

Avoiding extrapolation bias when using statistical models to make ecological prediction

PAUL B. CONN^{1,2} AND DEVIN S. JOHNSON¹, PETER L. BOVENG¹

¹*National Marine Mammal Laboratory, NOAA, National Marine Fisheries Service, Alaska*

Fisheries Science Center, 7600 Sand Point Way NE, Seattle, WA 98115 USA

¹ *Abstract.* We'll do this later

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⁴ *Species distribution model*

INTRODUCTION

⁵ In ecology and conservation, a common goal is to make predictions about an
⁶ unsampled random variable given a limited sample from the target population. For
⁷ instance, given a model (\mathcal{M}), estimated parameters ($\hat{\boldsymbol{\theta}}$), and a covariate vector \mathbf{x}_i , we often
⁸ desire to predict a new observation y_{new} at i . For instance, we might use a generalized
⁹ linear model (McCullagh and Nelder, 1989) or one of its extensions to predict species
¹⁰ density or occurrence in a new location, or to predict the future trend of a population.

¹¹ Early in their training, ecologists and statisticians are warned against extrapolating
¹² statistical relationships past the range of observed data. This caution is easily interpreted
¹³ in the context of single-variable linear regression analysis; one should be cautious in using
¹⁴ the fitted relationship to make predictions at some new point y_{new} whenever $x_{new} < \min(\mathbf{x})$
¹⁵ or $x_{new} > \max(\mathbf{x})$. But what about more complicated situations where there are multiple
¹⁶ explanatory variables, or when one uses a spatial regression model to account for the
¹⁷ residual spatial autocorrelation that is inevitably present in patchy ecological data

²Email: paul.conn@noaa.gov

18 (Lichstein et al., 2002)? How reliable are spatially- or temporally-explicit predictions in
19 sophisticated models for animal abundance and occurrence?

20 Statisticians have long struggled with the conditions under which fitted regression
21 models are capable of making robust predictions at new combinations of explanatory
22 variables. The issue is sometimes considered more of a philosophical problem than a
23 statistical one, and has even been likened to soothsaying (Ehrenberg and Bound, 1993). To
24 our mind, the reliability of predictions from statistical models is likely a function of several
25 factors, including (i) the intensity of sampling, (ii) spatial or temporal proximity of the
26 prediction location to locations where there are data, (iii) variability of the ecological
27 process, and (iv) the similarity of explanatory covariates in prediction locations when
28 compared to the ensemble of covariates for observed data locations.

29 Our aim in this paper is to investigate extrapolation bias in the generalized linear
30 model and its extensions, including generalized additive models (GAMs; Hastie and
31 Tibshirani, 1999; Wood, 2006) and spatial, temporal, or spatio-temporal regression models
32 (STRMs). In particular, we exploit some of the same ideas used in multiple linear
33 regression regarding leverage and outliers (Cook, 1979) to operationally define
34 “extrapolation” as making predictions that occur outside of a generalized independent
35 variable hull (gIVH) of observed data points. Application of the gIVH and related criterion
36 (e.g. prediction variance) can provide intuition regarding the reliability of predictions in
37 unobserved locations, and can aid in model construction. Also, since the gIVH can be
38 constructed solely with knowledge of sampled locations and explanatory covariates (i.e., it
39 does not necessarily require any observed response variables), it can also be used to help
40 guide survey design. We illustrate use of the gIVH on simulated count data, on a species
41 distribution model (SDM) for ribbon seals (*Histriophoca fasciata*) in the eastern Bering

42 Sea, and on a population trend model for Steller Sea Lions (*Phoca fasciata*).

43 THE GENERALIZED INDEPENDENT VARIABLE HULL (GIVH)

44 Extrapolation is often distinguished from interpolation. In a prediction context, we might
45 define (admittedly quite imprecisely) that extrapolation consists of making predictions that
46 are “outside the range of observed data” while interpolation consists of making predictions
47 “inside the range of observed data.” But what exactly do we mean by “outside the range of
48 observed data”? Predictions outside the range of observed covariates? Predictions for
49 locations that are so far from places where data are gathered that we are skeptical that the
50 estimated statistical relationship still holds? To help guide our choice of an operational
51 definition, we turn to early work on outlier detection in simple linear regression analysis.

52 In the context of outlier detection, Cook (1979) defined an independent variable hull
53 (IVH) as the smallest convex set containing all design points of a full-rank linear regression
54 model. Linear regression models are often written in matrix form, i.e.

