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 (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,

25   matrices, and arrays, and reserve subscripts for naming. Feel free to change notation when

26   describing the model to suit your purposes in reports or publications. For further details

27   regarding terminology, motivation, and statistical properties, please read the papers listed on

28   the GitHub main page.

29

30   **Overview**

31   VAST predicts variation in density across multiple locations s, time intervals t, for

32   multiple categories c. Categories could include either multiple species, and/or multiple

33   size/age/sex classes for each individual species. VAST approximates the covariance between

34   these multiple factors using a factor-model decomposition (Thorson et al. 2015a, 2016a), i.e.,

35   by summing across the contribution of multiple random effects (termed factors). If there is

36   only a single category, the model reduces to a standard univariate spatio-temporal model.

37   After estimating variation in density across space, time, and among categories, VAST

38   then predicts total abundance across a user-specified spatial domain. This is equivalent to an

39   "area-weighting" approach to index standardization, and the resulting prediction of total

40   abundance can be used an index of abundance.

41   In addition to spatial and spatio-temporal covariance among multiple categories,

42   VAST allows users to specify either density or catchability covariates. Both explain variation

43   in observed catch-rate data, but VAST predicts density (for use in calculating the abundance

44   index) using density covariates but not catchability covariates. Therefore, VAST "controls

45   for" catchability covariates when calculating an index (i.e., removes their estimated effect)

46   while "conditioning on" density covariates when calculating an index (i.e., uses them to

47   improve interpolated/extrapolated predictions of density).

48

49   **Linear predictors**

50   The model potentially includes two linear predictors (because it is designed to support delta-

51   models, which include two components). The first linear predictor $p_1(i)$ represents

52   encounter probability in a delta-model, or zero-inflation in a count-data model:

$$53 \quad p_1(i) = \underbrace{\beta_1^*(c_i) + \sum_{f=1}^{n_{\beta 1}} L_{\beta 1}(c_i, f)\beta_1(t_i, f)}_{Temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\omega 1}} L_{\omega 1}(c_i, f)\omega_1^*(s_i, f)}_{Spatial\ variation}$$

$$54 \quad + \underbrace{\sum_{f=1}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c_i, f)\varepsilon_1^*(s_i, f, t_i)}_{Spatio-temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\eta 1}} L_1(c_i, f)\eta_1(v_i, f)}_{Vessel\ effects}$$

$$55 \quad + \underbrace{\sum_{p=1}^{n_p} \Big(\gamma_1(c_i, t_i, p) + \sigma_{\xi 1}(c_i, p)\xi_1^*(s_i, c_i, p) \Big) X(i, t_i, p)}_{Habitat\ covariates} + \underbrace{\sum_{k=1}^{n_k} \lambda_1(k)\, Q(i, k)}_{Catchability\ covariate}$$

56   where $p_1(i)$ is the predictor for observation i, $\beta_1^*(t_i, f)$ represents temporal variation for time

57   t_i for factor f (of $n_{\beta 1}$ factors representing temporal variation), $L_{\beta 1}(c_i, f)$ is the loadings

58   matrix that generates temporal covariation among categories for this linear predictor, and

59    $\beta_2^*(c_i)$ represents the time-average for each category c_i. The number of factors $n_{\beta 1}$ can range

60   from zero to the number of categories n_c, $0 \le n_{\beta 1} \le n_c$, where $n_{\beta 1} = 0$ is equivalent to

61   eliminating all temporal terms from the model. By default, $n_{\beta 1} = n_c$, $\beta_1(t, f)$ is treated as a

62   fixed effect for each year t and factor f, and $\mathbf{L}_{\beta 1}$ is an identity matrix; this formulation is

63   equivalent to estimating a separate intercept $\beta_1(t_i, c) = \beta_1(t_i, f)$ for each category and year.

64   However, the intercepts can instead be treated as a random effect using the factor-model

65   formulation, which allows for sharing information among years and categories. When treated

66   as random, $\beta_1(t_i, f)$ is assigned a normal distribution with unit variance, such that $\mathbf{L}_{\beta 1}^T \mathbf{L}_{\beta 1}$ is

67   the covariance among categories for a given process (Thorson et al. 2015a). When treating

68   intercepts as random, and when there is only one category and using one factor ($n_{\beta 1} = 1$),

69   then $\mathbf{L}_{\beta 1}$ is a 1x1 matrix (i.e. a scalar) such $\mathbf{L}_{\beta 1}^2$ is the variance and the absolute value,

70    $abs(\mathbf{L}_{\beta 1})$ is the standard deviation for temporal variation.

