

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:

$$\begin{aligned}
p_1(i) = & \underbrace{\sum_{f=1}^{n_{\beta_1}} L_{\beta_1}(c_i, f) \beta_1(t_i, f)}_{\text{Temporal variation}} + \underbrace{\sum_{f=1}^{n_{\omega_1}} L_{\omega_1}(c_i, f) \omega_1(s_i, f)}_{\text{Spatial variation}} + \underbrace{\sum_{f=1}^{n_{\varepsilon_1}} L_{\varepsilon_1}(c_i, f) \varepsilon_1(s_i, f, t_i)}_{\text{Spatio-temporal variation}} \\
& + \underbrace{\sum_{f=1}^{n_{\eta_1}} L_1(c_i, f) \eta_1(v_i, f)}_{\text{Vessel effects}} + \underbrace{\sum_{p=1}^{n_p} (\gamma_1(c_i, t_i, p) + \sigma_1(c, p) \xi_1(s, c, p)) X(x_i, t_i, p)}_{\text{Habitat covariates}} \\
& + \underbrace{\sum_{k=1}^{n_k} \lambda_1(k) Q(i, k)}_{\text{Catchability covariate}}
\end{aligned}$$

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), and $L_{\beta_1}(c_i, f)$ is the loadings matrix that generates temporal covariation among categories for this linear predictor. 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 ($n_{\beta_1} = 1$), then \mathbf{L}_{β_1} is a 1x1 matrix (i.e. a scalar) such

69 $\mathbf{L}_{\beta 1}^2$ is the variance and the absolute value, $abs(\mathbf{L}_{\beta 1})$ is the standard deviation for temporal
70 variation.

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

84 Finally, $X(x_i, t_i, p)$ is an array of n_p measured density covariates that explain
85 variation in density for time t and knot x . VAST can include a separate, spatially-varying
86 effect of each habitat covariate p for each category c . The spatially varying slope is
87 $\gamma_1(c_i, t_i, p) + \sigma(c, p)\xi_n(s, c, p)$, where $\gamma_1(c_i, t_i, p)$ is the average effect of density covariate
88 $X(x_i, t_i, p)$ for category c , $\xi_n(s, c, p)$ represents spatial variation in that effect (which has a
89 mean of zero and standard deviation of one), and $\sigma(c, p)$ represents the estimated standard
90 deviation of spatial variation of covariate p for category c . $Q(i, k)$ is a matrix of n_k
91 measured catchability covariates that explain variation in catchability, and $\lambda_1(k)$ is the
92 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:

$$\begin{aligned}
 p_2(i) = & \underbrace{\sum_{f=1}^{n_{\beta 2}} L_{\beta 2}(c_i, f) \beta_2(t_i, f)}_{\text{Temporal variation}} + \underbrace{\sum_{f=1}^{n_{\omega 2}} L_{\omega 2}(c_i, f) \omega_2(s_i, f)}_{\text{Spatial variation}} + \underbrace{\sum_{f=1}^{n_{\varepsilon 2}} L_{\varepsilon 2}(c_i, f) \varepsilon_2(s_i, f, t_i)}_{\text{Spatio-temporal variation}} \\
 & + \underbrace{\sum_{f=1}^{n_{\eta 2}} L_2(c_i, f) \eta_2(v_i, f)}_{\text{Vessel effects}} + \underbrace{\sum_{p=1}^{n_p} (\gamma_2(c_i, t_i, p) + \sigma_2(c, p) \xi_2(s, c, p)) X(x_i, t_i, p)}_{\text{Density covariates}} \\
 & + \underbrace{\sum_{k=1}^{n_k} \lambda_2(k) Q(i, k)}_{\text{Catchability covariates}}
 \end{aligned}$$

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.

Number of overdispersion factors

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

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

115

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

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

118 For example, if the user inputs:

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

120

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

122 for both the first and second linear predictors.

123

124 **Link functions and observation error distributions**

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

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

127 the two linear predictors.

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

129 link function respectively.

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

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

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

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

$$134 \quad r_1(i) = \text{logit}^{-1}(p_1(i))$$

135 where $r_1(i)$ is the predictor encounter probability in a delta-model, or zero-inflation in a

136 count-data model, and $\text{logit}^{-1}(p_1(i))$ is the inverse-logit (a.k.a. logistic) function of

137 $p_1(i)$, and:

$$138 \quad r_2(i) = a_i \times \log^{-1}(p_2(i))$$

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:

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

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

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:

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

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.

