

REVIEW

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A guide to state–space modeling of ecological time series

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Abstract. State–space models (SSMs) are an important modeling framework for analyzing ecological time series. These hierarchical models are commonly used to model population dynamics, animal movement, and capture–recapture data, and are now increasingly being used to model other ecological processes. SSMs are popular because they are flexible and they model the natural variation in ecological processes separately from observation error. Their flexibility allows ecologists to model continuous, count, binary, and categorical data with linear or nonlinear processes that evolve in discrete or continuous time. Modeling the two sources of stochasticity separately allows researchers to differentiate between biological variation and imprecision in the sampling methodology, and generally provides better estimates of the ecological quantities of interest than if only one source of stochasticity is directly modeled. Since the introduction of SSMs, a broad range of fitting procedures have been proposed. However, the variety and complexity of these procedures can limit the ability of ecologists to formulate and fit their own SSMs. We provide the knowledge for ecologists to create SSMs that are robust to common, and often hidden, estimation problems, and the model selection and validation tools that can help them assess how well their models fit their data. We present a review of SSMs that will provide a strong foundation to ecologists interested in learning about SSMs, introduce new tools to veteran SSM users, and highlight promising research directions for statisticians interested in ecological applications. The review is accompanied by an in-depth tutorial that demonstrates how SSMs can be fitted and validated in R. Together, the review and tutorial present an introduction to SSMs that will help ecologists to formulate, fit, and validate their models.

Key words: Bayesian; diagnostic; fitting procedure; frequentist; model selection; state–space model; time series.

INTRODUCTION

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State–space models (SSMs) are a popular modeling framework for analyzing ecological time-series data. They are commonly used to model population dynamics

(Newman et al. 2014), including metapopulation dynamics (Ward et al. 2010), they have a long history in fisheries stock assessment (Aeberhard et al. 2018), and have been recently proposed as a means of analyzing sparse biodiversity data (Kindsvater et al. 2018). Moreover, they have been a favored approach in movement ecology for more than a decade (Patterson et al. 2008), and are increasingly used with biologging data (Jonsen et al. 2013). In addition, the flexibility of SSMs is advantageous when modeling complex capture–recapture data (King 2012). SSMs are also used in epidemiology (Dukic et al. 2012, Fasiolo et al. 2016) and disease ecology (Hobbs et al. 2015). These common uses of SSMs, and their many unique applications (e.g., investigating animal health from photographs [Schick et al. 2013], plant invasion [Damgaard et al. 2011], and host–parasitoid dynamics [Karban and de Valpine 2010]), demonstrate their widespread importance in ecology.

State–space models are popular for time series, in part because they directly model temporal autocorrelation in a way that helps differentiate process variation from observation error. SSMs are a type of hierarchical model (see Table 1 for definitions; Cressie et al. 2009) and their hierarchical structure accommodates the modeling of

two time series: (1) a state, or process, time series that is unobserved and attempts to reflect the true, but hidden, state of nature; and (2) an observation time series that consists of observations of, or measurements related to, the state time series. For example, actual fish population size over time would be the state time series, and incomplete and imprecise counts of fish sampled in a survey, or caught in a fishery, would be the observation time series. Process variation represents the stochastic processes that change the population size of a fish stock through time (e.g., the birth and death processes), and observation error reflects differences between the hidden state and the observed data due to randomness or imprecision in the sampling or survey methodology. These two stochastic components act at different levels of the model hierarchy, and the SSM framework allows them to be modeled separately. The assumptions that the hidden states are autocorrelated (e.g., that a large population in year t will likely lead to a large population in year $t + 1$), and that observations are independent once we account for their dependence on the states (Fig. 1a), allow SSMs to separate these two levels of stochasticity. When we fit a SSM to time series, we can often estimate the process and observation parameters, as well as the hidden states.

TABLE 1. Our definitions of important terms in the context of SSMs.

Term	Definition
Conditional likelihood (L_c)	Likelihood function of the parameters of the SSM conditional on the states. In contrast to the joint and marginal likelihoods, the function only includes the probability distribution of the observations (not that of the states) and use sufficient statistics for the state values (e.g., states are fixed to their estimated values)
Data stream	Distinct set of observations. The term is generally used when more than one source of data is used in a single model (e.g., a SSM that jointly models data from systematic survey and citizen science)
Hidden Markov model (HMM)	Class of SSMs with a finite number of discrete hidden states. For example, these discrete states could be categorical variables representing the behavioral modes of an animal (e.g., foraging, resting, traveling) or binary variables representing whether the individual is alive or dead
Hierarchical model	Class of statistical models that has multiple levels of stochasticity. They model randomness in the data and in the process. Linear mixed effects models (i.e., linear models with fixed and random effects) are a commonly used type of hierarchical model in ecology. SSMs are another type of hierarchical model
Joint likelihood (L_j)	Likelihood function of both hidden states and parameters, which summarizes the complete SSM. Although it is common to call this function a likelihood, this term can cause confusion because states, but not parameters, are often viewed as random variables and often cannot be jointly estimated with parameters by maximizing this function
Marginal likelihood (L_m)	Likelihood function of the parameters of the SSM, where the states have been marginalized (i.e., integrated out or summed over all possible state values)
Observation equation	Equation from a SSM that models how observations depend on hidden states. Synonymous, or closely related, terms used in the literature include observation model, and measurement equation or model
Observation error	Variation associated with the discrepancy between hidden states and observations. The observation error will often reflect the imprecision of the sampling methodology
Process equation	Equation from a SSM that models how unobserved states at a given time depend on past states. Synonymous, or closely related, terms used in the literature include: process model, state equation, state model, and transition equation
Process variation	Variation associated with the underlying process and hidden states. In ecology, process variation often represents biological variability
State	Unobserved random variable that generally represents a true attribute of the system. A SSM has at least one time series of hidden states (e.g., true population size through time or whether the individual is alive or dead during each sampling period). Synonymous, or closely related, terms used in the literature include: latent state and latent variable
State–space model (SSM)	Class of hierarchical models for time series that specifies the dynamic of the hidden states and their link to the observations (see Fig. 1a)

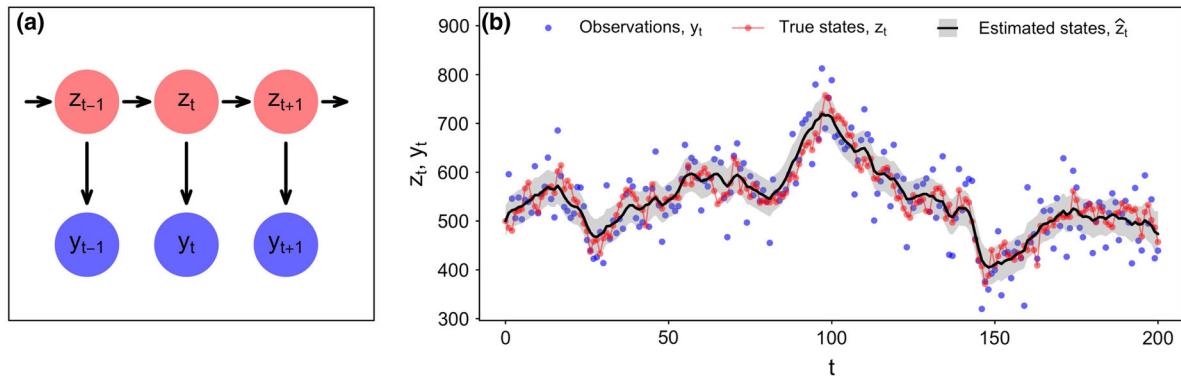


FIG. 1. The dependence structure and evolution of the two time series comprising a simple univariate state–space model. (a) Dependence relationships with arrows, demonstrating that once the dependence of the observations y_t on the states z_t is accounted for, the observations are assumed independent. (b) Our toy model (Eqs. 1, 2). The blue and red dots are the simulated observations and states, respectively. The black line and gray band are the estimated states and associated 95% confidence intervals. The true states, but not the observations, usually fall in the 95% confidence intervals. This demonstrates that the state estimates can be a closer approximation of the truth than the observations.

These estimates of the hidden states generally reflect the true state of nature better than the original observations (Fig. 1 b). For example, the estimates of the hidden states will generally reflect the true fish population size better than the survey- or fisheries-based counts.

The first SSMs, often referred as normal dynamic linear models (NDLMs), were a special case where the state and the observation time series were modeled with linear equations and normal distributions. Two seminal papers on NDLMs, Kalman (1960) and Kalman and Bucy (1961), provided an algorithmic procedure, the now-famous Kalman filter, for making inferences about the hidden states given imperfect observations and known parameters. These papers led to developments that revolutionized aerospace engineering in the 1960s and allowed the Apollo mission to correct the trajectory of a spacecraft going to the moon, given inaccurate observations of its location through time (Grewal and Mohinder 2010). The earliest applications of SSMs to ecological data, which used NDLMs and the Kalman filter, were in the 1980–90s and focused primarily on fisheries (Mendelsohn 1988, Sullivan 1992) and animal movement (Anderson-Sprecher and Ledolter 1991). The first animal movement SSMs were closely analogous to the original aerospace application in that they recreated the trajectory of an animal based on inaccurate observations. However, these ecological models required parameters to be estimated. Unlike a planned mission to the moon, we rarely have *a priori* knowledge of the intended speed and direction of an animal. Developments in the time-series literature made use of the Kalman filter to evaluate the likelihood function for unknown parameters, thus allowing calculation of maximum-likelihood parameter estimates in addition to state estimates (Harvey 1990). NDLMs, however, are a restricted class of SSMs and their applicability to many ecological time series, which have nonlinear and non-Gaussian structure, is limited.

Since their initial development, there have been important advancements in SSMs, and in their application in ecology. In the 1990s, the simultaneous popularization of Markov chain Monte Carlo methods (MCMC [Gilks et al. 1995]), including the freely available BUGS software (Lunn et al. 2009), and high-speed desktop computing considerably expanded the diversity of possible SSMs to include non-Gaussian and nonlinear formulations (e.g., Meyer and Millar [1999]). As a result, Bayesian ecological SSMs were developed for a variety of applications in the following decades, including capture–recapture models (e.g., Dupuis [1995], Gimenez et al. [2007], Royle [2008]) and formulations structured around matrix population models (Buckland et al. 2004). Further developments have advanced fitting procedures in both Bayesian and frequentist frameworks (de Valpine 2004, Ionides et al. 2015, Kristensen et al. 2016, Monnahan et al. 2017). These methods provide the means to fit increasingly complex SSMs with multiple hierarchical levels (e.g., Jonsen et al. [2005]) and integrate disparate data sets (e.g., Hobbs et al. [2015]).

However, although advancements in fitting SSMs have changed how we model time series in ecology, the computational burden required to fit some of these models is often high enough that comparisons between multiple SSMs can be difficult, and the complex structure of some SSMs complicates model validation and diagnostics. In the ecological literature, there has been a recent interest in model comparison and validation for hierarchical models or models for data sets with complex dependence structure (Hooten and Hobbs 2015, Roberts et al. 2017, Conn et al. 2018). In line with this, new validation tools for SSMs are being developed (Thygesen et al. 2017).

Although SSMs are powerful tools for modeling ecological time series, the fitting procedures may seem prohibitively complex to many practitioners. The

variety of inference procedures and tools that can be used to fit SSMs (Harvey 1990, Doucet et al. 2001, Durbin and Koopman 2012, Ionides et al. 2015, Kristensen et al. 2016) may bewilder all but the most quantitative ecologists, thus limiting the ability of many researchers to formulate, fit, and evaluate their own SSMs. Although there are some popular application-specific R (R Development Core Team 2019) packages with functions to fit specialized SSMs (e.g., MARSS for multivariate NDLMs [Holmes et al. 2012]; bsam, for animal movement [Jonsen et al. 2005]), few ecologists are aware of the full range of SSMs that can be fitted with such packages. In addition, these packages may be inadequate for the data-at-hand, especially when using SSMs to answer novel questions or with new data types. A further complication with the application of SSMs is the potential for estimability issues where some states or parameters cannot be estimated well, or at all, given the available data (Dennis et al. 2006, Knape 2008, Auger-Méthé et al. 2016). For example, such estimability issues may arise because the formulation of a SSM is too complex for the data (e.g., the time resolution of the process model is too fine relative to the time resolution of the observations). Although there has been some effort to provide a general, and easy-to-use, set of tools for ecologists to fit SSMs to their data (e.g., King et al. 2016, de Valpine et al. 2017), the available tools and array of choices may be overwhelming to those with little familiarity with SSMs. Given these challenges and the recent advancements in inference methods and model diagnostics, we believe the time is ripe to provide a review of these developments for scientists wanting to fit SSMs to ecological time series.

In this review, we first demonstrate the flexibility of SSMs through a set of examples (*Examples of Ecological SSMs*) and discuss how ecologists should consider SSMs as a default modeling technique for many of their time series (*SSMs as a Framework for Ecological Time Series*). Next, we review the different inference methods that can be used to fit a SSM to data (*Fitting SSMs*). We then discuss how one can assess whether a SSM suffers from estimability or identifiability issues (*Formulating an Appropriate SSM for Your Data*). Lastly, we describe model selection procedures (*Computationally Efficient Model Comparison Methods*) and diagnostic tools that can be used to verify whether a model is adequate (*Diagnostics and Model Validation for SSMs*), crucial steps that are often ignored. This review is accompanied by an in-depth tutorial that provides examples of how one can use R (R Development Core Team 2019) to fit, and validate, SSMs with various inference methods. We believe this review will give a strong foundation to ecologists interested in learning about SSMs and hope it will provide new tools to veteran SSM users interested in inference methods and model validation techniques.

EXAMPLES OF ECOLOGICAL SSMs

State–space models are flexible hierarchical models for time series, where observations are imperfect measures of temporally evolving hidden states. Through examples, we demonstrate that SSMs can model univariate or multivariate observations, as well as biological processes that evolve in discrete or continuous time steps. We also show that SSMs can be linear or nonlinear, and can use a variety of statistical distributions (e.g., normal, Poisson, multinomial). To show the structural flexibility of SSMs, we chose many examples from population and movement ecology, two fields that have been crucial in the development of these models. However, SSMs can be used to model time series from all branches of ecology.

A toy example: normal dynamic linear model

To formalize the description of SSMs, we start by describing a simple toy example. It models a time series of univariate observations, denoted y_t , made at discrete and evenly spaced points in time t ($t = 1, 2, \dots, T$). The time series of states, denoted z_t , is defined at the same time points t as the observations. Our model is a simple normal dynamic linear model (NDLM); thus process variance and observation error are modeled with Gaussian distributions and both time series are modeled with linear equations.

State–space models make two main assumptions. First, SSMs assume that the state time series evolves as a Markov process (Aeberhard et al. 2018). This Markov process, which is generally of first order, is a relatively simple way to incorporate temporal dependence. For our toy model, this means that the state at time t , z_t , depends only on the state at the previous time step, z_{t-1} . Second, SSMs assume that the observations are independent of one another once we account for their dependence on the states. More formally, we say that, given the corresponding state z_t , each observation y_t is conditionally independent of all other observations, y_s , $s \neq t$. Thus, any dependence between observations is the result of the dependence between hidden states (Aeberhard et al. 2018). For our toy model, this means that y_t is independent of y_{t-1} , and all other observations, once we account for the dependence of y_t on z_t (Fig. 1a). In a population dynamics context, this could be interpreted to mean that the values of observations are autocorrelated because the process driving them (i.e., the true population size of the animal) is autocorrelated through time. In contrast, the discrepancy between the true population size and the observation is not correlated in time. We can see this structure in the equations for our toy SSM:

$$z_t = \beta z_{t-1} + \varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}\left(0, \sigma_\varepsilon^2\right), \quad (1)$$

$$y_t = \alpha z_t + \eta_t, \quad \eta_t \sim \mathcal{N}\left(0, \sigma_\eta^2\right). \quad (2)$$

The autocorrelation in the states is captured by the parameter β . The observations are a function of the

states only and the parameter α allows the observation at time t to be a biased estimate of the state at time t . The process variation (ε_t) and observation error (η_t) are both modeled with normal distributions but have different standard deviations (σ_p^2 and σ_o^2). We have not defined the state at time 0, z_0 , and many authors will provide an additional equation, often referred as the initialization equation, which describes the probability of different values of z_0 (e.g., $z_0 \sim N(0, \sigma_{z_0}^2)$). For our toy example, we view z_0 as a fixed and unknown parameter.

The terminology used to refer to the process and observation equations varies in the literature. A process equation can be referred as a process model, state equation, state model, or transition equation. An observation equation can be referred as an observation model, measurement equation, or measurement model. In this paper, we generally use the terms “process equation” and “observation equation,” respectively, and we often describe SSMs with equations that combine a deterministic function with a stochastic component (e.g., Eqs. 1, 2).

To reveal the dependence structure further and understand how to fit SSMs to data, it can help to characterize a SSM in terms of probability distributions for the states and the observations, for example,

$$f(z_t|z_{t-1}, \boldsymbol{\theta}_p), \quad t = 1, \dots, T, \quad (3)$$

$$g(y_t|z_t, \boldsymbol{\theta}_o), \quad t = 1, \dots, T. \quad (4)$$

In the case of our toy model, f and g are two normal probability density functions, and $\boldsymbol{\theta}_p$ and $\boldsymbol{\theta}_o$ are vectors of parameters associated with each equation (i.e., $\boldsymbol{\theta}_p = (\beta, \sigma_p^2)$, $\boldsymbol{\theta}_o = (\alpha, \sigma_o^2)$). Eq. 3 describes the autocorrelation in state values as a first-order Markov process, and Eq. 4 describes how observations depend simply on the states. This definition also demonstrates that states are random variables and thus that SSMs are a type of hierarchical model.

One of the goals of fitting a SSM to data is typically to estimate unknown parameters. Here, to contrast them with the states, we refer to these as the fixed parameters and denote them together as $\boldsymbol{\theta}$. For example, here $\boldsymbol{\theta} = (\boldsymbol{\theta}_p, \boldsymbol{\theta}_o, z_0)$, thus α , β , σ_p^2 , σ_o^2 , z_0 in Eqs. 1, 2. A second important goal is to estimate the unobserved states, $\mathbf{z}_{1:T} = (z_1, z_2, \dots, z_T)$, where T is the length of the time series. The notation $1:t$, which we use throughout, refers to the sequence 1, 2, \dots , t . Fig. 1b shows how close estimates of the states ($\hat{\mathbf{z}}_{1:T}$) can be to their true values.

State-space models can be fitted using frequentist or Bayesian approaches to statistical inference. When using a Bayesian approach, a third level is added to the model hierarchy: the prior distribution(s) for the fixed parameters denoted by the probability density function, $\pi(\boldsymbol{\theta}|\boldsymbol{\lambda})$, where $\boldsymbol{\lambda}$ are known values called hyperparameters. Although we refer to $\boldsymbol{\theta}$ as fixed parameters to differentiate them from the states, in Bayesian inference $\boldsymbol{\theta}$ is a

vector of random variables. In *Fitting SSMs* and Appendix S2, we discuss how we can use these probabilistic descriptions of the model for inference.

This simple linear and normal model is a toy example that we will use throughout to explain the concepts associated with fitting and validating SSMs. We will also use this model in Appendix S1 to demonstrate how to use R to fit a SSM to data. Although the simplicity of this toy example makes it a helpful teaching tool, it is not a particularly useful model for ecology. We now turn to the description of a set of ecological SSMs.

