

□

In the first example, the system has a unique local solution $x(t) = \sigma(t,x)$ for all $x \in \Omega := [0,\infty)$ and for $0 \le t \le \frac{1}{x}$. In simple terms, the system blows up in a finite time at $m(x) = \frac{1}{x}$. Taking into account this example and Theorem 3, 2.5 in [38] and [39], respectively, one is led to the following observation.

Remark 4.2.3. Let Ω be a set and $t \to \sigma(t,x)$ be an Ω-invariant flow with Koopman-Lie generator $\mathcal{K}$. If $m_{inf} := \inf\{m(x) : x \in \Omega\} = 0$, then, for all $\lambda \in \mathbb{C}$ with $Re(\lambda) > 0$, $\mathcal{K}g_\lambda = \lambda g_\lambda$, where $0 \neq g_\lambda \in \mathcal{F}(\Omega, \mathbb{C})$ is given by $g_\lambda(x) = \exp(-\lambda m(x))$.

Proof. The Koopman-Lie operator is defined as

$$(\mathcal{K}g)(x) = \lim_{t\to 0}\frac{g(\sigma(t,x)) - g(x)}{t}$$

for those $g \in \mathcal{F}(\Omega, \mathbb{C})$ for which the limit exists for all $x \in \Omega$. Define

$$g_\lambda(x) := \exp(-\lambda m(x)).$$

Since $m_{inf} = 0$ and since λ has positive real part, it follows that $0 \neq g_\lambda \in \mathcal{F}(\Omega, \mathbb{C})$. Then, for all $x \in \Omega$ and $t > 0$,

$$\frac{g_\lambda(\sigma(t,x)) - g_\lambda(x))}{t} = \frac{\exp(-\lambda m(\sigma(t,x)) - \exp(-\lambda m(x))}{t}.$$

Since $m(\sigma(t,x)) = m(x) - t$ for $0 \le t < m(x)$, the above equation equals

$$\frac{\exp(-\lambda(m(x)-t)) - \exp(-\lambda m(x))}{t} = \frac{\exp(\lambda t) - 1}{t} \exp(-\lambda m(x)).$$

By taking the limit as $t \to 0^+$, this implies that $g_\lambda \in D(\mathcal{K})$ and $\mathcal{K} g_\lambda(x) = \lambda \exp(-\lambda m(x))$. Thus, if $Re(\lambda) > 0$, λ is an eigenvalue of $\mathcal{K}$ with eigenvector g_λ. □

The existence of Koopman-Lie eigenfunctions can be locally determined by using the Hartman-Grobman theorem [43]. It is a key result in the study of local behavior in ordinary differential equations. It asserts that close to a hyperbolic equilibrium point x_0, the nonlinear dynamics $x'(t) = f(x(t))$ is conjugate to the linear system $\dot{y} = Ay$ with the Jacobian matrix $A = [\frac{\partial f_i}{\partial x_j}|_{x_0}]$.

In [26], Matthew D. Kvalheim and S. Revzen extended the Hartman-Grobman theorem and proved the existence and uniqueness of global Koopman-Lie eigenfunctions for stable fixed points and periodic orbits.

In the next section, we will provide an algorithm for computing explicit Koopman-Lie eigenfunctions.

4.3. Computing the Koopman-Lie Invariant Subspace.

In the following, we expand the idea presented in the previous example towards an algorithm to help identify finite dimensional subspaces for Koopman-Lie operators and, therefore, to help compute explicit Koopman-Lie eigenfunctions. First, observe that $\mathcal{F}(\Omega, \mathbf{C})$ is a $\mathbf{C}$-algebra and that the Koopman-Lie operator

$$\mathcal{K} g = f \cdot \nabla g \tag{4.3.1}$$

is a *derivation*; i.e., for all sufficiently smooth $g_1, g_2 \in \mathcal{F}(\Omega, \mathbb{C})$,

$$\mathcal{K}(g_1 g_2) = \mathcal{K}(g_1)g_2 + g_1\mathcal{K}(g_2). \tag{4.3.2}$$

Setting $u = g_1 g_2$ and assuming that $u, \frac{1}{g_1} \in \mathcal{F}(\Omega, \mathbb{C})$, (4.3.2) implies that $g_1\mathcal{K}(g_2) = \mathcal{K}(u) - \mathcal{K}(g_1)g_2 = (\mathcal{K}(u)g_1 - \mathcal{K}(g_1)u)/g_1$ or

$$\mathcal{K}\left(\frac{u}{g_1}\right) = \frac{\mathcal{K}(u)g_1 - u\mathcal{K}(g_1)}{g_1^2}. \tag{4.3.3}$$

The following proposition follows immediately from (4.3.2) and (4.3.3).

Proposition 4.3.1. *Let $g_1, g_2, h_1, h_2 \in \mathcal{F}(\Omega, \mathbb{C})$ be sufficiently smooth. If*

$$\mathcal{K}(g_1) = g_1 h_1 \text{ and } \mathcal{K}(g_2) = g_2 h_2,$$

then

$$\mathcal{K}(g_1 g_2) = g_1 g_2 (h_1 + h_2) \text{ and } \mathcal{K}\left(\frac{g}{f}\right) = \frac{g_1}{g_2}(h_1 - h_2).$$

Lemma 4.3.2. *Let $f, \frac{1}{f} \in \mathcal{F}(\Omega, \mathbb{C})$ be sufficiently smooth.*

$$\mathcal{K}(f^n) = n f^{n-1}\mathcal{K}(f), \quad \text{for all } n \in \mathbb{Q}. \tag{4.3.4}$$

Proof. We will prove that 4.3.4 holds for all $n \in \mathbb{Z}$ using induction. Let $n > 0$, the base case is $n = 2$, then

$$\mathcal{K}(f^2) = \mathcal{K}(f \cdot f) = \mathcal{K}(f)f + f\mathcal{K}(f) = 2f\mathcal{K}(f).$$

Assume that the statement true for some natural number $n = k$, i.e.,

$$\mathcal{K}(f^k) = k f^{k-1}\mathcal{K}(f), \tag{4.3.5}$$

now, we need to show that the statement holds for $n = k + 1$,

$$\mathcal{K}(f^{k+1}) = \mathcal{K}(f^k \cdot f) = \mathcal{K}(f^k)f + \mathcal{K}(f)f^k = k f^{k-1}\mathcal{K}(f)f + \mathcal{K}(f)f^k = (k+1)f^k\mathcal{K}(f). \tag{4.3.6}$$

We will show the case where the Equation 4.3.4 holds for $-n < 0$,

$$\mathcal{K}(f \cdot \frac{1}{f}) = \frac{1}{f}\mathcal{K}(f) + f\mathcal{K}(\frac{1}{f}) \implies \mathcal{K}(\frac{1}{f}) = -\frac{1}{f^2}\mathcal{K}(f) \implies \mathcal{K}(f^{-1}) = -f^{-2}\mathcal{K}(f). \quad (4.3.7)$$

Suppose that Equation 4.3.4 holds for $-k < 0$, i.e.,

$$\mathcal{K}(f^{-k}) = -kf^{-k-1}\mathcal{K}(f), \quad (4.3.8)$$

the inductive hypothesis follows immediately from Equations 4.3.7, and 4.3.8

$$\mathcal{K}(f^{-k-1}) = \mathcal{K}(f^{-k}f^{-1}) = \mathcal{K}(f^{-k})f^{-1}+f^{-k}\mathcal{K}(f^{-1}) = -kf^{-k-2}\mathcal{K}(f)-f^{-k-2} = (-k-1)f^{-k-2}\mathcal{K}(f). \quad (4.3.9)$$

Now, we will address the case where the exponent is $\frac{n}{m}$, such that $m > n > 0$.

