## VAST model structure and user interface 1 **James Thorson** 2 3 **Purpose of document:** 4 5 R package VAST includes many different forms of documentation, which are documented on the package GitHub page. This "VAST model structure and user interface" 6 document is intended to complement these other resources by documenting and describing 7 the model structure (all model equations and notation). Please see reference documentation 8 for explanation of the user interface, and GitHub wiki for examples. 9 10 Package architecture: 11 VAST is developed as an R package available on GitHub. It depends upon helper 12 functions that are bundled in package FishStatsUtils, and these helper functions are installed 13 separately because they are also used by other spatio-temporal packages (e.g., EOFR). 14 VAST and FishStatsUtils use S3 objects to ease interpretation of objects that are commonly 15

abstraction:

16

17

- 18 1. High-level wrapper functions: New users are recommended to explore using
- 19 'FishStatsUtils::make\_settings' and 'FishStatsUtils::fit\_model' to run VAST, and to

saved to terminal (see Table 1 for list). VAST can be run using two primary levels of

- 20 explore results using 'plot' and 'summary'.
- 2. Mid-level utilities: Experienced users often run lower-level functions to accomplish basic
- tasks in spatial analysis, using `FishStatsUtils::make\_extrapolation\_info`,
- 'FishStatsUtils::make\_spatial\_info', 'VAST::make\_data', and 'VAST::make\_model'
- 24 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: 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matrices, and arrays, and reserve subscripts for naming (see Table 2 for summary of notation that may be slightly out-of-date). 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, multiple size/age/sex classes for each individual species, and/or a mix of biological, physical, and fishery variables describing an ecosystem. VAST approximates the covariance between these multiple categories and years using a factor-model decomposition (Thorson et al. 2015b, 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 variables at extrapolation-grid cells distributed within across a user-specified spatial domain. This allows derived quantities to be calculated by summing across extrapolation-grid cells (as an approximation to the integral across this spatial domain); this is

analogous 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).

VAST estimates the value of spatial variables at  $n_x$  knots, as well as additional boundary vertices such that the total number of spatial "vertices" is  $n_s$ . VAST specifically uses a k-means algorithm to identify the location of  $n_x$  knots to minimize the total distance between the location of knots and either data or extrapolation-grid cells. This distributes knots as a function of the spatial intensity of sampling data.

### Linear predictors

The model potentially includes two linear predictors (because it is designed to support delta-

models, 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:

$$p_1(i) = \underbrace{\beta_1(c_i, t_i)}_{Temporal \ variation} + \underbrace{\omega_1^*(s_i, c_i)}_{Spatial \ variation} + \underbrace{\varepsilon_1^*(s_i, c_i, t_i)}_{Spatio-temporal \ variation} + \underbrace{\eta_1(v_i, c_i)}_{Vessel \ effects}$$

70 + 
$$v_1(c_i, t_i)$$
 +  $\zeta_1(i)$  -  $v(c_i, t_i)$ 

Habitat covariates Catchability covariate Fishing impacts

where  $p_1(i)$  is the predictor for observation i, arising for category  $c_i$  at location  $s_i$  and time

 $t_i$ . Similarly, the second linear predictor  $p_2(i)$  represents positive catch rates in a delta-

model, or the count-data intensity function in a count-data model, where all variables and

parameters are defined similarly except using different subscripts (Thorson and Barnett 2017;

Thorson 2019). Model components are specified hierarchically to efficiently compute

correlated variation among categories and years as explained next.

#### Temporal variation

79 Regarding intercepts representing temporal variation:

80 
$$\beta_1(c_i, t_i) = \mu_{\beta_1}(c_i) + \sum_{f=1}^{n_{\beta_1}} L_{\beta_1}(c_i, f) \beta_1(t_i, f)$$

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. 2015b). When treating intercepts as random, and when there is only one category and using one factor  $(n_{\beta 1} = 1)$ , then  $\mathbf{L}_{\beta 1}$  is a 1x1 matrix (i.e. a scalar) such  $\mathbf{L}_{\beta 1}^2$  is the variance and the absolute value,  $abs(\mathbf{L}_{\beta 1})$  is the standard deviation for temporal variation.

By default 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 autocorrelation structure:

99 
$$\beta_1(t,f) \sim \begin{cases} Normal(0,1) & \text{if } t = t_{min} \\ Normal(\rho_{\beta 1}\beta_1(t-1,f),1) & \text{if } t > t_{min} \end{cases}$$

- 100 Where  $t_{min}$  is the index for the first modelled year and  $\rho_{\beta 1}$  and  $\rho_{\beta 2}$  are the estimated degree 101 of first-order autocorrelation in temporal variation (note that random effects have a variance 102 of one given that they are subsequently multiplied by loadings matrices that represent the 103 temporal covariance among factors). Options treating intercepts as a random effect include:
- 104 1. Independent among years –specifies  $\rho_{\beta 1} = 0$
- 105 2. Random walk –specifies  $\rho_{\beta 1} = 1$
- 3. Constant intercept –specifies  $\rho_{\beta 1} = 0$  and  $\sigma_{\beta 1}^2 = 0$  (i.e.,  $\beta_1(t)$  is constant for all t)
- 107 4. Autoregressive estimates  $\rho_{\beta 1}$  as a fixed effect
- and settings are defined identically for specifying  $\rho_{\beta 2}$ .

