- Smoothed factor analysis for identifying trends in multivariate time
- series

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2 Abstract

Ecological processes are rarely directly observable, and for most systems, variance parameters must be 13 estimated from data. State space models have become widely used in the environmental sciences, particularly for time series data, because of their ability to simultaneously estimate multiple sources of variation (process 15 or natural variability, and variance attributed to observations, associated with measurement and sampling errors). A common state space approach for using multivariate time series to identify underlying signals is 17 dynamic factor analysis. The conventional dynamic factor analysis model is flexible in that unseen processes 18 are modeled as random walks. Whereas this may be suitable for some situations, random walks may be too flexible for other cases. In this paper, we introduce a new class of models, where latent processes are modeled as smooth functions. We highlight two alternatives to the random walk approach, using basis splines and 21 Gaussian predictive process models. These models are applied to two long-term datasets from the west coast 22 of the United States: (1) a 35-year dataset of juvenile rockfishes from the west coast of the United States, and (2) a 39-year dataset of fisheries catches. Estimation and model selection is done in a Bayesian framework, 24 with code provided as an R package. For both applications we find that the smooth trend models have higher predictive accuracy and yield more precise predictions, compared to the conventional approach.

27 Key words

28 Dynamic factor analysis, smooth spline, B-spline, Gaussian process, Bayesian modeling, Stan

29 Introduction

Ecological data can be characterized by multiple sources of variability, including stochastic natural variation, and errors associated with data collection (observation, sampling, and measurement errors). Disentangling these sources of variability is often challenging, and necessitates the use of statistical methods, such as state space models. These approaches have become ubiquitous in ecology, particularly for time-series data (Auger-Méthé et al. 2020)—in part because these models allow researchers to make inferences about ecological processes that are not directly observable. Applications of these models include estimating population change over time (Clark and Bjørnstad 2004), movement dynamics (Patterson et al. 2008), and understanding spatiotemporal variation (Anderson and Ward 2019).

Estimating multiple sources of variation in state space models is numerically complex, and can be constrained explicitly or implicitly in ecological models via model assumptions. For example, discrete-time state-space models of population trajectories generally assume latent population size n_t at time t can be approximated by an autoregressive process in log-space, $x_{t+1} = f(x_t) + \epsilon_t$, where f() represents some function, $x_t = \log(n_t)$, and ϵ_t are normally distributed process deviations representing stochastic variability 42 of the natural system (Dennis et al. 2006). The autoregressive assumption is critical here; without such a constraint, the variance of the stochastic noise ϵ_t is not estimable in the presence of an observation or data model. Separating these sources of variability is critical to generating unbiased estimates of population trends or density dependence (Knape 2008). If inference is not dependent on parameters of ecological interest (e.g., growth rates, density dependence), a wide range of alternative semi-parametric approaches exist that can be used to model the trajectory of x_t , including generalized additive models (GAMs, Wood 2011) and Gaussian process models (Roberts et al. 2013). Because these models are not autoregressive with discrete time steps, the flexibility or 'wiggliness' of the model can be adjusted as part of the model fitting. In addition to their flexibility, these semi-parametric models may be better suited for situations when data are patchily distributed in time or unequally spaced, making estimation of process and observation errors more difficult. 52

Challenges posed by univariate time-series models also apply to multivariate time-series models, with the additional complexity that the number of latent time series may be variable, k = 1, ..., m, where m is the number of time series observed. At one extreme, k = m, and each time series corresponds to a unique latent state. Motivating questions in analyzing these kinds of data include estimating correlated latent processes or trends, or estimating effects of environmental covariates on sub-populations (Hovel et al. 2017). At the other extreme, k = 1, where each time series represents replicates or multiple measurements of the same trajectory of states, with optional offsets or coefficients included for each time series (e.g., offsets allowing for differing detectability). Applications focused on estimating a single trend from multivariate data include the development of ecological indicators. Models with intermediate numbers of latent states 1 < k < m require mapping of time series to latent trends. These may be specified a priori (Ward et al. 2010) or estimated within the modeling framework using dimension reduction techniques.

