Scalable finite mixture of regression models for community ecology

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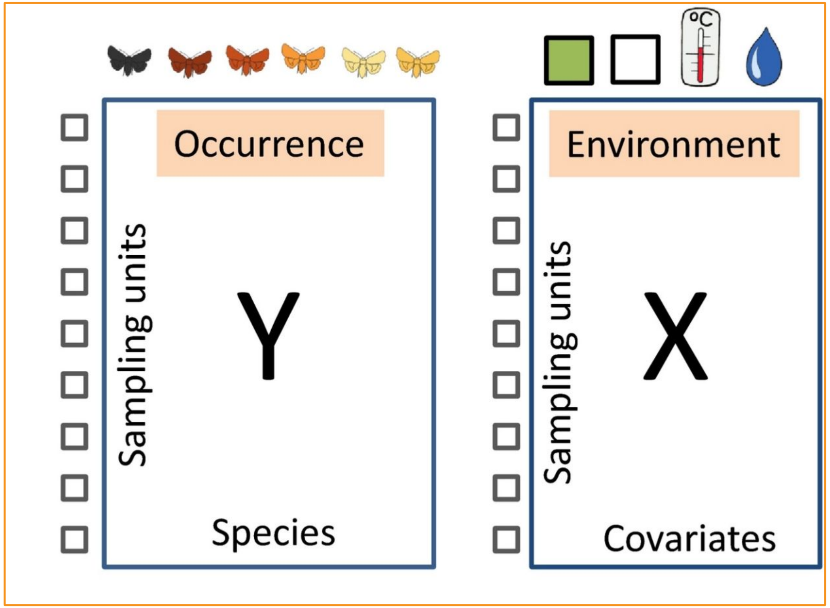
IBS-AR Conference 2025

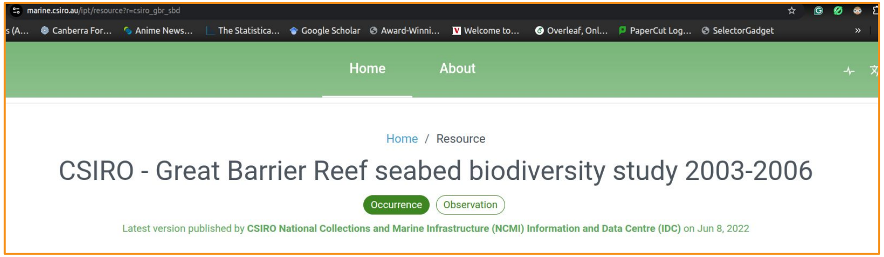
Community ecology data

- Multiple responses (potentially high-dimensional)
- Non-continuous responses with evident mean-variance relationship
- May have other data structures, but we will not worry about that in this presentation



