MULTI-SPECIES DISTRIBUTION MODELING USING PENALIZED MIXTURE OF REGRESSIONS

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Multi-species distribution modeling, which relates the occurrence of multiple species to environmental variables, is an important tool used by ecologists for both predicting the distribution of species in a community and identifying the important variables driving species co-occurrences. Recently, Dunstan, Foster and Darnell [Ecol. Model. 222 (2011) 955–963] proposed using finite mixture of regression (FMR) models for multi-species distribution modeling, where species are clustered based on their environmental response to form a small number of ’archetypal responses.’ As an illustrative example, they applied their mixture model approach to a presence–absence data set of 200 marine organisms, collected along the Great Barrier Reef in Australia. Little attention, however, was given to the problem of model selection—since the archetypes (mixture components) may depend on different but likely overlapping sets of covariates, a method is needed for performing variable selection on all components simultaneously. In this article, we consider using penalized likelihood functions for variable selection in FMR models. We propose two penalties which exploit the grouped structure of the covariates, that is, each covariate is represented by a group of coefficients, one for each component. This leads to an attractive form of shrinkage that allows a covariate to be removed from all components simultaneously. Both penalties are shown to possess specific forms of variable selection consistency, with simulations indicating they outperform other methods which do not take into account the grouped structure. When applied to the Great Barrier Reef data set, penalized FMR models offer more insight into the important variables driving species co-occurrence in the marine community (compared to previous results where no model selection was conducted), while offering a computationally stable method of modeling complex species–environment relationships (through regularization).

1. Introduction. Multi-species distribution modeling, which relates the occurrence of multiple species to environmental covariates, is an important tool
both for predicting how a species community will respond to changing environmental conditions and for identifying important environmental variables driving species co-occurrences [Ferrier and Guisan (2006), Ovaskainen, Hottola and Siitonen (2010), Pollock et al. (2014)]. To construct such models, statistical methods are required which can handle the underlying heterogeneity in species–environment relationships (i.e., different species in the same community can have very different environmental responses), while providing accurate predictions for rare species that may not be modeled reliably on their own (by borrowing strength across organisms in a community, Ferrier and Guisan (2006), Ovaskainen and Soininen (2011)).

Recently, Dunstan, Foster and Darnell (2011) proposed using finite mixture of regression [FMR, Wedel and DeSarbo (1995)] models for multi-species distribution modeling of presence–absence (binary) data, where species are clustered based on their environment response to form a small number of “archetypal responses.” The methodology was extended by Hui et al. (2013) and Dunstan et al. (2013) to handle count and biomass data, the latter being a nonnegative continuous value representing the combined weight of all individuals of each species. By clustering species into archetypes, and modeling each archetype using a generalized linear model [GLM, McCullagh and Nelder (1989)], these Species Archetype Models or SAMs offer a powerful approach to modeling heterogeneity in a community’s response to a set of covariates. Clustering species based on environmental response is also consistent with recent findings in ecology that groups of species tend to respond in a similar manner to environmental gradients [at least with the resolution of most multi-species data sets, Clark (2010)]. Moreover, Hui et al. (2013) showed SAMs offer strong predictive performance of rare species by borrowing strength from more prevalent species classified to the same archetype.

While these initial results for SAMs showed promise, little attention was given to the important issue of model selection. In their application of SAMs to a data set of presence–absence records collected for 200 species along the Great Barrier Reef off the northeast coast of Australia, Dunstan, Foster and Darnell (2011) used a heuristic version of BIC [Schwarz (1978)] to select the “types of covariates” to enter in the model, that is, physical habitat covariates, oceanographic measures or both. Also, both Hui et al. (2013) and Dunstan et al. (2013) a priori fixed the set of covariates to enter into their respective SAMs. In all three articles, the same set of covariates were entered into each archetype. This is a restrictive requirement, as it fails to account for the numerous (and unknown) ways which organisms react to their environment.

Since the component densities may depend on different but likely overlapping sets of covariates, a method is needed for performing variable selection on all components in an FMR model simultaneously. For SAMs especially, simultaneously performing variable selection over all archetypes is key to identifying which environmental variables are important in structuring the species community. On the other hand, given the number of candidate models is considerably larger than in
the standard GLM context, methods which require fitting all possible models, for example, information criteria, are impractical.

In this article, we consider using penalized likelihood methods for variable selection in FMR models and SAMs. Since each covariate in an FMR model is represented by a group of coefficients, one for each component (and whose true value may be zero), we propose two penalties which exploit this grouped structure. This leads to an attractive form of shrinkage that allows a covariate to be removed from all components simultaneously. The first penalty proposed is a modification of the group LASSO [Yuan and Lin (2006)] to FMR models, called MIXGL2 (since it is an $\ell_2$-norm penalty), which is applied across components on a per covariate basis. The second penalty, called MIXGL1, is based on the square root of the $\ell_1$-norm and allows the component densities to depend on different sets of covariates. In a diverging number of covariates settings (i.e., the number of parameters grows a slower rate than sample size), we demonstrate that MIXGL1 and MIXGL2 each possess a specific form of variable selection consistency. Furthermore, simulation studies show MIXGL2 and MIXGL1 outperform other penalties which do not take into account the grouped structure of the covariates, both in variable selection and prediction.