## 110 Spatial variation

109

111 Regarding spatial variation:

112 
$$\omega_1^*(s,c) = \sum_{f=1}^{n_{\omega_1}} L_{\omega_1}(c_i, f) \omega_1^*(s_i, f)$$

- where  $\omega_1^*(s_i, f)$  represents predicted spatial variation in the first linear predictor occurring at
- the location  $s_i$  of sample i for factor f (of  $n_{\omega 1}$  factors representing spatial variation), and
- 115  $L_{\omega 1}(c_i, f)$  is the loadings matrix that generates spatial covariation among categories for this
- 116 linear predictor.
- VAST specifies internally that the spatial and spatio-temporal Gaussian random fields
- 118 (GMRFs) have a variance of 1.0. By default VAST estimates their values at each of  $n_s$
- vertices as follows:

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

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. These GMRFs are then projected to calculate their value at

every location  $s_i$  using matrix **A** with  $n_i$  rows and  $n_s$  columns. Specifically, values are

125 projected as:

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

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 **A**.

130

131

135

124

#### Spatio-temporal variation

132 Regarding spatio-temporal the model by default specifies that each vector of spatio-temporal

random effects,  $\mathbf{\varepsilon}_1(f_1, f_2)$  and  $\mathbf{\varepsilon}_2(f_1, f_2)$  composed of  $\varepsilon_1(s, f_1, f_2)$  and  $\varepsilon_2(s, f_1, f_2)$  across

locations s, is independent for each factor representing covariation among categories  $(f_1)$  and

among years  $(f_2)$ . We describe the process for the 1<sup>st</sup> linear predictor, and an identical

process is used for the 2<sup>nd</sup> linear predictor (using different subscripts):

137 
$$\mathbf{\varepsilon}_1(f_1, f_2) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

Values are then projected as:

$$\mathbf{\varepsilon}_1^*(f_1, f_2) = \mathbf{A}_i \mathbf{\varepsilon}_1(f_1, f_2)$$

This is then projected across years and categories using loadings matrices  $\mathbf{L}_{\varepsilon_t 1}$  and  $\mathbf{L}_{\varepsilon_c 2}$ :

141 
$$\varepsilon_1'(s,c,t) = \sum_{f_1=1}^{n_{\varepsilon_{c1}}} \sum_{f_2=1}^{n_{\varepsilon_{t1}}} L_{\varepsilon_c1}(c,f_1) L_{\varepsilon_{t1}}(f_2,t) \varepsilon_1(s,f_1,f_2)$$

Using a factor-decomposition to approximate covariation among years is a generalization of empirical orthogonal function (EOF) analysis (Thorson et al. 2020). The user can also specify a vector-autoregressive structure:

145 
$$\varepsilon_{1}(s, c_{1}, t) = \begin{cases} \varepsilon'_{1}(s, c_{1}, t) & \text{if } t = t_{min} \\ \sum_{c_{2}=1}^{n_{c}} b(c_{1}, c_{2}) \varepsilon'_{1}(s, c_{2}, t - 1) & \text{if } t > t_{min} \end{cases}$$

- Where  $b(c_1, c_2)$  is the estimated impact of spatio-temporal variation in category  $c_2$  on spatiotemporal changes in category  $c_1$ :
- 148  $b(c_1, c_2) = \begin{cases} \sum_{f=1}^{n_b} \chi(c_1, f) \psi(f, c_2) + \rho_{\varepsilon_1}(c_1) & \text{if } c_1 = c_2 \\ \sum_{f=1}^{n_b} \chi(c_1, f) \psi(f, c_2) & \text{if } c_1 \neq c_2 \end{cases}$
- Where  $\chi(c_1, f)$  and  $\psi(f, c_2)$  represent elements of matrices **X** and  $\Psi$ , where the product  $\mathbf{X}\Psi$  is the typical interaction matrix in a cointegration model (Engle and Granger 1987), where  $\Psi$  projects dynamics to a low-dimensional subspace and **X** represents responses within that subspace. By default  $n_b = 0$  corresponding to  $\mathbf{X}\Psi = \mathbf{0}$ , and these terms drop out of the model; however, they allow a parsimonious representation of species interactions (Thorson et al. 2017, 2019). Meanwhile  $\rho_{\varepsilon 1}(c)$  is the estimated degree of first-order autocorrelation in temporal variation:
- 156 1. Random walk specifies  $\rho_{\varepsilon_1}(c) = 1$
- 157 2. Autoregressive estimates  $\rho_{\varepsilon 1}$  as a single fixed effect with the same value for all categories
- 159 3. Individual autoregressive -- estimates a separate value of  $\rho_{\varepsilon 1}(c)$  as a single fixed effect 160 for each category
- and settings are defined identically for specifying  $\rho_{\varepsilon 2}$ .

#### 163 Overdisperison

164 Regarding overdispersion:

165 
$$\eta_1(v_i, c_i) = \sum_{f=1}^{n_{\eta_1}} L_1(c_i, f) \eta_1(v_i, f)$$

where  $\eta_1(v_i, f)$  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  $\mathbf{L}_{\beta 1}$ , 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).