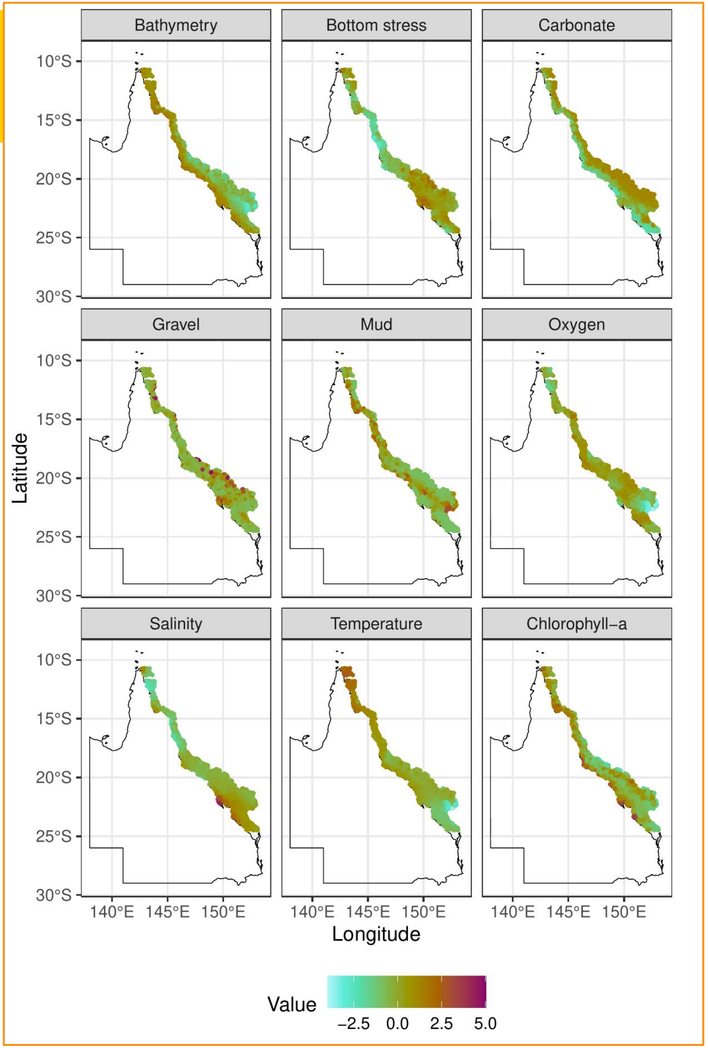
Community ecology data

- Great Barrier Reef Seabed biodiversity project



- For the purposes of this talk, we have:
  - Presence–absence (binary) responses
  - N = 1146 sites sampled
  - J = 235 species (median recorded prevalence = 31)

- For the purposes of this talk, we have:
  - Nine continuous environmental covariates
  - Standardized all to have mean zero and variance one



Species archetype models (SAMs)

- Aim: To understand how the assemblage distribution varies as a function of environment

- A starting point is to fit a stacked model e.g., separate binary logistic regression models to each species

Consider a set of species $j = 1, \ldots, J$ recorded at a set of observational units $i = 1, \ldots, N$, along with measured covariates $\boldsymbol{x}_i$. Then a stacked model is characterized by

$$
\begin{aligned}
g(\mu_{ij}) &= \eta_{ij} = \boldsymbol{x}_i^\top \boldsymbol{\beta}_j \\
[y_{ij}] &= \text{Exp-Fam}(\mu_{ij}, \boldsymbol{\phi}_j) \\
\ell(\boldsymbol{\Psi}) &= \sum_{j=1}^{J} \left(\sum_{i=1}^{N} \log f(y_{ij} | \mu_{ij}, \boldsymbol{\phi}_j) \right)
\end{aligned}
$$

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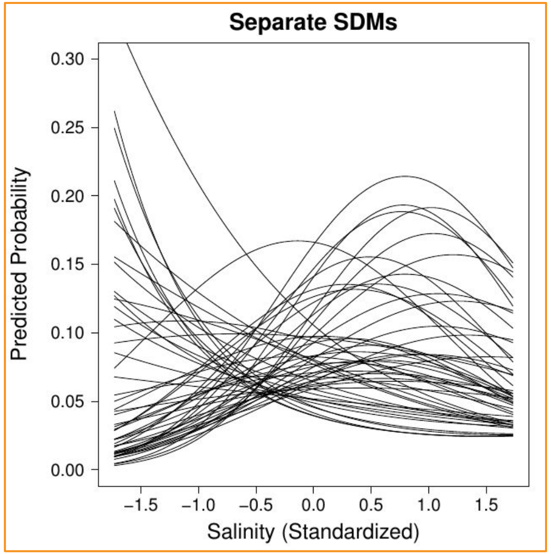

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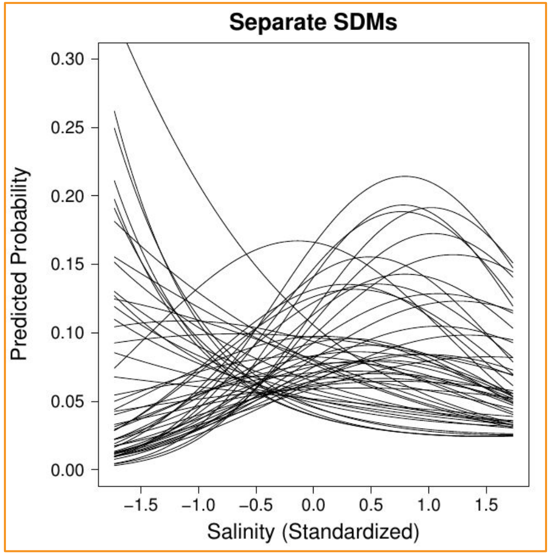