We apply both penalties to construct multi-species distribution models for the aforementioned Great Barrier Reef data set. This data set was collected as part of a larger biodiversity project aimed at identifying the key environmental variables important in structuring seabed biodiversity, as well as predicting future distributions of species communities along the Great Barrier Reef [Pitcher et al. (2007)]. It consists of presence-absence data of 200 species collected at 1189 sites, along with 13 environmental covariates. Compared to the results from unpenalized SAMs [Dunstan, Foster and Darnell (2011), Hui et al. (2013)], the penalized versions offer two advantages: (1) clearer insight is gained into species co-occurrence, as the penalties provide an automated way of identifying the variables informing each archetypal response; (2) the inclusion of penalties smooths the likelihood and leads to a more stable estimation procedure for SAMs.

We conclude this introduction by reviewing previous literature on penalized likelihood methods for FMR models. Khalili and Chen (2007) were the first to extend the LASSO [Tibshirani (1996)] and SCAD [Fan and Li (2001)] penalties to FMR models by applying these penalties on a per component basis, that is, each component has its own tuning parameter. For FMR models with a diverging number of covariates in each component, Khalili and Lin (2013) proposed elastic-net type penalties [i.e., a linear combination of a sparsity-inducing and a ridge penalty, Zou and Hastie (2005)], which were also applied on a per component basis. For mixtures of linear regression in particular, Städler, Bühlmann and van de Geer (2010) applied the adaptive LASSO [Zou (2006)] with one tuning parameter for the entire model. To date, no penalty has been proposed which exploits the grouped structure of the covariates in FMR models, something we investigate in this article.
2. Finite mixture of regression models. Consider a sample of observations \( \{(x_i, y_i); i = 1, \ldots, n\} \), where \( y_i \) is a univariate, independent and identically distributed response and \( x_i \) is a \( p \times 1 \) vector of covariates. We allow \( p \) to grow polynomially with sample size, that is, \( p^\nu/n \to 0 \) for some \( \nu > 1 \). The precise value of \( \nu \) is specified later on in Section 3.1. All covariates are assumed to have been standardized to mean zero and variance one. For an FMR model with \( K \) components, the conditional density function for observation \( i \) is given as follows:

\[
\begin{align*}
  h(y_i; x_i, \Psi) &= \sum_{k=1}^{K} \pi_k f(y_i; x_i, \mu_{ik}, \phi_k); \\
  g(\mu_{ik}) &= \beta_0 + \sum_{l=1}^{p} x_{il} \beta_{kl},
\end{align*}
\]

where \( \pi = (\pi_1, \ldots, \pi_K) \) denotes the mixing proportions satisfying \( \pi_k > 0, \sum_{k=1}^{K} \pi_k = 1 \) and \( f(y; x, \mu_k, \phi_k) \) is the \( k \)th component density assumed to come from the exponential family with mean \( \mu_k \) and dispersion parameter \( \phi_k \). For observation \( i \), the mean conditional on belonging to the \( k \)th component, \( \mu_{ik} \), is regressed against covariates \( x_i \) using a GLM with link function \( g(\cdot) \) and coefficients \( \{\beta_{kl}; l = 1, \ldots, p\} \).

Let \( \beta_l = (\beta_{l1}, \ldots, \beta_{lK}) \) be the vector of coefficients corresponding to covariate \( l \). Notice the coefficients are concatenated on a per covariate basis—this reflects the grouped structure of the covariates, that is, each covariate is represented by \( K \) coefficients, one for each component and whose true value may be zero. Finally, let \( \beta = (\beta_1, \ldots, \beta_p) \) be the \( K \times p \) matrix of regression coefficients, and \( \Psi = (\beta_1, \ldots, \beta_p, \beta_{01}, \ldots, \beta_{0K}, \phi, \pi) \) denote all the parameters in the FMR model, where \( \phi = (\phi_1, \ldots, \phi_K) \).

In this article, it is assumed the parameters in the FMR model in equation (1) are generically identifiable up to a permutation of the component labels [see condition (A1) in the Supplementary Material, Hui, Warton and Foster (2015b)]. Furthermore, we develop our asymptotic theory assuming the number of components \( K \) is known [analogous to Khalili and Lin (2013), Städler, Bühlmann and van de Geer (2010)], although for our application with SAMs we propose a BIC-type criterion to select the number of archetypes. General discussions regarding parameter identifiability for mixture models can be found in McLachlan and Peel (2004) and Frühwirth-Schnatter (2006), with the specific case of generic identifiability discussed in Follmann and Lambert (1991), Hennig (2000) and Grün and Leisch (2008), among others.

3. New penalties for variable selection. To exploit the grouped structure of covariates in FMR models and SAMs, we consider penalized likelihood methods using penalties which are applied across components on a per covariate basis,

\[
\ell_n^{\text{pen}}(\Psi) = \ell_n(\Psi) - n\lambda \sum_{l=1}^{p} P(\beta_l),
\]
where \( \ell_n(\Psi) = \sum_{i=1}^{n} \log(\sum_{k=1}^{K} \pi_k f(y_i; x_i, \mu_{ik}, \phi_k)) \) is the observed log-likelihood and \( \mathcal{P}(\mathbf{b}_l) \) denotes a penalty function which is nonnegative and satisfies \( \mathcal{P}(\mathbf{0}) = 0 \). Let \( \tilde{\mathbf{b}} = (\tilde{\beta}_1, \ldots, \tilde{\beta}_p) \) denote the unpenalized maximum likelihood estimates of \( \mathbf{b} \). We propose two penalty forms for \( \mathcal{P}(\mathbf{b}_l) \). The first is a modification of the group LASSO [Yuan and Lin (2006)] for FMR models.