Many statistical approaches have been proposed in recent years for clustering or estimating common 64 signals in multivariate time series (Liao 2005). Examples include clustering based on similarities among time series features (Sardá-Espinosa 2019), identifying common patterns in the frequency domain (Holan 66 and Ravishanker 2018), and clustering based on neural networks (Cherif et al. 2011). Application of these methods to ecological data has been limited, however, in part because many of these approaches identify clusters from raw data and ignore observation error. An alternative approach that has been used in ecology to map collections of multivariate time series to latent states, while accounting for observation error, is dynamic factor analysis (DFA) (Zuur et al. 2003b, 2003a). DFA is an extension of factor analysis for time 71 series data, and estimates a small number of unobserved processes, referred to as trends, that can describe observed data. Mapping time series to trends is done via estimated factor loadings—these allow each time 73 series to be modeled as a mixture of the estimated latent trends, rather than assigning each time series to a single trend. 75

To date, applications of DFA models in ecology and other fields have assumed that underlying trends are modeled as a random walk, $x_{t+1} = x_t + \epsilon_t$. The objective of this analysis is to introduce a new class of DFA models for multivariate time series. Just as the univariate autoregressive model described above can be approximated with smooth functions, DFA models may be extended to use smooth functions in lieu of autoregressive processes. Recent work has highlighted the application of hierarchical GAMs for multiple data sources (Pedersen et al. 2019). These approaches are flexible and likely to provide similar inference to DFA for single latent trend; however, these methods have not been extended to include more than one process. We illustrate two options for modeling smooth functions for latent trends: basis splines ('B-splines') and Gaussian process models. We compare both approaches to conventional autoregressive DFA models for two datasets on marine fishes from the west coast of the USA. All data and code for replicating our analysis are available on Github ($link\ here$) and Zenodo ($link\ here$), and in our existing R package 'bayesdfa' (Ward et al. 2019).

88 Methods

89 Dynamic Factor Model

The basic DFA model can be written as a multivariate state space model, consisting of a latent process model and observation or data model. In its simplest form, the process model is expressed as a random walk, $\mathbf{x}_{t+1} = \mathbf{x}_t + \mathbf{w}_t$, where $\mathbf{w}_t \sim \text{MVN}(\mathbf{0}, \mathbf{Q})$. For identifiability constraints, the covariance matrix \mathbf{Q} is generally constrained to be an identity matrix (Holmes et al. 2012, Zuur et al. 2003b). Additional features may be incorporated into the process model, including autoregressive or moving average coefficients, covariates, or deviations that are more extreme than that of the normal distribution (Ward et al. 2019). The observation model in a DFA is expressed as a linear combination of trends \mathbf{x}_t and a matrix of loadings coefficients \mathbf{Z} , $\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{B}\mathbf{d}_t + \mathbf{e}_t$. In addition to the trends and loadings, time-varying covariates \mathbf{d}_t may be optionally included and linked to the observations through estimated coefficients \mathbf{B} . The vector \mathbf{e}_t represents residual observation error, which is typically modeled as a diagonal matrix, $\mathbf{e}_t \sim \text{MVN}(\mathbf{0}, \mathbf{R})$, although off-diagonal elements may be estimated (Holmes et al. 2020). Further details of the Bayesian implementation of the DFA model and extensions are provided in Ward et al. (2019).

