

VAST model structure and user interface

James Thorson

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:

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

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

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

Similarly, $\omega_1^*(s_i, f)$ 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 $L_{\omega 1}(c_i, f)$ is the loadings matrix that generates spatial covariation among categories for this linear predictor. Similarly, $\varepsilon_1^*(s_i, f, t_i)$ represents predicted spatio-temporal variation in the first linear predictor for each factor f (of $n_{\varepsilon 1}$ factors representing spatio-temporal variation), and $L_{\varepsilon 1}(c_i, f)$ is the loadings matrix that generates spatio-temporal covariation for this predictor. $\eta_1(v_i, f)$ represents random variation in catchability among a grouping variable (tows or vessels) for each factor f (of $n_{\eta 1}$ factors representing overdispersion), and $L_1(c_i, f)$ is a loadings matrix that generates covariation in catchability among categories for this predictor. All loadings matrices are specified similarly to $\mathbf{L}_{\beta 1}$, 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).

Finally, $X(i, t_i, p)$ is an three-dimensional array of n_p measured density covariates that explain variation in density for time t and the location s_i where sampling occurred for sample i . VAST can include a separate, spatially-varying effect of each habitat covariate p for each category c . The spatially varying slope is $\gamma_1(c_i, t_i, p) + \sigma(c, p)\xi_n(s, c, p)$, 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 $\sigma(c, p)$ represents the estimated standard deviation of spatial variation of covariate p for category c . $Q(i, k)$ is a matrix of n_k measured catchability covariates that explain variation in catchability, and $\lambda_1(k)$ is the estimated impact of catchability covariates for this

linear predictor. By default, VAST specifies that $\gamma_1(c, t_1, p) = \gamma_1(c, t_2, p)$ for all years t_1 and t_2 , although users can relax this 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:

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

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

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

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

where `OverdispersionConfig[1]` controls n_{δ_1} , and `OverdispersionConfig[2]` controls n_{δ_2} , and a value of zero again “turns off” that component of random covariation in catchability.

For example, if the user inputs:

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

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

Link functions and observation error distributions

There are user-controlled options that control the observation error distribution and the link-functions used to calculate expected encounter probabilities and positive catch rates based on the two linear predictors.

The `ObsModel` vector has two components, controlling the observation error distribution and link function respectively.

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

There are currently four options for the link function. For the latest set of options see the R help documentation by typing into the R terminal `?VAST::Data_Fn`.

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

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

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:

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)
```

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
 186 generally can have one or more parameter governing dispersion, and the precise number and
 187 interpretation varies among observation models (i.e., the value of `ObsModel[1]`). For these
 188 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 spatial variable at all n_s vertices. Specifically, the correlation $\mathbf{R}_1(s, s + h)$ between location s and location $s + h$ for spatial and spatio-temporal terms included in the first linear predictor is approximated as following a Matern function:

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

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

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

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

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

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

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

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

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

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

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

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

Interpolating spatial variation from knots to the location of samples

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

$$\omega_1^*(f) = \mathbf{A}_i \omega_1(f)$$

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

1. *Piecewise constant*: Following the conventional for releases of VAST prior to 3.0.0, users can specify `fine_scale=FALSE`. Given this specification, spatial variables at location s are fixed equal to their value at the nearest “knot.” This involves specifying matrix \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 2013), users can specify `fine_scale=TRUE`. Given this specification, spatial variables at location s are interpolated using the triangulated mesh that is also used to approximate spatial variation. Specifically, matrix \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 spatio-temporal variation across time, using input:

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

Temporal structure on intercepts

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

275

276 *Temporal structure on spatio-temporal variation*

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

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

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

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

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

286

287 **Parameter estimation**

288 Parameters are estimated using maximum likelihood, where the maximum likelihood of fixed
 289 effects is obtained by integrating a joint likelihood function with respect to random effects
 290 (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.
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.:

$$p_1(g, c, t) = \underbrace{\sum_{f=1}^{n_{\beta 1}} L_{\beta 1}(c, f) \beta_1(t, f)}_{\text{Temporal variation}} + \underbrace{\sum_{f=1}^{n_{\omega 1}} L_{\omega 1}(x, f) \omega_1^*(s_g, f)}_{\text{Spatial variation}} + \underbrace{\sum_{f=1}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c, f) \varepsilon_1^*(s_g, f, t)}_{\text{Spatio-temporal variation}} \\ + \underbrace{\sum_{p=1}^{n_p} (\gamma_1(c, t, p) + \sigma_1(c, p) \xi_1^*(s, c, p)) X(g, t, p)}_{\text{Habitat covariates}}$$

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

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

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

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

