VAST model structure and user interface 1 2 **James Thorson** 3 **Purpose of document:** 4 5 R package VAST includes many different forms of documentation including: 6 1. Doxygen documentation that can accessed through the standard R-help interface when the 7 library is loaded within R; 2. the VAST decision tree and user guide (Thorson 2019) 8 3. two separate Rmarkdown "tutorials" that provide annotated code illustrating how to run 9 10 VAST for single- or multi-species example using real-world data; 4. a searchable "issue tracker" available through GitHub; and 11 5. peer-reviewed articles describing development and applications for each feature (see list 12 13 on GitHub). This "VAST model structure and user interface" document is intended to complement these 14 other resources by documenting and describing the model structure (all model equations and 15 notation) while linking it to user-options that are available via the R interface to package 16 VAST. 17 18 Package architecture: 19 20 VAST is developed as an R package available on GitHub. It depends upon helper functions that are bundled in package FishStatsUtils, and these helper functions are installed 21 separately because they are also used by other spatio-temporal packages (e.g., EOFR). 22

VAST and FishStatsUtils use S3 objects to ease interpretation of objects that are commonly

- saved to terminal (see Table 1 for list). VAST can be run using two primary levels ofabstraction:
- High-level wrapper functions: New users are recommended to explore using
 `FishStatsUtils::make_settings` and `FishStatsUtils::fit_model` to run VAST, and to
 explore results using `plot` and `summary`.
- 29 2. *Mid-level utilities*: Experienced users often run lower-level functions to accomplish basic
 30 tasks in spatial analysis, using `FishStatsUtils::make_extrapolation_info`,
- FishStatsUtils::make_spatial_info`, `VAST::make_data`, and `VAST::make_model`individually.
 - Updates to VAST are released using semantic-version numbering (e.g., version 3.2.0) and a battery of integrated tests (comparing results using updated code to saved results from earlier versions) are run prior to numbered releases to ensure that results are backwards compatible.

Model description:

In the following, I use mathematical notation similar to the C++ code used to define the model in TMB: I use parentheses to indicate a parameter or variable that is indexed by the specified indices, and I use subscripts for naming (e.g., to indicate different parameters for different model components). Notation is close to common recommendations, e.g., Edwards and Auger-Méthé (2019), although I use parentheses to indicate indices of vectors, matrices, and arrays, and reserve subscripts for naming. Feel free to change notation when describing the model to suit your purposes in reports or publications. For further details regarding terminology, motivation, and statistical properties, please read the papers listed on the GitHub main page.

Model Overview

VAST predicts variation in density across multiple locations s, time intervals t, for multiple categories c. Categories could include either multiple species, and/or multiple size/age/sex classes for each individual species. VAST approximates the covariance between these multiple factors using a factor-model decomposition (Thorson et al. 2015a, 2016a), i.e., by summing across the contribution of multiple random effects (termed factors). If there is only a single category, the model reduces to a standard univariate spatio-temporal model.

After estimating variation in density across space, time, and among categories, VAST then predicts total abundance across a user-specified spatial domain. This is equivalent to an "area-weighting" approach to index standardization, and the resulting prediction of total abundance can be used an index of abundance.

In addition to spatial and spatio-temporal covariance among multiple categories, VAST allows users to specify either density or catchability covariates. Both explain variation in observed catch-rate data, but VAST predicts density (for use in calculating the abundance index) using density covariates but not catchability covariates. Therefore, VAST "controls for" catchability covariates when calculating an index (i.e., removes their estimated effect) while "conditioning on" density covariates when calculating an index (i.e., uses them to improve interpolated/extrapolated predictions of density).

Linear predictors

The model potentially includes two linear predictors (because it is designed to support deltamodels, which include two components). The first linear predictor $p_1(i)$ represents encounter probability in a delta-model, or zero-inflation in a count-data model:

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$$p_{1}(i) = \underbrace{\beta_{1}^{*}(c_{i}) + \sum_{f=1}^{n_{\beta_{1}}} L_{\beta_{1}}(c_{i}, f)\beta_{1}(t_{i}, f)}_{Temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\omega_{1}}} L_{\omega_{1}}(c_{i}, f)\omega_{1}^{*}(s_{i}, f)}_{Spatial\ variation}$$

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$$+ \underbrace{\sum_{f=1}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c_i, f) \varepsilon_1^*(s_i, f, t_i)}_{Spatio-temporal \ variation} + \underbrace{\sum_{f=1}^{n_{\eta 1}} L_1(c_i, f) \eta_1(v_i, f)}_{Vessel \ effects}$$

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$$+ \sum_{p=1}^{n_p} \left(\gamma_1(c_i, t_i, p) + \sigma_{\xi_1}(c_i, p) \xi_1^*(s_i, c_i, p) \right) X(i, t_i, p) + \sum_{k=1}^{n_k} \lambda_1(k) Q(i, k)$$
Habitat covariates

where $p_1(i)$ is the predictor for observation i, $\beta_1^*(t_i, f)$ represents temporal variation for time t_i for factor f (of $n_{\beta 1}$ factors representing temporal variation), $L_{\beta 1}(c_i, f)$ is the loadings matrix that generates temporal covariation among categories for this linear predictor, and $\beta_2^*(c_i)$ represents the time-average for each category c_i . The number of factors $n_{\beta 1}$ can range from zero to the number of categories n_c , $0 \le n_{\beta 1} \le n_c$, where $n_{\beta 1} = 0$ is equivalent to eliminating all temporal terms from the model. By default, $n_{\beta 1} = n_c$, $\beta_1(t, f)$ is treated as a fixed effect for each year t and factor f, and $\mathbf{L}_{\beta 1}$ is an identity matrix; this formulation is equivalent to estimating a separate intercept $\beta_1(t_i, c) = \beta_1(t_i, f)$ for each category and year. However, the intercepts can instead be treated as a random effect using the factor-model formulation, which allows for sharing information among years and categories. When treated as random, $\beta_1(t_i, f)$ is assigned a normal distribution with unit variance, such that $\mathbf{L}_{\beta_1}^T \mathbf{L}_{\beta_1}$ is the covariance among categories for a given process (Thorson et al. 2015a). When treating intercepts as random, and when there is only one category and using one factor $(n_{\beta 1} = 1)$, then $L_{\beta 1}$ is a 1x1 matrix (i.e. a scalar) such $L_{\beta 1}^2$ is the variance and the absolute value, $abs(\mathbf{L}_{\beta 1})$ is the standard deviation for temporal variation.