102 Modeling trends as Gaussian processes

Conventional DFA models with trends modeled as random walks are flexible, but for some datasets these 103 models may be too complex. As a first alternative approach to the random walk model, we treat the trends as a Gaussian process. A discrete-time Gaussian process model of trends treats the vector representing the $k^{\rm th}$ 105 trend as a stochastic process, where \mathbf{x}_k is drawn from a multivariate normal distribution. As data in a DFA are generally standardized (mean 0, standard deviation 0), we can assume the mean of each trend to be 0, and 107 all inference about the Gaussian process centers around the covariance matrix, $\mathbf{x}_k \sim \text{MVN}(\mathbf{0}, \Sigma)$. Rather than estimate each element of Σ independently, smooth covariance functions or 'kernels' are chosen to represent the 109 covariance between points in time (typical choices include the exponential, Gaussian, and Matérn functions). For the purpose of our DFA modeling, we adopt a Gaussian kernel. With this kernel, the covariance 111 between points i and j at times t_i and t_j on trend k can be expressed as $cov(x_{i,k}, x_{j,k}) = \sigma_k^2 \exp\left(\frac{-(t_i - t_j)^2}{2\theta_k^2}\right)$, 112 where σ_k controls the magnitude of variation, and θ_k controls how smoothly correlation decreases as time 113 points become further apart. We allow each trend to have its own covariance parameters (θ_k, σ_k) , allowing 114 each to have differing degrees of smoothness. Because of potential computation issues in high dimensionality 115 problems such as spatial models (Latimer et al. 2009, Anderson and Ward 2019), we also allow this Gaussian 116 process model to be expressed as a Gaussian predictive process model. The difference between the predictive 117 process approach and the full Gaussian process model is that instead of modeling the \mathbf{x}_t themselves as 118

random variables, random variables are modeled at a subset of locations \mathbf{x}_k^* (referred to as 'knots') and projected to the locations of the data \mathbf{x}_k . If we assume $\mathbf{x}_k^* \sim \text{MVN}(\mathbf{0}, \Sigma^*)$, then this projection can be done as $x_k = \Sigma'_{k,k^*} \Sigma^{*-1} x_k^*$, where the matrix Σ'_{k,k^*} is the transpose of the matrix describing the covariance between x_k and x_k^* . The location of k^* can be spaced equally or depend on data; for the purposes of our DFA modeling, we assume that the k^* are equally spaced within each time series (with the endpoints also acting as knots).

25 Modeling trends as splines

As an alternative model of latent trends in a DFA, we use a series of smoothing functions, known as basis splines ('B-splines'). These models can be thought of as a special case of Gaussian process models (Kimeldorf 127 and Wahba 1970), and offer flexibility similar to the more familiar generalized additive models (Wood 2011). B-splines are represented as a series of piecewise polynomial functions, where higher order polynomials 129 result in more flexible curves (Hastie 1992). A common choice of the order of these polynomials is a cubic or 3rd degree, and will be the focus of our implementation for DFA models. An additional input to B-131 splines is the locations of the control points between polynomial segments—more control points translate 132 into a more flexible function, but also one with more parameters to estimate. Similar to Gaussian process 133 models, the locations of these control points are referred to as knots, and are generally selected within the 134 temporal domain of the data. For our applications to DFA, we assume knots to be uniformly distributed 135 over the time series. Uniform knot vectors may be appropriate for data collected at regular intervals, but for 136 observations more patchily distributed in time, distributing the knots based on quantiles or other metrics may be warranted. Mathematically, modeling the trends in a DFA with B-splines can be expressed as a linear 138 combination of the B-spline weights $\bf B$ and estimated coefficients $\bf a,\, x_k=aB$. The matrix $\bf B$ is generated from the raw data prior to estimation. In the DFA setting, ${f B}$ is shared across trends, but for trend-specific 140 variability, we allow the coefficients **a** to have a variance parameter unique to each trend, $\mathbf{a}_k \sim \text{Normal}(0, \sigma_k^2)$. 141