```

363 Options = c("SD_site_density"=0, "SD_site_logdensity"=0, "Calculate_Range"=0,
364 "Calculate_evenness"=0, "Calculate_effective_area"=0, "Calculate_Cov_SE"=0,
365 'Calculate_Synchrony'=0, 'Calculate_Coherence'=0)
366

```

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

$$369 \quad Z(c, t, m) = \sum_{x=1}^{n_x} \frac{(z(g, m) \times a(g, 1) \times d(g, c, t))}{I(c, t, 1)}$$

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

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

$$377 \quad D(c, t, l) = \sum_{x=1}^{n_x} \frac{a(x, l) \times d(x, c, t)}{I(c, t, l)} d(x, c, t)$$

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

$$380 \quad A(c, t, l) = \frac{I(c, t, l)}{D(c, t, l)}$$

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

383

384 **List of features**

385 I next provide a list of “features” organized as decisions that can be made by the analyst.

386 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;

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

5. Specify an “extrapolation grid” using input `SpatialDeltaGLMM::Prepare_Extrapolation_Data_Fn(..., Region)`, which is used to calculate the area associated with each knot a_x . This can be a user-specified extrapolation grid if `SpatialDeltaGLMM::Prepare_Extrapolation_Data_Fn(..., Region="User", input_grid=Input)`, where `Input` is a data frame supplied by the user.
6. Specifying a method for defining “knots”;
7. Specifying the number of “knots”;

- 411 8. Spatial variation being estimated (“turned on”) or ignored (“turned off”) for either linear
412 predictor #1 or #2;
- 413 9. Spatio-temporal variation being estimated (“turned on”) or ignored (“turned off”) for
414 either linear predictor #1 or #2;
- 415 10. Specifying that habitat covariates can affect linear predictors different ways including as:
- 416 a. a linear effect;
- 417 b. a spatially-varying effect; or
- 418 c. both linear and spatially-varying effects simultaneously.

419 *Multivariate analysis*

- 420 11. Including a “multivariate” structure with multiple responses that covary due to a specified
421 number of “factors” for spatial and spatio-temporal terms;
- 422 12. Rotate results prior to interpretation, using either:
- 423 a. principle components rotation; or
- 424 b. varimax rotation.

425 *Decisions regarding temporal structure*

- 426 13. Annual intercepts being structured over time, including:
- 427 a. estimated as fixed effects in every year;
- 428 b. fixed as fixed effect with the same value for all years;
- 429 c. estimated as a random effect with independent deviations in each year;
- 430 d. estimated as a random effect with first-order autoregressive structure; or
- 431 e. estimated as a random effect with a random-walk structure.
- 432 14. Spatio-temporal variation being structured over time, including:
- 433 a. estimated as independent deviations in each year;
- 434 b. estimated as following a first-order autoregressive structure over time;
- 435 c. estimated as following a random-walk structure over time; or

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

Derived quantities

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

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

- a. abundance indices;
- b. range shift;
- c. effective area occupied
- d. covariance among categories within a multivariate model; or