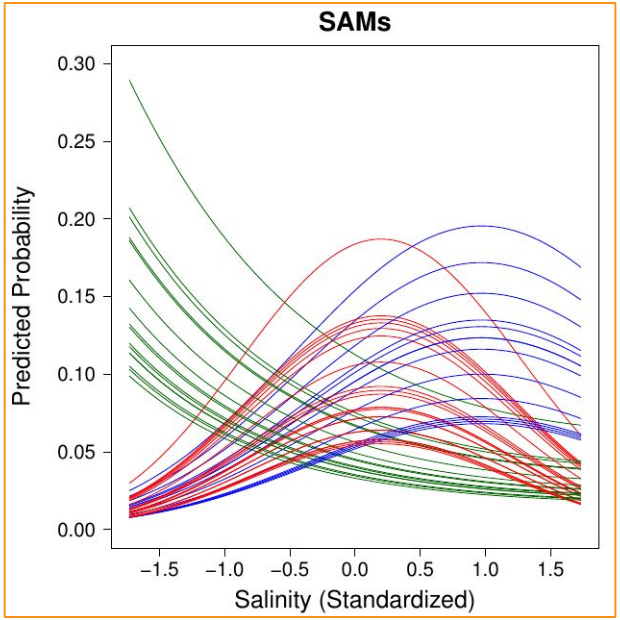

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- Aim: To understand how the assemblage distribution varies as a function of environment
- Cluster species with similar environmental responses into so-called archetypal responses

Consider a set of species $j = 1, \ldots, J$ recorded at a set of observational units $i = 1, \ldots, N$, along with covariates $\boldsymbol{x}_i$. Let $z_{jk} = 1$ if species $j = 1, \ldots, J$ belongs to archetype $k = 1, \ldots, K$ and zero otherwise. If we denote $\mu_{ijk} = \mathsf{E}(y_{ij}|\boldsymbol{x}_i, z_{jk} = 1)$, then a species archetypal model or SAM is characterized by

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\begin{aligned}
g(\mu_{ijk}) &= \alpha_j + \boldsymbol{x}_i^\top \boldsymbol{\beta}_k \\
[y_{ij}|z_{jk} = 1] &= \text{Exp-Fam}(\mu_{ijk}, \boldsymbol{\phi}_j) \\
\ell(\boldsymbol{\Psi}) &= \sum_{j=1}^{J} \log \left\{ \sum_{k=1}^{K} \omega_k \prod_{i=1}^{N} f(y_{ij}|\mu_{ijk}, \boldsymbol{\phi}_j) \right\}
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$$

Species archetype models (SAMs)

- Aim: To understand how the assemblage distribution varies as a function of environment

- Cluster species with similar environmental responses into so-called archetypal responses
    - A "partial" finite mixture of regression models

Consider a set of species $j = 1, \ldots, J$ recorded at a set of observational units $i = 1, \ldots, N$, along with covariates $\boldsymbol{x}_i$. Let $z_{jk} = 1$ if species $j = 1, \ldots, J$ belongs to archetype $k = 1, \ldots, K$ and zero otherwise. If we denote $\mu_{ijk} = \mathsf{E}(y_{ij}|\boldsymbol{x}_i, z_{jk} = 1)$, then a species archetypal model or SAM is characterized by

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\end{aligned}
$$

Species archetype models (SAMs)

- Unlike standard mixture models, partial finite mixture of regression models are more computationally burdensome to fit
  - Species-specific intercepts/dispersion parameters often done separately in a conditional maximization step (ECM)
  - Or update all parameters in a single M-step. This requires a single, large memory GLM which may not scale well with N and J (and K)

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\end{aligned}
$$

Approximate and scalable SAMs (asSAMs)

- Approximate each species-archetype contribution with a quadratic/normal approximation
  - Note the maximizer is species-specific!

For species $j = 1, \dots, J$, write $\boldsymbol{\theta}_{jk} = (\alpha_j^\top, \boldsymbol{\beta}_k^\top, \boldsymbol{\phi}_j^\top)^\top$, and let $L_{jk}(\boldsymbol{\theta}_{jk}) = \prod_{i=1}^N f(y_{ij}|\mu_{ijk}, \boldsymbol{\phi}_j)$.

Define $\boxed{\tilde{\boldsymbol{\theta}}_j = (\tilde{\boldsymbol{\alpha}}_j, \tilde{\boldsymbol{\beta}}_j, \tilde{\boldsymbol{\phi}}_j)} = \arg\max_{\boldsymbol{\alpha}_j, \boldsymbol{\beta}_k, \boldsymbol{\phi}_j} \log\{L_{jk}(\boldsymbol{\theta}_{jk})\}$, and $\boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j) = -\nabla^2 \log\{L_{jk}(\tilde{\boldsymbol{\theta}}_j)\}$.