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

55
56 where \mathbf{Y} give observed data, \mathbf{X} is a so-called design matrix that includes explanatory
57 variables (see e.g. Draper and Smith, 1966), and $\boldsymbol{\epsilon}$ represent normally distributed residuals
58 (here and throughout the paper, bold symbols will be used to denote vectors and
59 matrices). Under this formulation, the IVH is defined relative to the hat matrix,
60 $\mathbf{V}_{LR} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ (where the subscript “LR” denotes linear regression). Letting v
61 denote the maximum diagonal element of \mathbf{V}_{LR} , one can examine whether a new design

62 point, \mathbf{x}_0 is within the IVH. In particular, \mathbf{x}_0 is within the IVH whenever

63
$$\mathbf{x}'_0(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0 \leq v. \quad (1)$$

64 Cook (1979) used this concept to identify influential observations and possible outliers,

65 arguing that design points near the edge of the IVH are deserving of special attention.

66 Similarly, points outside the IVH should be interpreted with caution.

67 We simulated two sets of design data to help illustrate application of the IVH (Fig. 2).

68 In simple linear regression with one predictor variable, predictions on a hypothetical
69 response variable obtained at covariate values below the lowest observed value or above the
70 highest observed value are primarily outside of the IVH. We suspect this result conforms to
71 most ecologists intuition about what constitutes “extrapolating past the observed data.”

72 However, fitting a quadratic model exhibits more nuance; if there is a large gap between
73 design points, it is entirely possible that intermediate covariate values will also be outside
74 of the IVH and thus more likely to result in problematic predictions. Fitting a model with
75 two covariates and both linear and quadratic effects, the shape of the IVH is somewhat

76 more irregular, and even includes a hole in the middle of the surface when interactions are
77 modeled (Fig. 2). These simple examples highlight the sometimes counterintuitive nature
78 of the predictive inference problem, a problem that can only become worse as models with
79 more dimensions are contemplated (including those with temporal or spatial structure).

80 Fortunately, the ideas behind the IVH provide a potential way forward.

81 Cook’s (1979) formulation for the IVH is particular to linear regression analysis, which
82 assumes iid Gaussian error. Thus, it is not directly applicable to generalized models, such
83 as those including alternative error distributions (e.g., Poisson, binomial) or spatial random

84 effects. Further, the hat matrix is not necessarily well defined for models with more general
 85 spatial structure. However, since the hat matrix is proportional to prediction variance,
 86 Cook (1979) notes that design points with maximum prediction variance will be located on
 87 the boundary of the IVH. We therefore define a generalized independent variable hull
 88 (gIVH) as the set of all points \mathbf{x} (note that \mathbf{x} can include both observed and unobserved
 89 design points) such that

$$90 \quad \text{var}(\boldsymbol{\lambda}_x) \leq \max[\text{var}(\boldsymbol{\lambda}_X)], \quad (2)$$

91 where $\boldsymbol{\lambda}_x$ correspond to mean predictions at \mathbf{x} , and \mathbf{X} and $\boldsymbol{\lambda}_X$ denote observed design
 92 points and predictions at X , respectively.

93 Generalizations of the linear model are often written in the form

$$94 \quad Y_i \sim f_Y(g(\mu_i)), \quad (3)$$

95 where f_Y denotes a probability density or mass function (e.g. Bernoulli, Poisson), g gives
 96 an inverse link function, and μ_i is a linear predictor. For many such generalizations, it is
 97 possible to specify the μ_i as

$$98 \quad \boldsymbol{\mu} = \mathbf{X}_{aug}\boldsymbol{\beta}_{aug} + \boldsymbol{\epsilon}, \quad (4)$$

99 where the $\boldsymbol{\epsilon}$ represent Gaussian error, \mathbf{X}_{aug} denotes an augmented design matrix, and $\boldsymbol{\beta}_{aug}$
 100 denote an augmented vector of parameters. For instance, in a spatial model, $\boldsymbol{\beta}_{aug}$ might
 101 include both fixed effect parameters and spatial random effects in a reduced dimension
 102 subspace (see Appendix A for examples of how numerous types of models can be written in
 103 this form).

104 When models are specified as in Eq. 4, we can write prediction variance generically as

105 $\text{var}(\boldsymbol{\mu}_x) = \mathbf{x}\text{var}(\hat{\boldsymbol{\beta}}_{\text{aug}})\mathbf{x}',$ (5)

106 where it is understood that the exact form of \mathbf{x} and $\text{var}(\hat{\boldsymbol{\beta}}_{\text{aug}})$ depends on the model chosen
107 (i.e., GLM, GAM, or STRM; Appendix A). This expression for prediction variance is on
108 the linear predictor scale; if a non-identity link function is used, we can use the delta
109 method (Dorfman, 1938; Ver Hoef, 2012) to approximate prediction variance on the real
110 scale (i.e. the scale in which data are measured) as

111 $\text{var}(\boldsymbol{\lambda}_x) = \text{var}(g(\boldsymbol{\mu}_x)) = \boldsymbol{\Delta}\text{var}(\boldsymbol{\mu}_x)\boldsymbol{\Delta}',$ (6)

112 where $\boldsymbol{\Delta}$ is a matrix of partial derivatives $\partial g(\mu_r)/\partial \mu_c$ (r and c denoting rows and columns
113 of $\boldsymbol{\Delta}$, respectively). Under common univariate link functions (e.g. log, logit, probit), $\boldsymbol{\Delta}$ has
114 a diagonal form, while for multivariate links (e.g. multinomial logit) $\boldsymbol{\Delta}$ will be dense.