$$\begin{aligned}\mathcal{K}(f^n) = \mathcal{K}((f^{\frac{n}{m}})^m) &= (f^{\frac{n}{m}})^{m-1}\mathcal{K}(f^{\frac{n}{m}}) + f^{\frac{n}{m}}\mathcal{K}((f^{\frac{n}{m}})^{m-1}) \\ &= (f^{\frac{n}{m}})^{m-1}\mathcal{K}((f^{\frac{n}{m}})) + f^{\frac{n}{m}}\left[(f^{\frac{n}{m}})^{m-2}\mathcal{K}(f^{\frac{n}{m}}) + f^{\frac{n}{m}}\mathcal{K}((f^{\frac{n}{m}})^{m-2})\right]\end{aligned}$$

by repeating the process $m-1$ times, and using Equation 4.3.5, we obtain:

$$nf^{n-1}\mathcal{K}(f) = m(f^{\frac{n}{m}})^{m-1}\mathcal{K}(f^{\frac{n}{m}}) \implies \mathcal{K}(f^{\frac{n}{m}}) = \frac{n}{m}(f^{\frac{n}{m}})^{-m+1}f^{n-1}\mathcal{K}(f) = \frac{n}{m}f^{\frac{n}{m}-1}\mathcal{K}(f). \quad (4.3.10)$$

For $n > m > 0$, we can write $\frac{n}{m}$ as $\frac{n}{m} = q + \frac{r}{n}$, where $q \in \mathbb{Z}$, and $r < n$. Thus, applying this to the function $f^{\frac{n}{m}}$, we have $\mathcal{K}(f^{\frac{n}{m}}) = \frac{n}{m}f^{\frac{n}{m}-1}\mathcal{K}(f)$, which follows from the previously stated argument and equation 4.3.5. □

One of the interesting properties of Koopman-Lie eigenfunctions is:

Proposition 4.3.3. *Let $g_{\lambda_1}, g_{\lambda_1} \in \mathcal{F}(\Omega, \mathbb{C})$ be sufficiently smooth. If $(g_{\lambda_1}, \lambda_1)$ and $(g_{\lambda_2}, \lambda_2)$ are eigenfunction-eigenvalue pairs of $\mathcal{K}$, so are $(g_{\lambda_1}^{\alpha_1}g_{\lambda_2}^{\alpha_2}, \alpha_1\lambda_1 + \alpha_2\lambda_2)$, where $\alpha_1, \alpha_2 \in \mathbb{Q}$. Moreover, if $\{(g_{\lambda_i}, \lambda_i)\}_{i=1}^n$ eigenfunction-eigenvalue pairs of $\mathcal{K}$, so $(\prod_{i=1}^n g_{\lambda_i}, \sum_{i=1}^n \alpha_i\lambda_i)$, where α_i's $\in \mathbb{Q}$.*

Proof. By applying Lemma 4.3.2, then

$$\begin{aligned}\mathcal{K}(g_{\lambda_1}^{\alpha_1} g_{\lambda_2}^{\alpha_2}) &= g_{\lambda_1}^{\alpha_1}\mathcal{K}(g_{\lambda_2}^{\alpha_2}) + \mathcal{K}(g_{\lambda_1}^{\alpha_1}) g_{\lambda_2}^{\alpha_2} \\ &= g_{\lambda_1}^{\alpha_1}\alpha_2 g_{\lambda_2}^{\alpha_2-1}\mathcal{K}(g_{\lambda_2}) + g_{\lambda_2}^{\alpha_2}\alpha_1 g_{\lambda_1}^{\alpha_1-1}\mathcal{K}(g_{\lambda_1}) \\ &= g_{\lambda_1}^{\alpha_1}\alpha_2 g_{\lambda_2}^{\alpha_2-1}(\lambda_2 g_{\lambda_2}) + g_{\lambda_2}^{\alpha_1}\alpha_1 g_{\lambda_1}^{\alpha_1-1}(\lambda_1 g_{\lambda_1}) \\ &= (\alpha_1\lambda_1 + \alpha_2\lambda_2) g_{\lambda_1}^{\alpha_1} g_{\lambda_2}^{\alpha_2}.\end{aligned} \tag{4.3.11}$$

□

Now, we will define a relation between eigenfunctions. Let (g_λ, λ) be a pair of eigenfunction-eigenvalue, then the relation is defined, as

$$g_\mu \sim g_\lambda \text{ iff } g_\mu = \alpha g_\lambda^k,\ k \in \mathbb{Z}, \alpha \in \mathbb{R} \text{ and } \mu = k\lambda. \tag{4.3.12}$$

It can be easily seen that the relation in (4.3.12) is an equivalence relation. Therefore, the equivalence class is given by

$$[g_\lambda] = \{g_\mu : g_\mu = \alpha g_\lambda^k,\ k \in \mathbb{Z}, \alpha \in \mathbb{R} \text{ and } \mu = k\lambda\}. \tag{4.3.13}$$

The equivalence classes labeled 4.3.13 form a partition of the family of Koopman-Lie eigenfunctions.

In the next section, we introduce an algorithm for explicitly computing Lie-Koopman eigenfunctions. While this algorithm is effective in certain cases, a promising direction for future research is to extend it to a large class of dynamical systems. The algorithm is derived from Propositions 4.3.1 and 4.3.3.

4.4. Application of the Koopman-Lie Invariant Subspace Computation Algorithm

The following examples show how this algorithm can produce eigenfunction - eigenvalue pairs for the Koopman-Lie operator that then, in turn, can be used to solve the

Algorithm 4.5. Koopman-Lie eigenfunctions

Require: (1) $x'(t) = f(x(t))$, with initial condition and (2) library of measurements $\Theta := \begin{pmatrix} \theta_0 & \theta_1 & \theta_2 & \cdots & \theta_n \end{pmatrix}$.

for $i \leftarrow \{1, 2, \cdots, n\}$ **do**
    $h_i \leftarrow \frac{\nabla\theta_i \cdot f}{\theta_i}$
    $H[i] \leftarrow h_i$ ▷ *H is an array of h_i's*
    for $i, j \leftarrow \{1, 2, \cdots, n\}$ **do**
        $A[i, j] \leftarrow h_i + h_j$
        $B[i, j] \leftarrow h_i - h_j$
    end for
    for $a_{i,j}$ **in** A or $b_{i,j}$ **in** B **do** ▷ *c is constant*
        if $a_{i,j} := h_i + h_j = c$ **or** $b_{i,j} := h_i - hj = c$ **then**
            return $\lambda_{i,j} := (a_{i,j}, \psi_{i,j} := \theta_i\theta_j)$
                or $\lambda_{i,j} := (b_{i,j}, \psi_{i,j} := \frac{\theta_i}{\theta_j})$
    end for

underlying ordinary differential equation. This is done to demonstrate that the method works in some cases; the open problem is to determine its limitations and/or proper extensions.

Example 4.4.1. Consider

$$x'(t) = x(t), \; x(0) = x \in \Omega := \mathbb{R} \tag{4.4.1}$$

with associated Koopman-Lie operator

$$\mathcal{K}(g) = xg'(x)$$

for sufficiently smooth observations $g \in \mathcal{F}(\Omega, \mathbb{R})$. In order to find eigenfunctions and eigenvalues, we use **Algorithm 4.5.** which requires an initial library Θ of possible measurements like

$$\Theta := \left(1, \quad x, \quad x^2, \quad x^3, \quad x^{-1}, \quad e^{\lambda x}, \quad e^{\frac{\lambda}{x}}\right).$$

Table 4.1. Eigenfunctions of Example 4.4.1.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x	$x = \theta_1 h_1$	1
2	x^2	$2x^2 = \theta_2 h_2$	2
3	x^3	$3x^3 = \theta_3 h_3$	3
4	x^{-1}	$-x^{-1} = \theta_4 h_4$	-1
5	$e^{\lambda x}$	$e^{\lambda x}\lambda x = \theta_5 h_5$	λx
6	$e^{\frac{\lambda}{x}}$	$e^{\frac{\lambda}{x}}\left(\frac{-\lambda}{x}\right) = \theta_6 h_6$	$\frac{-\lambda}{x}$

The table shows that $\psi_k(x) := x^k$ are eigenfunctions to the eigenvalue k for $k \in \{-1, 0, 1, 2, 3\}$. By (4.3.13), all ψ_k are equivalent to $\psi_1(x) = x$. Now, let $\sigma(t, x) := x(t)$ be the unique solution of (4.4.1). Then

$$x(t) = \sigma(t, x) = \psi_1(\sigma(t, x) = e^{t\mathcal{K}}\psi_1(x) = e^t\psi_1(x) = e^t x.$$

Example 4.4.2. Consider

$$x'(t) = x^2(t),\ x(0) = x \in \Omega := \mathbb{R} \tag{4.4.2}$$

with associated Koopman-Lie operator

$$\mathcal{K}(g) = x^2 g'(x)$$

for sufficiently smooth observations $g \in \mathcal{F}(\Omega, \mathbb{R})$. **Algorithm 4.5.** with the same initial library Θ of measurements as in the previous example.