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$$\begin{aligned}
\log\{L_{jk}(\boldsymbol{\theta}_{jk})\} &= \sum_{i=1}^N \log\{f(y_{ij}|\mu_{ijk}, \boldsymbol{\phi}_j)\} \\
&\approx \sum_{i=1}^N \log\{f(y_{ij}|\tilde{\mu}_{ij}, \tilde{\boldsymbol{\phi}}_j)\} - \frac{1}{2}\left(\boldsymbol{\theta}_{jk} - \tilde{\boldsymbol{\theta}}_j\right)^\top \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)\left(\boldsymbol{\theta}_{jk} - \tilde{\boldsymbol{\theta}}_j\right),
\end{aligned}$$

where $\tilde{\mu}_{ij} = g^{-1}(\boldsymbol{u}_i^\top \tilde{\boldsymbol{\alpha}}_j + \boldsymbol{x}_i^\top \tilde{\boldsymbol{\beta}}_j)$.

Approximate and scalable SAMs (asSAMs)

- Approximate each species-archetype contribution with a quadratic/normal approximation
  - Note the maximizer is species-specific!

- After some algebraic manipulation and collecting terms that constant wrt parameters

$$
\begin{aligned}
\ell(\boldsymbol{\Psi}, \boldsymbol{\omega}) &= \sum_{j=1}^{J} \log \left(\sum_{k=1}^{K} \omega_k \exp \left[\log\{ L_{jk}(\boldsymbol{\theta}_{jk}) \} \right] \right) \\
&\approx C_0 + \sum_{j=1}^{J} \log \left[\sum_{k=1}^{K} \omega_k \exp \left\{ -\frac{1}{2} \left(\tilde{\boldsymbol{\theta}}_j - \boldsymbol{\theta}_{jk} \right)^\top \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j) \left(\tilde{\boldsymbol{\theta}}_j - \boldsymbol{\theta}_{jk} \right) \right\} \right] \\
&= C_1 + \sum_{j=1}^{J} \log \left[\sum_{k=1}^{K} \omega_k \mathcal{N} \left\{ \tilde{\boldsymbol{\theta}}_j | \boldsymbol{\theta}_{jk}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1} \right\} \right] \triangleq \ell_{\text{assam}}(\boldsymbol{\Psi}, \boldsymbol{\omega}), \qquad (1)
\end{aligned}
$$

Approximate and scalable SAMs (asSAMs)

- asSAM = finite mixture of multivariate normals with known covariance matrices

- asSAMs is *very* amenable to using EM-algorithm
  - M-step updates are all closed-form (details in manuscript)
  - Need a pre-step to form the quadratic/normal approximation, but we know how to do this!

- Model selection is easy/scalable
  - Choose K using BIC or some variation thereof
  - Archetypal (mixture) coefficients: Deploy sparse linear modelling ideas e.g., LASSO, SCAD, BAR etc...

$$\ell_{\text{assam}}(\boldsymbol{\Psi}, \boldsymbol{\omega}) = \sum_{j=1}^{J} \log \left[\sum_{k=1}^{K} \omega_k \mathcal{N} \left\{ \tilde{\boldsymbol{\theta}}_j | \boldsymbol{\theta}_{jk}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1} \right\} \right]$$

Application to Great Barrier Reef dataset

- Great Barrier Reef Seabed biodiversity project

- Recall:
    - Presence-absence (binary) responses
    - N = 1146 sites sampled
    - J = 235 species (median recorded prevalence = 31)

    - Nine continuous environmental covariates
    - Standardized all to have mean zero and variance one

- asSAMs application
    - All covariates included as linear terms only
    - Bernoulli distribution with logit link
    - BIC to choose K; BAR penalty to perform selection on archetypal coefficients (penalized asSAMs or pasSAMS)

ELSEVIER

Journal of Multivariate Analysis

Volume 168, November 2018, Pages 334-351

Broken adaptive ridge regression and its asymptotic properties

Linlin Dai [a], Kani Chen [b], Zhihua Sun [c], Zhenqiu Liu [d], Gang Li [e]

