**VAST model structure and user interface**

**James Thorson**

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

R package VAST includes many different forms of documentation, which are documented on the [package GitHub page](https://github.com/James-Thorson-NOAA/VAST#user-resources-for-learning-about-vast). 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). Please see reference documentation for explanation of the user interface, and GitHub wiki for examples.

**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: 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matrices, and arrays, and reserve subscripts for naming (see Table 2 for summary of notation that may be slightly out-of-date). 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 , time intervals , for multiple categories . Categories could include either multiple species, multiple size/age/sex classes for each individual species, and/or a mix of biological, physical, and fishery variables describing an ecosystem. 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 extrapolation-grid cells (as an approximation to the integral 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 knots, as well as additional boundary vertices such that the total number of spatial “vertices” is . VAST specifically uses a k-means algorithm to identify the location of 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 represents encounter probability in a delta-model, or zero-inflation in a count-data model:

where is the predictor for observation , arising for category at location and time . 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). Model components are specified hierarchically to efficiently compute correlated variation among categories and years as explained next.

**Temporal variation**

Regarding intercepts representing temporal variation:

where 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 as fixed effect for each category and year.

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. 2015b). 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.

By default the model specifies that each intercept and is a fixed effect. However, other settings specify the following autocorrelation 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). Options treating intercepts as a random effect include:

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

and settings are defined identically for specifying .

**Spatial variation**

Regarding spatial variation:

where 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.

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 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. These GMRFs are then projected to calculate their value at every location using matrix with rows and columns. Specifically, values are projected as:

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 .

**Spatio-temporal variation**

Regarding spatio-temporal the model by default specifies that each vector of spatio-temporal random effects, and composed of and across locations , is independent for each factor representing covariation among categories () and among years (). We describe the process for the 1st linear predictor, and an identical process is used for the 2nd linear predictor (using different subscripts):

Values are then projected as:

This is then projected across years and categories using loadings matrices and :

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

Where is the estimated impact of spatio-temporal variation in category on spatio-temporal changes in category :

Where and represent elements of matrices and , where the product is the typical interaction matrix in a cointegration model (Engle and Granger 1987), where projects dynamics to a low-dimensional subspace and represents responses within that subspace. By default corresponding to , and these terms drop out of the model; however, they allow a parsimonious representation of species interactions (Thorson et al. 2017, 2019). Meanwhile is the estimated degree of first-order autocorrelation in temporal variation:

1. *Random walk*  – specifies
2. *Autoregressive* – estimates as a single fixed effect with the same value for all categories
3. *Individual autoregressive* -- estimates a separate value of as a single fixed effect for each category

and settings are defined identically for specifying .

**Overdisperison**

Regarding overdispersion:

where 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).

**Density covariates**

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

where 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 . By default VAST estimates spatially-varying slope terms values at each vertex as follows:

Values are then predicted as e.g.:

**Catchability covariates**

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

Where is an element of matrix composed of measured catchability covariates that explain variation in catchability, is the estimated impact of catchability covariates for this linear predictor, is unit-variance spatial variation in that slope term such that has standard deviation , where spatial variation in detectability is specified as follows:

Values are then predicted as e.g.:

**Fishing impacts**

Fishing impacts are included to represent the effect of known human impacts on variables. They are not yet documented in detail here, but see Thorson et al. (2019) for details. By default this term is excluded (i.e., ) and it is only applicable within MICE or single-species production models following vector-autoregressive dynamics (i.e., Gompertz density dependence). Feel free to contact the package author if desiring more documentation.

**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:

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. 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 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 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., ).

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 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 2015), 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.

**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.

**Identifiability constraints**:

The model as described requires several identifiability constraints to ensure that the resulting Hessian is positive definite (and hence allow calculation of asymptotic standard errors):

1. All loadings matrices are defined to be lower-triangular (i.e., elements above the diagonal are fixed at 0);
2. When estimating spatial random fields and estimating a loadings matrix across years for spatio-temporal variation, it is helpful to impose a sum-to-zero constraint on factors of the loadings matrix . This ensures that spatial terms represent the distribution in an “average” year, defined as times when for all columns;
3. When estimating loadings across species and across years , the magnitude of these two matrices is confounded. The solution adopted here is to impose the constraint that for both linear predictors, such that the magnitude of can be interpreted similarly to other loadings matrices.