Handling nonlinearity

We use a set of simple univariate SSMs for population dynamics to demonstrate that even simple ecological models can rarely be blindly modeled as NDLMs. Jamieson and Brooks (2004) applied multiple SSMs to abundance estimates from North American ducks obtained through annual aerial counts. We start with one of their simplest models, for which the process equation is the stochastic logistic model of Dennis and Taper (1994). This model allows for density dependence, that is, a change in growth rate dependent on the abundance in the previous year:

$$z_t = z_{t-1} \exp(\beta_0 + \beta_1 z_{t-1} + \varepsilon_t), \quad \varepsilon_t \sim N(0, \sigma_p^2). \quad (5)$$

As in the toy example above, z_t denotes the true hidden state, in this case the number of ducks in year t . The parameter $\beta_0 > 0$ determines the median rate of population growth when population size is 0. The parameter $\beta_1 \leq 0$ determines how much the growth rate decreases with an increase in population size, with $\beta_1 = 0$ indicating no density dependence. The process variation, ε_t , is normally distributed and represents the random change in growth rate each year. The observations y_t are modeled as unbiased estimates of the true population size with a normally distributed error:

$$y_t = z_t + \eta_t, \quad \eta_t \sim N(0, \sigma_o^2). \quad (6)$$

Even though the observation equation is linear with a Gaussian error, the SSM is not a NDLM because of the exponent in the process equation (Eq. 5). Jamieson and Brooks (2004) also modeled the population size on a logarithmic scale, $w_t = \log(z_t)$, which resulted in the following formulation:

$$w_t = w_{t-1} + \beta_0 + \beta_1 \exp(w_{t-1}) + \varepsilon_t, \quad \varepsilon_t \sim N(0, \sigma_p^2), \quad (7)$$

$$y_t = \exp(w_t) + \eta_t, \quad \eta_t \sim N(0, \sigma_o^2). \quad (8)$$

Although such reconfiguration can sometimes linearize the model, in this case the model remains nonlinear. Jamieson and Brooks (2004) use a Bayesian

framework to fit this model; see their original paper for the description of the priors.

The modeling of density dependence has been extensively debated in the literature, and Jamieson and Brooks (2004) also explored an alternative process equation, a stochastic Gompertz model:

$$z_t = z_{t-1} \exp(\beta_0 + \beta_1 \log(z_{t-1}) + \varepsilon_t), \quad \varepsilon_t \sim \mathcal{N}(0, \sigma_p^2), \quad (9)$$

which assumes that the per-unit-abundance growth rate depends on the log abundance, $\log(z_{t-1})$, instead of the abundance, z_{t-1} (Dennis and Taper 1994). Such a model is often linearized as follows:

$$w_t = \beta_0 + (1 + \beta_1)w_{t-1} + \varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}(0, \sigma_p^2), \quad (10)$$

$$g_t = w_t + \eta_t, \quad \eta_t \sim \mathcal{N}(0, \sigma_o^2), \quad (11)$$

where $w_t = \log(z_t)$ and $g_t = \log(y_t)$ are the logarithms of the states and observations, respectively (e.g., Dennis et al. 2006). This linear version of the model is a NDLM that can be fitted with tools such as the Kalman filter (Dennis et al. 2006). This statistical convenience may have contributed to the uptake of the stochastic Gompertz SSM in the literature. However, it may not always be adequate to assume that the growth rate depends logarithmically on population density (Dennis and Taper 1994).

Many papers have extended these models to incorporate external covariates (e.g., Viljugrein et al. 2005, Sæther et al. 2008, Lindén and Knape 2009). For example, one could account for the influence of fluctuating availability of wetlands on the population size of ducks by including the number of ponds in year t , p_t , as a covariate in the process equation and modifying the Gompertz stochastic model as follows:

$$w_t = \beta_0 + (1 + \beta_1)w_{t-1} + \beta_2 p_t + \varepsilon_t, \quad \varepsilon_t \sim \mathcal{N}(0, \sigma_p^2). \quad (12)$$

This set of examples shows how easy it is to adapt and extend models in the SSM framework. Although even simple ecological models may only be linear with transformations and assumptions, Jamieson and Brooks (2004), Viljugrein et al. (2005), and Lindén and Knape (2009) showed that accounting for observation error improved the inference regardless of the process equation. For example, Viljugrein et al. (2005) demonstrated that using a SSM, rather than a model that ignores observation error, decreased the size of the bias in the estimates of density dependence. This decreased bias, and a better quantification of uncertainty, reduced the cases where one would erroneously conclude the presence of density dependence.

Joining multiple data streams

Integrating multiple sources of data, often referred as data streams, into a single model can offset their

individual limitations and reveal more complex ecological relationships (McClintock et al. 2017). To showcase how SSMs can extract the information provided by multiple data streams, we present a simplified version of a state-space stock assessment model described by Nielsen and Berg (2014). SSMs are often used in fisheries stock assessments (Aeberhard et al. 2018), where the first data stream, $C_{a,t}$, represents how many fish from each age class a are caught in the commercial fishery in each year t , and the second data stream, $I_{a,t,s}$, includes age-specific indices from distinct scientific surveys, s , which can occur in different years and only capture some portion of the age classes.

The hidden state in each year t is a vector combining the log-transformed stock sizes, $N_{a,t}$, and fishing mortality rates, $F_{a,t}$, for each age class: $\mathbf{z}_t = (\log N_{1,t}, \dots, \log N_{A,t}, \log F_{1,t}, \dots, \log F_{A,t})'$, where A represents the oldest age class. Just as for the toy example, the process equations describe the state in year t as a function of the state in year $t - 1$. However, unlike the toy model, we no longer have a single process equation. We have instead a set of equations describing recruitment, survival, and mortality:

$$\log(N_{1,t}) = \log(N_{1,t-1}) + \varepsilon_{N_{1,t}}, \quad (13)$$

$$\log(N_{a,t}) = \log(N_{a-1,t-1}) - F_{a-1,t-1} - M_{a-1,t-1} + \varepsilon_{N_{a,t}}, \quad 2 \leq a \leq A, \quad (14)$$

$$\log(F_{a,t}) = \log(F_{a,t-1}) + \varepsilon_{F_{a,t}}, \quad 1 \leq a \leq A, \quad (15)$$

where age and year specific log fishing mortality rates, $\log F_{a,t}$, are considered states that evolve as a random walk through time, but the equivalent natural mortality rate, $\log M_{a,t}$, is assumed known from outside sources. Although the main equation describing the population growth (Eq. 14) is based on demographic processes, the other equations (Eqs. 13, 15) are simply assuming that recruitment and fishing mortality are each correlated across years. The formulation of Eq. 14, and Eqs. 16, 17 below, are based on the well-known Baranov catch equation, which states that a cohort continuously decreases in size through time according to two sources of mortality (i.e., fishing and natural; see Aeberhard et al. [2018] for details). Derived from a continuous-time equation, the Baranov equation maps the surviving cohort size as depending exponentially on fishing and natural mortality rates. Thus, as shown here, the SSM can be modeled by expressing the age-specific stock size and mortality rates on the logarithmic scale.

The process variation for all of these equations are assumed to be Gaussian with zero mean, but they differ in their variance and covariance parameters. For recruitment and survival, the variation is assumed to be uncorrelated, that is, $\varepsilon_{N_{1,t}} \sim \mathcal{N}(0, \sigma_{N_{a=1}}^2)$, and $\varepsilon_{N_{a,t}} \sim \mathcal{N}(0, \sigma_{N_{a>1}}^2)$. However, for fishing mortality, the

yearly variation is assumed to be correlated across age classes (i.e., $\boldsymbol{\varepsilon}_{F_t} = (\varepsilon_{F_{1,t}}, \dots, \varepsilon_{F_{a,t}})' \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_F)$) due to age/size correlations in capture probability. The covariance matrix, $\boldsymbol{\Sigma}_F$, is assumed to have an autoregressive order 1, AR(1), correlation structure (i.e., each element $\Sigma_{a,\bar{a}} = \rho^{|a-\bar{a}|} \sigma_a \sigma_{\bar{a}}$, where ρ is the correlation coefficient and $|a-\bar{a}|$ is the absolute age difference).

The two different sets of data streams (i.e., the observed age-specific log-catches, $\log C_{a,t}$, and the age-specific log-indices from scientific surveys, $\log J_{a,t,s}$) are related to the time series of the unobserved states, \mathbf{z}_t , with the following observation equations:

$$\log C_{a,t} = \log\left(\frac{F_{a,t}}{K_{a,t}}(1 - e^{-K_{a,t}})N_{a,t}\right) + \eta_{a,t,c}, \quad (16)$$

$$\log J_{a,t,s} = \log\left(Q_{a,s}e^{-K_{a,s}\frac{D_s}{365}}N_{a,t}\right) + \eta_{a,t,s}, \quad (17)$$

where $K_{a,t}$ is the total mortality rate of age class a in year t (i.e., $K_{a,t} = M_{a,t} + F_{a,t}$), D_s is the number of days into the year when the survey s is conducted, and each $Q_{a,s}$ is a model parameter describing the catchability coefficient. The observation error terms, $\eta_{a,t,c}$ and $\eta_{a,t,s}$ are assumed to be Gaussian distributed and their variances are designed such that the catch data, and each scientific survey have their own covariance matrix. We can use different covariance structures for each matrix (e.g., independent catches across ages, but each survey index has an AR(1) correlation structure across ages; see Berg and Nielsen [2016] for other examples).

This example depicts how to harness more information from independent data streams. The observation equations (Eqs. 16, 17) account for the differences in how each data stream is related to a common set of states (i.e., stock sizes, $N_{a,t}$). In addition, the potentially more biased data stream (i.e., the fisheries catch data) provides direct information on the other set of states (i.e., fishing mortality rate, $F_{a,t}$), which would otherwise be difficult to estimate. This type of structure provides the opportunity to model more complex ecological mechanisms (e.g., Eqs. 13–15). SSMs that integrate multiple data streams have been used in other fields of ecology, including movement ecology (McClintock et al. 2017) and disease ecology (Hobbs et al. 2015).

Accounting for complex data structure

State-space models are well suited to handle the complex structure of many ecological data sets. For example, the first difference correlated random walk model (DCRW [Jonsen et al. 2005]), one of the earliest SSMs for animal movement, was developed to account for the peculiarities of Argos doppler shift location data (Jonsen et al. 2005). Argos tags are often used to track marine animals because they overcome some of the challenges associated with using conventional GPS units in an

aquatic environment. However, unlike most GPS data sets, Argos locations,

$$\mathbf{y}_i = \begin{bmatrix} y_{i,\text{lon}} \\ y_{i,\text{lat}} \end{bmatrix},$$

have large observation errors (mean error ranging from 0.5 to 36 km [Costa et al. 2010]), including large outliers. In addition, they are collected at irregular time intervals, i (i.e., when the animal is at the surface and the satellites are overhead), and have a quality rating that classifies each location into one of six categories q_i . All of these aspects of the data are incorporated in the simplified version of the DCRW presented below.

Although the observations are taken at irregular time intervals, the process equation models the true locations of the animal at regular time intervals t , $\mathbf{z}_t = \begin{bmatrix} z_{t,\text{lon}} \\ z_{t,\text{lat}} \end{bmatrix}$, for T time steps. The process equation assumes that the animal's location at time t is not only dependent on the previous location, \mathbf{z}_{t-1} , but also on the animal's previous displacement in each coordinate, $\mathbf{z}_{t-1} - \mathbf{z}_{t-2}$:

$$\mathbf{z}_t = \mathbf{z}_{t-1} + \gamma(\mathbf{z}_{t-1} - \mathbf{z}_{t-2}) + \boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}), \quad 1 \leq t \leq T, \quad (18)$$

where

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_{\varepsilon,\text{lon}}^2 & \rho\sigma_{\varepsilon,\text{lon}}\sigma_{\varepsilon,\text{lat}} \\ \rho\sigma_{\varepsilon,\text{lat}}\sigma_{\varepsilon,\text{lon}} & \sigma_{\varepsilon,\text{lat}}^2 \end{bmatrix}. \quad (19)$$

The parameter γ can take values between 0 and 1 (i.e., $0 \leq \gamma \leq 1$), and controls the degree of correlation between steps. Values close to 0 mean that the movement only depends on the previous location. Values close to 1 reflect strong correlation in both latitudinal and longitudinal displacements, and thus mean that the animal has a tendency to move at the same speed and in the same direction as the previous step. The covariance matrix for the process variation, $\boldsymbol{\Sigma}$, allows for covariance between longitude and latitude, but in many instances it is simpler to assume that $\rho = 0$.

The observation equation accounts for various characteristics of the Argos data:

$$\mathbf{y}_i = (1 - j_i)\mathbf{z}_{t-1} + j_i\mathbf{z}_t + \boldsymbol{\eta}_i, \quad \boldsymbol{\eta}_i \sim \mathcal{T}(\boldsymbol{\Psi} \circ \mathbf{S}_i, \mathbf{D}_i), \quad 1 \leq i \leq N, \quad (20)$$

where

$$\boldsymbol{\Psi} = \begin{bmatrix} \Psi_{\text{lon}} \\ \Psi_{\text{lat}} \end{bmatrix}, \quad (21)$$

$$\mathbf{S}_i = \begin{bmatrix} s_{\text{lon},q_i} \\ s_{\text{lat},q_i} \end{bmatrix}, \quad (22)$$

$$\mathbf{D}_i = \begin{bmatrix} df_{\text{lon},q_i} \\ df_{\text{lat},q_i} \end{bmatrix}, \quad (23)$$

and N is the number of observed Argos locations. Because data are taken at irregular time intervals, the

true location of the animal is linearly interpolated to the time of the observation, with j_i representing the proportion of the regular time interval between $t-1$ and t when the observation \mathbf{y}_i was made. Because the data often have outliers, the measurement errors are modeled with t distributions, which have fat tails. Finally, to model the differences in error size between the six quality categories, each category, q_i , is associated with unique bivariate t distributions: $T(\Psi \circ \mathbf{S}_i, \mathbf{D}_i)$. In particular, each category is associated with a unique scale parameter, s_{c,q_i} , and degrees of freedom, df_{c,q_i} , for each coordinate (i.e., $c = \text{lon or lat}$). Instead of estimating these 24 parameters, many researchers fix them to known values derived from field experiments (e.g., Jonsen et al. [2005]). To allow for discrepancies between these fixed values and the ones that may fit the data best, we can add a correction factor for each coordinate, ψ_c . Note that the Hadamard product, \circ , simply states that we perform entrywise multiplication of the correction factors to the scale parameters; that is, $\psi_c s_{c,q_i}$, for $c = (\text{lon}, \text{lat})$. Fig. 2 shows the DCRW fitted to a polar bear track, and Appendix S1: Section S2.3 provides the code to fit the model.

Data sets with unexplained outliers and data points with differing quality ratings are common in ecology, and the flexibility of SSMs allows one to account for these characteristics in the model directly, rather than arbitrarily discarding data.

Accommodating continuous-time processes

So far we have only described SSMs where the hidden state evolves in discrete time steps. However, many biological processes occur in continuous time and modeling them as such can facilitate the use of irregularly timed observations (Dennis and Ponciano 2014, McClintock et al. 2014). Using a simplified version of the movement model of Johnson et al. (2008), we showcase how SSMs can accommodate continuous-time process equations.

The SSM of Johnson et al. (2008) models the movement of an animal with a continuous-time correlated random walk. The process equation is formulated in terms of how changes in velocity v through time affect the location μ of an animal. Although the model describes an animal moving in two dimensions (e.g., latitude and longitude), for simplicity, we assume the velocity processes in each coordinate to be independent and only describe the process for one coordinate. Velocities at time t , denoted $v(t)$, are the first set of states. Change in velocity over time is described using a type of diffusion model called an Ornstein-Uhlenbeck (OU) process. At time $t + \Delta$, velocity is:

$$v(t + \Delta) = e^{-\beta\Delta} v(t) + \zeta(\Delta), \quad \zeta(\Delta) \sim N(0, \sigma_{\text{OU}}^2 (1 - e^{-2\beta\Delta}) / 2\beta), \quad \beta > 0, \quad (24)$$

where β represents how quickly the temporal correlation in velocity tends towards 0, and $\zeta(\Delta)$ is a random perturbation. As both increase, the autocorrelation in velocity

decreases. In addition, as the time difference (Δ) increases, the velocity value at time $t + \Delta$ depends less on the previous velocity value and more on the random perturbation. This assumption is often reasonable, as we expect an animal to continue at the same speed during a short period of time and be more likely to change speed over long time periods.

Although the core of the process model describes changes in velocity, the observations are locations. Thus, we have a second set of states, the locations $\mu(t)$, which are related to velocities as follows:

$$\mu(t + \Delta) = \mu(t) + \int_t^{t+\Delta} v(u) du. \quad (25)$$

Integrating the rate of change, here speed, over the time interval is often key to link continuous-time processes to ecological observations (e.g., to model oxygen concentration; Appling et al. [2018]). Such integration can be difficult to handle, but Johnson et al. (2008) solved Eq. 25 to show that the change in location in time Δ is simply:

$$\mu(t + \Delta) = \mu(t) + v(t) \left(\frac{1 - e^{-\beta\Delta}}{\beta} \right) + \xi(\Delta), \quad \xi(\Delta) \sim N\left(0, \frac{\sigma_{\text{OU}}^2}{\beta^2}\right). \quad (26)$$

Because Δ can take any nonnegative value, we can keep track of the states at any time intervals, thus easily accommodating observations, y_i , collected at irregular-spaced times, t_i . For the state, \mathbf{z}_i , the final process equations in matrix notation form are

$$\mathbf{z}_i = \begin{bmatrix} \mu_i \\ v_i \end{bmatrix} = \begin{bmatrix} 1 & (1 - e^{-\beta\Delta_i})/\beta \\ 0 & e^{-\beta\Delta_i} \end{bmatrix} \begin{bmatrix} \mu_{i-1} \\ v_{i-1} \end{bmatrix} + \boldsymbol{\eta}_i, \quad \boldsymbol{\eta}_i \sim N(\mathbf{0}, \boldsymbol{\Sigma}_p^2), \quad (27)$$

where μ_i and v_i are $\mu(t)$ and $v(t)$ at the time when the i th observation occurred, $\Delta_i = t_i - t_{i-1}$, and the variance-covariance matrix was solved to be

$$\boldsymbol{\Sigma}_p^2 = \begin{bmatrix} \frac{\sigma_{\text{OU}}^2}{\beta^2} & \frac{\sigma_{\text{OU}}^2}{2\beta^2} (1 - e^{-\beta\Delta_i})^2 \\ \frac{\sigma_{\text{OU}}^2}{2\beta^2} (1 - e^{-\beta\Delta_i})^2 & \sigma_{\text{OU}}^2 (1 - e^{-2\beta\Delta_i}) / 2\beta \end{bmatrix}. \quad (28)$$

The observation equation can be chosen as usual, for example, as simply adding normal error to the true location:

$$y_i = \mu_i + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma_o^2). \quad (29)$$

The SSM defined by Eqs. 27–29 is a linear Gaussian SSM and can therefore be fitted with a Kalman filter.