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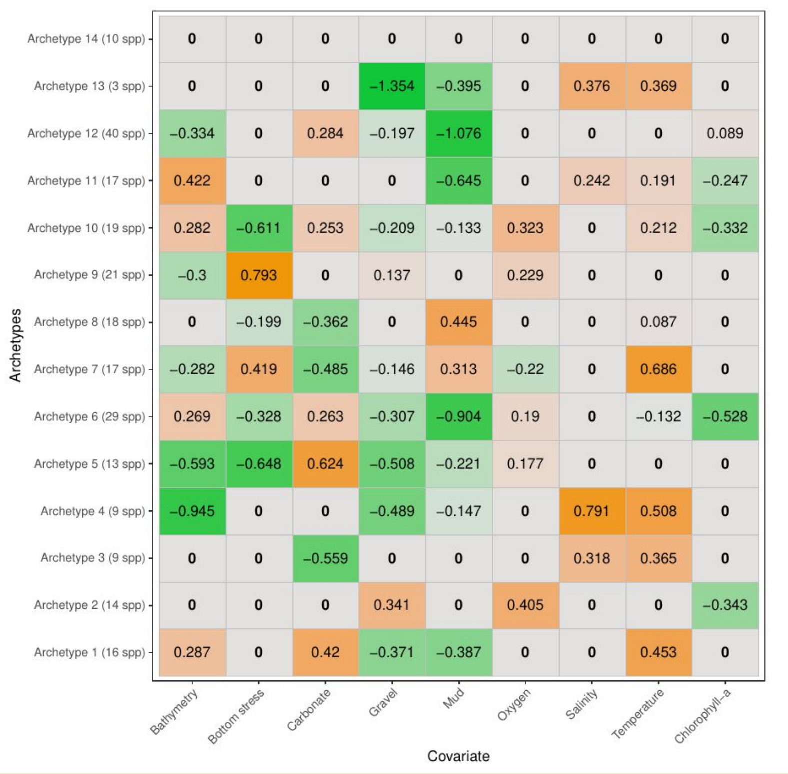
Application to Great Barrier Reef dataset

- Great Barrier Reef Seabed biodiversity project
- asSAMs application
  - K = 14 species archetypes chosen
  - All covariates important
  - Environment-agnostic archetype
  - Most species classified with high probability; this is typical of SAMs



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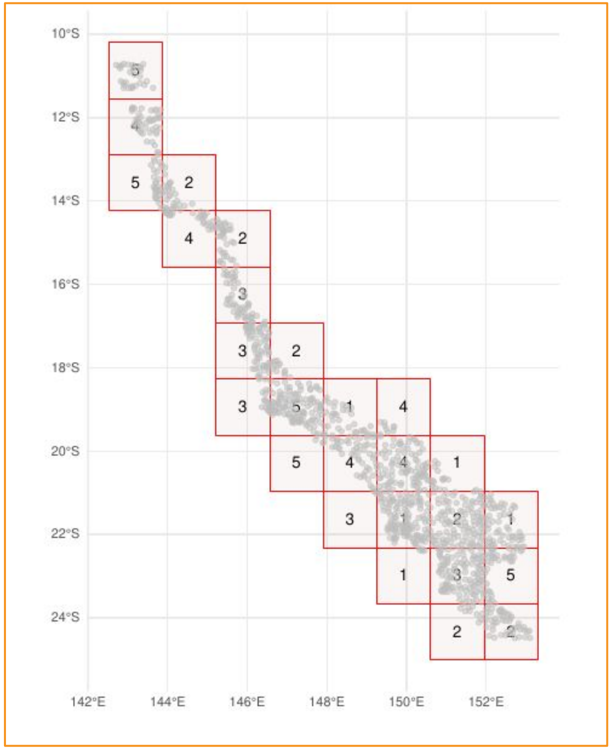
- 5-fold spatial cross-validation to compare predictions
  - Separate logistic regression models
  - Penalized asSAMs or pasSAMs
  - Unpenalized asSAMs i.e., no selection on archetypal coefficients
  - SAMs fitted `ecomix` (no approximations)