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, $b_i \in \{0, 1, 2, \dots\}$. VAST calculates the probability of these data as:

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

where `ObsModel[1]` controls the probability mass function $g\{B|r_2(i), \dots\}$ used (again, see `?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 approximates spatial and spatio-temporal variation as being piecewise-constant. 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). 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 each mesh vertex. 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:

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

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

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

```
217 # Turn of geometric anisotropy
218 Data = Data_Fn( ..., Aniso=FALSE )
219
```

220 VAST then specifies that the spatial and spatio-temporal Gaussian random fields each
 221 have a variance of 1.0. By default VAST specifies these as follows:

$$222 \quad \boldsymbol{\omega}_1(\cdot, f) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

$$223 \quad \boldsymbol{\omega}_2(\cdot, f) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

$$224 \quad \boldsymbol{\varepsilon}_1(\cdot, f, t) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

$$225 \quad \boldsymbol{\varepsilon}_2(\cdot, f, t) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

$$226 \quad \boldsymbol{\xi}_1(\cdot, c, p) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

$$227 \quad \boldsymbol{\xi}_2(\cdot, c, p) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

228 where $\boldsymbol{\omega}_1(\cdot, f)$ is the vector formed when subsetting $\omega_1(s, f)$ for a given f . Specifying a
 229 variance of 1.0 ensures that the covariance among categories is defined by the loadings
 230 matrix for that term.

231

232 **Structure on parameters among years:**

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

```
235 RhoConfig = c("Beta1"=0, "Beta2"=0, "Epsilon1"=0, "Epsilon2"=0)
236
```

237 *Temporal structure on intercepts*

238 By default (when $\text{RhoConfig}[1]=0$ and $\text{RhoConfig}[2]=0$) the model specifies that each
 239 intercept $\beta_1(t)$ and $\beta_2(t)$ is a fixed effect. However, other settings specify the following
 240 structure:

$$\beta_1(t+1) \sim \text{Normal}(\rho_{\beta_1}\beta_1(t), \sigma_{\beta_1}^2)$$

$$\beta_2(t+1) \sim \text{Normal}(\rho_{\beta_2}\beta_2(t), \sigma_{\beta_2}^2)$$

where RhoConfig[1] controls the specification of ρ_{β_1} :

1. *Independent among years* – RhoConfig[1]=1 specifies $\rho_{\beta_1} = 0$
 2. *Random walk* – RhoConfig[1]=2 specifies $\rho_{\beta_1} = 1$
 3. *Constant intercept* – 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* – RhoConfig[1]=4 estimates ρ_{β_1} as a fixed effect
- and settings are defined identically for RhoConfig[2] specifying ρ_{β_2} .

250

251 *Temporal structure on spatio-temporal variation*

252 By default (when RhoConfig[3]=0 and RhoConfig[4]=0), the model specifies that each spatio-
 253 temporal random effect $\varepsilon_1(s, f, t)$ and $\varepsilon_2(s, f, t)$ is independent among years. However,
 254 other settings specify the following structure

$$\varepsilon_1(s, f, t+1) \sim \text{MVN}(\rho_{\varepsilon_1}\varepsilon_1(s, f, t), \mathbf{R}_1)$$

$$\varepsilon_2(s, f, t+1) \sim \text{MVN}(\rho_{\varepsilon_2}\varepsilon_2(s, f, t), \mathbf{R}_2)$$

257 where RhoConfig[3] controls the specification of ρ_{ε_1} :

- 258 1. *Random walk* – RhoConfig[3]=2 specifies $\rho_{\varepsilon_1} = 1$
 - 259 2. *Autoregressive* – RhoConfig[3]=4 estimates ρ_{ε_1} as a fixed effect
- 260 and settings are defined identically for RhoConfig[4] specifying ρ_{ε_2} .

261

262 **Parameter estimation**

263 Parameters are estimated using maximum likelihood, where the maximum likelihood of fixed
 264 effects is obtained by integrating a joint likelihood function with respect to random effects

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

Combining multiple data types

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

Settings regarding 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. Estimated values of fixed and random effects are then used to predict density $d(x, c, t)$ as follows:

$$d(x, c, t) = r_1^*(x, c, t) \times r_2^*(x, c, t)$$

where $r_1^*(x, c, t)$ and $r_2^*(x, c, t)$ are identical to the values specified previously, except that catchability variables are excluded from their computation (i.e., $\eta_1(v, f) = 0$ and $\lambda_1(k) = 0$, etc.)

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

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

where $a(x, l)$ is the area associated with extrapolation-cell x for index l ; and n_x is the number of extrapolation-cells (Shelton et al. 2014; Thorson et al. 2015b). The user can also specify additional post-hoc calculations via the Options vector:

```
Options = c("SD_site_density"=0, "SD_site_logdensity"=0, "Calculate_Range"=0,
"Calculate_evenness"=0, "Calculate_effective_area"=0, "Calculate_Cov_SE"=0,
'Calculate_Synchrony'=0, 'Calculate_Coherence'=0)
```

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

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

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

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

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

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).