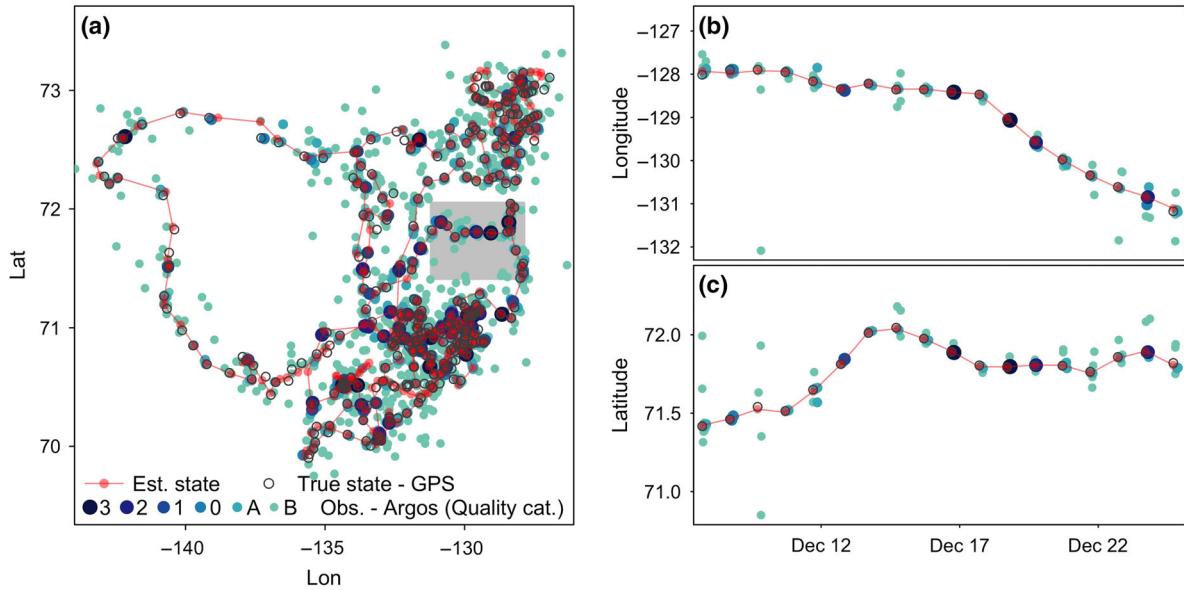


FIG. 2. The difference correlated random walk model (DCRW; Eqs. 18–23) fitted to a polar bear Argos track and validated with GPS data. Panel (a) Maps the observed Argos data with points in shades of blue and green (darker colors representing higher-quality observations), the estimated true locations in red, and the true locations of the bear (GPS data) with open circles. Panels (b) and (c) Show the longitudes and latitudes of a small subset of the time series (indicated by a gray box in the map). These panels highlight the temporal clustering of observations, which likely helped the state estimation procedures.

This model allows various extensions to include different aspects of animal movement. For example, Johnson et al. (2008) show how haul-out behavior of tagged seals can be incorporated using data on how long the tag has been dry (e.g., by making β an increasing function of dry time). To account for the large outliers associated with Argos data one can use a t distribution (see *Accounting for Complex Data Structure*), in which case the Kalman filter will no longer be adequate and other fitting methods will be required (Albertsen et al. 2015). Although continuous-time models can be more complex to understand, they are useful in a variety of contexts where data are collected at unequal time intervals and when ecological processes are intrinsically continuous (e.g., population dynamics [Dennis and Ponciano 2014]).

Integrating count and categorical data streams

The SSM framework provides the flexibility to create joint models that integrate different data types and link biological processes. Here, we use the model of Schick et al. (2013) to demonstrate how count and categorical data can be integrated in a single SSM for the health, monthly movement, and survival of North Atlantic right whales (*Eubalaena glacialis*).

Schick et al. (2013) extracted two types of data from photographic observations of individual whales. The first type, denoted $y_{i,t,k}$, is the number of sightings of individual i in geographic zone k and month t . The second type, denoted $H_{q,i,t}$ is the value for the q th visual health metric for individual i in month t . The six visual health metrics

(e.g., skin condition, entanglement status) are on ordinal scales, each with two or three levels. In addition, ancillary data (e.g., search effort, whale age) are used.

Three process equations model the health, survival, and monthly movement of each individual whale. Whale i in month t is characterized by its age $a_{i,t}$, health status $h_{i,t}$ (defined on an arbitrary, but positive, scale: (0,100)), and location $k_{i,t}$ (one of nine geographic zones). Health status, $h_{i,t}$, is modeled as a function of previous health status and age:

$$h_{i,t} = \beta_0 + \beta_1 h_{i,t-1} + \beta_2 a_{i,t-1} + \beta_3 a_{i,t-1}^2 + \varepsilon_{i,t}, \quad \varepsilon_{i,t} \sim N(0, \sigma^2). \quad (30)$$

When $\beta_2 > 0$ and $\beta_3 < 0$, the quadratic age term allows for the fact that health status, and thus survival probability, initially increases but declines with advanced age. Survival from month t to $t + 1$ is modeled as a Bernoulli process, with survival probability modeled with a logit link function:

$$\text{logit}(s_{i,k,t}) = \alpha_{0,k} + \alpha_1 h_{i,t}. \quad (31)$$

Here, $\alpha_{0,k}$ denotes the fixed effect for zone k and α_1 the relationship with health. Hence, survival probability depends on health and on the occupied zone, allowing researchers to identify the geographic zones associated with reduced survival.

Although a whale is assumed to stay in a single zone during the month, it can move between zones each

month. The monthly location of each individual $z_{i,t}$ is only known when the individual is sighted that month. The subscript t , throughout, represents the number of months since the beginning of the time series. For each month of the year (January, . . . , December), denoted $t^{(u)}$, the movement between zones is modeled with a transition matrix, where each element $m_{j,k,t^{(u)}}$ describes the probability of moving from zone j to zone k (i.e., $m_{j,k,t^{(u)}} = \Pr(z_{i,t^{(u)}+1} = k | z_{i,t^{(u)}} = j)$). As the complete geographic range of the whales is assumed to be covered by these zones, a living whale will be in one of the nine distinct zones at time $t + 1$, $\sum_{k=1}^9 m_{j,k,t^{(u)}} = 1$. The changes in transition probabilities between the months of the year, $t^{(u)}$, allow for the modeling of seasonal migration.

The model has two sets of observation equations. First, the number of sightings of whale i in location k and month t is modeled as a Poisson random variable.

$$y_{i,k,t} \sim \text{Pois}(\lambda_i E_{k,t}), \quad (32)$$

where $E_{k,t}$ denotes the search effort in zone k and month t and λ_i denotes the expected number of sightings of individual i per unit effort. The number of sightings of whale i is only modeled in months where the individual is alive based on state $s_{i,k,t}$ and in the appropriate monthly geographical zones according to state $z_{i,t}$. Second, each visual health metric is modeled as coming from a multinomial logit distribution. The probability of being in each level of the q th health metric depends on the true health status, $h_{i,t}$, and the model is structured so as to ensure that the ordinal aspect of the variables is respected (i.e., that lower values means lower health). For example, if the health metric $H_{q,i,t}$ has a three-level ordinal scale, the observation equations for this metric are

$$H_{q,i,t} \sim \text{Multinom}(1, \mathbf{p}_{q,i,t}), \quad (33)$$

$$\text{logit}(p_{q,i,t,1}) = \log\left(\frac{p_{q,i,t,1}}{p_{q,i,t,2} + p_{q,i,t,3}}\right) = c_{q,0,1} + c_{q,1,1}h_{i,t}, \quad (34)$$

$$\text{logit}(p_{q,i,t,1} + p_{q,i,t,2}) = \log\left(\frac{p_{q,i,t,1} + p_{q,i,t,2}}{p_{q,i,t,3}}\right) = c_{q,0,2} + c_{q,1,2}h_{i,t}, \quad (35)$$

$$p_{q,i,t,3} = 1 - p_{q,i,t,1} - p_{q,i,t,2}. \quad (36)$$

The vector $\mathbf{p}_{q,i,t}$ contains the probabilities with which an individual with true health $h_{i,t}$ is assigned a specific health level. Because $h_{i,t}$ is positive, forcing the parameters $c_{q,0,1} < c_{q,0,2}$ and $c_{q,1,1} < c_{q,1,2}$, and modeling cumulative probabilities (Eq. 35) ensure that the order of the levels is accounted for. The probabilistic nature of the

model allows health metrics to depend on the true health status but to be observed with error.

By integrating different data types, this SSM allows inference about various aspects of North Atlantic right whales. For example, we can learn which visual health metrics show the strongest links to underlying health, whether geographic regions (and thereby human activity) have an impact on survival, and at which times of the year movement to certain zones occurs. Although this joint model may seem complex at first sight, each of the individual hierarchical levels are relatively straightforward.

Capturing heterogeneity with random effects

SSMs can account for additional dependencies and heterogeneity in parameter values with random effects. This feature has been used to incorporate individual variation in capture–recapture models (Royle 2008, King 2012). Capture–recapture models, such as the Cormack–Jolly–Seber model, are often used to estimate survival probabilities and gain insight on the factors that may affect survival. They model data, where individuals are uniquely identifiable via artificial (e.g., rings) or natural marks (e.g., coloring [King 2012]). One of the first applications of SSMs to such data was by Royle (2008) to demonstrate how to model variation in survival and capture probabilities. Royle (2008) applied the model to a 7-yr study of European dippers (*Cinclus cinclus*).

Royle (2008) presents a SSM parameterization of a Cormack–Jolly–Seber model, where the observation $y_{i,t}$ represents whether individual i was capture during the t th sampling occasion (i.e., $y_{i,t} = 1$ means the individual was captured at time t) and the state $z_{i,t}$ describes whether individual i is dead or alive at time t (i.e., $z_{i,t} = 1$ means the individual was alive at time t). At the time of first capture, f_i , the state is considered fixed: $z_{i,f_i} = 1$. Afterward, the process and observation equations are both Bernoulli trials, representing the survival and capture processes for each individual i :

$$z_{i,t} \sim \text{Bernoulli}(\phi_{i,t-1} z_{i,t-1}), \quad f_i < t \leq T, \quad (37)$$

$$y_{i,t} \sim \text{Bernoulli}(p_{i,t} z_{i,t}), \quad f_i < t \leq T, \quad (38)$$

where T is the total number of sampling occasions, and $\phi_{i,t}$ is the probability of survival of individual i over the interval $(t, t + 1)$ if the individual was alive at time $t - 1$, and $p_{i,t}$ is the probability of capturing individual i during the t th sampling occasion if it is alive. These probabilities are multiplied by the state values. Thus, an individual’s probability of surviving to time t becomes 0 if the animal was dead at time $t - 1$ (i.e., $z_{t-1} = 0$) regardless of the value of $\phi_{i,t-1}$, which means that once the animal is dead it remains dead for the rest of the time series. Similarly, the probability of being captured at time t becomes 0 if the individual is dead at that time.

We could simplify the model by having a single overall survival probability ($\phi_{i,t} = \phi$) and a single capture probability ($p_{i,t} = p$). However, differences between sampling occasions and individuals (e.g., due to variations in environmental and body conditions) often warrant for temporal and individual variations in survival and capture probabilities. Royle (2008) modeled the variations in these probabilities as follows:

$$\text{logit}(\phi_{i,t}) = b_t + \beta_i, \quad \beta_i \sim N(0, \sigma_\beta^2), \quad (39)$$

$$\text{logit}(p_{i,t}) = a_t + \alpha_i, \quad \alpha_i \sim N(0, \sigma_\alpha^2), \quad (40)$$

where a_t and b_t are the fixed temporal effects (i.e., effects associated with each sampling occasion), α_i and β_i are the latent individual effects, and σ_α^2 and σ_β^2 are the variances for the random effects. Just as for generalized linear model, the logit link function ensures that probability parameters stay between 0 and 1. The fixed temporal effects require that we estimate $(T - 1) + (T - 2)$ additional parameters (for details, see Royle [2008]). In contrast, the individual random effects allow one to model heterogeneity in survival and capture probabilities with only two additional parameters.

State-space models are now commonly used to model capture–recapture data because their mechanistic structure allows one to incorporate additional complexity (King 2012). Using random effects to model variation in parameter values can be used in many other ecological applications.

Modeling discrete state values with hidden Markov models

Hidden Markov models (HMMs) are a special class of SSMs, where the states are discrete rather than continuous (generally categorical with a finite number of possible values [Langrock et al. 2012]). HMMs have gained popularity in ecology, where they are used to model capture–recapture data (e.g., Choquet and Gimenez 2012, Johnson et al. 2016) and animals that switch between distinct behavioral modes (Langrock et al. 2012). Recently, McClintock et al. (2020) have demonstrated that HMMs are widely applicable in ecology. Having discrete states in a SSM becomes important when choosing fitting procedures (see *Fitting Models with Discrete States*), and thus we provide a few examples.

The two main characteristics of HMMs are (1) each observation is assumed to be generated by one of N distributions, and (2) the hidden state sequence that determines which of the N distributions is chosen at time t is modeled as a Markov chain, where the probability of being in each mode at time t depends only on the state value at the previous time step (Langrock et al. 2012). The capture–recapture model presented in *Capturing Heterogeneity with Random Effects* is an HMM, because state $z_{i,t}$ can only have one of two discrete values: 0 if the individual is dead or 1 if alive. The state value directly

affects the observation equation (Eq. 38), and the observation, $y_{i,t}$, is generated by one of two distributions: $y_{i,t} \sim \text{Bernoulli}(0)$ if $z_{i,t} = 0$ or $y_{i,t} \sim \text{Bernoulli}(p_{i,t})$ if $z_{i,t} = 1$. As seen in the process equation (Eq. 37), the probability of being in each state at time t depends only on the state value at the previous time step. This process can be viewed as a Markov chain with the following transition probability matrix:

$$\mathbf{\Gamma} = \begin{bmatrix} 1 & 0 \\ 1 - \phi_{i,t-1} & \phi_{i,t-1} \end{bmatrix}, \quad (41)$$

where for each individual, the probability of staying dead (i.e., $\Pr(z_{i,t} = 0 | z_{i,t-1} = 0)$) is 1, that of resurrectoring (i.e., $\Pr(z_{i,t} = 1 | z_{i,t-1} = 0)$) is 0, that of dying (i.e., $\Pr(z_{i,t} = 0 | z_{i,t-1} = 1)$) is the probability that it did not survive (i.e., $1 - \phi_{i,t-1}$), and that of surviving (i.e., $\Pr(z_{i,t} = 1 | z_{i,t-1} = 1)$) is $\phi_{i,t-1}$.

In other contexts, the transition probabilities may be more flexible, allowing for transition between all states, and the SSM may include both discrete and continuous states. For example, the model presented in *Accounting for Complex Data Structure* was originally developed to model the movement of animals tracked with Argos data that switched between two behavioral modes (Jensen et al. 2005). Instead of having a single γ parameter that controls how correlated the steps are (e.g., Eq. 18), this model has two parameters, γ_{b_1} , each one associated with one of the behavioral modes, $b_t = 1$ or $b_t = 2$. When γ_1 is close to 0 and γ_2 is close to 1, the movement path switches between tortuous and directed movement. The switch between the behavioral modes is modeled with a simple Markov chain (i.e., $\Pr(b_t = j | b_{t-1} = i) = \alpha_{ij}$). Although here we could allow the animal to switch back and forth between the behavioral modes (i.e., no α_{ij} is set to 0), the transition out of a given mode always needs to sum to one (i.e., $\sum_{j=1}^2 \alpha_{ij} = 1$ for $i, j = 1, 2$).

SSMs AS A FRAMEWORK FOR ECOLOGICAL TIME SERIES

Time is one of the fundamental axes that shape ecological systems (Wolkovich et al. 2014) and time series are crucial to understand the complex processes and interactions that govern all aspects of ecology (e.g., Boero et al. 2015, Damgaard 2019). Although SSMs have a long history in only a few fields of ecology, the breadth of their applications has been expanding and could be extended to most ecological time series. SSMs provide a framework that can be used to understand the mechanisms underlying complex ecology systems and handle the large uncertainties associated with most ecological data and processes.

State–space models (SSM) have been increasingly used in plant ecology. Damgaard (2012) showed the usefulness of using SSMs to analyze plant cover data collected through quadrats (specifically through pin-point methods). Bell et al. (2015) demonstrated how SSMs could be used to estimate canopy processes (e.g., conductance

and transpiration) using imperfectly monitored stem sap flux data. Clark et al. (2011) used the SSM approach to model the growth, fecundity, and survival of more than 27,000 individual trees. They showed how these processes are linked with light competition and spatiotemporal variation in climate.

State-space models are now used for paleoecological research. For example, Tomé et al. (2020) used SSMs to identify the drivers of changes in the mass and diet of a small mammal during the late Pleistocene. They use three separate linear Gaussian SSMs to model temporal changes in mass (as estimated from molar size) and in two stable isotopes (extracted from jaw bone collagen) as responses to each other and of a set of covariates related to climate (e.g., maximum temperature) and community structure (e.g., species richness). Einarsson et al. (2016) developed a SSM for sediment core data. One process equation modeled the change in abundance of midge egg capsules. The other modeled the change in pigment concentration characterizing potential resources (e.g., diatoms). These process equations modeled the abundance of each group with a Gompertz population model (similar to the model in *Handling Nonlinearity*), modified to add the effect of the other group's abundance at the previous time step. The measurement equations modeled sediment mixing and its associated uncertainty. They use their model to show that the cyclic fluctuations in midges are likely driven by consumer–resource (a.k.a. exploiter–victim or predator–prey) interactions.

Detecting cyclicity in ecological time series can be challenging because of temporal autocorrelation, and Louca and Doebeli (2015) showed that SSMs can outperform statistical tests for cyclicity. For example, they showed that simpler models would often lead to erroneous conclusions that cycles are present; the SSM generally had an appropriate 5% rate of Type I errors, but simpler tests had rates as high as 79%. The midge example of Einarsson et al. (2016) further demonstrates the usefulness of SSMs to identify the mechanisms behind cycles in ecological time series. Similar SSMs have been used to investigate fluctuations in other ecological fields (e.g., host–parasitoid systems [Karban and de Valpine 2010]).

State-space models have been used in ecosystem ecology and biogeochemistry. For example, Appling et al. (2018) used a SSM to model changes in oxygen concentration in an aquatic ecosystem as a function of three important processes: ecosystem's gross primary production, respiration, and gas exchange rate with the atmosphere. The process equation of Appling et al. (2018) predicts the oxygen concentration at time t as a function of its previous value and its instantaneous rate of change (similar to the model in *Accommodating Continuous-Time Processes*). The rate of change is modeled through a mechanistic equation, which sums the three processes of interest. The study compared various versions of the model, including versions that were not SSMs (i.e., versions without measurement error or process variation), and showed that the best SSM formulation significantly

improved the accuracy and reduced the bias of estimates of gross primary productivity, respiration, and gas exchange. In some cases, the magnitude of the bias of the SSM was half as large as that of simpler models. The study of Jia et al. (2011) is one of the many examples of applications of SSMs in soil science. Jia et al. (2011) used linear SSMs with normally distributed error to model the effects of elevation and the physical and chemical properties of soil (e.g., clay content and organic carbon) on the total net primary productivity of managed grasslands. They showed that the SSMs described the spatial patterns of soil total net primary productivity better than classical regression methods.

The term SSM has been used broadly in ecology to represent various types of hierarchical models with complex dependence structure. In particular, the term has been used for occupancy models that are based on capture–recapture SSMs similar to the one described in *Capturing Heterogeneity with Random Effects* (e.g., Kéry et al. 2009, Mordecai et al. 2011). Although they have similar structure, many of them lack the specific temporal autocorrelation in process equation that we generally ascribe to SSM (Fig. 1a) and may be better thought of as a related, but different, type of hierarchical model. For some of these models, it may be worth adding the Markovian dependence of the state in the process equation. However, to our knowledge, there are no studies that compare these related hierarchical models to SSMs.

The ubiquity of SSMs in ecology may have been obscured as some complex SSMs that combine various statistical techniques have not been identified as SSMs. For example, Thorson et al. (2016) present a joint species distribution model that has temporal dynamics. Although not called a SSM, their model has the essential structure of a SSM (Fig. 1a). We view their model as a Gompertz SSM (similar to the model in *Handling Nonlinearity*) combined to dynamic factor analysis to reduce dimensions and Gaussian random fields to account for spatial autocorrelation. This complex multispecies model was used to demonstrate that the spatiotemporal patterns of butterflies from the same genus were significantly correlated and to identify dominant patterns in community dynamics of marine fish.

