**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 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 , time intervals , for multiple categories . 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 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 represents encounter probability in a delta-model, or zero-inflation in a count-data model:

where is the predictor for observation , represents temporal variation for time for factor (of factors representing temporal variation), is the loadings matrix that generates temporal covariation among categories for this linear predictor, and represents the time-average for each category . The number of factors can range from zero to the number of categories , , where is equivalent to eliminating all temporal terms from the model. By default, , is treated as a fixed effect for each year and factor , and is an identity matrix; this formulation is equivalent to estimating a separate intercept 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, is assigned a normal distribution with unit variance, such that 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 (), then is a 1x1 matrix (i.e. a scalar) such is the variance and the absolute value, is the standard deviation for temporal variation.

Similarly, represents predicted spatial variation in the first linear predictor occurring at the location of sample for factor (of factors representing spatial variation), and is the loadings matrix that generates spatial covariation among categories for this linear predictor. Similarly, represents predicted spatio-temporal variation in the first linear predictor for each factor (of factors representing spatio-temporal variation), and is the loadings matrix that generates spatio-temporal covariation for this predictor. represents random variation in catchability among a grouping variable (tows or vessels) for each factor (of factors representing overdispersion), and is a loadings matrix that generates covariation in catchability among categories for this predictor. All loadings matrices are specified similarly to , i.e., where factors have a variance of one such that 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, is an three-dimensional array of measured density covariates that explain variation in density for time *t* and the location where sampling occurred for sample . VAST can include a separate, spatially-varying effect of each habitat covariate for each category . The spatially varying slope is , where is the average effect of density covariate for category , represents spatial variation in that effect (which has a mean of zero and standard deviation of one), and represents the estimated standard deviation of spatial variation of covariate for category . is a matrix of measured catchability covariates that explain variation in catchability, and is the estimated impact of catchability covariates for this linear predictor. By default, VAST specifies that for all years and , although users can relax this constaint by specifying a different structure for Data\_Fn(…, Map=NewMap).

Similarly, the second linear predictor 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).

**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 , FieldConfig[2] controls , FieldConfig[3] controls , and FieldConfig[4] controls , 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 , and OverdispersionConfig[2] controls , 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:

where is the predictor encounter probability in a delta-model, or zero-inflation in a count-data model, and is the inverse-logit (a.k.a. logistic) function of , and:

where is the predicted biomass density for positive catch rates in a delta-model or mean-intensity function for a count-data model, is the exponential function of , and is the area-swept for observation , which enters as a linear offset for expected biomass given an encounter.

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

where is the predictor encounter probability and is a complementary log-log link of , and:

where is the predicted biomass given that the species is encountered. In this “Poisson-process” link function, is interpreted as the density in number of individuals per area such that is the predicted number of individuals encountered, and is interpreted as the average weight per individual. Area-swept 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 .

*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 can be any non-negative real number, and . VAST calculates the probability of these data as:

where ObsModel[1] controls the probability density function used for positive catch rates (see ?Data\_Fn for a list of options), where each options is defined to have with expectation and dispersion , where dispersion parameter 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 can be any whole number, . VAST calculates the probability of these data as:

where ObsModel[1] controls the probability mass function 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, is the “zero-inflation probability” (i.e., the proportion of habitat in the immediate vicinity of location and time that is never occupied), while is the expected value for probability mass function (i.e., the number of individuals that are in the vicinity of sampling in habitat that is occupied), and 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 user-specified “interior vertices,” as well as additional “boundary vertices” such that the total number of interior and boundary vertices is . 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 verticies. Specifically, the correlation between location and location for spatial and spatio-temporal terms included in the first linear predictor is approximated as following a Matern function:

where is a two-dimensional linear transformation representing geometric anisotropy (with a determinant of 1.0), is the Matern smoothness (fixed at 1.0), and governs the decorrelation distance for that first linear predictor ( is also separately estimated for the second linear predictor). By default, the two degrees of freedom in are estimated as fixed effects, but the user can specify isotropy (i.e., ) 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 vertices as follows:

where is the vector of length formed when subsetting for a given . 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 with rows and columns, row . Values are then predicted as e.g.:

where is the vector of length , containing the predicted value for spatial variation in the first linear predictor at every location , and other spatial variables are predicted similarly using matrix .

