

VAST model structure and user interface

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Purpose of document:

R package VAST includes many different forms of documentation including:

1. Doxygen documentation that can be accessed through the standard R-help interface when the library is loaded within R;
2. the VAST decision tree and user guide (Thorson 2019)
3. two separate Rmarkdown “tutorials” that provide annotated code illustrating how to run VAST for single- or multi-species example using real-world data;
4. a searchable “issue tracker” available through GitHub; and
5. peer-reviewed articles describing development and applications for each feature (see list on GitHub).

This “VAST model structure and user interface” document is intended to complement these other resources by documenting and describing the model structure (all model equations and notation) while linking it to user-options that are available via the R interface to package VAST.

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.

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 as 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 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:

$$\begin{aligned}
 p_1(i) = & \underbrace{\beta_1^*(c_i) + \sum_{f=1}^{n_{\beta_1}} L_{\beta_1}(c_i, f) \beta_1(t_i, f)}_{\text{Temporal variation}} + \underbrace{\sum_{f=1}^{n_{\omega_1}} L_{\omega_1}(c_i, f) \omega_1^*(s_i, f)}_{\text{Spatial variation}} \\
 & + \underbrace{\sum_{f=1}^{n_{\varepsilon_1}} L_{\varepsilon_1}(c_i, f) \varepsilon_1^*(s_i, f, t_i)}_{\text{Spatio-temporal variation}} + \underbrace{\sum_{f=1}^{n_{\eta_1}} L_1(c_i, f) \eta_1(v_i, f)}_{\text{Vessel effects}} \\
 & + \underbrace{\sum_{p=1}^{n_p} \left(\gamma_1(c_i, t_i, p) + \sigma_{\xi_1}(c_i, p) \xi_1^*(s_i, c_i, p) \right) X(i, t_i, p)}_{\text{Habitat covariates}} + \underbrace{\sum_{k=1}^{n_k} \lambda_1(k) Q(i, k)}_{\text{Catchability covariate}}
 \end{aligned}$$

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_{β_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_{β_1} can range from zero to the number of categories n_c , $0 \leq n_{\beta_1} \leq n_c$, 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}_{β_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 ($n_{\beta_1} = 1$),

69 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,
 70 $abs(\mathbf{L}_{\beta 1})$ is the standard deviation for temporal variation.

71 Similarly, $\omega_1^*(s_i, f)$ represents predicted spatial variation in the first linear predictor
 72 occurring at the location s_i of sample i for factor f (of $n_{\omega 1}$ factors representing spatial
 73 variation), and $L_{\omega 1}(c_i, f)$ is the loadings matrix that generates spatial covariation among
 74 categories for this linear predictor. Similarly, $\varepsilon_1^*(s_i, f, t_i)$ represents predicted spatio-
 75 temporal variation in the first linear predictor for each factor f (of $n_{\varepsilon 1}$ factors representing
 76 spatio-temporal variation), and $L_{\varepsilon 1}(c_i, f)$ is the loadings matrix that generates spatio-
 77 temporal covariation for this predictor. $\eta_1(v_i, f)$ represents random variation in catchability
 78 among a grouping variable (tows or vessels) for each factor f (of $n_{\eta 1}$ factors representing
 79 overdispersion), and $L_1(c_i, f)$ is a loadings matrix that generates covariation in catchability
 80 among categories for this predictor. All loadings matrices are specified similarly to $\mathbf{L}_{\beta 1}$, i.e.,
 81 where factors have a variance of one such that $\mathbf{L}^T \mathbf{L}$ represents the covariance among
 82 categories. The main difference is that spatial, spatio-temporal, and overdispersion factors
 83 can only be specified as random effects, while the intercepts can be specified as either
 84 random or fixed (where specifying as fixed “turns off” all factor-modelling for that intercept).