#### **Density covariates**

176 Regarding covariates affecting densities ("density" or "habitat" covariates):

177 
$$v_1(c_i, t_i) = \sum_{p=1}^{n_p} \left( \gamma_1(c_i, p) + \sigma_{\xi_1}(c_i, p) \xi_1^*(s_i, c_i, p) \right) X(i, t_i, p)$$

where  $X(i,t_i,p)$  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. By default VAST estimates spatially-varying slope terms values 185 at each vertex as follows: 186

$$\xi_1(c,p) \sim MVN(\mathbf{0},\mathbf{R}_1)$$

Values are then predicted as e.g.: 188

189 
$$\xi_1^*(c,p) = \mathbf{A}_i \xi_1(c,p)$$

190

191

#### **Catchability covariates**

- Finally, regarding covariates affecting the process of obtaining measurements ("catchability" 192 or "detectability" covariates): 193

194 
$$\zeta_1(i) = \sum_{k=1}^{n_k} \left( \lambda_1(k) + \sigma_{\varphi_1}(k) \varphi_1^*(s_i, k) \right) q_1(i, k)$$

Where  $q_1(i, k)$  is an element of matrix  $\mathbf{Q}_1$  composed of  $n_k$  measured catchability covariates 195 that explain variation in catchability,  $\lambda_1(k)$  is the estimated impact of catchability covariates 196 for this linear predictor,  $\varphi_1^*(s_i, k)$  is unit-variance spatial variation in that slope term such that 197  $\sigma_{\varphi 1}(k)\varphi_1^*(s_i,k)$  has standard deviation  $\sigma_{\varphi 1}(k)$ , where spatial variation in detectability is 198 specified as follows: 199

$$\mathbf{\phi}_1(k) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

Values are then predicted as e.g.: 201

$$\mathbf{\phi}_1^*(c,p) = \mathbf{A}_i \mathbf{\phi}_1(k)$$

203

204

205

#### **Fishing impacts**

- Fishing impacts are included to represent the effect of known human impacts on variables.
- They are not yet documented in detail here, but see Thorson et al. (2019) for details. By 206
- default this term is excluded (i.e.,  $\iota(c_i, t_i) = 0$ ) and it is only applicable within MICE or 207

single-species production models following vector-autoregressive dynamics (i.e., Gompertz density dependence). Feel free to contact the package author if desiring more documentation.

210

211

208

209

#### Link functions and observation error distributions

- There are currently four options for the link function. For the latest set of options see the R
- 213 help documentation by typing into the R terminal `?VAST::Data\_Fn`.
- 214 1. ObsModel[2]=0 applies a logit-link for the first linear predictor:

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

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

219 
$$r_2(i) = a_i \times \log^{-1}(p_2(i))$$

- 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.
- 224 2. ObsModel[2]=1 corresponds to a "Poisson-link" delta-model that approximates a Tweedie
- 225 distribution:

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

- 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. 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 for sampling data  $\mathbb{E}(B_i) = r_1(i) \times r_2(i)$ .
- *Continuous-valued data (e.g., biomass)*
- 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  $b_i \geq 0$ .
- VAST calculates the probability of these data as:

249 
$$\Pr(b_i = B) = \begin{cases} 1 - r_1(i) & \text{if } B = 0\\ r_1(i) \times g\{B | r_2(i), \sigma_m^2(c)\} & \text{if } B > 0 \end{cases}$$

- 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.
- 254 Discrete-valued data (e.g., abundance)

If using an observation model with discrete support (e.g., a Poisson, negative-binomial, 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:

258 
$$\Pr(B = b_i) = \begin{cases} (1 - r_1(i)) + g\{B = 0 | r_2(i), \dots\} & \text{if } B = 0 \\ r_1(i) \times g\{B = b_i | r_2(i), \dots\} & \text{if } B > 0 \end{cases}$$

where ObsModel[1] controls the probability mass function  $g\{B|r_2(i),...\}$  used (again, see ?Data\_Fn for a list of options), where I use ... to signify that these probability mass functions 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 individuals that are in the vicinity of sampling in habitat that is occupied), and  $g\{B=0|r_2(i),...\}$  is the probability of not encountering category c given that sampling occurs in occupied habitat (Martin et al. 2005).

#### **Settings regarding spatial smoothers**

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  $n_s$  verticies. 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:

282 
$$\mathbf{R}_1(s, s+h) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \times (\kappa_1|h\mathbf{H}|)^{\nu} \times K_{\nu}(\kappa_1|h\mathbf{H}|)$$

- where **H** is a two-dimensional linear transformation representing geometric anisotropy (with a determinant of 1.0),  $\nu$  is the Matern smoothness (fixed at 1.0), and  $\kappa_1$  governs the decorrelation distance for that first linear predictor ( $\kappa_2$  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**).
- There are also other options:
- 289 1. barrier effects: avoiding correlations traveling across land;
- 290 2. *spherical projections*: calculating distance based on spherical coordinates, to avoid sensitivity to chosen projection;
- 3. *stream-network distance*: calculating distance based on river distances in a stream network or other graphical spatial dependency (Hocking et al. 2018).

294

295

298

299

300

301

302

283

284

285

286

287

#### 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.
  - 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  $\mathbf{A}_i$  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 2015), 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  $\mathbf{A}_i$  has row i with value zero except for three cells, representing the vertices of the triangle containing location  $s_i$ .

#### **Structure on parameters among years:**

There are different user-controlled options for specifying structure for intercepts or spatiotemporal variation across time.