Application: 1-trend models of larval fish dynamics

As a first application of smooth factor analysis models, we apply DFA to a long term time series of larval fishes collected in Southern California (USA). The California Cooperative Oceanic Fisheries Investigations (CalCOFI) survey has been collecting physical and biological samples since 1949, to monitor annual, seasonal, and spatial changes to the California Current Ecosystem (Bograd et al. 2003). The CalCOFI data have been incorporated into models used to assess population status (MacCall 2003), and numerous publications have used time series of larval fishes from the CalCOFI survey as indicators of ecosystem state (Mcclatchie et al. 2008). These types of motivating questions also present an opportunity to apply DFA with both

conventional and smoothed trends to summarize ecosystem state indices. For this application, we focus on
the dynamics of three species of juvenile rockfishes: aurora rockfish (*Sebastes aurora*), shortbelly rockfish
(*S. jordani*), and bocaccio rockfish (*S. paucispinis*). For the purposes of this analysis, we restrict the time
series to data collected since 1985, when sampling has been consistent in space and time (Moser et al. 2001).
Though CalCOFI cruises are done throughout the year, we are primarily interested in estimating interannual
trends, and thus restrict our analysis to considering spring cruises from 1-April to 22-May when densities of
most rockfish species are highest (Mosek et al. 2000). All data were retrieved using the software R (R Core
Team 2020) and the 'rerddap' package (Chamberlain 2020).

With only three time series, we focus on identifying models estimating a single shared trend and 158 single observation error variance, shared across species. Other types of models, including hierarchical GAMs 159 (Pedersen et al. 2019) or models allowing estimated offsets may also be useful in this type of application. 160 Where the DFA model differs is that unlike models with random intercepts or additive offset terms, the 161 DFA factor loadings **Z** are multiplicative and may be close to zero. These cases may arise when a particular 162 time series has a low signal to noise ratio, or if there is low correspondence with the latent trends estimated among all other time series. In addition to estimating a conventional 1-trend DFA model with a latent 164 autoregressive process, we evaluate 1-trend B-spline and Gaussian process models. Because we have no a priori hypotheses about the complexity of these smoothed factor models, we evaluated a range of models for 166 each (Table 1), using equally spaced knots.

Application: 2-trend models of commercial fisheries catches

As a slightly more complex example of the smooth factor analysis model, we examine the performance of 2-trend models, using a dataset of commercial fisheries catches (landings) from the west coast of the USA. 170 This dataset consists of 13 species or groups reported annually over a 39 year period (1981–2019)(PFMC 2020). Landings on the west coast are dominated by Pacific hake (also Pacific whiting, Merluccius productus). 172 but also include substantial catches of rockfishes (Sebastes spp.) and flatfishes (e.g., Dover sole, Solea solea). Over the course of the last 4 decades, these species have experienced variability associated with population 174 dynamics and the environment, but the patterns of landings also reflects a dynamic fisheries management 175 process. Examples of changes include temporarily closing areas to fishing to protect species of conservation 176 concern, and implementing catch share programs. These processes, combined with environmental conditions 177 that have been positive for many species have resulted in many increasing populations (Warlick et al. 2018). Given these various management and ecological changes, it is important to summarize patterns of landings, 179 and identify common trends as indicators for management and ecosystem status (Harvey et al. 2018).

As with our previous example, we compared conventional DFA models to those modeling the trends with smooth functions. Preliminary model fitting suggested that 2-trend models were most supported by the data, and thus will be the focus of our analysis. In addition to modeling the 2-trend model with conventional DFA, we evaluated B-spline and Gaussian process models with equally spaced knots (Table 1). All models included a single observation error variance, shared across time series.

186 Estimation and model selection

We developed our smooth trend DFA model, extending an existing approach that implements conventional 187 DFA in a Bayesian framework (Ward et al. 2019). Estimation in the 'bayesdfa' package is done using Stan and the package R package 'rstan' (Stan Development Team 2016), which implements Markov chain Monte Carlo 189 (MCMC) using the No-U Turn Sampling (NUTS) algorithm (Hoffman and Gelman 2014, Carpenter et al. 2017). For each model considered, we ran 3 parallel MCMC chains for 4000 iterations each, discarding the first 191 50% of the samples. We assessed convergence using split-R and effective samples size (Gelman et al. 2013) 192 along with trace plots. Following previous approaches, we used the Leave One Out Information Criterion 193 (LOOIC, Vehtari et al. 2017, 2020) as a model selection tool (Ward et al. 2019), which approximates Leave 194 One Out Cross Validation. Preliminary model checks using LOOIC for the models included in our analysis indicated that many models had 1-4 data points that had high Pareto-k statistics (possibly because of model-196 misspecification or model flexibity, Vehtari et al. (2017)). To avoid re-fitting these models, we implemented moment matching in the loo package (Vehtari et al. 2020, Paananen et al. 2021). 198