85 Finally, $X(i, t_i, p)$ is an three-dimensional array of n_p measured density covariates
 86 that explain variation in density for time t and the location s_i where sampling occurred for
 87 sample i . VAST can include a separate, spatially-varying effect of each habitat covariate p
 88 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
 89 $\gamma_1(c_i, t_i, p)$ is the average effect of density covariate $X(i, t_i, p)$ for category c , $\xi_n(s_i, c_i, p)$
 90 represents spatial variation in that effect (which has a mean of zero and standard deviation of
 91 one), and $\sigma_{\xi 1}(c, p)$ represents the estimated standard deviation of spatial variation of
 92 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 constraint by specifying a different structure for `Data_Fn(..., Map=NewMap)`.

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:

$$\begin{aligned}
 p_2(i) = & \underbrace{\beta_2^*(c_i) + \sum_{f=1}^{n_{\beta 2}} L_{\beta 2}(c_i, f) \beta_2(t_i, f)}_{\text{Temporal variation}} + \underbrace{\sum_{f=1}^{n_{\omega 2}} L_{\omega 2}(c_i, f) \omega_2^*(s_i, f)}_{\text{Spatial variation}} \\
 & + \underbrace{\sum_{f=1}^{n_{\varepsilon 2}} L_{\varepsilon 2}(c_i, f) \varepsilon_2^*(s_i, f, t_i)}_{\text{Spatio-temporal variation}} + \underbrace{\sum_{f=1}^{n_{\eta 2}} L_2(c_i, f) \eta_2(v_i, f)}_{\text{Vessel effects}} \\
 & + \underbrace{\sum_{p=1}^{n_p} \left(\gamma_2(c_i, t_i, p) + \sigma_{\xi 2}(c_i, p) \xi_2^*(s_i, c_i, p) \right) X(i, t_i, p)}_{\text{Density covariates}} + \underbrace{\sum_{k=1}^{n_k} \lambda_2(k) Q(i, k)}_{\text{Catchability covariates}}
 \end{aligned}$$

where all variables and parameters are defined similarly except using different subscripts (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:

```
FieldConfig = c("Omega1"=1, "Epsilon1"=1, "Omega2"=1, "Epsilon2"=1)
```

where `FieldConfig[1]` controls $n_{\omega 1}$, `FieldConfig[2]` controls $n_{\varepsilon 1}$, `FieldConfig[3]` controls $n_{\omega 2}$, and `FieldConfig[4]` controls $n_{\varepsilon 2}$, and a value of zero “turns off” that component of spatial or spatio-temporal covariation.

113

114 **Number of overdispersion factors**

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

```
116 OverdispersionConfig = c("Eta1"=0, "Eta2"=0)
```

117

118 where `OverdispersionConfig[1]` controls n_{δ_1} , and `OverdispersionConfig[2]` controls n_{δ_2} ,

119 and a value of zero again “turns off” that component of random covariation in catchability.

120 For example, if the user inputs:

```
121 OverdispersionConfig = c("Eta1"=1, "Eta2"=1)
```

122

123 then there will be one random effect estimated for each unique level of `Data_Geostat$Vessel`

124 for both the first and second linear predictors.

125

126 **Link functions and observation error distributions**

127 There are user-controlled options that control the observation error distribution and the link-

128 functions used to calculate expected encounter probabilities and positive catch rates based on

129 the two linear predictors.

130 The `ObsModel` vector has two components, controlling the observation error distribution and

131 link function respectively.

```
132 ObsModel = c("PosDist"=2, "Link"=0)
```

133 There are currently four options for the link function. For the latest set of options see the R

134 help documentation by typing into the R terminal `?VAST::Data_Fn``.

135 1. `ObsModel[2]=0` applies a logit-link for the first linear predictor:

136
$$r_1(i) = \text{logit}^{-1}(p_1(i))$$

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

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

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 Tweedie 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. Area-swept 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 delta-models, 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:

161 There are different user-controlled options for observation models for available sampling
 162 data, which are controlled by `ObsModel_ez[1]`.

```
163 # Control observation error
164 ObsModel_ez = c("PosDist"=2, "Link"=0)
165
```

166 I distinguish between observation models for continuous-valued data (e.g., biomass, or
 167 numbers standardized to a fixed area), and observation models for count data (e.g., numbers
 168 treating area-swept as an offset). However, both are parameterized such that the expectation
 169 for sampling data $E(B_i) = r_1(i) \times r_2(i)$.