**DEFINITION 1.** For the FMR model defined in equation (1), the MIXGL2 estimates are given by maximizing the penalized log-likelihood function

\[
\ell_n^{\text{pen}}(\Psi) = \ell_n(\Psi) - n\lambda \sum_{l=1}^{p} \tilde{w}_l \sqrt{\sum_{k=1}^{K} \tilde{\beta}_{kl}^2},
\]

where \( \tilde{w}_l = (\sum_{k=1}^{K} \tilde{\beta}_{kl}^2)^{-\gamma/2} \) and \( \gamma > 0 \).

MIXGL2 possesses the group sparsity property, that is, it is nondifferentiable when \( \tilde{\beta}_{1l} = \cdots = \tilde{\beta}_{Kl} = 0 \) for covariate \( l \). This is an attractive property to have for variable selection in FMR models, as it encourages a covariate to be removed from all components simultaneously. Such a form of sparsity in the solution is useful for multi-species distribution modeling, as often there are numerous environmental covariates which are completely uninformative for all archetypes (a covariate is defined as completely uninformative if all its coefficients are truly zero). MIXGL2 is useful for screening these covariates out, potentially as a first stage in variable selection for SAMs.

The second penalty we propose is based on the square root of a weighted \( \ell_1 \)-norm.

**DEFINITION 2.** For the FMR model defined in equation (1), the MIXGL1 estimates are given by maximizing the penalized log-likelihood function

\[
\ell_n^{\text{pen}}(\Psi) = \ell_n(\Psi) - n\lambda \sum_{l=1}^{p} \tilde{w}_l \left| \sum_{k=1}^{K} \tilde{\beta}_{kl} \right|, \]

where \( \tilde{w}_l = |\tilde{\beta}_{kl}|^{-\gamma} \) and \( \gamma > 0 \).

MIXGL1 not only possesses the group sparsity property like MIXGL2, it also possesses individual coefficient sparsity analogous to the adaptive LASSO, that is, it is also nondifferentiable for all individual coefficients \( \beta_{kl} \). This individual sparsity allows MIXGL1 to remove covariates from only \( K' < K \) components. It is therefore well suited to species distribution modeling—since the archetypal responses typically depend on different sets of covariates, MIXGL1 can accommodate for differing mean structures in each archetype. Put another way, the set of variables that drive the co-occurrences of one group of species are usually slightly different to those that drive the co-occurrence of another group. The form
of MIXGL1 allows for this, while maintaining the ability to remove completely uninformative covariates from the entire SAM. Of course, the choice of which penalty also depends on the analysis objectives—sometimes, it is of interest to see which covariates affect any (or all) components, in which case MIXGL2 is more appropriate. Other times, we may want to know how each covariate affects the archetypes in the most compact way, in which case MIXGL1 is suitable.

Definition 2 is a special case of the Composite Absolute Penalty (CAP) family of penalties [Zhao, Rocha and Yu (2009)], although our work is the first to apply such a penalty to the FMR model context. Both MIXGL2 and MIXGL1 incorporate data-dependent weights based on the unpenalized estimates, \( \hat{\beta} \), with the severity of these weights controlled by \( \gamma \). The inclusion of weights builds on the idea of the adaptive LASSO and allows the penalized estimates to achieve desirable large sample properties as discussed in the next section. Finally, unlike the penalties in Khalili and Chen (2007) and Khalili and Lin (2013) which are applied on a per component basis, MIXGL1 and MIXGL2 do not depend on the mixing proportions. When penalization occurs on a per component basis, having penalties which are a function of \( \pi \) makes sense since it relates the severity of penalization to the “effective sample size” of each component. For penalization across components on a per covariate basis, specifically, the MIXGL1 and MIXGL2 penalties, the need to incorporate mixing proportions is less obvious.

3.1. Asymptotic properties. In this section, we consider the large sample behavior of the MIXGL2 and MIXGL1 estimators. As mentioned previously, we assume the number of components \( K \) is fixed and known a priori, but the number of covariates in each component grows with sample size \( n \). We shall use \( p_n \), as well as a subscript \( n \) in other quantities, for example, \( \lambda_n \) and \( \beta_n \), to reflect this. Let \( \Psi_0 = (\beta_{n,1}, \ldots, \beta_{n,p_n}, \phi_0, \pi_0) \) be parameter values corresponding to the true model, which is assumed to be identifiable. We can partition all the regression coefficients in the true model as follows:

**Definition 3.** The regression coefficients in the true model, \( (\beta_{n,1}^0, \ldots, \beta_{n,p_n}^0) \), can be partitioned into the following mutually exclusive sets:

- \( \mathcal{A}_n = \{(k,l) : \beta_{n,kl}^0 \neq 0\} \) denotes the set of truly nonzero coefficients.
- \( \mathcal{B}_n = \{(k,l) : \beta_{n,kl}^0 = 0, \|\beta_j^0\|_2 \neq 0\} \) denotes the set of zero coefficients belonging to partly uninformative covariates.
- \( \mathcal{C}_n = \{(k,l) : \beta_{n,kl}^0 = 0, \|\beta_j^0\|_2 = 0\} \) is the set of zero coefficients belonging to completely uninformative covariates.