The complexity of SSMs may prompt ecologists to ask: could we use a simpler alternative? In fisheries science, early papers on SSMs showed that they were particularly superior to simpler models when both the process variance and the observation error are large (e.g., de Valpine and Hastings 2002). When one of the sources of stochasticity is small, and the model dynamics are not too complex, simpler models that account for either just the process variance or observation error give adequate results (de Valpine and Hastings 2002). A key point, however, is that the simpler model performs adequately only if the model is well specified with regards to which source of stochasticity is most important. Thus, using a process variance-only model, is only suitable if we are certain that the observation error is negligible. Similarly, using an observation-

error-only model, is only suitable if we are certain that the process variation is small. Although simpler alternatives can be adequate in some contexts (see Bolker [2008: Chapter 11]), many studies have shown that SSMs provided better inference than simpler models (e.g., Jamieson and Brooks 2004, Jia et al. 2011, Louca and Doebeli 2015, Appling et al. 2018). For example, Lindén and Knape (2009) showed that, unlike SSMs, simpler models often had unreliable point and uncertainty estimates for environmental effects, and that the 95% confidence intervals excluded the true simulated value much more than 5% of the time (up to 30%). They showed that SSMs always outperformed the simpler alternatives. As such, we believe that SSMs, and their extensions, should be a default statistical modeling technique for many ecological time series. In the rest of the paper, we provide the tools that allow ecologists to apply these complex models adequately.

FITTING SSMs

The goals of fitting a SSM to data include estimating the parameters, θ , the states, z , or both. In ecology, we regularly need to estimate both, as we rarely know the value of θ *a priori* and estimating the states is often a primary goal of the analysis. In movement ecology, researchers often fit SSMs similar to that described in *Accounting for Complex Data Structure* because the states provide better estimates of the true locations of the animal than the data. In the SSM literature, a distinction is often drawn between three different types of state estimation processes based on the amount of observations used to inform the estimates (Shumway and Stoffer 2016). Using all of the observations, $y_{1:T}$, to estimate the states is referred to as “smoothing.” Smoothing is common with ecological SSMs, as we often have the complete data set in hand when we start the analysis. We denote the smoothed-state estimate as $\hat{z}_{t|1:T}$, with the subscript $t|1:T$ identifying that the state at time t is estimated using the observations from time 1 to T . In the original engineering application and in other fields, states are often estimated while data continue to be collected, so only observations up to and including time t , $y_{1:t}$, are used to estimate the state $\hat{z}_{t|1:t}$. This ubiquitous estimation procedure is referred to as “filtering.” Finally, we can use a subset of the observations that ends s time steps before time t , $y_{1:t-s}$, to predict the state at time t , $\hat{z}_{t|1:t-s}$, a procedure we refer to as “forecasting.” A common forecast is the one-step-ahead prediction, $\hat{z}_{t|1:t-1}$, which is also used within fitting algorithms (Appendix S2) and to validate models (*Diagnostics and Model Validation for SSMs*). Although these three types of state estimation processes are useful, the uncertainty associated with the state estimates tends to decrease for processes that use more observations (e.g., Shumway and Stoffer 2016).

The states are random variables, and thus have probability distributions. The states are sometimes referred to as random effects or latent variables. The fundamental differences in the procedures used to estimate states, as opposed to parameters (see *Frequentist Approach*), mean that

although we use estimation as an all-purpose term for both states and parameters, state estimation procedures are often referred as predictions, even when smoothing and filtering are used. The inferences about the states can include a variety of summary measures of their probability distributions. Above, the state estimates (e.g., $\hat{z}_{t|1:T}$) referred to point estimates such as the expected value. However, one can also calculate interval estimates (e.g., 95% confidence intervals) and single measures of uncertainty (e.g., standard deviations or variances).

Methods for fitting SSMs can be divided into the two main inferential approaches: frequentist and Bayesian. These approaches differ in their philosophies; see Bolker (2008) for a discussion. In brief, frequentist methods determine the probability of the data for a set of particular conditions (i.e., the hypothesis is fixed, but the data have a probability distribution). In contrast, Bayesian methods determine the probability that particular conditions exist given the data at hand (i.e., the data are fixed, but the hypothesis/parameters have probability distributions). The Bayesian approach requires the specification of prior beliefs for these distributions. Because of the early development of Bayesian computational methods for hierarchical models, historically it was easier to fit complex SSMs with a Bayesian approach and frequentist methods were limited to simple models (de Valpine 2012). As we will show, this is no longer true. There are now many accessible methods that allow one to fit complex SSMs with a frequentist approach (e.g., see *Laplace Approximation Methods* and *Sequential Monte Carlo Methods*). Thus, researchers can choose to work with their favored philosophical approach and/or based on the advantages of the algorithms available within each approach (see *When to Use Each Method?*).

In terms of fitting procedures, frequentists maximize the likelihood, and Bayesians focus on the posterior density. As we show below, despite these differences, both approaches involve high-dimensional integration, which is at the crux of the difficulties associated with fitting SSMs to data. The many tools developed for fitting SSMs are essentially different solutions to this high-dimensional integration problem.

Frequentist approach

When we fit a SSM with a frequentist approach, we search for the parameter values that maximize the likelihood, a method called maximum-likelihood estimation, with the resulting estimates called maximum likelihood estimates (MLEs). For our toy SSM (Eqs. 1, 2), the joint likelihood for θ and $z_{1:T}$ would be defined as:

$$L_j(\theta, z_{1:T}|y_{1:T}) = \prod_{t=1}^T g(y_t|z_t, \theta_o) f(z_t|z_{t-1}, \theta_p), \quad (42)$$

where T is the length of our time series and θ is a vector of (unknown) model parameters that contains the

parameters for the process equation, θ_p , and the observation equation, θ_o , and in this example the initial state, z_0 . Maximizing the joint likelihood with respect to both parameters and the states is challenging. Instead, one can use a process with two interrelated steps, each focused on estimating either the parameters or the states.

To estimate the parameters, we maximize the marginal likelihood, $L_m(\theta|y_{1:T})$:

$$\hat{\theta} = \arg \max_{\theta \in \Theta} L_m(\theta|y_{1:T}), \quad (43)$$

where

$$L_m(\theta|y_{1:T}) = \int L_j(\theta, z_{1:T}|y_{1:T}) dz_{1:T}. \quad (44)$$

Here, the key is that we integrate out the hidden states and thus have a function that only depends on the observations. The parameter estimates that result from maximizing the marginal likelihood have desired statistical properties (consistency and asymptotic normality; see Douc et al. 2011, de Valpine 2012), where the estimates are anticipated to improve with increasing sample size. Such properties would be hard to achieve when maximizing the joint likelihood, because the number of states to estimate generally increases with the number of observations.

To estimate the hidden states, we can use the conditional distribution of the states given the observations and the estimated parameter values, for example,

$$p(z_{1:T}|y_{1:T}, \hat{\theta}) = \frac{L_j(z_{1:T}|y_{1:T}, \hat{\theta})}{\int L_j(z_{1:T}|y_{1:T}, \hat{\theta}) dz_{1:T}}, \quad (45)$$

where $L_j(z_{1:T}|y_{1:T}, \hat{\theta})$ is similar to the right-hand side of Eq. 42, except that we use the MLEs for the parameters. Conditional distributions of the states, in particular the filtering distributions ($p(z_t|y_{1:t}, \hat{\theta})$; see Appendix S2 for an example), are at the base of filtering methods, such as the Kalman filter (*Kalman Filter*) and particle filter (*Sequential Monte Carlo Methods*). The means and variances of filtering densities can provide good point estimates and measures of uncertainty for state values (Appendix S2). As an approximation of the state estimates, one can also maximize $L_j(z_{1:T}|y_{1:T}, \hat{\theta})$ with respect to $\hat{z}_{1:T}$:

$$\hat{z}_{1:T} = \arg \max_{z_{1:T} \in Z^T} L_j(z_{1:T}|y_{1:T}, \hat{\theta}), \quad (46)$$

where Z^T is the set of all possible values for the states. This maximization treats the states as if they were equivalent to parameters in an ordinary likelihood (see Aeberhard et al. [2018] for more details) and is often used when the marginal likelihood is estimated with the Laplace approximation (see *Laplace Approximation Methods*). Although Eq. 46 treats the parameters as

known when estimating the states, one can propagate the parameter estimation variability when reporting the state estimate variance (e.g., see the `sdreport` function from R package *Template Model Builder* [TMB] [Kristensen et al. 2016]).

The marginal likelihood used to estimate the parameters, and thus the states, requires the computation of the high-dimensional integral found in Eq. 44. This computation is difficult to achieve for most SSMs and the frequentist inference methods now discussed are different ways to either evaluate the marginal likelihood (e.g., Kalman filter) or to approximate it (e.g., Laplace and simulation-based approximations).

Kalman filter.—For simple linear SSMs with Gaussian errors (i.e., NDLMs), the state estimates and marginal likelihood can be directly calculated using the Kalman filter (Kalman 1960). The Kalman filter provides an algorithm that, using only elementary linear algebra operations, sequentially updates the filtering mean and variance of the states (Harvey 1990, Durbin and Koopman 2012). Although the Kalman filter was developed to estimate the state values for models with known parameter values, its output can be used to evaluate the marginal likelihood and thus to find the MLE. The Kalman smoother is an analogous algorithm that uses backward recursion in time to obtain the mean and variance of each smoothing distribution (i.e., distribution of $z_{j|1:T}$; Harvey [1990], Durbin and Koopman [2012]). See Appendix S2 for a detailed example of the Kalman filter as applied to our toy model.

In Appendix S1: Section S1.3.1, we demonstrate how to use the R package `dml` (Petris 2010) to perform Kalman filtering and smoothing, as well as forecasting. It can also be used to find MLEs of unknown fixed parameters. The package is flexible enough to allow univariate and multivariate NDLMs, accounting for constant or time-varying distributions of states and observations. More details about Kalman filter and smoother and `dml` can be found in Petris et al. (2009) and Petris (2010). See also Shumway and Stoffer (2016: Chapter 6) for description of filtering, smoothing, forecasting, and maximum-likelihood estimation.

The Kalman filter is among the most broadly used algorithms to fit SSMs to ecological data. For example, it has been used in population ecology (e.g., Dennis et al. 2006), movement ecology (e.g., Johnson et al. 2008), community ecology (Ives et al. 2003), and plant ecology (Hooten et al. 2009). The main advantage of the Kalman filter is that it is fast and easy to calculate (de Valpine 2012). In addition, unlike most other methods that provide an approximation of the likelihood, the Kalman filter provides an exact evaluation of the marginal likelihood for linear and Gaussian SSMs (e.g., toy model [de Valpine 2002]).

Although the Kalman filter is an important algorithm for fitting SSMs to data, it does not work with nonlinear and non-Gaussian SSMs. Approximate techniques based on the Kalman filter are available for linear models

whose observations follow an exponential family distribution (e.g., Poisson, see Durbin and Koopman 2012: Chapter 9). Other approximate filtering and smoothing methods based on the Kalman filter, such as the extended Kalman filter and the unscented Kalman filter (e.g., Durbin and Koopman 2012: Chapter 10) are useful for some nonlinear and/or non-Gaussian SSMs. Such related methods have been used in ecology (e.g., Einarsson et al. 2016). However, for more complex, nonlinear, and non-Gaussian models, one must use one of the methods described below.

Laplace approximation methods.—The Laplace approximation is a commonly used tool for obtaining an approximation of the marginal likelihood of a SSM (Fournier et al. 2012, Kristensen et al. 2016). The general idea is that if the marginal likelihood (Eq. 44) is a well-behaved unimodal function, it can be approximated with a Normal density function. We can use this approximation to find the MLE. For a given set of parameter values, the Laplace approximation of the marginal likelihood requires the maximization of the joint likelihood (Eq. 42) with respect to the states. Thus, the parameter estimation process also returns an approximation of the state estimates. See Appendix S2 for details.

This method is flexible, and a variety of SSMs can be fitted using the Laplace approximation. However, the method assumes that the states can be locally approximated with a Gaussian distribution, which means that the states are assumed to have an unimodal distribution. Because the method uses the second derivative of the log-likelihood (Appendix S2), we cannot use the Laplace approximation with categorical states or other state distributions that are not twice differentiable. An important advantage of the Laplace approximation, over the simulation-based approaches described below, is the speed at which SSMs are fitted to data (see Auger-Méthé et al. 2017). Many software use the Laplace approximation approach (e.g., Fournier et al. 2012). We demonstrate in Appendix S1: Section S1.3.2 how TMB (Kristensen et al. 2016) is a particularly useful R package for SSMs. The Laplace approximation has been used in ecology, including in movement ecology (e.g., Auger-Méthé et al. 2017) and fisheries science (e.g., Aeberhard et al. 2018).

Sequential Monte Carlo methods.—Monte Carlo methods can be used to estimate the states and evaluate the integral needed to obtain the marginal likelihood. Monte Carlo methods are computer intensive sampling procedures that generate random samples from specific probability distributions, which can then be used to evaluate integrals. Although in this section we discuss Monte Carlo methods in the context of a frequentist inference approach, we will see in *Bayesian framework* that Monte Carlo methods are commonly used for Bayesian inference.

Sequential Monte Carlo methods, also referred to as particle filters, approximate the filtering distribution

through simulated sampling (de Valpine 2012). In the context of SSMs fitted with a frequentist approach, these Monte Carlo methods generally sample the state space by generating samples using the process equation and weighting the samples with the observation equation. Sequential importance sampling (Doucet et al. 2001) is a general procedure that can be used to generate N time series of the states, referred to as particles, and using their weighted average as the state estimates (see Appendices S1, S2 for details). However, sequential importance sampling is impractical for even moderately long time series (e.g., $T = 20$) because only a small proportion of the N randomly generated particles are generally supported by the observations. The reduced support for many of the particles, known as particle depletion, is a serious problem with sequential importance sampling that leads to state estimates with unacceptably large variances.

The bootstrap filter (Gordon et al. 1993) is a procedure designed to remedy particle depletion. The bootstrap filter assesses the weight of a particle through time and iteratively removes particles with low weights and replaces them with duplicates of particles with higher weights. There are various algorithms for the bootstrap filter; see Appendices S1, S2 for an example. Although simple bootstrap filters can reduce particle depletion, they do not completely solve the problem particularly for long time series. There are various remedies aimed at reducing particle depletion (de Valpine 2012), including more sophisticated importance sampling distributions that include information from the observations (Pitt and Shephard 1999) or changing the resampling methods (Liu and Chen 1998). Sequential Monte Carlo methods are also used for Bayesian inference and these methods are often built to reduce particle depletion (e.g., particle Markov chain Monte Carlo methods [Andrieu et al. 2010, Michaud et al. 2020]).

Sequential Monte Carlo methods, such as sequential importance sampling, can be used to estimate the likelihood. However, the likelihood maximization required for frequentist inference comes with additional challenges (e.g., to maximize the likelihood, one must explore what is often a complicated likelihood surface). In principle, it is possible to use a general-purpose optimization algorithm such as Nelder–Mead to maximize the likelihood computed by a simple particle filter. However, such an approach is usually prohibitively expensive. In addition, the stochastic ingredients of a particle filter make each of its runs different, making it hard to identify the precise peak of the likelihood surface (de Valpine 2012). Several methods have been proposed to overcome this difficulty (de Valpine 2012, Michaud et al. 2020).

Iterated filtering is an attractive method for maximizing the likelihood using particle filters (Ionides et al. 2015). This method repeatedly applies the particle filter but perturbs the fixed parameters of the model at each observation time step. These random perturbations

enhance performance and forestall particle depletion by continually reinjecting random variability into the filter. However, because it applies artificial perturbations to parameters, iterated filtering is not learning about the model of interest (i.e., model with fixed parameters), but about a modified model (i.e., model where fixed parameters have been transformed into state variables). Therefore, as filtering iterations proceed, one gradually cools (i.e., reduces the magnitude of) the artificial perturbations, so that the modified model approaches the model of interest as the iterations proceed. Because statistical inference hinges on identification of the global likelihood maximum, it is usually advisable to perform many independent iterated filtering computations, starting from widely dispersed starting points. See Appendix S2 for more detail. Iterated filtering, and other similar sequential Monte Carlo methods, can be easily implemented using the R packages *pomp* and *nimble* (see Appendix S1: Section S1.3.4; King et al. 2016, Michaud et al. 2020, de Valpine et al. 2017).

The main advantage of sequential Monte Carlo methods is that they are flexible, and thus can be used to conduct inference on any SSM (Michaud et al. 2020). Frequentist sequential Monte Carlo methods have been used in ecological fields such as bioenergetics (e.g., Fujiwara et al. 2005) and movement ecology (e.g., Breed et al. 2012). The main disadvantage of sequential Monte Carlo methods is that they can be computationally expensive.

Other methods.—The methods described above represent, in our view, the most commonly used methods to fit SSMs to ecological data in a frequentist framework. These methods are associated with comprehensive R packages that facilitate their implementation. However, many other methods exist (see de Valpine [2012] for a review of frequentist methods). Of note, Kitagawa (1987) provided a general algorithm for non-Gaussian SSMs similar to the Kalman filter, but that approximates the nonnormal distributions by discretizing them (e.g., through piecewise linear functions). It can be viewed as discretizing the continuous state space and reformulating the model as a HMM (Pedersen et al. 2011). de Valpine and Hastings (2002) demonstrated how flexible this approach was to fit nonlinear non-Gaussian population dynamics models. The main advantages of this approach are that it can be computationally efficient for models with a few state dimensions and does not require Monte Carlo methods (de Valpine 2012). This approach appears particularly promising for population modeling, where the states are counts, and thus the state space is already discretized (Besbeas and Morgan 2019). Pedersen et al. (2011) demonstrated that although this method is general and can provide results similar to the Laplace approximation and Bayesian methods, it is computationally limited to problems with only a few state dimensions. This limitation arises from the

curse of dimensionality, where even if each dimension has a manageable number of cells (e.g., 1,000 cells), the number of values needed to be stored become impractical as the number of dimension increases (e.g., three dimensions would result in $1,000^3 = 10^9$ cells; see de Valpine 2012).

Bayesian framework

When we fit a SSM with a Bayesian approach, the function of interest (also known as the target distribution) is the posterior distribution for the states and parameters given the observations:

$$p(\boldsymbol{\theta}, \mathbf{z}_{1:T} | \mathbf{y}_{1:T}, \boldsymbol{\lambda}) = \frac{L_j(\boldsymbol{\theta}, \mathbf{z}_{1:T} | \mathbf{y}_{1:T}) \pi(\boldsymbol{\theta} | \boldsymbol{\lambda})}{\iint L_j(\boldsymbol{\theta}, \mathbf{z}_{1:T} | \mathbf{y}_{1:T}) \pi(\boldsymbol{\theta} | \boldsymbol{\lambda}) d\mathbf{z}_{1:T} d\boldsymbol{\theta}}, \quad (47)$$

where $L_j(\boldsymbol{\theta}, \mathbf{z}_{1:T} | \mathbf{y}_{1:T})$ is the joint likelihood (i.e., $p(\mathbf{y}_{1:T} | \boldsymbol{\theta}, \mathbf{z}_{1:T})$; see for example, Eq. 42), and $\pi(\boldsymbol{\theta} | \boldsymbol{\lambda})$ is the prior distribution(s) for the parameters with fixed hyperparameters, $\boldsymbol{\lambda}$. Eq. 47 is an application of Bayes' theorem ($p(\boldsymbol{\theta} | \mathbf{y}) = \frac{p(\mathbf{y} | \boldsymbol{\theta}) p(\boldsymbol{\theta})}{p(\mathbf{y})}$) and the denominator of Eq. 47 represents the probability of the data (i.e., the marginal likelihood, which is the probability of the data for all possible values of the states and parameters). In Bayesian analyses, both the states, $\mathbf{z}_{1:T}$, and what we have been referring to as fixed parameters, $\boldsymbol{\theta}$, are considered random variables. The posterior distribution is a complete characterization of these random variables given the data and prior information. As such, the first inferential goal of a Bayesian analysis is often to evaluate the posterior distribution. Although point estimates for the parameters and the states are not necessarily the primary goal of a Bayesian analysis, they can be obtained by summarizing the center of the posterior distribution (e.g., mean or mode of the posterior distribution). Similarly, we can use the posterior distribution to obtain interval estimates and single measures of variation.

