VAST model structure and user interface

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Purpose of document:

R package VAST includes many different forms of documentation, which are documented on the package GitHub page. 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.

Package architecture:

VAST is developed as an R package available on GitHub. It depends upon helper functions that are bundled in package FishStatsUtils, and these helper functions are installed separately because they are also used by other spatio-temporal packages (e.g., EOFR). VAST and FishStatsUtils use S3 objects to ease interpretation of objects that are commonly saved to terminal (see Table 1 for list). VAST can be run using two primary levels of abstraction:

1. *High-level wrapper functions*: New users are recommended to explore using \`FishStatsUtils::make_settings\` and \`FishStatsUtils::fit_model\` to run VAST, and to explore results using \`plot\` and \`summary\`.
2. *Mid-level utilities*: Experienced users often run lower-level functions to accomplish basic tasks in spatial analysis, using \`FishStatsUtils::make_extrapolation_info\`, \`FishStatsUtils::make_spatial_info\`, \`VAST::make_data\`, and \`VAST::make_model\` individually.

Updates to VAST are released using semantic-version numbering (e.g., version 3.2.0) and a battery of integrated tests (comparing results using updated code to saved results from earlier versions) are run prior to numbered releases to ensure that results are backwards compatible.

Model description:

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

Model Overview

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

After estimating variation in density across space, time, and among categories, VAST then predicts variables at extrapolation-grid cells distributed within across a user-specified spatial domain. This allows derived quantities to be calculated by summing across this spatial domain; this is analogous to an "area-weighting" approach to index standardization, and the resulting prediction of total abundance can be used an index of abundance.

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

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

Linear predictors

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

$$p_1(i) = \underbrace{\mu_{\beta 1}(c_i) + \beta_1(c_i, t_i)}_{\mathit{Temporal\ variation}} + \underbrace{\omega_1^*(s_i, c_i)}_{\mathit{Spatial\ variation}} + \underbrace{\varepsilon_1^*(s_i, c_i, t_i)}_{\mathit{Spatio-temporal\ variation}} + \underbrace{\eta_1(v_i, c_i)}_{\mathit{Vessel\ effects}}$$

$$+ \underbrace{\nu_1(c_i, t_i)}_{\mathit{Habitat\ covariates}} + \underbrace{\zeta_1(i)}_{\mathit{Catchability\ covariate}}$$

where $p_1(i)$ is the predictor for observation i, arising for category c_i at location s_i and time t_i. Similarly, the second linear predictor $p_2(i)$ represents positive catch rates in a delta-model, or the count-data intensity function in a count-data model, where all variables and parameters are defined similarly except using different subscripts (Thorson and Barnett 2017; Thorson 2019). Model components are specified hierarchically to generate a correlation among categories and years as explained next.

Temporal variation

Regarding intercepts representing temporal variation:

$$\beta_1(c,t) = \sum_{f=1}^{n_{\beta 1}} L_{\beta 1}(c_i, f)\beta_1(t_i, f)$$

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

By default the model specifies that each intercept $\beta_1(c,t)$ and $\beta_2(c,t)$ is a fixed effect. However, other settings specify the following autocorrelation structure:

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

$$\beta_2(t,f) \sim \begin{cases} Normal(0,1) & \text{if } t = t_{min} \\ Normal\big(\rho_{\beta 2}\beta_2(t-1,f),1\big) & \text{if } t > t_{min} \end{cases}$$

Where t_{min} is the index for the first modelled year and $\rho_{\beta 1}$ and $\rho_{\beta 2}$ are the estimated degree of first-order autocorrelation in temporal variation (note that random effects have a variance of one given that they are subsequently multiplied by loadings matrices that represent the temporal covariance among factors). Options include:

1. *Independent among years* –specifies $\rho_{\beta 1} = 0$
2. *Random walk* –specifies $\rho_{\beta 1} = 1$
3. *Constant intercept* –specifies $\rho_{\beta 1} = 0$ and $\sigma_{\beta 1}^2 = 0$ (i.e., $\beta_1(t)$ is constant for all t)
4. *Autoregressive* –estimates $\rho_{\beta 1}$ as a fixed effect

and settings are defined identically for specifying $\rho_{\beta 2}$.