#### **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.

#### **Identifiability constraints:**

- The model as described requires several identifiability constraints to ensure that the resulting

  Hessian is positive definite (and hence allow calculation of asymptotic standard errors):
- 1. All loadings matrices are defined to be lower-triangular (i.e., elements above the diagonal are fixed at 0);
- 2. When estimating spatial random fields  $\omega_1^*(s,c)$  and estimating a loadings matrix across years for spatio-temporal variation, it is helpful to impose a sum-to-zero constraint on factors of the loadings matrix  $L_{\varepsilon_t 1}(f_2,t)$ . This ensures that spatial terms represent the distribution in an "average" year, defined as times t when  $L_{\varepsilon_t 1}(f_2,t)=0$  for all columns;
  - 3. When estimating loadings across species  $L_{\varepsilon_c 1}(c,f_1)$  and across years  $L_{\varepsilon_t 1}(f_2,t)$ , the magnitude of these two matrices is confounded. The solution adopted here is to impose the constraint that  $\sum_{f=1}^{n_f} \sum_{t=1}^{n_t} L_{\varepsilon_t}(f,t) = 1$  for both linear predictors, such that the magnitude of  $L_{\varepsilon_c 1}(c,f_1)$  can be interpreted similarly to other loadings matrices.
  - The model also has issues arising from "label switching," i.e., where any column of any loadings matrix could be multiplied by negative-one (and similarly for the associated factor) without any change in the model predicts and likelihood. This implies that the negative log-likelihood has a series of local minima that all have the same properties. We do not address "label switching" because it does not have any practical effect on maximum-likelihood estimation or resulting predictions, but we note that it gives rise to numerical complexities when tuning or interpreting mixing for conventional samplers within a Bayesian estimation paradigm.

### Combining multiple data types

VAST can be used to combine encounter/non-encounter, count, and biomass-sampling data.

353 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

(2019) 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 1st

observation. The user then specifies multiple observation errors via input ObsModel\_ez:

```
# Control observation error
ObsModel_ez = cbind( "PosDist"=c(13,14,2), "Link"=c(1,1,1) )
360
```

361

362

363

364

365

354

355

356

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.

366

367

## Relationship to other named models

- VAST can be configured to be identical to (or closely mimic) many models that have
- previously been published in ecology and fisheries:
- 370 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).
- 373 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. 2015b), although it permits the
- use of a delta-model (i.e., separate analysis of encounters and positive catch rates).
- 376 3. 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 use of a delta-model.

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. 2015a). 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.:

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

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.:

402 
$$p_1(g,c,t) = \underbrace{\beta_1^*(c) + \sum_{f=1}^{n_{\beta_1}} L_{\beta_1}(c,f)\beta_1(t,f)}_{Temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\omega_1}} L_{\omega_1}(x,f)\omega_1^*(g,f)}_{Spatial\ variation}$$

$$+ \sum_{\substack{f=1\\ Spatio-temporal\ variation}}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c,f)\varepsilon_{1}^{*}(g,f,t) + \sum_{\substack{p=1\\ P=1}}^{n_{p}} \left(\gamma_{1}(c,t,p) + \sigma_{\xi 1}(c,p)\xi_{1}^{*}(g,c,p)\right)X(g,t,p)$$

- where  $p_2(g, c, t)$  is predicted similar, and these linear predictors are used in turn to predict 404
- $r_1(g,c,t)$  and  $r_2(g,c,t)$ , where their product is predicted biomass-density d(g,c,t) at every 405
- extrapolation-grid cell g, category c, and time t. 406
- By default, density is used to predict total abundance for the entire domain (or a 407
- subset of the domain) for a given species: 408

409 
$$I(c,t,l) = \sum_{x=1}^{n_x} (a(g,l) \times d(g,c,t))$$

- where a(g, l) is the area associated with extrapolation-grid cell g for index l; and. The user 410
- can also specify additional post-hoc calculations via the Options vector: 411
- Options = c("SD\_site\_density"=0, "SD\_site\_logdensity"=0, "Calculate\_Range"=0, 412
- "Calculate\_evenness"=0, "Calculate\_effective\_area"=0, "Calculate\_Cov\_SE"=0, 'Calculate\_Synchrony'=0, 'Calculate\_Coherence'=0) 413
- 414
- 1. Distribution shift RhoConfig[3]=1 turns on calculation of the centroid of the 416
- population's distribution: 417

418 
$$Z(c,t,m) = \sum_{x=1}^{n_x} \frac{(z(g,m) \times a(g,1) \times d(g,c,t))}{I(c,t,1)}$$

- where z(q, m) is a matrix representing location for each extrapolation-grid cell (by 419
- default z(q, m) is the location in Eastings and Northings of each knot), representing 420
- movement North-South and East-West). This model-based approach to estimating 421
- distribution shift can account for differences in the spatial distribution of sampling, unlike 422
- conventional sample-based estimators (Thorson et al. 2016b). 423

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

426 
$$D(c,t,l) = \sum_{x=1}^{n_x} \frac{a(x,l) \times d(x,c,t)}{I(c,t,l)} d(x,c,t)$$

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 reference documentation for details regarding user
  interface).

435

436

- I next provide a list of "features" organized as decisions that can be made by the analyst.
- 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.