71   Similarly, $\omega_1^*(s_i, f)$ represents predicted spatial variation in the first linear predictor

72   occurring at the location s_i of sample i for factor f (of $n_{\omega 1}$ factors representing spatial

73   variation), and $L_{\omega 1}(c_i, f)$ is the loadings matrix that generates spatial covariation among

74   categories for this linear predictor. Similarly, $\varepsilon_1^*(s_i, f, t_i)$ represents predicted spatio-

75   temporal variation in the first linear predictor for each factor f (of $n_{\varepsilon 1}$ factors representing

76   spatio-temporal variation), and $L_{\varepsilon 1}(c_i, f)$ is the loadings matrix that generates spatio-

77   temporal covariation for this predictor. $\eta_1(v_i, f)$ represents random variation in catchability

78   among a grouping variable (tows or vessels) for each factor f (of $n_{\eta 1}$ factors representing

79   overdispersion), and $L_1(c_i, f)$ is a loadings matrix that generates covariation in catchability

80   among categories for this predictor. All loadings matrices are specified similarly to $\mathbf{L}_{\beta 1}$, i.e.,

81   where factors have a variance of one such that $\mathbf{L}^T\mathbf{L}$ represents the covariance among

82   categories. The main difference is that spatial, spatio-temporal, and overdispersion factors

83   can only be specified as random effects, while the intercepts can be specified as either

84   random or fixed (where specifying as fixed "turns off" all factor-modelling for that intercept).

85   Finally, $X(i, t_i, p)$ is an three-dimensional array of n_p measured density covariates

86   that explain variation in density for time t and the location s_i where sampling occurred for

87   sample i. VAST can include a separate, spatially-varying effect of each habitat covariate p

88   for each category c. The spatially varying slope is $\gamma_1(c_i, t_i, p) + \sigma_{\xi 1}(c, p)\xi_n(s, c, p)$, where

89    $\gamma_1(c_i, t_i, p)$ is the average effect of density covariate $X(i, t_i, p)$ for category c, $\xi_n(s_i, c_i, p)$

90   represents spatial variation in that effect (which has a mean of zero and standard deviation of

91   one), and $\sigma_{\xi 1}(c, p)$ represents the estimated standard deviation of spatial variation of

92   covariate p for category c. $Q(i, k)$ is a matrix of n_k measured catchability covariates that

93   explain variation in catchability, and $\lambda_1(k)$ is the estimated impact of catchability covariates

94   for this linear predictor. By default, VAST specifies that $\gamma_1(c, t_1, p) = \gamma_1(c, t_2, p)$ for all

95   years t_1 and t_2, although users can relax this constaint by specifying a different structure for

96   `Data_Fn(…, Map=NewMap)`.

97   Similarly, the second linear predictor $p_2(i)$ represents positive catch rates in a delta-

98   model, or the count-data intensity function in a count-data model:

99    $$p_2(i) = \beta_2^*(c_i) + \underbrace{\sum_{f=1}^{n_{\beta 2}} L_{\beta 2}(c_i, f)\beta_2(t_i, f)}_{Temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\omega 2}} L_{\omega 2}(c_i, f)\omega_2^*(s_i, f)}_{Spatial\ variation}$$

100   $$+ \underbrace{\sum_{f=1}^{n_{\varepsilon 2}} L_{\varepsilon 2}(c_i, f)\varepsilon_2^*(s_i, f, t_i)}_{Spatio-temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\eta 2}} L_2(c_i, f)\eta_2(v_i, f)}_{Vessel\ effects}$$

101   $$+ \underbrace{\sum_{p=1}^{n_p} \Big(\gamma_2(c_i, t_i, p) + \sigma_{\xi 2}(c_i, p)\xi_2^*(s_i, c_i, p)\Big) X(i, t_i, p)}_{Density\ covariates} + \underbrace{\sum_{k=1}^{n_k} \lambda_2(k)\, Q(i, k)}_{Catchability\ covariates}$$

102   where all variables and parameters are defined similarly except using different subscripts

103   (Thorson and Barnett 2017; Thorson 2019).

104

105   **Number of spatial and spatio-temporal factors**

106   The user controls the number of spatial and spatio-temporal factors used for each component

107   via input:

108   `FieldConfig = c("Omega1"=1, "Epsilon1"=1, "Omega2"=1, "Epsilon2"=1)`
109

110   where `FieldConfig[1]` controls $n_{\omega 1}$, `FieldConfig[2]` controls $n_{\varepsilon 1}$, `FieldConfig[3]` controls

111   $n_{\omega 2}$, and `FieldConfig[4]` controls $n_{\varepsilon 2}$, and a value of zero "turns off" that component of

112   spatial or spatio-temporal covariation.

113

Number of overdispersion factors

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

```
OverdispersionConfig = c("Eta1"=0, "Eta2"=0)
```
117

118   where `OverdispersionConfig[1]` controls $n_{\delta 1}$, and `OverdispersionConfig[2]` controls $n_{\delta 2}$,

119   and a value of zero again "turns off" that component of random covariation in catchability.

120   For example, if the user inputs:

```
OverdispersionConfig = c("Eta1"=1, "Eta2"=1)
```
122

123   then there will be one random effect estimated for each unique level of `Data_Geostat$Vessel`

124   for both the first and second linear predictors.

125

Link functions and observation error distributions

127   There are user-controlled options that control the observation error distribution and the link-

128   functions used to calculate expected encounter probabilities and positive catch rates based on

129   the two linear predictors.