As formalized below, the group sparsity property of MIXGL2 allows it to asymptotically set all coefficients belonging to set \( \mathcal{C}_n \) to zero, while the combined group and individual coefficient sparsity property of MIXGL1 allows it to asymptotically set all coefficients belonging to sets \( \mathcal{B}_n \) and \( \mathcal{C}_n \) to zero.

For both penalties, assume the following regularity conditions are satisfied:
\( \lambda_n a_n = o_p(n^{-1/2}) \),
\( \lambda_n a_n = o_p(n^{-1/2} p_n^{-1}) \),
\( p_n^2 / (\lambda_n^2 b_n) = o_p(n) \),
\( p_n^4 / n \to 0 \),
\( (C') p_n^5 / n \to 0 \),

where for the MIXGL2 penalty, \( a_n = \max \{ \tilde{w}_{n,l}; l \in A_n \} \) and \( b_n = \min \{ \tilde{w}^2_{n,l}; l \in C_n \} \), and, analogously for the MIXGL1 penalty, \( a_n = \max \{ \tilde{w}_{kl}; (k,l) \in A_n \} \) and \( b_n = \min \{ \tilde{w}_{kl}; (k,l) \in B_n \cup C_n \} \). Conditions (A) and (A') ensure the existence of penalized likelihood estimates which are asymptotically unbiased, while condition (B) ensures an appropriate degree of shrinkage. The rate of growth of the number of covariates in conditions (C) and (C') is the same as Khalili and Lin (2013), and we believe it to be appropriate in many applications of species distribution modeling in ecology, that is, the number of environmental variables recorded is usually small compared to the number of sites visited.

We first consider the asymptotic behavior of the MIXGL2 estimator:

**Theorem 1** (Oracle property—MIXGL2). Assume conditions (A)–(C) hold. Then there exists a local maximizer \( \hat{\Psi}_n \) of \( \ell_n^{\text{pen}}(\Psi_n) \) in Definition 1 which satisfies the following:

- **Estimation consistency:** \( \| \hat{\Psi}_n - \Psi_n^0 \| = O_p(\sqrt{p_n/n}) \).
- **Covariate selection consistency:** \( P(\hat{\beta}_{n,c_n} = 0) \to 1 \).
- **Asymptotic normality:** If conditions (A') and (C') are also satisfied, then

\[
\sqrt{n} \Gamma_n I_n(\Psi_n^0, C_n^c) \frac{1}{2}(\hat{\Psi}_n, C_n^c - \Psi_n^0, C_n^c) \xrightarrow{d} N(0, G),
\]

where \( \hat{\Psi}_n, c_n^c = (\hat{\beta}_{n,c_n^c}, \hat{\beta}_{n,01}, \ldots, \hat{\beta}_{n,0K}, \hat{\pi}_n) \), \( \Gamma_n \) is a \( q \times |C_n^c| \) matrix such that \( \Gamma_n G_n \xrightarrow{p} G \), and \( I_n(\Psi_n^0, C_n^c) \) is the Fisher information matrix knowing \( C_n^c \).

All proofs have been relegated to the Supplementary Material [Hui, Warton and Foster (2015b)]. Theorem 1 states MIXGL2 is covariate selection consistent, that is, it will asymptotically remove completely uninformative covariates from the FMR model. On the other hand, if the true model contains partly uninformative covariates (\( B_n \neq \emptyset \)), MIXGL2 will in the large sample limit retain these covariates in all components. This makes sense because MIXGL2 does not possess individual coefficient sparsity. By contrast, if we consider the asymptotic behavior of the MIXGL1 estimator, then we have the following:

**Theorem 2** (Oracle property—MIXGL1). Assume conditions (A)–(C) hold. Then there exists a local maximizer \( \hat{\Psi}_n \) of \( \ell_n^{\text{pen}}(\Psi_n) \) in Definition 2 which satisfies the following:

- **Estimation consistency:** \( \| \hat{\Psi}_n - \Psi_n^0 \| = O_p(\sqrt{p_n/n}) \).
• Coefficient selection consistency: \( P(\hat{\beta}_{n,B_n\cup C_n} = 0) \to 1 \).
• Asymptotic normality: If conditions \((A')\) and \((C')\) are also satisfied, then
\[
\sqrt{n} \Gamma_n I_n(\Psi^0_{n,A_n})^{1/2} (\hat{\Psi}_{n,A_n} - \Psi^0_{n,A_n}) \xrightarrow{d} N(0, G),
\]
where \( \hat{\Psi}_{n,A_n} = (\hat{\beta}_{n,A_n}, \hat{\beta}_{n,01}, \ldots, \hat{\beta}_{n,0K}, \hat{\phi}_n, \hat{\pi}_n) \), \( \| \cdot \| \) denotes the \( \ell_2 \)-norm, \( \Gamma_n \) is a \( q \times |A_n| \) matrix such that \( \Gamma_n \Gamma_n' \to_p G \), and \( I_n(\Psi^0_{n,A_n}) \) is the Fisher information matrix knowing \( A_n \).