115 Unlike Cook's original formulation, the gIVH for nonidentity link functions often
116 involve unknown parameters. For example, using Eq. 6 with a log link function means that
117 diagonal entries of $\boldsymbol{\Delta}$, $\exp \boldsymbol{\mu}$, include $\boldsymbol{\beta}$. Further, the exact form of $\text{var}(\hat{\boldsymbol{\beta}}_{\text{aug}})$ differs
118 depending on the underlying model structure and estimation procedure. In the following
119 treatment, we shall focus on Bayesian analysis; although it is not necessarily needed to fit
120 GLMs and GAMs, it puts different models into a common analysis framework and allows
121 us to specify informative probability distributions for unknown parameters. Specifically,
122 our solution is to impose a probability distribution for unknown parameters, $[\boldsymbol{\theta}]$, and to

123 compute prediction variance as

$$124 \quad var(\boldsymbol{\lambda}_x) = \int_{\boldsymbol{\theta}} var(\boldsymbol{\lambda}_x | \boldsymbol{\theta}) [\boldsymbol{\theta}] d\boldsymbol{\theta}. \quad (7)$$

125 If data have already been collected or a pilot study has been conducted, a posterior
126 distribution can be substituted for $[\boldsymbol{\theta}]$; otherwise, informative priors that encompass the
127 likely range of model parameters can be considered. Judicious choices of priors can at
128 times limit the influence of priors on calculation of the gIVH. For example, if we specify a
129 Zellner's g-prior (Zellner, 1986) on the vector of regression coefficients,
130 $[\boldsymbol{\beta}] = MVN(\mathbf{0}, (\tau_\beta X'X)^{-1})$, then priors are automatically scaled to the level of the gathered
131 covariates, and the only remaining task is to investigate sensitivity to τ_β . Some care must
132 be taken with prior distributions if Eq. 7 is used for calculation of prediction variance. For
133 instance, standard "non-informative" or "flat" priors may place substantial mass on
134 implausible values. When using the gIVH or prediction variance to help guide sampling
135 design (see ?, for an example using prediction variance), we suggest using informative prior
136 distributions.

137 We propose to use the gIVH in much the same manner as Cook (1979). In particular,
138 we use the gIVH to differentiate whether spatial predictions are interpolations (predictive
139 design points lying inside the gIVH) or extrapolations (predictive design points lying
140 outside the gIVH). The gIVH, together with prior or posterior prediction variance, seem
141 ideally situated to diagnosing potential extrapolation issues as it does not necessarily need
142 to rely on gathered response data. Thus, it may prove useful when formulating survey
143 designs since one can examine whether or not prediction points lie within the gIVH
144 without ever collecting response data there. Further, one can compare prediction variance

¹⁴⁵ in places one has data to places where predictions are desired to gauge the relative amount
¹⁴⁶ of information that predictions are being based on.

¹⁴⁷ **EXAMPLES**

¹⁴⁸ We used simulation to investigate the usefulness of the gIVH when (i) designing animal
¹⁴⁹ count surveys, and (ii) limiting the scope of inference when fitting models to count data
¹⁵⁰ that have already been collected. We also applied the gIVH to examining the robustness of
¹⁵¹ a species distribution model (SDM) of ribbon seals in the eastern Bering Sea, and to time
¹⁵² series projections of Steller sea lion population trends.

¹⁵³ *Simulation study I: study design*

¹⁵⁴ To investigate the utility of the gIVH in comparing alternative animal survey designs, we
¹⁵⁵ first generated animal abundance over a 30×30 grid assuming that animal density was
¹⁵⁶ homogeneous in each grid cell. Animal abundance was generated as a function of four
¹⁵⁷ hypothetical spatially autocorrelated habitat variables (Appendix B). We systematically
¹⁵⁸ examined designs where abundance is modeled as a function of 1-4 of these covariates
¹⁵⁹ (representing a low to a high degree of understanding about animal habitat utilization and
¹⁶⁰ preference). Three possible sampling configurations were initially compared: (1) a 6×6
¹⁶¹ regular grid ($n = 36$ sampling locations); (2) a convenience sample of $n = 60$ observations
¹⁶² where the probability of sampling was greater for cells closer to a “base of operations”
¹⁶³ (reflecting the principle that greater sample sizes are usually possible if logistics are easier);
¹⁶⁴ and (3) a $n = 36$ sample obtained by stratifying the predictive covariate(s) (Appendix B).