Table 4.2. Eigenfunctions of Example 4.4.2.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x	$x^2 = \theta_1 h_1$	x
2	x^2	$2x^3 = \theta_2 h_2$	$2x$
3	x^3	$3x^4 = \theta_3 h_3$	$3x$
4	x^{-1}	$-1 = \theta_4 h_4$	$-x$
5	$e^{\lambda x}$	$e^{\lambda x}\lambda x^2 = \theta_5 h_5$	λx^2
6	$e^{\frac{\lambda}{x}}$	$-\lambda e^{\frac{\lambda}{x}} = \theta_6 h_6$	$-\lambda$

Observe that $\theta_6(x) = e^{\frac{\lambda}{x}}$ is an eigenfunction for the eigenvalue $-\lambda$. Thus, $\psi_\lambda(x) := e^{\frac{-\lambda}{x}}$ is an eigenfunction for the eigenvalue λ. If $\sigma(t,x) := x(t)$ denotes the unique solution of (4.4.2), then

$$e^{\frac{-\lambda}{x(t)}} = \psi_\lambda(x(t)) = \psi_\lambda(\sigma(t,x) = e^{t\mathcal{K}}\psi_\lambda(x) = e^{\lambda t}\psi_\lambda(x) = e^{\lambda t}e^{\frac{-\lambda}{x}}$$

So, $e^{\frac{-\lambda}{x(t)}} = e^{t\lambda}e^{\frac{-\lambda}{x}}$ or

$$x(t) = \frac{x}{1-tx}$$

for $t \in [0, m(x)$, where $m(x) = \infty$ if $x \leq 0$ and $m(x) = 1/x$ if $x > 0$. □

We can also use the Taylor and Laurent series to determine the eigenfunctions. Consider the following power series expansion: $\psi(x) = \sum_{n=-\infty}^{\infty} c_n x^n$, then

$$\begin{aligned} \nabla\psi(x)\cdot f(x) &= \lambda\psi(x) \\ \sum_{n=-\infty}^{\infty} nc_n x^{n+1} &= \lambda \sum_{n=-\infty}^{\infty} c_n x^n \end{aligned} \tag{4.4.3}$$

where $c_n = 0$ for $n > 0$ and $c_n = \frac{(-\lambda)^{-n}}{(-n)!}c_0$ for $n \leq 0$. Therefore,

$$\begin{aligned} \psi(x) =& \sum_{n=0}^{\infty} c_{-n}x^{-n} = \sum_{n=0}^{\infty} \frac{(-\lambda)^n}{(n)!}c_0 x^{-n} \\ =& c_0 \sum_{n=0}^{\infty} \frac{(-\lambda)^n}{n!x^n} = c_0 e^{\frac{-\lambda}{x}}. \end{aligned}$$

Example 4.4.3. Consider

$$x'(t) = x^2(t) + \alpha^2, x(0) = x \in \Omega := \mathbb{C}, \tag{4.4.4}$$

where $\alpha > 0$ and $x(0) = x \in \mathbb{C}$. For sufficiently smooth observations $g \in \mathcal{F}(\Omega, \mathbb{C})$, the associated Koopman-Lie operator is given by

$$\mathcal{K}(g) = (x^2 + \alpha^2)g'(x).$$

Consider the initial library as follows: $\Theta := \{1, x, x + c, x + i\alpha, x - i\alpha\}$.

Table 4.3. Eigenfunctions of Example 4.4.3.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x	$x^2 + \alpha^2 = \theta_1 h_1$	$\frac{x^2+\alpha^2}{x}$
2	$x + c$	$x^2 + \alpha^2 = \theta_2 h_2$	$\frac{x^2+\alpha^2}{x+c}$
3	$x + i\alpha$	$x^2 + \alpha^2 = \theta_3 h_3$	$x - i\alpha$
4	$x - i\alpha$	$x^2 + \alpha^2 = \theta_4 h_4$	$x + i\alpha$

It follows from Corollary 4.3.2 that

$$\psi(x) := \theta_4(x)/\theta_3(x) = \frac{x + i\alpha}{x - i\alpha}$$

is the eigenfunction to the eigenvalue $2i\alpha = h_4(x) - h_3(x)$. If $\sigma(t, x) := x(t)$ denotes the unique solution of (4.4.4), then

$$\frac{x(t) + i\alpha}{x(t) - i\alpha} = \psi(x(t)) = \psi(\sigma(t, x) = e^{t\mathcal{K}}\psi(x) = e^{2i\alpha t}\psi(x) = e^{2i\alpha t}\frac{x + i\alpha}{x - i\alpha}.$$

This implies that

$$\frac{x(t) + i\alpha}{x(t) - i\alpha} = e^{2i\alpha t}\frac{x + i\alpha}{x - i\alpha}.$$

Therefore,

$$x(t) = \alpha \frac{ix + \alpha + e^{2i\alpha t}(ix - \alpha)}{e^{2i\alpha t}(x + i\alpha) - x + i\alpha}. \tag{4.4.5}$$

Equivalently,

$$x(t) = \alpha \tan\left(\alpha t + \tan^{-1}(\frac{x}{\alpha})\right)$$

for $t \in [0, m(x))$, where $m(x) = \frac{1}{\alpha}\left(\frac{\pi}{2} - \tan^{-1}(\frac{x}{\alpha})\right)$. □

Example 4.4.4. Consider

$$x_1'(t) = 4x_1(t) - 2x_2(t), x_1(0) = x_1$$

$$x_2'(t) = 3x_1(t) - 3x_2(t), x_2(0) = x_2.$$

Equivalently, consider

$$x'(t) = Ax(t), x(0) = x$$

with $x(t) = (x_1(t), x_2(t)), x = (x_1, x_2)$, and

$$A = \begin{pmatrix} 4 & -2 \\ 3 & -3 \end{pmatrix}.$$

The associated Koopman-Lie operator is given by

$$\mathcal{K}g = (4x_1 - 2x_2) \cdot \frac{\partial g}{\partial x_1} + (3x_1 - 3x_2) \cdot \frac{\partial g}{\partial x_2},$$

Algorithm 4.5. requires an initial library of possible measurements like

$$\Theta := \begin{pmatrix} 1 & x_1 & x_2 & ax_1 + bx_2 \end{pmatrix}. \tag{4.4.6}$$

Table 4.4. Eigenfunctions of Example 4.4.4.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1	$4x_1 - 2x_2 = \theta_1 h_1$	$\frac{4x_1-2x_2}{x_1}$
2	x_2	$3x_1 - 3x_2 = \theta_2 h_2$	$\frac{3x_1-3x_2}{x_2}$
3	$ax_1 + bx_2$	$(4a+3b)x_1 - (2a+3b)x_2 = \theta_3 h_3$	$\frac{(4a+3b)x_1-(2a+3b)x_2}{ax_1+bx_2}$