occurring at the location s_i of sample i for factor f (of $n_{\omega 1}$ factors representing spatial

Similarly, $\omega_1^*(s_i, f)$ represents predicted spatial variation in the first linear predictor

variation), and $L_{\omega 1}(c_i, f)$ is the loadings matrix that generates spatial covariation among categories for this linear predictor. Similarly, $\varepsilon_1^*(s_i, f, t_i)$ represents predicted spatiotemporal variation in the first linear predictor for each factor f (of $n_{\varepsilon 1}$ factors representing spatio-temporal variation), and $L_{\varepsilon 1}(c_i, f)$ is the loadings matrix that generates spatiotemporal covariation for this predictor. $\eta_1(v_i, f)$ represents random variation in catchability among a grouping variable (tows or vessels) for each factor f (of $n_{\eta 1}$ factors representing overdispersion), and $L_1(c_i, f)$ is a loadings matrix that generates covariation in catchability among categories for this predictor. All loadings matrices are specified similarly to $L_{\beta 1}$, i.e., where factors have a variance of one such that $\mathbf{L}^T \mathbf{L}$ represents the covariance among categories. The main difference is that spatial, spatio-temporal, and overdispersion factors can only be specified as random effects, while the intercepts can be specified as either random or fixed (where specifying as fixed "turns off" all factor-modelling for that intercept). Finally, $X(i, t_i, p)$ is an three-dimensional array of n_p measured density covariates that explain variation in density for time t and the location s_i where sampling occurred for sample i. VAST can include a separate, spatially-varying effect of each habitat covariate p for each category c. The spatially varying slope is $\gamma_1(c_i, t_i, p) + \sigma_{\xi_1}(c, p)\xi_n(s, c, p)$, where $\gamma_1(c_i, t_i, p)$ is the average effect of density covariate $X(i, t_i, p)$ for category $c, \xi_n(s_i, c_i, p)$ represents spatial variation in that effect (which has a mean of zero and standard deviation of one), and $\sigma_{\xi_1}(c,p)$ represents the estimated standard deviation of spatial variation of covariate p for category c. Q(i, k) is a matrix of n_k measured catchability covariates that explain variation in catchability, and $\lambda_1(k)$ is the estimated impact of catchability covariates for this linear predictor. By default, VAST specifies that $\gamma_1(c,t_1,p)=\gamma_1(c,t_2,p)$ for all years t_1 and t_2 , although users can relax this constaint by specifying a different structure for

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Data_Fn(..., Map=NewMap).

Similarly, the second linear predictor $p_2(i)$ represents positive catch rates in a deltamodel, or the count-data intensity function in a count-data model:

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$$p_2(i) = \underbrace{\beta_2^*(c_i) + \sum_{f=1}^{n_{\beta_2}} L_{\beta_2}(c_i, f)\beta_2(t_i, f)}_{Temporal \ variation} + \underbrace{\sum_{f=1}^{n_{\omega_2}} L_{\omega_2}(c_i, f)\omega_2^*(s_i, f)}_{Spatial \ variation}$$

$$+ \underbrace{\sum_{f=1}^{n_{\varepsilon 2}} L_{\varepsilon 2}(c_i, f) \varepsilon_2^*(s_i, f, t_i)}_{Spatio-temporal \ variation} + \underbrace{\sum_{f=1}^{n_{\eta 2}} L_2(c_i, f) \eta_2(v_i, f)}_{Vessel \ effects}$$

$$+ \underbrace{\sum_{p=1}^{n_p} \left(\gamma_2(c_i, t_i, p) + \sigma_{\xi_2}(c_i, p) \xi_2^*(s_i, c_i, p) \right) X(i, t_i, p)}_{Density\ covariates} + \underbrace{\sum_{k=1}^{n_k} \lambda_2(k)\ Q(i, k)}_{Catchability\ covariates}$$

- where all variables and parameters are defined similarly except using different subscripts
- 121 (Thorson and Barnett 2017; Thorson 2019).

Number of spatial and spatio-temporal factors

- The user controls the number of spatial and spatio-temporal factors used for each component
- via input:

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- FieldConfig = c("Omega1"=1, "Epsilon1"=1, "Omega2"=1, "Epsilon2"=1)
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- where FieldConfig[1] controls $n_{\omega 1}$, FieldConfig[2] controls $n_{\varepsilon 1}$, FieldConfig[3] controls
- 129 $n_{\omega 2}$, and FieldConfig[4] controls $n_{\varepsilon 2}$, and a value of zero "turns off" that component of
- spatial or spatio-temporal covariation.

Number of overdispersion factors

The user controls the number of catchability factors used for each component via input:

134 OverdispersionConfig = c("Eta1"=0, "Eta2"=0)

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- where OverdispersionConfig[1] controls $n_{\delta 1}$, and OverdispersionConfig[2] controls $n_{\delta 2}$,
- and a value of zero again "turns off" that component of random covariation in catchability.
- 138 For example, if the user inputs:
- OverdispersionConfig = c("Eta1"=1, "Eta2"=1)

- then there will be one random effect estimated for each unique level of Data_Geostat\$Vessel
- for both the first and second linear predictors.