165 *Simulation study II: Limiting scope of inference*

166 We conducted a simulation study to investigate whether the gIVH (and accompanying
167 prediction variance) was useful in diagnosing prediction biases when analyzing animal
168 count data. For each of 100 simulations, we generated animal abundance over a 30×30
169 grid assuming that animal density was homogeneous in each grid cell. Animal abundance
170 was generated as a function of four hypothetical habitat covariates (Appendix B). For each
171 simulated landscape, we randomly selected 60 grid cells for sampling, assuming that
172 sampling quadrats encompassed 10% of the area of each selected grid cell. For ease of
173 presentation and analysis, we assumed detection probability was 100% in each quadrat.
174 Once animal counts were simulated, three different estimation models were fitted to the
175 data: a GLM, a GAM, and an STRM (Appendix B). The GLM and STRM expressed
176 log-density as a function of linear and quadratic covariate effects, while the GAM used a
177 kernel smoother with 4 knots for each covariate (Appendix B). Each model was provided
178 with three of the four covariates used to generate the data.

179 For each simulated data set and model structure, we calculated (1) gIVH_{int} , the gIVH
180 resulting from integrating over prior parameter variance (i.e. using Eq. ?? with informative
181 priors), and (2) gIVH_{post} , the gIVH arising from posterior predictive variance (i.e. posterior
182 variance when data are actually analyzed). We then calculated posterior predictions of
183 animal abundance within and outside of each gIVH in order to gauge bias as a function of
184 whether or not inference is constrained to the gIVH. Specifically, the performance of the
185 gIVH_{int} criterion in diagnosing extrapolation bias is a test of whether it is useful in
186 designing animal count surveys, while the performance of gIVH_{post} may help decide its
187 utility in limiting the scope of landscape-based inference once data have been collected and

188 analyzed.

189 *Ribbon seal SDM*

190 As part of an international effort, researchers with the U.S. National Marine Fisheries
191 Service conducted aerial surveys over the eastern Bering Sea in 2012 and 2013. Agency
192 scientists used infrared video to detect seals that were on ice, and simultaneous automated
193 digital photographs provided information on species identity. Here, we use spatially
194 referenced count data from photographed ribbon seals, *Phoca fasciata* (Fig. 1) on a subset
195 of 10 flights flown over the Bering Sea in April 2012. These flights were limited to a one
196 week period so that both sea ice conditions and seal distributions could be assumed to be
197 static.

198 Our objective with this dataset will be to model seal counts on transects through 25km
199 by 25km grid cells as a function of habitat covariates and possible spatial autocorrelation.
200 Estimates of apparent abundance can then be obtained by summing predictions across grid
201 cells. Figure 3 shows the transects flown and the number of ribbon seals encountered in
202 each cell, and Figure 5 show explanatory covariates gathered to help predict ribbon seal
203 abundance. These data are described in fuller detail by Conn et al. (In Press), who extend
204 the modeling framework of STRMs to account for incomplete detection and species
205 misidentification errors (see e.g. Conn et al., In Press). Since our focus in this paper is on
206 illustrating spatial modeling concepts, we devote our efforts to the comparably easier
207 problem of estimating apparent abundance (i.e., uncorrected for vagaries of the detection
208 process).

209 Inspection of ribbon seal data (Fig. 3) immediately reveals a potential issue with
210 spatial prediction: abundance of ribbon seals appears to be maximized in the southern

211 and/or southeast quadrant of the surveyed area. Predicting abundance in areas further
 212 south and east may thus prove problematic. To illustrate, let Y_i denote the ribbon seal
 213 count (Y_i) obtained in sampled grid cell i . Suppose that counts arise according to a
 214 log-Gaussian Cox process, such that

$$Y_i \sim \text{Poisson}(\lambda_i) \text{ and} \quad (8)$$

$$\log(\lambda_i) = \log(P_i) + \mathbf{X}_i\boldsymbol{\beta} + \eta_i + \epsilon_i,$$

215 where P_i gives the proportion of area photographed in grid cell i (recall also that \mathbf{X}_i
 216 denotes a vector covariates for cell i , $\boldsymbol{\beta}$ are regression coefficients, η_i represents a spatially
 217 autocorrelated random effect, and ϵ_i is normally distributed *iid* error).

218 We could fit any number of predictive models to these data, but we start with a simple
 219 generalized linear model where we ignore the spatial random effect, η_i , and use the full
 220 suite of predictor covariates (Fig. 5) to fit Eq. 8 to our data. In particular, we fit a model
 221 with linear effects of all predictor variables, and with an additional quadratic term for ice
 222 concentration (seal density is often maximized at an intermediate value of ice
 223 concentration; see Ver Hoef et al., 2013; Conn et al., In Press). To enable comparison with
 224 more complicated types of models, we formulated a generalized Bayesian strategy for
 225 parameter estimation (see Appendix S1). For simplicity, we generated posterior predictions
 226 of ribbon seal abundance across the landscape as

$$N_i \sim \text{Poisson}(A_i\lambda_i), \quad (9)$$

227 where A_i gives the proportion of suitable habitat in cell i (ribbon seals do not inhabit land

228 masses).