As for the frequentist framework, the fitting procedures are complicated by high-dimensional integrals and it is common to avoid calculating the integral and the posterior distribution explicitly. Instead, quantities of interest are generally approximated using Monte Carlo methods (see also *Sequential Monte Carlo Methods*), where large samples of states and parameters are randomly drawn from the posterior distribution. For example, one can approximate the point estimate of a parameter with the sample mean of the draws from the posterior distribution (often referred as the posterior mean). Simulating independent draws from Eq. 47 is typically impossible. However, there are various algorithms that can approximate the posterior distribution with large samples of dependent draws. In particular, Markov Chain Monte Carlo (MCMC) methods are a

broad class of algorithms that obtain samples from the target distribution (here the posterior distribution Eq. 47), by sampling from a Markov chain rather than sampling from the target itself. This Markov chain needs to have an invariant distribution (i.e., the probability distribution remains unchanged as samples are drawn) equal to the target distribution (Geyer 2011), a quality that is dependent on the initial condition of the chain and the transition probabilities, and relates to the importance of chain convergence as a diagnostic in MCMC sampling. MCMC algorithms fall into two broad families: Metropolis–Hastings samplers (which include Gibbs samplers) and Hamiltonian Monte Carlo.

Metropolis–Hastings samplers.—Metropolis–Hastings samplers are at the base of most MCMC algorithms used to sample the posterior distribution in a Bayesian analysis. Metropolis–Hastings samplers are iterative algorithms that construct an appropriate Markov chain to sample the target distribution. The general idea is that for each step j of the chain, we use a proposal distribution to generate a candidate value for the variable of interest (e.g., a parameter value). The probability that this candidate value is selected for that step rather than the previous value of the chain is based on the relative fit of the model with that candidate value compared to the previous value of the chain (see Appendix S2 for details).

In the context of SSMs, we have a multivariate posterior distribution for the states and the parameters. Using Metropolis–Hastings algorithms to sample for more than one random variables is complex, but there are various implementation tools to do so. For example, for each iteration j of the chain, one can first sample sequentially all parameter values, and then sequentially sample the state values (Newman et al. 2014; see also Appendix S2). If groups of variables are related, they can be sampled simultaneously from a multivariate distribution rather than sequentially. In practice, states and parameters are often correlated, and thus it may be difficult to implement an efficient MCMC sampler that does not require very long simulations before convergence (Newman et al. 2014).

Gibbs samplers are commonly used Metropolis–Hastings samplers for multivariate distributions, where the proposal distributions are conditional distributions of the target distribution and thus the candidate values are always accepted (Geyer 2011; see also Appendix S2). For NDLMs, the entire sequence $\mathbf{z}_{0:T}$ can be simulated at once from its conditional distribution, given the data $\mathbf{y}_{1:T}$ and the time-invariant parameter $\boldsymbol{\theta}$, using the forward filtering backward sampling algorithm described in Carter and Kohn (1994). The forward filtering backward sampling algorithm can also be used to conduct inference for the SSMs that are conditionally linear and Gaussian. However, Gibbs samplers for nonlinear and non-Gaussian models often require sampling from each conditional distribution sequentially (see Prado and

West 2010: Chapter 4.5, for an overview). A drawback of this particular Gibbs sampler design is that consecutive draws of $\mathbf{z}_{0:T}^j$ and $\mathbf{z}_{0:T}^{j-1}$ tend to be highly correlated, slowing the convergence and deteriorating the quality of the Monte Carlo approximations. Despite these drawbacks, Metropolis–Hastings samplers, including Gibbs samplers, are commonly used to fit ecological SSMs because they are flexible and freely available software to implement these algorithms have been available since the 1990s (Meyer and Millar 1999). They have been used to fit many of the original models described in *Examples of Ecological SSMs*, including the population models of Viljugrein et al. (2005), the movement model of Jonsen et al. (2005), the health and survival model of Schick et al. (2013), and the capture–recapture model of Royle (2008).

Combining sequential Monte Carlo methods (*Sequential Monte Carlo Methods*) within MCMC algorithms can help alleviate some of the efficiency problems produced by generic MCMC algorithms (Michaud et al. 2020). In these combined algorithms, a sequential Monte Carlo algorithm draws the states, and an MCMC algorithm draws the parameters. Particle MCMC methods (Andrieu et al. 2010) are particularly useful for SSMs (Michaud et al. 2020). Some particle filters, such as the bootstrap filter (*Sequential Monte Carlo Methods* and Appendix S2), can return unbiased estimates of the marginal likelihood (Eq. 44). At each iteration j , a particle MCMC algorithm will estimate the marginal likelihood and use it to draw a full state sequence (i.e., one sample particle will be used for $\mathbf{z}_{1:T}^j$). Although particle MCMCs may still suffer from poor mixing when the likelihood estimates are highly variable, these algorithms tend to reduce the correlations between successive draws of the states (Michaud et al. 2020). Custom-made particle MCMC algorithms have been used to fit different ecological SSMs, including population models (e.g., Knappe and de Valpine 2012, White et al. 2016) and complex models for range expansion (Osada et al. 2019). The recent implementation of such algorithms in R packages such as *pomp* and *nimble* will facilitate their uptake (Michaud et al. 2020).

There are a few important general Bayesian software and R packages that can be easily used to fit ecological SSMs using Metropolis–Hastings samplers. Generating draws from the posterior distributions can be done using software from the BUGS (Bayesian analysis using Gibbs sampling; see Lunn et al. 2013) project and their associated R packages: *WinBUGS* can be called in R via *R2WinBUGS* (Lunn et al. 2000), *OpenBUGS* via *BRugs* (Lunn et al. 2009), and *MultiBUGS* R interface is in development (Goudie et al. 2017). Gimenez et al. (2009a) provide a tutorial on how to fit ecological models (including some of the SSMs of *Handling Nonlinearity*) with *WinBUGS* in R. *JAGS* (just another Gibbs sampler; Plummer 2003) is an alternative to BUGS project software that is written for UNIX, thus preferred by Mac and Linux users. *JAGS* is available through the R

package *rjags* (Plummer 2018). The R package *nimble* (de Valpine et al. 2017) is a recent alternative to JAGS and BUGS software that is more transparent in how the sampling is performed. *nimble* allows users to write custom Gibbs samplers that perform block updating or implement a variety of other techniques including particle MCMC (de Valpine et al. 2017, Michaud et al. 2020). All these software allow one to write general models in a language based on BUGS. The user can set up the sampler in R, and once compiled, can use it to simulate draws to make inference about states and parameters. See Appendix S1: Sections S1.3.5 and S1.3.6 for detailed examples in JAGS and *nimble*.

Hamiltonian Monte Carlo.—An efficient alternative to Metropolis–Hastings sampling is provided by Hamiltonian Monte Carlo (HMC) methods, which have gained popularity in recent years thanks in part to their implementation in the Stan software (Stan Development Team 2012). These methods are inspired by analogies drawn from physics and rely heavily on deep differential geometric concepts, which are beyond the scope of this review. HMC can be a more efficient sampler than Metropolis–Hastings, as fewer iterations are typically required and fewer rejections occur. This is achieved by the addition of a momentum variable that helps the Markov chain to remain within the typical set of the target distribution, rather than conducting random walk to explore the target distribution as is frequently done by Metropolis–Hastings samplers. Interested readers can read the introduction for ecologists by Monnahan et al. (2017) and explore the statistical details in Neal (2011) or Betancourt (2017). Conducting inference for general SSMs via HMC is possible when all parameters and states are continuous or when the posterior distribution can be marginalized over any discrete parameters or states. Continuous distributions are required because density gradients of the target distribution are required to direct the sampling through the typical set of the target distribution (Betancourt 2017, Monnahan et al. 2017). Unlike Metropolis–Hastings samplers, HMC methods draw samples from the joint posterior distribution directly and can scale well to high-dimensional spaces. General SSMs can be fitted either by defining the posterior as in Eq. 47 or by marginalization over the state process to derive the posterior distribution of the time-invariant parameters only, $p(\theta|y_{1:T}, \lambda)$.

One of the most popular software that uses Hamiltonian Monte Carlo is Stan, available in R through the package *rstan* (Stan Development Team 2018). See Appendix S1: Sections S1.3.7 and S2.3.2 for detailed examples using *rstan*. Monnahan et al. (2017) showed that Stan can fit ecological SSMs more efficiently than Gibbs software like JAGS. Although the parameterization of the SSM affects Stan's efficiency, it can reduce computing time by orders of magnitude (Monnahan et al. 2017). Other advantages of Stan over JAGS include better

diagnostics for when the algorithms is unable to explore the entire posterior, which could result in biased inference (Monnahan et al. 2017). The main disadvantage of HMC is that one cannot easily work with discrete parameters, which makes it harder to have SSMs with discrete latent states (e.g., counts, categories; Monnahan et al. [2017]). We discuss methods to work around this limitation in *Fitting Models with Discrete States*. The use of HMC is increasing in ecology (Monnahan et al. 2017), and HMC has been recently used to fit ecological SSMs (e.g., in ecosystem ecology [Appling et al. 2018], and in fisheries science [Best and Punt 2020]).

Other algorithms.—The algorithms and software just discussed are the most commonly used to fit SSMs to ecological data in a Bayesian framework. For a more general introduction on how to develop statistical algorithms to fit Bayesian ecological models, please refer to Hooten and Hefley (2019). However, the development of Bayesian sampling algorithms is an active field of research. New methods, such as variational inference, appear particularly promising for fitting SSMs (e.g., Ong et al. [2018]).

Convergence diagnostics.—Regardless of the sampling method, it is important to assess whether it has reached the target posterior distribution. Convergence between multiple chains usually indicates that they have reached the invariant distribution. As such, multiple approaches have been developed to assess whether chain convergence has been achieved. In general, samples from the first iterations are discarded, as these likely occurred before the chain has reached the target distribution (Gelman and Shirley [2011], but see Geyer [2011]). In the Metropolis–Hastings setting, this period is referred to as “burn-in.” A somewhat similar initial period, referred as the “warm-up,” is discarded with HMC. Then, as a first step, convergence within and between chains can be assessed visually via traceplots (see Appendix S1). More formal metrics exist. The Gelman–Rubin metric, \hat{R} (Gelman and Rubin [1992]; see Brooks and Gelman [1998] for the multivariate analogue), is one of the most popular multichain diagnostics. Although $\hat{R} < 1.1$ generally indicates convergence (Gelman et al. 2013), recent research indicates that a threshold closer to one may be more suitable in some scenarios (Vats and Knudson 2018). Note that pseudo-convergence can occur in many different scenarios. For example, the sampler can get caught in one mode if the target distribution has multiple modes that are not well connected by the Markov chain dynamics (Geyer 2011). Running the chain for a long period can help limit these pseudo-convergence problems (Geyer 2011). A detailed summary of convergence methods is available in Cowles and Carlin (1996), and further research on convergence diagnostics includes Boone et al. (2014), VanDerwerken and Schmidler (2017), and Vats and Knudson (2018). Both JAGS and BUGS project software, as well as the R package *coda*

(Plummer et al. 2006), provide several methods to assess convergence.

Priors.—Selection of priors is a significant part of a Bayesian analysis because priors affect the resulting posterior distribution (Robert 2007). Several approaches can be taken depending on the information available about the model parameters and the philosophy of the modeler. Ecologists often use “noninformative” priors. These priors (e.g., a uniform distribution over the parameter space) are often thought to be objective and are generally chosen with the goal of maximizing the influence of the data on the posterior. However, noninformative priors may still have important effects on the posterior, and they should not be used naively (Gelman et al. 2017, Lemoine 2019). For example, Lele (2020) showed that noninformative priors could significantly influence the parameter and state estimates of ecological SSMs. Alternatively, ecologists can use informative priors, which are created using knowledge of the parameters or previously collected data (e.g., Meyer and Millar [1999], Dunham and Grand [2016]). As there are many advantages to using informative priors, they are increasingly used in ecological models (Hooten and Hobbs 2015). For example, informative priors can be used to supplement SSMs with limited time-series data (Chaloupka and Balazs 2007) and can improve state estimates (Dunham and Grand 2016). In most cases, noninformative and informative priors are used in the same model on different parameters. For technical reasons, it can sometimes be advantageous to use conjugate priors (i.e., priors with the same distribution as the conditional posterior distribution or the posterior distribution). Kass and Wasserman (1996) and Millar (2002) have summarized priors typically used in fisheries models, including many SSMs. Lemoine (2019) advocates for the use of weakly informative priors as default in ecology and provides a guide to their implementation. More generally, Robert (2007) and Gelman et al. (2013) provide a thorough review of available priors, selection, and examples for a variety of models.

Information reduction approaches

Although not commonly used with SSMs, information reduction approaches, such as synthetic likelihood or approximate Bayesian computation (ABC), appear promising to fit complex, highly nonlinear, ecological SSMs (Fasiolo et al. 2016). These methods bypass the calculation of the exact likelihood (Csilléry et al. 2010, Fasiolo et al. 2016). Instead, these methods generate samples from the model and transform them into a vector of summary statistics that describe the data in the simplest manner possible (Csilléry et al. 2010, Fasiolo et al. 2016). The simulated summary statistics are then compared to observed summary statistics using a predefined distance measure (Fasiolo et al. 2016). Information reduction approaches smooth the likelihood, reducing some of the common implementation problems encountered with

other fitting methods. However, the results from information reduction approaches are often imprecise and, thus, may be most useful in the model development phase (Fasiolo et al. 2016, Fasiolo and Wood 2018). Interested readers are referred to Csilléry et al. (2010), Fasiolo et al. (2016), and Fasiolo and Wood (2018).

Fitting models with discrete states

Depending on the complexity of the SSM and one’s favored inferential approach, having discrete states can either facilitate or complicate the fitting process. A SSM with a single time series of categorical states, generally referred as an HMM (*Modeling discrete state values with Hidden Markov models*), can be relatively easily fitted with a frequentist approach. The key advantage of these HMMs is their mathematical simplicity: what would be a high-dimensional integration in a SSM with continuous state values (e.g., Eq. 44) is now a simple sum. As such, having a finite number of possible state values (i.e., discrete states) significantly simplifies the analysis (Langrock et al. 2012). The mathematical simplicity of HMMs makes them highly attractive, and various efficient tools and R packages have been developed to fit HMMs to data. We refer readers interested in HMMs to McClintock et al. (2020) and Zucchini et al. (2016).

Although one can use Metropolis–Hastings samplers (*Metropolis–Hastings Samplers*) to fit HMMs with a Bayesian approach (e.g., Zucchini et al. 2016), these algorithms are far less efficient than those used to fit HMMs in a frequentist framework. In addition, HMC algorithms (Hamiltonian Monte Carlo) do not generally allow sampling of discrete states. However, recent work has demonstrated the gain in speed that can be made by marginalizing the latent states and how this can be implemented with Gibbs sampling (e.g., JAGS) and HMC software (e.g., Stan [Leos-Barajas and Michelot 2018, Betancourt et al. 2020, Yackulic et al. 2020]). Marginalizing the states means that when we estimate the parameter values, we do not sample the hidden states at each iteration, but rather track the likelihood of being in any given state (Yackulic et al. 2020). One can then estimate the states values using the conditional distribution (Eq. 45) or approximations of it (see Yackulic et al. [2020] for more details), or algorithms that are commonly used with frequentist HMMs, such as the Viterbi algorithm (Zucchini et al. 2016, Leos-Barajas and Michelot 2018). This two-step approach used when marginalizing the states has many parallels with the frequentist approach described in *Frequentist Approach*, where we first estimate the parameters using the marginal likelihood and subsequently estimate the hidden states based on the estimated parameter values.

Although there are many efficient tools to fit simple HMMs with a frequentist approach, it can be more challenging to fit SSMs that combined both continuous and

discrete states. Just as for Bayesian methods, some of the computationally efficient methods (e.g., Laplace approximation method described in *Laplace Approximation Methods*) do not allow for discrete states. One can use instead frequentist methods that rely on sampling the states (e.g., sequential Monte Carlo methods described in *Sequential Monte Carlo Methods*). One could potentially develop algorithms that marginalize the discrete and continuous states with different approaches.

For Bayesian SSMs with discrete states, one additional consideration is label-switching (Jonsen et al. 2013). The labels given to the N discrete states are arbitrary, and thus there are $N!$ potential label assignments (Zucchini et al. 2016). The different label permutations result in the same model. Thus, when the MCMC chains have reached convergence, all possible labels will have been assigned to each state and inference on the states will be difficult. For example, we will no longer be able to take the mean of the posterior distribution to estimate the states because all $\hat{z}_{t,1:T} \approx N/2$. One solution is to impose constraints on the parameters that would be violated when labels are permuted (Zucchini et al. 2016). For example, in the two-behavior movement model described in *Modeling discrete state values with Hidden Markov models* we would constrain $\gamma_1 \leq \gamma_2$.

When to use each method?

Choosing from this multitude of fitting methods can appear daunting, but can be guided by a choice of inference framework and the limitations of each methodology. In Table 2, we list the methods just discussed, with some pros and cons. We simply state the associated inferential framework (frequentist vs. Bayesian), and we let the readers decide their favorite inferential framework. In general, there are more computationally efficient methods for simple models in the frequentist framework (e.g., Kalman filter and Laplace approximation), but such generalization cannot be made for more complex models.

In some cases, it may also be easier to use one of the more specific ecological SSM R packages. For example, the package MARSS (which stands for multivariate auto-regressive state-space; Holmes et al. [2012, 2018]) can be useful to model multiple populations, if these can be reasonably formulated with a linear and normal SSM. Those interested in fisheries stock assessment SSMs should look at the package stockassessment (available on GitHub;¹⁴ Nielsen and Berg [2014]). Those interested in SSMs for animal movement should explore bsam (Jonsen et al. 2005, Jonsen 2016), crawl (Johnson et al. 2008, Johnson and London 2018), and momentHMM (McClintock and Michelot 2018).

FORMULATING AN APPROPRIATE SSM FOR YOUR DATA

SSMs are powerful tools, but their inherent flexibility can tempt ecologists to formulate models that are far too complex for the available data. The model structure or the characteristics of the specific data set may make it impossible to estimate every parameter reliably. In such cases, parameter estimates will no longer provide key information on the underlying biological process and state estimates may become unreliable (e.g., Auger-Méthé et al. [2016]). Formulation of SSMs needs to be guided by the inference objectives and the available data. In this section, we discuss how to assess whether a model is adequate for your data and how one can alleviate potential estimation problems.

Identifiability, parameter redundancy, and estimability

When we estimate the parameters of a model, denoted here as $M(\theta)$, we often want to find the set of parameter values, θ , that results in the best fit to the data. For this to be possible, the model needs to be identifiable. Identifiability refers to whether or not there is a unique representation of the model. A model is globally identifiable if $M(\theta_1) = M(\theta_2)$ implies that $\theta_1 = \theta_2$. For example, in a frequentist framework, an identifiable model would have only a single θ value that would maximize the likelihood (Fig. 3a). A model is locally identifiable if there exists a neighborhood of θ where this is true (Fig. 3b). Otherwise a model is nonidentifiable (Fig. 3c; Rothenberg [1971], Cole et al. [2010]).