List of features

- 443 Basic features in a generalized linear model (GLM)
- 1. Specifying one of several possible distributions for data, including for:
- 445 a. Count data using a Poisson, negative-binomial, Conway-Maxwell-Poisson, or 446 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.
- 2. Specifying one of several possible link functions for predicting data given linear
- 450 predictors including:
- a. A conventional delta-model;
- b. A Poisson-link delta model.
- 453 3. Including dynamic habitat covariates or not;
- 454 4. Including catchability covariates or not;
- Basic features in a spatio-temporal generalized linear mixed model (GLMM)
- 456 5. Specify an "extrapolation grid" using input
- 457 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
- 459 FishStatsUtils::make extrapolation info(..., Region="User", input grid=Input),
- where Input is a data frame supplied by the user.
- 461 6. Specifying a method for defining "knots";
- 462 7. Specifying the number of "knots";
- 8. Spatial variation being estimated ("turned on") or ignored ("turned off") for either linear
- 464 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.
- 471 *Multivariate analysis*

11. Including a "multivariate" structure with multiple responses that covary due to a specified 472 number of "factors" for spatial and spatio-temporal terms; 473 12. Rotate results prior to interpretation, using either: 474 a. principle components rotation; or 475 b. varimax rotation. 476 Decisions regarding temporal structure 477 13. Annual intercepts being structured over time, including: 478 a. estimated as fixed effects in every year; 479 480 b. fixed as fixed effect with the same value for all years; c. estimated as a random effect with independent deviations in each year; 481 d. estimated as a random effect with first-order autoregressive structure; or 482 e. estimated as a random effect with a random-walk structure. 483 14. Spatio-temporal variation being structured over time, including: 484 a. estimated as independent deviations in each year; 485 b. estimated as following a first-order autoregressive structure over time; 486 c. estimated as following a random-walk structure over time; or 487 d. estimated as following a vector-autoregressive structure involving a matrix of 1st 488 order autoregressive interactions. 489 Derived quantities 490 491 15. Specifying spatial strata for use when calculating derived quantities; 16. Calculating one of many possible "univariate derived quantities", including: 492 a. abundance indices; 493 494 b. range shift; c. effective area occupied 495 d. covariance among categories within a multivariate model; or 496

- e. synchrony among categories.
- 498 17. Calculating "multivariate derived quantities" that are derived from estimates for multiple
- categories in a multivariate model, e.g., where one category represents a standardized diet
- sample (e.g., prey biomass per predator biomass in a stomach-content sample) and
- another category represents a biomass-density sample (e.g., predator biomass in a bottom-
- trawl sample) such that their product represents predator-expanded consumption.
- 503 Unusual circumstances and special cases
- 18. Specifying separate distributions for different data sets (e.g., when multiple surveys
- providing different data types are available);
- 506 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);
- 509 20. Specifying multiple "seasons" (e.g., when modelling data with both annual and monthly
- spatio-temporal variation).

## 512 Common problems

- 513 There are two basic problems that are often encountered during spatio-temporal delta-
- 514 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  $\beta_1(c,t) \to \infty$  and/or
- 517  $\varepsilon_1(s,c,t) \to \infty$  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
- that category c and year t;
- 520 2. *Bounds*: Some parameter(s) hits a bound;
- 521 These problems can be solved by:

- 1. Encounter rates: constraining terms that vary among years (e.g., intercept  $\beta$  and spatiotemporal 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% encounter rates and fix corresponding intercepts for encounter probability to an extremely high value.
- 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.
- 533 2. *Bounds*: Please try running the model without estimating standard errors or a final newton step:

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

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

538

539

532

#### How to implement basic model changes

- There are a few basic model types that users often want to fit using VAST. I briefly describe
- 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,
- 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
- should then turn off the last two elements of the FieldConfig vector (i.e.,
- 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 positive catch rates (i.e., RhoConfig[2]=3). Finally, the user should "jitter" their presence observations by a very small amount (i.e., add a random normal deviation with a very small standard deviation, rnorm(n=1,mean=0,sd=0.001), to each observation for which b\_i=1). This will result in VAST estimating a logistic regression model for encounter/non-encounter data, except with one additional parameter estimated ( $\sigma_M$ ), 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).

### **Acknowledgements**

I thank K. Kristensen, H. Skaug, and the developers of Template Model Builder, without which this research and resulting R package VAST would not be possible. I also thank the many collaborators who have contributed to developing features (see <a href="https://github.com/nwfsc-assess/geostatistical\_delta-GLMM/wiki/Applications">https://github.com/nwfsc-assess/geostatistical\_delta-GLMM/wiki/Applications</a>), as well as the funding sources that have supported development (see <a href="https://github.com/James-Thorson-NOAA/VAST#funding-and-support-for-the-tool">https://github.com/James-Thorson-NOAA/VAST#funding-and-support-for-the-tool</a>). In particular, I think C. Monnahan and M. Rudd for contributing substantially to coding new features, and A. Gruss for identifying indexing errors in several (little used) features. I also thank the many volunteers and NOAA scientists who have served on sampling vessels that provided data to test these methods. Finally, I think A. Grüss and S. Hoyle for providing edits to this document.

#### Works cited

573

584

585

586

587

588

589

590

591

592

593 594

598

599

- 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.
- Engle, R.F., and Granger, C.W. 1987. Co-integration and error correction: representation, estimation, and testing. Econom. J. Econom. Soc.: 251–276.
- Gelman, A., and Hill, J. 2007. Data analysis using regression and multilevel/hierarchical
   models. Cambridge University Press, Cambridge, UK.
- Godefroid, M., Boldt, J.L., Thorson, J.T., Forrest, R., Gauthier, S., Flostrand, L., Ian Perry,
   R., Ross, A.R.S., and Galbraith, M. 2019. Spatio-temporal models provide new
   insights on the biotic and abiotic drivers shaping Pacific Herring (Clupea pallasi)
   distribution. Prog. Oceanogr. 178: 102198. doi:10.1016/j.pocean.2019.102198.
  - Grüss, A., and Thorson, J.T. 2019. Developing spatio-temporal models using multiple data types for evaluating population trends and habitat usage. ICES J. Mar. Sci. **76**(6): 1748–1761. doi:10.1093/icesjms/fsz075.
    - 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.
- Hocking, D.J., Thorson, J.T., O'Neil, K., and Letcher, B.H. 2018. A geostatistical state-space model of animal densities for stream networks. Ecol. Appl. 28(7): 1782–1796.
   doi:10.1002/eap.1767.
  - 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.
- 604 Lindgren. 2012. Continuous domain spatial models in R-INLA. ISBA Bull. 19(4): 14–20.
- 605 Lindgren, F., and Rue, H. 2015. Bayesian spatial modelling with r-inla. J. Stat. Softw. **63**(19): 1–25. doi:10.18637/jss.v063.i19.
- Lindgren, 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.

