# Deep Learning-based Approaches for State Space Models:
# A Selective Review

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**Abstract**

State-space models (SSMs) offer a powerful framework for dynamical system analysis, wherein the temporal dynamics of the system are assumed to be captured through the evolution of the latent states, which govern the values of the observations. This paper provides a selective review of recent advancements in deep neural network-based approaches for SSMs, and presents a unified perspective for discrete time deep state space models and continuous time ones such as latent neural Ordinary Differential and Stochastic Differential Equations. It starts with an overview of the classical maximum likelihood based approach for learning SSMs, reviews variational autoencoder as a general learning pipeline for neural network-based approaches in the presence of latent variables, and discusses in detail representative deep learning models that fall under the SSM framework. Very recent developments, where SSMs are used as standalone architectural modules for improving efficiency in sequence modeling, are also examined. Finally, examples involving mixed frequency and irregularly-spaced time series data are presented to demonstrate the advantage of SSMs in these settings.

## 1   Introduction

Latent space modeling is a widely used technical framework that aims to capture the essential features and patterns of complex data through low-dimensional representations, and it plays a central role in many learning tasks such as representation learning, link prediction, and dynamical system analysis. Within the domain of dynamical system analysis, a latent space framework assumes that the dynamics of the underlying system is governed by a low-dimensional *latent state* process, which dictates the evolution of the observed data. By separating the state evolution from the observation processes, the resulting *state space models* (SSMs) fully characterize the underlying patterns and structural dependencies of the system.

The state space modeling paradigm represents a well-established framework with a long and rich history. It was originally developed for the study of dynamical systems and control problems, such as predicting system behaviors and designing control strategies in engineering, where understanding the evolution of hidden states and their impact on observable outputs is crucial for system stability and optimization (Friedland, 2005; Zadeh and Desoer, 2008; Aoki, 2013; Kumar and Varaiya, 2015). The original SSM formalism focused on systems governed by linear dynamics under a Gaussianity assumption (Kalman, 1960; Kalman and Bucy, 1961). Over time, the framework has been extended to accommodate nonlinear dynamics and non-Gaussian data, enhancing its versatility for a wide range of real-world applications. However, the presence of nonlinearity when coupled with high-dimensionality presents significant challenges, partly due to the limitations of available technical tools. Advances in deep learning has led to renewed interest in modeling dynamical systems via SSMs; in particular, the flexible parameterization via neural networks and the variational autoencoder (VAE, Kingma and Welling, 2013)-based learning pipeline have addressed some of the limitations of earlier methods.

The main objective of this paper is to review recent advancements in deep learning techniques for SSMs, in the context of sequence modeling. Given the well-established SSM framework for dynamical systems,

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Section 2 provides an overview of the model formulation, including its general-form representation that encompasses the state and the observation equations. Classical strategies that leverage maximum likelihood estimation to learn SSM parameters from data are presented, and the roles of key tools such as filtering and smoothing are highlighted. As a technical preliminary, we also provide a brief review of VAE and its corresponding pipeline for modeling sequential data, which have become the standard approach for training neural network-based SSMs.

Section 3 reviews work in the literature, wherein the model formulation corresponds to an SSM with the state and observation equations parameterized with neural networks, and employs deep learning-based approaches to handle the learning task. Arguably, up until 2018, the models remain somewhat closely aligned with the classical framework. This alignment manifests either in the exact model formulation, such as the assumption of states evolving in *discrete time* with fixed intervals, reviewed in Section 3.1, or in key techniques for learning SSM parameters, including filtering and smoothing (see Section 3.4). However, a notable shift occurred thereafter, with the model formulation being increasingly flexible (e.g., states are assumed to evolve in continuous time) and VAE-based pipelines becoming the predominant strategy for learning (Sections 3.2 and 3.3). A key distinction between the two learning strategies lies in how they handle latent states. In the classical framework, filters and smoothers are employed to recursively update the distribution of latent states, using either closed-form updates or Monte Carlo approximations. In contrast, VAEs leverage an encoder and a decoder, wherein the encoder learns an approximate posterior of the latent states conditional on the observations, while the decoder reconstructs the data from latent states sampled from the former. Learning is done by maximizing a variational lower bound of the data likelihood. VAEs learn the SSM's dynamics in an end-to-end manner, by updating the neural network weights that are used for parameterizing the encoder and the decoder; they can handle more complex dependencies and relationships that are cumbersome or challenging to capture by classical filtering and smoothing techniques.

The material presented in Sections 2 and 3 focuses on SSM being a modeling framework for time series data, covering both classical approaches and deep learning based ones. Section 4 shifts focus and considers SSMs as modules for *input-output mapping* embedded within neural network architectures. This line of work, emerging since 2021, represents a stream of effort dedicated to enhance the models' capabilities to handle long-range dependencies in sequence modeling, such as GPT-style language models (e.g., Radford et al., 2018). In particular, compared with Transformers (Vaswani et al., 2017), its ability to efficiently model dependencies across long input sequences allows for significant reductions in memory and computational requirements. For the material presented in Section 4, the SSMs are not used as a postulated model for the data generative process, but rather they are standalone technical tools for handling sequence data.

The paper concludes by providing concrete examples that showcase a formulation akin to the SSM form is both beneficial and convenient for selected tasks, such as modeling mixed frequency and irregularly-spaced time series data. Finally, it is worth noting that this review does not cover the extensive body of work on SSMs for *control* problems, which constitute a separate topic on their own.

**Notation.** Boldface letters are used to denote multivariate random processes indexed by $t$. Specifically, $\boldsymbol{z}_t$ denotes the $d$-dimensional *latent* (state) process and $\boldsymbol{x}_t$ the $p$-dimensional *observation* process with $t$ taking values in a discrete index set $\mathcal{T} = \{0, 1, 2, \cdots, T\}$. In the case of a continuous index set $\mathcal{T} = [0, T]$, we use $\boldsymbol{z}(t), \boldsymbol{x}(t)$ to denote the processes and $\boldsymbol{z}_t, \boldsymbol{x}_t$ their values sampled at $t$. $\boldsymbol{u}_t$ and $\boldsymbol{\epsilon}_t$ denote $d$- and $p$-dimensional shock/noise processes associated with the state and observation processes, respectively, and $\boldsymbol{u}(t)$ and $\boldsymbol{\epsilon}(t)$ are analogously defined. The trajectory of a process from time $s$ to time $t$ is denoted by $\boldsymbol{x}_{s:t} := \{\boldsymbol{x}_s, \cdots, \boldsymbol{x}_t\}$. Deterministic multivariate functions of appropriate dimensions are denoted by the lower case letters $f(\cdot), g(\cdot)$ and $h(\cdot)$, possibly indexed by $t$ if they are time-varying. Matrices are denoted by capital latters (e.g., $A, B$). Finally, lower case Greek letters denote the parameters of appropriate dimensions of a distribution or a function; e.g., $\theta, \phi$, etc.

## 2 Overview of State Space Models

SSMs are a versatile modeling framework extensively used across various scientific domains, particularly for analyzing time series data. They have a hierarchical structure encompassing two multivariate processes: (i)

a $d$-dimensional *latent state* process $z_t \in \mathcal{Z}$ that captures the dynamics of the evolution of the system, and (ii) a $p$-dimensional *observation* process $x_t \in \mathcal{X}$ comprising of the measurements, whose values are dictated by the latent state. In this review, we focus on cases where both processes take continuous values, namely, $\mathcal{Z} \subseteq \mathbb{R}^d, \mathcal{X} \subseteq \mathbb{R}^p$, and thus models wherein $\mathcal{Z}$ and $\mathcal{X}$ correspond to discrete valued spaces, such as the Hidden Markov Model, are outside the scope of this review. The index $t$ of the latent and observation processes can take values in a discrete index set $\mathcal{T} := \{0, \cdots, T\}$, or a continuous one $\mathcal{T} := [0, T]$.

A functional specification of the SSM relates the processes $z_t$ and $x_t$ through equations that depend on processes of *independent shocks or noises*; specifically, assuming 1-lag Markovian dynamics

$$\text{initial state:} \quad z_0 = f_0(u_0; \theta); \tag{2.1a}$$
$$\text{state equation:} \quad z_t = f_t(z_{t-1}, u_t; \theta), \quad t > 0; \tag{2.1b}$$
$$\text{observation equation:} \quad x_t = g_t(z_t, \epsilon_t; \theta), \quad t \geq 0, \tag{2.1c}$$

where $f_0, f_t, g_t$ are deterministic multivariate functions of appropriate dimensions, and $\{u_t\}, \{\epsilon_t\}$ sequences of independent and identically distributed random variables of shocks/noises. $\theta$ collects the parameters associated with the state/observation equations, although they do not actually have shared parameters. This specification is often encountered in the engineering and natural sciences literature, wherein subject matter theoretical considerations dictate the functional form of $f$ and $g$. Some illustrative examples are presented next.

1. **Discrete time linear Gaussian SSM.** It represents an important and extensively studied class of SSMs; see detailed expositions in the books by Harvey (1990); Hannan and Deistler (2012); Durbin and Koopman (2012). Its specification under a time-invariant setting is given in the form of (2.1a)-(2.1c) with $f_t(z_{t-1}, u_t) = Az_{t-1} + u_t$, $g_t(z_t, \epsilon_t) = Cz_t + \epsilon_t$; $A$ and $C$ are matrices of appropriate dimensions, and $u_t \sim \mathcal{N}(0, Q), \epsilon_t \sim \mathcal{N}(0, R)$. For this model the parameters are $\theta := (A, Q, C, R)$.

2. **Nonlinear dynamical systems.** In discrete time, they are described by the set of equations (2.1a)-(2.1c), while in continuous time by a set of differential equations. Concretely, a specific instance can be defined by the following coupled stochastic differential equations:

$$dz(t) = f(z(t))dt + \sigma(z(t))dw^z(t),$$
$$dx(t) = g(z(t))dt + dw^x(t),$$

where $f(\cdot), \sigma(\cdot)$ and $g(\cdot)$ are measurable multivariate functions (on the appropriate filtration), while $w^x(t)$ and $w^z(t)$ are standard multivariate Wiener processes. This model underpins the extensive literature on the multifaceted mathematical problem of nonlinear filtering (Kalman and Bucy, 1961; Bain and Crisan, 2009; Davis and Marcus, 1981; Lototsky et al., 1997); see also Appendix C.

The main learning task involves estimating the parameter $\theta$ of the model and the latent process $z_t$, given a sequence of observations $\{x_t, t \in \mathcal{T}\}$—collectively known as *system identification*. The learning of the latent process $z_t$ itself is referred to as the *state estimation/identification* problem. Note that when $f$ and $g$ are known (i.e., both their functional form and the parameter $\theta$ are given)—which is often the case in engineering and other physical systems—the state identification problem has been extensively studied as an independent topic on its own in the literature.

## 2.1 An overview of SSM learning

For an SSM learning task, one has access to observations of the system's trajectory over time. In the case of a discrete time SSM, these observations are collected directly from the recursive generation mechanism, i.e., $x_1, \cdots, x_T$. In the continuous case, they correspond to a realization of the underlying continuous trajectory *sampled* at discrete time points; i.e., $x_{t_1}, \cdots, x_{t_n}, t_i \in [0, T]$. To highlight key concepts, the remainder of this section provides an overview of learning frameworks focusing on the discrete time case. The continuous time case can be handled analogously with some necessary modifications, which will be discussed in more detail as specific models are introduced in Section 3.

The model in (2.1a)-(2.1c) can be alternatively defined through the following probabilistic specification

$$\text{initial state:} \quad \boldsymbol{z}_0 \sim p_\theta(\boldsymbol{z}_0); \tag{2.2a}$$

$$\text{state equation:} \quad \boldsymbol{z}_t \mid (\boldsymbol{z}_0 = \boldsymbol{z}_0, \cdots, \boldsymbol{z}_{t-1} = \boldsymbol{z}_{t-1}) \sim p_\theta(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}); \tag{2.2b}$$

$$\text{observation equation:} \quad \boldsymbol{x}_t \mid (\boldsymbol{z}_0 = \boldsymbol{z}_0, \cdots \boldsymbol{z}_t = \boldsymbol{z}_t, \boldsymbol{x}_0 = \boldsymbol{x}_0, \cdots, \boldsymbol{x}_{t-1} = \boldsymbol{x}_{t-1}) = \boldsymbol{x}_t|\boldsymbol{z}_t \sim p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t). \tag{2.2c}$$

Given an identifiable SSM[1], $\theta$ is typically learned by maximum likelihood estimation methods, i.e., $\max p_\theta(\mathbb{x}_{1:T})$, or equivalently $\widehat{\theta} := \operatorname{argmax} \log p_\theta(\mathbb{x}_{1:T})$. Based on the specification in (2.2a)-(2.2c), the marginal distribution (likelihood) of the observed trajectory $\mathbb{x}_{1:T}$ (jointly over time) can be written as

$$p_\theta(\mathbb{x}_{1:T}) = \int_{\mathcal{Z}} p_\theta(\mathbb{x}_{1:T}, \mathbb{z}_{0:T}) \mathrm{d}\mathbb{z}_{0:T} = \int \cdots \int_{\mathcal{Z}} p_\theta(\mathbb{x}_{1:T}, \mathbb{z}_{0:T}) \mathrm{d}\boldsymbol{z}_0 \mathrm{d}\boldsymbol{z}_1 \cdots \mathrm{d}\boldsymbol{z}_T, \tag{2.3}$$

i.e., it can be obtained by "averaging" the joint density $p_\theta(\cdot, \cdot)$ of the observed trajectory and the latent states, over all possible sequences of the latent state process. However, to compute the likelihood in (2.3) poses two challenges: (i) the high-dimensional nature of the integral, whose computational complexity increases exponentially as the number of observations points $T$ increases, and (ii) the fact that for most distributions $p_\theta$, one needs to resort to numerical/sampling methods to evaluate each term. In addition, as with many other statistical methods, optimization-related issues involving the complex likelihood in (2.3) are still present, although we do not segregate this aspect within the scope of this paper. Performing the computation in (2.3) in a *recursive* manner addresses the first challenge, but the second one persists and requires further attention, as illustrated next.

To compute the likelihood in (2.3), one can express the integral as follows, by applying the recursion:

$$p_\theta(\mathbb{x}_{1:T}) = p_\theta(\mathbb{x}_{1:T-1})p_\theta(\boldsymbol{x}_T|\mathbb{x}_{1:T-1}) = \cdots = \prod_{t=1}^{T} p_\theta(\boldsymbol{x}_t|\mathbb{x}_{1:t-1}), \tag{2.4}$$

with $p_\theta(\boldsymbol{x}_t|\mathbb{x}_{1:t-1})$ being the *one-step predictive likelihood*. This predictive likelihood based on (2.2a)-(2.2c) can be rewritten as

$$p_\theta(\boldsymbol{x}_t|\mathbb{x}_{1:t-1}) = \int_{\mathcal{Z}} p_\theta(\boldsymbol{x}_t, \boldsymbol{z}_t|\mathbb{x}_{1:t-1}) \mathrm{d}\boldsymbol{z}_t = \int_{\mathcal{Z}} p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t) p_\theta(\boldsymbol{z}_t|\mathbb{x}_{1:t-1}) \mathrm{d}\boldsymbol{z}_t, \tag{2.5}$$

where $p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t)$ corresponds to the probabilistic mechanism of the observation equation, and $p_\theta(\boldsymbol{z}_t|\mathbb{x}_{1:t-1})$ to the *posterior predictive* density of the latent state. Given the Markovian dynamics of the SSM, the posterior predictive distribution can be calculated using the Chapman-Kolmogorov equation; i.e.,

$$p_\theta(\boldsymbol{z}_t|\mathbb{x}_{1:t-1}) = \int_{\mathcal{Z}} p_\theta(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}) p_\theta(\boldsymbol{z}_{t-1}|\mathbb{x}_{1:t-1}) \mathrm{d}\boldsymbol{z}_{t-1}. \tag{2.6}$$

The calculations in (2.5) and (2.6) require calculating the posterior distribution $p_\theta(\boldsymbol{z}_t|\mathbb{x}_{1:t})$, which is referred to as the *filtering* distribution in the literature; they proceed *forward* in time and do not leverage the $\mathbb{x}_{t+1:T}$ data. To obtain better estimates of the latent state $\boldsymbol{z}_t$, it is advantageous to utilize the full trajectory $\mathbb{x}_{1:T}$ and compute the *smoothing* density $p_\theta(\boldsymbol{z}_t|\mathbb{x}_{1:T})$, which can be accomplished by running the recursive calculation *backwards* in time, as elaborated in Section 2.2.

The key takeaway from this brief derivation is that by applying recursion, one can avoid the challenge of evaluating high-dimensional integrals related to the time dimension when calculating the likelihood. However, the evaluation of various filtering and posterior predictive distributions that are present in each term still poses challenges, with the exception of selected SSMs, wherein their special specification significantly simplifies the underlying calculations. The most "famous" such case is the discrete linear Gaussian SSM for which the nature and properties of the Gaussian distribution (fully parameterized by the mean and covariance, whose conditional distributions also remain Gaussian) mitigate the computational challenges. For all

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[1]If $\theta \neq \theta'$, then $p_\theta(\mathbb{x}_{1:T}) \neq p_{\theta'}(\mathbb{x}_{1:T})$, namely the set on which the two likelihoods differ, has a positive measure (in the usual measure theoretic sense).

other *non-Gaussian and nonlinear* SSMs, calculating the likelihood remains a significant challenge, particularly when the state dimension $d$ and the observation dimension $p$ are moderate to high, due to the need to evaluate the integrals involved.

The classical framework follows one of the two routes to address the challenge of the integral noted above: (i) assuming that the filtering and predictive densities of the latent states can be approximated satisfactorily by Gaussian distributions, which simplifies both the calculations and the optimization problem for obtaining the maximum likelihood estimate of $\theta$; or (ii) using particle filtering and Monte Carlo methods to evaluate the integrals involved. While the second route is more general, it still requires specifying the distribution and/or the functional form of the SSM, and tends to perform rather poorly for large $p$ and $d$. Irrespective of the route adopted, the maximum likelihood estimation can be based either on *marginalization* or a *data augmentation* strategy, as discussed in Section 2.2.

The deep learning framework enables flexible parameterization of the state and observation equations using neural networks. A key feature of most approaches in this framework is the use of a VAE-based learning pipeline: the encoder approximates the posterior distribution $p_\theta(z_{1:T}|x_{1:T})$, the decoder emulates the data generative process, and the model parameters are learned in an end-to-end fashion by optimizing an evidence lower bound that approximates the log-likelihood. Further, the encoder/decoder distributions are assumed to be Gaussian, wherein the mean and the covariance—typically assumed to be diagonal—of the latent states/observations are parameterized by neural networks. This Gaussian assumption simplifies the learning and optimization process, allowing efficient computation of the variational evidence lower bound (details in Section 2.3).

## 2.2 Classical approaches of maximum likelihood based learning of SSMs

For MLE-based learning of the model parameters $\theta$, there are two dominant strategies: the first one is based on *marginalization* of the latent states, treating them as nuisance parameters, and the optimization focuses only on the model parameters $\theta$; the second one is based on *data augmentation*, wherein the latent states are considered auxiliary variables and estimated jointly with the model parameters $\theta$.