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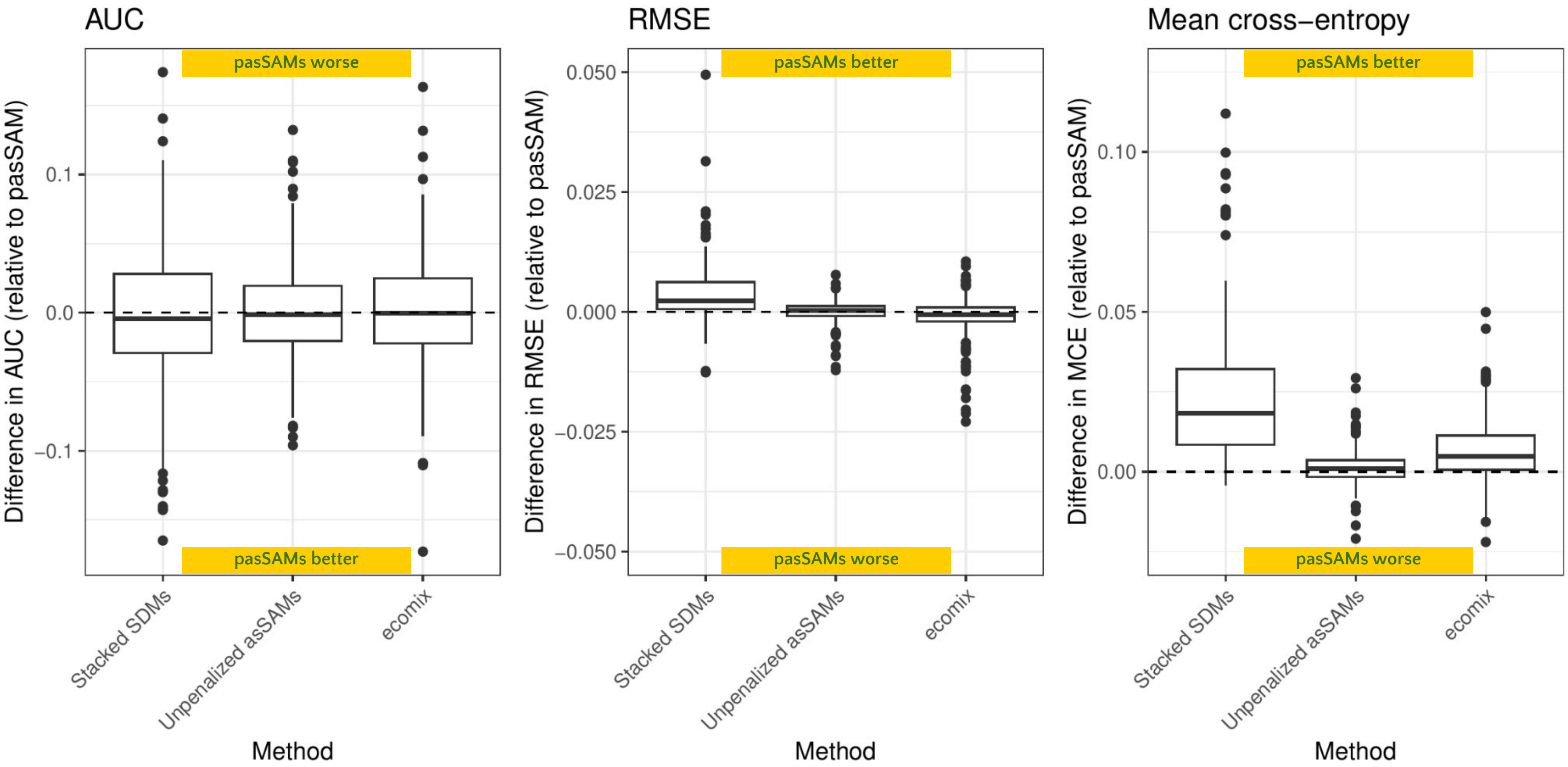


Application to Great Barrier Reef dataset

- Great Barrier Reef Seabed biodiversity project

- asSAMs application
  - K = 14 species archetypes chosen
  - All covariates important
  - Environment-agnostic archetype
  - Most species classified with relatively high probability

- 5-fold spatial cross-validation to compare predictions
  - Separate logistic regression models
  - Penalized asSAMs or pasSAMs
    - ~5.7 mins per fold
  - Unpenalized asSAMs i.e., no selection on archetypal coefficients
    - ~42 seconds per fold
  - SAMs fitted `ecomix` (no approximations)
    - ~56 mins per fold