An obvious case of nonidentifiability is when a model is overparameterized and can be reparameterized with a smaller set of parameters. For example, if two parameters only appear as a product in a model (e.g., $y = \alpha\beta x$); that model could be reparameterized with a single parameter replacing that product (e.g., $y = \gamma x$, where $\gamma = \alpha\beta$). The parameter redundancy of the original model will result in nonidentifiability (Catchpole and Morgan 1997) and nonidentifiability caused by the inherent structure of a model is referred to as intrinsic parameter redundancy (Gimenez et al. 2004) or structural nonidentifiability (Cobelli and DiStefano 1980). Regardless of the amount or quality of data, it is impossible to estimate all the parameters in such a model.

Having a structurally identifiable model does not guarantee that one can estimate its parameters with the data at hand. Nonidentifiability can be caused by a specific data set with, for example, missing or sparse data (Gimenez et al. 2004). This problem is known as extrinsic parameter redundancy (Gimenez et al. 2004) or practical nonidentifiability (Raue et al. 2009). A parameter is defined as practically nonidentifiable if it has a confidence interval that is infinite (Raue et al. 2009). It is also possible for a data set to create estimation problems with an otherwise structurally and practically identifiable model, a phenomenon referred to as statistical inestimability (Campbell and Lele 2014). If a model is

¹⁴<https://github.com/fishfollower/SAM>

TABLE 2. Comparison of the fitting methods discussed in *Fitting SSMs*.

Method	Framework	Pros	Cons	R package
Kalman filter and MLE	Frequentist	Efficient and exact	Only applicable to linear Gaussian SSMs	dlm, MARSS
Laplace approximation	Frequentist	Efficient and flexible	States need to be approximable with a continuous unimodal distribution (e.g., no discrete states)	TMB
Particle filter and iterated filtering	Frequentist	Flexible	Can be slow and sensitive to starting values	pomp, nimble
MCMC-MH	Bayesian	Flexible	Can be slow and sensitive to convergence problems	rjags, nimble, R2WinBUGS, BRugs
MCMC-HMC	Bayesian	Efficient and flexible	Require continuous parameters and states or marginalization	rstan
Information reduction	Bayesian	Flexible and fewer estimation problems	Can be slow and imprecise	EasyABC

Notes: HMC, Hamiltonian Monte Carlo; MCMC, Markov chain Monte Carlo; MH, Metropolis–Hastings; MLE, maximum-likelihood estimate.

statistical inestimable, a confidence interval for a parameter will be extremely large but not infinite. This often occurs because the model is very similar to a submodel that is parameter redundant for a particular data set, which is known as near redundancy (Catchpole et al. 2001, Cole et al. 2010).

Having a nonidentifiable model (either structurally or practically) leads to several problems. First, there will be a flat ridge in the likelihood of a parameter redundant model (Catchpole and Morgan 1997), resulting in more than one set of MLEs. However, despite the parameter redundancy, numerical methods for parameter estimation usually converge to a single set of MLEs. Therefore, without further diagnostics, one may not realize that the MLEs are not unique. Second, the Fisher information matrix will be singular (Rothenberg 1971) and therefore the standard errors will be undefined in a nonidentifiable model. However, the exact Fisher information matrix is rarely known and standard errors are typically approximated using a Hessian matrix. The Hessian describes the local curvature of a multiparameter likelihood surface. The Hessian is generally evaluated numerically, which

can lead to explicit (but incorrect) estimates of standard errors. Third, many model selection methods (see *Computationally Efficient Model Comparison Methods*) are based on the assumption that a model is identifiable and that the penalty for complexity is a function of the number of unique and estimable parameters (Gimenez et al. 2004). If a model is statistically inestimable or near redundant, these three problems may also occur, as the model is close to being nonidentifiable. For example the log-likelihood profile will be almost flat.

Checking for identifiability and estimability should become part of the model-fitting process and several methods are available to do so. A clear sign of problems is a flat log-likelihood profile (Fig. 3c), and plotting the log-likelihood profile for each parameter can serve as a diagnostic for this (Fig. 3; Dennis et al. [2006], Raue et al. [2009], Auger-Méthé et al. [2016]). Correlation between parameters can also be indicative of estimation problems, and it may be useful to inspect the log-likelihood or posterior surface of pairs of parameters (Campbell and Lele 2014, Auger-Méthé et al. 2016). Depending on model complexity and computation time,

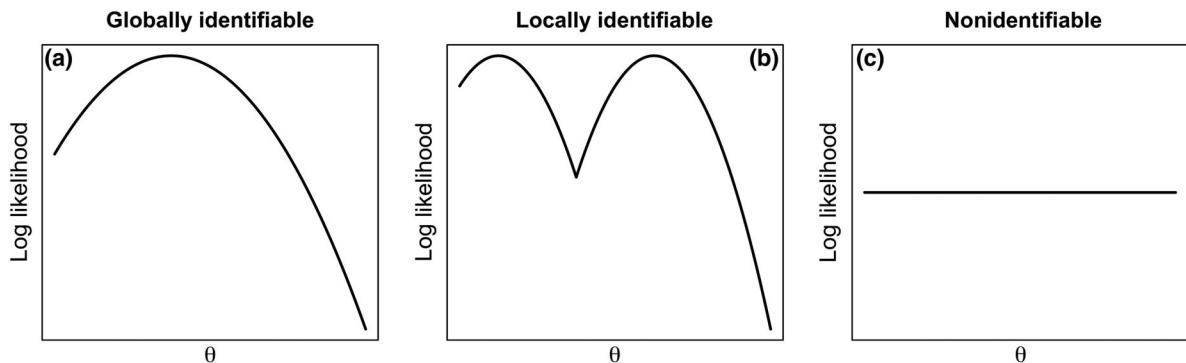


Fig. 3. Examples of log-likelihood profiles for a parameter θ under various identifiability scenarios: (a) globally identifiable, (b) locally identifiable, and (c) nonidentifiable model.

simulations can be an easy way to investigate the estimability of SSMs (Auger-Méthé et al. 2016). For a specified SSM and a known set of parameters, one simulates the state process and observation time series, and then estimates the parameters and states. One then compares estimated parameter and state values with the known true values. Parameter estimates from nonidentifiable models will usually be biased with large variances.

In addition to these simple checks, three advanced methods to assess estimability and identifiability problems exist. First, data cloning has been shown to be useful with ecological models (Peacock et al. 2017). Data cloning involves using Bayesian methodology with a likelihood based on K copies of the data (clones). The posterior variance of a parameter will tend towards K times the asymptotic variance of the parameter, so that if a parameter is identifiable, the posterior variance will tend to zero as K tends to infinity. If a parameter is not identifiable, the posterior variance will tend to a fixed (nonzero) value (Lele et al. 2010). Campbell and Lele (2014) show how this method can be extended to find estimable parameter combinations in nonidentifiable models.

Second, one can use the fact that the Hessian matrix in a nonidentifiable model will be singular at the MLE. As a singular matrix has at least one zero eigenvalue, the Hessian method involves finding the eigenvalues of the Hessian matrix. If the Hessian matrix is found numerically, the eigenvalues for a singular matrix may be close to zero rather than exactly zero. Therefore, if any of the eigenvalues are zero or close to zero, the model is deemed nonidentifiable or parameter redundant, at least for that particular data set (Viallefont et al. 1998). The Hessian matrix will also have eigenvalues close to zero if the model is statistically inestimable or near redundant (Catchpole et al. 2001).

Third, one can use the symbolic method. This method uses the concept that a model can be represented by an exhaustive summary, which is a vector of parameter combinations that uniquely define the model. For example, this vector could be $\mathbf{k} = (L_m(\boldsymbol{\theta}|y_1), L_m(\boldsymbol{\theta}|y_{1:2}), \dots, L_m(\boldsymbol{\theta}|y_{1:T}))'$, where the first element is the marginal likelihood (Eq. 44) for the first observation (y_1), the second element is the marginal likelihood for the first two observations ($y_{1:2}$), etc. This straightforward exhaustive summary works well for HMMs (Cole 2019), but can be impractical for SSMs with continuous states as it involves integration. Suitable, but more complex to derive, exhaustive summaries for SSMs are given in Cole and McCrea (2016). To investigate identifiability, we form a derivative matrix by differentiating each term of the exhaustive summary vector with respect to each parameter. Then, we find the rank of this matrix. The rank of a matrix is the number of columns that are linearly independent. Because each column of the derivative matrix is associated with one of the parameters, the rank is the number of estimable parameters (or parameter combinations). If the rank is less than the number of parameters, then the model is nonidentifiable or

parameter redundant (Catchpole and Morgan 1997, Cole et al. 2010). This method can be used to investigate practical identifiability as well as structural identifiability by choosing an exhaustive summary that includes the specific data set (Cole et al. 2012). In some more complex models, the computer can run out of memory calculating the rank of the derivative matrix. Cole et al. (2010) and Cole and McCrea (2016) provide symbolic algebra methods for overcoming this issue. The alternative is a hybrid symbolic-numerical method, which involves finding the derivative matrix using symbolic algebra, but then finding the rank at five random points in the parameter space (Choquet and Cole 2012).

Each of the numerical methods (log-likelihood profile, simulation, data cloning, Hessian method) can be inaccurate. They are also not able to distinguish between estimability, practical identifiability, and structural identifiability when applied to a specific data set, although in some cases a large simulated data set could be used to test structural identifiability. Being able to distinguish between these problems is useful, as it can help us assess whether gathering more data will help. The symbolic method is accurate, but is more complicated to use, as it involves using a symbolic algebra package. Code for assessing estimability using simulations and the Hessian method is given in Appendix S1: Section S1.4. Code for the symbolic algebra method is given in Appendix S3.

In Bayesian analysis, identifiability and estimability issues have a different focus because priors can affect our capacity to differentiate between parameters (Cressie et al. 2009). In general, parameters are said to be weakly identifiable when the posterior distribution significantly overlaps with the prior (Garrett and Zeger 2000, Gimenez et al. 2009b). If priors are well informed by previous data or expert knowledge, their strong influence on the posterior distribution is no longer an identifiability/estimability issue but one of the benefits of Bayesian analysis. However, misusing informed priors (e.g., when the information is not reliable) may hide identifiability issue or cause the estimability problems (Yin et al. 2019). Thus, one should choose priors with great care. To help ensure that the data inform the model and that the posterior is well behaved, Gelfand and Sahu (1999) suggested using informative priors that are not too precise (see *Priors* for other considerations). Weak identifiability can result in multiple implementation issues, including slow convergence (Gimenez et al. 2009). Diagnostics for parameter identifiability in the Bayesian framework include some of the tools described above and the visual or numerical assessment of the overlap between priors and posterior distributions (Garrett and Zeger 2000, Gimenez et al. 2009b).

Remedies for identifiability issues

When we fit a SSM to our data, we hope that it will provide accurate and precise estimates of our parameters and states. But how can we achieve these goals? First, we need to have a structurally identifiable model. Second,

one needs a data set appropriate for the model and vice versa; otherwise one can face estimation problems even with structurally identifiable models. Generally, we assume that having more data will allow us to estimate parameters and states better. However, as discussed below, increasing the length of the time series may not be the best way to improve estimation.

Reformulate the SSM.—To create a structurally identifiable model, one should start by avoiding overparameterization. As mentioned above, models where some parameters only appear as products of each other should be simplified. The same holds for models where parameters only appear as sums (e.g., $y = (\alpha + \beta)x$), or differences, or fractions. Models where the magnitude of two sources of error are simply additive are also problematic (e.g., $Y \sim N(X, \sigma^2)$ and $X \sim N(\mu, \tau^2)$, will result in $Y \sim N(\mu, \sigma^2 + \tau^2)$, where σ and τ cannot be uniquely identified). As such, one needs to check that none of the parameters are confounded and carefully inspect the combination of the sources of variability in all hierarchical models, including SSMs (see below). Some of the tools discussed above can help construct structurally identifiable models. In particular, the symbolic method can be used to identify the parameters that are confounded in a nonidentifiable model, and thus can be used to select estimable parameter combinations. This involves solving a set of partial differential equations formed from the same derivative matrix used to check identifiability (Catchpole et al. 1998, Cole et al. 2010).

Make simplifying assumptions when data are limited.—A full model may be too complex for the data at hand and it may be advantageous to make simplifying assumptions. For example, when the data available for older age classes are limited, researchers can have difficulties fitting the fisheries stock assessment model presented in *Joining Multiple Data Streams*. To help the estimation process, one can create a cumulative age class, A^+ , that accounts for all fish older than a certain age (Nielsen and Berg 2014). To allow fish to remain in the cumulative age class, we need to add the following equation to the model

$$\begin{aligned} \log(N_{A^+,t}) &= \log(N_{A^+-1,t-1} e^{-F_{A^+-1,t-1} - M_{A^+-1,t-1}} \\ &+ N_{A^+,t-1} e^{-F_{A^+,t-1} - M_{A^+,t-1}}) + \varepsilon_{N_{A^+,t}}. \end{aligned} \quad (48)$$

The similar size of these older fish makes them more likely to be caught by the same type of fishing gear, and thus their catchability and fishing mortality can be further assumed to equal that of the previous age class ($Q_{A^+,s} = Q_{A^+-1,s}$ and $F_{A^+,t} = F_{A^+-1,t}$). Although this appears to add complexity, creating this cumulative age class and equating some terms reduces the number of

states and parameters to estimate. However, some simplifying assumptions may result in estimation problems. For example, the original DCRW model of Jonsen et al. (2005) has a single correction factor rather than one per coordinate ($\psi = \psi_{\text{lon}} = \psi_{\text{lat}}$, see *Accounting For Complex Data Structure*). The common correction factor can result in estimation problems because longitude and latitude often differ in the degree of correction they need (Auger-Méthé et al. 2017). As long as they are biologically reasonable, such simplifying assumptions can be useful in a wide range of fields, including in community ecology, where SSMs can link multiple species to common latent variables and thus reduce the dimension of the model (Thorson et al. 2016).

Estimate measurement errors externally.—SSMs can be associated with significant estimability problems, particularly when trying to estimate the two main sources of variability (Knape 2008, Auger-Méthé et al. 2016). As a result, researchers often fix some of the parameters to known values, or use informed priors if they are working in a Bayesian framework. In particular, many use fixed values for the measurement errors and use for them independent estimates of measurement errors (e.g., Jonsen et al. [2005]). Although such methods can alleviate estimation problems (Knape 2008), one must be careful not to use biased or misspecified values.

Integrate additional data.—Covariates that provide additional information about a state or a process (e.g., survival) may be a means of overcoming identifiability problems. Polansky et al. (2021) showed that nonidentifiability in the estimation of a fecundity and observation correction parameter could be overcome by including a covariate in the model for fecundity.

Similarly, identifiability issues can be overcome by combining a SSM with a model for another data set that has parameters in common with the SSM. For example, in integrated population models, SSMs for time series of census data are combined with capture–recapture data (Besbeas et al. 2002, Abadi et al. 2010). Adding additional data sources can be extremely useful, but may not remove all identifiability issues. Methods for checking identifiability in integrated models are discussed in Cole and McCrea (2016).

Use replicated observations.—Having replicated observations through time (e.g., two independent population surveys) can help differentiate process variation from observation error, improve the parameter estimates' accuracy, and improve the capacity of model selection methods to identify the correct observation distribution (Dennis et al. 2010, Knape et al. 2011). In many instances, such replicated observations have already been collected, but are aggregated. For example, in population monitoring studies, subsamples (e.g., transect portions) are often aggregated into one overall estimate of abundance. Dennis et al. (2010) demonstrated that using

these as replicates, rather than aggregating them, can improve the estimates. One can also take advantage of time series with multiple data sources to estimate the errors of each data source (e.g., double-tagged individuals in movement SSMs [Winship et al. 2012]). For animal movement models, individuals can be also seen as replicates of the same process, but often the SSMs are fitted separately to each individual track. To improve inference, one can create a population model, where each individual track is linked to a distinct state time series but all share the same parameters (Jonsen 2016). Although the gains that can be made with replications are significant, one must understand the assumptions of models for replicated data. Simple population models for replicated data sets may assume that the replicates are independent (Dennis et al. 2010). However, many temporally varying factors (e.g., weather) may affect the sampling conditions and/or the behavior of animals and result in correlations between replicates. Knape et al. (2011) demonstrated how to account for such dependence in population dynamics models. For animal movement, one may want to consider whether it is appropriate to assume that the behavioral mechanism driving movement is identical across individuals and, if not, may want to modify the model accordingly. However, as the gains that can be made with replications far surpass those that could be made with longer time series (Dennis et al. 2010), one should consider using replication in models and when designing studies. For example, Knape et al. (2011) suggested that in some cases managers may want to sample a population twice every second year rather than once a year. As SSMs are becoming the prime method to fit ecological time series, such study design issues should be explored further.

Match temporal resolution for states and observations.—The temporal resolution of the data can affect the parameter and state estimates, and it is important to define a model at a resolution that is appropriate for the data. In many cases, adequate temporal span or resolution is more important than increased data quantity. For example, if a model describes a long-term cycle, then collecting data from more individuals is unlikely to make parameters estimable if the data set is not long enough to span the cycle being described (Peacock et al. 2017). If developing a model to classify a movement path into distinct behavioral modes, one must sample the movement track at a high enough frequency so that multiple locations are recorded in each movement bout (Postlethwaite and Dennis 2013). If one has a data set with locations every 8 h, it would be challenging to estimate behavioral states lasting <16–24 h. One can use pilot data, simulations, and data cloning to identify the temporal (and spatial) scale of sampling appropriate for the model, in something akin to a power analysis (Peacock et al. 2017). Overall, finding an appropriate model for your data, or collecting the appropriate data for your questions, can be an iterative process where one assesses

the estimability of different models under different data conditions.

COMPUTATIONALLY EFFICIENT MODEL COMPARISON METHODS

Model comparison (or selection) can be used to compare the relative fit of models representing multiple working hypotheses, and to identify the model among these that best describes the data (see *Diagnostics and Model Validation for SSMs* for methods to evaluate the absolute fit of a model). Because different model structures can affect the estimated states and parameters (Knape et al. 2011), model comparison can be extremely useful in helping to refine state estimates (Auger-Méthé et al. 2017). Model comparison is common in ecology and has been used to compare SSMs (e.g., Siple and Francis [2016]). However, it is not uncommon for users to fit only a single SSM, likely because of the computational burden of fitting complex SSMs and some of the known limitations of applying model selection methods to SSMs (Jonsen et al. 2013). With the improved efficiency of fitting algorithms and advancements in model selection measures, model comparison of SSMs is becoming more attainable.

One common view is that ecological systems are so complex that it is impossible to develop a model that truly describes them, and that the goal of model selection is to find the best approximation of the truth (Burnham and Anderson 2002). Under this paradigm, a useful way to compare models is to assess how well they can be used to predict new data. Comparing the out-of-sample predictive accuracy of models can be done with cross-validation. However, it is rarely done with ecological SSMs because it requires fitting the same model multiple times, and thus can add significant computational burden to the analysis. Many advocate cross-validation as the best method for model selection (Gelman et al. 2014, Link et al. 2017), and gains in efficiency of fitting algorithms are making its use increasingly feasible. We discuss cross-validation as a model selection, and validation, method in *Diagnostics and Model Validation for SSMs*. Here, we focus on what can be considered approximations of predictive accuracy. In particular, we discuss information criteria measures used with frequentist and Bayesian approaches.