Irrespective of the selected strategy, both approaches require solving the state estimation problem. Due to the Markovian dynamics governing the latent state's evolution, this involves two key learning subtasks: (i) *filtering* and *prediction*, which estimate the posterior distribution of the latent variable $z_t$ and $z_{t+1}, t \in \mathcal{T}$ given an observed trajectory up to time $t$ (i.e., $x_{1:t}$), and (ii) *smoothing* which estimates the posterior distribution of the latent state $z_t$ at time $t$, given a full observed trajectory $x_{1:T}$.

**Marginalization.** The first strategy is based in obtaining the MLE $\widehat{\theta}$ by directly optimizing the marginal log-likelihood, namely,

$$\widehat{\theta} = \mathrm{argmax}_\theta \ \log p_\theta(x_{1:T}) = \sum_{t=1}^{T} \log \int_{\mathcal{Z}} p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t) p_\theta(\boldsymbol{z}_t|x_{1:t-1}) \mathrm{d}\boldsymbol{z}_t,$$

where the state variables are integrated out (marginalized) and $\theta$ is the only parameter to be estimated. Optimizing the marginalized likelihood requires an iterative algorithm, often based on gradient ascent. The algorithm computes a sequence of iterates $\theta^{(k)}$ until a stopping criterion is satisfied. The update rule is given by $\theta^{(k+1)} = \theta^{(k)} + \lambda^{(k)}\alpha^{(k)}$, where $\alpha^{(k)}$ denotes an ascent direction and $\lambda^{(k)}$ the step size. Typically ascent directions can be the gradient of the log-likelihood function evaluated at the previous iterate $\theta^{(k)}$, namely, $\alpha^{(k)} = \nabla_\theta \log p_{\theta^{(k)}}(x_{1:T})$, or a Newton direction $\alpha^{(k)} = \left(H(\theta^{(k)})\right)^{-1}\nabla_\theta \log p_{\theta^{(k)}}(x_{1:T})$, with $H(\theta^{(k)})$ denoting the Hessian matrix of the log-likelihood evaluated at $\theta^{(k)}$. By Fisher's identity, the gradient can be expressed as $\nabla_\theta \log p_\theta(x_{1:T}) = \int_{\mathcal{Z}} \nabla_\theta \log p_\theta(z_{1:T}, x_{1:T}) p_\theta(z_{1:T}|x_{1:T}) \mathrm{d}z_{1:T}$. This expression of the gradient (and analogously that of the Hessian) involves the filtering and smoothing distributions of the latent state, which is detailed later in the exposition of the E-step in the data augmentation approach. However, except for linear Gaussian SSMs, computing the gradient and the Hessian of the log-likelihood is computationally intractable, requiring approximations such as Sequential Monte Carlo (SMC) methods, as discussed in detail in work by Liu and Chen (1998); Olsson et al. (2008); Poyiadjis et al. (2011); Nemeth et al. (2016); Kantas et al. (2015).

**Data augmentation.** The second strategy leverages data augmentation, wherein the latent states are treated as auxiliary variables and hence must be "imputed" to obtain a complete data likelihood, given by

$$p_\theta(\varkappa_{1:T}, \mathbb{z}_{0:T}) = p_\theta(\boldsymbol{z}_0) \prod_{t=1}^{T} p_\theta(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}) \prod_{t=1}^{T} p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t),$$

that in turn is used to estimate the model parameters $\theta$. In this approach, the Expectation-Maximization (EM) algorithm provides an iterative procedure to obtain the MLE $\widehat{\theta}$. In the E-step, the expected log-likelihood of the observed data and latent states is computed, based on the conditional distribution of the latent states given an observed data trajectory evaluated at the previous set of model parameters $\theta^{(k)}$:

$$L(\theta, \theta^{(k)}) := \mathbb{E}_{(\mathbb{z}|\varkappa;\theta^{(k)})}\Big[\log p_\theta(\varkappa_{1:T}, \mathbb{z}_{1:T})\Big] = \int_{\mathcal{Z}} \log p_\theta(\varkappa_{1:T}, \mathbb{z}_{1:T}) p_{\theta^{(k)}}(\mathbb{z}_{1:T}|\varkappa_{1:T}) \mathrm{d}\mathbb{z}_{1:T}. \qquad \text{(E-step)}$$

In the M-step, the model parameters are updated by

$$\theta^{(k+1)} = \mathrm{argmax}_\theta \, L(\theta, \theta^{(k)}). \qquad \text{(M-step)}$$

Depending on the analytical form of the log-likelihood function, gradient ascent type algorithms are typically used to solve the (M-step).

Next, a basic strategy on how to compute the quantities appearing in (E-step) is outlined. Specifically, the posterior conditional density can be expressed based on *filtering densities* $p_\theta(\boldsymbol{z}_t|\varkappa_{1:t})$[2] as follows:

$$p_\theta(\mathbb{z}_{1:T}|\varkappa_{1:T}) = p_\theta(\boldsymbol{z}_T|\varkappa_{1:T}) \prod_{t=1}^{T-1} p_\theta(\boldsymbol{z}_t|\varkappa_{1:t}, \boldsymbol{z}_{t+1}),$$

with the backward-in-time Markov transition density given by

$$p_\theta(\boldsymbol{z}_t|\varkappa_{1:T}, \boldsymbol{z}_{t+1}) = \frac{p_\theta(\boldsymbol{z}_{t+1}|\boldsymbol{z}_t)p_\theta(\boldsymbol{z}_t|\varkappa_{1:t})}{p_\theta(\boldsymbol{z}_{t+1}|\varkappa_{1:t})}. \qquad (2.7)$$

It can be seen that to compute the posterior density for *any* latent state sequence in (2.7), given the observed data trajectory, one needs to be able to compute the *filtering* distribution $p_\theta(\boldsymbol{z}_t|\varkappa_{1:t})$ and the *predictive* distribution $p_\theta(\boldsymbol{z}_{t+1}|\varkappa_{1:t})$. Start from the prior distribution $p_\theta(\boldsymbol{z}_0)$, these quantities can be obtained via the following recursive calculations for $t = 1, \cdots, T$:

- calculate the predictive distribution—conditioning on $\varkappa_{1:t-1}$—by the Chapman-Kolomogorov equation given in (2.6), namely $p_\theta(\boldsymbol{z}_t|\varkappa_{1:t-1}) = \int_{\mathcal{Z}} p_\theta(\boldsymbol{z}_t|\boldsymbol{z}_{t-1})p_\theta(\boldsymbol{z}_{t-1}|\varkappa_{1:t-1})\mathrm{d}\boldsymbol{z}_{t-1}$;
- given $\boldsymbol{x}_t$, use Bayes' rule to update the predictive distribution by

$$p_\theta(\boldsymbol{z}_t|\varkappa_{1:t}) = \frac{1}{C_t} p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t)p_\theta(\boldsymbol{z}_t|\varkappa_{1:t-1}), \qquad (2.8)$$

 with the normalizing constant $C_t = \int_{\mathcal{Z}} p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t)p_\theta(\boldsymbol{z}_t|\varkappa_{1:t-1})\mathrm{d}\boldsymbol{z}_t$.

The above recursion runs *forward in time*, which however, only utilizes observations up to the current time point $t$ and hence does not take advantage of the fact that future observations at $t+1, \cdots, T$ are available. To this end, improved estimates of the states can be obtained by also computing the *smoothing* posterior density $\boldsymbol{z}_t$ given the complete observed trajectory $\varkappa_{1:T}$, which can be computed for any $t < T$ as follows:

$$p_\theta(\boldsymbol{z}_t|\varkappa_{1:T}) = p_\theta(\boldsymbol{z}_t|\varkappa_{1:t}) \int_{\mathcal{Z}} \Big[\frac{p_\theta(\boldsymbol{z}_{t+1}|\boldsymbol{z}_t)p_\theta(\boldsymbol{z}_{t+1}|\varkappa_{1:T})}{p_\theta(\boldsymbol{z}_{t+1}|\boldsymbol{x}_{1:t})}\Big]\mathrm{d}\boldsymbol{z}_{t+1}; \qquad (2.9)$$

it involves both the predictive and the filtering densities. To obtain the smoothing distribution for all time points $t \in \mathcal{T}$, one first calculates the predictive and filtering densities forward in time; subsequently, starting from time $T$, one calculates the smoothing densities according to (2.9) backwards in time, as the smoothing

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[2]by conditioning arguments and the Markovian nature of the state dynamics

density $p_\theta(\boldsymbol{z}_{t+1}|\boldsymbol{x}_{1:T})$ has become available. The above forward-backward scheme is referred to in the literature as the *fixed-interval smoothing* (Kitagawa, 1987). More complex smoothing procedures are presented and reviewed in Briers et al. (2010); Doucet et al. (2009).

For the class of of linear Gaussian SSMs, the filtering, prediction and smoothing densities correspond to Gaussian distributions whose parameters can be computed *explicitly* in a *recursive* manner. Therefore, the sequence of latent states $\boldsymbol{z}_{1:T}$ can be obtained by the famous Kalman filter algorithm (Kalman, 1960, see details in Appendix A).

For nonlinear, non-Gaussian SSMs, the corresponding filtering, predictive and smoothing densities *do not* possess closed forms. To address this, two primary strategies are commonly employed. The first is based on Sequential Monte Carlo (SMC) methods (also known as particle filters). The key idea is that the distribution of interest can be approximated by a large collection of random samples (termed "particles" in the corresponding literature). These particles are propagated over time using importance sampling and resampling mechanisms, allowing for efficient approximation of the required posterior distributions. For a detailed exposition of such methods related to the state identification/estimation problem, see Andrieu et al. (2004); Kitagawa (1988); Schön et al. (2015) and references therein. The second strategy aims to approximate the densities by linearizing them around their mean and covariance matrix from the previous time update, and then apply the update rules of the original Kalman filter. This gives rise to the Extended Kalman Filter (EKF) algorithm (Anderson and Moore, 2005). However, while EKF is widely used, it can provide unreliable state estimates in the presence of strong nonlinearities. As alternatives, *Gaussian* filters and the *unscented* Kalman filter (UKF) (Julier and Uhlmann, 2004; Wan and Van Der Merwe, 2000) have been proposed. The Gaussian filter approximates the predictive and the filtering distributions by *matching* their first two moments (mean and covariance); in particular, it minimizes the Kullback-Leibler divergence between the true posterior and the corresponding Gaussian approximation, with the integrals calculated using numerical methods such as quadrature or Monte Carlo sampling. The UKF, a variant of the Gaussian filter, employs deterministically chosen *"sigma"* points to approximate the moments of these distributions, by computing weighted averages based on these points. A brief exposition of the Gaussian, the unscented Kalman and the extended Kalman Filter is given in Appendix B.

*Remark* 1. In continuous time SSMs defined by ordinary or stochastic differential equations, the estimates of the latent states are obtained by solving the filter's corresponding differential equation; see, learning of latent neural ODE model and a discussion of the nonlinear filtering problem for the SDE model in Appendix C. This approach contrasts with the discrete time case, where prediction and filtering are distinct steps.

*Remark* 2. The presentation thus far has focused on maximum likelihood based approaches for learning SSM. While Bayesian type computations (namely, the posteriors) are extensively used in the filtering, smoothing and prediction steps, Bayesian estimation of the model parameters which requires specification of prior distributions on $\theta$ is not widely adopted, especially for non-linear, non-Gaussian SSMs, primarily due to the inherent complexity of the learning problem. Representative work for linear Gaussian SSMs include Durbin and Koopman (2000) and references therein.

## 2.3  Deep learning framework for SSMs

Deep learning (DL) offers a highly flexible framework to extend classical approaches and model more complex dynamics. Broadly, DL approaches can be categorized into two streams: (1) "partially DL" approaches, where neural networks are used only for parameterizing selected parts of the state and/or the observation equations, yet the overall learning process follows along the lines of the classical framework (see, e.g., works in Section 3.4), and (2) "fully DL" approaches where all model components are parameterized by neural networks, *and* the parameters are learned with a VAE-based pipeline. The latter has become the *de facto* approach for training complex SSMs.

We begin the exposition with a brief overview of the VAE strategy (Kingma and Welling, 2013), a general approach for training complex models with latent variables in an "end-to-end" manner. With a slight abuse of notation, let $\boldsymbol{z}$ generically denote the latent variable and $\boldsymbol{x}$ the observed one. Their joint distribution is given by $p_\theta(\boldsymbol{x}, \boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z})p_\theta(\boldsymbol{z})$, where $\theta$ denotes the learnable parameters of the generative process and

$p_\theta(\boldsymbol{z})$ is the prior distribution, typically selected as the standard Gaussian distribution. Instead of maximizing the data log-likelihood $\log p_\theta(\boldsymbol{x}, \boldsymbol{z})$ directly, the training objective becomes to maximize its evidence lower bound (ELBO), given by

$$\log p_\theta(\boldsymbol{x}) \geq \log p_\theta(\boldsymbol{x}) - \mathrm{KL}\big(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,\|\, p_\theta(\boldsymbol{z}|\boldsymbol{x})\big) = \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\big(\log p_\theta(\boldsymbol{x}|\boldsymbol{z})\big) - \mathrm{KL}\big(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,\|\, p_\theta(\boldsymbol{z})\big),$$

where $q_\phi(\boldsymbol{z}|\boldsymbol{x})$ is the encoder (or the recognition/inference model, equivalently), which approximates the true-but-intractable posterior distribution $p_\theta(\boldsymbol{z}|\boldsymbol{x})$, and $p_\theta(\boldsymbol{x}|\boldsymbol{z})$ is the decoder (also known as the generative model) that captures the generative process given $\boldsymbol{z}$. Both the encoder and the decoder are usually parameterized by neural networks, which are jointly trained by minimizing the negative ELBO with respect to the trainable parameters $\phi$ and $\theta$. This objective can be interpreted as the sum of the reconstruction error and the KL regularization term, with the Kullback-Leibler (KL) divergence preventing the learned encoder distribution to deviate drastically from the prior distribution.

Next, we elaborate on how the VAE strategy is utilized for modeling sequential data. When both the observable and the latent variables are *sequences* of the form $\varkappa_{1:T}, \mathbb{z}_{0:T}$, the ELBO for the corresponding data log-likelihood can be expressed in a timestep-wise form as:

$$\log p_\theta(\varkappa) \geq \mathbb{E}_{q_\phi(\mathbb{z}|\varkappa)}\Big( \log p_\theta(\varkappa|\mathbb{z}) \Big) - \mathrm{KL}\Big( q_\phi(\mathbb{z}|\varkappa) \,\|\, p_\theta(\mathbb{z}) \Big) \tag{2.10}$$

$$= \mathbb{E}_{q_\phi(\mathbb{z}|\varkappa)}\bigg\{ \sum_{t=1}^{T} \Big[ \log p_\theta(\boldsymbol{x}_t \,|\, \boldsymbol{z}_t) - \mathrm{KL}\Big( q_\phi(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}, \varkappa) \,\|\, p_\theta(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}) \Big) \Big] - \mathrm{KL}\Big( q_\phi(\boldsymbol{z}_0|\varkappa) \,\|\, p_\theta(\boldsymbol{z}_0) \Big) \bigg\},$$

wherein the encoder distribution is factorized as $q_\phi(\mathbb{z}|\varkappa) = q_\phi(\boldsymbol{z}_0)\prod q_\phi(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}, \varkappa)$, with each term approximating the true posterior $p_\theta(\boldsymbol{z}_t|\boldsymbol{z}_{1:t-1}, \varkappa)$ and further assumed to be Gaussian. For the decoder, it emulates the generative model, and the conditional distribution satisfies

$$p_\theta(\varkappa_{1:T}, \mathbb{z}_{1:T} \,|\, \boldsymbol{z}_0) \equiv p_\theta(\boldsymbol{z}_0)\prod_{t=1}^{T} p_\theta(\boldsymbol{x}_t|\boldsymbol{z}_t)p(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}).$$

Specifically, under the Gaussianity assumption, the conditional distribution of an observation is $\boldsymbol{x}_t|\boldsymbol{z}_t \sim \mathcal{N}(\boldsymbol{\mu}_t^x := \mu_\theta(\boldsymbol{z}_t), \Sigma_t^x := \Sigma_\theta(\boldsymbol{z}_t))$, where $\mu_\theta(\cdot), \Sigma_\theta(\cdot)$ are functions of $\boldsymbol{z}_t$, and their outputs correspond to the mean and the covariance, respectively, with the latter usually assumed to be diagonal. The reconstruction error can thus be calculated accordingly based on the negative log-likelihood loss:

$$\sum_{t=1}^{T} \Big( \log \big|\Sigma_t^x\big| + \big(\boldsymbol{x}_t - \boldsymbol{\mu}_t^x\big)^\top \big(\Sigma_t^x\big)^{-1} \big(\boldsymbol{x}_t - \boldsymbol{\mu}_t^x\big) \Big);$$

with the corresponding "reconstructed trajectory" given by $\widehat{\boldsymbol{x}}_t \equiv \boldsymbol{\mu}_t^x, \forall\, t$, namely, the mean of the estimated conditional distribution. In practice, instead of obtaining the full distribution, it is often the case that only the reconstructed "mean" is obtained, and the reconstruction error is typically calculated using the mean-squared-error between $\boldsymbol{x}_t$ and $\widehat{\boldsymbol{x}}_t$'s. This is equivalent to imposing the additional assumption that the conditional distribution $\boldsymbol{x}_t|\boldsymbol{z}_t$ is isotropic.

The encoder and decoder are trained jointly by minimizing the negative ELBO, which allows the model to simultaneously learn the latent process dynamics and the state-observation link function.

*Remark* 3. The exact implementation of the inference/recognition network that parameterizes $q_\phi(\boldsymbol{z}_t|\boldsymbol{z}_{t-1}, \varkappa)$ often varies depending on the specific task and the model architecture. In some cases, additional approximation may be introduced to simplify certain steps (e.g., see Hasan et al. (2021) reviewed in Section 3.3). Similarly, for the decoder, the conditional distribution of the observations may be operationalized differently, with the inputs to the neural networks potentially incorporating extra dependence on past observations (e.g, Chung et al., 2015), albeit this deviates from the specification of observation equation.

# 3 Deep Learning-based State-Space Models

This section reviews SSM-based modeling frameworks where deep learning techniques play a central role in facilitating the learning process. These models, similarly to the classical framework reviewed in Section 2, incorporate a latent component that governs the system's dynamics that can be potentially complex. Observed

processes are linked to the latent states via a general link function, typically parameterized by a neural network. These deep learning-based approaches can be further segmented into two main categories based on the latent process evolution: (1) latent states are assumed to evolve in discrete-time (e.g., Krishnan et al., 2015; Karl et al., 2017; Rangapuram et al., 2018); and (2) latent states are modeled as continuous-time processes, such as ODE-based (Rubanova et al., 2019; Biloš et al., 2021) and SDE-based ones (Jia and Benson, 2019; Duncker et al., 2019; Hasan et al., 2021; Deng et al., 2021).

Throughout this section, we separate $\theta$—the parameter governing the generative model—into $\theta_f$ and $\theta_g$ that respectively represent the parameters governing the state and the observation equations; note that they also coincide with the trainable parameters in the decoder. The trainable parameters in the encoder are collectively denoted by $\phi$.