199 Results

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For our application of smooth dynamic factor models to the CalCOFI juvenile rockfish dataset, we found 200 that the full rank Gaussian process DFA model had slightly lower LOOIC values compared to alternative 201 models (Table 1), with most performing better than the conventional DFA model. Varying the number of 202 knots for the B-spline and Gaussian process models resulted in similar predictions and data support between 203 the two smooth trend approaches (Table 1). Varying the number of knots did allow for greater flexibility, 204 however, allowing for more complex models to better capture recent variability in rockfish densities (Fig. 1). 205 Trend 1 can be seen as largely capturing the variability in the timeseries of aurora rockfish, which had the loading that was largest in magnitude (0.6, 90% credible interval = 0.04-2.14). Bocaccio rockfish also loaded 207 positively on trend 1, though the effect was weaker (0.53, 90% credible interval = -1.07-2.31). The loading for shortbelly rockfish was smallest in magnitude (0.25, 90% credible interval = -1.44-1.66). 209

When smooth-trend B-spline and Gaussian predictive process models were applied to commercial fish-

eries landings data, the model with the lowest LOOIC was the B-spline model with 6 knots. The first trend 211 exhibited nearly linear change from 1981–2001 and was relatively stationary from 2001–2019 (Fig. 2). The second trend represented change from the early 1990s, with the strongest change occurring 2010-present. 213 Estimates of the loadings from this B-spline model indicated many species or species groups loaded negatively on trend 1 (lingcod, sablefish, rockfishes), but Arrowtooth flounder and Pacific whiting had opposite 215 loadings (Fig. 2). Trend 2 from this model appeared to contrast species with relatively stationary catches before declining in 2010 (e.g., Arrowtooth flounder, Atheresthes stomas) versus Petrale sole (Eopsetta jor-217 dani)—one of the only non-whiting species that has experienced positive catches since 2010. Predictions 218 across all models appeared to characterize the trends of most species, and trends from the B-spline model 219 generated more precise predictions relative to the random walk, although neither model was able to capture 220 the variability in Pacific whiting catches since 2000 (Fig. 3). 221

While low dimensional Gaussian process and B-spline models perform similarly (Table 1), comparing higher order models highlights an interesting contrast between these two smooth approaches. As more knots are added to the B-spline model of fisheries landings, the wiggliness of the estimated trends generally increases (Fig. 4). The opposite is generally true of the Gaussian process model for this application, with trends becoming smoother as more knots are added (Fig. 4). Estimates of θ_k for this Gaussian process model are relatively large (8.32, 4.4), allowing correlation between neighboring points to decrease slowly and neighboring points further away to have a larger effect. In contrast, the full rank Gaussian process model was most supported for the CalCOFI data – this model had a relatively small value of $\theta_k = 1.12$, allowing correlation between adjacent points to decrease rapidly, translating into greater flexibility.

Discussion

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Dynamic factor analysis (DFA) represents a flexible approach for using state space models to capture latent 232 processes in multivariate time series (Zuur et al. 2003b, 2003a). For some ecological processes – particularly 233 those with high variability - random walks may be too constraining, while for others, using a random walk 234 may be overly complex. Examples of cases where random walks may overfit trends may exist when there 235 are large temporal gaps between observations, or data are collected from systems with high signal to noise 236 ratios. As alternatives to the conventional random walk, we illustrate how DFA trends may be modeled using Gaussian process models or B-splines. Both of these alternatives are flexible in that their smoothness may be 238 specified a priori by the user, and compared via model selection. As the variability of latent trends is nearly always fixed in a conventional DFA for identifiability (Holmes et al. 2012, Zuur et al. 2003b), adopting 240 an alternative model of the trend does not limit inference or change the meaning of other parameters (e.g., loadings).