Frequentist approach

The most common model comparison measure in ecology is Akaike's Information Criterion (AIC; Aho et al. [2014]). AIC was derived to estimate the expected and relative distance between the fitted model and the unknown true data-generating mechanism (Burnham and Anderson 2002), and can be viewed as -2 times an approximation of the predictive accuracy of the model (Gelman et al. 2014):

$$AIC = -2\log L(\hat{\theta}_{mle}|\mathbf{y}) + 2k, \tag{49}$$

where $L(\hat{\theta}_{mle}|\mathbf{y})$ is the likelihood of the model at the MLE (i.e., the probability of the observed data given the model) and k is the number of parameters estimated. The model with the lowest AIC, thus the shortest distance from the truth, is considered the best model. Models with more parameters will be more flexible and will tend to fit the existing data better by chance alone. Thus, AIC penalizes a model for its number of estimated parameters to compensate for overfitting.

There are many issues related to using AIC with SSMs, and some have cautioned against this practice (e.g., Jonsen et al. [2013]). We identified five different concerns. The first three concerns are related to the fact that the states of a SSM can be considered as random effects. First, using AIC to understand whether including random effects improves the model is difficult because some of the models may have parameters at the boundary of parameter space (Bolker et al. 2009). For example, testing whether or not there is process variance in SSMs (e.g., comparing our toy model to a model with no process variance, where $\sigma_p = 0$) could result in boundary problems, and is not recommended. Second, when you have random effects, it is difficult to quantify the effective number of parameters (Bolker et al. 2009). For SSMs, it is difficult to know to what extent the states should be counted as estimated parameters and contribute to k . However, if all of the compared SSMs have the same number of states and no additional random effects, these two issues should be less problematic. In such cases, we would expect any bias in the penalty k to be the same across models and thus have little effect on the difference in AIC across models. Third, one must decide whether the marginal likelihood or the conditional likelihood should be used when calculating AIC of a model with random effects (Müller et al. 2013). In contrast to the marginal likelihood, where we integrate out the states (Eq. 44), the conditional likelihood considers the states as known $L_c(\theta_o|\mathbf{z}_{1:T}, \mathbf{y}_{1:T}) = \prod_{t=1}^T g(y_t|z_t, \theta_o)$. When the conditional likelihood is used in the AIC framework, both the parameter and state estimates are plugged in and different approaches can be used to account for the number of states (Vaida and Blanchard 2005, Müller et al. 2013). This conditional AIC is a measure of the model’s ability to predict new observations that share the same latent states, whereas the marginal AIC does not assume that the latent states are shared with the new observations and measures the model’s ability to predict new observations from the same process (Vaida and Blanchard 2005). For example, for a SSM describing the population dynamics of a fish species, we would interpret the conditional AIC as assessing the ability to predict another survey of the same population during the same time period. The marginal AIC would be assessing the ability of the model to predict a survey from a similar

population of the same species. To our knowledge the marginal likelihood has always been used with SSMs fitted in a frequentist framework. In most SSMs, the number of states increases with the sample size (i.e., with the length of the time series). Because frequentist model selection methods rely on asymptotic properties, which can be attained when the sample size is large compared to the number of quantities estimated, conditional AIC may be unreliable for most SSMs. This characteristic may explain why potential advantages of using the conditional likelihood remain uninvestigated in the frequentist SSM literature (the conditional likelihood is used in Bayesian information criteria; see *Bayesian approaches* for a discussion). The fourth source of concern is related to the problems associated with using AIC to choose the number of components in mixture models, which are particularly relevant for choosing the number of states in HMMs (Jonsen et al. 2013). Pohle et al. (2017) outline solutions to this HMM-specific problem.

The final concern, which is specific to cases with small sample size, is one that has been studied in the SSM literature. When the sample size n is small and the number of parameters k is relatively large (e.g., when $k \approx n/2$), the $2k$ penalty is inadequate and AIC has a tendency to favor more complex SSMs (Cavanaugh and Shumway 1997). Many use the corrected AIC (AIC_c) for small sample size (Burnham and Anderson 2002). However, Cavanaugh and Shumway (1997) noted that AIC_c may be inadequate for many SSMs, and suggested an alternative: the bootstrap-corrected measure, AICb. AICb has been used for ecological SSMs (Ward et al. 2010, Siple and Francis 2016), especially by users of the R package MARSS (Holmes et al. 2012). This package for estimating the parameters of linear multivariate auto-regressive SSMs with Gaussian errors (i.e., multivariate NDLMs) has a function that calculates various versions of AICb. AICb was developed in the context of linear Gaussian SSMs, but is thought to be relatively robust to violations to normality (Cavanaugh and Shumway 1997). We can describe AICb as

$$AICb = -2\log L_m(\hat{\theta}_{mle}|\mathbf{y}_{1:T}) + 2\left(\frac{1}{N} \sum_{i=1}^N -2\log \frac{L_m(\hat{\theta}^i|\mathbf{y}_{1:T})}{L_m(\hat{\theta}_{mle}|\mathbf{y}_{1:T})}\right), \tag{50}$$

where $\hat{\theta}^i$ is the i th bootstrap replicate of $\hat{\theta}$, N is the number of replicates, and $L_m(\hat{\theta}^i|\mathbf{y}_{1:T})$ is the marginal likelihood of the model with the bootstrapped parameter sets given the original data. This bootstrap replicate can be achieved by simulating a time series from our model with $\hat{\theta}_{mle}$ and estimating the parameters using this new time series. AICb was shown to outperform AIC and AIC_c when used with SSMs that had relatively small sample size for the number of parameter estimated (Cavanaugh and Shumway 1997). The disadvantage of AICb is that

it requires fitting the model N times. In the case of models that are computationally demanding to fit, one may need to continue to rely on AIC_c when sample sizes are small. Although AIC_c tends to erroneously choose more complex models compared to AIC_b , it is better than AIC and many other metrics for SSMs with small sample size (Cavanaugh and Shumway 1997). Another similar computationally intensive AIC variant for SSMs fitted to small samples has been developed by Bengtsson and Cavanaugh (2006), but its use in ecology has been limited by some of its constraints (e.g., Ward et al. 2010). For large data sets, some ecologists prefer to use BIC over AIC because AIC tends to choose more complex models as sample size increases. However, these two measures are used to achieve different inferential goals, and choosing between them is largely a philosophical question (see Aho et al. 2014, Hooten and Hobbs 2015).

Overall, AIC and its small sample alternatives can be used with SSMs in many instances, especially when the number of states and random effects are the same. AIC has been used for decades with SSMs (Harvey 1990), and simple simulation studies have shown that AIC can be used to reliably select between SSMs (Auger-Méthé et al. 2017). Further research on the capacity of AIC to compare the predictive abilities of SSMs when the number of states or random effects vary, and research on how to account for the number of states in the penalty term would be useful. In the meantime, one should be aware of the limitations outlined above, and interpret the results accordingly.

Other frequentist methods may be used to select between SSMs. For example, likelihood ratio tests can be used to select between nested models, especially when conducting planned hypothesis testing (e.g., Karban and de Valpine 2010). However, likelihood ratio tests will suffer from some of the same issues as the those highlighted for AIC . Newman et al. (2014) also highlighted the potential use of score tests, transdimensional simulated annealing, and other methods. To our knowledge, these alternative methods have not been used in the SSM literature, but may be the focus of future research.

Bayesian approaches

Two Bayesian information criteria, the deviance information criteria (DIC, see Appendix S4) and the Watanabe–Akaike information criterion (WAIC), are popular with hierarchical models, and have been used with SSMs. They replace the information criteria based on MLEs, such as AIC , which do not have a clear interpretation for Bayesians (Hooten and Hobbs 2015). DIC and WAIC are similar to AIC , but they both use information from the posterior and estimate the effective number of parameters using data-based bias correction rather than a fixed rule. These data-based methods attempt to account for the effects of priors and the hierarchical

structure (e.g., the characteristics of the random effects) on the flexibility of the model.

Although DIC has been used to select ecological SSMs (e.g., Michielsens et al. 2006), and MCMC sampler software (e.g., JAGS [Plummer 2003]) and R packages like *rjags* (Plummer 2018) have functions that compute it easily, this information criterion is known to have many drawbacks that hinder its suitability for SSMs. DIC performs better when the number of effective parameters is much smaller than the sample size (Hooten and Hobbs 2015), a condition likely uncommon with SSMs because the number of latent states scales with the sample size. In addition, DIC is known to be problematic for mixture models, can poorly estimate the effective number of parameters (e.g., can return negative numbers), relies on approximate posterior normality, and is not fully Bayesian because its measure of fit relies on the posterior mean of θ (i.e., a point estimate; see Appendix S4) instead of the entire posterior distribution (Gelman et al. 2014, Hooten and Hobbs 2015, Kai and Yokoi 2019). These limitations may explain why Chang et al. (2015), in contrast to Wilberg and Bence (2008), showed that DIC had difficulties selecting amongst ecological SSMs.

Many now favor WAIC, a recently developed Bayesian information criterion (Gelman et al. 2014, Hooten and Hobbs 2015)

$$WAIC = -2 \sum_{i=1}^T \log \int p(y_i | \theta) p(\theta | \mathbf{y}) d\theta + 2p_{waic}. \quad (51)$$

The first component of WAIC is a measure of fit that, unlike DIC, uses the entire posterior distribution for θ rather than a point estimate. As such, we can consider this measure of fit as truly Bayesian. There are different ways to estimate the effective number of parameters, p_{waic} . Gelman et al. (2014) recommend using $\sum_{i=1}^T \text{Var}_{\text{post}}(\log p(y_i | \theta))$, as it gives results closer to the leave-one-out cross-validation. In our formulation of WAIC (Eq. 51), we used a -2 multiplier, as it helps highlight the similarity to AIC (Eq. 49). However, this multiplier may obscure how WAIC is a measure of the predictive accuracy of the model, and some researchers prefer not using it (e.g., Vehtari et al. 2017). See Appendix S4 for how Eq. 51 is calculated in practice.

WAIC has been used to compare ecological SSMs (e.g., Baldwin et al. 2018, Ferretti et al. 2018) and can be computed using the R package *loo* (Vehtari et al. 2017). Recent reviews of Bayesian model comparison methods favor WAIC over DIC (Gelman et al. 2014, Hooten and Hobbs 2015) because it is a fully Bayesian metric, it is not affected by parameterization, and will not return negative values for the effective number of parameters. However, WAIC has a few shortcomings, and new approximations of predictive accuracy have been recently proposed (e.g., Pareto-smoothed importance sampling leave-one-out cross-validation [Vehtari et al.

2017]). Both parts of WAIC are computed by using the sum over each data point i , and thus rely on partitioning the data into disjoint, ideally conditionally independent, pieces (Gelman et al. 2014). Naively partitioning can be problematic with SSMs, because the time-series nature of the data generally results in dependence structures (see Appendix S4 for a potential solution). Although AIC and DIC rely on a point estimate rather than summing over each data point, they also assume conditional independence.

Just as for AIC, we could use either the conditional or marginal likelihood with DIC and WAIC (Kai and Yokoi 2019, Merkle et al. 2019). With the Bayesian approach, the likelihood is generally defined as fully conditional on both parameters and latent states and both are generally sampled when sampling the posterior. Thus, the conditional likelihood is usually used with Bayesian metrics even though this is rarely specified (Millar 2018, Merkle et al. 2019). Although computing the marginal likelihood version of these Bayesian metrics is more computationally expensive, their conditional counterparts are often unreliable (Millar 2009, 2018, Merkle et al. 2019). In particular, DIC and WAIC were shown to select the true underlying SSM more reliably when the marginal likelihood is used (Kai and Yokoi 2019).

As Gelman et al. (2014) noted, we are asking close to the impossible from these information criteria measures: an unbiased estimate of out-of-sample prediction error based on data used to fit the model that works for all model classes and requires minimum computation. As such, metrics such as WAIC can be unreliable estimates of the predictive ability of ecological models (Link et al. 2017). Although further research is needed to assess when WAIC is appropriate for SSMs and to identify data partitioning schemes that resolve some of the potential biases, WAIC based on the marginal likelihood is likely the best information criterion for Bayesian SSMs at this point. Future work should explore how promising new approximation methods (see Vehtari et al. 2017, Bürkner et al. 2020) perform with ecological SSMs. If the models are relatively inexpensive to fit, then one can bypass many of the shortcomings of WAIC, and other approximations of predictive ability, by comparing models using more computer intensive cross-validation methods (Gelman et al. 2014, Link et al. 2017, Vehtari et al. 2017). Cross-validation will also require one to partition data intelligently, but this may be more easily implemented with blocking (Gelman et al. 2014, Roberts et al. 2017).

Other methods could be used to compare models in a Bayesian framework (e.g., Newman et al. [2014]). For example, reversible-jump MCMC has been used to compare SSMs (McClintock et al. 2012), but is known to be difficult to implement (Hooten and Hobbs 2015). The importance of multiple covariates in a model (e.g., the effect of temperature and precipitation on bird

survival) can be assessed by multiplying coefficients in a model by indicator variables which when equal to one include the covariate and when equal to zero exclude the covariate (O'Hara and Sillanpää 2009). Such techniques have been used to compare ecological SSMs (Sanderlin et al. 2019), but such an approach is designed for nested models only. Posterior predictive loss approaches appear to be suitable for time-series data (Hooten and Hobbs 2015) and have been used to compare ecological SSMs (Mills Flemming et al. 2010). Although these alternative approaches may not be as commonly used to compare ecological SSMs, and will have drawbacks, many of them warrant further exploration.

Model averaging

Model averaging can combine the strength of several models and account for model uncertainty, something model selection cannot offer (Buckland et al. 1997, Hooten and Hobbs 2015). Wintle et al. (2003) argued against using a single model to make predictions because uncertainty about model structure is often high in ecology, and alternative models can have prediction differences with important repercussions for management decisions. When one selects a single model, and presents the parameter and state estimates based on this best model, one implicitly assumes that the model is true and that the uncertainty is only in the estimation process (Buckland et al. 1997, Wintle et al. 2003). One can instead use model averaging, where, for example, each model is weighted and the predictions are a weighted sum across the plausible models (Wintle et al. 2003). Both the parameters and the predictions could be averaged, but this must be done with care and we would generally caution against averaging parameters. In many cases, differences in model structure result in changing the meaning of parameters, thus making their average nonsensical (Dormann et al. 2018). Model averaging has been used in a few studies applying SSMs to ecological data (e.g., Maunder and Deriso 2011, Moore and Barlow 2011) and was shown to provide unbiased estimates (Wilberg and Bence 2008). However, simulation studies have shown that model averaging may not always provide more accurate point estimates than the best SSMs (Wilberg and Bence 2008, Chang et al. 2015). In addition, although model averaging generally reduces prediction errors compared to each of the contributing models, these gains can be counteracted by factors such as uncertainty in the model weights and covariance between models (Dormann et al. 2018). In addition, calculating weights using parametric methods such as AIC can perform poorly (Dormann et al. 2018). We refer interested readers to a recent review by Dormann et al. (2018), which provides an in-depth discussion of model averaging in ecology.

DIAGNOSTICS AND MODEL VALIDATION FOR SSMs

Although model selection can help us identify which of the fitted models best describes the data, it rarely provides an assessment of the absolute fit of that model. As such, the selected model could be a poor representation of the data-generating process (i.e., could poorly describe the ecological process and/or measurement process) and relative measures of fit, such as AIC, do not quantify how closely the model matches the data. Thus, before interpreting model results, it is crucial to carry out some of the following model diagnostics. First, it is essential to examine whether estimated parameters seem biologically reasonable. For example, our understanding of the system may stipulate that a response variable should increase with a covariate. A model with parameter estimates inconsistent with such *a priori* understanding or with unrealistic effect sizes will be suspect. Second, it is important to assess the influence of individual observations on estimated parameters. For example, outliers can have a strong influence on parameter estimates. Third, one should examine whether the model assumptions are reasonable. For example, with SSMs, assumptions are made about the probability distributions for states and observations (e.g., Eqs. 1, 2 assume both are normal). Fourth, it is important to examine the goodness of fit, which defines how well the model describes the data used to fit the model. At the individual-observation level, goodness of fit measures how far an observation is from its predicted value (e.g., $|y_t - \hat{y}_t|$, $t = 1, \dots, T$). At the model level, it summarizes the overall fit of a model to all observations (e.g., the average squared errors). Fifth, one ought to assess the model's predictive accuracy, or how well the model predicts an outcome for an observation that was not used to fit the model (e.g., via cross-validation). With time-series models, including SSMs, one can use the first t observations to fit the model, and then use the model to predict the $t + 1$ observation, or fit the model to all T observations and see how well future observations are predicted.

Challenges with SSMs

For simple statistical models, such as linear regression, diagnostics for most of the above features are well established. Diagnostics for SSMs, however, can be challenging for two reasons. First, observations are temporally dependent. Many diagnostics rely on response or conventional residuals, which we define as follows for our toy model:

$$e_{t|1:T} = y_t - \hat{y}_{t|1:T}, \quad (52)$$

where $\hat{y}_{t|1:T}$ is the predicted observation at time t given all observations. This predicted value depends on the smoothed-state estimate at time t , $\hat{z}_{t|1:T}$, and the

observation equation. For example, for our toy model (Eqs. 1, 2), $\hat{y}_{t|1:T} = E[y_t | y_{1:T}] = \alpha \hat{z}_{t|1:T}$. Harvey (1990) notes that these response residuals are not serially independent. Their use can impair one's capacity to identify model misspecification (Harvey 1990), and can have negative consequences for model inference and further model diagnosis (e.g., inflated goodness of fit [Thygesen et al. 2017]). Second, as for most hierarchical models, we generally do not have direct observations of the hidden states, z_t ; thus one cannot directly compare predicted states with their "true" values.

Because of these challenges, researchers often fail to check the absolute fit of SSMs, and thus risk making conclusions based on a misspecified model or risk having biased parameter and state estimates. Here, we provide a list of tools to help researchers perform this essential model-checking step. We start with the tools commonly used to assess Bayesian hierarchical models. These tools can be easily used with frequentist and Bayesian SSMs alike, but have important limitations. We then discuss the tools that have been the focus of model validation developments for SSMs, which specifically address the issue of temporal dependence in the residuals. We end with methods relying on out-of-sample validation (e.g., cross-validation), which we believe is the gold standard for assessing the predictive ability of a model, and we hope will become the focus of future developments for SSMs. This order also reflects an increased division between the data used to estimate the model parameters and hidden states and the data used to perform the diagnostics.