## 3.1 Discrete-time deep state space models

These models extend classical SSMs by representing the state and the observation equations through neural network parameterization, rather than using predefined parametric forms for $f$ and $g$. Such an approach allows for flexible modeling of the complex dynamics in time series data, and the formulation can be viewed as a direct neural variant of linear SSMs.

Krishnan et al. (2015, 2017) consider a data generating process (DGP) wherein the latent state $z_t$ is modeled as a Markov process, and its conditional distribution on its past is explicitly assumed Gaussian:

$$\text{initial state:} \quad z_0 \sim \mathcal{N}(\boldsymbol{\mu}_0, \Sigma_0) \tag{3.1a}$$

$$\text{state equation:} \quad z_t \,|\, (z_{t-1} = z_{t-1}) \sim \mathcal{N}\Big(f_{\theta_f}(z_{t-1}, \Delta_t), \Sigma_{\theta_f}(z_{t-1}, \Delta_t)\Big) \tag{3.1b}$$

$$\text{observation equation:} \quad \boldsymbol{x}_t = g_{\theta_g}(z_t) + \boldsymbol{\epsilon}_t. \tag{3.1c}$$

$f(\cdot,\cdot), \Sigma(\cdot,\cdot)$ and $g(\cdot)$ respectively define the dynamics of the latent process and the observation equation, and $\Delta_t$ corresponds to the time elapsed between $t-1$ and $t$. To learn the parameters associated with the model, the authors consider variational inference as outlined in Section 2.3, with a loss in the form of (2.10). Specifically, the true posterior factorizes as $p(\mathbb{z}|\mathbb{x}) = p(z_0|\mathbb{x}) \prod_{t=1}^{T} p(z_t|z_{t-1}, \mathbb{x})$, where $p(z_t|z_{t-1}, \mathbb{x}) \equiv p(z_t|z_{t-1}, \mathbb{x}_{t:T})$ due to $z_t \perp\!\!\!\perp \mathbb{x}_{1:t-1} \,|\, z_{t-1}$. The encoder distribution $q_\phi$ is selected to approximate this true posterior, namely,

$$q_\phi(\mathbb{z}|\mathbb{x}) := q_\phi(z_0|\mathbb{x}) \prod_{t=1}^{T} q_\phi(z_t|z_{t-1}, \mathbb{x}_{t:T}), \tag{3.2}$$

$$\text{where} \quad q_\phi(z_t|z_{t-1}, \mathbb{x}) \sim \mathcal{N}\Big(\mu_\phi(z_{t-1}, \mathbb{x}_{t:T}), \Sigma_\phi(z_{t-1}, \mathbb{x}_{t:T})\Big). \tag{3.3}$$

Both $\mu_\phi(\cdot)$ and $\Sigma_\phi(\cdot)$ are parametrized by neural networks with the output of $\Sigma_\phi(\cdot)$ further assumed diagonal. The ELBO loss can be written as

$$\sum_{t=1}^{T} \mathbb{E}_{q_\phi(z_t|\mathbb{x})} \log p_{\theta_g}(\boldsymbol{x}_t|z_t) - \mathrm{KL}\Big(q_\phi(z_0|\mathbb{x}) \,\big\|\, p(z_0)\Big) - \sum_{t=1}^{T} \mathbb{E}_{q_\phi(z_{t-1}|\mathbb{x})}\Big[\mathrm{KL}\Big(q_\phi(z_t|z_{t-1}, \mathbb{x}_{t:T}) \,\big\|\, p_{\theta_f}(z_t|z_{t-1})\Big)\Big], \tag{3.4}$$

where $p_{\theta_f}(z_t|z_{t-1})$, $p_{\theta_g}(\boldsymbol{x}_t|z_t)$ are decoder distributions dictated by the latent state dynamics (3.1b) and the observation equation specification (3.1c), and the functions involved are parameterized by neural networks. Exhibit 1 outlines the forward pass of the training pipeline.

*Remark* 4. The approximate posterior distribution in (3.2)—operationalized via the inference network in (3.3)–corresponds to a variant of the smoothing step in the classical Kalman filter; see, e.g., (2.9) and references in Briers et al. (2010). In practice, other choices of the inference network have been considered, such as the ones based on the entire observed trajectory $\mathbb{x}$ that correspond to a fixed interval smoother, namely, $\mu_\phi$ and $\Sigma_\phi$ are in the form of $\mu_\phi(z_{t-1}, \mathbb{x})$ and $\Sigma_\phi(z_{t-1}, \mathbb{x})$, or those depending on left-only information (i.e., $\mu_\phi(z_{t-1}, \mathbb{x}_{1:t})$ and $\Sigma_\phi(z_{t-1}, \mathbb{x}_{1:t})$). Other mean-field type specifications let the inference network only operate on (a subset of) $\mathbb{x}$ while ignoring $z_{t-1}$, that is, $\mu_\phi(\mathbb{x}), \Sigma_\phi(\mathbb{x})$ (Krishnan et al., 2017), or the "neighborhood-only" ones with $\mu_\phi(\boldsymbol{x}_t)$ and $\Sigma_\phi(\boldsymbol{x}_t, \boldsymbol{x}_{t-1})$ (Gao et al., 2016; Archer et al., 2016).

**Exhibit 1:** Outline of the forward pass based on Krishnan et al. (2017)

**Input:** observed time series $\varkappa := \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_T\}$; inference networks $\mu_\phi, \Sigma_\phi$, state transition $f_{\theta_f}, \Sigma_{\theta_f}$ and $g_{\theta_g}$ in the observation equation

1. [`encode`] run $\{\boldsymbol{x}_t, t = 1, \cdots, T\}$ through the inference network, which gives the approximate posterior distributions $q_\phi(\varkappa|\varkappa)$ in the form of $\mathcal{N}(\boldsymbol{\mu}_t^z, \Sigma_t^z)$'s, $t = 1, \cdots, T$;

2. [`sampling`] sample $\widetilde{\boldsymbol{z}}_t$'s from the encoded distributions $\mathcal{N}(\boldsymbol{\mu}_t^z, \Sigma_t^z)$'s,

3. [`decode`] obtain the conditional likelihood $p_\theta(\varkappa|\varkappa) = \prod_{t=1}^T p(\boldsymbol{x}_t|\boldsymbol{z}_t)$ according to the observation equation, using $\widetilde{\boldsymbol{z}}_t$'s as the plug-in, namely

$$p(\boldsymbol{x}_t|\boldsymbol{z}_t = \widetilde{\boldsymbol{z}}_t) \sim \mathcal{N}\big(\text{mean network}_{\theta_g}(\widetilde{\boldsymbol{z}}_t), \text{cov network}_{\theta_g}(\widetilde{\boldsymbol{z}}_t)\big), \quad t = 1, \cdots, T.$$

4. [`loss`] calculate the loss function according to (3.4).

In the method reviewed above, the state transition enters into the loss function only through the KL term as $p_{\theta_f}(\boldsymbol{z}_t|\boldsymbol{z}_{t-1})$. In the decoding step, the conditional likelihood $p_{\theta_g}(\boldsymbol{x}_t|\boldsymbol{z}_t)$ is computed by plugging in the corresponding $\widetilde{\boldsymbol{z}}_t$'s, effectively sidelining the role of the state transition. To address this, Karl et al. (2017) propose embedding the state transition into the decoding step itself. Concretely, instead of directly using sampled $\widetilde{\boldsymbol{z}}_{t-1}$'s to obtain the conditional likelihood, the state transition equation generates $\widehat{\boldsymbol{z}}_t$'s, which are subsequently used to compute the conditional likelihood. This approach preserves the generative model's full dynamics during decoding, enabling the gradient from the reconstruction error term to backpropagate through the state transition. It is operationalized leveraging a similar idea to that of the reparametrization trick in VAEs (Kingma and Welling, 2013): a "stochastic" parameter $\boldsymbol{\beta}_t$ is introduced, which encompasses both the unknown parameters in the transition equation and the shock (namely, $\boldsymbol{u}_t$). The inference network, in this case, encodes the posterior distribution of $\boldsymbol{\beta}_t$, rather than that of $\boldsymbol{z}_t$. During the sampling stage, stochastic parameters are drawn from the inference network-learned encoder distributions, which are then passed to the decoding stage and enable deterministic state transition yielding the $\widehat{\boldsymbol{z}}_t$'s. Empirically, enforcing state transitions within the generative process enables this method to capture latent system dynamics fairly accurately, although specific parameterization choices are often application-dependent.

Several other concurrent works, such as Fraccaro et al. (2017); Li and Mandt (2018) that are reviewed in Girin et al. (2021), explore variations of discrete-time "deep" state space models tailored to specific tasks. Note that the main focus of Girin et al. (2021) is to consider VAE as a learning paradigm for dynamical systems that evolve at discrete time points; hence it also includes selected RNN-style "hybrid" models, featuring a *deterministic* internal state sequence $\{\boldsymbol{h}_t\}$ that propagates forward the system information and interacts with the *stochastic* state $\boldsymbol{z}_t$. For further details, interested readers are directed to references therein.

## 3.2 Latent neural ODEs

Before introducing the latent neural ODE framework, we first present the neural ODE one as a general tool, in which the hidden unit dynamics of a neural network are modeled with ordinary differential equations (ODE). As it will be seen in the sequel, the technical components adopted in neural ODE are extensively used for latent neural ODE-based modeling.

**Preliminaries: neural ODEs.** The neural ODE model, introduced by Chen et al. (2018), models the instantaneous change of the hidden units in a neural network using a function $f_\theta(\mathbf{h}_t, t)$. The motivation comes from the fact that neural networks can be viewed as a sequence of transformations applied to the hidden units, based on which connections can be established to the discretization of continuous transformations.

To set the stage, consider a neural network-based supervised learning setting where the output $\boldsymbol{y} \approx \text{DNN}(\boldsymbol{x})$. With a slight abuse of notation, let $t$ index the layers of the network. For a neural network with layers $\{0, ..., T\}$, let $\mathbf{h}_t$ be the vector of hidden neurons at layer $t$; a forward pass of the neural network effectively conducts the transformation $\boldsymbol{x} \to \mathbf{h}_0 \to \cdots \to \mathbf{h}_T \to \boldsymbol{y}$. In particular, for a residual network-type architecture (ResNet; He et al., 2016) wherein all hidden layers having the same size, the sequential update between

hidden layers is given by $\mathbf{h}_{t+1} = \mathbf{h}_t + f_\theta(\mathbf{h}_t, t)$. This recursive update is similar to the Euler discretization scheme used to numerically obtain solutions of ODEs.

As the step size approaches zero, the dynamics of the hidden units—now viewed as a continuous process—can be represented through the following ODE: $\frac{\mathrm{d}\mathbf{h}(t)}{\mathrm{d}t} = f_\theta(\mathbf{h}(t), t)$, with the dependency of $f_\theta(\cdot, \cdot)$ on $t$ made explicit. The quantity of interest is given by $\mathbf{h}_{t_1}$ for some $t_1$, which can be interpreted as the "final" hidden unit, which is subsequently mapped to the output $\boldsymbol{y}$ of ultimate interest; this mapping step is usually through a small shallow network. In particular, $\mathbf{h}_{t_1}$ can be expressed as $\mathbf{h}_{t_1} := \int_{t_0}^{t_1} f_\theta(\mathbf{h}(t), t)\mathrm{d}t$, with boundary condition $\mathbf{h}(t_0) \equiv \mathbf{h}_{t_0}$ that corresponds to some initial transformation of the input $\boldsymbol{x}$[3]. The integration is typically performed using an off-the-shelf ODE solver, which is treated as a black box, In practice, the state at $t_1$ is computed as $\mathbf{h}_{t_1} = \text{ODESolve}(\mathbf{h}_{t_0}, f_\theta, (t_0, t_1))$. The end-to-end training involves optimizing the loss with respect to the parameters $\theta, t_0, t_1$ (and potentially the parameters of the final small shallow network that maps $\mathbf{h}_{t_1}$ to $\boldsymbol{y}$). Given the continuous nature of the hidden units in this framework, backpropagation is carried out using the adjoint method (Pontryagin et al., 1962), as detailed in Chen et al. (2018), Appendix B.

The general setup of neural ODEs builds upon the connection between residual networks (ResNet) and the Euler discretization, treating the hidden units/layers as a continuous process. This approach can be viewed as a continuous approximation of traditional neural network architectures, where instead of discrete layers indexed by integers, the propagation of information between hidden units occurs in a continuous manner. While this framework can potentially reduce memory requirements and enhance computational efficiency, it may seem unintuitive from a purely modeling perspective. However, in time series settings where there is an actual underlying process evolving over time, the neural ODE framework becomes particularly relevant especially when combined with a posited latent process, as mentioned briefly in Chen et al. (2018), Section 5 and investigated in-depth in Rubanova et al. (2019).

**Back to the latent neural ODE model.** Let $t_0, \cdots, t_n$ denote the observation timestamps. Under the latent neural ODE framework, the following DGP is assumed for the system:

$$
\begin{aligned}
\text{initial state:} \quad & \boldsymbol{z}(t_0) \sim p(\boldsymbol{z}_{t_0}), \\
\text{state equation:} \quad & \frac{\mathrm{d}\boldsymbol{z}(t)}{\mathrm{d}t} = f_{\theta_f}(\boldsymbol{z}(t)), \\
\text{observation equation:} \quad & \boldsymbol{x}(t) = g_{\theta_g}(\boldsymbol{z}(t)) + \boldsymbol{\epsilon}(t).
\end{aligned}
\tag{3.5}
$$

The latent process $\boldsymbol{z}(t)$ is modeled according to an ODE governed by a time invariant function $f_{\theta_f}(\cdot)$, which is parameterized through some neural network with parameters $\theta_f$. The observation model defined by the link function $g_{\theta_g}(\cdot)$ is parameterized through some shallow neural network or even a simple linear layer. The forward pass of the VAE-based training pipeline is summarized in Exhibit 2, and the prior distribution $p(\boldsymbol{z}_{t_0})$ is typically selected to be a multivariate standard Gaussian.

Referring to the generic description in (2.10), it can be easily seen that in the current setting, only the KL term associated with the initial state $\boldsymbol{z}_0$ is present, due to the noiseless nature of the assumed state dynamics. Specifically, the encoder compresses the observed trajectory $\boldsymbol{x}$ into $\boldsymbol{z}_{t_0}$, and the ODE solver solves the corresponding initial-value problem, generating the $\boldsymbol{z}_{t_i}$'s during decoding. The authors further discuss different choices for the encoder module (i.e., the recognition network), including using an RNN or an ODE-RNN; for additional details, we refer interested readers to Rubanova et al. (2019).

Within the same modeling framework wherein the latent dynamics (state equation) are specified through an ODE, subsequent work by Biloš et al. (2021) considers directly modeling the *solution* of the ODE through a neural network (referred to as the "neural flows"). Specifically, let $F_{\theta_f}(t, \boldsymbol{z}_{t_0})$ be the solution to the initial value problem

$$
\frac{\mathrm{d}\boldsymbol{z}(t)}{\mathrm{d}t} = f(\boldsymbol{z}(t), t), \quad \boldsymbol{z}(t_0) = \boldsymbol{z}_{t_0};
$$

---

[3]In the common supervised learning context, let $(\boldsymbol{x}, \boldsymbol{y})$ denote the input-output pair. As a concrete example in the context of image classification, $\mathbf{h}_{t_0} \equiv \mathbf{h}(t_0)$ can be the output of the initial convolution layer, $\mathbf{h}_{t_1}$ is the output after a series such operations, and is passed to the final linear classifier (e.g., linear and softmax) after average pooling.

**Exhibit 2:** Outline of the forward pass based on latent neural ODE (Rubanova et al., 2019)

**Input:** observed time series $\varkappa := \{\boldsymbol{x}_{t_0}, \cdots, \boldsymbol{x}_{t_n}\}$

1. [encode] run $\{(\boldsymbol{x}_{t_i}, t_i), i = 0, \cdots, n\}$ through the inference network backwards in time, which gives rise to the mean and variance of the approximate posterior $q_\phi(\boldsymbol{z}_{t_0}|\varkappa, \{t_0, \cdots, t_n\})$ in the form of $\mathcal{N}(\boldsymbol{\mu}_{t_0}^z, \Sigma_{t_0}^z)$;

2. [sampling] sample $\widetilde{\boldsymbol{z}}_{t_0}$ from the encoded distribution $\mathcal{N}(\boldsymbol{\mu}_{t_0}^z, \Sigma_{t_0}^z)$;

3. [decode]

    (3.1) solve the initial value problem with $\boldsymbol{z}_{t_0} \equiv \widetilde{\boldsymbol{z}}_{t_0}$ and obtain $\widehat{\boldsymbol{z}}_{t_1}, \cdots, \widehat{\boldsymbol{z}}_{t_n}$ based on the ODE, namely

$$\widehat{\boldsymbol{z}}_{t_1}, \cdots, \widehat{\boldsymbol{z}}_{t_n} = \text{ODESolve}\big(\widetilde{\boldsymbol{z}}_{t_0}, f_{\theta_f}, (t_0, t_1, \cdots, t_n)\big);$$

    (3.2) obtain the posterior conditional data likelihood based on the observation equation in (3.5); that is,

$$p(\boldsymbol{x}_{t_i}|\boldsymbol{z}_{t_i} = \widehat{\boldsymbol{z}}_{t_i}) \sim \mathcal{N}\big(\text{mean network}_{\theta_g}(\widehat{\boldsymbol{z}}_{t_i}), \text{cov network}_{\theta_g}(\widehat{\boldsymbol{z}}_{t_i})\big), \quad i = 0, \cdots, n.$$

4. [loss] $\sum_{t=1}^T \mathbb{E}_{q_\phi(\boldsymbol{z}_{t_0}|\varkappa, \{t_0, \cdots, t_n\})} \log p_\theta(\boldsymbol{x}_{t_i}|\boldsymbol{z}_{t_i}) - \text{KL}\big(q_\phi(\boldsymbol{z}_{t_0}|\varkappa, \{t_0, \cdots, t_n\}) \,\|\, p(\boldsymbol{z}_{t_0})\big);$

---

the solution is parameterized by a neural network, under the assumption that it is smooth and invertible. These conditions ensure the solution's uniqueness. In this approach, the neural network directly learns the function $F_{\theta_f}(\cdot, \cdot)$ which is the solution of an (unknown) ODE that captures the dynamics, rather than the instantaneous changes $f$. The training pipeline is similar to the one outlined above; however, at the decoding stage, instead of using an ODE solver to obtain the $\boldsymbol{z}_{t_i}$'s, they are directly computed as $\boldsymbol{z}_{t_i} := F_{\theta_f}(t_i, \boldsymbol{z}_{t_0})$, effectively bypassing the need for a numerical ODE solver. Empirically, the neural flow-based approach achieves comparable performance to the latent neural ODE on several real datasets in terms of model accuracy, but with significantly reduced wall-clock time during training.

## 3.3   Latent neural SDEs

In this subsection, we present the formulation of neural SDEs that incorporate stochastic dynamics, along with their model training pipeline. Further, we highlight key differences in encoding and decoding procedures between neural ODEs and SDEs.