Concluding remarks

- Manuscript in review; https://github.com/fhui28/assam

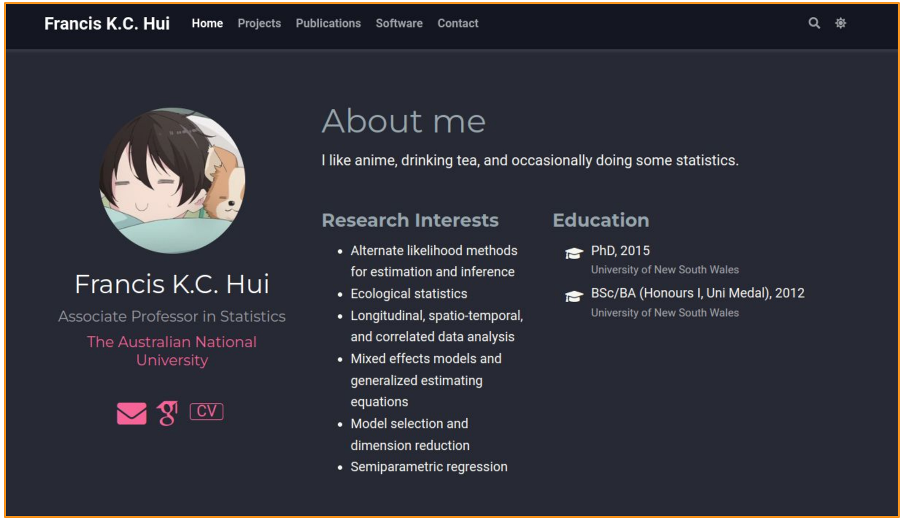
- The package allows:
  - A number of response types
  - Fast approximate bootstrap for uncertainty quantification
  - Specific-specific effects besides intercepts e.g., sampling effort, survey effect
  - Specific-specific spatial fields

- Future extensions to semi-parametric/ML-based archetypal responses

Thanks for listening!

Questions?

- francis.hui@anu.edu.au
- https://francishui.netlify.app/



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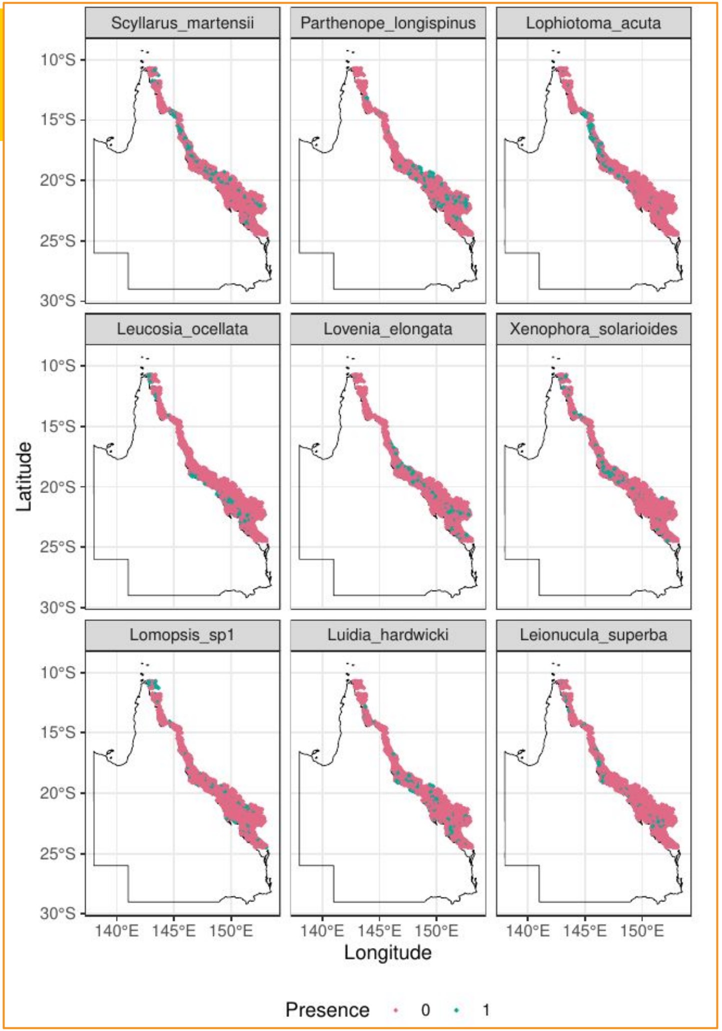
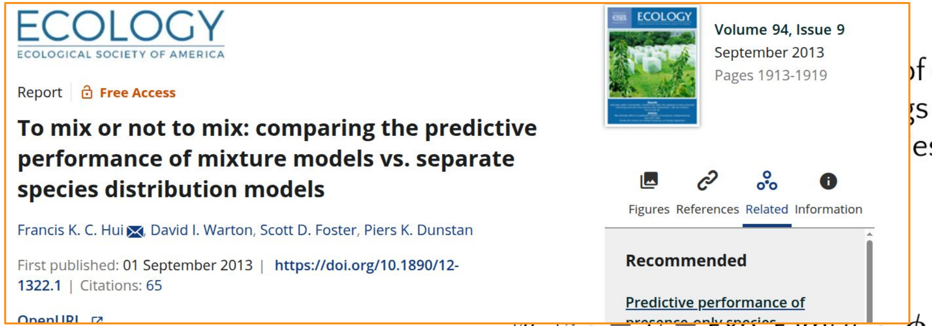