The model also has issues arising from “label switching,” i.e., where any column of any loadings matrix could be multiplied by negative-one (and similarly for the associated factor) without any change in the model predicts and likelihood. This implies that the negative log-likelihood has a series of local minima that all have the same properties. We do not address “label switching” because it does not have any practical effect on maximum-likelihood estimation or resulting predictions, but we note that it gives rise to numerical complexities when tuning or interpreting mixing for conventional samplers within a Bayesian estimation paradigm.

**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 (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 “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 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).

The calculation of these and other derived quantities can be turned on and off using input Options to function make\_data (see reference documentation for details regarding user interface).

**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).

**Acknowledgements**

I thank K. Kristensen, H. Skaug, and the developers of Template Model Builder, without which this research and resulting R package VAST would not be possible. I also thank the many collaborators who have contributed to developing features (see <https://github.com/nwfsc-assess/geostatistical_delta-GLMM/wiki/Applications>), as well as the funding sources that have supported development (see <https://github.com/James-Thorson-NOAA/VAST#funding-and-support-for-the-tool>). In particular, I think C. Monnahan and M. Rudd for contributing substantially to coding new features, and A. Gruss for identifying indexing errors in several (little used) features. I also thank the many volunteers and NOAA scientists who have served on sampling vessels that provided data to test these methods. Finally, I think A. Grüss and S. Hoyle for providing edits to this document.

**Works cited**

Edwards, A.M., and Auger‐Méthé, M. 2019. Some guidance on using mathematical notation in ecology. Methods Ecol. Evol. **10**(1): 92–99. doi:10.1111/2041-210X.13105.

Engle, R.F., and Granger, C.W. 1987. Co-integration and error correction: representation, estimation, and testing. Econom. J. Econom. Soc.: 251–276.

Gelman, A., and Hill, J. 2007. Data analysis using regression and multilevel/hierarchical models. Cambridge University Press, Cambridge, UK.

Godefroid, M., Boldt, J.L., Thorson, J.T., Forrest, R., Gauthier, S., Flostrand, L., Ian Perry, R., Ross, A.R.S., and Galbraith, M. 2019. Spatio-temporal models provide new insights on the biotic and abiotic drivers shaping Pacific Herring (Clupea pallasi) distribution. Prog. Oceanogr. **178**: 102198. doi:10.1016/j.pocean.2019.102198.

Grüss, A., and Thorson, J.T. 2019. Developing spatio-temporal models using multiple data types for evaluating population trends and habitat usage. ICES J. Mar. Sci. **76**(6): 1748–1761. doi:10.1093/icesjms/fsz075.

Grüss, A., Thorson, J.T., Babcock, E.A., and Tarnecki, J.H. 2018. Producing distribution maps for informing ecosystem-based fisheries management using a comprehensive survey database and spatio-temporal models. ICES J. Mar. Sci. **75**(1): 158–177. doi:10.1093/icesjms/fsx120.

Grüss, A., Thorson, J.T., Sagarese, S.R., Babcock, E.A., Karnauskas, M., Walter, J.F., and Drexler, M. 2017. Ontogenetic spatial distributions of red grouper (Epinephelus morio) and gag grouper (Mycteroperca microlepis) in the U.S. Gulf of Mexico. Fish. Res. **193**(Supplement C): 129–142. doi:10.1016/j.fishres.2017.04.006.

Hocking, D.J., Thorson, J.T., O’Neil, K., and Letcher, B.H. 2018. A geostatistical state-space model of animal densities for stream networks. Ecol. Appl. **28**(7): 1782–1796. doi:10.1002/eap.1767.

Kass, R.E., and Steffey, D. 1989. Approximate Bayesian inference in conditionally independent hierarchical models (parametric empirical bayes models). J. Am. Stat. Assoc. **84**(407): 717–726. doi:10.2307/2289653.

Kristensen, K., Nielsen, A., Berg, C.W., Skaug, H., and Bell, B.M. 2016. TMB: Automatic differentiation and Laplace approximation. J. Stat. Softw. **70**(5): 1–21. doi:10.18637/jss.v070.i05.

Lindgren. 2012. Continuous domain spatial models in R-INLA. ISBA Bull. **19**(4): 14–20.

Lindgren, F., and Rue, H. 2015. Bayesian spatial modelling with r-inla. J. Stat. Softw. **63**(19): 1–25. doi:10.18637/jss.v063.i19.

Lindgren, Rue, H., and Lindström, J. 2011. An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach. J. R. Stat. Soc. Ser. B Stat. Methodol. **73**(4): 423–498. doi:10.1111/j.1467-9868.2011.00777.x.