The extension of the neural ODE framework to an SDE setting has been considered in a series of concurrent papers across diverse contexts. For example, Tzen and Raginsky (2019) shows that similar to neural ODEs, neural SDEs can be viewed as the limiting regime of Deep Latent Gaussian Models (Rezende et al., 2014) as the number of layers goes to infinity, with the step size and layer-to-layer transformation noise variance going to zero (see also Peluchetti and Favaro, 2020). Liu et al. (2020) considers SDE as a "noisy" counterpart to ODE, which coincides with certain regularization mechanisms and sometimes offers greater robustness than a deterministic formulation; see also Wang et al. (2019). Li et al. (2020) generalizes the adjoint sensitivity method (e.g., Pearlmutter, 1995) to enable backpropagation through an SDE solver for neural network training. In these works, instead of using a deterministic function to model the continuous process, a diffusion term that carries stochasticity is additionally incorporated.

Representative work on using neural SDEs to model latent processes in the context of time series include Duncker et al. (2019); Jia and Benson (2019); Hasan et al. (2021); Deng et al. (2021). We anchor our review based on Hasan et al. (2021) which considers a more "standard" setup, and discuss the other approaches in Section 3.3.1.

To this end, under the latent neural SDE framework, the system dynamics are defined as follows:

$$\text{state equation:} \quad \mathrm{d}\boldsymbol{z}(t) = f_{\theta_f}\big(\boldsymbol{z}(t)\big)\mathrm{d}t + \sigma\big(\boldsymbol{z}(t)\big)\mathrm{d}\boldsymbol{w}(t), \tag{3.6a}$$

$$\text{observation equation:} \quad \boldsymbol{x}(t) = g_{\theta_g}\big(\boldsymbol{z}(t)\big) + \boldsymbol{\epsilon}(t), \tag{3.6b}$$

where $\boldsymbol{w}(t)$ denotes a $d$-dimensional standard Wiener process; $f : \mathbb{R}^d \mapsto \mathbb{R}^d$ is a time-invariant drift function, $\sigma : \mathbb{R}^d \mapsto \mathbb{R}^{d \times d}$ the diffusion coefficient and $\boldsymbol{\epsilon}(t)$ and i.i.d. noise process. The $f$ and $\sigma$ functions are

assumed to be globally Lipschitz and satisfy a linear growth condition ensuring that the state equation admits a unique solution (see discussion in Appendix C). The system is identifiable up to some equivalence class whose elements are given by $(\tilde{f}, \tilde{\sigma}, \tilde{g}) \sim (f, \sigma, g)$ with $(\tilde{f}, \tilde{\sigma}, \tilde{g})$ being a solution to the system. This holds provided that there exists an invertible function $\varphi$ such that for any solution $z(t)$ to (3.6a), $\varphi(z(t))$ is also a solution to the SDE in the same form as (3.6a) but with drift and diffusion coefficients $\tilde{f}$ and $\tilde{\sigma}$, where $\tilde{f}(z) = (f \circ \varphi^{-1})(z), \forall z \in \mathbb{R}^d$. Further, under certain regularity conditions, there exists an element in the equivalence class such that $\tilde{\sigma}$ is isotropic, i.e., $\tilde{\sigma}(z) = I_d, \forall z \in \mathbb{R}^d$; see Hasan et al. (2021), Proposition 1 and Theorem 2. Thus, it suffices to consider latent dynamics governed by a "simplified" SDE with an isotropic diffusion term: $dz(t) = f_{\theta_f}(z(t))dt + dw(t)$ and focus on recovering $(f, g)$ with learnable parameters $\theta := \{\theta_f, \theta_g\}$.

Next, we briefly describe the construction of the encoder, the decoder and the corresponding training pipeline. First, note that for any pairs of $(x_t, x_{t+\Delta t})$ and $(z_t, z_{t+\Delta t})$,

$$p(z_t, z_{t+\Delta t} \,|\, x_t, x_{t+\Delta t}) = p(z_{t+\Delta t}|x_{t+\Delta t}, z_t)p(z_t|x_t, x_{t+\Delta t}). \tag{3.7}$$

Leveraging (3.7), the *true* posterior distribution can be *approximately* decomposed as[4]

$$p_\theta(\mathbb{z}|\mathbb{x}) \approx p_\theta(z_{t_n}|z_{t_{n-1}}, x_{t_n}) \cdots p_\theta(z_{t_1}|z_{t_0}, x_{t_1})p(z_{t_0}|x_{t_0}), \tag{3.8}$$

where $z_{t_i}$ depends only on $(z_{t_{i-1}}, x_{t_i}), \forall i$. The authors consider a further approximation by using an encoder $q_\phi(z_t|x_t)$ that omits the "autoregressive" component, allowing $z_t$ to be inferred solely based on $x_t$. This approximation is reasonably tight as long as the noise term $\epsilon_t$ in the observation equation is small, and it becomes exact if $\epsilon_t \equiv 0$ and $g(\cdot)$ is injective. Such an approximation gives rise to the following encoder in practice:

$$q_\phi(\mathbb{z}|\mathbb{x}) \approx \prod_{i=0}^{n} q_\phi(z_{t_i}|x_{t_i}); \qquad z_{t_i} \,|\, x_{t_i} \sim \mathcal{N}\Big(\mu_{t_i}^z := \mu_\phi(x_{t_i}), \Sigma_{t_i}^z := \Sigma_\phi(x_{t_i})\Big), \tag{3.9}$$

where $\mu_\phi(\cdot), \Sigma_\phi(\cdot)$ are parameterized by neural networks. On the other hand, the joint distribution factorizes as

$$p\big((x_t, x_{t+\Delta t}), (z_t, z_{t+\Delta t})\big) = p(x_{t+\Delta t}|z_{t+\Delta t})p(x_t|z_t)p(z_{t+\Delta t}|z_t)p(z_t);$$

therefore, the probabilistic decoder can be decomposed as

$$p_\theta(\mathbb{x}|\mathbb{z}) = p(z_{t_0}) \prod_{i=1}^{n} \Big(p_{\theta_g}(x_{t_i}|z_{t_i})p_{\theta_f}(z_{t_i}|z_{t_{i-1}})\Big),$$

where $p_{\theta_f}(z_{t_i}|z_{t_{i-1}})$ describes the SDE dynamics, and $p_{\theta_g}(x_{t_i}|z_{t_i})$ the observation model. Specifically, if the $t_i$'s are equally-spaced with $\Delta t := t_i - t_{i-1}, \forall i$, it follows that

$$z_{t+\Delta t} \,|\, z_t \sim \mathcal{N}\Big(z_t + f_{\theta_f}(z_t)\Delta t, (\Delta t)I_d\Big), \tag{3.10}$$

using the approximation $z_{t+\Delta t} \approx z_t + f_{\theta_f}(z_t)\Delta t + w_{t+\Delta t} - w_t$, where $(w_{t+\Delta t} - w_t)$ is distributed as a multivariate Gaussian with variance $(\Delta t)I_d$. The forward pass is summarized in Exhibit 3.

*Remark* 5 (Comparison with the latent neural ODE). We briefly highlight several differences in the training pipeline between the latent neural ODE and the SDE models. First note that in the latent ODE case, the encoding procedure compresses the information in the observed trajectory $\mathbb{x}$ into $z_{t_0}$. After the parameters of the posterior distribution $q_\phi(z_{t_0}|\mathbb{x})$ are learned, a $z_{t_0}$ is sampled from the learned distribution and serves as the initial value of the ODE problem during decoding. In contrast, for the latent SDE, encoding produces $q_\phi(z_{t_i}|x_{t_i})$'s that approximate their respective true posterior counterpart for *every* $t_i$, $i = 0, \cdots, n$. Further, at the decoding stage, in the ODE case, the $z_{t_i}$'s are obtained *deterministically* by solving an initial value problem. Whereas in the SDE case, samples $\tilde{z}_{t_i}$'s are first drawn from the corresponding encoded distributions; subsequently, $\hat{z}_{t_i}$'s are obtained based on the sampled $\tilde{z}_{t_{i-1}}$'s (see Exhibit 3) following the state transition equation, and they incorporate stochasticity due to the presence of the diffusion term $w_t$ in the posited model dynamics. These $\hat{z}_{t_i}$'s are then used for reconstructing the conditional data distribution.

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[4]We elaborate on how this is derived. First note that the 1st term on the RHS of (3.7) uses the fact that $z_{t+\Delta t} \perp\!\!\!\perp x_t \,|\, z_t$. For the 2nd term on the RHS, (Hasan et al., 2021, equation 11) in fact uses an approximation $p(z_t|x_t, x_{t+\Delta t}) \approx p(z_t|x_t)$ which disregards the dependency on $x_{t+\Delta t}$ and gives $p(z_t, z_{t+\Delta t} \,|\, x_t, x_{t+\Delta t}) \approx p(z_{t+\Delta t}|x_{t+\Delta t}, z_t)p(z_t|x_t)$. Applying this $(t, \Delta t)$ "paired relationship" on consecutive observations gives $p_\theta(\mathbb{z}|\mathbb{x}) = p_\theta(z_{t_0} \,|\, \mathbb{x}) \prod p_\theta\big(z_{t_i} \,|\, z_{t_i-1}, \mathbb{z}_{1:(t_i-1)}, x_{t_i}, \mathbb{x}_{1:(t_i-1)}, \mathbb{x}_{(t_i+1):t_n}\big) = p_\theta\big(z_{t_0} \,|\, x_{t_0}, \mathbb{x}_{1:t_n}\big) \prod p_\theta\big(z_{t_i} \,|\, z_{t_i-1}, x_{t_i}, \mathbb{x}_{(t_i+1):t_n}\big) \approx p_\theta(z_{t_0}|x_{t_0}) \prod p_\theta\big(z_{t_i} \,|\, z_{t_i-1}, x_{t_i}\big)$.

**Exhibit 3:** Outline of the forward pass based on the latent neural SDE (Hasan et al., 2021)

**Input:** observed time series $\boldsymbol{x}_{t_0}, \cdots, \boldsymbol{x}_{t_n}$

1. [encode] run $\{\boldsymbol{x}_{t_i}, i = 0, \cdots, n\}$ through the inference network in parallel w.r.t. $i$, which gives rise to the mean and variance $(\boldsymbol{\mu}_{t_i}^z, \Sigma_{t_i}^z)$'s of the the approximate posteriors $q_\phi(\boldsymbol{z}_{t_i}|\boldsymbol{x}_{t_i})$'s;

2. [sampling] sample $\widetilde{\boldsymbol{z}}_{t_i}$'s from the corresponding encoded distributions $\mathcal{N}(\boldsymbol{\mu}_{t_i}^z, \Sigma_{t_i}^z)$;

3. [decode]
   (3.1) for each sampled $\widetilde{\boldsymbol{z}}_{t_i}, i = 0, \cdots, (n-1)$, obtain the "next" $\widehat{\boldsymbol{z}}_{t_{i+1}}$ based on (3.10) via a stochastic draw;
   (3.2) obtain the posterior $p(\boldsymbol{x}_{t_i}|\boldsymbol{z}_{t_i}), i = 1, \cdots, n$ based on the observation equation in (3.6b); that is,

$$p(\boldsymbol{x}_{t_i}|\boldsymbol{z}_{t_i} = \widehat{\boldsymbol{z}}_{t_i}) \sim \mathcal{N}\big(\text{mean network}_{\theta_g}(\widehat{\boldsymbol{z}}_{t_i}), \text{cov network}_{\theta_g}(\widehat{\boldsymbol{z}}_{t_i})\big), \quad i = 0, \cdots, n.$$

4. [loss] calculate the ELBO loss given (generically) in (2.10), by plugging in the approximated encoder (3.9) and decoder (3.10).

*Remark* 6. Note that under the classical framework, to operationalize learning the parameters of latent continuous time SDEs, it is necessary to compute the *continuous time analogue* of the posterior distribution $p(\boldsymbol{z}_t|\boldsymbol{x}_{0:s})$ required in the filtering $(s \leq t)$ and smoothing $(s = T)$ steps, which is generally a very involved task, as detailed in Appendix C. In contrast, under the deep learning framework, with a VAE based learning pipeline, it requires an approximation of the true posterior distribution to simplify computations, as outlined above (see (3.8) and (3.9)). Crucially, it bypasses the need to solve an SDE—required in certain approaches under the classical framework—thereby significantly simplifying the process.

### 3.3.1 Other latent neural SDE-based models

Next, we briefly discuss additional representative works that model latent dynamics with SDEs.

In Duncker et al. (2019), the observable $\boldsymbol{x}_t$'s depend on the latent states through a generalized linear link function with a known parametric form (but unknown parameters), and the latent dynamics follow an SDE, wherein the drift term is modeled by a Gaussian process.

In Jia and Benson (2019), a hybrid flow-plus-jump system is proposed to handle events with either discrete types or continuous-value features. In that setting, the latent state $\boldsymbol{z}(t)$ governs the system, while $\boldsymbol{x}_t$ corresponds to the "embedding" vector of the observed event sampled from $\boldsymbol{x}(t) \sim p(\boldsymbol{x}|\boldsymbol{z}(t))$[5]. The probability of an event happening satisfies

$$\mathbb{P}\big(\text{event happens in } [t, t + \mathrm{d}t) \,|\, \mathcal{H}_t\big) := \lambda(\boldsymbol{z}(t))\mathrm{d}t, \qquad \mathcal{H} := \{(t_i, \boldsymbol{x}_{t_i})\},$$

where $\lambda(\boldsymbol{z}(t))$ is the conditional intensity function and $\mathcal{H}_t$ the subset of events up to $t$ (excluded). Further, let $N(t)$ be the number of events up to time $t$, and the latent dynamics is given as a follows, with a flow component $f_\theta(\cdot, \cdot)$ and a jump one $\nu_\theta(\cdot, \cdot, \cdot)$ (for a technical presentation of SDEs with jumps see Bass (2004)):

$$\mathrm{d}\boldsymbol{z}(t) = f_\theta\big(\boldsymbol{z}(t), t\big)\mathrm{d}t + \nu_\theta\big(\boldsymbol{z}(t), \boldsymbol{x}(t), t\big)\mathrm{d}N(t). \tag{3.11}$$

Note that with the dynamics postulated in (3.11), the latent process "interacts" with the observable process through the jump component, evolving *deterministically* until a stochastic event occurs. Notably, the learning of various system components (e.g., $\lambda(\boldsymbol{z}(t), p(\boldsymbol{x}|\boldsymbol{z}(t)), f_\theta(\cdot), \nu_\theta(\cdot))$ parameterized by neural networks does not rely on a VAE-based training pipeline. Instead, the authors leverage the adjoint method developed in Chen et al. (2018), with special attention given to the jump term. Interested readers are referred to the original paper for further details.

In Deng et al. (2021), the decoding from the latent states $\boldsymbol{z}_t$ to the observable $\boldsymbol{x}_t$ leverages continuously-

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[5]In the case of discrete event types, the support of $\boldsymbol{x}(t)$ is a finite set of one-hot encodings; in the case where the events are characterized by real-valued features, $p(\boldsymbol{x}|\boldsymbol{z}(t))$ is parameterized with a mixture of Gaussian whose parameters depend on $\boldsymbol{z}(t)$.

indexed normalizing flows[6] (Papamakarios et al., 2021) modeled as follows:

$$\boldsymbol{x}_t = G_\theta(\mathbf{o}_t, \boldsymbol{z}_t, t),$$

where $\mathbf{o}_t$ is a $k$-dimensional "base" process with closed-form transition density (e.g., a Wiener process or an Ornstein–Uhlenbeck (OU) process), and $G_\theta(\cdot, \boldsymbol{z}_t, t)$ is a normalizing flow (e.g., Kobyzev et al., 2020) that transforms the base process into the more complex one through invertible mappings. The dynamics of $\boldsymbol{z}_t$ are modeled as an SDE similar to that in Hasan et al. (2021). It is worth noting that the starting point of Deng et al. (2021) differs slightly from the other works reviewed thus far: from a modeling perspective, instead of treating the latent process as the governing component of the system that drives the evolution of the observable process, the latent process is incorporated primarily for expressiveness. Specifically, built upon Deng et al. (2020) where the process is modeled as $\boldsymbol{x}_t = G_\theta(\mathbf{o}_t, t)$—which omits the latent process and only includes the base process, the additional inclusion of the latent process $\boldsymbol{z}_t$ enhances the model's representation capacity, thereby potentially reduce the inductive bias. At the conceptual level, connections can be drawn to classical statistical modeling where a factor-augmented structure is leveraged (e.g., Bernanke et al., 2005; Bai et al., 2016; Lin and Michailidis, 2020a).

## 3.4 Additional related approaches

We highlight selected works that, while adhering closely to classical approaches, leverage deep learning tools—such as neural networks for function parameterization—to enable more flexible model specification.

An example of this approach is detailed in Rangapuram et al. (2018). Let $x_t^j \in \mathbb{R}$ be the $j$-th coordinate of the observation process, whose corresponding noise process is given by $\epsilon_t^j$. With a slight abuse of notation, let $\boldsymbol{z}_t^{(j)}$ be the latent state and $\boldsymbol{c}_t^{(j)}$ the covariates associated with $x_t^j$ –both potentially multivariate. A discrete-time linear system of the following form is considered:

$$\begin{aligned}
\boldsymbol{z}_0^{(j)} &\sim \mathcal{N}(\boldsymbol{\mu}_0, \Sigma_0), \ \ \Sigma_0 \text{ is diagonal}, \\
\boldsymbol{z}_t^{(j)} &= F_t^{(j)} \boldsymbol{z}_{t-1}^{(j)} + G_t^{(j)} \boldsymbol{u}_t^{(j)}, \\
x_t^j &= b_t^{(j)} + H_t^{(j)} \boldsymbol{z}_t^{(j)} + \epsilon_t^j, \ \ \epsilon_t^j \sim \mathcal{N}(\mathbf{0}, r_t^{(j)}),
\end{aligned}$$

with time-varying parameters $\theta_t^{(j)} := (\boldsymbol{\mu}_0, \Sigma_0, F_t^{(j)}, G_t^{(j)}, b_t^{(j)}, H_t^{(j)}, r_t^{(j)})$, parameterized through $\theta_t^{(j)} = f_\phi(\mathbb{c}_{1:t}^{(j)})$. The mapping $f_\phi$ is shared across all $j$'s and is parameterized by an RNN, and the parameter $\phi$ is learned by maximizing the log-likelihood of the observations. In particular, in the Gaussian case, the likelihood can be decomposed as in (2.4), and the corresponding terms can be calculated using the Kalman filter. The authors also briefly discuss using a VAE to optimize the lower bound, when the Gaussian assumption does not hold; see Appendix A of the paper for details. Notably, the time-varying parameters are handled by neural networks, which conveniently provide the necessary mapping for each time step as a result of the inner workings of RNNs. A similar idea is adopted in Revach et al. (2022), where an RNN is used to parameterize the Kalman gain to perform recursive filtering for the real-time state estimation problem.