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 are fixed equal to their value at the nearest “knot.” This involves specifying matrix such that row has value zero except for one cell containing a value of one for the knot closest to sample .
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 are interpolated using the triangulated mesh that is also used to approximate spatial variation. Specifically, matrix has row with value zero except for three cells, representing the vertices of the triangle containing location .

**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 and is a fixed effect. However, other settings specify the following factor-model structure:

Where is the index for the first modelled year and and 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). RhoConfig[1] controls the specification of :

1. *Independent among years* – RhoConfig[1]=1 specifies
2. *Random walk*  – RhoConfig[1]=2 specifies
3. *Constant intercept* – RhoConfig[1]=3 specifies and (i.e., is constant for all )
4. *Autoregressive* – RhoConfig[1]=4 estimates as a fixed effect

and settings are defined identically for RhoConfig[2] specifying .

*Temporal structure on spatio-temporal variation*

By default (when RhoConfig[3]=0 and RhoConfig[4]=0), the model specifies that each vector of spatio-temporal random effects, and composed of and across locations , is independent among years. However, other settings specify the following structure

where and are the estimated degree of first-order autocorrelation in temporal variation, RhoConfig[3] controls the specification of :

1. *Random walk*  – RhoConfig[3]=2 specifies
2. *Autoregressive* – RhoConfig[3]=4 estimates as a fixed effect

and settings are defined identically for RhoConfig[4] specifying .

**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 and biomass-per-individual , 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 “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 at location is accomplished using matrix with rows and columns. Values are predicted as e.g.:

where is the vector of length , containing the predicted value for spatial variation in the first linear predictor at every location , and other spatial variables are predicted similarly using matrix . Predicted values for random effects are then plugged into the linear predictor, e.g.:

where is predicted similar, and these linear predictors are used in turn to predict and , where their product is predicted biomass-density at every extrapolation-grid cell , category , and time .

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

where is the area associated with extrapolation-grid cell for index ; 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:

where is a matrix representing location for each extrapolation-grid cell (by default 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).

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

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

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:
   1. Count data using a Poisson, negative-binomial, Conway-Maxwell-Poisson, or Poisson-lognormal distribution, including zero-inflated versions of each;
   2. 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:
   1. A conventional delta-model;
   2. 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)*

1. Specify an “extrapolation grid” using input FishStatsUtils::make\_extrapolation\_info(..., Region), which is used to calculate the area associated with each knot . 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.
2. Specifying a method for defining “knots”;
3. Specifying the number of “knots”;
4. Spatial variation being estimated (“turned on”) or ignored (“turned off”) for either linear predictor #1 or #2;
5. Spatio-temporal variation being estimated (“turned on”) or ignored (“turned off”) for either linear predictor #1 or #2;
6. Specifying that habitat covariates can affect linear predictors different ways including as:
   1. a linear effect;
   2. a spatially-varying effect; or
   3. both linear and spatially-varying effects simultaneously.

*Multivariate analysis*

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

*Decisions regarding temporal structure*

1. Annual intercepts being structured over time, including:
   1. estimated as fixed effects in every year;
   2. fixed as fixed effect with the same value for all years;
   3. estimated as a random effect with independent deviations in each year;
   4. estimated as a random effect with first-order autoregressive structure; or
   5. estimated as a random effect with a random-walk structure.
2. Spatio-temporal variation being structured over time, including:
   1. estimated as independent deviations in each year;
   2. estimated as following a first-order autoregressive structure over time;
   3. estimated as following a random-walk structure over time; or
   4. estimated as following a vector-autoregressive structure involving a matrix of 1st order autoregressive interactions.

*Derived quantities*

1. Specifying spatial strata for use when calculating derived quantities;
2. Calculating one of many possible “univariate derived quantities”, including:
   1. abundance indices;
   2. range shift;
   3. effective area occupied
   4. covariance among categories within a multivariate model; or
   5. synchrony among categories.
3. 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*

1. Specifying separate distributions for different data sets (e.g., when multiple surveys providing different data types are available);
2. 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);
3. 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 in year , then and/or for that year. If there is 0% encounter rate in year , then and/or and there is no information to estimate or for that category and year ;
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 and spatio-temporal variation ). This can be done in many different ways that are each idiosyncratic and require some special justification. The easiest options are:
   1. 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.
   2. 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.
   3. Four other options are listed on the [wiki](https://github.com/nwfsc-assess/geostatistical_delta-GLMM/wiki/What-to-do-with-a-species-with-0%25-or-100%25-encounters-in-any-year).
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 (), plus one additional parameter per category (), 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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