170 *Continuous-valued data (e.g., biomass)*

171 If using an observation model with continuous support (e.g., a normal, lognormal, gamma, or
 172 Tweedie models), then data b_i can be any non-negative real number, $b_i \in \mathcal{R}$ and $b_i \geq 0$.

173 VAST calculates the probability of these data as:

$$174 \quad \Pr(b_i = B) = \begin{cases} 1 - r_1(i) & \text{if } B = 0 \\ r_1(i) \times g\{B|r_2(i), \sigma_m^2(c)\} & \text{if } B > 0 \end{cases}$$

175 where `ObsModel[1]` controls the probability density function $g\{B|r_2(i), \sigma_m^2(c)\}$ used for
 176 positive catch rates (see `?Data_Fn` for a list of options), where each options is defined to have
 177 with expectation $r_2(i)$ and dispersion $\sigma_m^2(c)$, where dispersion parameter $\sigma_m^2(c)$ varies
 178 among categories by default.

179 *Discrete-valued data (e.g., abundance)*

180 If using an observation model with discrete support (e.g., a Poisson, negative-binomial,
 181 Conway-Maxwell Poisson, or lognormal-Poisson models), then data b_i can be any whole
 182 number, $b_i \in \{0, 1, 2, \dots\}$. VAST calculates the probability of these data as:

$$183 \quad \Pr(B = b_i) = \begin{cases} (1 - r_1(i)) + g\{B = 0|r_2(i), \dots\} & \text{if } B = 0 \\ r_1(i) \times g\{B = b_i|r_2(i), \dots\} & \text{if } B > 0 \end{cases}$$

184 where `ObsModel[1]` controls the probability mass function $g\{B|r_2(i), \dots\}$ used (again, see
 185 `?Data_Fn` for a list of options), where I use \dots 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 $g\{B = b_i | r_2(i), \dots\}$ (i.e., the number of individuals that are in the vicinity of sampling in habitat that is occupied), and $g\{B = 0 | r_2(i), \dots\}$ 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, the user specifies a number of knots n_x :

```
# Number of knots
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

212 spatial variable at all n_s vertices. Specifically, the correlation $\mathbf{R}_1(s, s + h)$ between
 213 location s and location $s + h$ for spatial and spatio-temporal terms included in the first linear
 214 predictor is approximated as following a Matern function:

$$215 \quad \mathbf{R}_1(s, s + h) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \times (\kappa_1|h\mathbf{H}|)^{\nu} \times K_{\nu}(\kappa_1|h\mathbf{H}|)$$

216 where \mathbf{H} is a two-dimensional linear transformation representing geometric anisotropy (with
 217 a determinant of 1.0), ν is the Matern smoothness (fixed at 1.0), and κ_1 governs the
 218 decorrelation distance for that first linear predictor (κ_2 is also separately estimated for the
 219 second linear predictor). By default, the two degrees of freedom in \mathbf{H} are estimated as fixed
 220 effects, but the user can specify isotropy (i.e., $\mathbf{H} = \mathbf{I}$) by specifying:

```
221 # Turn of geometric anisotropy
222 Data = Data_Fn( ..., Aniso=FALSE )
223
```

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

$$227 \quad \boldsymbol{\omega}_1(f) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

$$228 \quad \boldsymbol{\omega}_2(f) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

$$229 \quad \boldsymbol{\epsilon}_1(f, t) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

$$230 \quad \boldsymbol{\epsilon}_2(f, t) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

$$231 \quad \boldsymbol{\xi}_1(c, p) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

$$232 \quad \boldsymbol{\xi}_2(c, p) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

233 where $\boldsymbol{\omega}_1(f)$ is the vector of length n_s formed when subsetting $\omega_1(s, f)$ for a given f .

234 Specifying a variance of 1.0 ensures that the covariance among categories is defined by the
 235 loadings matrix for that term.

236

237 **Interpolating spatial variation from knots to the location of samples**

238 Starting with VAST release 3.0.0, users can choose between two options for smoothing
 239 spatial variation. Both options involve specifying a matrix \mathbf{A}_i with n_i rows and n_s columns,
 240 row i . Values are then predicted as e.g.:

$$241 \quad \boldsymbol{\omega}_1^*(f) = \mathbf{A}_i \boldsymbol{\omega}_1(f)$$

242 where $\boldsymbol{\omega}_1^*(f)$ is the vector of length n_i , containing the predicted value $\omega_1^*(s_i, f)$ for spatial
 243 variation in the first linear predictor at every location s_i , and other spatial variables are
 244 predicted similarly using matrix \mathbf{A}_i .

- 245 1. *Piecewise constant*: Following the conventional for releases of VAST prior to 3.0.0,
 246 users can specify `fine_scale=FALSE`. Given this specification, spatial variables at location
 247 s are fixed equal to their value at the nearest “knot.” This involves specifying matrix \mathbf{A}_i
 248 such that row i has value zero except for one cell containing a value of one for the knot
 249 closest to sample i .
- 250 2. *Bilinear interpolation*: Following standard practices using the software R-INLA
 251 (Lindgren 2012; Lindgren and Rue 2013), users can specify `fine_scale=TRUE`. Given this
 252 specification, spatial variables at location s are interpolated using the triangulated mesh
 253 that is also used to approximate spatial variation. Specifically, matrix \mathbf{A}_i has row i with
 254 value zero except for three cells, representing the vertices of the triangle containing
 255 location s_i .

256

257 **Structure on parameters among years:**

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

```
260 RhoConfig = c("Beta1"=0, "Beta2"=0, "Epsilon1"=0, "Epsilon2"=0)
```

261

262 *Temporal structure on intercepts*

By default (when $\text{RhoConfig}[1]=0$ and $\text{RhoConfig}[2]=0$) 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 factor-model structure:

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

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

Where t_{\min} is the index for the first modelled year and ρ_{β_1} and ρ_{β_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). $\text{RhoConfig}[1]$ controls the specification of ρ_{β_1} :

1. *Independent among years* – $\text{RhoConfig}[1]=1$ specifies $\rho_{\beta_1} = 0$
 2. *Random walk* – $\text{RhoConfig}[1]=2$ specifies $\rho_{\beta_1} = 1$
 3. *Constant intercept* – $\text{RhoConfig}[1]=3$ specifies $\rho_{\beta_1} = 0$ and $\sigma_{\beta_1}^2 = 0$ (i.e., $\beta_1(t)$ is constant for all t)
 4. *Autoregressive* – $\text{RhoConfig}[1]=4$ estimates ρ_{β_1} as a fixed effect
- and settings are defined identically for $\text{RhoConfig}[2]$ specifying ρ_{β_2} .

Temporal structure on spatio-temporal variation

By default (when $\text{RhoConfig}[3]=0$ and $\text{RhoConfig}[4]=0$), the model specifies that each vector of spatio-temporal random effects, $\boldsymbol{\varepsilon}_1(f, t)$ and $\boldsymbol{\varepsilon}_2(f, t)$ composed of $\varepsilon_1(s, f, t)$ and $\varepsilon_2(s, f, t)$ across locations s , is independent among years. However, other settings specify the following structure

$$\boldsymbol{\varepsilon}_1(f, t) \sim \begin{cases} \text{MVN}(\mathbf{0}, \mathbf{R}_1) & \text{if } t = t_{\min} \\ \text{MVN}(\rho_{\varepsilon_1}\boldsymbol{\varepsilon}_1(f, t-1), \mathbf{R}_1) & \text{if } t > t_{\min} \end{cases}$$

$$\epsilon_2(f, t) \sim \begin{cases} MVN(\mathbf{0}, \mathbf{R}_2) & \text{if } t = t_{min} \\ MVN(\rho_{\epsilon_2} \epsilon_2(f, t-1), \mathbf{R}_2) & \text{if } t > t_{min} \end{cases}$$

where ρ_{ϵ_1} and ρ_{ϵ_2} are the estimated degree of first-order autocorrelation in temporal

variation, `RhoConfig[3]` controls the specification of ρ_{ϵ_1} :

1. *Random walk* – `RhoConfig[3]=2` specifies $\rho_{\epsilon_1} = 1$
2. *Autoregressive* – `RhoConfig[3]=4` estimates ρ_{ϵ_1} as a fixed effect

and settings are defined identically for `RhoConfig[4]` specifying ρ_{ϵ_2} .

291

292 **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.

306

307 **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 (n.d.) 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) )
```