*Remark* 7 (Connection to time-varying linear Gaussian SSMs). The model presented above exemplifies a *time-varying linear* Gaussian SSM, where the parameters are flexibly parameterized with neural networks. In contrast, in classical approaches (see Appendix A), additional modeling assumptions are often imposed on these parameters, such as that they evolve according to a Markov chain and hence become piecewise linear, to make their estimation tractable. This highlights the advantage of neural network based parameterization to enhance flexibility in modeling.

In Masti and Bemporad (2021), a non-linear state-space model is proposed in the form[7]

$$\boldsymbol{z}_{t+1} = f(\boldsymbol{z}_t, \boldsymbol{u}_{t+1}), \qquad \boldsymbol{x}_t = g(\boldsymbol{z}_t, \boldsymbol{\epsilon}_t).$$

---

[6] The main idea of a normalizing flow is to express the joint distribution of some (generic) $\boldsymbol{y}$ as the transformation of some (generic) $\boldsymbol{x}$, i.e., $\boldsymbol{y} = T(\boldsymbol{x})$ with $\boldsymbol{x} \sim p_{\text{base}}(\boldsymbol{x})$ coming from some simple base distribution (e.g,. multivariate normal); $T$ is invertible and differentiable, and usually comprises of a sequence of transformations $T = T_K \circ \cdots \circ T_1$.

[7] For simplicity, the control variable from the original model is omitted

At the core of the proposed framework, the problem is recast as solving for $f$ and $e, d$, where $\boldsymbol{z}_t :=$ $e(\varkappa_{t-k:t-1}), k > 1$, with $e(\cdot)$ being the "encoder" that performs dimensionality reduction, while the decoder $d(\cdot)$ reconstructs $\varkappa_{t-k':t}, k' < k$[8]. Here, $f$ handles state transitions and propagates information from $t$ to $t+1$. The functions $f, e, d$ are jointly learned by minimizing the loss that comprises of two components: one for reconstruction error based on observed data, and another based on the discrepancy between the state estimates respectively from state transitions and from the encoder, for the same time point.

A similar approach within the scope of factor models can be found in the deep dynamic factor model by Andreini et al. (2020), where factor (or state) dynamics are modeled as a linear VAR process. Related work on deep factor models is also explored in Wang et al. (2019).

## 4 SSMs as Components of an Input-Output System

In this section, we diverge from the discussion in previous sections and consider the body of work where SSMs are utilized as input-output mapping modules.

The advent of Transformers (Vaswani et al., 2017) led to the development of language models with enhanced capabilities, including BERT (Devlin et al., 2018), T5 (Raffel et al., 2020) and the GPT family (Radford et al., 2018; Brown et al., 2020). However, these models suffer from computational complexity that scales quadratically with the length of the input sequence, which becomes a severe bottleneck when processing long sequences. In response to this challenge, various alternatives to traditional sequence modeling paradigms such as CNNs, RNNs, and Transformers have emerged (e.g., Dai et al., 2019; Kitaev et al., 2020), though they still face computational and learning-related limitations.

Recent works, such as those in Gu et al. (2021, 2022); Smith et al. (2023); Gu and Dao (2023); Dao and Gu (2024), have focused on enhancing long-range sequence modeling performance across a range of application domains. These recent SSM-based approaches can overcome some of the bottlenecks of previous models, and excel in modeling tasks involving very long sequences.

At a high level, the sequence modeling task can be generically cast as establishing a mapping from the input sequence $\{\boldsymbol{x}_{t-L+1}, \cdots, \boldsymbol{x}_t\}$ with context length $L$ to the output sequence $\{\boldsymbol{x}_{t+1}, \cdots, \boldsymbol{x}_{t+L'}\}$ of length $L'$. For the line of work in question, by treating the SSMs as input-output systems and incorporating them into neural network architectures, efficient processing of long input sequences becomes achievable. In contrast to the work reviewed in Sections 2 and 3, where the models are postulated as having an inherent latent component, here SSMs are not associated with specific latent state-driven DGPs. Instead, they serve as stand-alone input-output mapping modules that propagate information. This approach is implemented with Linear State-Space Layers (LSSLs) as the operating unit, and the technical development focuses on the efficient computation and learning of these SSM-enabled modules.

### 4.1 The main building block: linear state-space layers (LSSLs)

Gu et al. (2021) introduces LSSLs as a new paradigm that integrates popular tools from sequence modeling, including recurrence, convolution and differential equations.

Concretely, let $\boldsymbol{u}(t) \in \mathbb{R}^{d_{\text{in}}}$ denote the input, $\boldsymbol{v}(t) \in \mathbb{R}^{d_{\text{out}}}$ the output and $\boldsymbol{z}(t)$ the $d$-dimensional latent state. A continuous-time linear state-space model is defined by

$$\frac{\mathrm{d}\boldsymbol{z}(t)}{\mathrm{d}t} = A\boldsymbol{z}(t) + B\boldsymbol{u}(t), \qquad \boldsymbol{v}(t) = C\boldsymbol{z}(t) + D\boldsymbol{u}(t). \tag{4.1}$$

After discretization, the system in (4.1) possesses a *recurrent* form given by:

$$\boldsymbol{z}_t = \bar{A}\boldsymbol{z}_{t-1} + \bar{B}\boldsymbol{u}_t, \qquad \boldsymbol{v}_t = C\boldsymbol{z}_t + D\boldsymbol{u}_t, \tag{4.2}$$

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[8]In the original paper, given the presence of the control variable, the input to the encoder encompasses also past information of the control variable, whereas the reconstruction target always only encompasses the observation $\boldsymbol{x}_t$'s.

where $\bar{A}$ and $\bar{B}$ are approximations of $A$ and $B$ using the bilinear method (Tustin, 1947), respectively:

$$\bar{A} := (I - \tfrac{\Delta}{2}A)^{-1}(I + \tfrac{\Delta}{2}A), \qquad \bar{B} := (I - \tfrac{\Delta}{2}A)^{-1}\Delta B. \tag{4.3}$$

Here, $\Delta$ is the timescale at which the input $\boldsymbol{u}(t)$ is discretized and thus $\boldsymbol{u}_t = \boldsymbol{u}(\Delta \cdot t)$; $\boldsymbol{v}_t$ and $\boldsymbol{z}_t$ are analogously defined. Unrolling the recurrence in (4.2) leads to

$$\boldsymbol{v}_t = C\bar{A}^t\bar{B}\boldsymbol{u}_0 + C\bar{A}^{t-1}\bar{B}\boldsymbol{u}_1 + \cdots + C\bar{B}\boldsymbol{u}_t + D\boldsymbol{u}_t.$$

In particular, for a discrete input sequence $\{\boldsymbol{u}_t\}$ of length $L$, based on the connection between a linear time-invariant system and continuous convolution[9], the following holds with an SSM convolution kernel $\bar{K}$ and convolution operator $*$:

$$\boldsymbol{v} = \bar{K} * \boldsymbol{u} + D\boldsymbol{u}, \quad \text{where } \bar{K} \in \mathbb{R}^L := \mathcal{K}_L(\bar{A}, \bar{B}, C) := (C\bar{B}, C\bar{A}\bar{B}, \cdots, C\bar{A}^{L-1}\bar{B}). \tag{4.4}$$

The representation in (4.4) corresponds to the *convolutional* form, which can be computed efficiently using the fast Fourier transform (FFT).

Equations (4.1),(4.2) and (4.4) represent different perspectives of an LSSL, each contributing to its versatility and enabling this paradigm to leverage a combination of advantages. Specifically, as with many other continuous-time models, LSSLs naturally adapt to different timescales, and their connection to differential equations ensures that the trajectory is mathematically tractable. On the other hand, being a recurrent model, they are "stateful" and hence allow for fast autoregressive generation. Finally, the convolutional representation enables parallelizable training. The authors further establish explicit connections between LSSLs and convolutions, with the timescale $\Delta$ viewed as controlling the width of the convolution kernel. A similar connection can be established with RNNs, where the gating heuristics are linked to $\Delta$ and can be derived from ODE approximations.

The trainable parameters in an LSSL are $A, B, C, D$, and the timescale $\Delta \in \mathbb{R}$. When both $\boldsymbol{u}(t)$ and $\boldsymbol{v}(t)$ are 1-dimensional, an LSSL effectively forms a sequence to sequence map $\mathbb{R}^L \mapsto \mathbb{R}^L$ as a single-input-single-output (SISO) system, with $B \in \mathbb{R}^{d\times 1}, C \in \mathbb{R}^{1\times d}$ and $D \in \mathbb{R}^{1\times 1}$. Multi-dimensional outputs can be easily accommodated with $C \in \mathbb{R}^{d_{\text{out}}\times d}, D \in \mathbb{R}^{d_{\text{out}}\times 1}$. When the input is multi-dimensional with $d_{\text{in}} > 1$, multiple copies of LSSLs are used to process each input dimension independently. Finally, LSSLs can be stacked to form deep LSSLs, akin to the modules in Transformers.

It is worth noting that the basic form of LSSLs does not perform particularly well and inherits some of the challanges of recurrence and convolution, such as vanishing gradients. To overcome this, the authors leverage the HiPPO framework (Gu et al., 2020) that introduces continuous-time memorization. Specifically, by utilizing a class of structured matrices $A$[10], the state $\boldsymbol{z}(t)$ can effectively "memorize" the history of the input $\boldsymbol{u}(t)$. This approach significantly enhances the LSSL's performance, particularly in tasks involving long-sequence modeling.

In summary, an LSSL is a sequence modeling module, whose design primarily concerns 1-dimensional sequences. It maps an input sequence $\boldsymbol{u}(t)$ to the output sequence $\boldsymbol{v}(t)$ via the latent state $\boldsymbol{z}(t)$, by emulating a linear continuous-time SSM representation in discrete time. Multi-dimensional input/output can be handled with necessary modifications/adaptations.

## 4.2 Structured state-spaces (S4)

Despite its appealing properties, the computation of LSSLs remains a bottleneck in practice. As pointed out in Gu et al. (2022), with state dimension $d$ and context length $L$, computing the latent state requires $O(d^2L)$ operations, while memory usage scales as $O(dL)$. In addition, although a theoretically-efficient algorithm

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[9]For a linear time-invariant system, let $h(t)$ be the impulse response function. The output $\boldsymbol{v}(t)$ in response to the input $\boldsymbol{u}(t)$ then satisfy $\boldsymbol{v}(t) = \sum_j \boldsymbol{u}(t-\tau_j)h(t-\tau_j)$; taking $\tau_j \to 0$, $\boldsymbol{v}(t) = \int_{-\infty}^{\infty} \boldsymbol{u}(\tau)h(t-\tau)\mathrm{d}\tau$, i.e., $\boldsymbol{v}(t) = h(t) * \boldsymbol{u}(t)$. For further details, see Oppenheim et al. (1983).

[10]Known as the "HiPPO" matrix. Specifically, for $A \in \mathbb{R}^{d\times d}$, a HiPPO-LegS (short for "scaled Legendre measure") matrix is given by $A_{ij} = -(2i+1)^{1/2}(2j+1)^{1/2}$ if $i > j$; $i+1$ if $i = j$ and 0 otherwise.

exists, it is not numerically stable. The special form of the HiPPO matrix $A$ restricts the use of convolution techniques. Gu et al. (2022) addresses these limitations and enhances the practical applicability of LSSLs, focusing on improving both memory and computational efficiency. The primary setting considered involves both the input $u(t)$ and the output $v(t)$ being 1-dimensional, i.e., a single-input, single-output (SISO) SSM. In addition, $D$, see (4.1) and (4.2), is omitted hereafter (or equivalently, assume $D = 0$), due to the fact that the term $Du$ can be viewed as a skip connection and thus is easy to compute.

The major technical advancement involves considering the generating function on the coefficients of the convolution kernel $\bar{K}$ and imposing a special structure on the state matrix $A$. These two elements together enable stable and efficient computation, in the steps where repeated matrix multiplication of $\bar{A}$ is required (see, e.g., equation (4.4)). Concretely, the key steps can be outlined as follows:

1. Instead of directly computing $\bar{K}$, its spectrum is computed through the truncated generating function $\widetilde{\mathcal{K}}_L(\phi; \bar{A}, \bar{B}, C) := \sum_{\ell=0}^{L-1} C\bar{A}^\ell \bar{B}\phi^\ell$ evaluated at the roots of unity $\phi := \{\exp(2\pi i\ell/L) : \ell = 1, \cdots, L\}$. The filter $\bar{K}$ is then recovered by applying the inverse FFT in $O(L\log L)$ operations. Crucially, using the properties of the truncated generating function, that is, by letting $\widetilde{C}$ collect the constant terms, we can express it as[11]

$$\widetilde{\mathcal{K}}_L(\phi; \bar{A}, \bar{B}, C) = \widetilde{C}(I - \bar{A}\phi)^{-1}\bar{B} \quad \overset{\text{discretize}}{=} \quad \frac{2\Delta}{1+\phi}\widetilde{C}\Big[2\frac{1-\phi}{1+\phi} - \Delta A\Big]^{-1}B. \qquad (4.5)$$

This approach involves matrix inversion rather than calculating a matrix power series, and thus it reduces to obtaining the inverse efficiently.

2. Let the state matrix $A$ be a structured one, in the form of the sum of diagonal-plus-low-rank (DPLR) matrices, that is $A := \Lambda - PQ^*$ with $\Lambda$ being diagonal, $P, Q \in \mathbb{R}^{d\times r}$ for some small $r$. Using the Woodbury identity (Woodbury, 1950), for $r = 1$, $P, Q$ become vectors and (4.5) satisfies

$$\widetilde{K}_L(\phi; \bar{A}, \bar{B}, C) = \frac{2}{1+\phi}\Big[\widetilde{C}^*\kappa_\Lambda(\phi)B - \widetilde{C}^*\kappa_\Lambda(\phi)P\big[1 + Q^*\kappa_\Lambda(\phi)P\big]^{-1}Q^*\kappa_\Lambda(\phi)B\Big],$$

where $\kappa_\Lambda(\phi) := (\frac{2}{\Delta}\frac{1-\phi}{1+\phi} - \Lambda)^{-1}$ (Gu et al., 2022, Lemma C.3). This reduces the calculation to $\tilde{O}(d+L)$ operations and $O(d+L)$ space, as $Q^*\kappa_\Lambda(\phi)P$ can be handled with Cauchy matrix-vector multiplication (Gu et al., 2022, Appendix C.3, Proposition 5).

The above techniques allow for the efficient calculation of the convolution filter $\bar{K}$. For the recurrence in (4.2), it can computed in $O(d)$ operations with a DPLR matrix. By considering matrix $A$ in DPLR form, S4 is (near-)optimal for both the recurrent (4.2) and the convolutional (4.4) representations of the LSSLs. Depending on the exact setting, the former is typically used for online generation, while the latter is used for offline training with equally-spaced observations, taking advantage of the the parallelizable nature of the FFT.

*Remark* 8 (Some additional results). We briefly outline some other results established in Gu et al. (2022), focusing on the motivation behind adopting a DPLR form for the state matrix $A$.

- Conjugation is an equivalence relation for SSMs (Gu et al., 2022, Lemma 3.1). Two SSMs that are conjugate to each other provide the same $u \mapsto v$ mapping, but with a change of basis in the state $z$, effectively allowing the system to be "reparametrized". The HiPPO matrices (Gu et al., 2020, 2021) have a normal[12]-plus-low-rank (NPLR) form (as shown in Theorem 1), and can be conjugated into a DPLR form. This has two important implications: (1) from a computation perspective, it suffices to focus on the complexities of the SSMs whose $A$ is in DPLR form; (2) practically, the SSM can be initialized with $A$ set to a specific HiPPO matrix (e.g., the HiPPO-LegS shown in footnote 10), with $\Lambda, P, Q$ being the actual learnable parameters associated with it.

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[11]this is due to $\widetilde{\mathcal{K}}_L(\phi; \bar{A}, \bar{B}, C) = \sum_{\ell=0}^{L-1} C\bar{A}^\ell \bar{B}\phi^\ell = C(I - \bar{A}^L\phi^L)(I - \bar{A}\phi)^{-1}\bar{B} = \widetilde{C}(I - \bar{A}\phi)^{-1}\bar{B}$; the last equality holds since $\phi^L = 1$ by definition and $\widetilde{C}$ collects the constant term

[12]A complex square matrix $A$ is normal if it commutes with its conjugate transpose $A^*$.

- When $A$ is diagonal, the computation of the generating function reduces to calculating a Cauchy kernel, which is a well-studied problem with stable numerical algorithms (see Appendix C.3, Proposition 5). The DPLR form can be viewed as a relaxation of the diagonal case, adopted because the diagonalization of the HiPPO matrix is unstable. This instability makes the naive application of a diagonal parameterization prone to numerical issues, thus necessitating the DPLR approach.

## 4.3 Simplified state-spaces (S5)

Smith et al. (2023) extend S4 along the following two directions: (1) in the case where the input/output are multi-dimensional, instead of using multiple SISO SSMs followed by a "mixing layer" to combine the features, a multi-input-multi-output (MIMO) SSM is used; this reduces the combined latent state size $(d_{\text{in}} \cdot d)$ to some $\tilde{d}$, which can be much smaller; and (2) instead of taking the frequency domain approach with generating functions, S5 utilizes parallel scan (Blelloch, 1990) which yields the same computational complexity as S4, yet operates solely in the time domain via recurrence. At a high level, a parallel scan computes the linear recurrence in (4.2) in parallel via the following steps:

1. Precompute $c_k \equiv (c_{k,a}, c_{k,b}) := (\bar{A}, \bar{B}\boldsymbol{u}_k)$ for $k = 1, \cdots, L$, and let $r_0 = (I, 0)$. Define a binary associative operator $\bullet$ used for combining the elements $q_i \bullet q_j = (q_{j,a} \odot q_{i,a}, q_{j,a} \otimes q_{i,b} + q_{j,b})$, where $\odot, \otimes, +$ are matrix-matrix multiplication, matrix-vector multiplication and elementwise addition, respectively.

2. A reduction (or upsweep) step giving rise to the "upsweep tree". Let $c_k$ be the leaves; each element is obtained by pairwise operations as defined by the operator. This steps gives the partial "prefix" scan results.

3. A downsweep step that completes the scan. Let $r_0$ be the foot. Based on the above outputs, complete the scan by passing each node's own value to the left child; the right child is obtained by applying the operator between the node itself and the left child in the (mirrored) upsweep tree.

Given sufficient number of processors, the parallel time scales logarithmically with $L$ (Smith et al., 2023); see also Appendix H therein for a concrete example for a sequence of length $4$.