- 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., Adams, G., and Holsman, K. 2019. Spatio-temporal models of intermediate complexity for ecosystem assessments: A new tool for spatial fisheries management. Fish Fish. **20**(6): 1083–1099. doi:10.1111/faf.12398.
- 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., Ciannelli, L., and Litzow, M.A. 2020. Defining indices of ecosystem variability using biological samples of fish communities: A generalization of empirical orthogonal functions. Prog. Oceanogr. **181**: 102244. doi:10.1016/j.pocean.2019.102244.
- Thorson, J.T., and Haltuch, M.A. 2018. Spatiotemporal analysis of compositional data: increased precision and improved workflow using model-based inputs to stock assessment. Can. J. Fish. Aquat. Sci. **76**(3): 401–414. doi:10.1139/cjfas-2018-0015.
- 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., Munch, S.B., and Swain, D.P. 2017. Estimating partial regulation in spatiotemporal models of community dynamics. Ecology **98**(5): 1277–1289. doi:10.1002/ecy.1760.
  - 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., Olden, J.D., and Schindler, D.E. 2018. Spatial heterogeneity contributes more to portfolio effects than species variability in bottom-associated marine fishes. Proc R Soc B **285**(1888): 20180915. doi:10.1098/rspb.2018.0915.
- Thorson, J.T., Shelton, A.O., Ward, E.J., and Skaug, H.J. 2015a. Geostatistical deltageneralized 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.

672 673 674	Thorson, Scheuerell, M.D., Shelton, A.O., See, K.E., Skaug, H.J., and Kristensen, K. 2015b. Spatial factor analysis: a new tool for estimating joint species distributions and correlations in species range. Methods Ecol. Evol. <b>6</b> (6): 627–637. doi:10.1111/2041-
675	210X.12359.
676	Tierney, L., Kass, R.E., and Kadane, J.B. 1989. Fully exponential Laplace approximations to
677	expectations and variances of nonpositive functions. J. Am. Stat. Assoc. 84(407):
678	710–716.
679	
680	

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	
683			
684			
685			
686			

Table 2 – Definition of mathematical notation, including the symbol used, its type (Index, Data, fixed effects "FE", random effects "RE", intermediate quantity computed internally "IQ", and derived quantities that are outputted for users "DQ"), and its dimension

Table 2A – Indices

Index name	Symbol
Observation number	i
Extrapolation-grid cell	g
Knot number	x
Vertex number (including internal knots and boundary vertices)	S
Time interval number	t
Category number	С
Factor number	f
Habitat covariate number for 1st linear predictor	$p_1$
Habitat covariate number for 2 <sup>nd</sup> linear predictor	$p_2$
Catchability covariate number for 1st linear predictor	$k_1$
Catchability covariate number for 2 <sup>nd</sup> linear predictor	$k_2$
Stratum number	l
Index number for measures of center-of-gravity	m
Index number for other book-keeping	Z

Table 2B – Data

Index name	Symbol	Dimensions
Sample response	$b_i$	$n_i$
Time interval for each sample	$t_i$	$n_i$
Category for each sample	$c_i$	$n_i$
Overdispersion level for each sample	$v_i$	$n_i$

Area covered by each sample	$a_i$	$n_i$
Bilinear interpolation from vertices to samples	$\mathbf{A}_{is}$	$n_i \times 3$
Bilinear interpolation from vertices to extrapolation- grid cells	$\mathbf{A}_{gs}$	$n_g \times 3$
Distance between two vertices	d(s,s')	$n_s \times n_s$
Habitat covariates affecting 1 <sup>st</sup> linear predictor for each sampling location, time, and variable	$X_1(i,t,p_1)$	$n_i \times n_t \times n_{p1}$
Habitat covariates affecting 2 <sup>nd</sup> linear predictor for each sampling location, time, and variable	$X_2(i,t,p_2)$	$n_i \times n_t \times n_{p2}$
Habitat covariates affecting 1 <sup>st</sup> linear predictor for each extrapolation-grid cell, time, and variable	$X_1(g,t,p_1)$	$n_g \times n_t \times n_{p1}$
Habitat covariates affecting 2 <sup>nd</sup> linear predictor for each extrapolation-grid cell, time, and variable	$X_2(g,t,p_2)$	$n_g \times n_t \times n_{p2}$
Catchability covariates affecting 1 <sup>st</sup> linear predictor for each sample and variable	$Q_1(i,k_1)$	$n_i \times n_{k1}$
Catchability covariates affecting 2 <sup>nd</sup> linear predictor for each sample and variable	$Q_2(i,k_2)$	$n_i \times n_{k2}$
Area associated with extrapolation-grid cell in each stratum	a(g, l)	$n_g \times n_l$
Statistic for each location used to calculate center of gravity and range edges	z(s,m)	$n_s \times n_m$