- 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 $\beta_p(c, t) \rightarrow \infty$ 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% 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::Optimize( ..., 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).

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

511 many volunteers and NOAA scientists who have served on sampling vessels that provided
512 data to test these methods. Finally, I think A. Grüss and S. Hoyle for providing edits to this
513 document.

514

515

516 Works cited

- 517 Edwards, A.M., and Auger-Méthé, M. 2019. Some guidance on using mathematical notation
518 in ecology. *Methods Ecol. Evol.* **10**(1): 92–99. doi:10.1111/2041-210X.13105.
- 519 Gelman, A., and Hill, J. 2007. Data analysis using regression and multilevel/hierarchical
520 models. Cambridge University Press, Cambridge, UK.
- 521 Grüss, A., and Thorson, J. In press. Developing spatio-temporal models using multiple data
522 types for evaluating population trends and habitat usage. *ICES J. Mar. Sci.*
- 523 Grüss, A., Thorson, J.T., Babcock, E.A., and Tarnecki, J.H. 2018. Producing distribution
524 maps for informing ecosystem-based fisheries management using a comprehensive
525 survey database and spatio-temporal models. *ICES J. Mar. Sci.* **75**(1): 158–177.
526 doi:10.1093/icesjms/fsx120.
- 527 Grüss, A., Thorson, J.T., Sagarese, S.R., Babcock, E.A., Karnauskas, M., Walter, J.F., and
528 Drexler, M. 2017. Ontogenetic spatial distributions of red grouper (*Epinephelus*
529 *morio*) and gag grouper (*Mycteroperca microlepis*) in the U.S. Gulf of Mexico. *Fish.*
530 *Res.* **193**(Supplement C): 129–142. doi:10.1016/j.fishres.2017.04.006.
- 531 Kass, R.E., and Steffey, D. 1989. Approximate bayesian inference in conditionally
532 independent hierarchical models (parametric empirical bayes models). *J. Am. Stat.*
533 *Assoc.* **84**(407): 717–726. doi:10.2307/2289653.
- 534 Kristensen, K., Nielsen, A., Berg, C.W., Skaug, H., and Bell, B.M. 2016. TMB: Automatic
535 Differentiation and Laplace Approximation. *J. Stat. Softw.* **70**(5): 1–21.
536 doi:10.18637/jss.v070.i05.
- 537 Lindgren, F. 2012. Continuous domain spatial models in R-INLA. *ISBA Bull.* **19**(4): 14–20.
- 538 Lindgren, F., and Rue, H. 2013. Bayesian spatial and spatiotemporal modelling with r-inla. *J.*
539 *Stat. Softw.* Available from [http://inla.googlecode.com/hg-](http://inla.googlecode.com/hg-history/fd1c0951196f7e7b6d57e2ea84c541981fcb3bf4/r-inla.org/papers/jss/lindgren.pdf)
540 [history/fd1c0951196f7e7b6d57e2ea84c541981fcb3bf4/r-](http://inla.googlecode.com/hg-history/fd1c0951196f7e7b6d57e2ea84c541981fcb3bf4/r-inla.org/papers/jss/lindgren.pdf)
541 inla.org/papers/jss/lindgren.pdf [accessed 23 February 2014].
- 542 Lindgren, F., Rue, H., and Lindström, J. 2011. An explicit link between Gaussian fields and
543 Gaussian Markov random fields: the stochastic partial differential equation approach.
544 *J. R. Stat. Soc. Ser. B Stat. Methodol.* **73**(4): 423–498. doi:10.1111/j.1467-
545 9868.2011.00777.x.
- 546 Martin, T.G., Wintle, B.A., Rhodes, J.R., Kuhnert, P.M., Field, S.A., Low-Choy, S.J., Tyre,
547 A.J., and Possingham, H.P. 2005. Zero tolerance ecology: improving ecological
548 inference by modelling the source of zero observations. *Ecol. Lett.* **8**(11): 1235–1246.
- 549 R Core Team. 2017. R: A Language and Environment for Statistical Computing. R
550 Foundation for Statistical Computing, Vienna, Austria. Available from
551 <https://www.R-project.org/>.