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In both of our case studies comparing smooth DFA models to conventional ones, we found that using 243 smooth functions to model DFA trends resulted in models with higher predictive ability (as measured with LOOIC). Our two case studies contrast two datasets with different degrees of variability. The CalCOFI 245 dataset on juvenile rockfish abundance represents data with relatively high variability – both because of the sampling process, and because the nature of fish recruitment is stochastic. In comparing conventional 1-trend 247 DFA versus smooth trend DFA models to the CalCOFI data, the conventional random walk had difficulty in capturing extremes (Fig. 1), while the B-spline and Gaussian process models generally did better (Table 249 1). Our second example consisted of applying DFA models to time series of fisheries catches; this data is generally less variable than the CalCOFI data because catches are aggregated across space and individual 251 vessels. Like the CalCOFI example, we found that smooth trend DFA models were better supported over 252 the conventional random walk, however the models receiving the most support were lower dimension models 253 (e.g. B-spline with 6 knots, Table 1). For both of our case studies knot locations were assigned uniformly, 254 and these results would be expected to change slightly if the knot locations were adjusted. For models 255 with missing data, or datasets with unevenly distributed replicate samples, it may be important to consider 256 non-uniform knot vectors.

Because of their flexibility, applications of LOOIC or related model selection tools to state-space models, including the DFA models in our analysis, may result in poor diagnostics (e.g. high Pareto-k statistics). Though not explored here, alternative approaches for evaluating predictive performance may be used, including the expected log posterior density (ELPD) (Vehtari et al. 2020, 2017). Rather than performing parameter estimation once per model, as was done in our analysis, calculating ELPD is more computationally challenging because with cross-validation, a model must be fit once per fold. With this added cost comes new opportunities, in that cross validation methods specific to time series data may be more easily applied. Commonly used approximations like LOOIC represent an approximation to cross validation where each data point is held out in turn. An alternative approach for time series data is that the observations in each time step can be treated as a fold, and held out in turn. Extensions of this time series approach include leave-future-out cross-validation, where data points are only used to predict future observations, not historical ones (Bürkner et al. 2020). While the specific tool used to assess model performance may be tailored to the research questions being addressed, the types of flexible trend models included in our analysis represent a robust approach for DFA that may also be considered in hindcasting or forecasting scenarios.

Tables

Table 1. Approximate Leave One Out Information Criterion (LOOIC, with standard errors in parentheses)
for each of the models applied to our cases studies (CalCOFI time series of juvenile rockfishes, and the time
series of commercial groundfish landings from the west coast of the USA). The B-spline models are generated
with basis splines, and the Gaussian predictive process models are generated using a Gaussian covariance
function. For each model, knots (or locations of control points) are assumed to be uniformly spaced over the
time series. To aid in interpretation, the minimum LOOIC value across models has been subtracted from
each case study.

Trend.model	Knots	CalCOFI	Landings
Random walk	NA	16.46 (12.37)	27.56 (49.21)
B-spline	6	13.61 (12.14)	0 (54.64)
B-spline	12	16.73 (12.28)	2.46 (50.72)
B-spline	18	14.56 (11.99)	17.01 (49.72)
B-spline	24	11.34 (12)	30.74 (48.22)
B-spline	30	10.06 (12.07)	49.94 (47.68)
Gaussian process	6	13.95 (12.41)	3.3 (53.64)
Gaussian process	12	15.13 (12.33)	3.34 (53.81)
Gaussian process	18	14.53 (12.29)	6.24 (53.31)
Gaussian process	24	13.79 (12.39)	6.26 (53.38)
Gaussian process	30	13.32 (12.68)	6.75 (53.26)
Gaussian process	Full rank	0 (13.59)	4.48 (53.42)

