**VAST model structure and user interface**

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**Purpose** **of document**:

R package VAST includes many different forms of documentation including:

1. Doxygen documentation that can accessed through the standard R-help interface when the library is loaded within R;
2. the VAST decision tree and user guide (currently in review at Fisheries Research)
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). 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 , is an intercept for category and year , represents spatial variation at location for factor (of factors representing spatial variation), and is the loadings matrix that generates spatial covariation among categories for this linear predictor. Similarly, represents spatio-temporal variation 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. is an array of measured density covariates that explain variation in density for time *t* and knot *x* and is the estimated impact of density covariates by 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 et al. In press, Thorson and Barnett 2017). The spatial, spatio-temporal, and overdispersion loadings matrices are designed such that is the covariance among categories for a given process (Thorson et al. 2015a), and when there is only one category is a 1x1 matrix (i.e. a scalar) such that its absolute value is the standard deviation for a given process. This model therefore reduces to a single-species spatio-temporal model (e.g., Thorson et al. 2015b) when only one category is available.

**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” function 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 In press). This Poisson-link function should only be used for delta-models, and not for count-data models.

**Observation models**:

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

# Control observation error

ObsModel = 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 approximates spatial and spatio-temporal variation as being piecewise-constant. To do so, the user specifies a number of knots n\_x:

# Number of knots

n\_x = 1000

VAST then uses a k-means algorithm to identify the location of n\_x knots to minimize the total distance between the location of available data and the location of the nearest knot. This distributes knots as a function of the spatial intensity of sampling data.

VAST then uses a stochastic partial differential equation (SPDE) approximation to the probability density function for spatial and spatio-temporal variation (Lindgren et al. 2011). This SPDE approximation involves generating a triangulated mesh that has a vertex of a triangle at each knot, and VAST generates this triangulated mesh using package *R-INLA* (Lindgren 2012). Outputs from this triangulated mesh can then be used to calculate the precision (inverse-covariance) matrix for a multivariate normal probability density function for the value of a spatial variable at each mesh vertex. Specifically, the correlation 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 each have a variance of 1.0. By default VAST specifies these as follows:

where is the vector formed when subsetting for a given , and is the variance of , where other parameters are defined similarly. Specifying a variance of 1.0 ensures that the covariance among categories is defined by the loadings matrix for that term. However, VAST allows spatio-temporal variance to be specified differently as discussed in the section titled “Structure on parameters among years”.

**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 structure:

where 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 spatio-temporal random effect and is independent among years. However, other settings specify the following structure

where 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.

**Relationship to other named models**

VAST can be configured to be identical to (or closely mimic) many models that have previously been published in ecology and fisheries:

1. *Spatial Gompertz model*:If intercepts are constant across years, spatio-temporal variation follows an autoregressive process, and only one category is modelled, then VAST is identical to a spatio-temporal Gompertz model (Thorson et al. 2014).
2. *Spatial factor analysis*:If only one year is analysed and multiple categories are modelled, VAST is similar to spatial factor analysis (Thorson et al. 2015a), although it permits the use of a delta-model (i.e., separate analysis of encounters and positive catch rates).
3. *Spatial dynamic factor analysis*: If intercepts are constant among years, spatio-temporal variation follows an autoregressive process, and multiple categories are modelled, then VAST is similar to spatial dynamic factor analysis (Thorson et al. 2016a), although VAST allows separate estimates of spatial vs. spatio-temporal covariation and also the use of a delta-model.

**Settings regarding derived quantities**

After a nonlinear minimizer has identified the value of fixed effects that maximizes the Laplace approximation to the marginal likelihood, Template Model Builder predicts the value of random effects that maximizes the joint likelihood conditional on these fixed effects. Estimated values of fixed and random effects are then used to predict density as follows:

where and are identical to the values specified previously, except that catchability variables are excluded from their computation (i.e., and , etc.)

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

Options = c("SD\_site\_density"=0, "SD\_site\_logdensity"=0, "Calculate\_Range"=0, "Calculate\_evenness"=0, "Calculate\_effective\_area"=0, "Calculate\_Cov\_SE"=0, 'Calculate\_Synchrony'=0, 'Calculate\_Coherence'=0)

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

where is a matrix representing location for each knot (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.

*Basic features in a generalized linear model (GLM)*

1. Specifying one of several possible distributions for data;
2. Specifying one of several possible link functions for predicting data given linear predictors;
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 SpatialDeltaGLMM::Prepare\_Extrapolation\_Data\_Fn(..., Region), which is used to calculate the area associated with each knot . 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.
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;

*Derived quantities*

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

*Non-standard decisions regarding temporal structure*

1. Annual intercepts being estimated as fixed effects in every year, fixed at the same value for all years, or estimated as a random effect with independent deviations in each year, a first-order autoregressive structure, or a random-walk structure.
2. Spatio-temporal variation being estimated as independent deviations in each year, following a first-order autoregressive structure over time, or following a random-walk structure over time.

*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 principle components rotation or varimax rotation;

*Unusual circumstances and spatial cases*

1. Specifying separate distributions for different data sets (e.g., when multiple surveys 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::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 (), 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. In press, 2017).

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