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Link functions and observation error distributions

- There are user-controlled options that control the observation error distribution and the link-
- functions used to calculate expected encounter probabilities and positive catch rates based on
- the two linear predictors.
- 148 The ObsModel vector has two components, controlling the observation error distribution and
- link function respectively.
- 150 ObsModel = c("PosDist"=2, "Link"=0)
- 151 There are currently four options for the link function. For the latest set of options see the R
- help documentation by typing into the R terminal `?VAST::Data Fn`.
- 153 1. ObsModel[2]=0 applies a logit-link for the first linear predictor:

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$$r_1(i) = \text{logit}^{-1}(p_1(i))$$

- where $r_1(i)$ is the predictor encounter probability in a delta-model, or zero-inflation in a
- 156 count-data model, and $logit^{-1}(p_1(i))$ is the inverse-logit (a.k.a. logistic) function of
- 157 $p_1(i)$, and:

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$$r_2(i) = a_i \times \log^{-1}(p_2(i))$$

- where $r_2(i)$ is the predicted biomass density for positive catch rates in a delta-model or
- mean-intensity function for a count-data model, $log^{-1}(p_2(i))$ is the exponential function

- of $p_2(i)$, and a_i is the area-swept for observation i, which enters as a linear offset for expected biomass given an encounter.
- 2. ObsModel[2]=1 corresponds to a "Poisson-link" delta-model that approximates a Tweediedistribution:

$$r_1(i) = 1 - \exp(-a_i \times \exp(p_1(i)))$$

where $r_1(i)$ is the predictor encounter probability and $1 - \exp(-a_i \times \exp(p_1(i)))$ is a complementary log-log link of $p_1(i) + \log(a_i)$, and:

$$r_2(i) = \frac{a_i \times \exp(p_1(i))}{r_1(i)} \times \exp(p_2(i))$$

where $r_2(i)$ is the predicted biomass given that the species is encountered. In this "Poisson-process" link function, $\exp(p_1(i))$ is interpreted as the density in number of individuals per area such that $a_i \times \exp(p_1(i))$ is the predicted number of individuals encountered, and $\exp(p_2(i))$ is interpreted as the average weight per individual. Areaswept a_i therefore enters as a linear offset for the expected number of individuals encountered (Thorson 2018). This Poisson-link function should only be used for deltamodels, and not for count-data models, but can also be used to combine encounter, count, and biomass-sampling data (see section below for details).

Observation models:

There are different user-controlled options for observation models for available sampling

data, which are controlled by ObsModel_ez[1].

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# Control observation error
ObsModel_ez = c("PosDist"=2, "Link"=0)
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I distinguish between observation models for continuous-valued data (e.g., biomass, or numbers standardized to a fixed area), and observation models for count data (e.g., numbers

- treating area-swept as an offset). However, both are parameterized such that the expectation
- 187 for sampling data $\mathbb{E}(B_i) = r_1(i) \times r_2(i)$.
- 188 *Continuous-valued data (e.g., biomass)*
- 189 If using an observation model with continuous support (e.g., a normal, lognormal, gamma, or
- Tweedie models), then data b_i can be any non-negative real number, $b_i \in \mathcal{R}$ and $b_i \geq 0$.
- 191 VAST calculates the probability of these data as:

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$$\Pr(b_i = B) = \begin{cases} 1 - r_1(i) & \text{if } B = 0\\ r_1(i) \times g\{B | r_2(i), \sigma_m^2(c)\} & \text{if } B > 0 \end{cases}$$

- where ObsModel[1] controls the probability density function $g\{B|r_2(i), \sigma_m^2(c)\}$ used for
- positive catch rates (see ?Data_Fn for a list of options), where each options is defined to have
- with expectation $r_2(i)$ and dispersion $\sigma_m^2(c)$, where dispersion parameter $\sigma_m^2(c)$ varies
- among categories by default.
- 197 *Discrete-valued data (e.g., abundance)*
- 198 If using an observation model with discrete support (e.g., a Poisson, negative-binomial,
- 199 Conway-Maxwell Poisson, or lognormal-Poisson models), then data b_i can be any whole
- number, $b_i \in \{0,1,2,...\}$. VAST calculates the probability of these data as:

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$$\Pr(B = b_i) = \begin{cases} (1 - r_1(i)) + g\{B = 0 | r_2(i), \dots\} & \text{if } B = 0 \\ r_1(i) \times g\{B = b_i | r_2(i), \dots\} & \text{if } B > 0 \end{cases}$$

- where ObsModel[1] controls the probability mass function $g\{B|r_2(i),...\}$ used (again, see
- 203 ?Data_Fn for a list of options), where I use ... to signify that these probability mass functions
- 204 generally can have one or more parameter governing dispersion, and the precise number and
- interpretation varies among observation models (i.e., the value of ObsModel[1]). For these
- count-data models, $(1 r_1(i))$ is the "zero-inflation probability" (i.e., the proportion of
- habitat in the immediate vicinity of location s_i and time t_i that is never occupied), while $r_2(i)$
- is the expected value for probability mass function $g\{B=b_i|r_2(i),...\}$ (i.e., the number of
- 209 individuals that are in the vicinity of sampling in habitat that is occupied), and $g\{B = A\}$

 $0|r_2(i),...$ } is the probability of not encountering category c given that sampling occurs in occupied habitat (Martin et al. 2005).

Settings regarding spatial domain

- VAST estimates the value of spatial variables at a user-defined number of knots. To do so,
- 215 the user specifies a number of knots n x:
- 216 # Number of knots
- $217 n_x = 1000$

- VAST then uses a k-means algorithm to identify the location of n_x knots to minimize the total distance between the location of available data and the location of the nearest knot. This distributes knots as a function of the spatial intensity of sampling data.
- VAST then uses a stochastic partial differential equation (SPDE) approximation to the probability density function for spatial and spatio-temporal variation (Lindgren et al. 2011). This SPDE approximation involves generating a triangulated mesh that has a vertex of a triangle at each knot, and VAST generates this triangulated mesh using package R-INLA (Lindgren 2012). This mesh includes all n_x user-specified "interior vertices," as well as additional "boundary vertices" such that the total number of interior and boundary vertices is n_s . Outputs from this triangulated mesh can then be used to calculate the precision (inverse-covariance) matrix for a multivariate normal probability density function for the value of a spatial variable at all n_s vertices. Specifically, the correlation $\mathbf{R}_1(s,s+h)$ between location s and location s h for spatial and spatio-temporal terms included in the first linear predictor is approximated as following a Matern function:

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$$\mathbf{R}_1(s, s+h) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \times (\kappa_1|h\mathbf{H}|)^{\nu} \times K_{\nu}(\kappa_1|h\mathbf{H}|)$$

where **H** is a two-dimensional linear transformation representing geometric anisotropy (with a determinant of 1.0), ν is the Matern smoothness (fixed at 1.0), and κ_1 governs the

decorrelation distance for that first linear predictor (κ_2 is also separately estimated for the second linear predictor). By default, the two degrees of freedom in **H** are estimated as fixed effects, but the user can specify isotropy (i.e., **H** = **I**) by specifying:

239 # Turn of geometric anisotropy
240 Data = Data_Fn(..., Aniso=FALSE)

VAST then specifies that the spatial and spatio-temporal Gaussian random fields at each have a variance of 1.0. By default VAST estimates their values at each of n_s vertices as follows:

$$\mathbf{\omega}_{1}(f) \sim MVN(\mathbf{0}, \mathbf{R}_{1})$$

$$\mathbf{\omega}_{2}(f) \sim MVN(\mathbf{0}, \mathbf{R}_{2})$$

$$\mathbf{\varepsilon}_{1}(f,t) \sim MVN(\mathbf{0},\mathbf{R}_{1})$$

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$$\mathbf{\varepsilon}_2(f,t) \sim MVN(\mathbf{0},\mathbf{R}_2)$$

$$\boldsymbol{\xi}_{1}(c,p) \sim MVN(\boldsymbol{0},\boldsymbol{R}_{1})$$

$$\boldsymbol{\xi}_{2}(c,p) \sim MVN(\mathbf{0},\mathbf{R}_{2})$$

where $\omega_1(f)$ is the vector of length n_s formed when subsetting $\omega_1(s, f)$ for a given f.

Specifying a variance of 1.0 ensures that the covariance among categories is defined by the

loadings matrix for that term.

Interpolating spatial variation from knots to the location of samples

Starting with VAST release 3.0.0, users can choose between two options for smoothing spatial variation. Both options involve specifying a matrix \mathbf{A}_i with n_i rows and n_s columns,

row i. Values are then predicted as e.g.:

$$\mathbf{\omega}_1^*(f) = \mathbf{A}_i \mathbf{\omega}_1(f)$$

- where $\mathbf{\omega}_{1}^{*}(f)$ is the vector of length n_{i} , containing the predicted value $\omega_{1}^{*}(s_{i}, f)$ for spatial variation in the first linear predictor at every location s_{i} , and other spatial variables are predicted similarly using matrix \mathbf{A}_{i} .
- 1. *Piecewise constant*: Following the conventional for releases of VAST prior to 3.0.0,

 users can specify fine_scale=FALSE. Given this specification, spatial variables at location

 s are fixed equal to their value at the nearest "knot." This involves specifying matrix A_i

 such that row i has value zero except for one cell containing a value of one for the knot

 closest to sample i.
- 2. Bilinear interpolation: Following standard practices using the software R-INLA
 (Lindgren 2012; Lindgren and Rue 2013), users can specify fine_scale=TRUE. Given this
 specification, spatial variables at location s are interpolated using the triangulated mesh
 that is also used to approximate spatial variation. Specifically, matrix A_i has row i with
 value zero except for three cells, representing the vertices of the triangle containing
 location s_i.

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Structure on parameters among years:

- 276 There are different user-controlled options for specifying structure for intercepts or spatio-
- temporal variation across time, using input:

- 280 Temporal structure on intercepts
- By default (when RhoConfig[1]=0 and RhoConfig[2]=0) the model specifies that each
- intercept $\beta_1(c,t)$ and $\beta_2(c,t)$ is a fixed effect. However, other settings specify the following
- 283 factor-model structure:

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$$\beta_1(t,f) \sim \begin{cases} Normal(0,1) & \text{if } t = t_{min} \\ Normal(\rho_{\beta 1}\beta_1(t-1,f),1) & \text{if } t > t_{min} \end{cases}$$

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$$\beta_2(t,f) \sim \begin{cases} Normal(0,1) & \text{if } t = t_{min} \\ Normal(\rho_{\beta_2}\beta_2(t-1,f),1) & \text{if } t > t_{min} \end{cases}$$

- Where t_{min} is the index for the first modelled year and $\rho_{\beta 1}$ and $\rho_{\beta 2}$ are the estimated degree
- of first-order autocorrelation in temporal variation (note that random effects have a variance
- of one given that they are subsequently multiplied by loadings matrices that represent the
- temporal covariance among factors). RhoConfig[1] controls the specification of $\rho_{\beta 1}$:
- 290 1. Independent among years RhoConfig[1]=1 specifies $ho_{\beta 1}=0$
- 291 2. Random walk RhoConfig[1]=2 specifies $\rho_{\beta 1}=1$
- 292 3. Constant intercept RhoConfig[1]=3 specifies $\rho_{\beta 1}=0$ and $\sigma_{\beta 1}^2=0$ (i.e., $\beta_1(t)$ is
- 293 constant for all t)

- 294 4. Autoregressive RhoConfig[1]=4 estimates $\rho_{\beta 1}$ as a fixed effect
- and settings are defined identically for RhoConfig[2] specifying ρ_{R2} .
- 297 Temporal structure on spatio-temporal variation
- By default (when RhoConfig[3]=0 and RhoConfig[4]=0), the model specifies that each vector
- of spatio-temporal random effects, $\mathbf{\varepsilon}_1(f,t)$ and $\mathbf{\varepsilon}_2(f,t)$ composed of $\mathbf{\varepsilon}_1(s,f,t)$ and
- 300 $\varepsilon_2(s, f, t)$ across locations s, is independent among years. However, other settings specify
- 301 the following structure

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$$\mathbf{\varepsilon}_{1}(f,t) \sim \begin{cases} MVN(\mathbf{0}, \mathbf{R}_{1}) & \text{if } t = t_{min} \\ MVN(\rho_{\varepsilon 1}\mathbf{\varepsilon}_{1}(f, t - 1), \mathbf{R}_{1}) & \text{if } t > t_{min} \end{cases}$$

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$$\mathbf{\varepsilon}_{2}(f,t) \sim \begin{cases} MVN(\mathbf{0}, \mathbf{R}_{2}) & \text{if } t = t_{min} \\ MVN(\rho_{\varepsilon 2}\mathbf{\varepsilon}_{2}(f, t - 1), \mathbf{R}_{2}) & \text{if } t > t_{min} \end{cases}$$

- where $\rho_{\varepsilon 1}$ and $\rho_{\varepsilon 2}$ are the estimated degree of first-order autocorrelation in temporal
- variation, RhoConfig[3] controls the specification of $\rho_{\varepsilon 1}$:
- 306 1. Random walk RhoConfig[3]=2 specifies $\rho_{\varepsilon 1} = 1$
- 307 2. Autoregressive RhoConfig[3]=4 estimates $\rho_{\varepsilon 1}$ as a fixed effect

and settings are defined identically for RhoConfig[4] specifying $\rho_{\varepsilon 2}$.