- 552 Searle, S.R., Casella, G., and McCulloch, C.E. 1992. Variance components. John Wiley &
553 Sons, Hoboken, New Jersey.
- 554 Shelton, A.O., Thorson, J.T., Ward, E.J., and Feist, B.E. 2014. Spatial semiparametric models
555 improve estimates of species abundance and distribution. *Can. J. Fish. Aquat. Sci.*
556 **71**(11): 1655–1666. doi:10.1139/cjfas-2013-0508.
- 557 Skaug, H., and Fournier, D. 2006. Automatic approximation of the marginal likelihood in
558 non-Gaussian hierarchical models. *Comput. Stat. Data Anal.* **51**(2): 699–709.
- 559 Thorson, J.T. 2018. Three problems with the conventional delta-model for biomass sampling
560 data, and a computationally efficient alternative. *Can. J. Fish. Aquat. Sci.* **75**(9):
561 1369–1382. doi:10.1139/cjfas-2017-0266.
- 562 Thorson, J.T. 2019. Guidance for decisions using the Vector Autoregressive Spatio-Temporal
563 (VAST) package in stock, ecosystem, habitat and climate assessments. *Fish. Res.* **210**:
564 143–161. doi:10.1016/j.fishres.2018.10.013.

- Thorson, J.T., and Barnett, L.A.K. 2017. Comparing estimates of abundance trends and distribution shifts using single- and multispecies models of fishes and biogenic habitat. *ICES J. Mar. Sci.* **74**(5): 1311–1321. doi:10.1093/icesjms/fsw193.
- Thorson, J.T., Ianelli, J.N., Larsen, E.A., Ries, L., Scheuerell, M.D., Szuwalski, C., and Zipkin, E.F. 2016a. Joint dynamic species distribution models: a tool for community ordination and spatio-temporal monitoring. *Glob. Ecol. Biogeogr.* **25**(9): 1144–1158. doi:10.1111/geb.12464.
- Thorson, J.T., and Kristensen, K. 2016. Implementing a generic method for bias correction in statistical models using random effects, with spatial and population dynamics examples. *Fish. Res.* **175**: 66–74. doi:10.1016/j.fishres.2015.11.016.
- Thorson, J.T., and Minto, C. 2015. Mixed effects: a unifying framework for statistical modelling in fisheries biology. *ICES J. Mar. Sci. J. Cons.* **72**(5): 1245–1256. doi:10.1093/icesjms/fsu213.
- Thorson, J.T., Pinsky, M.L., and Ward, E.J. 2016b. Model-based inference for estimating shifts in species distribution, area occupied and centre of gravity. *Methods Ecol. Evol.* **7**(8): 990–1002. doi:10.1111/2041-210X.12567.
- Thorson, J.T., Rindorf, A., Gao, J., Hanselman, D.H., and Winker, H. 2016c. Density-dependent changes in effective area occupied for sea-bottom-associated marine fishes. *Proc R Soc B* **283**(1840): 20161853. doi:10.1098/rspb.2016.1853.
- Thorson, J.T., Scheuerell, M.D., Shelton, A.O., See, K.E., Skaug, H.J., and Kristensen, K. 2015a. Spatial factor analysis: a new tool for estimating joint species distributions and correlations in species range. *Methods Ecol. Evol.* **6**(6): 627–637. doi:10.1111/2041-210X.12359.
- Thorson, J.T., Shelton, A.O., Ward, E.J., and Skaug, H.J. 2015b. Geostatistical delta-generalized linear mixed models improve precision for estimated abundance indices for West Coast groundfishes. *ICES J. Mar. Sci. J. Cons.* **72**(5): 1297–1310. doi:10.1093/icesjms/fsu243.
- Thorson, J.T., Skaug, H.J., Kristensen, K., Shelton, A.O., Ward, E.J., Harms, J.H., and Benante, J.A. 2014. The importance of spatial models for estimating the strength of density dependence. *Ecology* **96**(5): 1202–1212. doi:10.1890/14-0739.1.
- Tierney, L., Kass, R.E., and Kadane, J.B. 1989. Fully exponential Laplace approximations to expectations and variances of nonpositive functions. *J. Am. Stat. Assoc.* **84**(407): 710–716.