130   The `ObsModel` vector has two components, controlling the observation error distribution and

131   link function respectively.

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

133   There are currently four options for the link function. For the latest set of options see the R

134   help documentation by typing into the R terminal `` `?VAST::Data_Fn` ``.

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

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

137   where $r_1(i)$ is the predictor encounter probability in a delta-model, or zero-inflation in a

138   count-data model, and $logit^{-1}(p_1(i))$ is the inverse-logit (a.k.a. logistic) function of

139      $p_1(i)$, and:

140 $$r_2(i) = a_i \times \log^{-1}(p_2(i))$$

141   where $r_2(i)$ is the predicted biomass density for positive catch rates in a delta-model or

142   mean-intensity function for a count-data model, $log^{-1}(p_2(i))$ is the exponential function

143   of $p_2(i)$, and a_i is the area-swept for observation i, which enters as a linear offset for

144   expected biomass given an encounter.

145 2. `ObsModel[2]=1` corresponds to a "Poisson-link" delta-model that approximates a Tweedie

146   distribution:

147 $$r_1(i) = 1 - \exp(-a_i \times \exp(p_1(i)))$$

148   where $r_1(i)$ is the predictor encounter probability and $1 - \exp(-a_i \times \exp(p_1(i)))$ is a

149   complementary log-log link of $p_1(i) + \log(a_i)$, and:

150 $$r_2(i) = \frac{a_i \times \exp(p_1(i))}{r_1(i)} \times \exp(p_2(i))$$

151   where $r_2(i)$ is the predicted biomass given that the species is encountered. In this

152   "Poisson-process" link function, $\exp(p_1(i))$ is interpreted as the density in number of

153   individuals per area such that $a_i \times \exp(p_1(i))$ is the predicted number of individuals

154   encountered, and $\exp(p_2(i))$ is interpreted as the average weight per individual. Area-

155   swept a_i therefore enters as a linear offset for the expected number of individuals

156   encountered (Thorson 2018). This Poisson-link function should only be used for delta-

157   models, and not for count-data models, but can also be used to combine encounter, count,

158   and biomass-sampling data (see section below for details).

159

160 **Observation models**:

161 There are different user-controlled options for observation models for available sampling

162 data, which are controlled by `ObsModel_ez[1]`.

```
# Control observation error
ObsModel_ez = c("PosDist"=2, "Link"=0)
```

166 I distinguish between observation models for continuous-valued data (e.g., biomass, or

167 numbers standardized to a fixed area), and observation models for count data (e.g., numbers

168 treating area-swept as an offset). However, both are parameterized such that the expectation

169 for sampling data $\mathbb{E}(B_i) = r_1(i) \times r_2(i)$.

Continuous-valued data (e.g., biomass)

171 If using an observation model with continuous support (e.g., a normal, lognormal, gamma, or

172 Tweedie models), then data b_i can be any non-negative real number, $b_i \in \mathcal{R}$ and $b_i \geq 0$.

173 VAST calculates the probability of these data as:

174
$$\mathrm{Pr}(b_i = B) = \begin{cases} 1 - r_1(i) & \text{if } B = 0 \\ r_1(i) \times g\{B | r_2(i), \sigma_m^2(c)\} & \text{if } B > 0 \end{cases}$$

175 where `ObsModel[1]` controls the probability density function $g\{B | r_2(i), \sigma_m^2(c)\}$ used for

176 positive catch rates (see `?Data_Fn` for a list of options), where each options is defined to have

177 with expectation $r_2(i)$ and dispersion $\sigma_m^2(c)$, where dispersion parameter $\sigma_m^2(c)$ varies

178 among categories by default.

Discrete-valued data (e.g., abundance)

180 If using an observation model with discrete support (e.g., a Poisson, negative-binomial,

181 Conway-Maxwell Poisson, or lognormal-Poisson models), then data b_i can be any whole

182 number, $b_i \in \{0,1,2,...\}$. VAST calculates the probability of these data as:

183
$$\mathrm{Pr}(B = b_i) = \begin{cases} \left(1 - r_1(i)\right) + g\{B = 0 | r_2(i), ...\} & \text{if } B = 0 \\ r_1(i) \times g\{B = b_i | r_2(i), ...\} & \text{if } B > 0 \end{cases}$$

184 where `ObsModel[1]` controls the probability mass function $g\{B | r_2(i), ...\}$ used (again, see

185 `?Data_Fn` for a list of options), where I use … to signify that these probability mass functions

186   generally can have one or more parameter governing dispersion, and the precise number and

187   interpretation varies among observation models (i.e., the value of `ObsModel[1]`). For these

188   count-data models, $(1 - r_1(i))$ is the "zero-inflation probability" (i.e., the proportion of

189   habitat in the immediate vicinity of location s_i and time t_i that is never occupied), while $r_2(i)$

190   is the expected value for probability mass function $g\{B = b_i | r_2(i), ... \}$ (i.e., the number of

191   individuals that are in the vicinity of sampling in habitat that is occupied), and $g\{B =$

192    $0 | r_2(i), ... \}$ is the probability of not encountering category c given that sampling occurs in

193   occupied habitat (Martin et al. 2005).