Parameter estimation

Parameters are estimated using maximum likelihood, where the maximum likelihood of fixed effects is obtained by integrating a joint likelihood function with respect to random effects (Searle et al. 1992, Gelman and Hill 2007, Thorson and Minto 2015). This integral is approximated using the Laplace approximation (Skaug and Fournier 2006), as implemented in Template Model Builder (Kristensen et al. 2016). The likelihood is then optimized in the R statistical environment (R Core Team 2017), and standard errors are obtained using a generalization of the delta method (Kass and Steffey 1989). Derived quantities calculated via a nonlinear transformation of random effects can be bias-corrected using the epsilon-method (Tierney et al. 1989, Thorson and Kristensen 2016). Depending upon user-specified options, different parameters will be either fixed (estimated via maximizing the log-likelihood) or random (integrated across when calculating the log-likelihood). Please use R function 'ThorsonUtilities::list_parameters (Obj)' to see a list of estimated parameters (where 'Obj' is the compiled VAST object), including which are fixed or random.

Combining multiple data types

VAST can be used to combine encounter/non-encounter, count, and biomass-sampling data. This involves specifying a Poisson-link delta model which predicts each data type from numbers density $\exp(p_1(i))$ and biomass-per-individual $\exp(p_2(i))$, see Grüss and Thorson (In press) for details. This approach is specified by associating each observation with a given error distribution using input e_i where e.g. e_i[1] is the error-distribution for the $1^{\rm st}$ observation. The user then specifies multiple observation errors via input ObsModel_ez:

ObsModel_ez = cbind("PosDist"=c(13,14,2), "Link"=c(1,1,1))

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In this specification, e_i[1]==1 indicates that the first observation follows a Bernoulli distribution for encounter/non-encounter data, e_i[1]==2 indicates that this observation follows a lognormal-Poisson distribution for count data, and e_i[1]==3 indicates that it follows a gamma distribution for biomass-sampling data. This specification can be modified to include different combinations of these same data types.

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Relationship to other named models

use of a delta-model.

- VAST can be configured to be identical to (or closely mimic) many models that have previously been published in ecology and fisheries:
- 1. *Spatial Gompertz model*: If intercepts are constant across years, spatio-temporal variation follows an autoregressive process, and only one category is modelled, then VAST is identical to a spatio-temporal Gompertz model (Thorson et al. 2014).
- 2. Spatial factor analysis: If only one year is analysed and multiple categories are modelled,
 VAST is similar to spatial factor analysis (Thorson et al. 2015a), although it permits the

use of a delta-model (i.e., separate analysis of encounters and positive catch rates).

- 35. Spatial dynamic factor analysis: If intercepts are constant among years, spatio-temporal variation follows an autoregressive process, and multiple categories are modelled, then

 VAST is similar to spatial dynamic factor analysis (Thorson et al. 2016a), although

 VAST allows separate estimates of spatial vs. spatio-temporal covariation and also the
 - 4. *Empirical orthogonal function analysis*: VAST can be configured to replicates empirical orthogonal function analysis, e.g., as commonly used by physical oceanographers to summarize physical conditions to produce an annual index and spatial map associated

with a positive phase of the resulting index. However, I will wait to document this until the associated paper is published.

Predicting variables across the spatial domain and calculating derived

quantities

After a nonlinear minimizer has identified the value of fixed effects that maximizes the Laplace approximation to the marginal likelihood, Template Model Builder predicts the value of random effects that maximizes the joint likelihood conditional on these fixed effects. It then uses the predicted values of random effects to predict each spatial variable at each of n_g "extrapolation-grid cells" that are used to summarize the spatial domain of sampling (Shelton et al. 2014; Thorson et al. 2015b). Predicting random effects at extrapolation-grid cell g at location s_g is accomplished using matrix \mathbf{A}_g with n_g rows and n_s columns. Values are predicted as e.g.:

$$\mathbf{\omega}_1^*(f) = \mathbf{A}_a \mathbf{\omega}_1(f)$$

where $\mathbf{\omega}_1^*(f)$ is the vector of length n_i , containing the predicted value $\mathbf{\omega}_1^*(s_g, f)$ for spatial variation in the first linear predictor at every location s_g , and other spatial variables are predicted similarly using matrix \mathbf{A}_g . Predicted values for random effects are then plugged into the linear predictor, e.g.:

376
$$p_1(g,c,t) = \underbrace{\beta_1^*(c) + \sum_{f=1}^{n_{\beta_1}} L_{\beta_1}(c,f)\beta_1(t,f)}_{Temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\omega_1}} L_{\omega_1}(x,f)\omega_1^*(g,f)}_{Spatial\ variation}$$

$$+ \sum_{\substack{f=1\\ Spatio-temporal\ variation}}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c,f) \varepsilon_1^*(g,f,t) + \sum_{\substack{p=1\\ P=1}}^{n_p} \Big(\gamma_1(c,t,p) + \sigma_{\xi 1}(c,p) \xi_1^*(g,c,p) \Big) X(g,t,p)$$

where $p_2(g, c, t)$ is predicted similar, and these linear predictors are used in turn to predict $r_1(g, c, t)$ and $r_2(g, c, t)$, where their product is predicted biomass-density d(g, c, t) at every extrapolation-grid cell g, category c, and time t.

By default, density is used to predict total abundance for the entire domain (or a subset of the domain) for a given species:

383
$$I(c,t,l) = \sum_{x=1}^{n_x} \left(a(g,l) \times d(g,c,t) \right)$$

where a(g, l) is the area associated with extrapolation-grid cell g for index l; and. The user can also specify additional post-hoc calculations via the Options vector:

1. *Distribution shift* — RhoConfig[3]=1 turns on calculation of the centroid of the population's distribution:

392
$$Z(c,t,m) = \sum_{x=1}^{n_x} \frac{(z(g,m) \times a(g,1) \times d(g,c,t))}{I(c,t,1)}$$

where z(g,m) is a matrix representing location for each extrapolation-grid cell (by default z(g,m) is the location in Eastings and Northings of each knot), representing movement North-South and East-West). This model-based approach to estimating distribution shift can account for differences in the spatial distribution of sampling, unlike conventional sample-based estimators (Thorson et al. 2016b).