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.

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:

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).
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. 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.:

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

where $\boldsymbol{\omega}_1^*(f)$ is the vector of length n_i , containing the predicted value $\omega_1^*(s_g, f)$ 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.:

$$\begin{aligned}
358 \quad p_1(g, c, t) = & \underbrace{\beta_1^*(c) + \sum_{f=1}^{n_{\beta 1}} L_{\beta 1}(c, f) \beta_1(t, f)}_{\text{Temporal variation}} + \underbrace{\sum_{f=1}^{n_{\omega 1}} L_{\omega 1}(x, f) \omega_1^*(g, f)}_{\text{Spatial variation}} \\
359 \quad & + \underbrace{\sum_{f=1}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c, f) \varepsilon_1^*(g, f, t)}_{\text{Spatio-temporal variation}} + \underbrace{\sum_{p=1}^{n_p} \left(\gamma_1(c, t, p) + \sigma_{\xi 1}(c, p) \xi_1^*(g, c, p) \right) X(g, t, p)}_{\text{Habitat covariates}}
\end{aligned}$$

360 where $p_2(g, c, t)$ is predicted similar, and these linear predictors are used in turn to predict
361 $r_1(g, c, t)$ and $r_2(g, c, t)$, where their product is predicted biomass-density $d(g, c, t)$ at every
362 extrapolation-grid cell g , category c , and time t .

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

$$365 \quad I(c, t, l) = \sum_{x=1}^{n_x} (a(g, l) \times d(g, c, t))$$

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

```

368 Options = c("SD_site_density"=0, "SD_site_logdensity"=0, "Calculate_Range"=0,
369 "Calculate_evenness"=0, "Calculate_effective_area"=0, "Calculate_Cov_SE"=0,
370 'Calculate_Synchrony'=0, 'Calculate_Coherence'=0)
371

```

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

$$374 \quad Z(c, t, m) = \sum_{x=1}^{n_x} \frac{(z(g, m) \times a(g, 1) \times d(g, c, t))}{I(c, t, 1)}$$

375 where $z(g, m)$ is a matrix representing location for each extrapolation-grid cell (by
376 default $z(g, m)$ is the location in Eastings and Northings of each knot), representing
377 movement North-South and East-West). This model-based approach to estimating
378 distribution shift can account for differences in the spatial distribution of sampling, unlike
379 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:

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

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 1).

List of features

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.

Basic features in a generalized linear model (GLM)

1. Specifying one of several possible distributions for data, including for:
 - a. Count data using a Poisson, negative-binomial, Conway-Maxwell-Poisson, or 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.