Martin, T.G., Wintle, B.A., Rhodes, J.R., Kuhnert, P.M., Field, S.A., Low-Choy, S.J., Tyre, A.J., and Possingham, H.P. 2005. Zero tolerance ecology: improving ecological inference by modelling the source of zero observations. Ecol. Lett. **8**(11): 1235–1246.

R Core Team. 2017. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria. Available from https://www.R-project.org/.

Searle, S.R., Casella, G., and McCulloch, C.E. 1992. Variance components. John Wiley & Sons, Hoboken, New Jersey.

Shelton, A.O., Thorson, J.T., Ward, E.J., and Feist, B.E. 2014. Spatial semiparametric models improve estimates of species abundance and distribution. Can. J. Fish. Aquat. Sci. **71**(11): 1655–1666. doi:10.1139/cjfas-2013-0508.

Skaug, H., and Fournier, D. 2006. Automatic approximation of the marginal likelihood in non-Gaussian hierarchical models. Comput. Stat. Data Anal. **51**(2): 699–709.

Thorson, J.T. 2018. Three problems with the conventional delta-model for biomass sampling data, and a computationally efficient alternative. Can. J. Fish. Aquat. Sci. **75**(9): 1369–1382. doi:10.1139/cjfas-2017-0266.

Thorson, J.T. 2019. Guidance for decisions using the Vector Autoregressive Spatio-Temporal (VAST) package in stock, ecosystem, habitat and climate assessments. Fish. Res. **210**: 143–161. doi:10.1016/j.fishres.2018.10.013.

Thorson, J.T., Adams, G., and Holsman, K. 2019. Spatio-temporal models of intermediate complexity for ecosystem assessments: A new tool for spatial fisheries management. Fish Fish. **20**(6): 1083–1099. doi:10.1111/faf.12398.

Thorson, J.T., and Barnett, L.A.K. 2017. Comparing estimates of abundance trends and distribution shifts using single- and multispecies models of fishes and biogenic habitat. ICES J. Mar. Sci. **74**(5): 1311–1321. doi:10.1093/icesjms/fsw193.

Thorson, J.T., Ciannelli, L., and Litzow, M.A. 2020. Defining indices of ecosystem variability using biological samples of fish communities: A generalization of empirical orthogonal functions. Prog. Oceanogr. **181**: 102244. doi:10.1016/j.pocean.2019.102244.

Thorson, J.T., and Haltuch, M.A. 2018. Spatiotemporal analysis of compositional data: increased precision and improved workflow using model-based inputs to stock assessment. Can. J. Fish. Aquat. Sci. **76**(3): 401–414. doi:10.1139/cjfas-2018-0015.

Thorson, J.T., Ianelli, J.N., Larsen, E.A., Ries, L., Scheuerell, M.D., Szuwalski, C., and Zipkin, E.F. 2016a. Joint dynamic species distribution models: a tool for community ordination and spatio-temporal monitoring. Glob. Ecol. Biogeogr. **25**(9): 1144–1158. doi:10.1111/geb.12464.

Thorson, J.T., and Kristensen, K. 2016. Implementing a generic method for bias correction in statistical models using random effects, with spatial and population dynamics examples. Fish. Res. **175**: 66–74. doi:10.1016/j.fishres.2015.11.016.

Thorson, J.T., and Minto, C. 2015. Mixed effects: a unifying framework for statistical modelling in fisheries biology. ICES J. Mar. Sci. J. Cons. **72**(5): 1245–1256. doi:10.1093/icesjms/fsu213.

Thorson, J.T., Munch, S.B., and Swain, D.P. 2017. Estimating partial regulation in spatiotemporal models of community dynamics. Ecology **98**(5): 1277–1289. doi:10.1002/ecy.1760.

Thorson, J.T., Pinsky, M.L., and Ward, E.J. 2016b. Model-based inference for estimating shifts in species distribution, area occupied and centre of gravity. Methods Ecol. Evol. **7**(8): 990–1002. doi:10.1111/2041-210X.12567.

Thorson, J.T., Rindorf, A., Gao, J., Hanselman, D.H., and Winker, H. 2016c. Density-dependent changes in effective area occupied for sea-bottom-associated marine fishes. Proc R Soc B **283**(1840): 20161853. doi:10.1098/rspb.2016.1853.

Thorson, J.T., Scheuerell, M.D., Olden, J.D., and Schindler, D.E. 2018. Spatial heterogeneity contributes more to portfolio effects than species variability in bottom-associated marine fishes. Proc R Soc B **285**(1888): 20180915. doi:10.1098/rspb.2018.0915.