**Diagonal state space.** Similar to S4 where the efficient computation requires a specific parameterization of $A$ (e.g., a DPLR form), S5 parameterizes $A$ as a diagonal matrix[13]. Initialization of the state matrix is done with the HiPPO-N matrix, that is, the normal part of the HiPPO-LegS matrix (see footnote 10). Recall that all HiPPO matrices have an NPLR form (Gu et al., 2022); specifically, in the case of HiPPO-LegS, it has the following decomposition:

$$ A_{\text{LegS},ij} := \begin{cases} -(2i+1)^{\frac{1}{2}}(2j+1)^{\frac{1}{2}} & i > j, \\ i+1 & i = j, \\ 0 & \text{otherwise}; \end{cases} \quad \overset{\text{decomp.}}{=} A_{\text{LegS}}^{\text{Normal}} + P_{\text{LegS}} P_{\text{LegS}}^{\top}, $$

where $P_{\text{LegS}} \in \mathbb{R}^{d \times 1}$ is rank-1:

$$ P_{\text{LegS},i} := (i + \tfrac{1}{2})^{\frac{1}{2}}, \quad \text{and} \quad A_{\text{LegS},ij}^{\text{Normal}} := - \begin{cases} (i+\tfrac{1}{2})^{\frac{1}{2}}(j+\tfrac{1}{2})^{\frac{1}{2}} & i \neq j, \\ \tfrac{1}{2} & i = j; \end{cases} . $$

This normal portion $A_{\text{LegS}}^{\text{Normal}}$ can be diagonalized stably (Gupta et al., 2022; Gu et al., 2022), though diagonalization of the full matrix $A_{\text{LegS}}$ suffers from some instability issues.

## 4.4 Selective-scan state-spaces (Mamba)

In the SSM used thus far for mapping the input $\boldsymbol{u}(t)$ to the output $\boldsymbol{v}(t)$, the model parameters (e.g., $A, B, C, D$) are time-invariant. However, Gu and Dao (2023) argue that the invariance in the dynamics restricts the model's ability to "selectively" incorporate contextual information, limiting its capacity to update

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[13]This is also a requirement for using parallel scan to compute efficiently.

hidden states based on input-specific cues. To address this, an SSM with a selection mechanism is proposed, called Mamba, where the parameters are functions of the input and (4.2) is extended to the following form:

$$\boldsymbol{z}_t = \bar{A}(\boldsymbol{u}_t)\boldsymbol{z}_{t-1} + \bar{B}(\boldsymbol{u}_t)\boldsymbol{u}_t, \qquad \boldsymbol{v}_t = C(\boldsymbol{u}_t)\boldsymbol{z}_t.$$

Notably, instead of having fixed $\bar{A}, \bar{B}, C$, they are now functions of $\boldsymbol{u}_t$ and thus become context-aware, and the SSM now corresponds to a time-varying system. Following the discretization rule in (4.3) or its zero-order hold (ZOH) alternative, given by

$$\bar{A} := \exp(\Delta A), \qquad \bar{B} := (\Delta A)^{-1}\big(\exp(\Delta A) - I\big) \cdot \Delta B, \tag{4.6}$$

the input-dependent state transition matrix $\bar{A}(\boldsymbol{u}_t)$ is operationalized "indirectly" via the discretization time scale $\Delta$ that becomes a function of $\boldsymbol{u}_t$, given in the form of $\Delta(\boldsymbol{u}_t) := \mathrm{softplus}\big(c + \mathrm{Linear}(\boldsymbol{u}_t)\big)$[14]. Meanwhile, $A$ remains an input-independent structured matrix, while $B$ and $C$ are assumed linear functions of $\boldsymbol{u}_t$ that directly govern the magnitude of the input $\boldsymbol{u}_t$'s influence on the latent state $\boldsymbol{z}_t$, and that of the state $\boldsymbol{z}_t$ on the output $\boldsymbol{v}_t$, respectively. In the special case where the state dimension is 1, connections between the selective SSM recurrence and the gating mechanism used in RNN can be further established. Further, $\Delta$ can be interpreted as controlling the amount of emphasis on the current input $\boldsymbol{u}_t$: a small $\Delta$ corresponds to the case where the current input is considered transient and thus "unselected", whereas a larger $\Delta$ places more emphasis on the current input, rather than the context that is contained in the state. Similar to S5, Mamba leverages parallel scanning and emphasizes the recurrence perspective of the SSM, with the state matrix $A$ assumed to have a diagonal structure.

*Remark* 9. To compute selective state spaces efficiently with parallel scan, the authors consider additional techniques that fully leverage modern GPU capabilities. These include using kernel fusion to reduce memory I/O operations, performing discretization and recurrence calculations directly in GPU SRAM while loading the "raw" parameters from GPU HBM[15], and leveraging recomputation to avoid saving intermediate states needed for backpropagation, thereby reducing memory requirements. The specific implementation details are omitted here; readers interested in a comprehensive explanation are encouraged to consult the original paper.

To conclude this section, it is worth noting that modern structured SSMs represent an active area of research in the deep learning community. On the theoretical front, Cirone et al. (2024) proposes a continuous-time framework that establishes connections between Linear Controlled Differential equations (Linear CDEs) with SSMs, such as S4 and Mamba. The framework provides an explicit characterization of the "uniform closure"[16], along with insights into the efficiency, stability, and expressiveness of these systems in relation to their specific structured transition matrices or architectures stability and expressiveness of the system in relation to the specific structured transition matrix or the architectures adopted. Empirically, SSM-based architectures such as Linear Attention (Katharopoulos et al., 2020) that can be viewed as a degenerate linear SSM (Gu and Dao, 2023), and more recent models such as RetNet (Sun et al., 2023) have gained popularity as efficient alternatives to standard Transformers that suffer from quadratic computational complexity. Additional connections between Transformers and SSMs are explored in the follow-up work Mamba-2 (Dao and Gu, 2024). S4/S5/Mamba-style architectures have also found applications across other areas, including spatio-temporal modeling (Smith et al., 2024), vision (Zhu et al., 2024) and graph learning (Wang et al., 2024).

# 5    Applications to Selected Modeling Tasks

In this section, we discuss selected modeling tasks for time series data facilitated by an SSM formulation.

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[14]$\mathrm{softplus}(x) := \log\big(1 + \exp(x)\big)$. In the expression, $c$ is some (hyper)-parameter; we also omit the "broadcast$_D$" operation in the original paper (Algorithm 2), which effectively creates identical $D$ copies along the "extra" dimension so that the tensor shape is suitable for subsequent operations.

[15]SRAM and HBM are shorthand for "static random-access memory" and "high-bandwidth memory", respectively.

[16]The uniform closure describes the set of functions from compact subsets of the input space to $\mathbb{R}$ (the output space) that can be uniformly approximated at an arbitrary precision by a Linear CDE" (see Section 4 of Cirone et al. (2024))

## 5.1 Mixed-frequency data modeling and nowcasting

Mixed-frequency data involves two groups of related time series that evolve at different sampling frequencies. Modeling such data is primarily concerned with prediction tasks tailored to these time series. For instance, consider a scenario with two blocks of variables—one observed at a low frequency and the other at a high frequency. The goal is to forecast both blocks while simultaneously performing *nowcasting* for the low-frequency block by incorporating the progressively available high-frequency data. This modeling task is particularly relevant in macroeconomic applications, such as predicting key quarterly indicators like Gross Domestic Product (GDP) using monthly economic and financial variables.

Formally, let $\boldsymbol{x}_t \in \mathbb{R}^p$ denote the high-frequency block of variables and $\boldsymbol{y}_{t'} \in \mathbb{R}^q$ the low-frequency one, indexed by $t$ and $t'$, respectively. The *frequency ratio* $r$ defines the relative granularity between two collections; for example, $r = 3$ for quarterly/monthly time series. By construction, $\boldsymbol{x}_{rt'}$ and $\boldsymbol{y}_{t'}$ correspond to observations at the same physical timestamp. The prediction $\widehat{\boldsymbol{y}}_{T'+1}$ at time period $(T' + 1)$ for the low-frequency block, may be based either on *forecast* or a *nowcast*, depending on the data available up to $T'$ for the low-frequency block and up to $T$ for the high-frequency block, where $rT' \leq T \leq (r+1)T'$ is always satisfied. A *forecast* pertains to the case where $T \equiv rT'$, whereas a *nowcast* uses $T = rT' + h$ for some $1 \leq h \leq r$. For example, predicting quarterly GDP for the quarter ending in March, a forecast is based on data available up to the preceding December for both blocks of variables, whereas a nowcast is based on data up to the preceding December for the quarterly variables, and up to the preceding January, February or March for the monthly variables, depending on the corresponding *vintage* of the nowcast.

The state-space model is a popular framework for handling this modeling task, as seen in works by Giannone et al. (2008); Schorfheide and Song (2015); Gefang et al. (2020); Ankargren et al. (2020). At a high level, these approaches model the system dynamics through a state-space representation with the latent state $\boldsymbol{z}_t$ evolving at the high-frequency; the exact dependency of the low and the high-frequency blocks on the states vary, depending on the specific approach in question, as briefly discussed next.

Giannone et al. (2008) model the high-frequency block $\boldsymbol{x}_t$ and the latent state $\boldsymbol{z}_t \in \mathbb{R}^d$ as a joint system according to a dynamic factor model that effectively adopts a linear state-space representation and assume the low-frequency variable evolution is modeled with a regression structure as:

$$\boldsymbol{z}_t = A\boldsymbol{z}_{t-1} + \boldsymbol{u}_t; \tag{high-freq}$$
$$\boldsymbol{x}_t = C\boldsymbol{z}_t + \boldsymbol{\epsilon}_t, \quad \text{with} \ \ \mathbb{E}(\boldsymbol{\epsilon}_t) = 0, \mathbb{E}(\boldsymbol{\epsilon}_t \boldsymbol{\epsilon}_t') = \Sigma_\epsilon;$$
$$y_{j,t'} = \alpha_k + \boldsymbol{\beta}_j^\top \boldsymbol{z}_{rt'} + \varepsilon_{j,t'}, \quad \forall \, j = 1, \cdots, q. \tag{low-freq}$$

The latent state $\boldsymbol{z}_t$ is a low-dimensional object when compared with $\boldsymbol{x}_t$, that is, $d \ll p$, and can be interpreted as the latent factors. The estimation proceeds in two steps:

1. Latent states $\boldsymbol{z}_t$ are extracted based on the high-frequency variables $\boldsymbol{x}_t$ using a two-step approach (Doz et al., 2011) comprising of PCA–OLS and a Kalman Smoother step, which gives rise to the estimated states $\widehat{\boldsymbol{z}}_t$ and the system parameters $\widehat{\theta} := (\widehat{A}, \widehat{C}, \widehat{\Sigma}_\epsilon)$.

2. Once the $\widehat{\boldsymbol{z}}_t$'s are extracted, parameters in the low-frequency equation can be estimated with the plug-in estimates of the states, based on available observations.

During prediction, future state estimates are obtained via Kalman filtering, enabling forecasts and nowcasts for both high- and low-frequency variables.

Schorfheide and Song (2015) propose a joint modeling framework for high and the low-frequency variables, linked through a partially observed state. Concretely, the state vector is defined as $\tilde{\boldsymbol{z}}_t := [(\tilde{\boldsymbol{z}}_t^{\text{obs}})^\top, (\tilde{\boldsymbol{z}}_t^{\text{unobs}})^\top]^\top$, with the high and low frequency blocks satisfying

$$\boldsymbol{x}_t \equiv \tilde{\boldsymbol{z}}_t^{\text{obs}}; \qquad \boldsymbol{y}_{t'} \equiv \tilde{\boldsymbol{y}}_{rt'} \ \ \text{and} \ \ \tilde{\boldsymbol{y}}_t \equiv \text{agg}(\tilde{\boldsymbol{z}}_{rt'}^{\text{unobs}}, ..., \tilde{\boldsymbol{z}}_{(r-1)t'+1}^{\text{unobs}}).$$

In other words, the model assumes that the high-frequency block coincides with the observed part of the state; there is an *unobserved* high-frequency process $\tilde{\boldsymbol{y}}_t$, and its every $r$th observation corresponds to the

observed low-frequency one. The actual modeling then boils down to handling the dynamics of a system evolving at the high frequency. To this end, the partially observed latent process is assumed to be an autoregressive dynamic one with $\ell$ lags, that is, $\tilde{z}_t = \Phi_1 \tilde{z}_{t-1} + \cdots + \Phi_\ell \tilde{z}_{t-\ell} + \boldsymbol{\xi}_t$. By letting $\boldsymbol{z}_t := [\tilde{z}_t^\top, \cdots, \tilde{z}_{t-\ell+1}^\top]^\top$, $M_t :=$ some "selection" matrix, $\Lambda :=$ aggregation matrix[17], the system dynamics can be written according to the following state-space representation:

$$\text{state equation:} \quad \boldsymbol{z}_t = A\boldsymbol{z}_{t-1} + \boldsymbol{u}_t, \;\; \boldsymbol{u}_t \sim \mathcal{N}(0, \Sigma_u),$$
$$\text{observation equation:} \quad \begin{bmatrix} \boldsymbol{x}_t \\ \tilde{\boldsymbol{y}}_t \end{bmatrix} = M_t \Lambda \boldsymbol{z}_t + \boldsymbol{\zeta}_t.$$

The parameter $\theta := (A, \Sigma_u)$ is estimated via Gibbs sampling that draws from the posterior conditional distributions $\mathbb{P}(\theta \,|\, \{\boldsymbol{z}_t\}_{t=1}^T, \{\boldsymbol{x}_t, \tilde{\boldsymbol{y}}_t\}_{t=1}^T)$ and $\mathbb{P}(\{\tilde{z}_t\}_{t=1}^T \,|\, \theta, \{\boldsymbol{x}_t, \boldsymbol{y}_t\}_{t=1}^T)$ at each iteration. Specifically, by imposing conjugate priors, $\mathbb{P}(\theta | \cdot)$ has a closed-form and becomes easy to draw samples from; on the other hand, drawing samples from $\mathbb{P}(\{\tilde{z}_t\}_{t=1}^T | \cdot)$ requires a simulation smoother (Durbin and Koopman, 2002). At prediction phase, for each draw of the state $(\theta, \{\boldsymbol{z}_t\}_{t=1}^T)$ from the posterior distribution, one can obtain the $h$-step-ahead prediction of $\{\hat{\boldsymbol{z}}_t\}_{t=T+1}^{T+h}$ according to the state equation, which then gives the corresponding estimate $\hat{\boldsymbol{x}}_t$ and $\tilde{\boldsymbol{y}}_t$'s. Point estimate and credible intervals can be readily obtained by summarizing estimates from multiple draws.

*Remark* 10 (Other modeling approaches for mixed frequency data). Alternative frameworks, such as mixed data sampling (MIDAS) regression (Ghysels et al., 2007) and vector-autoregression (VAR) model-based ones that require frequency-alignment (McCracken et al., 2015) are also considered for modeling mixed-frequency data. A notable benefit of SSM-based approaches is their ability to maintain consitency and uniqueness in the postulated dynamics across forecasting and nowcasting vintages. In contrast, MIDAS regression and VAR-based approaches require a collection of models, each tailored to a specific forecast or nowcast vintage. We refer interested readers to (Lin and Michailidis, 2023, Section 1.1 and Appendix A) for a brief juxtaposition and references therein for additional details.

*Remark* 11 (Multi-rate time series). Multi-rate time series (Hamilton, 2020; Reinsel, 2003) generalize the concept of mixed-frequency data by incorporating *multiple blocks* of variables sampled at varying frequencies, rather than being restricted to just high- and low-frequency blocks. Approaches leveraging a latent space representation to address the challenges posed by different sampling rates and complex temporal dynamics include classical ones that use the extended Kalman filter (Armesto et al., 2008; Safari et al., 2014), and more recently neural network-based ones (Che et al., 2018).

## 5.2 Irregularly-spaced time series modeling and imputation

Time series with irregular-spaced observations arise in various application domains including electronic health records, biology and ecology (Reinsel, 2003). Traditionally, techniques such as linear/polynomial fitting, spline interpolation, time scale aggregation (e.g., binning, averaging) and SSM have been employed to handle such data (Reinsel, 2003; Hamilton, 2020). More recently, neural network-based approaches have emerged, which can be broadly segmented into three categories: (1) preprocessing the input, by either mapping observations on a regularly-spaced grid through discretization of the time interval (Marlin et al., 2012; Lipton et al., 2016), or through interpolation (Shukla and Marlin, 2019); (2) using one of the regular neural network architectures (e.g., RNN or transformers) for time series modeling, with input augmented by information on missingness and intervals (Che et al., 2018), or incorporating specialized modules such as "time attention" that additionally incorporate a "time attention" mechanisms that explicitly leverage temporal embeddings (Shukla and Marlin, 2020); and (3) modeling the latent space in continuous time, leveraging frameworks like neural ODEs (Rubanova et al., 2019; Yildiz et al., 2019), which are naturally agnostic to the time scale. The remainder of this subsection focuses on representative approaches from the third category.

The modeling framework proposed by Rubanova et al. (2019), detailed in Section 3.2, focuses on the application of neural ODE for irregularly-spaced time series in tasks such interpolation (i.e., imputation) and extrapolation (i.e., forecasting), respectively. At a high level, once the model is trained and yields estimated

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[17]both $M_t$ and $\Lambda$ can be pre-determined through frequency mismatch and the pre-specified aggregation/transformation schema

parameters $(\widehat{\theta}_f, \widehat{\theta}_g)$, the latent state trajectory can be computed by solving an initial value problem based on sampled initial value $\widetilde{z}_{t_0}$ from its encoded distribution at desired time points:

$$\widehat{z}_{t_1}, \widehat{z}_{t'_1}, \cdots, \widehat{z}_{t'_m} = \text{ODESolve}\big(\widetilde{z}_{t_0}, f_{\widehat{\theta}_f}, (t'_1, \cdots, t'_m)\big).$$

Here, $\{t'_1, \cdots, t'_m\}$ represent timestamps of interest at inference time—either imputation or prediction, distinct from the available ones $\{t_1, \cdots, t_n\}$ used for training the model. Once estimates of the latent states are available, the corresponding $\widehat{x}_{t'_i}$'s can be readily obtained through the observation equation (3.5). For both imputation and forecasting tasks, the training process follows the VAE-based pipeline outlined in Exhibit 2, with slight variations in how encoding and decoding are handeled. Specifically,

- For imputation, both encoding and the reconstruction error calculation are conducted based on the available time points $\{t_1, \cdots, t_n\}$;

- For forecasting, the observed time points are *partitioned* in two halves: $\{t_1, \cdots, t_{\lfloor n/2 \rfloor}\}$ and $\{t_{\lfloor n/2 \rfloor+1}, \cdots, t_n\}$; encoding is done by traversing the first half $\{t_1, \cdots, t_{\lfloor n/2 \rfloor}\}$ backwards in time, and decoding is done by solving the ODE forward at the second half $\{t_{\lfloor n/2 \rfloor+1}, \cdots, t_n\}$, based on which the reconstruction error is calculated.

In a variation to Rubanova et al. (2019), Yildiz et al. (2019) introduce a Bayesian neural second-order ODE to mitigate the incapability of a first-order ODE model to capture higher-order dynamics. Specifically, the latent state is modeled as:

$$\frac{\mathrm{d}^2 z_t}{\mathrm{d}^2 t} = h_{\theta_h}(z_t, \frac{\mathrm{d} z_t}{\mathrm{d} t}),$$

where $h_{\theta_h} : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}^d$ is parameterized by a neural network. By considering the state as a tuple $z_t := (s_t, v_t)$ with $s_t$ and $v_t$ representing its position and velocity, the above equation can be equivalently written as a system of coupled first-order ODEs, namely,

$$\frac{\mathrm{d} s_t}{\mathrm{d} t} = v_t, \qquad \frac{\mathrm{d} v_t}{\mathrm{d} t} = h_{\theta_h}(s_t, v_t),$$

$$\Rightarrow \quad s_t = s_0 + \int_0^t v_\tau \mathrm{d}\tau, \ \ v_t = v_0 + \int_0^t h_{\theta_h}(s_\tau, v_\tau)\mathrm{d}\tau.$$

The observation $x_t$ depends only on the state position $s_t$'s, and the velocity $v_t$ serves as an auxiliary variable. Finally, model training, imputation and/or forecasting steps largely stay the same as the ones outlined for Rubanova et al. (2019).