Theorem 2 states MIXGL1 is coefficient selection consistent, that is, it will asymptotically remove completely uninformative covariates and zero coefficients belonging to partly uninformative covariates from the FMR model. This is a stronger form of selection consistency compared to MIXGL2, and is a desirable property in terms of identifying the truly important covariates facilitating species co-occurrence.

To compute the MIXGL2 and MIXGL1 estimates, we use an estimation procedure combining the Expectation Maximization [EM, Dempster, Laird and Rubin (1977)] algorithm with a local quadratic approximation [LQA, Fan and Li (2001)]. Details regarding this estimation procedure, and a proof that it possesses the desired ascent property, may be found in the Supplementary Material [Hui, Warton and Foster (2015b)]. To select the tuning parameters \((\lambda_n, \gamma)\), we use a BIC-type criterion [see Zhang, Li and Tsai (2010) for the use of information criteria in selecting tuning parameters],
\[
\text{BIC}_{\lambda_n,\gamma} = -2\ell_n(\hat{\Psi}_n) + \log(n) \dim(\hat{\beta}_n),
\]
where \( \dim(\hat{\beta}_n) \) denotes the number of nonzero estimates in \( \hat{\beta}_n \). Note \( \hat{\Psi}_n \) and \( \dim(\hat{\beta}_n) \) both depend on \( \lambda_n \) and \( \gamma \), for example, as \( \lambda_n \) increases, more values of \( \hat{\beta}_n \) are shrunk to zero. For our simulations and applications, we select from \( \gamma \in \{0.5, 1, 2\} \).

4. Application. We apply MIXGL1 and MIXGL2 to Species Archetype Models and the Great Barrier Reef data set introduced in Section 1. To recap, the data set consists of presence–absence data of 200 species at 1189 sites, along with 13 environmental covariates. Five of these covariates were descriptors of physical habitat: depth (BATHY), bottom stress (BSTRESS), percent gravel (GRAVEL), percent mud (MUD), percent carbonate (CARBON), and the other eight covariates were oceanographic measures: mean and intra-annual standard deviation of temperature (T.AV, T.SD), mean and intra-annual standard deviation of oxygen concentration (O2.AV, O2.SD), mean and intra-annual standard deviation of salinity (S.AV, S.SD), mean and intra-annual standard deviation of K490 (K490.AV, K490.SD). K490 is measure of turbidity based on light penetration and is related to the presence of light scattering particles in the water.

To model the 200 species separately using a GLM (say) would be a difficult task, especially since 164 out of 200 species are present at less than 5\% of the sites. Such
sparsity in the response (in the sense that most species are rarely observed) is characteristic of multi-species data and motivates methods such as SAMs which are able to borrow strength across species. On the other hand, while the applications of SAMs in Dunstan, Foster and Darnell (2011) and Dunstan et al. (2013) were mainly for illustrative purposes, the goal in this article is to perform (consistent) variable selection in order to identify the key drivers of species co-location.

Let $Y$ denote the multi-species response matrix collected at $i = 1, \ldots, n$ sites for $j = 1, \ldots, s$ species, with $[Y]_{ij} = 1$ if species $j$ was found at site $i$ and 0 otherwise. For the Great Barrier Reef data set, $n = 1189$ and $s = 200$. Let $x_i$ be the vector of environmental covariates at site $i$. SAMs are an extension of FMR models in (1) to the case of product Bernoulli component densities:

$$h(y_j; x_i, \Psi) = \sum_{k=1}^{K} \pi_k \left( \prod_{i=1}^{n} \mu_{ijk}^{y_{ij}} (1 - \mu_{ijk})^{1-y_{ij}} \right);$$

(2)

$$\logit(\mu_{ijk}) = \beta_{0j} + \sum_{l=1}^{p} x_{il} \beta_{kl}.$$ 

Note in (2), the intercepts $\beta_{0j}$ are species-specific instead of component-specific. As discussed in Dunstan et al. (2013), this is so that species are clustered solely on the shape of their environmental responses and not as well on the prevalence.

For each of the 13 covariates, we fitted linear and quadratic terms, resulting in 26 terms available for selection in each archetype. We used MIXGL2 and MIXGL1 to perform variable selection, with the tuning parameters chosen using $\text{BIC}_{\lambda n, \gamma}$ defined in Section 3.1, and $\log(n)$ replaced by $\log(s)$ as the model complexity penalty. The reason for this replacement is because the fundamental observational unit in SAMs is a species instead of a site [see Dunstan, Foster and Darnell (2011) and also the Discussion in Section 6]. For a fixed $K$, the combined EM plus LQA algorithm used for fitting penalized FMR models can be straightforwardly extended to the case of SAMs [see the Supplementary Material for details, Hui, Warton and Foster (2015b)]. To select the number of archetypes, we considered a candidate range $K = [1, 20]$ and used another BIC-type criterion [see Sections 6.8–6.9, McLachlan and Peel (2004), on using information criteria for selecting $K$],

$$\text{BIC}_K = -2 \ell_n(\hat{\Psi}(K)_n) + \log(s) \dim(\hat{\Psi}(K)_n),$$

where $\dim(\hat{\Psi}(K)_n)$ denotes the number of nonzero parameters in the SAM with $K$ archetypes. The model selection procedure thus proceeds as follows: for each candidate $K$, the best penalized SAM is selected using $\text{BIC}_{\lambda n, \gamma}$. Afterward, the final model is selected from these “best penalized SAMs” using $\text{BIC}_K$.