Thorson, J.T., Shelton, A.O., Ward, E.J., and Skaug, H.J. 2015a. Geostatistical delta-generalized linear mixed models improve precision for estimated abundance indices for West Coast groundfishes. ICES J. Mar. Sci. J. Cons. **72**(5): 1297–1310. doi:10.1093/icesjms/fsu243.

Thorson, J.T., Skaug, H.J., Kristensen, K., Shelton, A.O., Ward, E.J., Harms, J.H., and Benante, J.A. 2014. The importance of spatial models for estimating the strength of density dependence. Ecology **96**(5): 1202–1212. doi:10.1890/14-0739.1.

Thorson, Scheuerell, M.D., Shelton, A.O., See, K.E., Skaug, H.J., and Kristensen, K. 2015b. Spatial factor analysis: a new tool for estimating joint species distributions and correlations in species range. Methods Ecol. Evol. **6**(6): 627–637. doi:10.1111/2041-210X.12359.

Tierney, L., Kass, R.E., and Kadane, J.B. 1989. Fully exponential Laplace approximations to expectations and variances of nonpositive functions. J. Am. Stat. Assoc. **84**(407): 710–716.

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 |

Table 2 – Definition of mathematical notation, including the symbol used, its type (Index, Data, fixed effects “FE”, random effects “RE”, intermediate quantity computed internally “IQ”, and derived quantities that are outputted for users “DQ”), and its dimension

Table 2A – Indices

|  |  |
| --- | --- |
| Index name | Symbol |
| Observation number |  |
| Extrapolation-grid cell |  |
| Knot number |  |
| Vertex number (including internal knots and boundary vertices) |  |
| Time interval number |  |
| Category number |  |
| Factor number |  |
| Habitat covariate number for 1st linear predictor |  |
| Habitat covariate number for 2nd linear predictor |  |
| Catchability covariate number for 1st linear predictor |  |
| Catchability covariate number for 2nd linear predictor |  |
| Stratum number |  |
| Index number for measures of center-of-gravity |  |
| Index number for other book-keeping |  |

Table 2B – Data

|  |  |  |
| --- | --- | --- |
| Index name | Symbol | Dimensions |
| Sample response |  |  |
| Time interval for each sample |  |  |
| Category for each sample |  |  |
| Overdispersion level for each sample |  |  |
| Area covered by each sample |  |  |
| Bilinear interpolation from vertices to samples |  |  |
| Bilinear interpolation from vertices to extrapolation-grid cells |  |  |
| Distance between two vertices |  |  |
| Habitat covariates affecting 1st linear predictor for each sampling location, time, and variable |  |  |
| Habitat covariates affecting 2nd linear predictor for each sampling location, time, and variable |  |  |
| Habitat covariates affecting 1st linear predictor for each extrapolation-grid cell, time, and variable |  |  |
| Habitat covariates affecting 2nd linear predictor for each extrapolation-grid cell, time, and variable |  |  |
| Catchability covariates affecting 1st linear predictor for each sample and variable |  |  |
| Catchability covariates affecting 2nd linear predictor for each sample and variable |  |  |
| Area associated with extrapolation-grid cell in each stratum |  |  |
| Statistic for each location used to calculate center of gravity and range edges |  |  |

Table 2C – Coefficients, indicating whether they are fixed effects (FE), random effects (RE) or whether their treatment depends upon user settings (FE/RE)