Table 2C - Coefficients, indicating whether they are fixed effects (FE), random effects (RE)

or whether their treatment depends upon user settings (FE/RE)

Coefficient name	Symbol	Type	Dimensions
Factor values for intercept for 1st linear predictor	$\beta_1(f,t)$	FE/RE	$n_{\beta 1} \times n_t$
Factor values for intercept for 2st linear predictor	$\beta_2(f,t)$	FE/RE	$n_{\beta 2} \times n_t$
Loadings matrix for intercepts for 1st linear predictor	$L_{\beta 1}(c,f)$	FE	$n_c \times n_{\beta 1}$
Loadings matrix for intercepts for 2 <sup>nd</sup> linear predictor	$L_{\beta 2}(c,f)$	FE	$n_c \times n_{\beta 2}$
Loadings matrix for spatial covariation for 1 <sup>st</sup> linear predictor	$L_{\omega 1}(c,f)$	FE	$n_c \times n_{\omega 1}$

Loadings matrix for spatial covariation for 2 <sup>nd</sup> linear predictor	$L_{\omega 2}(c,f)$	FE	$n_c \times n_{\omega 2}$
Loadings matrix for spatio-temporal covariation across categories for 1 <sup>st</sup> linear predictor	$L_{\varepsilon 1}(c,f)$	FE	$n_c \times n_{\varepsilon 1}$
Loadings matrix for spatio-temporal covariation across categories for 2 <sup>nd</sup> linear predictor	$L_{\varepsilon 2}(c,f)$	FE	$n_c \times n_{\varepsilon 2}$
Loadings matrix for spatio-temporal covariation across time for 1 <sup>st</sup> linear predictor	$L_{arepsilon 1}^{time}(t,f)$	FE	$n_t \times n_{\varepsilon 1}^{time}$
Loadings matrix for spatio-temporal covariation across time for 2 <sup>nd</sup> linear predictor	$L_{\varepsilon 2}^{time}(t,f)$	FE	$n_t \times n_{\varepsilon 2}^{time}$
Loadings matrix for overdispersion covariation for 1 <sup>st</sup> linear predictor	$L_1(c,f)$	FE	$n_c \times n_{\eta 1}$
Loadings matrix for overdispersion covariation for 2 <sup>nd</sup> linear predictor	$L_2(c,f)$	FE	$n_c \times n_{\eta 2}$
Impact of habitat covariates on 1st linear predictor	$\gamma_1(c,t,p)$	FE	$n_c \times n_t \times n_p$
Impact of habitat covariates on 2 <sup>nd</sup> linear predictor	$\gamma_2(c,t,p)$	FE	$n_c \times n_t \times n_p$
Impact of catchability covariates on 1st linear predictor	$\lambda_1(k)$	FE	$n_k$
Impact of catchability covariates on 2 <sup>nd</sup> linear predictor	$\lambda_2(k)$	FE	$n_k$
Parameters governing residual variation	$\sigma_m^2(c,z)$	FE	$n_c \times 2$
Decorrelation rate for 1st linear predictor	$\kappa_1$	FE	1
Decorrelation rate for 2 <sup>nd</sup> linear predictor	$\kappa_2$	FE	1
Autocorrelation for intercepts of 1st linear predictor	$\rho_{\beta 1}$	FE	1
Autocorrelation for intercepts of 2 <sup>nd</sup> linear predictor	$ ho_{eta 2}$	FE	1
Conditional variance for intercepts of 1st linear predictor	$\sigma_{\!eta 1}^2$	FE	1
Conditional variance for intercepts of 2 <sup>nd</sup> linear predictor	$\sigma_{\!eta 2}^2$	FE	1
Autocorrelation for spatio-temporal covariation of 1 <sup>st</sup> linear predictor	$ ho_{arepsilon 1}$	FE	1
Autocorrelation for spatio-temporal covariation of 2 <sup>nd</sup> linear predictor	$ ho_{arepsilon 2}$	FE	1
Parameters governing geometric anisotropy	h(z)	FE	2
Spatial factors for 1st linear predictor	$\omega_1(s,f)$	RE	$n_s \times n_{\omega 1}$
Spatial factors for 2 <sup>nd</sup> linear predictor	$\omega_2(s,f)$	RE	$n_s \times n_{\omega 2}$

Spatio-temporal factors for 1 <sup>st</sup> linear predictor	$\varepsilon_1(s,f,f)$	RE	$n_s \times n_{arepsilon_1} \  imes n_{arepsilon_1}^{time}$
Spatio-temporal factors for 2 <sup>nd</sup> linear predictor	$\varepsilon_2(s,f,f)$	RE	$n_s \times n_{\varepsilon 1} \\ \times n_{\varepsilon 1}^{time}$
Overdispersion factors for 1st linear predictor	$\eta_1(v,f)$	RE	$n_v \times n_{\eta 1}$
Overdispersion factors for 2 <sup>nd</sup> linear predictor	$\eta_2(v,f)$	RE	$n_v \times n_{\eta 2}$