Looking at θ_3, we now find numbers λ, a, b such that

$$4a + 3b = \lambda a \text{ and } -2a - 3b = \lambda b.$$

In other words, we find the eigenvalues λ and corresponding eigenvectors (a, b) of the matrix

$$A^T = \begin{pmatrix} 4 & 3 \\ -2 & -3 \end{pmatrix}.$$

Since $(\lambda I - A^T) = \begin{pmatrix} \lambda - 4 & -3 \\ 2 & \lambda + 3 \end{pmatrix}$ has determinant $\lambda^2 - \lambda - 6$, it follows that $\lambda = 3$ is an eigenvalue with eigenvector $(a, b) = (3, -1)$ and that $\lambda = -2$ is an eigenvalue with eigenvector $(a, b) = (1, -2)$. Therefore, by the table above, if $\theta_4(x) = 3x_1 - x_2$ and $\theta_5(x) = x_1 - 2x_2$, then $\mathcal{K}\theta_4 = 3\theta_4$ and $\mathcal{K}\theta_5 = -2\theta_5$. Since

$$\psi(x_1(t), x_2(t)) = \psi(\sigma(t, (x_1, x_2)) = e^{t\mathcal{K}}\psi(x_1, x_2)$$

it follows that

$$3x_1(t) - x_2(t) = \theta_4(x_1(t), x_2(t)) = e^{3t}\theta_4(x_1, x_2) = e^{3t}(3x_1 - x_2)$$

and

$$x_1(t) - 2x_2(t) = \theta_5(x_1(t), x_2(t)) = e^{-2t}\theta_5(x_1, x_2) = e^{-2t}(x_1 - 2x_2).$$

This yields

$$x_1(t) = \frac{1}{5}\big((6e^{3t} - e^{-2t})x_1 + (-2e^{3t} + 2e^{-2t})x_2\big)$$
$$x_2(t) = \frac{1}{5}\big((3e^{3t} - 3e^{-2t})x_1 + (-e^{3t} + 6e^{-2t})x_2\big).$$

$\square$

We can also use the invariant subspace method outlined in Example 4.4.4 to treat a system of linear ODEs with constant coefficients

$$x'(t) = Ax(t), x(0) = x \tag{4.4.7}$$

with $x(t) = (x_1(t), x_2(t)), x = (x_1, x_2)$, and

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

The associated Koopman-Lie operator is given by

$$\mathcal{K}g = (ax_1 + bx_2)\frac{\partial g}{\partial x_1} + (cx_1 + dx_2)\frac{\partial g}{\partial x_2}.$$

If we choose $\mathcal{M}$ to be the linear span $< g_1, g_2 > \subset \mathcal{F}(\mathbb{R}^2, \mathbb{R})$, where $g_1(x_1, x_2) := x_1$, $g_2(x_1, x_2) := x_2$, then,

$$\mathcal{K}g_1 = \mathbf{K}(1,0)_{\mathcal{M}} = (a,b)_{\mathcal{M}} = ag_1 + bg_2,$$

$$\mathcal{K}g_2 = \mathbf{K}(0,1)_{\mathcal{M}} = (c,d)_{\mathcal{M}} = cg_1 + dg_2,$$

and $\mathbf{K} := \mathcal{K}|_{\mathcal{M}}$ is a linear map from $\mathcal{M}$ into $\mathcal{M}$ given by

$$\mathbf{K} = A^T = \begin{pmatrix} a & c \\ b & d \end{pmatrix}, \tag{4.4.8}$$

and

$$e^{t\mathbf{K}} = \begin{pmatrix} f_{1,1}(t) & f_{1,2}(t) \\ f_{2,1}(t) & f_{2,2}(t) \end{pmatrix} \tag{4.4.9}$$

can be computed explicitly with standard linear algebra or complex analysis methods. This yields that

$$\mathcal{T}(t)g_1 = e^{t\mathbf{K}}(1,0)_{\mathcal{M}} = (f_{1,1}(t), f_{1,2}(t))_{\mathcal{M}} = f_{1,1}(t)g_1 + f_{2,1}(t)g_2$$

$$\mathcal{T}(t)g_2 = e^{t\mathbf{K}}(0,1)_{\mathcal{M}} = (f_{2,1}(t), f_{2,2}(t))_{\mathcal{M}} = f_{2,1}(t)g_1 + f_{2,2}(t)g_2.$$

Since

$$\mathcal{T}(t)g(x) = g(\sigma(t,x)) = g(x_1(t), x_2(t)),$$

where $x_1(t)$ and $x_2(t)$ are the unique solutions of (4.4.7) with initial value $x = (x_1, x_2)$, it follows that

$$x_1(t) = g_1(x_1(t), x_2(t)) = \mathcal{T}(t)g_1(x_1, x_2) = f_{1,1}(t)x_1 + f_{2,1}(t)x_2,$$

$$x_2(t) = g_2(x_1(t), x_2(t)) = \mathcal{T}(t)g_2(x_1, x_2) = f_{2,1}(t)x_1 + f_{2,2}(t)x_2.$$

□

There are many methods for computing the matrix exponential, such as using the Jordan canonical form or operator splitting methods, as detailed in the article "Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later" by C. Moler and C. V. Loan [32], and in the book The Theory of Differential Equations by Kelley and Peterson [21].

Example 4.4.5. In Example 4.2.4, instead of using the invariant subspace method, we will apply **Algorithm 4.5.**. Consider

$$\begin{aligned} x'_1(t) &= \alpha x_1(t) \\ x'_2(t) &= \beta(x_2(t) - x_1^2(t)) \end{aligned} \tag{4.4.10}$$

with initial $(x_1(0), x_2(0)) = (x_1, x_2) \in \mathbb{R}^2$ and associated Koopman-Lie operator

$$\mathcal{K}g = \alpha x_1 \frac{\partial g}{\partial x_1} + \beta(x_2 - x_1^2)\frac{\partial g}{\partial x_2}.$$

To find the eigenfunctions and eigenvalues, we apply **Algorithm 4.5.**, which relies on an initial library of potential measurements, such as:

$$\Theta := \begin{pmatrix} 1 & x_1 & x_2 & x_1x_2 & x_1^2 & c_1x_2 + c_2x_1^2 \end{pmatrix}.$$

Table 4.5. Eigenfunctions of Example 4.4.5.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1	$\alpha x_1 = \theta_1 h_1$	α
2	x_2	$\beta(x_2 - x_1^2) = x_2\big(\beta - \beta\frac{x_1^2}{x_2}\big) = \theta_2 h_2$	$\beta - \beta\frac{x_1^2}{x_2}$
3	x_1x_2	$x_1x_2\big(\beta - \beta\frac{x_1^2}{x_2} + \alpha\big) = \theta_3 h_3$	$\beta - \beta\frac{x_1^2}{x_2} + \alpha$
4	x_1^2	$2x_1x_1' = 2\alpha x_1^2 = \theta_4 h_4$	2α
5	$c_1x_2 + c_2x_1^2$	$\beta c_1x_2 + (2\alpha c_2 - c_1\beta)x_1^2 = \theta_5 h_5$	$\frac{\beta c_1x_2 + (2\alpha c_2 - c_1\beta)x_1^2}{c_1x_2 + c_2x_1^2}$

It follows from Corollary 4.3.2 that $\psi_1 = \theta_1$ and $\psi_2 = \theta_4$ are the eigenfunctions to the eigenvalues α and 2α, respectively. Looking at θ_5, we will find λ, c_1,and c_2 such that

$$\beta c_1 = \lambda c_1 \text{ and } -\beta c_1 + 2\alpha c_2 = \lambda c_2.$$

In other words, we find the eigenvalues λ and corresponding eigenvectors (c_1, c_2) of the matrix

$$\begin{pmatrix} \beta & 0 \\ -\beta & 2\alpha \end{pmatrix}.$$

It follows that $\lambda = \beta$ is an eigenvalue with eigenvector $(c_1, c_2) = (1, \frac{\beta}{2\alpha - \beta})$ and that $\lambda = 2\alpha$ is an eigenvalue with eigenvector $(c_1, c_2) = (0, 1)$. Therefore, by the table above, if $\theta_5(x) = x_2 + \frac{\beta}{2\alpha-\beta}x_1^2$ and $\theta_4(x) = x_1^2$, then $\mathcal{K}\theta_5 = \beta\theta_5$ and $\mathcal{K}\theta_4 = 2\alpha\theta_4$. Since

$$\psi(x_1(t), x_2(t)) = \psi(\sigma(t, (x_1, x_2)) = e^{t\mathcal{K}}\psi(x_1, x_2),$$

it follows that

$$x_2(t) + \frac{\beta}{2\alpha - \beta}x_1^2(t) = \theta_5(x_1(t), x_2(t)) = e^{\beta t}\theta_5(x_1, x_2) = e^{\beta t}(x_2 + \frac{\beta}{2\alpha - \beta}x_1^2)$$

and

$$x_1^2(t) = \theta_4(x_1(t), x_2(t)) = e^{2\alpha t}\theta_4(x_1, x_2) = e^{2\alpha t}x^2.$$