There is another line of work that does not leverage directly an SSM formulation, albeit the notion of latent process dynamics is still present. For example, De Brouwer et al. (2019) utilize an RNN to implicitly model the latent state dynamics through GRU operations[18], which when coupled with an ODE enables continuous-time modeling for irregularly-spaced time series. In subsequent work, Yuan et al. (2023) combine an SSM formulation with the ODE-RNN architecture in De Brouwer et al. (2019) to address the same modeling task. Detailed explanations if these two approaches can be found in the respective references.

## 6  Concluding Remarks

As noted in this review, classical approaches to estimating the SSM parameters rely on recursion. To handle non-linearities and/or non-Gaussianity in the SSM specification, approximations (e.g., extended Kalman or other filters) or sampling techniques (e.g., sequential Monte Carlo; SMC) are needed in the filtering and smoothing steps. Note that although SMC can handle arbitrary functional/distribution specification of

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[18]Gated Recurrent Units (GRUs) are designed to model sequences efficiently by using update and reset gates to manage information flow. The update gate controls the amount of past information retained, while the reset gate the amount of past information ignores, allowing the model to manage long-term dependencies effectively.

the SSM, it can do so effectively only in low-dimensional settings. On the other hand, neural network-based approaches allow for flexible parameterization of the state and the observation equations. With VAE being the dominant learning paradigm, the learning pipeline requires an encoder and a decoder; the former is usually operationalized with additional approximations (e.g., mean field approximation) to simplify the calculation of the $q_\phi(z_t|x)$'s, which are designed to approximate the true posterior $p(z_t|x)$'s. Both the encoder and the decoder distributions are typically assumed Gaussian. Note that while VAE is usually trained end-to-end, the underlying modules for the encoder/decoder networks (such as RNNs) often inherently rely on recursive computations.

It is worth noting that the discrete time linear SSM has also been extensively studied in the econometrics literature (Stock and Watson, 2012), and is referred to as the exact Dynamic Factor Model, with the additional assumption of a diagonal covariance matrix of the error term in the state equation. A focus in that stream of literature is to allow cross-sectional dependence in the error term of the observation equation, giving rise to the approximate Dynamic Factor Model (see review paper by Stock and Watson (2016) and references therein). Extensions addressing in addition temporal dependence in observation errors are provided in Lin and Michailidis (2020b).

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# A Discrete Time Linear Gaussian SSM

This section first provides an overview of the key steps involved in estimating the model parameters based on the EM algorithm, wherein linearity and Gaussianity lead to closed form expressions for the E-step. Further, explicit expressions can be obtained for the M-step under the assumption that the model parameters are *time invariant*. Finally, a variant of the SSM with piecewise linear parameters is discussed, highlighting the added challenges in estimation introduced by the dynamically evolving parameters.

A *general* form of the model under consideration is given by

$$\text{state equation:} \quad \boldsymbol{z}_t = A_t \boldsymbol{z}_{t-1} + \boldsymbol{u}_t, \tag{A.1a}$$

$$\text{observation equation:} \quad \boldsymbol{x}_t = C_t \boldsymbol{z}_t + \boldsymbol{\epsilon}_t, \tag{A.1b}$$

where $A_t \in \mathbb{R}^{d \times d}$ and $C_t \in \mathbb{R}^{p \times d}$ specify the autoregressive dynamics and the relationships between the latent state and the observed variables, respectively, and

$$\begin{pmatrix} \boldsymbol{u}_t \\ \boldsymbol{\epsilon}_t \end{pmatrix} \overset{iid}{\sim} \mathcal{N}\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} Q_t & 0 \\ 0 & R_t \end{pmatrix} \right).$$

Note that the equation shown in (A.1a) assumes the state to be a lag-1 vector autoregressive process. More lags can be accommodated in a straightforward manner, by rewriting a lag-d autoregressive process in its lag-1 form (see details in Lütkepohl (2005)).

The computations in the E-step involve the following updates of (see also Section (2.2)): (i) the *filtering step*, which calculates the posterior distribution of the latent state given the observed trajectory up to time $t$—$p_\theta(\boldsymbol{z}_t | \boldsymbol{x}_{1:t})$ in (2.8), (ii) the *prediction step*, which calculates the predictive distribution of the next latent state given the observed trajectory up to time $t - 1$—$p_\theta(\boldsymbol{z}_t | \boldsymbol{x}_{1:t-1})$, and (iii) the *smoothing step* that updates the posterior distribution of the latent state given all the data—$p_\theta(\boldsymbol{z}_t | \boldsymbol{x}_{1:T})$ in (2.9).

Let $\boldsymbol{z}_{t|s} := \mathbb{E}(\boldsymbol{z}_t | \boldsymbol{x}_{1:s})$ and $P_{t|s} := \text{Cov}(\boldsymbol{z}_t | \boldsymbol{x}_{1:s})$, $s, t = 0, 1, 2, \cdots, T$. For the linear Gaussian SSM, all three distributions computed during the E-step are *Gaussian*, whose means and covariance matrices can be sequentially updated based on the following recursive formulas, for *given* values of the model parameters $\theta_t = (A_t, C_t, Q_t, R_t)$. Concretely,

- Filtering step:

$$\boldsymbol{z}_{t|t} = \boldsymbol{z}_{t|t-1} + K_t(\boldsymbol{x}_t - C_t \boldsymbol{z}_{t|t-1}),$$
$$P_{t|t} = (I - K_t C_t) P_{t|t-1},$$

  where $K_t$ corresponds to the *Kalman gain* matrix given by

$$K_t = P_{t|t-1} C_t^\top (C_t P_{t|t-1} C_t^\top + R_t)^{-1}.$$

- Prediction step:

$$\boldsymbol{z}_{t|t-1} = A_t \boldsymbol{z}_{t-1|t-1},$$
$$P_{t|t-1} = A_t P_{t-1|t-1} A^\top + Q_t.$$

- Smoothing step:

$$\boldsymbol{z}_{t|T} = \boldsymbol{z}_{t|t} + H_t(\boldsymbol{z}_{t+1|T} - \boldsymbol{z}_{t+1|t}),$$
$$P_{t|T} = P_{t|t} + H_t(P_{t+1|T} - P_{t+1|t}) H_t^\top,$$

  with $H_t = P_{t|t} A_t^\top P_{t+1|t}^{-1}$ being the Kalman smoother gain.

Derivations of these formulas, collectively known as the Kalman filter algorithm, can be found in standard references (e.g., in Harvey, 1990; Durbin and Koopman, 2012).

While the Kalman filter algorithm solves the state identification problem for the general form of the linear Gaussian SSM, estimation of the parameters $\theta_t$ is intractable without additional simplification in the model specification, due to the fact that a single observation is available for each value of the time varying parameter. To overcome this limitation, the most widely used version of the model assumes *time invariant* parameters; i.e., $\theta_t \equiv \theta = (A, C, Q, R)$. In that case, the M-step computations yield closed form expressions for the model parameters $\theta$, due to the Gaussian nature of the expected log-likelihood $L(\theta, \theta^{(k)})$ given in (M-step). Specifically, the M-step estimates are then given by (Shumway and Stoffer, 1982):

$$\widehat{A} = \Big(\sum_{t=1}^{T} V_{t,t-1|T}\Big)\Big(\sum_{t=1}^{T} P_{t-1|T} + z_{t-1|T} z_{t-1|T}^{\top}\Big)^{-1} \quad , \quad \widehat{C} = \Big(\sum_{t=1}^{T} x_t z_{t|T}^{\top}\Big)\Big(\sum_{t=1}^{T} P_{t|T} + z_{t|T} z_{t|T}^{\top}\Big)^{-1},$$

$$\widehat{Q} = \frac{1}{T}\Big(\sum_{t=1}^{T}(P_{t|T} + z_{t|T} z_{t|T}^{\top}) - \widehat{A} V_{t,t-1|T}\Big) \quad , \quad \widehat{R} = \frac{1}{T}\Big(\sum_{t=1}^{T} x_t x_t^{\top} - \widehat{C} z_{t|T} x_t^{\top}\Big),$$

where $V_{t,t-1|T} := \mathrm{Cov}(z_t, z_{t-1}|x_{1:T})$ and can be computed recursively based on the updates of the quantities from the Kalman filter as follows:

$$V_{t,t-1|T} = P_{t|t} J_{t-1}^{\top} + J_t(V_{t+1,t|T} - A P_{t-1|t-1}) J_{t-1}^{\top}, \quad t = 1, \cdots, T-1,$$

with $J_t = P_{t|t} A^{\top}(P_{t+1|t})^{-1}$ and $V_{T,T-1|T} = (I - K_T C) A P_{T-1|T-1}$.

Finally, note that another estimation strategy for $\theta$ based on the likelihood marginalization approach is given in (Shumway and Stoffer, 2000, Chapter 6).

**Linear Gaussian Switching SSM.** This variant exhibits richer dynamics compared to the time-invariant model, while parameter estimation remains feasible, albeit significantly more technically involved. The model includes an *additional latent state* variable $S_t$ that takes values in a finite state space $S_t \in \mathcal{S} = \{s_1, \cdots, s_M\}$ and follows Markovian dynamics governed by a transition kernel $\mathcal{P}_S := \mathbb{P}(S_t|S_{t-1})$. Each state $s_m \in \mathcal{S}$ has its associated transition and covariance matrices $(A_{s_m}, C_{s_m}, Q_{s_m}, R_{s_m})$. The state and observation equations of this model variant are given by

$$z_t = A_{S_t} z_{t-1} + u_{S_t},$$
$$x_t = C_{S_t} z_t + \epsilon_{S_t}.$$

This model combines the linear dynamics of Gaussian SSMs, with a discrete structure of Hidden Markov Models for the time varying parameters.

The model has been studied in the systems engineering (Chang and Athans, 1978), econometrics (Hamilton, 1989) and statistics (Shumway and Stoffer, 1991) literature. Parameter learning is based on the EM algorithm. Note that in the filtering step, the posterior distribution of the *augmented* latent state $(z_t, S_t)$ given an observed trajectory needs to be computed. As shown in Chang and Athans (1978), even with a *known* transition kernel $\mathcal{P}_S$, this posterior distribution corresponds to a Gaussian mixture distribution with $M^T$ components, where $T$ is the length of the observed trajectory. As such, direct computation is intractable. In addition, predicting $z_t$ not only depends on the extra state variable $S_t$, but also on its value at time $t-1$, and this further increases the computational burden; i.e., $z_{t|t}(m, m') := \mathbb{E}(z_t|x_{1:t}, S_t = m, S_{t-1} = m')$, $m, m' \in \mathcal{S}$, and analogously for $P_{t|t}(m, m') := \mathrm{Cov}(z_t|x_{1:t}, S_t = m, S_{t-1} = m')$. To render the computations in the E-step manageable, Kim (1994) and Bar-Shalom et al. (2004) introduce appropriate approximations, originally proposed in Harrison and Stevens (1976), enabling computations whose complexity is linear in $M$ rather $M^T$. They also derive the corresponding filtering, prediction and smoothing updates for state identification and maximum likelihood estimators for the model parameters. Alternatively, Ghahramani and Hinton (2000) leverage a variational approach, using a tractable distribution that eliminates some of the dependencies between the original state $z_t$ and the extra state $S_t$ to approximate the posterior distribution in the filtering step. A number of Bayesian approaches have also been proposed for estimating this model's parameters, including Carter and Kohn (1994, 1996); Kim and Nelson (1998, 1999); Ghahramani and Hinton (2000); Frühwirth-Schnatter (2001); Petetin et al. (2021).

**The discrete process SSM.** A more involved variant of the discrete time linear Gaussian SSM, known as the discrete process model (Roesser, 1975; Kitagawa and Gersch, 2012), is defined as

$$z_t = Az_{t-1} + u_t,$$
$$x_t \sim p_\theta(x_t|z_t), \quad x_t \in \mathbb{Z}^p,$$

where the state equation is linear, and the observation process takes discrete values, so that it can handle binary or count data. Parameter learning is based on the EM algorithm. However, the presence of a nonlinear, non-Gaussian observation equation introduces complications, necessitating the use of the general learning framework discussed in Section 2.2, instead of the straightforward updates offered by the Kalman filter; see Kitagawa (1987, 1988) for further details.

# B The Extended Kalman, the Gaussian and the Unscented Kalman filters

This section outlines three key filtering techniques—Extended Kalman Filter (EKF), Gaussian Filter, and Unscented Kalman Filter (UKF)—commonly used for nonlinear state-space models. It highlights their respective methodologies, and briefly discusses their strengths, and limitations in approximating the posterior distributions required in state identification.

We consider a discrete time non-linear SSM with *additive Gaussian* state and observation noise, given by

$$\text{initial state:} \quad z_0 = f(u_0; \theta); \tag{B.1a}$$
$$\text{state equation:} \quad z_t = f(z_{t-1}; \theta) + u_t, \tag{B.1b}$$
$$\text{observation equation:} \quad x_t = g(z_t; \theta) + \epsilon_t, \tag{B.1c}$$

where $\{u_t\}, \{\epsilon_t\}$ are sequences of Gaussian independent and identically distributed random variables of shocks/noises, with

$$\begin{pmatrix} u_t \\ \epsilon_t \end{pmatrix} \overset{iid}{\sim} \mathcal{N}\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} Q & 0 \\ 0 & R \end{pmatrix} \right).$$

For ease of presentation, we further assume that $f, g$ are deterministic *time invariant* multivariate functions of appropriate dimensions.

**Extended Kalman filter.** The key idea underlying this filter is to assume that the posterior distributions appearing in the filtering, prediction and smoothing steps are *approximately Gaussian*, whose means and covariance matrices are obtained by *linearizing* the state and observation functions using first-order Taylor expansions.

Let $J_f(\cdot) := \frac{\partial f}{\partial z}$ and $J_g(\cdot) := \frac{\partial g}{\partial z}$ be the Jacobians. The recursive formulas for the filtering, prediction and smoothing steps are then given by:

- Filtering step:

$$z_{t|t} = z_{t|t-1} + K_t\big(x_t - g(z_{t|t-1})\big),$$
$$P_{t|t} = \big(I - K_t J_g(z_{t|t-1})\big)P_{t|t-1},$$

  where $K_t = P_{t|t-1}J_g^\top(z_{t|t-1})\big[J_g(z_{t|t-1})P_{t|t-1}J_g^\top(z_{t|t-1}) + R\big]^{-1}$.

- Prediction step:

$$z_{t|t-1} = f(z_{t-1|t-1}),$$
$$P_{t|t-1} = J_f(z_{t-1|t-1})P_{t-1|t-1}J_f^\top(z_{t-1|t-1}) + Q.$$

- Smoothing step:

$$z_{t|T} = z_{t|t} + H_t(z_{t+1|T} - z_{t+1|t}),$$
$$P_{t|T} = P_{t|t} + H_t(P_{t+1|T} - P_{t+1|t})H_t^\top,$$

  with $H_t = P_{t|t}J_f^\top(z_{t|t})P_{t+1|t}^{-1}$.

It can be seen that the filtering, smoothing and prediction updates of the EKF for the posited Gaussian additive model, follow closely those for the Kalman filter for the linear Gaussian model. Specifically, the coefficient matrices $A$ and $C$ are replaced by the functions $f$ and $g$, respectively, in the updates of the mean $z_{t|s}$, and by the Jacobian matrices $J_f$ and $J_g$ of the $f$ and $g$ functions evaluated at the corresponding expectation $z_{t|s}$, for the updates of the covariances $P_{t|s}$.

*Remark* 12. The EKF updates presented above use first-order Taylor expansions of the functions $f$ and $g$. Second-order Taylor expansions have also be considered in the literature (Gelb, 1974; Roth and Gustafsson, 2011), although they become computationally expensive for larger size SSMs. Further, iterative EKF schemes (Gelb, 1974; Bell and Cathey, 1993) involve an additional pass after an initial set of latent states estimates, and use the same EKF updates to enhance accuracy.

*Remark* 13. In the case where the error/noise terms do no enter the model in an additive form, analogous EKF updates can be derived for the general nonlinear SSM given in (2.1a)-(2.1c), with Gaussian state and observation error terms. At the high level, key modifications include: (i) in expressions involving the functions $f(z, u)$ and $g(x, \epsilon)$, the noise variables should be set to zero; (ii) the Jacobian matrices $J_f$ and $J_g$ incorporate the error terms and when evaluated, a value of zero is also used for the corresponding error terms.

The main advantage of the EKF over more general SMC methods is its relative simplicity. Linearization is a standard way of constructing approximations to non-linear systems, making EKF easy to apply. Further, when the degree of non-linearity of the SSM is mild, EKF performs well, especially with advanced iterative schemes. However, if the system exhibits strong nonlinearities in the state and observation equations, EKF performance may degrade significantly.

**Gaussian filters.** To accommodate *strong* non-linearities, this family of filters was proposed in Ito and Xiong (2000); Wu et al. (2006). The starting point is once again that the posterior distributions required in the E-step are assumed to be *approximately Gaussian*. Hence, the means $z_{t|t}$ and the covariance matrices $P_{t|t}$ of the approximating Gaussian distributions need to be computed as shown next.