2. Range expansion — RhoConfig[5]=1 turns on calculation of effective area occupied. This involves calculating biomass-weighted average density:

400
$$D(c,t,l) = \sum_{x=1}^{n_x} \frac{a(x,l) \times d(x,c,t)}{I(c,t,l)} d(x,c,t)$$

Effective area occupied is then calculated as the area required to contain the population at this average density:

$$A(c,t,l) = \frac{I(c,t,l)}{D(c,t,l)}$$

This effective-area occupied estimator can then be used to monitor range expansion or contraction or density-dependent range expansion (Thorson et al. 2016c).

The calculation of these and other derived quantities can be turned on and off using input

Options to function make_data (see Table 2).

List of features

408

- I next provide a list of "features" organized as decisions that can be made by the analyst.
- 411 Although this is somewhat redundant with the explanations provided above, this list might be
- useful for some readers to provide a high-level overview of different options that are
- available. This "feature set" is also provided as a high-level summary of what VAST is
- designed to be capable of doing; any software replacing VAST would ideally include this
- same set of features.
- 416 Basic features in a generalized linear model (GLM)
- 417 1. Specifying one of several possible distributions for data, including for:
- a. Count data using a Poisson, negative-binomial, Conway-Maxwell-Poisson, or
- 419 Poisson-lognormal distribution, including zero-inflated versions of each;
- b. Continuous-valued data that include zeros using a delta-model with a lognormal
- or gamma distribution for positive values.
- 422 2. Specifying one of several possible link functions for predicting data given linear
- 423 predictors including:
- a. A conventional delta-model;
- b. A Poisson-link delta model.

- 426 3. Including dynamic habitat covariates or not;
- 4. Including catchability covariates or not;
- 428 Basic features in a spatio-temporal generalized linear mixed model (GLMM)
- 429 5. Specify an "extrapolation grid" using input
- FishStatsUtils::make_extrapolation_info(..., Region), which is used to calculate the
- area associated with each knot a_x . This can be a user-specified extrapolation grid if
- FishStatsUtils::make_extrapolation_info(..., Region="User", input_grid=Input),
- where Input is a data frame supplied by the user.
- 434 6. Specifying a method for defining "knots";
- 435 7. Specifying the number of "knots";
- 8. Spatial variation being estimated ("turned on") or ignored ("turned off") for either linear
- 437 predictor #1 or #2;
- 9. Spatio-temporal variation being estimated ("turned on") or ignored ("turned off") for
- either linear predictor #1 or #2;
- 10. Specifying that habitat covariates can affect linear predictors different ways including as:
- a. a linear effect;
- b. a spatially-varying effect; or
- c. both linear and spatially-varying effects simultaneously.
- 444 Multivariate analysis
- 11. Including a "multivariate" structure with multiple responses that covary due to a specified
- number of "factors" for spatial and spatio-temporal terms;
- 12. Rotate results prior to interpretation, using either:
- a. principle components rotation; or
- b. varimax rotation.
- 450 Decisions regarding temporal structure

451	13. Annua	al intercepts being structured over time, including:	
452	a.	estimated as fixed effects in every year;	
453	b.	fixed as fixed effect with the same value for all years;	
454	c.	estimated as a random effect with independent deviations in each year;	
455	d.	estimated as a random effect with first-order autoregressive structure; or	
456	e.	estimated as a random effect with a random-walk structure.	
457	14. Spatio-temporal variation being structured over time, including:		
458	a.	estimated as independent deviations in each year;	
459	b.	estimated as following a first-order autoregressive structure over time;	
460	c.	estimated as following a random-walk structure over time; or	
461	d.	estimated as following a vector-autoregressive structure involving a matrix of 1st	
462		order autoregressive interactions.	
463	Derived quantities		
464	15. Specifying spatial strata for use when calculating derived quantities;		
465	16. Calculating one of many possible "univariate derived quantities", including:		
466	a.	abundance indices;	
467	b.	range shift;	
468	c.	effective area occupied	
469	d.	covariance among categories within a multivariate model; or	
470	e.	synchrony among categories.	
471	17. Calcul	lating "multivariate derived quantities" that are derived from estimates for multiple	
472	catego	ories in a multivariate model, e.g., where one category represents a standardized diet	
473	sampl	e (e.g., prey biomass per predator biomass in a stomach-content sample) and	
474	another category represents a biomass-density sample (e.g., predator biomass in a bottom-		
475	trawl s	sample) such that their product represents predator-expanded consumption.	

- 476 Unusual circumstances and special cases
- 477 18. Specifying separate distributions for different data sets (e.g., when multiple surveys
- 478 providing different data types are available);
- 479 19. Specifying that some data are predicted based on summing linear predictors across
- multiple variables (e.g., when modelling density for different size classes, and specifying
- that some data are aggregated measurements of multiple sizes-classes);
- 482 20. Specifying multiple "seasons" (e.g., when modelling data with both annual and monthly
- 483 spatio-temporal variation).

485

Common problems

- There are two basic problems that are often encountered during spatio-temporal delta-
- 487 GLMMs:
- 1. *Encounter rates*: Some combination of categories and year has 0% or 100% encounter
- rate. If there is 100% encounter rate for category c in year t, then $\beta_1(c,t) \rightarrow \infty$ and/or
- 490 $\varepsilon_1(s,c,t) \to \infty$ for that year. If there is 0% encounter rate in year t, then $\beta_1(c,t) \to -\infty$
- and/or $\varepsilon_1(s,c,t) \to -\infty$ and there is no information to estimate $\beta_2(c,t)$ or $\varepsilon_2(s,c,t)$ for
- 492 that category c and year t;
- 493 2. *Bounds*: Some parameter(s) hits a bound;
- These problems can be solved by:
- 1. Encounter rates: constraining terms that vary among years (e.g., intercept β and spatio-
- temporal variation $\varepsilon(s, t, p)$). This can be done in many different ways that are each
- idiosyncratic and require some special justification. The easiest options are:
- a. If there is a small number of years with 100% encounter rate, try ObsMode1[2]=3.
- This indicates that VAST should check for species-years combinations with 100%

- 500 encounter rates and fix corresponding intercepts for encounter probability to an extremely high value. 501
 - b. If there is a small number of years with either 100% of 0% encounter rate, add temporal structure to intercepts and spatio-temporal terms using RhoConfig options.
 - c. Four other options are listed on the wiki.