Spatial variation

Regarding spatial variation:

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

where $\omega_1^*(s_i,f)$ represents predicted spatial variation in the first linear predictor occurring at the location s_i of sample i for factor f (of $n_{\omega 1}$ factors representing spatial variation), and $L_{\omega 1}(c_i,\ f)$ is the loadings matrix that generates spatial covariation among categories for this linear predictor.

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

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

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

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. These GMRFs are then projected to calculate their value at every location s_i using matrix **A** with n_i rows and n_s columns. Values are then predicted as e.g.:

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

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

Spatio-temporal variation

Regarding spatio-temporal variation:

$$\varepsilon_1^*(s,c,t) = \sum_{f=1}^{n_{\varepsilon_c 1}} L_{\varepsilon_c 1}(c_i,f)\varepsilon_1^*(s_i,f,t_i)$$

where $\varepsilon_1^*(s_i,f,t_i)$ represents predicted spatio-temporal variation in the first linear predictor for each factor f_1 representing covariance among species (of $n_{\varepsilon_c 1}$ factors) and each factor f_2 representing covariance among years (of $n_{\varepsilon_t 1}$ such factors). Meanwhile and $L_{\varepsilon_c 1}(c_i,f_1)$ is the loadings matrix that generates spatio-temporal covariation among species, and $L_{\varepsilon_t 1}(t_i,f_2)$ is the loadings matrix that generates spatio-temporal covariation among years.

By default, the model specifies that each vector of spatio-temporal random effects, $\boldsymbol{\varepsilon}_1(f_1, f_2)$ and $\boldsymbol{\varepsilon}_2(f_1, f_2)$ composed of $\varepsilon_1(s, f_1, f_2)$ and $\varepsilon_2(s, f_1, f_2)$ across locations s, is independent for each factor representing covariation among categories (f_1) and among years (f_2). We describe the process for the 1st linear predictor, and an identical process is used for the 2nd linear predictor (using different subscripts):

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

Values are then predicted as e.g.:

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

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

$$\varepsilon_1'(s, c, t) = \sum_{f_1=1}^{n_{\varepsilon_c 1}} \sum_{f_2=1}^{n_{\varepsilon_t 1}} L_{\varepsilon_c 1}(c, f_1) L_{\varepsilon_t 1}(f_2, t) \varepsilon_1(s, f_1, f_2)$$

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

$$\varepsilon_1(s, c_1, t) = \begin{cases} \varepsilon_1'(s, c_1, t) & \text{if } t = t_{min} \\ \sum_{c_2=1}^{n_c} b(c_1, c_2) \varepsilon_1'(s, c_2, t-1) & \text{if } t > t_{min} \end{cases}$$

Where $b(c_1, c_2)$ is the estimated impact of spatio-temporal variation in category c_2 on spatio-temporal changes in category c_1:

$$b(c_1, c_2) = \begin{cases} \sum_{f=1}^{n_b} \chi(c_1, f) \psi(f, c_2) + \rho_{\varepsilon 1}(c_1) & \text{if } c_1 = c_2 \\ \sum_{f=1}^{n_b} \chi(c_1, f) \psi(f, c_2) & \text{if } c_1 \neq c_2 \end{cases}$$

Where $\chi(c_1, f)$ and $\psi(f, c_2)$ represent elements of matrices $\mathbf{X}$ and $\mathbf{\Psi}$, where the product $\mathbf{X\Psi}$ is the typical interaction matrix in a cointegration model (Engle and Granger 1987), where $\mathbf{\Psi}$ projects dynamics to a low-dimensional subspace and $\mathbf{X}$ represents responses within that subspace. By default $n_b = 0$ corresponding to $\mathbf{X\Psi} = \mathbf{0}$, and these terms drop out of the model; however, they allow a parsimonious representation of species interactions (Thorson et al. 2017, 2019). Meanwhile $\rho_{\varepsilon 1}(c)$ is the estimated degree of first-order autocorrelation in temporal variation:

1. *Random walk* – specifies $\rho_{\varepsilon 1}(c) = 1$
2. *Autoregressive* – estimates $\rho_{\varepsilon 1}$ as a single fixed effect with the same value for all categories
3. *Individual autoregressive* -- estimates a separate value of $\rho_{\varepsilon 1}(c)$ as a single fixed effect for each category

and settings are defined identically for specifying $\rho_{\varepsilon 2}$.