|  |  |  |  |
| --- | --- | --- | --- |
| Coefficient name | Symbol | Type | Dimensions |
| Factor values for intercept for 1st linear predictor |  | FE/RE |  |
| Factor values for intercept for 2st linear predictor |  | FE/RE |  |
| Loadings matrix for intercepts for 1st linear predictor |  | FE |  |
| Loadings matrix for intercepts for 2nd linear predictor |  | FE |  |
| Loadings matrix for spatial covariation for 1st linear predictor |  | FE |  |
| Loadings matrix for spatial covariation for 2nd linear predictor |  | FE |  |
| Loadings matrix for spatio-temporal covariation across categories for 1st linear predictor |  | FE |  |
| Loadings matrix for spatio-temporal covariation across categories for 2nd linear predictor |  | FE |  |
| Loadings matrix for spatio-temporal covariation across time for 1st linear predictor |  | FE |  |
| Loadings matrix for spatio-temporal covariation across time for 2nd linear predictor |  | FE |  |
| Loadings matrix for overdispersion covariation for 1st linear predictor |  | FE |  |
| Loadings matrix for overdispersion covariation for 2nd linear predictor |  | FE |  |
| Impact of habitat covariates on 1st linear predictor |  | FE |  |
| Impact of habitat covariates on 2nd linear predictor |  | FE |  |
| Impact of catchability covariates on 1st linear predictor |  | FE |  |
| Impact of catchability covariates on 2nd linear predictor |  | FE |  |
| Parameters governing residual variation |  | FE |  |
| Decorrelation rate for 1st linear predictor |  | FE | 1 |
| Decorrelation rate for 2nd linear predictor |  | FE | 1 |
| Autocorrelation for intercepts of 1st linear predictor |  | FE | 1 |
| Autocorrelation for intercepts of 2nd linear predictor |  | FE | 1 |
| Conditional variance for intercepts of 1st linear predictor |  | FE | 1 |
| Conditional variance for intercepts of 2ndlinear predictor |  | FE | 1 |
| Autocorrelation for spatio-temporal covariation of 1st linear predictor |  | FE | 1 |
| Autocorrelation for spatio-temporal covariation of 2nd linear predictor |  | FE | 1 |
| Parameters governing geometric anisotropy |  | FE | 2 |
| Spatial factors for 1st linear predictor |  | RE |  |
| Spatial factors for 2nd linear predictor |  | RE |  |
| Spatio-temporal factors for 1st linear predictor |  | RE |  |
| Spatio-temporal factors for 2nd linear predictor |  | RE |  |
| Overdispersion factors for 1st linear predictor |  | RE |  |
| Overdispersion factors for 2nd linear predictor |  | RE |  |

Table 2D – Variable calculated internally

|  |  |  |
| --- | --- | --- |
| Coefficient name | Symbol | Dimensions |
| 1st linear predictor |  |  |
| 2nd linear predictor |  |  |
| 1st link-transformed predictor |  |  |
| 2nd link-transformed predictor |  |  |
| Spatio-temporal variation for 1st linear predictor at each extrapolation-grid cell |  |  |
| Spatio-temporal variationfor 2nd linear predictor at each extrapolation-grid cell |  |  |
| Spatio-temporal variation for 1st linear predictor at each sample |  |  |
| Spatio-temporal variationfor 2nd linear predictor at each sample |  |  |
| Spatial variation for 1st linear predictor at each extrapolation-grid cell |  |  |
| Spatial variation for 2nd linear predictor at each extrapolation-grid cell |  |  |
| Spatial variation for 1st linear predictor at each sample |  |  |
| Spatial variation for 2nd linear predictor at each sample |  |  |
| Intercept for 1st linear predictor |  |  |
| Intercept for 2st linear predictor |  |  |
| Spatial correlation matrix among vertices for 1st linear predictor |  |  |
| Spatial correlation matrix among vertices for 2nd linear predictor |  |  |
| Anisotropy matrix |  |  |

Table 2E – Derived quantities

|  |  |  |
| --- | --- | --- |
| Coefficient name | Symbol | Dimensions |
| Predicted density for each sample |  |  |
| Predicted density for each extrapolation-grid cell |  |  |
| Index of abundance |  |  |
| Center of gravity |  |  |
| Average density |  |  |
| Effective area occupied |  |  |
| Rotation matrix for spatial covariation for 1st linear predictor |  |  |
| Rotation matrix for spatial covariation for 2ndlinear predictor |  |  |
| Rotation matrix for spatio-temporal covariation for 1st linear predictor |  |  |
| Rotation matrix for spatio-temporal covariation for 2nd linear predictor |  |  |
| Rotation matrix for overdispersion covariation for 1st linear predictor |  |  |
| Rotation matrix for overdispersion covariation for 2ndlinear predictor |  |  |
| Rotated loadings matrix for spatial covariation for 1st linear predictor |  |  |
| Rotated loadings for spatial covariation for 2nd linear predictor |  |  |
| Rotated loadings for spatio-temporal covariation for 1st linear predictor |  |  |
| Rotated loadings for spatio-temporal covariation for 2nd linear predictor |  |  |
| Rotated loadings for overdispersion covariation for 1st linear predictor |  |  |
| Rotated loadings for overdispersion covariation for 2nd linear predictor |  |  |
| Rotated spatial factors for 1st linear predictor |  |  |
| Rotated spatial factors for 2nd linear predictor |  |  |
| Rotated spatio-temporal factors for 1st linear predictor |  |  |
| Rotated spatio-temporal factors for 2nd linear predictor |  |  |
| Rotated overdispersion factors for 1st linear predictor |  |  |
| Rotated overdispersion factors for 2nd linear predictor |  |  |