194

195   **Settings regarding spatial domain**

196   VAST estimates the value of spatial variables at a user-defined number of knots. To do so,

197   the user specifies a number of knots `n_x`:

```
198    # Number of knots
199    n_x = 1000
```

200

201   VAST then uses a k-means algorithm to identify the location of `n_x` knots to minimize the

202   total distance between the location of available data and the location of the nearest knot. This

203   distributes knots as a function of the spatial intensity of sampling data.

204   VAST then uses a stochastic partial differential equation (SPDE) approximation to the

205   probability density function for spatial and spatio-temporal variation (Lindgren et al. 2011).

206   This SPDE approximation involves generating a triangulated mesh that has a vertex of a

207   triangle at each knot, and VAST generates this triangulated mesh using package *R-INLA*

208   (Lindgren 2012). This mesh includes all n_x user-specified "interior vertices," as well as

209   additional "boundary vertices" such that the total number of interior and boundary vertices is

210   n_s. Outputs from this triangulated mesh can then be used to calculate the precision (inverse-

211   covariance) matrix for a multivariate normal probability density function for the value of a

212 spatial variable at all n_s verticies. Specifically, the correlation $\mathbf{R}_1(s, s+h)$ between

213 location s and location $s+h$ for spatial and spatio-temporal terms included in the first linear

214 predictor is approximated as following a Matern function:

215
$$\mathbf{R}_1(s, s+h) = \frac{1}{2^{\nu-1}\Gamma(n)} \times (\kappa_1|h\mathbf{H}|)^\nu \times K_\nu(\kappa_1|h\mathbf{H}|)$$

216 where $\mathbf{H}$ is a two-dimensional linear transformation representing geometric anisotropy (with

217 a determinant of 1.0), ν is the Matern smoothness (fixed at 1.0), and κ_1 governs the

218 decorrelation distance for that first linear predictor (κ_2 is also separately estimated for the

219 second linear predictor). By default, the two degrees of freedom in $\mathbf{H}$ are estimated as fixed

220 effects, but the user can specify isotropy (i.e., $\mathbf{H} = \mathbf{I}$) by specifying:

```
221  # Turn of geometric anisotropy
222  Data = Data_Fn( …, Aniso=FALSE )
223
```

224   VAST then specifies that the spatial and spatio-temporal Gaussian random fields at

225 each have a variance of 1.0. By default VAST estimates their values at each of n_s vertices as

226 follows:

227
$$\boldsymbol{\omega}_1(f) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

228
$$\boldsymbol{\omega}_2(f) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

229
$$\boldsymbol{\varepsilon}_1(f, t) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

230
$$\boldsymbol{\varepsilon}_2(f, t) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

231
$$\boldsymbol{\xi}_1(c, p) \sim MVN(\mathbf{0}, \mathbf{R}_1)$$

232
$$\boldsymbol{\xi}_2(c, p) \sim MVN(\mathbf{0}, \mathbf{R}_2)$$

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

234 Specifying a variance of 1.0 ensures that the covariance among categories is defined by the

235 loadings matrix for that term.

236

237 **Interpolating spatial variation from knots to the location of samples**

238   Starting with VAST release 3.0.0, users can choose between two options for smoothing

239   spatial variation. Both options involve specifying a matrix $\mathbf{A}_i$ with n_i rows and n_s columns,

240   row i. Values are then predicted as e.g.:

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

242   where $\boldsymbol{\omega}_1^*(f)$ is the vector of length n_i, containing the predicted value $\omega_1^*(s_i, f)$ for spatial

243   variation in the first linear predictor at every location s_i, and other spatial variables are

244   predicted similarly using matrix $\mathbf{A}_i$.

245   1. *Piecewise constant*: Following the conventional for releases of VAST prior to 3.0.0,

246   users can specify `fine_scale=FALSE`. Given this specification, spatial variables at location

247   s are fixed equal to their value at the nearest "knot." This involves specifying matrix $\mathbf{A}_i$

248   such that row i has value zero except for one cell containing a value of one for the knot

249   closest to sample i.

250   2. *Bilinear interpolation*: Following standard practices using the software R-INLA

251   (Lindgren 2012; Lindgren and Rue 2013), users can specify `fine_scale=TRUE`. Given this

252   specification, spatial variables at location s are interpolated using the triangulated mesh

253   that is also used to approximate spatial variation. Specifically, matrix $\mathbf{A}_i$ has row i with

254   value zero except for three cells, representing the vertices of the triangle containing

255   location s_i.