Figure 1 shows a plot of coefficients estimates for the two penalized SAMs, with exact values of the coefficients provided in the Supplementary Material [Hui, Warton and Foster (2015b)]. Using $\text{BIC}_K$, MIXGL2 and MIXGL1 produced SAMs with $K = 9$ and 10 archetypes, respectively [note Dunstan, Foster and Darnell (2011) chose $K = 11$ archetypes when applying unpenalized SAMs.
FIG. 1. Map of coefficients for penalized SAMs with MIXGL2 (left) and MIXGL1 penalties (right). Empty circles indicate coefficients shrunk to exactly 0. Based on BIC\(_K\), the former chose \(K = 9\) archetypes while the latter chose \(K = 10\) archetypes.

To the same data set. Compared with the unpenalized SAM in Dunstan, Foster and Darnell (2011), penalized variable selection offers much more insight into the drivers of seabed biodiversity. Both models indicated the five physical habitat covariates were informative for almost all archetypes (Figure 1—bottom 10 rows in both plots), meaning these variables are important in structuring the entire marine species assemblage. In contrast, MIXGL1 and MIXGL2 deemed several of the oceanographic measures to be either completely or close to completely uninformative, for example, the quadratic terms T.SD\(^2\) and S.SD\(^2\). It is also in these oceanographic covariates where the archetypal responses were largely differentiated for the MIXGL1 model. For example, archetype 2 was the only archetype where the four terms corresponding to mean and intra-annual standard deviation of oxygen were informative. That is, the co-occurrence of species classified to this archetype could be partly attributed to their shared environmental response to oxygen. Also, archetypes 2 to 6 all had coefficients for mean annual temperature which were substantially different from zero. However, species in archetypes 3 and 6 tend to occupy regions of higher temperatures, while species classified to archetype 2, 4 and 5 tend to occur in relatively cooler regions.

For prediction purposes, maps were constructed for each archetype showing how the probability of presence on the linear predictor scale varies spatially along the entire Great Barrier Reef. That is, for archetype \(k = 1, \ldots, K\), these were constructed using the linear predictor,

\[
\hat{\eta}_{ik} = \frac{\sum_{j=1}^{s} \hat{\tau}_{jk} \hat{\beta}_{0j}}{\sum_{j=1}^{s} \hat{\tau}_{jk}} + \sum_{l=1}^{p} x_{il} \hat{\beta}_{kl},
\]
which were then mapped across all sites in the Barrier Reef region. To clarify, we chose to map the linear predictors \( \hat{\eta}_{ik} \) directly rather than convert them to probabilities, as this generally makes it easier to identify any differences between the archetypes. Note the intercept used in the predicted maps is a weighted average of all species-specific intercepts, with weights proportional to the posterior probabilities of belonging to archetype \( k \). These maps are provided in the Supplementary Material [Hui, Warton and Foster (2015b)]. Note that maps could also be constructed for each species, although for managerial purposes maps constructed on a per archetype basis tend to be more useful, since managing an archetype is equivalent to simultaneously managing all the species classified into the archetype [Dunstan, Foster and Darnell (2011)].

Both MIXGL2 and MIXGL1 produced some similar maps, for example, archetype 4 in both models exhibited a high probability of presence from the central to the southeast region of the reef toward the Coral sea, with the probability decreasing sharply toward land. Also, species in archetype 9 for both models tend to be found with relatively high probability toward the southeast Queensland coast. Given the differing properties of MIXGL2 and MIXGL1, however, it was not surprising to also observe some notable differences between the two sets of maps, for example, archetype 2 for the MIXGL2 fit displayed relatively high probabilities of presence in a small region on the southeast region of the Barrier Reef, where percent gravel was rather high. However, no corresponding archetype was observed for the MIXGL1 fit—while archetypes 4 and 7 also had positive linear terms for percent gravel (Figure 1—right), the environmental response of species in these two components tends to be driven more by other covariates. This suggests incorporating a penalty such as MIXGL1, which allows different mean structures in each archetype and leads to more precise differentiation of the sources of species co-occurrences.

5. Simulation study. A small simulation was performed to assess the finite sample performance of the MIXGL1 and MIXGL2 in FMR models in equation (1). The number of covariates in each component was determined as \( p_n = \lceil 4n^{1/4} \rceil - 5 \), where \( \lceil \cdot \rceil \) is the ceiling function [see also Khalili and Lin (2013)]. Covariates \( \{x_i; i = 1, \ldots, n\} \) were generated from a standard multivariate Gaussian distribution with correlation structure \( \text{Cor}(x_{ir}, x_{is}) = 0.5^{|r-s|} \). Responses were then simulated from a \( K = 2 \) binomial FMR model with trial size 10, using the four models below:

- Model I: \( (\beta_{01}, \beta_1) = (1, 0.7, 2, -2, 1.5, 0, 0, 0, \ldots) \),
- Model II: \( (\beta_{02}, \beta_2) = (-0.5, 2, 0, 0, 0, 1, -2, 0.5, \ldots) \),
- Model III: \( (\beta_{02}, \beta_2) = (-0.5, 2, 0, 0, 1, -2, 0.5, 0, \ldots) \),
- Model IV: \( (\beta_{02}, \beta_2) = (-0.5, 2, 1, -2, 0.5, 0, 0, \ldots) \),

where “...” indicates extra zeros. The models are designed such that, as we move from models I to IV, the number of partly uninformative covariates decreases. We
considered combinations of $\pi_1 = 0.5, 0.7$ and $n = 100, 200, 400$, with the latter corresponding to $p_n = 7, 9, 12$ covariates (excluding intercept) in each component, respectively. 500 data sets were generated for each combination. We assumed $K = 2$ was known in advance.

We compared MIXGL1 and MIXGL2 to three penalties proposed previously for FMR models: adaptive LASSO [ADL, Städler, Bühlmann and van de Geer (2010)], MIXLASSO-$\ell_2$, and MIXSCAD-$\ell_2$ [Khalili and Lin (2013)]. The latter two penalties are linear combinations of the ridge and LASSO (SCAD) penalty. ADL penalizes coefficients separately, while MIXLASSO-$\ell_2$ and MIXSCAD-$\ell_2$ penalize on a per component basis. Performance was assessed using mean sensitivity (proportion of true nonzeros estimated to be nonzero) and specificity (proportion of true zeros estimated to be zero), and predicted log-likelihood. The latter was calculated using an independent test data set of $n = 10,000$ observations, with higher values implying better predictions. Note that to remove variation across the different data sets, we centered the predicted log-likelihood values by subtracting the average obtained across the different methods in each data set. Also, to deal with the problem of label-switching prior to calculating sensitivity and specificity [see Section 4.9, McLachlan and Peel (2004)], we permuted the estimated coefficients so as to minimize the $\ell_2$-norm between the estimated and true coefficients.

For brevity, we only present results for $\pi_1 = 0.5$. Similar outcomes were observed for $\pi_1 = 0.7$, and these results are provided in the Supplementary Material [Hui, Warton and Foster (2015b)].

MIXGL1 performed consistently well, with sensitivity and specificity largely unaffected by the number of completely uninformative covariates (Table 1). Compared to MIXGL1, the three methods which did not penalize on a per-covariate basis had lower specificity indicative of overfitting. The result makes sense given the group sparsity property of MIXGL1 and MIXGL2—for all four models, there was a proportion of coefficients which always belonged to completely uninformative covariates. Therefore, penalties which can remove a covariate from all components simultaneously were much better at shrinking these coefficients to zero. As the number of partly uninformative covariates decreased, the performance of MIXGL2 dramatically improved, especially in specificity. Another interesting trend observed when Transitioning from models I to IV, in this simulation at least, was a slight but noticeable decline in specificity for ADL and MIXSCAD-$\ell_2$ (indicating overfitting). Finally, MIXLASSO-$\ell_2$ had the highest sensitivity in most models, but significantly lower specificity than all the other methods tested, which suggested a substantial amount of overfitting.

The trends in sensitivity and specificity (Table 1) were similarly observed in predictive performance. MIXGL1 predicted the best overall, while as we move from models I to IV and decrease the number of partly uninformative covariates, predictions from MIXGL2 improved significantly (Figure 2). There is also a slight decreasing trend in predictive log-likelihood for ADL and MIXSCAD-$\ell_2$, which
TABLE 1
Mean sensitivity/specificity for various sample sizes and \( \pi_1 = 0.5 \). Transitioning from models I to IV, the proportion of completely uninformative covariates increases

| n   | Model | MIXGL1 | MIXGL2 | ADL | MIXLASSO-\( \ell_2 \) | MIXSCAD-\( \ell_2 \) |
|-----|-------|--------|--------|-----|----------------------|----------------------|
| 100 | I     | 0.962/0.948 | 0.947/0.940 | 0.958/0.897 | 0.991/0.170 | 0.978/0.690 |
|     | II    | 0.962/0.962 | 0.959/0.373 | 0.956/0.855 | 0.992/0.128 | 0.975/0.683 |
|     | III   | 0.966/0.972 | 0.957/0.747 | 0.950/0.832 | 0.989/0.160 | 0.970/0.647 |
|     | IV    | 0.957/0.980 | 1/0.970 | 0.965/0.825 | 0.981/0.183 | 0.970/0.635 |
| 200 | I     | 0.983/0.986 | 0.960/0.320 | 0.994/0.948 | 0.998/0.388 | 0.996/0.826 |
|     | II    | 0.986/0.983 | 0.954/0.651 | 0.987/0.935 | 0.999/0.430 | 0.993/0.819 |
|     | III   | 0.985/0.985 | 0.956/0.864 | 0.994/0.911 | 0.999/0.415 | 0.995/0.803 |
|     | IV    | 0.985/0.989 | 1/1 | 0.987/0.908 | 0.995/0.392 | 0.991/0.782 |
| 400 | I     | 0.998/0.992 | 0.979/0.636 | 0.999/0.961 | 1/0.546 | 1/0.918 |
|     | II    | 0.999/0.991 | 0.978/0.761 | 0.999/0.958 | 1/0.576 | 0.999/0.901 |
|     | III   | 0.999/0.995 | 0.981/0.884 | 0.999/0.940 | 1/0.561 | 0.999/0.897 |
|     | IV    | 0.999/0.992 | 1/1 | 0.997/0.942 | 1/0.543 | 0.998/0.895 |

appeared to coincide with a slight drop in specificity. In the Supplementary Material [Hui, Warton and Foster (2015b)], we present an additional simulation conducted with mixtures of linear regression, \( K = 4 \), and more covariates, with similar results to those observed above despite the larger number of components.