- 404 2. Specifying one of several possible link functions for predicting data given linear
405 predictors including:
- 406 a. A conventional delta-model;
 - 407 b. A Poisson-link delta model.
- 408 3. Including dynamic habitat covariates or not;
- 409 4. Including catchability covariates or not;
- 410 *Basic features in a spatio-temporal generalized linear mixed model (GLMM)*
- 411 5. Specify an “extrapolation grid” using input
412 `FishStatsUtils::make_extrapolation_info(..., Region)`, which is used to calculate the
413 area associated with each knot a_x . This can be a user-specified extrapolation grid if
414 `FishStatsUtils::make_extrapolation_info(..., Region="User", input_grid=Input)`,
415 where Input is a data frame supplied by the user.
- 416 6. Specifying a method for defining “knots”;
- 417 7. Specifying the number of “knots”;
- 418 8. Spatial variation being estimated (“turned on”) or ignored (“turned off”) for either linear
419 predictor #1 or #2;
- 420 9. Spatio-temporal variation being estimated (“turned on”) or ignored (“turned off”) for
421 either linear predictor #1 or #2;
- 422 10. Specifying that habitat covariates can affect linear predictors different ways including as:
- 423 a. a linear effect;
 - 424 b. a spatially-varying effect; or
 - 425 c. both linear and spatially-varying effects simultaneously.
- 426 *Multivariate analysis*
- 427 11. Including a “multivariate” structure with multiple responses that covary due to a specified
428 number of “factors” for spatial and spatio-temporal terms;

429 12. Rotate results prior to interpretation, using either:

430 a. principle components rotation; or

431 b. varimax rotation.

432 *Decisions regarding temporal structure*

433 13. Annual intercepts being structured over time, including:

434 a. estimated as fixed effects in every year;

435 b. fixed as fixed effect with the same value for all years;

436 c. estimated as a random effect with independent deviations in each year;

437 d. estimated as a random effect with first-order autoregressive structure; or

438 e. estimated as a random effect with a random-walk structure.

439 14. Spatio-temporal variation being structured over time, including:

440 a. estimated as independent deviations in each year;

441 b. estimated as following a first-order autoregressive structure over time;

442 c. estimated as following a random-walk structure over time; or

443 d. estimated as following a vector-autoregressive structure involving a matrix of 1st

444 order autoregressive interactions.

445 *Derived quantities*

446 15. Specifying spatial strata for use when calculating derived quantities;

447 16. Calculating one of many possible “univariate derived quantities”, including:

448 a. abundance indices;

449 b. range shift;

450 c. effective area occupied

451 d. covariance among categories within a multivariate model; or

452 e. synchrony among categories.

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.

Unusual circumstances and special cases

18. Specifying separate distributions for different data sets (e.g., when multiple surveys providing different data types are available);

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);

20. Specifying multiple “seasons” (e.g., when modelling data with both annual and monthly spatio-temporal variation).

Common problems

There are two basic problems that are often encountered during spatio-temporal delta-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 $\varepsilon_1(s, c, t) \rightarrow \infty$ for that year. If there is 0% encounter rate in year t , then $\beta_1(c, t) \rightarrow -\infty$ and/or $\varepsilon_1(s, c, t) \rightarrow -\infty$ and there is no information to estimate $\beta_2(c, t)$ or $\varepsilon_2(s, c, t)$ for that category c and year t ;
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 `ObsModel[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% or 0% encounter rate, add temporal structure to intercepts and spatio-temporal terms using `RhoConfig` options.
 - c. Four other options are listed on the [wiki](#).
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.

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 (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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623 Table 1 – 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 measuring distribution shifts	(Thorson et al. 2016b)
SD_observation_density	Calculate standard error for response variable measured in each sample	-
Calculate_effective_area	Calculate effective area occupied for use in measuring range expansion/contraction	(Thorson et al. 2016c)
Calculate_Cov_SE	Calculate standard error for correlation / covariance among categories	(Godefroid et al. In review)
Calculate_Synchrony	Calculate reduction in variance associated with asynchrony among species and/or locations	(Thorson et al. 2018)
Calculate_Coherence	Calculate the Gini coefficient for axes of covariation among categories	-
Calculate_proportion	Convert indices to a proportion in a multivariate model; breaks	(Thorson and Haltuch 2018)

	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 using a MICE-in-space model	(Thorson et al. In review)
Estimate_B0	Option to calculate unfished density using a MICE-in-space model	(Thorson et al. In 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 combinations of category and year that are never encountered and therefore should be treated as having zero abundance; Useful for compositional-expansion	(Thorson and Haltuch 2018)
simulate_random_effects	Option governing behaviour of bootstrap simulator; determines whether simulator re-simulates	(Thorson et al. In review)

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

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