229 Fitting this model to our data,

230 *Steller sea lion trends*

231 **DISCUSSION**

232 A number of authors have explored optimal knot placement in spatial models. In the
233 context of predictive process modeling (where a covariance function is specified over a
234 group of knots; see Banerjee et al., 2008), Finley et al. (2009) and Gelfand et al. (2013)
235 considered near-optimal knot placement by minimizing spatially averaged prediction
236 variance. Gelfand et al. knot selection

237 Using GAs to select knot placement using

238 Contrast with posterior loss (e.g., Jay's linex loss function estimator)

239 Contrast with cross validation

240 David Miller (the evil one)/Simon Wood stuff on edge effects

241 Contrast with other approaches- Gelfand et al. Bayesian analysis - intrinsic CAR in
242 SDM Chakraborty et al. '10 - spatial abundance modeling - ordinal Latimer et al. 2009 -
243 spatial predictive process modelling in SPDs

244 Can't be complacent... still possible to get poor/biased results, e.g. if $\tau_\epsilon \rightarrow 0$. Can't
245 resolve pathological problems.

246 Presence-absence data, other link functions (e.g. probit)

247 extensions to models w/ secondary observation process, measurement error

248 much attention has been given to collinearity in multiple linear regression - suggest
249 researchers give as much attention to predictive extrapolation bias in predictive models

250 For predictions with spatial , our experience is that predictions outside the minimum
251 convex polygon where data are obtained can sometimes be more problematic than
252 predictions within the polygon. Spatial prediction surfaces may have a tendency to bend
253 up or down in these areas, resulting in “edge effects” that can lead to positive prediction
254 bias when a log link function is employed (Ver Hoef and Jansen, 2007).

255 In the context of polynomial response surface design, Box and Draper (1959) showed
256 that when one wishes to reduce predictive variance, but also has uncertainty about the
257 functional form of the response surface to be estimated, that the “optimal” strategy in
258 terms of bias and variance combined is often to concentrate on minimizing bias alone. For
259 this purpose, a first order orthogonal design is required; in spatial applications without
260 only easting and northing covariates, this would imply some type of systematic sample. “. .
261 . conclusions obtained by minimizing variance error only and assuming the postulated
262 model to be correct are likely to be wrong in many practical design situations.” (Draper
263 and Smith 1966, pp 18-19).

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306 Inference and Decision Techniques: Essays in Honor of Bruno de Finetti.
307 North-Holland/Elsevier.
- 308 FIGURE 1. A ribbon seal, *Phoca fasciata*; the focus of spatial modeling efforts in this
309 paper.
- 310 FIGURE 2. Examples IVHs constructed from simulated data. In panels A and B, the
311 investigator plans to model a hypothetical (unmeasured) response variable using a linear
312 regression model as a function of a single covariate, x , obtained at a number of design
313 points (denoted with an “x”). Using x as a simple linear effect (A), only predictions less

than the minimum observed value of x or greater than the maximum value of x are outside the IVH (shaded area), as scaled prediction variance in these areas (solid line) are greater than the maximum scaled prediction variance for observed data (dashed line). Using both linear and quadratic effects of x , some intermediate points are also outside the IVH; predictions at these points should also be viewed with some caution. Panels C & D show a more complicated IVH when the investigator wishes to relate an unmeasured response variable to linear and quadratic effects of two covariates, x and y , either without interactions (C) or with interactions (D). Any potential predictions in the shaded area are outside of the IVH.

FIGURE 3. Aerial surveys over the Bering Sea in spring of 2012 (blue lines) overlayed on a tesselated surface composed of 25km by 25km grid cells. Gray indicates land, and colored pixels indicate ribbon seal encounters (yellow: 1-2 seals; orange: 3-4 seals; magenta: 5-9 seals; red: 10-15 seals). On average, photographs covered approximately 2.6km^2 (0.4%) of each surveyed grid cell.

FIGURE 4. Potential covariates gathered to help explain and predict ribbon seal abundance in the eastern Bering Sea. Covariates include distance from mainland (`dist_mainland`), distance from 1000m depth contour (`dist_shelf`), average remotely sensed sea ice concentration while surveys were being conducted (`ice_conc`), and distance from the southern sea ice edge (`dist_edge`). All covariates except ice concentration were standardized to have a mean of 1.0 prior to plotting and analysis.