Posterior predictive measures

Posterior predictive checking is a common Bayesian method to quantify the discrepancies between the data and the model (Gelman et al. 2013, Conn et al. 2018). It has been used to verify the fit of SSMs to ecological data (e.g., Hobbs et al. 2015). The idea behind posterior predictive checking is that if the model fits the data well, then data generated from the model should have characteristics similar to those of the observed data (Gelman et al. 2013). These posterior predictive checks often involve calculating a posterior predictive P value, p_B :

$$p_B = \Pr(T(\mathbf{y}^i, \boldsymbol{\theta}) \geq T(\mathbf{y}, \boldsymbol{\theta}) | \mathbf{y}), \quad (53)$$

where each \mathbf{y}^i is a time series that has been simulated from the fitted model (i.e., representing a replicate time series that could have been observed from the model), \mathbf{y} is the observed data, $\boldsymbol{\theta}$ contains the model parameters, and $T(\mathbf{y}, \boldsymbol{\theta})$ is a test quantity summarizing the data (e.g., the mean) or a discrepancy function (e.g., χ^2 measure). This P value is similar to the one used in frequentist inference. It measures the probability, under the model of interest, of finding a test quantity as extreme as that associated with the data. Posterior predictive checks use

three steps: (1) sample a set of posterior θ values, (2) simulate one y^i from each, and (3) calculate the test quantity for each y^i . We estimate the P value with the proportion of the replicates that have a test quantity value greater or equal to that of the real data. Posterior predictive P values near 0 or 1 indicate that the pattern observed with the data would be unlikely if the model were true. Thus, unlike P values associated with classic statistical tests used to reject null hypotheses (e.g., t -test), we are seeking a posterior predictive P value close to 0.5 not smaller than 0.05. The relevance of the P value largely depends on the choice of test quantity. Hobbs et al. (2015) used the mean and standard deviation of the observed data, as well as a discrepancy function $\left(T(\mathbf{y}, \theta) = \sum_{t=1}^T (y_t - \hat{y}_{t|1:T})^2 = \sum_{t=1}^T e_{t|1:T}^2\right)$ that measures the disagreement between the SSM and the data. Newman et al. (2014) and Conn et al. (2018) provide lists of important alternative functions. Although we described posterior predictive checks in a Bayesian framework and have defined the test quantity as a function of \mathbf{y} , King et al. (2015) have applied similar concepts in a frequentist framework, using test quantities that describe characteristics of the estimated hidden states, \mathbf{z} (e.g., autocorrelation function at lag 1 of the states).

Although common, posterior predictive P values have important limitations (Conn et al. 2018). Because they use the data twice, once to fit the model and once to test the model fit, they tend to be conservative (i.e., tend to return value closer to 0.5 than to 0 or 1), and often have insufficient power to detect lack of fit. One can alter the method described above and generate all the observation replicates using only a single sample from the posterior parameter distribution. This method was shown to have better theoretical properties (e.g., better Type I error rate control), and to detect lack of fit more reliably for some ecological hierarchical models (Conn et al. 2018). Following King et al. (2015), we recommend assessing discrepancies between the SSM and the data by looking at where $T(\mathbf{y}, \theta)$ falls in the frequency distribution of $T(\mathbf{y}^i, \theta)$ (Fig. 4a, d). This graphical method is also more useful in assessing the ecological importance of the discrepancies than looking at the P value, and can provide a better sense of why the model may be inappropriate for the data (Conn et al. 2018).

Posterior predictive checks are also useful to assess the validity of model assumptions (Gelman et al. 2013). We can use a single sample from the posterior distribution of the hidden states to assess the assumptions associated with the process equation (Thygesen et al. 2017). For example, we can sample a time series of state \mathbf{z}^i from the posterior state distribution of our toy model to calculate the process variation as $\varepsilon_t^i = z_t^i - \beta z_{t-1}^i$, and verify whether the ε_t^i are normally distributed with a mean of 0 as assumed by Eq. 1. Departures from the assumed distribution (e.g., if the mean of the process variation is far

from 0), indicate that the model is not adequate for the data. This method is generally recommended for assessing the assumptions of Bayesian hierarchical models (Gelman et al. 2013), but Thygesen et al. (2017) used the Laplace approximation implemented in TMB to create a posterior distribution of the states for non-Bayesian models.

One-step-ahead residuals and their extensions

The model diagnostic that has received the most attention in the SSM literature is the one-step-ahead residuals (Harvey 1990, Thygesen et al. 2017), also known as recursive residuals (Frühwirth-Schnatter 1996). Unlike the response residuals (Eq. 52), the one-step-ahead residuals should not have temporal dependence when the model is adequate because the residual for the t th observation uses the expected observation at time t given observations only up to time $t-1$:

$$e_{t|1:t-1} = y_t - \hat{y}_{t|1:t-1}. \quad (54)$$

Effectively, for response residuals (Eq. 52) we use the smoothed estimates of states, $\hat{z}_{t|1:T}$, to predict the observation at time t , whereas for one-step-ahead residuals, we use the prediction of the states, $\hat{z}_{t|1:t-1}$. In the context of a Kalman filter, we can calculate $\hat{y}_{t|1:t-1}$ using the one-step-ahead forecast prediction that is already calculated as part of the recursive algorithm. As more information is available for fitting the model as t increases, the variance of prediction residuals will tend to decrease with t . To account for this change in variance, it is useful to scale the prediction residuals by their standard deviations (a procedure equivalent to calculating standardized Pearson residuals):

$$\tilde{e}_{t|1:t-1} = \frac{e_{t|1:t-1}}{sd(e_{t|1:t-1})}. \quad (55)$$

For the special case of SSMs with normally distributed states and observations, such standardized residuals are independent and identically distributed with a standard normal distribution and can be used to test a variety of assumptions. Diagnostic procedures include qq-normal plots to check for normality, autocorrelation function plots to see if the residuals are independent, and plots of the residuals against observed values to check for non-constant variance.

For nonnormal SSMs, the probability distribution of these standardized one-step-ahead residuals are not standard normal, making the exploration of residuals harder. Probability scores (P scores), and their transformed version, prediction quantile residuals, are useful alternatives (Frühwirth-Schnatter 1996, Thygesen et al. 2017). A P score, u_t , is the cumulative distribution function for the predicted observations evaluated at the t th observed value:

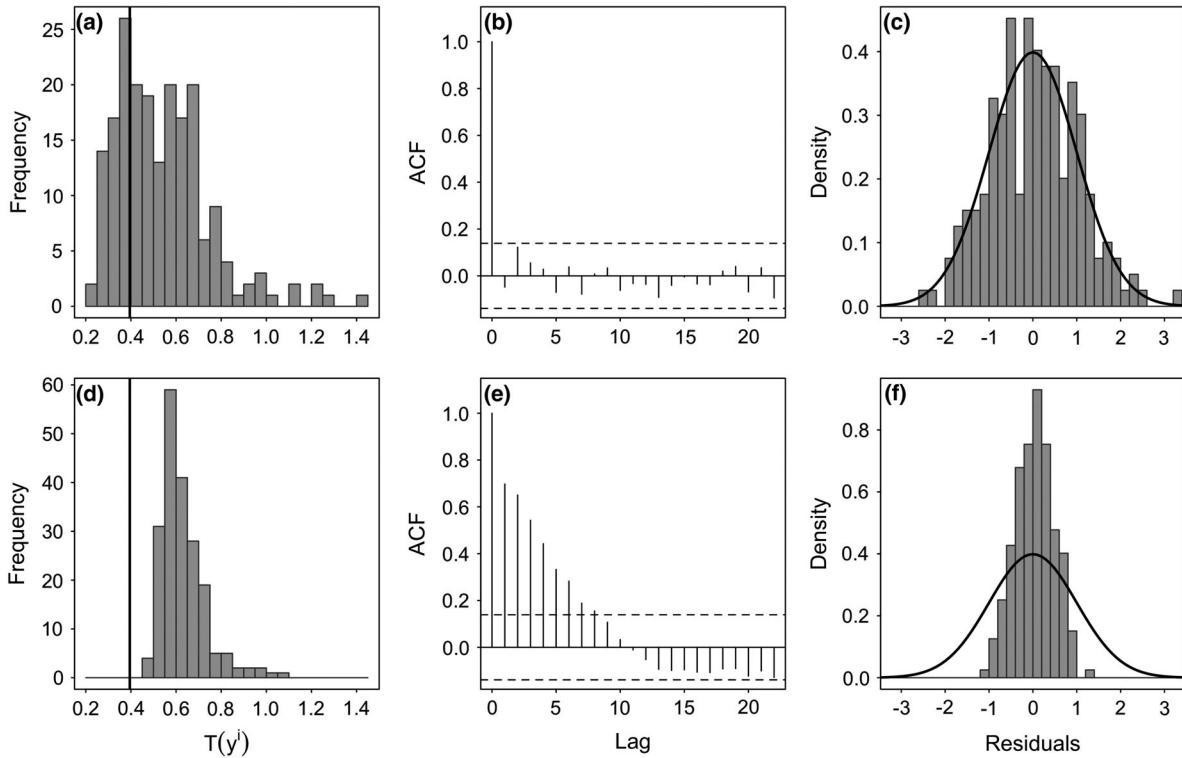


FIG. 4. Examples of diagnostic plots for a well-specified (a, b, c) and a misspecified model (d, e, f). The data for all plots were simulated from the toy model (Eqs. 1, 2) with $\alpha = \beta = 1$ and the $\sigma_p = \sigma_o = 0.1$. The correctly specified model used the correct known values of α and β , and estimated σ_p and σ_o . Although the misspecified model also used the correct known values of α and β , it wrongly assumed a value of $\sigma_o = 0.5$ and then estimated σ_p . (a), (d) A frequentist version of the posterior predictive check, where the test quantity is the standard deviation of the observations, $T(\mathbf{y}) = \sqrt{\sum_{t=1}^T (y_t - \bar{y})^2 / (T - 1)}$. The histograms represent the frequency of test quantity for 200 data sets simulated using the estimated parameters with the original data set. The vertical bar is the test quantity for the original data set. (b), (e) The autocorrelation function (ACF) of the one-step-ahead residuals. (c), (f) Comparison of the distribution of the observed one-step-ahead residuals (histograms) to a standard normal probability density function (curves).

$$u_t = F_{Y_t|y_{1:t-1}}(y_t) = \Pr(Y_t \leq y_t | Y_{1:t-1} = y_{1:t-1}). \quad (56)$$

If $F_{Y_t|y_{1:t-1}}$ describes the cumulative distribution function of the true model, then the resulting u_t are uniformly distributed (Conn et al. 2018). Deviations from uniformity suggest model misspecification. As this is simply an application of the probability integral transformation (i.e., if Y has the cumulative density function F_Y , then $F_Y(Y)$ is distributed with $\text{Uniform}(0,1)$ [Smith 1985]), these are a specific case of probability integral transform (PIT) residuals (Warton et al. 2017). To get normally distributed residuals, we can transform the P scores to prediction quantile residuals, v_t , as follows:

$$v_t = \Phi^{-1}(u_t), \quad (57)$$

where Φ^{-1} is the inverse of the standard normal cumulative distribution function (also known as the standard normal quantile function). When the model is true, v_t should be an independent sample from a standard normal. Thus, we can assess whether the data fit the model

assumptions using the same diagnostic procedures available for standardized one-step-ahead prediction residuals in the case of normally distributed SSMs (see Fig. 4b, c, e, f and Newman et al. [2014], Thygesen et al. [2017]).

P scores and prediction quantile residuals can be difficult to estimate for nonnormal SSMs because their calculation requires knowledge of the cumulative distribution function (cdf) for $Y_t|y_{1:t-1}$, which in many cases will not be known nor have an analytical form. However, Thygesen et al. (2017) developed methods for approximating the cdf based on the Laplace approximation that can be implemented easily in TMB. Because this method depends on the Laplace approximation, it is important to assess the accuracy of this approximation (see Appendix S1: Section S1.2.3). The quantile residuals of Thygesen et al. (2017) are applicable to a broad range of frequentist SSMs, although there are some limitations in using them with multivariate time series. We are not aware of equivalent methods for as broad a range of Bayesian SSMs, although some exist for a limited class (Frühwirth-Schnatter 1996, Gamerman et al. 2013).

Cross-validation

Although one-step-ahead residuals and their extensions remove data when calculating the expected value of the observation at time t , they use the complete data set to estimate the model parameters. Thus, these residuals cannot be used to assess the predictive ability of the model fully. Assessing the predictive ability of a model is thought to be best achieved with out-of-sample data, where two independent data sets are used: one to fit (or train) the model and one to validate (or test or evaluate) it (Hooten and Hobbs 2015). Although rarely done with SSMs, there are examples where independent information on the true values of the hidden states was collected (e.g., Auger-Méthé et al. 2017; Appendix S1: Section S2.2), a data stream was used as validation data (e.g., Hobbs et al. 2015), or part of a time series was selected as a validation time period (e.g., Holdo et al. 2009).

When using a single subset of the data as validation, we can only assess the predictive ability for those specific observations. Instead, one can use cross-validation methods that look at the predictive ability of all data points by sequentially leaving out small subsets of the data (Hooten and Hobbs 2015). k -fold cross-validation is a ubiquitous statistical method, where k groups of similar size sequentially serve as the validation data set, and the remaining $k-1$ groups are collectively used as the training set. Leave one out is a common version that leaves each of the data points out sequentially. To assess the predictive ability of the model, we can use score or discrepancy functions, such as the mean-squared prediction error (MSPE) for group k :

$$\text{MSPE}_k = \sum_{i=1}^n (\mathbf{y}_{i,k,\text{oos}} - \hat{\mathbf{y}}_{i,k,\text{oos}})^2 / n, \quad (58)$$

where we assume that T/k is an integer n , oos means out of sample, $\mathbf{y}_{i,k,\text{oos}}$ is the i th observation in subsample k , and $\hat{\mathbf{y}}_{i,k,\text{oos}}$ is the expected observation based on the model fitted to the data set without sample k . As an overall value, we can then average the k MSPE_k . Such functions directly assess the predictive ability of the model and thus are intuitive measures of how good a model is.

As mentioned in *Computationally Efficient Model Comparison Methods*, cross-validation is also often deemed the preferred method for model comparison (Gelman et al. 2014, Hooten and Hobbs 2015). The model set can be ranked based on predictive accuracy, with better models having lower prediction error (e.g., lower MSPE or its square root, RMSPE [Hooten and Hobbs 2015]). Although cross-validation can be implemented relatively easily, it can be computationally demanding (Link and Sauer 2016, Vehtari et al. 2017). Cross-validation generally requires refitting the models k times, which can be a daunting task with Bayesian models (but see Hooten and Hobbs 2015, for suggested

solutions). In addition, cross-validation assumes that the training and evaluation data sets are independent (Roberts et al. 2017). The main challenge with using cross-validation with SSMs is that, because of the temporal dependency in the data, removing only a few data points will underestimate the prediction error and removing many will lead to propagation of error (Newman et al. 2014).

Despite these drawbacks cross-validation is a powerful tool, which has been promoted for use with complex ecological models (Link et al. 2017). At present, there are few cross-validation methods specifically designed to handle the dependency structure of SSMs (Ansley and Kohn 1987, de Jong 1988). These are appropriate for only a restricted set of SSMs and appear to be rarely used. However, the time-series literature (e.g., Tashman 2000, Bergmeir and Benítez 2012, Bürkner et al. 2020) and the suggestions of Roberts et al. (2017) on block cross-validation methods to account for dependence structure in ecological data are useful starting points for the development and evaluation of such methods for SSMs. Cross-validation methods for time series include procedures analogous to the one-step-ahead residuals (*One-step-ahead Residuals and Their Extensions*), but where model parameters differ across the k folds and are estimated using only observations prior to the expected values (Hyndman and Athanasopoulos 2018). One may need to consider additional modifications, such as whether one should use a rolling window for the training data set (Tashman 2000).

The topic of model validation for SSM is one that has been relatively poorly studied, with a few notable exceptions (e.g., Frühwirth-Schnatter 1996, King et al. 2015, Thygesen et al. 2017). Because of the additional parameter identifiability and estimability problems discussed in *Formulating an Appropriate SSM for Your Data*, we believe this topic deserves more attention. Beyond the tools we have outlined, SSM developers and users can gain inspiration from the tools developed for hierarchical models (PIT-trap residuals [Warton et al. 2017]). For researchers using Bayesian SSMs, we point readers towards the review of Conn et al. (2018) on model-checking methods for Bayesian hierarchical models. Finally, we would like to remind readers that, although it is crucial to perform a model validation step, passing this step does not mean that the model is representing the truth. It simply means that one could not find difference between the data-generating system and the model. This could be due to a low sample size or the conservative nature of some of the methods described.

CONCLUSION

Through a diverse set of examples, we have demonstrated that SSMs are flexible models for time series that can be used to answer a broad range of ecological questions. They can be used to model univariate or

multivariate time series. SSMs can be linear or nonlinear, and have discrete or continuous time steps. They can have normal or nonnormal sources of stochasticity, and thus can model continuous, count, binary, or categorical data. They are particularly useful when one has significant process variation and observation error. Accounting for these sources of uncertainty can substantially affect management decisions, making SSMs the perfect modeling tool in many contexts (e.g., Jamieson and Brooks 2004, Hobbs et al. 2015).

As we have outlined, a variety of tools to fit SSMs to data exist. Historically, many researchers wrote SSMs so they could be fitted with the Kalman filter and its extensions. However, the diversity of fitting procedures available now allows researchers to create models that are more representative of the structure of their data and the ecological processes they are interested in. In addition, flexible fitting tools now exist in both the frequentist and Bayesian frameworks, allowing researchers to choose their preferred inferential framework rather than have their model dictate the framework they can use. Within each inferential framework, the choice of a fitting procedure will be a compromise between flexibility and efficiency. In particular, highly efficient fitting methods (e.g., Laplace approximation and Hamiltonian Monte Carlo) have more restrictions than their slower alternatives (e.g., particle filter and Gibbs samplers).

Although these tools provide the means to fit complex SSMs, it is crucial to formulate the model appropriately. As discussed, SSMs can suffer from parameter estimability problems, but various tools exist to assess whether this is the case and to identify the type of study design or model simplification that will resolve these problems. In general, making use of replication or including covariates can help reduce some of the common estimation problems.

Researchers often forgo doing model selection and validation with SSMs, but we advocate that these should become part of every SSM user's workflow. Model misspecification can affect ecological inferences and the accuracy of state estimates. Although no model selection measure is perfect for SSMs, AIC and WAIC can be useful. Although model validation is also difficult with SSMs, posterior predictive measures and one-step-ahead residuals and their extensions are relatively easy ways to assess whether the model describes the data well and whether some of the model assumptions are met. Cross-validation methods are often computationally expensive, but provide one of the best ways to select and evaluate models when correlation is handled appropriately.

Although there are many tools already available to fit, compare, and validate SSMs, five topics warrant further research. First, although we advocate that SSMs be a default framework to model many ecological time series, it is important to pinpoint the conditions under which simpler alternatives perform adequately (e.g., when do models without observation error provide reliable parameter and state estimates?). Such research should account for

the additional identifiability and estimability issues that comes with fitting SSMs and the types of data sets that allow SSMs to return reliable estimates. Second, as SSMs are often the primary tools used to analyze time series, it is important to explore the data-collection designs that optimize the estimation of SSMs, so that the best data possible are collected. Third, there is a need for further developments of computationally efficient model selection procedures for SSMs. Using the marginal likelihood with AIC and WAIC appears most adequate for SSMs, especially if one has a single observation time series. However, we should explore when the conditional likelihood can be used and whether it affects the predictive accuracy of the states and parameters differently. To facilitate the uptake of WAIC based on the marginal likelihood, new R functions that automatically calculate this information criterion should be written. In addition, it would be helpful to explore how newer tools to approximate predictive ability (e.g., Vehtari et al. 2017, Bürkner et al. 2020) perform with SSMs. Fourth, although there have been a few important advances in model validation methods for SSMs, this remains a relatively untouched research area. Given the increasing use of SSMs in management, it is crucial that a broader range of validation methods be developed for these complex models. Fifth, with the increasing efficiency of fitting procedures, cross-validation is becoming a feasible procedure to assess predictive accuracy and compare models. As such, the time is ripe to start developing proper cross-validation procedures that will account for dependencies in the data.

Overall, we provided a review of the topics needed to formulate and fit SSMs to ecological data, and Appendix S1 provides an extensive set of examples of methods to facilitate this process. We hope this guide will help researchers develop and apply SSMs to their own data, and foster the development of SSMs in multiple fields of ecology.

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SUPPORTING INFORMATION

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Data (Auger-Méthé and Derocher 2021) are available from the Dryad Digital Repository. <https://doi.org/10.5061/dryad.4qrfj6q96>