This yields,

$$\begin{aligned} x_1(t) =& x_1 e^{\alpha t} \\ x_2(t) =& x_2 e^{\beta t} - \frac{\beta}{2\alpha - \beta}x_1^2\big(e^{2\alpha t} - e^{\beta t}\big). \end{aligned} \tag{4.4.11}$$

□

Example 4.4.6. Consider the system

$$\begin{aligned} x_1'(t) &= x_1(t)x_2(t) \\ x_2'(t) &= x_2^2(t) - x_2(t) \end{aligned} \tag{4.4.12}$$

where $(x_1(0), x_2(0)) = (x_1, x_2) \in \Omega := \mathbb{R}^2$ and with associated Koopman-Lie operator

$$\mathcal{K}g = x_1 x_2 \frac{\partial g}{\partial x_1} + (x_2^2 - x_2)\frac{\partial g}{\partial x_2}. \tag{4.4.13}$$

We apply **Algorithm 4.5.** along with an initial library of possible measurements,

$$\Theta := \begin{pmatrix} 1 & x_1 & x_2 & x_1x_2 & x_2^2 & x_2 - 1 & x_1^2 \end{pmatrix}.$$

Table 4.6. Eigenfunctions of Example 4.4.6.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1	$x_1x_2 = \theta_1 h_1$	x_2
2	x_2	$x_2^2 - x_2 = x_2(x_2-1) = \theta_2 h_2$	$x_2 - 1$
3	x_1x_2	$x_1x_2(2x_2-1) = \theta_3 h_3$	$2x_2 - 1$
4	x_2^2	$2x_2x_2' = 2x_2^2(x_2-1) = \theta_4 h_4$	$2x_2 - 2$
5	$x_2 - 1$	$x_2^2 - x_2 = x_2(x_2-1) = \theta_5 h_5$	x_2

It follows from Corollary 4.3.2 that $\psi_1 := \frac{\theta_1}{\theta_2} = \frac{x_1}{x_2}$ and $\psi_2 := \frac{\theta_2}{\theta_5} = \frac{x_2}{x_2-1}$ are the eigenfunctions to the eigenvalues 1 and -1, respectively. It is clear that $\psi_1 = \psi_3^{-1}$ and follows from Equation 4.3.13 that $\psi_1 \sim \psi_3$.

Now, solving the following equation

$$\psi(\sigma(t,(x_1,x_2)) = e^{t\mathcal{K}}\psi(x_1,x_2) \tag{4.4.14}$$

where $\sigma(t,(x_1,x_2)) := (x_1(t), x_2(t))$. So,

$$\begin{aligned} \psi_1(\sigma(t,(x_1,x_2)) =& e^{t\mathcal{K}}\psi_1(x_1,x_2) \\ \frac{x_1(t)}{x_2(t)} =& e^t\frac{x_1}{x_2} \end{aligned} \tag{4.4.15}$$

and

$$\begin{aligned} \psi_2(\sigma(t,(x_1,x_2)) =& e^{t\mathcal{K}}\psi_2(x_1,x_2) \\ \frac{x_2(t)}{x_2(t)-1} =& e^{-t}\frac{x_2}{x_2-1}. \end{aligned} \tag{4.4.16}$$

By solving Equations 4.4.15 and 4.4.16, then the solution can be written as

$$\begin{aligned} x_1(t) =& \frac{x_1}{e^{-t}x_2 + 1 - x_2} \\ x_2(t) =& \frac{e^{-t}x_2}{e^{-t}x_2 - x_2 + 1}. \end{aligned} \tag{4.4.17}$$

□

Example 4.4.7. Consider the system

$$x_1'(t) = x_1(t)x_2(t) - x_1(t)$$
$$x_2'(t) = x_2^2(t) - x_1(t) + x_2(t) \tag{4.4.18}$$

where $(x_1(0), x_2(0)) = (x_1, x_2) \in \Omega := \mathbb{R}^2$ and with associated Koopman-Lie operator

$$\mathcal{K}g = (x_1x_2 - x_1)\frac{\partial g}{\partial x_1} + (x_2^2 - x_1 + x_2)\frac{\partial g}{\partial x_2}. \tag{4.4.19}$$

The initial library of possible measurements

$$\Theta := \begin{pmatrix} 1 & x_1 & x_1x_2 & x_1 - x_2 & ax_1 + bx_2 \end{pmatrix}.$$

Table 4.7. Eigenfunctions of Example 4.4.7.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1	$x_1x_2 - x_1 = \theta_1 h_1$	$x_2 - 1$
2	x_1x_2	$2x_1x_2^2 - x_1^2 = \theta_2 h_2$	$\frac{2x_1x_2^2 - x_1^2}{x_1x_2}$
3	$x_1 - x_2$	$x_2x_1 - x_2^2 - x_2 = \theta_3 h_3$	$\frac{x_2(x_1-x_2-1)}{x_1-x_2}$
4	$x_1 - x_2 - 1$	$x_2(x_1 - x_2 - 1) = \theta_4 h_4$	x_2
5	$ax_1 + bx_2$	$a(x_1x_2 - x_1) + b(x_2^2 - x_1 + x_2) = \theta_5 h_5$	$\frac{a(x_1x_2-x_1)+b(x_2^2-x_1+x_2)}{ax_1+bx_2}$

Looking at θ_5, we have $h_5 = \frac{a(x_1x_2-x_1)+b(x_2^2-x_1+x_2)}{ax_1+bx_2} = x_2 + 1 + \frac{(-2a-b)x_1}{ax_1+bx_2}$. By sitting $b = -2a$, in particular, choose $a = 1$ and $b = -2$. Therefore, $\theta_5 = x_1 - 2x_2$ and $h_5 = x_2 + 1$.

It follows from Corollary 4.3.2 that $\psi_1 := \frac{\theta_1}{\theta_4} = \frac{x_1}{x_1-x_2-1}$ and $\psi_2 := \frac{\theta_1}{\theta_5} = \frac{x_1}{x_1-2x_2}$ are the eigenfunctions to the eigenvalues -1 and -2, respectively.

Since

$$\psi(\sigma(t,(x_1,x_2))) = e^{t\mathcal{K}}\psi(x_1,x_2) \tag{4.4.20}$$

where $\sigma(t,(x_1,x_2)) := (x_1(t), x_2(t))$. It follows that

$$\begin{aligned} \psi_1(\sigma(t,(x_1,x_2)) =& e^{t\mathcal{K}}\psi_1(x_1,x_2) \\ \frac{x_1(t)}{x_1(t)-x_2(t)-1} =& e^{-t}\frac{x_1}{x_1-x_2-1} \end{aligned} \tag{4.4.21}$$

and

$$\begin{aligned} \psi_2(\sigma(t,(x_1,x_2)) =& e^{t\mathcal{K}}\psi_2(x_1,x_2) \\ \frac{x_1(t)}{x_1(t)-2x_2(t)} =& e^{-2t}\frac{x_1}{x_1-2x_2}. \end{aligned} \tag{4.4.22}$$

By solving Equations 4.4.21 and 4.4.22, then the solution can be written as

$$\begin{aligned} x_2(t) =& \frac{\frac{x_1}{x_1-x_2-1} - \frac{x_1^2}{(x_1-x_2-1)(x_1-2x_2)}e^{-2t}}{-\frac{x_1}{x_1-x_2-1} + \frac{2x_1}{x_1-2x_2}e^{-t} - \frac{2x_1^2}{(x_1-x_2-1)(x_1-2x_2)}e^{-2t}} \\ x_1(t) =& \frac{x_2+1}{1-\frac{x_1-x_2-1}{x_1}e^{t}}. \end{aligned} \tag{4.4.23}$$

□

In the next section, we will explore one of the most important applications of Koopman-Lie eigenfunctions, specifically the Koopman-Lie eigenfunction with eigenvalue $\lambda = 0$, commonly known as the Hamiltonian function and denoted by H.