# Table 2D – Variable calculated internally

Coefficient name	Symbol	Dimensions
1 <sup>st</sup> linear predictor	$p_1(i)$	$n_i$
2 <sup>nd</sup> linear predictor	$p_2(i)$	$n_i$
1 <sup>st</sup> link-transformed predictor	$r_1(i)$	$n_i$
2 <sup>nd</sup> link-transformed predictor	$r_2(i)$	$n_i$
Spatio-temporal variation for 1 <sup>st</sup> linear predictor at each extrapolation-grid cell	$\varepsilon_1(g,c,t)$	$n_g \times n_c \times n_t$
Spatio-temporal variation for 2 <sup>nd</sup> linear predictor at each extrapolation-grid cell	$\varepsilon_2(g,c,t)$	$n_g \times n_c \times n_t$
Spatio-temporal variation for 1 <sup>st</sup> linear predictor at each sample	$\varepsilon_1(i,c,t)$	$n_i \times n_c \times n_t$
Spatio-temporal variation for 2 <sup>nd</sup> linear predictor at each sample	$\varepsilon_2(i,c,t)$	$n_i \times n_c \times n_t$
Spatial variation for 1 <sup>st</sup> linear predictor at each extrapolation-grid cell	$\omega_1(g,c)$	$n_g \times n_c$
Spatial variation for 2 <sup>nd</sup> linear predictor at each extrapolation-grid cell	$\omega_2(g,c)$	$n_g \times n_c$
Spatial variation for 1st linear predictor at each sample	$\omega_1(i,c)$	$n_i \times n_c$
Spatial variation for 2 <sup>nd</sup> linear predictor at each sample	$\omega_2(i,c)$	$n_i \times n_c$
Intercept for 1st linear predictor	$\beta_1(c,t)$	$n_c \times n_t$
Intercept for 2 <sup>st</sup> linear predictor	$\beta_2(c,t)$	$n_c \times n_t$
Spatial correlation matrix among vertices for 1 <sup>st</sup> linear predictor	$\mathbf{R}_1$	$n_s \times n_s$

Spatial correlation matrix among vertices for 2 <sup>nd</sup> linear predictor	$\mathbf{R}_2$	$n_s \times n_s$
Anisotropy matrix	Н	$2 \times 2$

# Table 2E – Derived quantities

Coefficient name	Symbol	Dimensions
Predicted density for each sample	$d^*(i,c,t)$	$n_i \times n_c \times n_t$
Predicted density for each extrapolation-grid cell	$d^*(g,c,t)$	$n_g \times n_c \times n_t$
Index of abundance	I(c,t,l)	$n_c \times n_t \times n_l$
Center of gravity	Z(c,t,m)	$n_c \times n_t \times n_m$
Average density	D(c,t,l)	$n_c \times n_t \times n_l$
Effective area occupied	A(c,t,l)	$n_c \times n_t \times n_l$
Rotation matrix for spatial covariation for 1 <sup>st</sup> linear predictor	$\mathbf{B}_{\omega 1}$	$n_c \times n_c$
Rotation matrix for spatial covariation for 2 <sup>nd</sup> linear predictor	$\mathbf{B}_{\omega 2}$	$n_c \times n_c$
Rotation matrix for spatio-temporal covariation for 1 <sup>st</sup> linear predictor	$\mathbf{B}_{arepsilon 1}$	$n_c \times n_c$
Rotation matrix for spatio-temporal covariation for 2 <sup>nd</sup> linear predictor	$\mathbf{B}_{arepsilon 2}$	$n_c \times n_c$
Rotation matrix for overdispersion covariation for 1 <sup>st</sup> linear predictor	$\mathbf{B}_1$	$n_c \times n_c$
Rotation matrix for overdispersion covariation for 2 <sup>nd</sup> linear predictor	$\mathbf{B}_2$	$n_c \times n_c$
Rotated loadings matrix for spatial covariation for 1 <sup>st</sup> linear predictor	$L^*_{\omega 1}(c,f)$	$n_c \times n_{\omega 1}$
Rotated loadings for spatial covariation for 2 <sup>nd</sup> linear predictor	$L^*_{\omega 2}(c,f)$	$n_c \times n_{\omega 2}$
Rotated loadings for spatio-temporal covariation for 1 <sup>st</sup> linear predictor	$L^*_{\varepsilon 1}(c,f)$	$n_c \times n_{\varepsilon 1}$
Rotated loadings for spatio-temporal covariation for 2 <sup>nd</sup> linear predictor	$L^*_{\varepsilon 2}(c,f)$	$n_c \times n_{\varepsilon 2}$
Rotated loadings for overdispersion covariation for 1 <sup>st</sup> linear predictor	$L_1^*(c,f)$	$n_c \times n_{\eta 1}$

Rotated loadings for overdispersion covariation for 2 <sup>nd</sup> linear predictor	$L_2^*(c,f)$	$n_c \times n_{\eta 2}$
Rotated spatial factors for 1st linear predictor	$\omega_1^*(s,f)$	$n_s \times n_{\omega 1}$
Rotated spatial factors for 2 <sup>nd</sup> linear predictor	$\omega_2^*(s,f)$	$n_s \times n_{\omega 2}$
Rotated spatio-temporal factors for 1st linear predictor	$\varepsilon_1^*(s,f,t)$	$n_s \times n_{\varepsilon 1} \times n_t$
Rotated spatio-temporal factors for 2 <sup>nd</sup> linear predictor	$\varepsilon_2^*(s,f,t)$	$n_s \times n_{\varepsilon 1} \times n_t$
Rotated overdispersion factors for 1st linear predictor	$\eta_1^*(v,f)$	$n_v \times n_{\eta 1}$
Rotated overdispersion factors for 2 <sup>nd</sup> linear predictor	$\eta_2^*(v,f)$	$n_v \times n_{\eta 2}$