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506 2. Bounds: Please try running the model without estimating standard errors or a final 507 newton step:

```
508
         # Specify derived quantities to calculate
509
         TMBhelper::fit_tmb( ..., getsd=FALSE, newtonsteps=0 )
```

Then check what parameters are being estimated near an upper or lower boundary. 510

How to implement basic model changes

- There are a few basic model types that users often want to fit using VAST. I briefly describe 513 how these can be done here.
- 1. Fitting encounter/non-encounter data: If the user wishes to use only the first component of a delta-model, i.e., to fit a binomial model to simply predict encounter probabilities, 516 517 then, the ObsModel vector should be set to c("PosDist"=[Make Choice], "Link"=0), where [Make Choice] can be any option for continuous data (i.e., 0, 1, or 2). The user 518 should then turn off the last two elements of the FieldConfig vector (i.e., 519 520 FieldConfig[3]=0 and FieldConfig[4]=0) such that there is no spatial or spatio-temporal variability in positive catch rates, and also turn off annual variation in the intercept for 521 positive catch rates (i.e., RhoConfig[2]=3). Finally, the user should "jitter" their presence 522 observations by a very small amount (i.e., add a random normal deviation with a very 523 small standard deviation, rnorm(n=1, mean=0, sd=0.001), to each observation for which 524 b_i=1). This will result in VAST estimating a logistic regression model for 525

encounter/non-encounter data, except with one additional parameter estimated (σ_M), plus one additional parameter per category ($\beta_2(c)$), where these additional parameters have no impact on other parameters, are not meant to be interpreted statistically or biologically, and are an artefact of using VAST (which is designed to fit a delta-model) to encounter/non-encounter data. This feature has been used to estimate species distributions for use in ecosystem models (Grüss et al. 2017, 2018).

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Works cited

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- Edwards, A.M., and Auger-Méthé, M. 2019. Some guidance on using mathematical notation in ecology. Methods Ecol. Evol. **10**(1): 92–99. doi:10.1111/2041-210X.13105.
- Gelman, A., and Hill, J. 2007. Data analysis using regression and multilevel/hierarchical
 models. Cambridge University Press, Cambridge, UK.
- Grüss, A., and Thorson, J. In press. Developing spatio-temporal models using multiple data types for evaluating population trends and habitat usage. ICES J. Mar. Sci.
- Grüss, A., Thorson, J.T., Babcock, E.A., and Tarnecki, J.H. 2018. Producing distribution maps for informing ecosystem-based fisheries management using a comprehensive survey database and spatio-temporal models. ICES J. Mar. Sci. **75**(1): 158–177. doi:10.1093/icesjms/fsx120.
- Grüss, A., Thorson, J.T., Sagarese, S.R., Babcock, E.A., Karnauskas, M., Walter, J.F., and
 Drexler, M. 2017. Ontogenetic spatial distributions of red grouper (Epinephelus
 morio) and gag grouper (Mycteroperca microlepis) in the U.S. Gulf of Mexico. Fish.
 Res. 193(Supplement C): 129–142. doi:10.1016/j.fishres.2017.04.006.
 - Kass, R.E., and Steffey, D. 1989. Approximate bayesian inference in conditionally independent hierarchical models (parametric empirical bayes models). J. Am. Stat. Assoc. **84**(407): 717–726. doi:10.2307/2289653.
- Kristensen, K., Nielsen, A., Berg, C.W., Skaug, H., and Bell, B.M. 2016. TMB: Automatic Differentiation and Laplace Approximation. J. Stat. Softw. **70**(5): 1–21. doi:10.18637/jss.v070.i05.
- Lindgren, F. 2012. Continuous domain spatial models in R-INLA. ISBA Bull. **19**(4): 14–20.
- Lindgren, F., and Rue, H. 2013. Bayesian spatial and spatiotemporal modelling with r-inla. J.
 Stat. Softw. Available from http://inla.googlecode.com/hg-history/fd1c0951196f7e7b6d57e2ea84c541981fcb3bf4/r-inla.org/papers/jss/lindgren.pdf [accessed 23 February 2014].
- Lindgren, F., Rue, H., and Lindström, J. 2011. An explicit link between Gaussian fields and
 Gaussian Markov random fields: the stochastic partial differential equation approach.
 J. R. Stat. Soc. Ser. B Stat. Methodol. 73(4): 423–498. doi:10.1111/j.1467 9868.2011.00777.x.
- Martin, T.G., Wintle, B.A., Rhodes, J.R., Kuhnert, P.M., Field, S.A., Low-Choy, S.J., Tyre,
 A.J., and Possingham, H.P. 2005. Zero tolerance ecology: improving ecological
 inference by modelling the source of zero observations. Ecol. Lett. 8(11): 1235–1246.
- R Core Team. 2017. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria. Available from https://www.R-project.org/.
- Searle, S.R., Casella, G., and McCulloch, C.E. 1992. Variance components. John Wiley &
 Sons, Hoboken, New Jersey.
- Shelton, A.O., Thorson, J.T., Ward, E.J., and Feist, B.E. 2014. Spatial semiparametric models improve estimates of species abundance and distribution. Can. J. Fish. Aquat. Sci.
 71(11): 1655–1666. doi:10.1139/cjfas-2013-0508.
- 585 Skaug, H., and Fournier, D. 2006. Automatic approximation of the marginal likelihood in non-Gaussian hierarchical models. Comput. Stat. Data Anal. **51**(2): 699–709.
- Thorson, J.T. 2018. Three problems with the conventional delta-model for biomass sampling data, and a computationally efficient alternative. Can. J. Fish. Aquat. Sci. **75**(9): 1369–1382. doi:10.1139/cjfas-2017-0266.
- Thorson, J.T. 2019. Guidance for decisions using the Vector Autoregressive Spatio-Temporal (VAST) package in stock, ecosystem, habitat and climate assessments. Fish. Res. **210**: 143–161. doi:10.1016/j.fishres.2018.10.013.