4.5. Applications of Koopman-Lie Eigenfunctions

The Hamiltonian function is highly useful in various fields of physics and mathematics, particularly in classical mechanics, quantum mechanics, and even in modern applications like optimization and control theory.

In particular, the Hamiltonian function H can be used to assess the quality of the splitting method discussed in Chapter 3. The relative error E_r can be measured by:

$$E_r = \frac{|H(\sigma(t,x)) - H(\sigma(0,x))|}{|H(\sigma(0,x))|}. \tag{4.5.1}$$

In this section, we will use Algorithm 4.5., Lemma 4.3.2 and Proposition 4.3.3, to derive the Hamiltonian function for both the Lotka-Volterra model and the Kermack-McKendrick model.

The **Lotka-Volterra model (LV2D)** is a predator-prey model that describes how two interacting species evolve over time —- one acting as the predator and the other as the prey. The system is governed by the following set of differential equations:

$$\begin{aligned} x'(t) &= \alpha x(t) - \beta x(t)y(t) \\ y'(t) &= \delta x(t)y(t) - \gamma y(t), \end{aligned} \tag{4.5.2}$$

where $x(t)$, $y(t)$ represent the populations of the prey and the predator, respectively, and the parameters $\alpha, \beta, \delta, \gamma$ correspond the prey's growth rate, the rate of predation, the predator's growth rate per prey consumed, and the natural death rate of the predator in the absence of prey, respectively.

The initial $(x_1(0), x_2(0)) = (x_1, x_2) \in \Omega := \mathbb{R}^2_+$ and with associated Koopman-Lie operator

$$\mathcal{K}g = (\alpha x_1 - \beta x_1 x_2)\frac{\partial g}{\partial x_1} + (\delta x_1 x_2 - \gamma x_2)\frac{\partial g}{\partial x_2}. \tag{4.5.3}$$

To find the Hamiltonian function, we use **Algorithm 4.5.** and the initial library of possible measurements

$$\Theta := \begin{pmatrix} 1 & x_1^\gamma & x_2^\alpha & e^{\delta x} & e^{\beta y} \end{pmatrix}.$$

Table 4.8. Hamiltonian function of LV2D.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1^γ	$\gamma x_1^{\gamma-1} x_1(\alpha - \beta x_2) = x_1^\gamma(\gamma\alpha - \gamma\beta x_2) = \theta_1 h_1$	$\gamma\alpha - \gamma\beta x_2$
2	x_2^α	$\alpha x_2^{\alpha-1} x_2(\delta x_1 - \gamma) = \theta_2 h_2$	$\alpha\delta x_1 - \alpha\gamma$
3	$e^{\delta x_1}$	$\delta e^{\delta x_1} x_1(\alpha - \beta x_2) = \theta_3 h_3$	$\delta\alpha x_1 - \delta\beta x_1 x_2$
4	$e^{\beta x_2}$	$\beta e^{\beta x_2} x_2(\delta x_1 - \gamma) = \theta_4 h_4$	$\beta\delta x_1 x_2 - \beta\gamma x_2$

Notice that $(h_3 + h_4) - (h_1 + h_2) = 0$. Thus, the Koopman-Lie eigenfunction corresponding to the eigenvalue $\lambda = 0$ is derived from Propositions 4.3.1, 4.3.3 , and Algorithm 4.5. is given by

$$H(x_1, x_2) = \frac{e^{\delta x_1} e^{\beta x_2}}{x_1^\gamma x_2^\alpha} \tag{4.5.4}$$

Remark 4.5.1. Equation 4.5 is equivalent to the standard Hamiltonian function derived using the integral method. Let

$$x'(t) = F_1(x(t), y(t)) = F_{11}(x(t))F_{12}(y(t))$$

$$y'(t) = F_2(x(t), y(t)) = F_{21}(x(t))F_{22}(y(t))$$

with initial conditions $(x(0), y(0)) = (x_1, y_1) \in \Omega)$. Then there exists a function $H(x, y)$ such that $H(x(t), y(t)) = H(x(0), y(0))$, for all $\bar{x} = (x, y) \in \Omega$ and $0 \leq t < m(\bar{x})$, where

$$H(x, y) = \int \frac{F_{21}(x)}{F_{11}(x)}\, dx - \int \frac{F_{12}(y)}{F_{22}(y)}\, dy, \tag{4.5.5}$$

and

$$H(\sigma(t, \bar{x})) = c = e^{t\mathcal{K}} H(x, y) \implies \mathcal{K}H(x, y) = 0.$$

Proof. Since the system is separable, we can rewrite it as follows

$$\frac{dx}{dy} = \frac{F_{11}(x)F_{12}(y)}{F_{21}(x)F_{22}(y)},$$

integrating both sides:

$$\int \frac{F_{21}(x)}{F_{11}(x)}\,dx = \int \frac{F_{12}(y)}{F_{22}(y)}\,dy + C \implies \int \frac{F_{21}(x)}{F_{11}(x)}\,dx - \int \frac{F_{12}(y)}{F_{22}(y)}\,dy = C.$$

Now apply (4.5.5)to the Lotka-Volterra system

$$x'(t) = \alpha x(t) - \beta x(t)y(t)$$

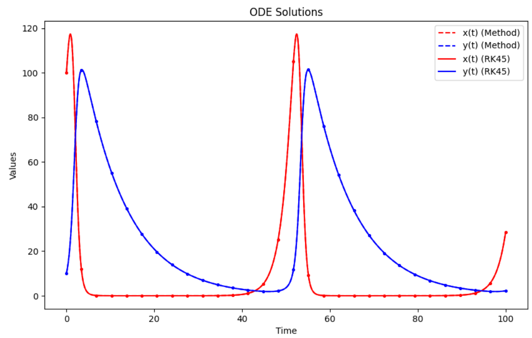
$$y'(t) = \delta x(t)y(t) - \gamma y(t),$$

with initial $(x(0), y(0)) = (x, y) \in \Omega$. By sitting $F_{11}(x) = x$, $F_{12}(y) = \alpha - \beta y$, $F_{21}(x) = \delta x - \gamma$, and $F_{22}(y) = y$, then we have

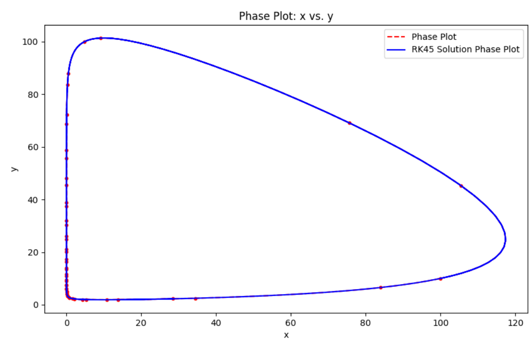
$$\begin{aligned} H(x,y) &= \int \frac{F_{21}(x)}{F_{11}(x)}\,dx - \int \frac{F_{12}(y)}{F_{22}(y)}\,dy \\ &= \int \frac{\delta x - \gamma}{x}dx - \int \frac{\alpha - \beta y}{y}dy \\ &= \gamma \ln|x| + \delta x - \alpha \ln|y| + \beta y. \end{aligned}$$

□

Now, using Equation 4.5, for given initial conditions: $\alpha = 0.5$, $\beta = 0.02$, $\delta = 0.01$, $\gamma = 0.1$, $x(0) = 100$, $y(0) = 10$, considering the number of iterations $n = 1000$ and total time $t = 100$, we compare the approximation of the solution obtained by the splitting methods $\sigma(t, (x, y))$ and the Runge-Kutta method (RK45) $\tilde{\sigma}(t, (x, y))$, which results in the following:



(a) ODE solution.



(b) Phase plot.

Figure 4.1. Comparison of the third-order method and RK45 for the LV model.

Table 4.9. The E_r of the third-order approximation is compared with $E_{\tilde{r}}$ of RK45 for the LV model.