Overdisperison

Regarding overdispersion:

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

where $\eta_1(v_i, f)$ represents random variation in catchability among a grouping variable (tows or vessels) for each factor f (of $n_{\eta 1}$ factors representing overdispersion), and $L_1(c_i, f)$ is a loadings matrix that generates covariation in catchability among categories for this predictor. All loadings matrices are specified similarly to $\mathbf{L}_{\beta 1}$, i.e., where factors have a variance of one such that $\mathbf{L}^T\mathbf{L}$ represents the covariance among categories. The main difference is that spatial, spatio-temporal, and overdispersion factors can only be specified as random effects, while the intercepts can be specified as either random or fixed (where specifying as fixed "turns off" all factor-modelling for that intercept).

Density covariates

Regarding covariates affecting densities (“density” or “habitat” covariates):

$$\nu_1(c_i,t_i) = \sum_{p=1}^{n_p} \left(\gamma_1(c_i,p) + \sigma_{\xi 1}(c_i,p)\xi_1^*(s_i,c_i,p)\right) X(i,t_i,p)$$

where $X(i,t_i,p)$ is an three-dimensional array of n_p measured density covariates that explain variation in density for time *t* and the location s_i where sampling occurred for sample i. VAST can include a separate, spatially-varying effect of each habitat covariate p for each category c. The spatially varying slope is $\gamma_1(c_i,t_i,p) + \sigma_{\xi 1}(c,p)\xi_n(s,c,p)$, where $\gamma_1(c_i,\ t_i,p)$ is the average effect of density covariate $X(i,t_i,p)$ for category c, $\xi_n(s_i,c_i,p)$ represents spatial variation in that effect (which has a mean of zero and standard deviation of one), and $\sigma_{\xi 1}(c,p)$ represents the estimated standard deviation of spatial variation of covariate p for category c. By default VAST estimates spatially-varying slope terms values at each vertex as follows:

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

Values are then predicted as e.g.:

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

Catchability covariates

Finally, regarding covariates affecting the process of obtaining measurements (“catchability” or “detectability” covariates):

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

Where $q_1(i,k)$ is an element of matrix $\mathbf{Q}_1$ composed of n_k measured catchability covariates that explain variation in catchability, $\lambda_1(k)$ is the estimated impact of catchability covariates for this linear predictor, $\varphi_1^*(s_i,k)$ is unit-variance spatial variation in that slope term such that

$\sigma_{\varphi 1}(k)\varphi_1^*(s_i,k)$ has standard deviation $\sigma_{\varphi 1}(k)$, where spatial variation in detectability is specified as follows:

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

Values are then predicted as e.g.:

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

Link functions and observation error distributions

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:

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

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

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

   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:

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

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

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

where $r_2(i)$ is the predicted biomass given that the species is encountered. In this "Poisson-process" link function, $\exp\big(p_1(i)\big)$ is interpreted as the density in number of individuals per area such that $a_i \times \exp\big(p_1(i)\big)$ is the predicted number of individuals encountered, and $\exp\big(p_2(i)\big)$ 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. 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, $b_i \in \{0,1,2,\ldots\}$. VAST calculates the probability of these data as:

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

where `ObsModel[1]` controls the probability mass function $g\{B | r_2(i), \ldots\}$ used (again, see `?Data_Fn` for a list of options), where I use … to signify that these probability mass functions generally can have one or more parameter governing dispersion, and the precise number and interpretation varies among observation models (i.e., the value of `ObsModel[1]`). For these count-data models, $\big(1 - r_1(i)\big)$ 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 $g\{B = b_i | r_2(i), \ldots\}$ (i.e., the number of individuals that are in the vicinity of sampling in habitat that is occupied), and $g\{B = 0 | r_2(i), \ldots\}$ is the probability of not encountering category *c* given that sampling occurs in occupied habitat (Martin et al. 2005).

Settings regarding spatial smoothers

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

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

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

There are also other options:

1. *barrier effects*: avoiding correlations traveling across land;
2. *spherical projections*: calculating distance based on spherical coordinates, to avoid sensitivity to chosen projection;
3. *stream-network distance*: calculating distance based on river distances in a stream network or other graphical spatial dependency (Hocking et al. 2018).