- Prediction step. The key assumption made is that the posterior distribution of the random variable $z_{t-1}|x_{t-1}$ is Gaussian with mean $z_{t-1|t-1}$ and covariance matrix $P_{t-1|t-1}$, i.e., $p_\theta(z_{t-1}|x_{t-1}) = \mathcal{N}(z_{t-1|t-1}, P_{t-1|t-1})$. Using the state equation $z_t = f(z_{t-1}) + u_t$, the *Gaussian approximation* of the predicted density of the state $z_t|x_{1:t-1}$ compute the first two moments as follows:

$$z_{t|t-1} = \mathbb{E}_{p_\theta(z_{t-1}|x_{1:t-1})}(z_t|x_{1:t-1}) = \int_{\mathbb{R}^d} f(z_{t-1})p_\theta(z_{t-1}|x_{1:t-1})\mathrm{d}z_{t-1},$$

$$P_{t|t-1} = \mathrm{Cov}(z_t|x_{1:t-1}) = Q + \int_{\mathbb{R}^d} (f(z_{t-1}) - z_{t-1|t-1})(f(z_{t-1}) - z_{t-1|t-1})^\top p_\theta(z_{t-1}|x_{1:t-1})\mathrm{d}z_{t-1}.$$

- Filtering step. The starting point is to use the *Gaussian approximation* of the predicted density that we obtained from the prediction step; namely, $p_\theta(z_t|x_{t-1}) = \mathcal{N}(z_{t|t-1}, P_{t|t-1})$. Then, combined with the observation equation $x_t = g(z_t) + \epsilon_t$, we can obtain a Gaussian approximation of the distribution of $z_{t|t}$. However, this is computationally challenging (Ito and Xiong, 2000). Instead, an efficient moment-matching based strategy approximates the *joint* conditional distribution of the latent state and the observation $[z_t, x_t]^\top|x_{1:t-1}$ as Gaussian. Subsequently, using a conditioning argument together with the properties of the Gaussian distribution, we can obtain the first two moments of the quantity of interest, namely $z_t|[x_t, x_{1:t-1}] = z_t|x_{1:t}$. Consider the joint conditional distribution of $[z_t, x_t]^\top|x_{1:t-1}$

$$\begin{pmatrix} z_t \\ x_t \end{pmatrix} \Big| x_{1:t-1} \sim \mathcal{N}\left( \begin{pmatrix} z_{t|t-1} \\ \widehat{x}_{t|t-1} \end{pmatrix}, \begin{pmatrix} P_{t|t-1} & \Sigma_{zx,t} \\ \Sigma_{xz,t} & \Sigma_{xx,t} \end{pmatrix} \right).$$

It can be seen that the following quantities need to be computed: (i) the expected value of the observation measurement, denoted by $\widehat{x}_{t|t-1}$; (ii) its covariance matrix, denoted by $\Sigma_{xx,t}$ of $x_t$, and (iii) the cross-covariance of $x_t$ with $z_t$, denoted by $\Sigma_{zx,t}$. Note that the expected value of $z_t|x_{1:t-1}$ has already

been obtained from the prediction step. We then have

$$\widehat{\boldsymbol{x}}_{t|t-1} = \int_{\mathbb{R}^d} g(\boldsymbol{z}_{t-1}) p_\theta(\boldsymbol{z}_t|\boldsymbol{\varkappa}_{1:t-1}) \mathrm{d}\boldsymbol{z}_t,$$

$$\Sigma_{xx,t} = R + \int_{\mathbb{R}^d} (g(\boldsymbol{z}_{t-1}) - \widehat{\boldsymbol{x}}_{t|t-1})(g(\boldsymbol{z}_{t-1}) - \widehat{\boldsymbol{x}}_{t|t-1})^\top p_\theta(\boldsymbol{z}_t|\boldsymbol{\varkappa}_{1:t-1}) \mathrm{d}\boldsymbol{z}_t,$$

$$\Sigma_{zx,t} = \int_{\mathbb{R}^d} (\boldsymbol{z}_t - \boldsymbol{z}_{t|t-1})(g(\boldsymbol{z}_{t-1}) - \widehat{\boldsymbol{x}}_{t|t-1})^\top p_\theta(\boldsymbol{z}_t|\boldsymbol{\varkappa}_{1:t-1}) \mathrm{d}\boldsymbol{z}_t.$$

Finally, based on these quantities and the formulas for the conditional expected value and covariance of a multivariate Gaussian distribution, we get the filtering updates:

$$\boldsymbol{z}_{t|t} = \boldsymbol{z}_{t|t-1} + K_t(\boldsymbol{x}_t - \widehat{\boldsymbol{x}}_{t|t-1}),$$
$$P_{t|t} = P_{t|t-1} - K_t \Sigma_{xx,t} K_t^\top,$$

where $K_t = \Sigma_{zx,t} \Sigma_{xx,t}^{-1}$.

- Smoothing step: Analogous derivations to those in the filtering step lead to the following recursive updates (Sarkka and Hartikainen, 2010)

$$\boldsymbol{z}_{t|T} = \boldsymbol{z}_{t|t-1} + H_t(\boldsymbol{z}_{t+1|T} - \boldsymbol{z}_{t+1|t}),$$
$$P_{t|T} = P_{t|t} + H_t(P_{t+1|T} - P_{t+1|t})H_t^\top,$$

where $H_t = L_{t,t+1} P_{t+1|t}^{-1}$, and $L_{t,t+1} = \mathrm{Cov}(\boldsymbol{z}_t - \boldsymbol{z}_{t|t}, f(\boldsymbol{z}_t) - \boldsymbol{z}_{t+1|t})$; the latter is computed based on the Gaussian filtering distribution with mean $\boldsymbol{z}_{t|t}$ and covariance $P_{t|t}$.

A key difference compared to the EKF is that in the filtering step, instead of $g(\boldsymbol{z}_{t|t-1})$ (that appears on the RHS of the filtering update), an *approximation* based on $\widehat{\boldsymbol{x}}_{t|t-1}$ is used, and analogously for the quantities that appear in the Kalman gain matrix $K_t$.

Implementing the Gaussian filter involves calculating five integrals, two during the prediction step and three during the filtering step. These integrals can be computed efficiently with established numerical integration methods like Gauss-Hermite quadrature (Ito and Xiong, 2000) or cubature (Wu et al., 2006), and/or Monte Carlo techniques.

**Unscented Kalman filter.** It is based on the Gaussian filter's moment-matching approach, with a key distinction lying in how the integrals in the prediction and filtering steps are computed. The main idea is to compute the required integrals using a weighted sum of carefully chosen "sigma" points based on the unscented transform (Julier and Uhlmann, 2004), designed to match the mean and covariance of the distribution at time $t-1$. Note that unlike Monte Carlo methods, these sigma points are selected deterministically. In the prediction step, the selected sigma points are transformed based on the function $f$, based on which the mean and covariance of the updated posterior distribution are computed. Analogous steps are used for computing the filtering update (see Julier and Uhlmann, 2004, for more details).

Unlike the EKF, the Gaussian filter and its UKF variant do not require differentiability of the $f$ and $g$ functions, and avoid computing Jacobian matrices. However, both can be computationally more expensive than the EKF, especially for larger scale SSMs. However, empirical evidence suggests that they typically yield better performance, especially for strongly nonlinear systems.

# C   Nonlinear SDE based SSMs

This section provides a brief review regarding SSMs defined by nonlinear SDEs. Given the complexity of such a model, we note that under the classical framework, the system identification problem—that encompasses both state identification and parameter estimation—has not been considered in an "integrated" fashion in the literature. On the other hand, the following two problems: (i) the state identification problem for *fixed*

*and known* model parameters, and (ii) the parameter estimation problem for an observed SDE in the form of $\mathrm{d}\boldsymbol{x}_t = g(\boldsymbol{x}_t)\mathrm{d}t + \mathrm{d}\boldsymbol{w}^x(t)$ (note the absence of a latent state) have been studied in their respective context. Arguably, at the conceptual level, one can perform estimation akin to an EM algorithm, by alternating between the state identification and parameter estimation, with the latter considering an augmented system wherein the latent variables are imputed by the former.

To this end, the remainder of the section provides a brief review of the state identification problem, emphasizing the technical requirements that filters satisfy and also presenting the Kalman filter updates for linear SDE based SSMs. Additionally, it briefly discusses and references the limited literature on the parameter estimation for observed nonlinear SDE-based models.

**The state identification problem.** Let $(\Omega, \mathcal{F}, \{\mathcal{F}_t\}_{t\in\mathbb{R}_+}, \mathbb{P})$ denote a filtered probability space and consider a $(d+p)$ dimensional process $[\boldsymbol{z}_t, \boldsymbol{x}_t]^\top$, adapted to the filtration $\mathcal{F}_t$. The SSM is defined by the following two stochastic differential equations:

$$\text{state equation:} \quad \mathrm{d}\boldsymbol{z}(t) = f(\boldsymbol{z}(t))\mathrm{d}t + \sigma(\boldsymbol{z}(t))\mathrm{d}\boldsymbol{w}^z(t), \tag{C.1a}$$

$$\text{observation equation:} \quad \mathrm{d}\boldsymbol{x}(t) = g(\boldsymbol{z}(t))\mathrm{d}t + \mathrm{d}\boldsymbol{w}^x(t), \tag{C.1b}$$

where $f(\cdot) : \mathbb{R}^d \to \mathbb{R}^d$, $\sigma(\cdot) : \mathbb{R}^d \to \mathbb{R}^d$, and $g(\cdot) : \mathbb{R}^d \to \mathbb{R}^p$ are $\mathcal{F}$-measurable functions and $\boldsymbol{w}^z, \boldsymbol{w}^x$ independent $\mathbb{R}^d$ and $\mathbb{R}^p$-valued standard Wiener processes, respectively. In addition, the initial value of the latent state $\boldsymbol{z}_0$ is a random variable drawn from a distribution which is independent of the Wiener processes $\boldsymbol{w}^z$ and $\boldsymbol{w}^x$. Further, it is assumed that $f, \sigma$ are globally Lipschitz functions and $g$ satisfies the linear growth condition $\|g(x)\|_2^2 = c(1 + \|x\|_2^2)$ for some constant $c > 0$. The former condition ensures pathwise uniqueness of the solution, while the latter ensures that the solution of (C.1b) does not explode in finite time almost surely (Ikeda and Watanabe, 2014).

The state estimation (filtering) problem (for given $f, \sigma, g$) is then defined by determining the probability distribution of the state $\boldsymbol{z}(t)$ conditional on the filtration generated by observations $\varkappa_{0:t} := \{\boldsymbol{x}(\tau), \tau \in [0, t]\}$. Concretely, the goal is to calculate the probability kernel

$$\pi_{t|s}(\mathrm{d}z, \varkappa_{0:s}) := \mathbb{P}(\boldsymbol{z}(t) \in \mathrm{d}z \mid \varkappa_{0:s}).$$

Recall from Section 2.1 that the state estimation problem comprises of the following three tasks: learning $\pi_{t|s}(\mathrm{d}z, \varkappa_{0:s})$ for (i) $s = t$ (*filtering* problem), (ii) $s > t$ (*smoothing* problem) and (iii) $s < t$ (*prediction* problem) (Bain and Crisan, 2009). For the filtering problem, the kernel $\pi_{t|t}$ satisfies the Kushner-Stratonovich stochastic differential equation (SDE).

Specifically, for a bounded twice differentiable function $h : \mathbb{R}^d \to \mathbb{R}$, let $\mathfrak{V}_t h$ denote the infinitesimal generator of the process $\boldsymbol{z}$, given by

$$\mathfrak{V}_t h := \sum_{i=1}^d f_i(\boldsymbol{z})\frac{\partial h(\boldsymbol{z})}{\partial \boldsymbol{z}_i} + \frac{1}{2} \sum_{i,j=1}^d \sigma_{i,j}(\boldsymbol{z})\frac{\partial^2 h(\boldsymbol{z})}{\partial \boldsymbol{z}_i \partial \boldsymbol{z}_j}.$$

The Kushner-Stratonovich *nonlinear* SDE for $h$ is then given by

$$\mathrm{d}\pi_{t|t}(h, \varkappa_{0:t}) = \pi_{t|t}(\mathfrak{V}_t h, \varkappa_{0:t}) + \left[\pi_{t|t}(hg, \varkappa_{0:t}) - \pi_{t|t}(hg, \varkappa_{0:t})\pi_{t|t}(h, \varkappa_{0:t})\right]\left(\mathrm{d}\boldsymbol{x}(t) - \pi_{t|t}(h, \varkappa_{0:t})\right), \tag{C.2}$$

where $hg$ is short-hand for $h(\boldsymbol{z})g(\boldsymbol{z}) := \sum_{j=1}^p h(\boldsymbol{z})g_j(\boldsymbol{z})$, with $g_j : \mathbb{R}^d \to \mathbb{R}$ and the product computed in a coordinate-wise manner. The expression in the last parenthesis can be interpreted as an *innovation* term, namely the difference between the observed signal $\boldsymbol{x}_t$ and its expected value. The Kushner-Stratonovich SDE is a nonlinear one, which in general poses significant challenges in solving it. To that end, an unnormalized version of $\pi_{t|t}(\cdot)$ has been considered that gives rise to a *linear* SDE, which is typically easier to solve. Define for the function $h$ the kernel $q_{t|t}(h, \varkappa_{0:s}) := \mathbb{E}_{\mathbb{Q}}(h(\boldsymbol{z}_t)|\varkappa_{0:t})$, such that under the measure $\mathbb{Q}$ (obtained by Girsanov's theorem from the original measure $\mathbb{P}$, and using the Kallianpur-Streibel formula), its expectation is finite. It can be shown that $\pi_{t|t}(h, \varkappa_{0:t}) = q_{t|t}(h, \varkappa_{0:t})/q_{t|t}(\mathbf{1}, \varkappa_{0:t})$ where $\mathbf{1}$ denotes the constant function $h(\boldsymbol{z}) = 1$. Then, the Zakai SDE for the function $h$ is given by

$$\mathrm{d}q_{t|t}(h, \varkappa_{0:t}) = q_{t|t}(\mathfrak{V}_t h, \varkappa_{0:t})\mathrm{d}t + q_{t|t}(hg, \varkappa_{0:t})\mathrm{d}\boldsymbol{x}_t.$$

The counterparts of the Kushner-Stratonovich and Zakai SDEs for the prediction and the smoothing tasks are more involved and provided in Pardoux (1981); Steinberg et al. (1994). Further, the smoothing task is more technically involved, since it requires the introduction of backward stochastic integration.

The characterization of the solutions and their uniqueness of the Kushner-Stratonovich and Zakai equations has been the topic of theoretical investigation (Rozovskii, 1991; Bain and Crisan, 2009), since it is of central importance for their solution by numerical methods. Note that in general $\pi_{t|t}(\cdot, \varkappa_{0:s})$ (the solution to (C.2)) is an *infinite dimensional* process (LeGland, 2005; Ocone and Pardoux, 2006). The most notable exception is the Kalman-Bucy filter (Kalman and Bucy, 1961) used for the state identification problem of an SSM whose specification is given by a *linear SDE*.

**SSMs based on Linear SDEs and the Kalman-Bucy filter.** In this case, (C.1a)-(C.1b) become

$$\text{state equation:} \quad \mathrm{d}\boldsymbol{z}(t) = A\boldsymbol{z}(t)\mathrm{d}t + Q\mathrm{d}\boldsymbol{w}^z(t) \tag{C.3a}$$

$$\text{observation equation:} \quad \mathrm{d}\boldsymbol{x}(t) = C\boldsymbol{z}(t)\mathrm{d}t + \mathrm{d}\boldsymbol{w}^x(t), \tag{C.3b}$$

with matrix coefficients $A, Q \in \mathbb{R}^{d \times d}$, and $C \in \mathbb{R}^{d \times p}$.

The conditional distribution $\pi_{t|t}(\cdot, \varkappa_{0:s})$ of the latent state $\boldsymbol{z}_t$ given an observed trajectory, corresponds to a multivariate (finite dimensional) Gaussian distribution, characterized by its first and second moments alone. Specifically, for coordinate $j = 1, \cdots, d$ of the state $\boldsymbol{z}(t)$, define its conditional mean as $\boldsymbol{z}_{t|s}^j := \mathbb{E}(\boldsymbol{z}^j(t)|\varkappa_{0:s})$ and its conditional covariance matrix by $P_{t|s}^{jk} := \mathbb{E}(\boldsymbol{z}^j(t)\boldsymbol{z}^k(t)|\varkappa_{0:s}) - \boldsymbol{z}_{t|s}^j \boldsymbol{z}_{t|s}^k$. The $d$-dimensional vector $\boldsymbol{z}_{t|t}$ then satisfies the following SDE

$$\mathrm{d}\boldsymbol{z}_{t|t} = A\boldsymbol{z}_{t|t}\mathrm{d}t + K_t\big(\mathrm{d}\boldsymbol{x}(t) - C\boldsymbol{z}_{t|t}\mathrm{d}t\big),$$

and the $d \times d$ matrix $P_{t|t}$ satisfies the *deterministic* matrix Ricatti equation (ODE)

$$\mathrm{d}P_{t|t} = QQ^\top \mathrm{d}t + A\boldsymbol{z}_{t|t}\mathrm{d}t + AP_{t|t}\mathrm{d}t + P_{t|t}A^\top \mathrm{d}t - P_{t|t}C^\top C P_{t|t}\mathrm{d}t,$$

with $K_t = P_{t|t}C^\top$ being the Kalman gain matrix. Of note, the SDE for the conditional mean and the ODE for the conditional variance are also satisfied for linear SSMs with time-varying coefficient matrices $A_t, C_t, R_t$ (recall that these parameters are assumed to be known in the context of state identification).

**Model parameter estimation for observed diffusion processes.** The starting point is that, for sufficiently small time increments $\Delta t$ and under certain regularity conditions (Kloeden and Platen, 1992), the distribution of the increment $\boldsymbol{x}(t + \Delta t) - \boldsymbol{x}(t)$ is *approximately* Gaussian, whose mean and variance are determined by the Euler-Maruyama approximation (Maruyama, 1955) (an extension of the Euler method for ordinary differential equations)

$$\boldsymbol{x}(t + \Delta t) \approx \boldsymbol{x}(t) + g_\theta(\boldsymbol{x}(t))\Delta t + \sqrt{\Delta t}\, \boldsymbol{\epsilon}_t,$$

with $\boldsymbol{\epsilon}_t \sim \mathcal{N}(0, I)$; $g_\theta(\cdot)$ is a function parameterized by $\theta \in \mathbb{R}^m$. Assuming that the continuous process is observed *without error* at discrete times $0 = t_0 < t_1 < \cdots < t_n$, it gives rise to an *observed trajectory* of the underlying process $\{\boldsymbol{x}_{t_i}\}_{i=0}^n$. The log-likelihood of the parameter $\theta$ given the data is given by

$$L(\theta; \{\boldsymbol{x}_{t_i}\}_{i=0}^n) = \sum\nolimits_{i=0}^n \ell_i(\theta), \quad \ell_i := \log\big(\mathcal{K}_{\Delta t_i}(\boldsymbol{x}_{t_i}, \boldsymbol{x}_{t_i-1}; \theta)\big),$$

wherein $\mathcal{K}_{\Delta t_i}(\cdot, \cdot; \theta)$ denotes the transition kernel for two consecutive observations. Note that $\mathcal{K}_{\Delta t_i}$ corresponds to the discrete time analogue for the observation process of the $\pi_{t|s}$ kernel for the state process discussed in the context of the state identification problem.

However, in almost all cases, this transition kernel and thus its log-likelihood are analytically intractable. Hence, obtaining the maximum likelihood estimate of $\theta$ is particularly challenging, even though its theoretical properties under ergodicity assumptions are well established (Gobet, 2002). A number of directions for computing estimates of $\theta$ have been investigated in the literature. One direction focuses on the method of moments, or solving estimating equations (Gourieroux et al., 1993; Gallant and Long, 1997). Another direction considers closed form asymptotic expansions to the transition kernels $\mathcal{K}_{\Delta t_i}$ (Aït-Sahalia, 2004;

Chang and Chen, 2011). A third direction aims to augment the observed trajectories through imputation at additional time points, so that a satisfactory complete-data approximation of the likelihood function can be written down and subsequently use Markov Chain Monte Carlo methods to impute the additional data and also obtain samples from the posterior distribution of the parameter $\theta$ (Elerian et al., 2001; Eraker, 2001; Roberts and Stramer, 2001). Additional details on these three broad directions are available in the review paper by Sørensen (2004). Another line of work leverages Monte Carlo techniques for exact simulation of sample paths from the diffusion model (Beskos and Roberts, 2005) and then obtain a Monte Carlo estimate of $\theta$ (Beskos et al., 2006; Blanchet and Zhang, 2020; Craigmile et al., 2023).