256

257   **Structure on parameters among years**:

258   There are different user-controlled options for specifying structure for intercepts or spatio-

259   temporal variation across time, using input:

260   ```
RhoConfig = c("Beta1"=0, "Beta2"=0, "Epsilon1"=0, "Epsilon2"=0)
```
261

262    *Temporal structure on intercepts*

263    By default (when RhoConfig[1]=0 and RhoConfig[2]=0) the model specifies that each

264    intercept $\beta_1(c,t)$ and $\beta_2(c,t)$ is a fixed effect. However, other settings specify the following

265    factor-model structure:

266
$$\beta_1(t,f) \sim \begin{cases} Normal(0,1) & \text{if } t = t_{min} \\ Normal(\rho_{\beta 1}\beta_1(t-1,f),1) & \text{if } t > t_{min} \end{cases}$$

267
$$\beta_2(t,f) \sim \begin{cases} Normal(0,1) & \text{if } t = t_{min} \\ Normal(\rho_{\beta 2}\beta_2(t-1,f),1) & \text{if } t > t_{min} \end{cases}$$

268    Where $t_{min}$ is the index for the first modelled year and $\rho_{\beta 1}$ and $\rho_{\beta 2}$ are the estimated degree

269    of first-order autocorrelation in temporal variation (note that random effects have a variance

270    of one given that they are subsequently multiplied by loadings matrices that represent the

271    temporal covariance among factors). RhoConfig[1] controls the specification of $\rho_{\beta 1}$:

272    1. *Independent among years* – RhoConfig[1]=1 specifies $\rho_{\beta 1} = 0$

273    2. *Random walk* – RhoConfig[1]=2 specifies $\rho_{\beta 1} = 1$

274    3. *Constant intercept* – RhoConfig[1]=3 specifies $\rho_{\beta 1} = 0$ and $\sigma_{\beta 1}^2 = 0$ (i.e., $\beta_1(t)$ is

275       constant for all $t$)

276    4. *Autoregressive* – RhoConfig[1]=4 estimates $\rho_{\beta 1}$ as a fixed effect

277    and settings are defined identically for RhoConfig[2] specifying $\rho_{\beta 2}$.

278

279    *Temporal structure on spatio-temporal variation*

280    By default (when RhoConfig[3]=0 and RhoConfig[4]=0), the model specifies that each vector

281    of spatio-temporal random effects, $\boldsymbol{\varepsilon}_1(f,t)$ and $\boldsymbol{\varepsilon}_2(f,t)$ composed of $\varepsilon_1(s,f,t)$ and

282    $\varepsilon_2(s,f,t)$ across locations $s$, is independent among years. However, other settings specify

283    the following structure

284
$$\boldsymbol{\varepsilon}_1(f,t) \sim \begin{cases} MVN(\mathbf{0},\mathbf{R}_1) & \text{if } t = t_{min} \\ MVN(\rho_{\varepsilon 1}\boldsymbol{\varepsilon}_1(f,t-1),\mathbf{R}_1) & \text{if } t > t_{min} \end{cases}$$

285
$$\boldsymbol{\varepsilon}_2(f,t)\sim\begin{cases}MVN(\mathbf{0},\mathbf{R}_2) & \text{if } t = t_{min}\\ MVN(\rho_{\varepsilon 2}\boldsymbol{\varepsilon}_2(f,t-1),\mathbf{R}_2) & \text{if } t > t_{min}\end{cases}$$

286 where $\rho_{\varepsilon 1}$ and $\rho_{\varepsilon 2}$ are the estimated degree of first-order autocorrelation in temporal

287 variation, RhoConfig[3] controls the specification of $\rho_{\varepsilon 1}$:

288 1. *Random walk* – RhoConfig[3]=2 specifies $\rho_{\varepsilon 1} = 1$

289 2. *Autoregressive* – RhoConfig[3]=4 estimates $\rho_{\varepsilon 1}$ as a fixed effect

290 and settings are defined identically for RhoConfig[4] specifying $\rho_{\varepsilon 2}$.

291

## 292 **Parameter estimation**

293 Parameters are estimated using maximum likelihood, where the maximum likelihood of fixed

294 effects is obtained by integrating a joint likelihood function with respect to random effects

295 (Searle et al. 1992, Gelman and Hill 2007, Thorson and Minto 2015). This integral is

296 approximated using the Laplace approximation (Skaug and Fournier 2006), as implemented

297 in Template Model Builder (Kristensen et al. 2016). The likelihood is then optimized in the

298 R statistical environment (R Core Team 2017), and standard errors are obtained using a

299 generalization of the delta method (Kass and Steffey 1989). Derived quantities calculated via

300 a nonlinear transformation of random effects can be bias-corrected using the epsilon-method

301 (Tierney et al. 1989, Thorson and Kristensen 2016). Depending upon user-specified options,

302 different parameters will be either fixed (estimated via maximizing the log-likelihood) or

303 random (integrated across when calculating the log-likelihood). Please use R function

304 `ThorsonUtilities::list_parameters( Obj )` to see a list of estimated parameters (where `Obj` is

305 the compiled VAST object), including which are fixed or random.

306

## 307 **Combining multiple data types**

308 VAST can be used to combine encounter/non-encounter, count, and biomass-sampling data.

309 This involves specifying a Poisson-link delta model which predicts each data type from

310 numbers density $\exp(p_1(i))$ and biomass-per-individual $\exp(p_2(i))$, see Grüss and Thorson

311 (In press) for details. This approach is specified by associating each observation with a given

312 error distribution using input `e_i` where e.g. `e_i[1]` is the error-distribution for the 1st

313 observation. The user then specifies multiple observation errors via input `ObsModel_ez`:

```
314  # Control observation error
315  ObsModel_ez = cbind( "PosDist"=c(13,14,2), "Link"=c(1,1,1) )
316
```

317 In this specification, `e_i[1]==1` indicates that the first observation follows a Bernoulli

318 distribution for encounter/non-encounter data, `e_i[1]==2` indicates that this observation

319 follows a lognormal-Poisson distribution for count data, and `e_i[1]==3` indicates that it

320 follows a gamma distribution for biomass-sampling data. This specification can be modified

321 to include different combinations of these same data types.

322

Relationship to other named models

324 VAST can be configured to be identical to (or closely mimic) many models that have

325 previously been published in ecology and fisheries:

326 1. *Spatial Gompertz model*: If intercepts are constant across years, spatio-temporal variation

327 follows an autoregressive process, and only one category is modelled, then VAST is

328 identical to a spatio-temporal Gompertz model (Thorson et al. 2014).

329 2. *Spatial factor analysis*: If only one year is analysed and multiple categories are modelled,

330 VAST is similar to spatial factor analysis (Thorson et al. 2015a), although it permits the

331 use of a delta-model (i.e., separate analysis of encounters and positive catch rates).

332 3. *Spatial dynamic factor analysis*: If intercepts are constant among years, spatio-temporal

333 variation follows an autoregressive process, and multiple categories are modelled, then

334   VAST is similar to spatial dynamic factor analysis (Thorson et al. 2016a), although

335   VAST allows separate estimates of spatial vs. spatio-temporal covariation and also the

336   use of a delta-model.

337   4. *Empirical orthogonal function analysis*: VAST can be configured to replicates empirical

338   orthogonal function analysis, e.g., as commonly used by physical oceanographers to

339   summarize physical conditions to produce an annual index and spatial map associated

340   with a positive phase of the resulting index. However, I will wait to document this until

341   the associated paper is published.

342

Predicting variables across the spatial domain and calculating derived quantities

345   After a nonlinear minimizer has identified the value of fixed effects that maximizes the

346   Laplace approximation to the marginal likelihood, Template Model Builder predicts the value

347   of random effects that maximizes the joint likelihood conditional on these fixed effects. It

348   then uses the predicted values of random effects to predict each spatial variable at each of n_g

349   "extrapolation-grid cells" that are used to summarize the spatial domain of sampling (Shelton

350   et al. 2014; Thorson et al. 2015b). Predicting random effects at extrapolation-grid cell g at

351   location s_g is accomplished using matrix $\mathbf{A}_g$ with n_g rows and n_s columns. Values are

352   predicted as e.g.:

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

354   where $\boldsymbol{\omega}_1^*(f)$ is the vector of length n_i, containing the predicted value $\omega_1^*(s_g, f)$ for spatial

355   variation in the first linear predictor at every location s_g, and other spatial variables are

356   predicted similarly using matrix $\mathbf{A}_g$. Predicted values for random effects are then plugged

357   into the linear predictor, e.g.:

$$358 \quad p_1(g,c,t) = \underbrace{\beta_1^*(c) + \sum_{f=1}^{n_{\beta 1}} L_{\beta 1}(c,f)\beta_1(t,f)}_{Temporal\ variation} + \underbrace{\sum_{f=1}^{n_{\omega 1}} L_{\omega 1}(x,f)\omega_1^*(g,f)}_{Spatial\ variation}$$

$$359 \quad + \underbrace{\sum_{f=1}^{n_{\varepsilon 1}} L_{\varepsilon 1}(c,f)\varepsilon_1^*(g,f,t)}_{Spatio-temporal\ variation} + \underbrace{\sum_{p=1}^{n_p} \Big(\gamma_1(c,t,p) + \sigma_{\xi 1}(c,p)\xi_1^*(g,c,p) \Big) X(g,t,p)}_{Habitat\ covariates}$$

360   where $p_2(g,c,t)$ is predicted similar, and these linear predictors are used in turn to predict

361     $r_1(g,c,t)$ and $r_2(g,c,t)$, where their product is predicted biomass-density $d(g,c,t)$ at every

362   extrapolation-grid cell g, category c, and time t.

363   By default, density is used to predict total abundance for the entire domain (or a

364   subset of the domain) for a given species:

$$365 \quad I(c,t,l) = \sum_{x=1}^{n_x} \Big(a(g,l) \times d(g,c,t) \Big)$$

366   where $a(g,l)$ is the area associated with extrapolation-grid cell g for index l; and. The user

367   can also specify additional post-hoc calculations via the `Options` vector:

```
368   Options = c("SD_site_density"=0, "SD_site_logdensity"=0, "Calculate_Range"=0,
369   "Calculate_evenness"=0, "Calculate_effective_area"=0, "Calculate_Cov_SE"=0,
370   'Calculate_Synchrony'=0, 'Calculate_Coherence'=0)
371
```

372   1. *Distribution shift* — `RhoConfig[3]=1` turns on calculation of the centroid of the

373   population's distribution:

$$374 \quad Z(c,t,m) = \sum_{x=1}^{n_x} \frac{\big(z(g,m) \times a(g,1) \times d(g,c,t) \big)}{I(c,t,1)}$$

375   where $z(g,m)$ is a matrix representing location for each extrapolation-grid cell (by

376   default $z(g,m)$ is the location in Eastings and Northings of each knot), representing

377   movement North-South and East-West). This model-based approach to estimating

378   distribution shift can account for differences in the spatial distribution of sampling, unlike

379   conventional sample-based estimators (Thorson et al. 2016b).

380   2. *Range expansion* – `RhoConfig[5]=1` turns on calculation of effective area occupied. This

381   involves calculating biomass-weighted average density:

382
$$D(c,t,l) = \sum_{x=1}^{n_x} \frac{a(x,l) \times d(x,c,t)}{I(c,t,l)} d(x,c,t)$$

383   Effective area occupied is then calculated as the area required to contain the population at

384   this average density:

385
$$A(c,t,l) = \frac{I(c,t,l)}{D(c,t,l)}$$

386   This effective-area occupied estimator can then be used to monitor range expansion or

387   contraction or density-dependent range expansion (Thorson et al. 2016c).

388

List of features

390   I next provide a list of "features" organized as decisions that can be made by the analyst.

391   Although this is somewhat redundant with the explanations provided above, this list might be

392   useful for some readers to provide a high-level overview of different options that are

393   available. This "feature set" is also provided as a high-level summary of what VAST is

394   designed to be capable of doing; any software replacing VAST would ideally include this

395   same set of features.

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

397   1. Specifying one of several possible distributions for data, including for:

398   a. Count data using a Poisson, negative-binomial, Conway-Maxwell-Poisson, or

399   Poisson-lognormal distribution, including zero-inflated versions of each;

400   b. Continuous-valued data that include zeros using a delta-model with a lognormal

401   or gamma distribution for positive values.

402   2. Specifying one of several possible link functions for predicting data given linear

403   predictors including:

404   a.   A conventional delta-model;

405   b.   A Poisson-link delta model.

406   3.   Including dynamic habitat covariates or not;

407   4.   Including catchability covariates or not;

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

409   5.   Specify an "extrapolation grid" using input

410   `FishStatsUtils::make_extrapolation_info(..., Region)`, which is used to calculate the

411   area associated with each knot a_x. This can be a user-specified extrapolation grid if

412   `FishStatsUtils::make_extrapolation_info(..., Region="User", input_grid=Input)`,

413   where `Input` is a data frame supplied by the user.

414   6.   Specifying a method for defining "knots";

415   7.   Specifying the number of "knots";

416   8.   Spatial variation being estimated ("turned on") or ignored ("turned off") for either linear

417   predictor #1 or #2;

418   9.   Spatio-temporal variation being estimated ("turned on") or ignored ("turned off") for

419   either linear predictor #1 or #2;

420   10. Specifying that habitat covariates can affect linear predictors different ways including as:

421   a.   a linear effect;

422   b.   a spatially-varying effect; or

423   c.   both linear and spatially-varying effects simultaneously.

424   *Multivariate analysis*

425   11. Including a "multivariate" structure with multiple responses that covary due to a specified

426   number of "factors" for spatial and spatio-temporal terms;

427   12. Rotate results prior to interpretation, using either:

428   a.   principle components rotation; or

429   b. varimax rotation.

430 *Decisions regarding temporal structure*

431 13. Annual intercepts being structured over time, including:

432   a. estimated as fixed effects in every year;

433   b. fixed as fixed effect with the same value for all years;

434   c. estimated as a random effect with independent deviations in each year;

435   d. estimated as a random effect with first-order autoregressive structure; or

436   e. estimated as a random effect with a random-walk structure.

437 14. Spatio-temporal variation being structured over time, including:

438   a. estimated as independent deviations in each year;

439   b. estimated as following a first-order autoregressive structure over time;

440   c. estimated as following a random-walk structure over time; or

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

442   order autoregressive interactions.

443 *Derived quantities*

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

445 16. Calculating one of many possible "univariate derived quantities", including:

446   a. abundance indices;

447   b. range shift;

448   c. effective area occupied

449   d. covariance among categories within a multivariate model; or

450   e. synchrony among categories.

451 17. Calculating "multivariate derived quantities" that are derived from estimates for multiple

452 categories in a multivariate model, e.g., where one category represents a standardized diet

453 sample (e.g., prey biomass per predator biomass in a stomach-content sample) and

454   another category represents a biomass-density sample (e.g., predator biomass in a bottom-

455   trawl sample) such that their product represents predator-expanded consumption.

456   *Unusual circumstances and special cases*

457   18. Specifying separate distributions for different data sets (e.g., when multiple surveys

458   providing different data types are available);

459   19. Specifying that some data are predicted based on summing linear predictors across

460   multiple variables (e.g., when modelling density for different size classes, and specifying

461   that some data are aggregated measurements of multiple sizes-classes);

462   20. Specifying multiple "seasons" (e.g., when modelling data with both annual and monthly

463   spatio-temporal variation).

464

465   **Common problems**

466   There are two basic problems that are often encountered during spatio-temporal delta-

467   GLMMs:

468   1. *Encounter rates*: Some combination of categories and year has 0% or 100% encounter

469   rate. If there is 100% encounter rate for category c in year t, then $\beta_1(c,t) \to \infty$ and/or

470    $\varepsilon_1(s,c,t) \to \infty$ for that year. If there is 0% encounter rate in year t, then $\beta_1(c,t) \to -\infty$

471   and/or $\varepsilon_1(s,c,t) \to -\infty$ and there is no information to estimate $\beta_2(c,t)$ or $\varepsilon_2(s,c,t)$ for

472   that category c and year t;

473   2. *Bounds*: Some parameter(s) hits a bound;

474   These problems can be solved by:

475   1. *Encounter rates*: constraining terms that vary among years (e.g., intercept β and spatio-

476   temporal variation $\varepsilon(s,t,p)$). This can be done in many different ways that are each

477   idiosyncratic and require some special justification. The easiest options are:

478   a. If there is a small number of years with 100% encounter rate, try `ObsModel[2]=3`.

479   This indicates that VAST should check for species-years combinations with 100%

480   encounter rates and fix corresponding intercepts for encounter probability to an

481   extremely high value.

482   b. If there is a small number of years with either 100% of 0% encounter rate, add

483   temporal structure to intercepts and spatio-temporal terms using `RhoConfig`

484   options.

485   c. Four other options are listed on the wiki.

486 2. *Bounds*: Please try running the model without estimating standard errors or a final

487   newton step:

```
488    # Specify derived quantities to calculate
489    TMBhelper::fit_tmb( ..., getsd=FALSE, newtonsteps=0 )
490    Then check what parameters are being estimated near an upper or lower boundary.
```

491

How to implement basic model changes

493 There are a few basic model types that users often want to fit using VAST. I briefly describe

494 how these can be done here.

495 1. *Fitting encounter/non-encounter data*: If the user wishes to use only the first component

496   of a delta-model, i.e., to fit a binomial model to simply predict encounter probabilities,

497   then, the `ObsModel` vector should be set to `c("PosDist"=[Make Choice], "Link"=0)`,

498   where [Make Choice] can be any option for continuous data (i.e., 0, 1, or 2). The user

499   should then turn off the last two elements of the `FieldConfig` vector (i.e.,

500   `FieldConfig[3]=0` and `FieldConfig[4]=0`) such that there is no spatial or spatio-temporal

501   variability in positive catch rates, and also turn off annual variation in the intercept for

502   positive catch rates (i.e., `RhoConfig[2]=3`). Finally, the user should "jitter" their presence

503   observations by a very small amount (i.e., add a random normal deviation with a very

504   small standard deviation, `rnorm(n=1,mean=0,sd=0.001)`, to each observation for which

505   `b_i=1`). This will result in VAST estimating a logistic regression model for

506   encounter/non-encounter data, except with one additional parameter estimated (σ_M), plus

507   one additional parameter per category ($\beta_2(c)$), where these additional parameters have no

508   impact on other parameters, are not meant to be interpreted statistically or biologically,

509   and are an artefact of using VAST (which is designed to fit a delta-model) to

510   encounter/non-encounter data. This feature has been used to estimate species

511   distributions for use in ecosystem models (Grüss et al. 2017, 2018).

512

522

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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.

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

Grüss, A., and Thorson, J. In press. Developing spatio-temporal models using multiple data types for evaluating population trends and habitat usage. ICES J. Mar. Sci.

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.

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

Lindgren, F., and Rue, H. 2013. Bayesian spatial and spatiotemporal modelling with r-inla. J. Stat. Softw. Available from http://inla.googlecode.com/hg-history/fd1c0951196f7e7b6d57e2ea84c541981fcb3bf4/r-inla.org/papers/jss/lindgren.pdf [accessed 23 February 2014].

Lindgren, F., 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.

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

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

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

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

586   Thorson, J.T., Pinsky, M.L., and Ward, E.J. 2016b. Model-based inference for estimating
587   shifts in species distribution, area occupied and centre of gravity. Methods Ecol. Evol.
588   **7**(8): 990–1002. doi:10.1111/2041-210X.12567.

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

592   Thorson, J.T., Scheuerell, M.D., Shelton, A.O., See, K.E., Skaug, H.J., and Kristensen, K.
593   2015a. Spatial factor analysis: a new tool for estimating joint species distributions and
594   correlations in species range. Methods Ecol. Evol. **6**(6): 627–637. doi:10.1111/2041-
595   210X.12359.

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

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

603   Tierney, L., Kass, R.E., and Kadane, J.B. 1989. Fully exponential Laplace approximations to
604   expectations and variances of nonpositive functions. J. Am. Stat. Assoc. **84**(407):
605   710–716.

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