Interpolating spatial variation from knots to the location of samples

Starting with VAST release 3.0.0, users can choose between two options for smoothing spatial variation.

1. *Piecewise constant*: Following the conventional for releases of VAST prior to 3.0.0, users can specify `fine_scale=FALSE`. Given this specification, spatial variables at location s are fixed equal to their value at the nearest “knot.” This involves

specifying matrix $\mathbf{A}_i$ such that row i has value zero except for one cell containing a value of one for the knot closest to sample i.

2. *Bilinear interpolation*: Following standard practices using the software R-INLA (Lindgren 2012; Lindgren and Rue 2015), users can specify `fine_scale=TRUE`. Given this specification, spatial variables at location s are interpolated using the triangulated mesh that is also used to approximate spatial variation. Specifically, matrix $\mathbf{A}_i$ has row i with value zero except for three cells, representing the vertices of the triangle containing location s_i.

Structure on parameters among years:

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

Parameter estimation

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

`ThorsonUtilities::list_parameters( Obj )` to see a list of estimated parameters (where `Obj` is the compiled VAST object), including which are fixed or random.

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 $\exp\big(p_1(i)\big)$ and biomass-per-individual $\exp\big(p_2(i)\big)$, see Grüss and Thorson (2019) for details. This approach is specified by associating each observation with a given error distribution using input `e_i` where e.g. `e_i[1]` is the error-distribution for the 1st observation. The user then specifies multiple observation errors via input `ObsModel_ez`:

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

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. 2015b), 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. 2015a). Predicting random effects at extrapolation-grid cell g at location s_g is accomplished using matrix $\mathbf{A}_g$ with n_g rows and n_s columns. Values are predicted as e.g.:

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

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.:

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

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

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:

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

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:

```
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:

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

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

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

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

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

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

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

The calculation of these and other derived quantities can be turned on and off using input `Options` to function `make_data` (see Table 2).

List of features

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;

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

5. Specify an "extrapolation grid" using input `FishStatsUtils::make_extrapolation_info(..., Region)`, which is used to calculate the area associated with each knot a_x. This can be a user-specified extrapolation grid if `FishStatsUtils::make_extrapolation_info(..., Region="User", input_grid=Input)`, where `Input` is a data frame supplied by the user.
6. Specifying a method for defining "knots";
7. Specifying the number of "knots";
8. Spatial variation being estimated ("turned on") or ignored ("turned off") for either linear predictor #1 or #2;
9. Spatio-temporal variation being estimated ("turned on") or ignored ("turned off") for either linear predictor #1 or #2;
10. Specifying that habitat covariates can affect linear predictors different ways including as:

    a. a linear effect;
    b. a spatially-varying effect; or
    c. both linear and spatially-varying effects simultaneously.

Multivariate analysis

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

Decisions regarding temporal structure

13. Annual intercepts being structured over time, including:
    a. estimated as fixed effects in every year;
    b. fixed as fixed effect with the same value for all years;
    c. estimated as a random effect with independent deviations in each year;
    d. estimated as a random effect with first-order autoregressive structure; or
    e. estimated as a random effect with a random-walk structure.
14. Spatio-temporal variation being structured over time, including:
    a. estimated as independent deviations in each year;
    b. estimated as following a first-order autoregressive structure over time;
    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 $\beta_1(c,t) \rightarrow \infty$ 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% of 0% encounter rate, add temporal structure to intercepts and spatio-temporal terms using `RhoConfig` options.
    c. Four other options are listed on the wiki.
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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Table 1 – List of S3 objects defined in package VAST (or its primary dependency FishStatsUtils), listing S3 methods defined for each class as well as the intended purpose of each method.

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

661 Table 2 – List of slots in vector `Options`.

Slot name	What it does	Examples of usage
SD_site_density	Calculate standard error for each knot or extrapolation-grid cell (very slow with fine_scale=TRUE)	-
SD_site_logdensity	Calculate standard error for each knot or extrapolation-grid cell (very slow with fine_scale=TRUE)	-
Calculate_Range	Calculate center of gravity for use in 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. 2019)
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. 2019)
Estimate_B0	Option to calculate unfished density using a MICE-in-space model	(Thorson et al. 2019)
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. 2019)

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