Time	$H(x, y)$	$H(\tilde{x}, \tilde{y})$	E_r	$E_{\tilde{r}}$
0	0	0	0	0
10	1.12606e-07	2.88435e-06	2.734427e-07	7.00409473e-06
20	1.12605e-07	3.2169266e-05	2.7344142e-07	7.811685e-05
30	1.126074e-07	3.32956e-05	2.734453e-07	8.085194e-05
40	1.12631638e-07	3.62404905e-05	2.7350418e-07	8.800303e-05
50	1.0991952e-07	3.44472265e-05	2.6691832e-07	8.3648437e-05
60	1.94687623e-07	3.735858e-05	4.727613e-07	9.071814e-05
70	1.946644e-07	6.1164952e-05	4.72704934e-07	0.00014853
80	1.9466613e-07	7.3077776e-05	4.727091e-07	0.0001774553
90	1.946782904e-07	6.93063451e-05	4.727386e-07	0.0001682971
100	1.952592e-07	6.925106e-05	4.74149332e-07	0.000168163

According to the Table 4.9., we observe that the third-order approximation achieves accuracy comparable to RK45 when the number of iterations n is sufficiently large. We also compare the Lie-Trotter, Strang, third-order, and sixth-order methods to RK45.

Table 4.10. Relative error of different approximations for the LV model at $t = 100$.

Method	$n = 100$	$n = 1000$	$n = 10000$
Lie-Trotter	0.491634141	0.027463401243	0.0023093248
Strang	0.03299725522	0.0002932121	2.933394141e-06
Third order	0.018645393334	4.74149332e-07	3.619100108e-11
Sixth order	7.57745275e-07	1.7469835e-13	3.8956654e-14
RK45	0.00016816282452	0.000168163	0.000168162825

Remark 4.5.2. We observed that increasing the number of iterations and the order improves the accuracy of the approximation. The third- and sixth-order methods give better accuracy for larger values of n.

The **Kermack-McKendrick model (SIR)**, is a mathematical framework used to describe the spread of infectious diseases within a population. The dynamics of the model are described by a system of ordinary differential equations:

$$x'_1(t) = -\alpha x_1(t)x_2(t) \tag{4.5.6}$$

$$x'_2(t) = \alpha x_1(t)x_2(t) - \beta x_2(t) \tag{4.5.7}$$

$$x'_3(t) = \beta x_2(t) \tag{4.5.8}$$

where $(x_1(0), x_2(0), x_3(0)) = (x_1, x_2, x_3) \in \Omega := \mathbb{R}^3_+$ and $x_1(t), x_2(t)$, and $x_3(t)$ are the number of susceptible, infectious, and recovered individuals at time t, respectively. The parameter α is the transmission rate (the rate at which susceptible individuals become infected), and β is the recovery rate (the rate at which infectious individuals recover).

The associated Koopman-Lie operator

$$\mathcal{K}g = -\alpha x_1 x_2 \frac{\partial g}{\partial x_1} + (\alpha x_1 x_2 - \beta x_2)\frac{\partial g}{\partial x_2} + \beta x_2 \frac{\partial g}{\partial x_3}. \tag{4.5.9}$$

Using **Algorithm 4.5.** and the initial library of possible measurements

$$\Theta := \begin{pmatrix} 1 & x_1^{\alpha} & x_1^{\beta} & x_2^{\alpha} & e^{\alpha x_1} & e^{\alpha x_2} & e^{\alpha x_3} & e^{\beta x_1} & e^{\beta x_2} & e^{\beta x_3} \end{pmatrix}$$

Table 4.11. Hamiltonian function of the Kermack-McKendrick model (SIR).

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1^{α}	$-\alpha^2 x_2 x_1^{\alpha} = \theta_1 h_1$	$-\alpha^2 x_2$
2	x_1^{β}	$-\alpha\beta x_2 x_1^{\beta} = \theta_2 h_2$	$-\alpha\beta x_2$
3	x_2^{α}	$\alpha(\alpha x_1 - \beta) x_2^{\alpha} = \theta_3 h_3$	$\alpha^2 x_1 - \alpha\beta$
4	$e^{\alpha x_1}$	$-\alpha^2 x_1 x_2 e^{\alpha x_1} = \theta_4 h_4$	$-\alpha^2 x_1 x_2$
5	$e^{\alpha x_2}$	$\alpha x_2(\alpha x_1 -) e^{2} = \theta_5 h_5$	$\alpha^2 x_2 x_1 - \alpha\beta x_2$
6	$e^{\alpha x_3}$	$\alpha\beta x_2 e^{\alpha x_3} = \theta_6 h_6$	$\alpha\beta x_2$
7	$e^{\beta x_1}$	$-\alpha\beta x_1 x_2 e^{\beta x_1} = \theta_7 h_7$	$-\alpha\beta x_1 x_2$
8	$e^{\beta x_2}$	$(\alpha\beta x_1 x_2 - \beta^2 x_2) e^{\beta x_2} = \theta_8 h_8$	$\alpha\beta x_1 x_2 - \beta^2 x_2$
9	$e^{\beta x_3}$	$\beta^2 x_2 e^{\beta x_3} = \theta_9 h_9$	$\beta^2 x_2$

Notice that $h_2 - (h_1 + h_2) = 0$. Thus, the Hamiltonian function is given by

$$H(x_1, x_2, x_3) = \frac{x_1^{\beta}}{e^{\alpha x_1} e^{\alpha x_2}} \tag{4.5.10}$$

For the given initial conditions: $\alpha = 0.5$, $\beta = 0.3$, $x(0) = 0.99$, $y(0) = 0.01$, $z(0) = 0.01$, considering the number of iterations $n = 1000$ and the total time $t = 100$,

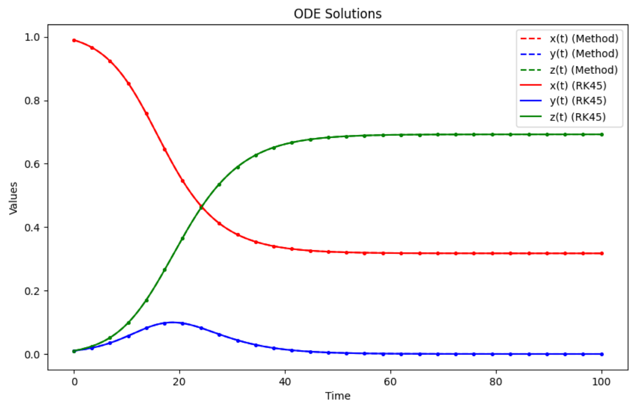


Figure 4.2. Comparison of the third-order method and RK45 for the SIR model.

Table 4.12. The E_r of the third-order approximation is compared with $E_{\tilde{r}}$ of RK45 for the SIR model.

Time	E_r	$E_{\tilde{r}}$
0	0	0
10	2.310943e-12	2.512172e-09
20	8.812683e-13	2.350606e-09
30	1.353481e-12	1.159298e-09
40	4.966314e-13	1.666694e-09
50	4.729473e-13	2.270360e-09
60	4.920415e-13	2.350518e-09
70	4.981002e-13	2.410142e-09
80	4.995690e-13	2.427375e-09
90	5.004870e-13	2.431035e-09
100	4.995690e-13	2.432801e-09

Table 4.13. Relative errors for different approximations for the SIR model at $t = 100$.