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.
2. Specifying one of several possible link functions for predicting data given linear predictors including:
 - a. A conventional delta-model;
 - b. A Poisson-link delta model.
3. Including dynamic habitat covariates or not;
4. Including catchability covariates or not;

364 *Basic features in a spatio-temporal generalized linear mixed model (GLMM)*

365 5. Specify an “extrapolation grid” using input

366 `SpatialDeltaGLMM::Prepare_Extrapolation_Data_Fn(..., Region)`, which is used to
367 calculate the area associated with each knot a_x . This can be a user-specified
368 extrapolation grid if `SpatialDeltaGLMM::Prepare_Extrapolation_Data_Fn(...,`
369 `Region="User", input_grid=Input)`, where `Input` is a data frame supplied by the user.

370 6. Specifying a method for defining “knots”;

371 7. Specifying the number of “knots”;

372 8. Spatial variation being estimated (“turned on”) or ignored (“turned off”) for either linear
373 predictor #1 or #2;

374 9. Spatio-temporal variation being estimated (“turned on”) or ignored (“turned off”) for
375 either linear predictor #1 or #2;

376 10. Specifying that habitat covariates can affect linear predictors different ways including as:

377 a. a linear effect;

378 b. a spatially-varying effect; or

379 c. both linear and spatially-varying effects simultaneously.

380 *Multivariate analysis*

381 11. Including a “multivariate” structure with multiple responses that covary due to a specified
382 number of “factors” for spatial and spatio-temporal terms;

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

384 a. principle components rotation; or

385 b. varimax rotation.

386 *Decisions regarding temporal structure*

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

388 a. estimated as fixed effects in every year;

- 389 b. fixed as fixed effect with the same value for all years;
- 390 c. estimated as a random effect with independent deviations in each year;
- 391 d. estimated as a random effect with first-order autoregressive structure; or
- 392 e. estimated as a random effect with a random-walk structure.
- 393 14. Spatio-temporal variation being structured over time, including:
- 394 a. estimated as independent deviations in each year;
- 395 b. estimated as following a first-order autoregressive structure over time;
- 396 c. estimated as following a random-walk structure over time; or
- 397 d. estimated as following a vector-autoregressive structure involving a matrix of 1st
- 398 order autoregressive interactions.

399 *Derived quantities*

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

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

- 402 a. abundance indices;
- 403 b. range shift;
- 404 c. effective area occupied
- 405 d. covariance among categories within a multivariate model; or
- 406 e. synchrony among categories.

407 17. Calculating “multivariate derived quantities” that are derived from estimates for multiple

408 categories in a multivariate model, e.g., where one category represents a standardized diet

409 sample (e.g., prey biomass per predator biomass in a stomach-content sample) and

410 another category represents a biomass-density sample (e.g., predator biomass in a bottom-

411 trawl sample) such that their product represents predator-expanded consumption.

412 *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 $\beta_p(c, t) \rightarrow \infty$ and/or $\varepsilon_p(s, c, t) \rightarrow \infty$ for that year. If there is 0% encounter rate in year t , then $\beta_p(c, t) \rightarrow -\infty$ and/or $\varepsilon_p(s, c, t) \rightarrow -\infty$ and there is no information to estimate $\beta_r(c, t)$ or $\varepsilon_r(s, c, t)$ 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%

436 encounter rates and fix corresponding intercepts for encounter probability to an
437 extremely high value.

438 b. If there is a small number of years with either 100% of 0% encounter rate, add
439 temporal structure to intercepts and spatio-temporal terms using RhoConfig
440 options.

441 c. Four other options are listed on the [wiki](#).

442 2. *Bounds*: Please try running the model without estimating standard errors or a final
443 newton step:

```
444 # Specify derived quantities to calculate  
445 TMBhelper::Optimize( ..., getsd=FALSE, newtonsteps=0 )  
446 Then check what parameters are being estimated near an upper or lower boundary.
```

447

448 **How to implement basic model changes**

449 There are a few basic model types that users often want to fit using VAST. I briefly describe
450 how these can be done here.

451 1. *Fitting encounter/non-encounter data*: If the user wishes to use only the first component
452 of a delta-model, i.e., to fit a binomial model to simply predict encounter probabilities,
453 then, the ObsModel vector should be set to c("PosDist"=[Make Choice], "Link"=0),
454 where [Make Choice] can be any option for continuous data (i.e., 0, 1, or 2). The user
455 should then turn off the last two elements of the FieldConfig vector (i.e.,
456 FieldConfig[3]=0 and FieldConfig[4]=0) such that there is no spatial or spatio-temporal
457 variability in positive catch rates, and also turn off annual variation in the intercept for
458 positive catch rates (i.e., RhoConfig[2]=3). Finally, the user should “jitter” their presence
459 observations by a very small amount (i.e., add a random normal deviation with a very
460 small standard deviation, rnorm(n=1, mean=0, sd=0.001), to each observation for which
461 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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