FIGURE 5 Posterior median estimates of ribbon seal apparent abundance across the eastern Bering sea for (A) a generalized linear model (GLM), (B) a generalized additive model (GAM), (C) a GLM with known zero data, and (D) a GAM with known zero data. Highlighted cells indicate those where predictive covariate values are outside of the

³³⁸ generalized independent variable hull.

FIGURES



FIG 1

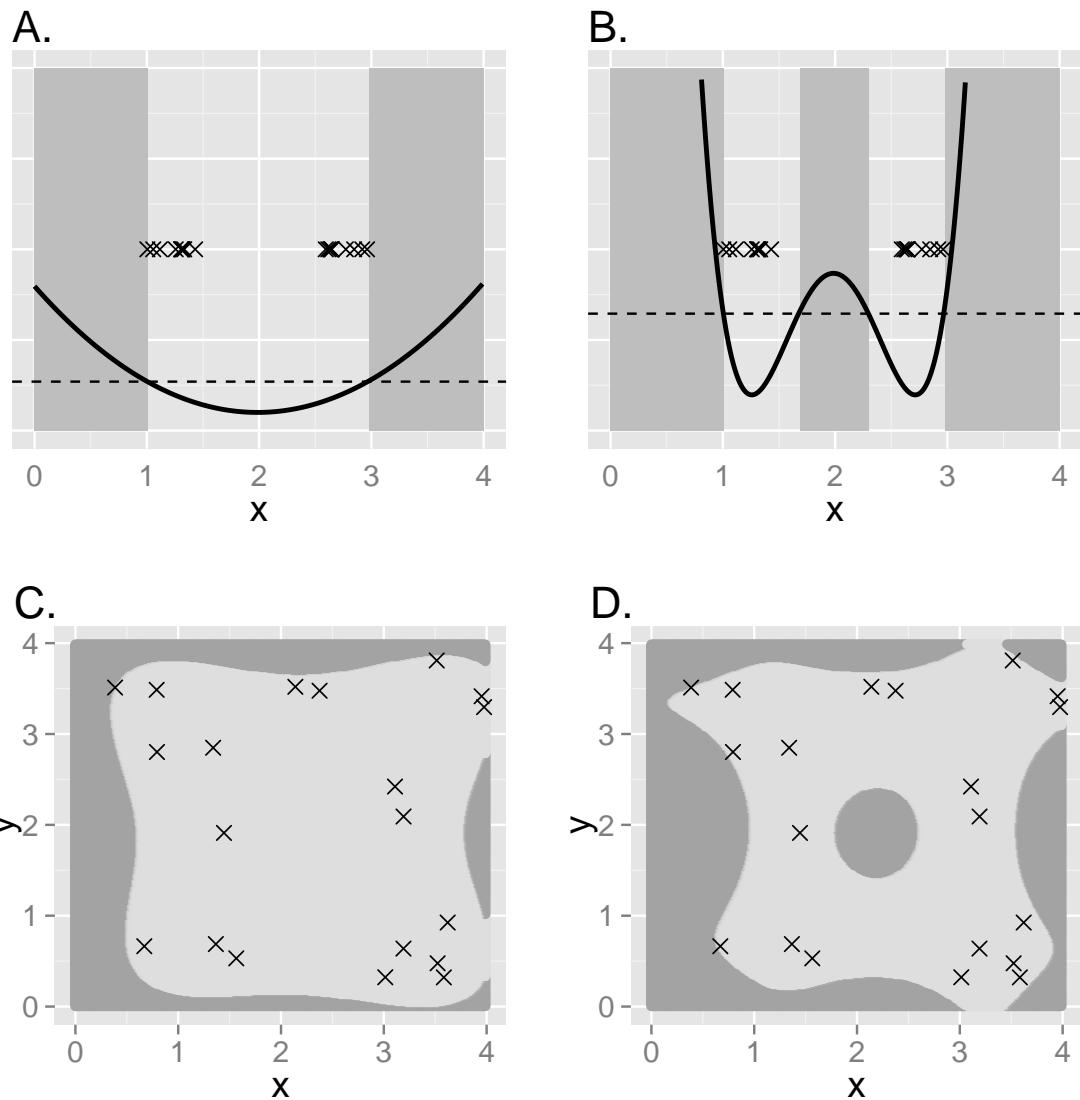


FIG 2

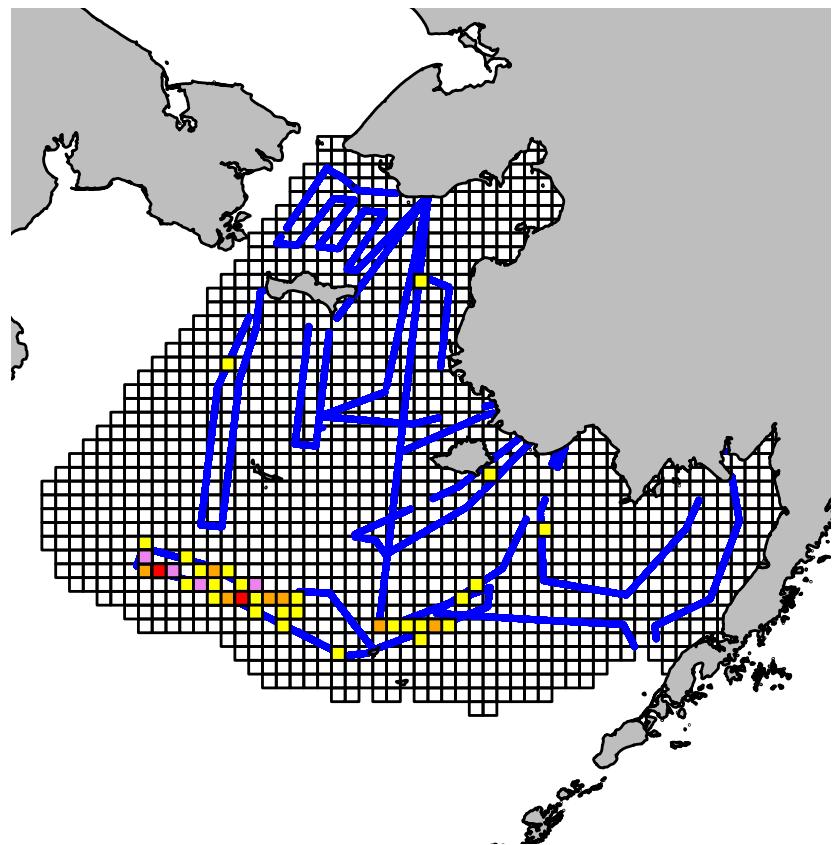


FIG 3

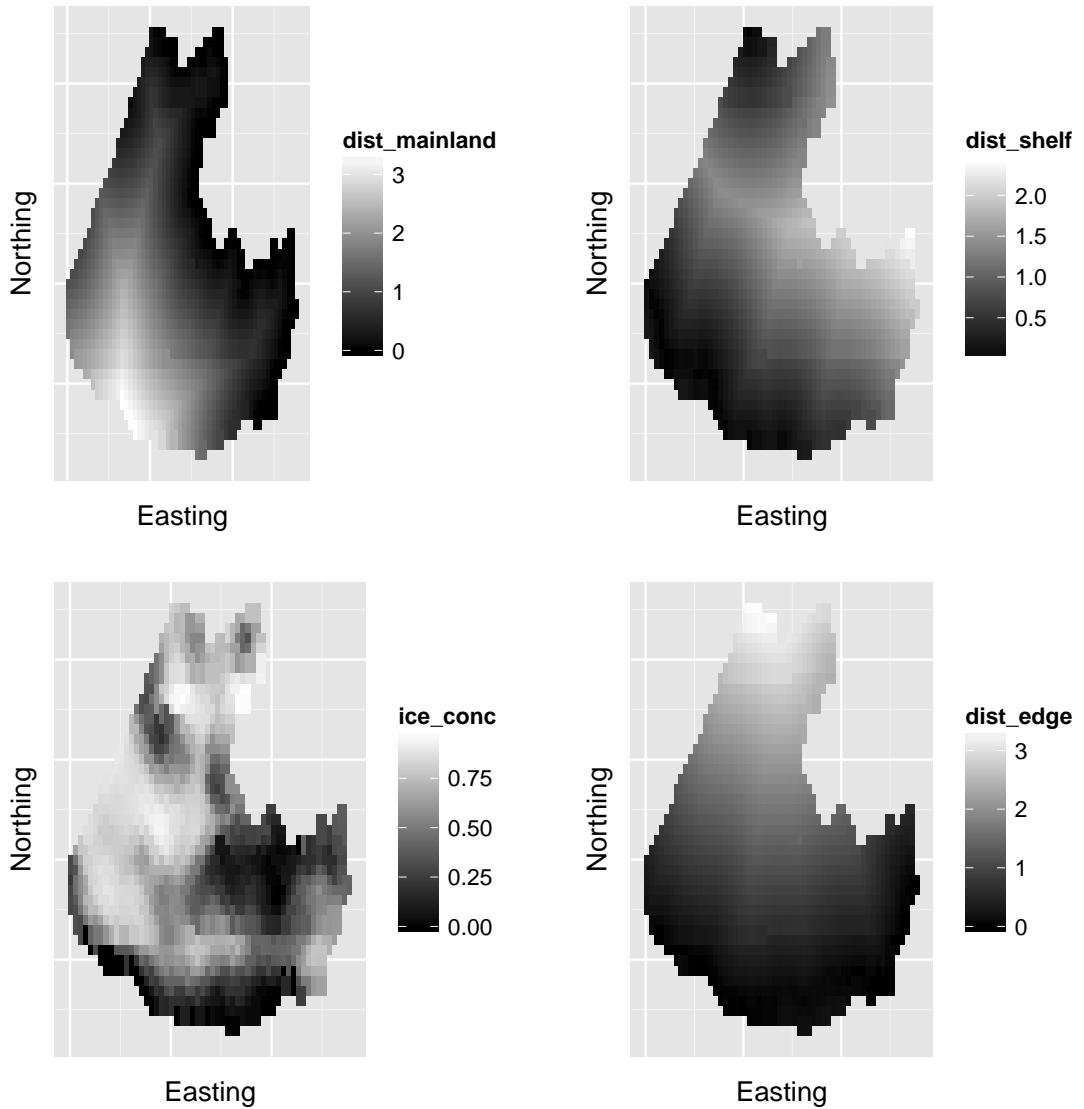


FIG 4

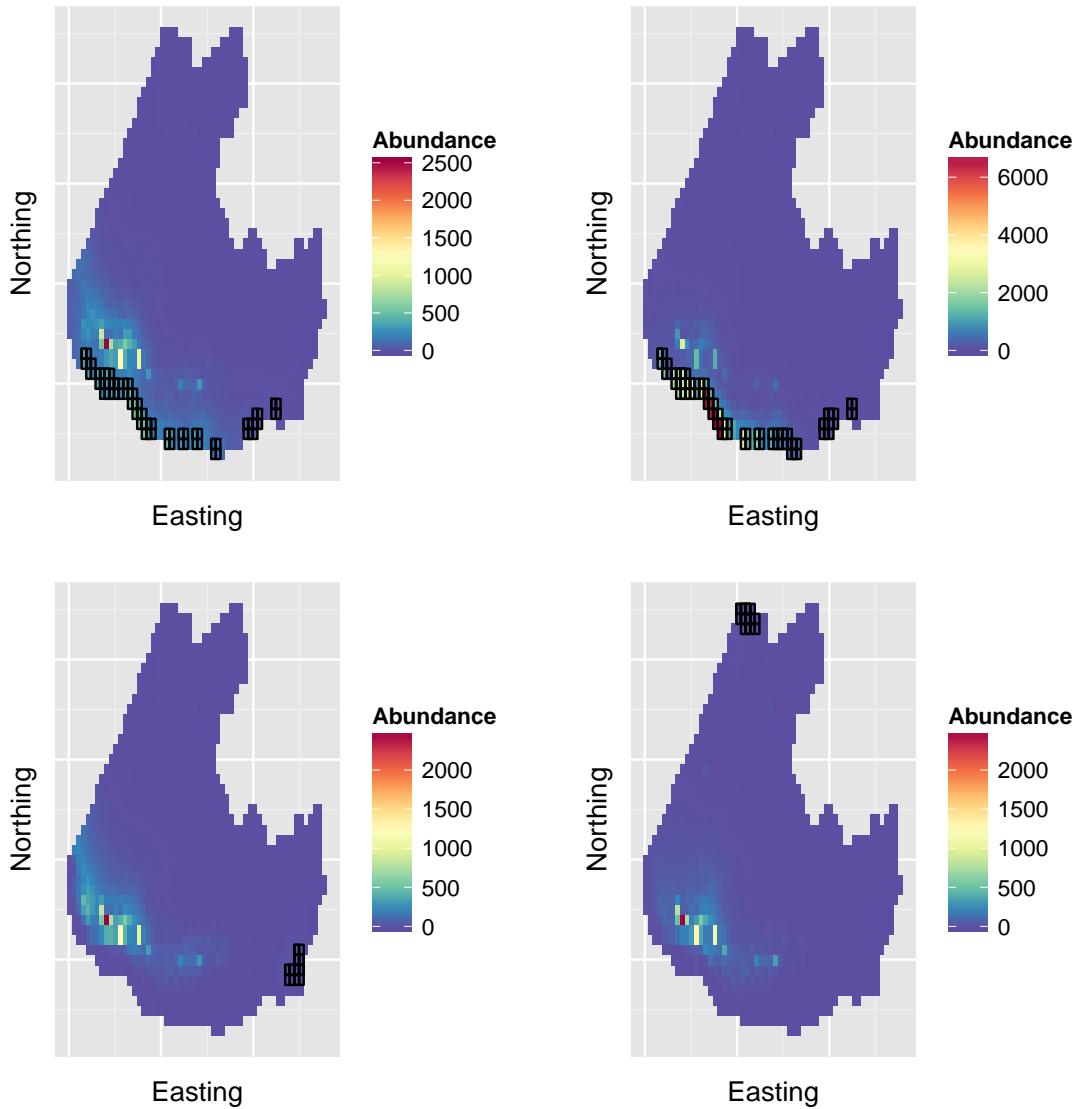


FIG 5