Figure Captions

Figure 1. Standardized densities of juvenile shortbelly rockfish collected in the CalCOFI survey, and estimates
of latent trends for three candidate models, representing a range of flexibility in splines compared to the
conventional random walk. In addition to the conventional DFA model with a latent random walk (included
in all panels for reference), predictions from a full rank Gaussian process model, and B-spline model with
12 knots and 24 knots are shown. The posterior mean from each model is shown as a solid line, and 90%
credible intervals are shown with ribbons.

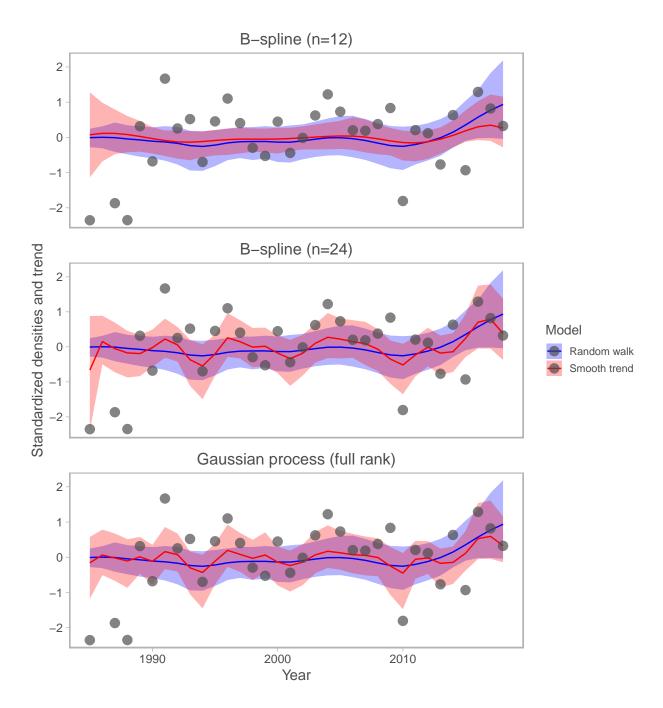
Figure 2. Estimated trends and loadings from the 2-trend DFA model applied to commercial groundfish landings off the west coast of the United States. The model results with highest LOOIC is shown, a model that allows trends to be approximated with B-spines (6 knots). The posterior mean for each trend is shown, with ribbons representing 90% credible intervals. The loadings of each species on each trend are shown as points, with lines representing 90% credible intervals.

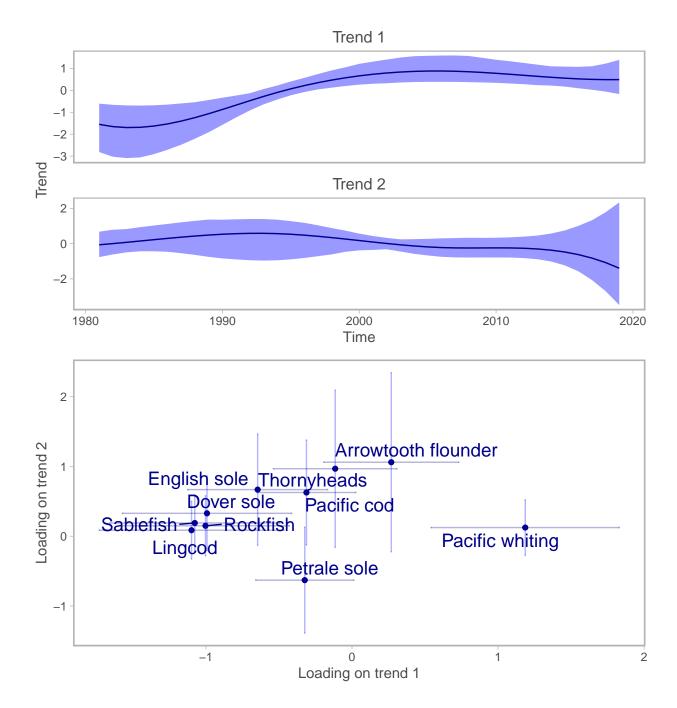
Figure 3. Estimated landings for 2 species included in our analysis, with contrasting trends (lingcod,
Pacific whiting). Posterior means and 90% credible intervals (ribbons) for two candidate models are shown:
a B-spline trend model with 6 knots, and a random walk model representing the conventional DFA.