6. Discussion. Species in a community exhibit significant heterogeneity in their occurrence patterns. A major source of this heterogeneity is due to species responses being driven by different but potentially overlapping sets of environmental covariates. In the context of multi-species distribution modeling using SAMs, this

![Fig. 2](image-url)

**Fig. 2.** Predicted log-likelihood (centered) as a function of a simulation model for \( \pi_1 = 0.5 \). The methods shown are the following: MIXGL1 (○), MIXGL2 (△), ADL (+), MIXLASSO-\( \ell_2 \) (×), MIXSCAD-\( \ell_2 \) (♦). As we move from models I to IV, the proportion of completely uninformative covariates increases. Note the different scales on the y-axis for the three figures.
means we require a method of variable selection which can consistently identify the covariates responsible for shaping each archetypal response (and thus shaping species co-occurrences within each archetype). In this article, we proposed two penalties, MIXGL2 and MIXGL1, which exploit the grouped structure of covariates in FMR models and SAMs. By penalizing across components on a per covariate basis, these penalties can remove a covariate simultaneously from all components of an FMR model. Both penalties were shown to possess specific forms of selection consistency, with simulations indicating they outperform other penalties which do not take into account the grouped structure of covariates. Applying penalized SAMs to the Great Barrier Reef data set offered clearer insight into the variables structuring seabed biodiversity, while providing a relatively simple idea of how the species assemblage as a whole responds to the environment.

While we have demonstrated that penalized SAMs can help to unravel how the distribution of a species community depends on environmental covariates, imposing a penalty on the likelihood also offers computational advantages. Given the high dimensionality \( (s/n) \) being a nonnegligible ratio) and heterogeneity in environmental responses of multi-species data sets, the likelihood for a SAM is expected to be “bumpy” with numerous local maxima. The estimates obtained from applying the EM algorithm to an unpenalized SAM may therefore depend heavily on the starting point, and may correspond to a local instead of the (one of \( K! \) equivalent) global maximum. Adding a penalty to the likelihood can help to resolve this problem by smoothing the likelihood surface and making the global maxima more apparent.

As an illustration of this, we considered two models fitted to the Great Barrier Reef data set: (1) the MIXGL1 penalized SAM with \( K = 10 \) and the tuning parameter fixed at the final value used in Section 4; (2) an unpenalized SAM, that is, \( \lambda = 0 \), with \( K = 10 \) and the 26 covariate terms included in each archetype. Each model was fitted 50 times using the same estimation procedure as in Section 4, each time using a random starting point generated by simulated posterior probabilities for each species from a Dirichlet distribution with hyperparameters all set to 1. Figure 3 shows a comparative boxplot of the resulting log-likelihood values. Importantly, the variability of the log-likelihood values for the penalized SAM was smaller compared to the unpenalized SAM (ratio of variance = 1.510; \( F \)-test \( p \)-value < 0.01). The reduction in variability can be attributed to the MIXGL1 penalty smoothing the SAM likelihood surface, removing some of the “bumps and small hills” and leading to a more stable estimation algorithm.

In future work, we hope to extend penalized SAMs to multi-species presence-only data, particularly given the commonality of such data and recently shown equivalences between point process models and Poisson/Logistic GLMs [Fithian and Hastie (2013), Warton and Shepherd (2010)]. Whether the consistency and oracle properties of MIXGL1 and MIXGL2 hold in this context should be considered. Also, other penalties which exploit the grouped structure of the covariates should be considered [e.g., the sparse group LASSO, Simon et al. (2013)].
In our application to the Barrier Reef data set, MIXGL2 and MIXGL1 did not take into account the hierarchical structure of polynomials, for example, the linear term for intra-annual standard deviation of K490 (K490.SD) was removed while the quadratic term remained in the model. While this still makes sense ecologically (i.e., given all covariates were centered, then the values of K490.SD where species are most likely to be found was around the average value observed in the data set), a penalty which explicitly obeys this hierarchical principle would be preferred, such as the fused lasso [Tibshirani et al. (2005)]. Finally, the validity of BIC or any other information criterion for choosing the tuning parameter in MIXGL1 and MIXGL2 remains an open question. In particular, whether the model complexity penalty for SAMs should be modified to log(s) (as was done in this article to reflect the fundamental observational unit being a species), remain as log(n) or perhaps be something else [see, e.g., Hui, Warton and Foster (2015a)] warrants further investigation.

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SUPPLEMENTARY MATERIAL

Supplement to “Multi-species distribution modeling using penalized mixture of regressions” (DOI: 10.1214/15-AOAS813SUPP; .pdf). Material includes technical proofs, details on estimation procedure and additional simulation and application results.

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