Thorson, J.T., and Barnett, L.A.K. 2017. Comparing estimates of abundance trends and distribution shifts using single- and multispecies models of fishes and biogenic habitat. ICES J. Mar. Sci. **74**(5): 1311–1321. doi:10.1093/icesjms/fsw193.

- Thorson, J.T., Ianelli, J.N., Larsen, E.A., Ries, L., Scheuerell, M.D., Szuwalski, C., and Zipkin, E.F. 2016a. Joint dynamic species distribution models: a tool for community ordination and spatio-temporal monitoring. Glob. Ecol. Biogeogr. **25**(9): 1144–1158. doi:10.1111/geb.12464.
- Thorson, J.T., and Kristensen, K. 2016. Implementing a generic method for bias correction in statistical models using random effects, with spatial and population dynamics examples. Fish. Res. **175**: 66–74. doi:10.1016/j.fishres.2015.11.016.
- Thorson, J.T., and Minto, C. 2015. Mixed effects: a unifying framework for statistical modelling in fisheries biology. ICES J. Mar. Sci. J. Cons. **72**(5): 1245–1256. doi:10.1093/icesjms/fsu213.
- Thorson, J.T., Pinsky, M.L., and Ward, E.J. 2016b. Model-based inference for estimating shifts in species distribution, area occupied and centre of gravity. Methods Ecol. Evol. **7**(8): 990–1002. doi:10.1111/2041-210X.12567.
- Thorson, J.T., Rindorf, A., Gao, J., Hanselman, D.H., and Winker, H. 2016c. Density-dependent changes in effective area occupied for sea-bottom-associated marine fishes. Proc R Soc B **283**(1840): 20161853. doi:10.1098/rspb.2016.1853.
- Thorson, J.T., Scheuerell, M.D., Shelton, A.O., See, K.E., Skaug, H.J., and Kristensen, K. 2015a. Spatial factor analysis: a new tool for estimating joint species distributions and correlations in species range. Methods Ecol. Evol. **6**(6): 627–637. doi:10.1111/2041-210X.12359.
- Thorson, J.T., Shelton, A.O., Ward, E.J., and Skaug, H.J. 2015b. Geostatistical delta-generalized linear mixed models improve precision for estimated abundance indices for West Coast groundfishes. ICES J. Mar. Sci. J. Cons. **72**(5): 1297–1310. doi:10.1093/icesjms/fsu243.
- Thorson, J.T., Skaug, H.J., Kristensen, K., Shelton, A.O., Ward, E.J., Harms, J.H., and Benante, J.A. 2014. The importance of spatial models for estimating the strength of density dependence. Ecology **96**(5): 1202–1212. doi:10.1890/14-0739.1.
- Tierney, L., Kass, R.E., and Kadane, J.B. 1989. Fully exponential Laplace approximations to expectations and variances of nonpositive functions. J. Am. Stat. Assoc. **84**(407): 710–716.

Table 1 – List of S3 objects defined in package VAST (or its primary dependency FishStatsUtils), listing S3 methods defined for each class as well as the intended purpose of each method.

S3 object	S3 methods	Purpose
VAST::make_data	print	De-clutter terminal output
VAST::make_model	print	De-clutter terminal output
FishStatsUtils::make_extrapolation_info	print	De-clutter terminal output
	plot	Simple organization for plotting options
FishStatsUtils::make_spatial_info	print	De-clutter terminal output
	print	Simple organization for plotting options
FishStatsUtils::fit_model	print	De-clutter terminal output
	plot	Simple organization for plotting options
	summary	Interface to access derived quantities that
		users may want

Table 2-List of slots in vector Options.

Slot name	What it does	Examples of usage
SD_site_density	Calculate standard error for each knot	-
	or extrapolation-grid cell (very slow	
	with fine_scale=TRUE)	
SD_site_logdensity	Calculate standard error for each knot	-
	or extrapolation-grid cell (very slow	
	with fine_scale=TRUE)	
Calculate_Range	Calculate center of gravity for use in	(Thorson et al.
	measuring distribution shifts	2016b)
SD_observation_density	Calculate standard error for response	_
	variable measured in each sample	
Calculate_effective_area	Calculate effective area occupied for	(Thorson et al.
	use in measuring range	2016c)
	expansion/contraction	
Calculate_Cov_SE	Calculate standard error for	(Godefroid et al. In
	correlation / covariance among	review)
	categories	
Calculate_Synchrony	Calculate reduction in variance	(Thorson et al.
	associated with asynchrony among	2018)
	species and/or locations	
Calculate_Coherence	Calculate the Gini coefficient for axes	-
	of covariation among categories	
Calculate_proportion	Convert indices to a proportion in a	(Thorson and
	multivariate model; breaks	Haltuch 2018)
Calculate_proportion		,

	separability across categories and	
	therefore users typically use an	
	approximation to calculate input	
	sample size	
normalize_GMRF_in_CPP	Option to potentially speed up GMRF	-
	calculations, although early testing	
	didn't indicate substantial	
	improvements (could be explored	
	more)	
Calculate_Fratio	Option to calculate exploitation rate	(Thorson et al. In
	using a MICE-in-space model	review)
Estimate_B0	Option to calculate unfished density	(Thorson et al. In
	using a MICE-in-space model	review)
Project_factors	Project factors to extrapolation-grid;	-
	Useful to visualize factors when using	
	fine_scale=TRUE	
treat_nonencounter_as_zero	Option to internally track	(Thorson and
	combinations of category and year	Haltuch 2018)
	that are never encountered and	
	therefore should be treated as having	
	zero abundance; Useful for	
	compositional-expansion	
simulate_random_effects	Option governing behaviour of	(Thorson et al. In
	bootstrap simulator; determines	review)
	whether simulator re-simulates	

	random-effects conditional on fixed
	effects (default) or not.
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633	