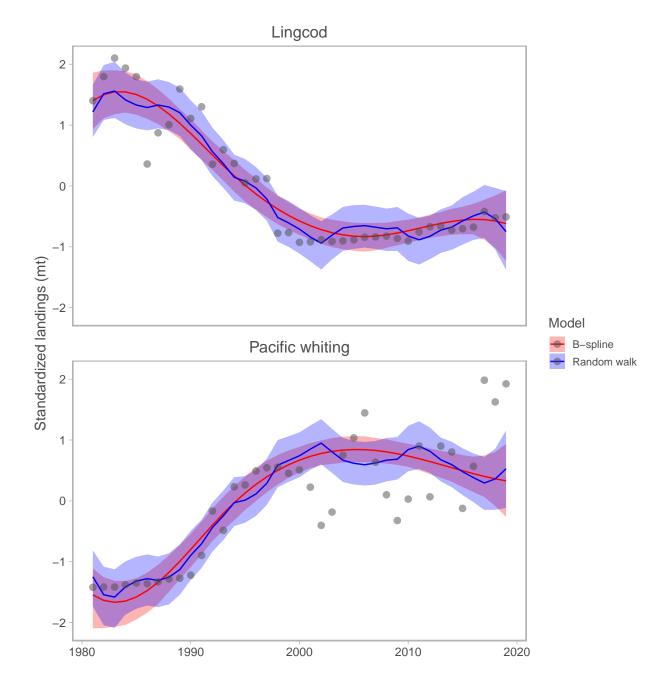
Figure 4. Estimated trends for the 2-trend model of fisheries landings on the west coast of the USA.

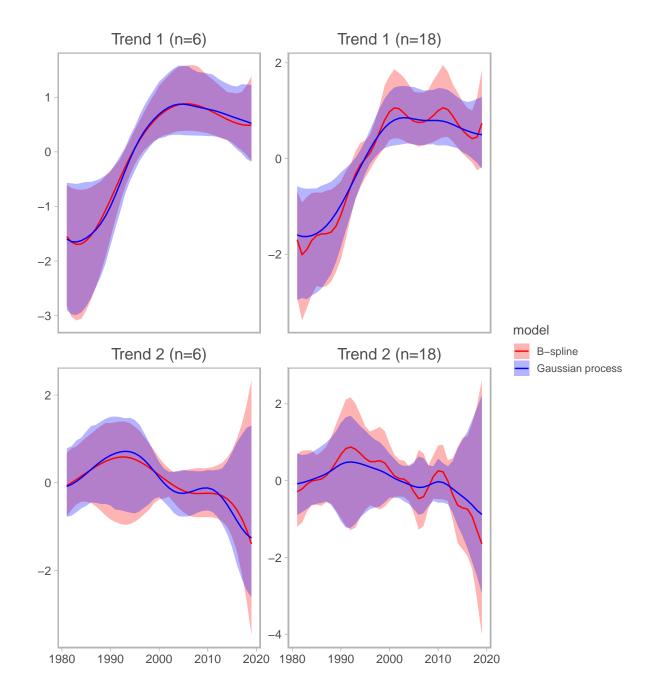
Shown are results for the B-spline and Gaussian process models with 6 and 18 knots (or control points).

Solid lines represent the posterior means and 90% credible intervals are shown as ribbons.









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