Method	$n = 100$	$n = 1000$	$n = 10000$
Lie-Trotter	0.000471	0.000049	1.313878e-05
Strang	6.887782e-06	6.889311e-08	1.458724e-09
Third order	9.376734e-09	4.995690e-13	3.121159e-15
Sixth order	1.578939e-14	4.773537e-15	3.231317e-14
Runge-Kutta (RK45)	2.432801e-09	2.432801e-09	2.512172e-09

Moreover, we can use Proposition 4.3.3 and Algorithm 4.5. to find Hamiltonian functions in higher dimensions. For example, consider the Lotka-Volterra model in three dimensions (LV3D):

$$x'_1(t) = x_1(t)(1 - x_2(t))$$

$$x'_2(t) = x_2(t)(x_1(t) - x_3(t))$$

$$x'_3(t) = x_3(t)(x_2(t) - 1)$$

where $(x_1(0), x_2(0), x_3(0)) = (x_1, x_2, x_3) \in \Omega := \mathbb{R}^3_+$ and with associated Koopman-Lie operator

$$\mathcal{K}g = (x_1 - x_1x_2)\frac{\partial g}{\partial x_1} + (x_1x_2 - x_2x_3)\frac{\partial g}{\partial x_2} + (x_2x_3 - x_3)\frac{\partial g}{\partial x_3}. \tag{4.5.11}$$

The initial library of possible measurements

$$\Theta := \begin{pmatrix} 1 & x_1 & x_2 & x_3 & e^{x_1} & e^{x_2} & e^{x_3} \end{pmatrix}$$

Table 4.14. Hamiltonian function of LV3D.

i	θ_i	$\mathcal{K}\theta_i = \theta_i h_i$	h_i
0	1	0	0
1	x_1	$x_1(1 - x_2) = \theta_1 h_1$	$1 - x_2$
2	x_2	$x_2(x_1 - x_3) = \theta_2 h_2$	$x_1 - x_3$
3	x_3	$x_3(x_2 - 1) = \theta_3 h_3$	$x_2 - 1$
4	e^{x_1}	$e^{x_1}(x_1 - x_1x_2) = \theta_4 h_4$	$x_1 - x_1x_2$
5	e^{x_2}	$e^{x_2}(x_2x_1 - x_2x_3) = \theta_5 h_5$	$x_2x_1 - x_2x_3$
6	e^{x_3}	$e^{x_3}(x_3x_2 - x_3) = \theta_6 h_6$	$x_3x_2 - x_3$

Notice that $(h_4 + h_5 + h_6) - h_2 = 0$. Thus, the Hamiltonian function is given by

$$H(x_1, x_2) = \frac{e^{x_1}e^{x_2}e^{x_3}}{x_2}.$$

For the given initial conditions: $x(0) = 1$, $y(0) = 0.5$, $z(0) = 2.0$, considering the number of iterations $n = 10000$ and total time $t = 100$. The relative error E_r of the third-order approximation is compared with the relative error $E_{\tilde{r}}$ of RK45, as shown in the table below.

Table 4.15. The E_r of the third-order approximation is compared with $E_{\tilde{r}}$ of RK45 for the LV3D model.

Time	E_r	$E_{\tilde{r}}$
0	0	0
10	6.509697e-12	3.525271e-06
20	4.169277e-10	2.434830e-06
30	4.439513e-10	1.394332e-06
40	3.136666e-11	8.461986e-07
50	2.383949e-11	5.630829e-07
60	1.185222e-10	4.091040e-06
70	3.322321e-10	2.198812e-06
80	6.381623e-11	3.484594e-07
90	7.620545e-11	2.968360e-06
100	2.582701e-10	4.961482e-06

We show that the relative error E_r is smaller for the third-order approximation than for the Runge-Kutta method, indicating better accuracy. Similarly, we compare the Lie-Trotter, Strang, third-, and sixth-order methods with the Runge-Kutta method.

Table 4.16. Relative errors for different approximations for the LV3D model at $t = 10$.

Method	$n = 100$	$n = 1000$	$n = 10000$
Lie-Trotter	0.275905	0.000824	0.000053
Strang	0.000884	0.000012	2.379111e-08
Third order	2.527004e-06	6.509697e-12	1.287392e-15
Sixth order	4.175656e-11	6.866090e-15	1.120031e-13
RK45	4.850160e-06	3.525271e-06	3.595274e-07

Appendix A.

The main reference used in this appendix is [33].

Definition A.0.1. A topological space Ω is called a **Hausdorff space** if for each pair x_1, x_2 of distinct points of Ω, there exist neighborhoods U_1, and U_2 of x_1 and x_2, respectively, that are disjoint.

Definition A.0.2. A topological space Ω is said to be locally compact at x if there is some compact subspace K of Ω that contains a neighborhood of x. If Ω is locally compact at each of its points, Ω is simply said to be **locally compact**.

Note that a compact space is automatically locally compact. For example, the space $\mathbb{R}^n$ is locally compact Hausdorff space; the point x lies in some basis element $(a_1, b_1) \times \cdots \times (a_n, b_n)$, which, in turn, is contained within the compact subspace $[a_1, b_1] \times \cdots \times [a_n, b_n]$.

An alternative formulation of local compactness, one that is more intrinsically 'local,' is equivalent to our definition when Ω is Hausdorff.

Theorem A.0.3. *Let Ω be a Hausdorff space. Then Ω is locally compact if and only if given x in Ω, and given a neighborhood U of x, there is a neighborhood V of x such that $\overline{V}$ is compact and $\overline{V} \subset U$.*

Definition A.0.4. Let Ω be a locally compact Hausdorff space equipped with the *supremum norm* of a function g on Ω, denoted $\|g\|_\infty$, is defined as:

$$\|g\|_\infty = \sup_{x \in \Omega} |g(x)|.$$

Theorem A.0.5. *The space*

$$C_m(\Omega) := \{g \in C_b(\Omega) \mid \lim_{x \to \partial_m(\Omega)} g(x) = 0\}$$

is a Banach space when equipped with the supremum norm

$$\|g\|_\infty := \sup_{x\in\Omega} |g(x)|. \tag{A.0.1}$$

Proof. We verify that $C_m(\Omega)$ is a vector space, and then we show completeness under the supremum norm. To show that $C_m(\Omega)$ is a vector space, we check closure under addition and scalar multiplication.

Let $g, h \in C_m(\Omega)$. Then, for any sequence $x_n \to \partial_m(\Omega)$,

$$\lim_{x_n\to\partial_m(\Omega)} g(x_n) = 0, \qquad \lim_{x_n\to\partial_m(\Omega)} h(x_n) = 0.$$

Then, $\lim\limits_{x_n\to\partial_m(\Omega)} (g(x_n) + h(x_n)) = 0$. Thus, $g + h \in C_m(\Omega)$.

Now, for any $\lambda \in \mathbb{R}$ and $g \in C_m(\Omega)$, we have $\lim_{x_n\to\partial_m(\Omega)} g(x_n) = 0$. Therefore, we get $\lim_{x_n\to\partial_m(\Omega)} \lambda g(x_n) = \lambda \cdot 0 = 0$. Thus, $\lambda g \in C_m(\Omega)$, proving closure under scalar multiplication.

To show that $C_m(\Omega)$, is complete, we must prove that every Cauchy sequence $\{g_n\}$ in $C_m(\Omega)$ converges to a function $g \in C_m(\Omega)$. Since $\{g_n\}$ is Cauchy; for every $\epsilon > 0$, there exists N such that for all $n, k \geq N$, $\|g_n - g_k\|_\infty < \epsilon$. Since $C_b(\Omega)$ is complete, there exists $g \in C_b(\Omega)$ such that $\lim_{n\to\infty} \|g_n - g\|_\infty = 0$. Thus, $g_n \to g$ uniformly in $C_b(\Omega)$. Since each g_n satisfies, $\lim\limits_{x\to\partial_m(\Omega)} g_n(x) = 0$. For any $\epsilon > 0$, there exists n_0 such that for all $n \geq n_0$,

$$\sup_{x\in\Omega} |g_n(x) - g(x)| < \frac{\epsilon}{2}.$$

Since $g_{n_0}(x) \to 0$ as $x \to \partial_m$, we can choose x close to ∂_m so that $|g_{n_0}(x)| < \frac{\epsilon}{2}$. Thus,

$$|g(x)| \leq |g(x) - g_{n_0}(x)| + |g_{n_0}(x)| < \epsilon.$$

Since ϵ was arbitrary, it follows that $\lim_{x\to\partial_m(\Omega)} g(x) = 0$. Thus, $g \in C_m(\Omega)$. $\square$

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Vita

Ibrahem AlJabea was born in Jordan. He completed his undergraduate studies at Al-Bayt University in June 2005. He earned a Master of Science in Mathematics from Memorial University in June 2018. In August 2019, he began his mathematics studies at Louisiana State University, where he earned his Master of Science in 2022. He is currently a Ph.D. candidate in Mathematics and is expected to receive his degree in May 2025.