Species archetype models (SAMs)

- Aim: To understand how each species' distribution varies as a function of environment

- Cluster species with similar environmental responses into so-called archetypal responses
  - Simpler interpretation and easier to deploy for ecologist/policy makers
  - Borrow strength across species


ECOLOGY
ECOLOGICAL SOCIETY OF AMERICA

Volume 94, Issue 9
September 2013
Pages 1913-1919

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To mix or not to mix: comparing the predictive performance of mixture models vs. separate species distribution models

Francis K. C. Hui, David I. Warton, Scott D. Foster, Piers K. Dunstan

First published: 01 September 2013 | https://doi.org/10.1890/12-1322.1 | Citations: 65

Figures References Related Information

Recommended

Predictive performance of


Finite Mixture of Regression Modeling for High-Dimensional Count and Biomass Data in Ecology

Published: 16 May 2013

Volume 18, pages 357–375, (2013) Cite this article

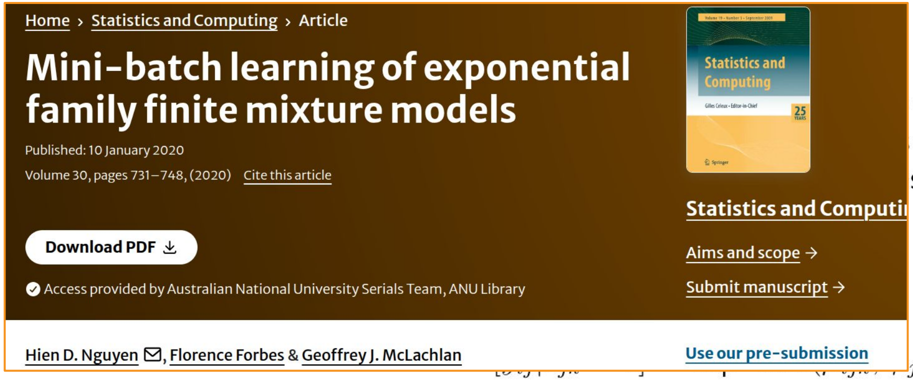
Journal of Agricultural, Biological, and Environ

$$[y_{ij}|z_{jk}=1] = \text{Exp-Fam}(\mu_{ijk}, \phi_j)$$

$$\ell(\Psi) = \sum_{j=1}^{J} \log\left\{\sum_{k=1}^{K} \omega_k \prod_{i=1}^{N} f(y_{ij}|\mu_{ijk}, \phi_j)\right\}$$

Species archetype models (SAMs)

- Unlike standard mixture models, partial finite mixture of regression models are more computationally burdensome to fit
  - Some ways to get around this, but not easy to generalize if we have random effects, smooth covariate terms etc…



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Species archetype models (SAMs)

- Unlike standard mixture models, partial finite mixture of regression models are more computationally burdensome to fit
  - Some ways to get around this, but not easy to generalize if we have random effects, smooth covariate terms etc...

- Unlike (partial) finite mixture of regressions model in other settings, we have multiple observations per "object" we wish to cluster (N sites within each species)

Consider a set of species $j = 1, \dots, J$ recorded at a set of observational units $i = 1, \dots, N$, along with covariates $\boldsymbol{x}_i$. Let $z_{jk} = 1$ if species $j = 1, \dots, J$ belongs to archetype $k = 1, \dots, K$ and zero otherwise. If we denote $\mu_{ijk} = \mathsf{E}(y_{ij}|\boldsymbol{x}_i, z_{jk} = 1)$, then a species archetypal model or SAM is characterized by

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- Aim: To understand how each species' distribution varies as a function of environment

- Cluster species with similar environmental responses into so-called archetypal responses
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  - Borrow strength across species
  - A "partial" finite mixture of regression models

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Approximate and scalable SAMs (asSAMs)

- Inference via bootstrapping
  - Uncertainty due to making the quadratic/normal approximation
  - Uncertainty due to sampling variability given on the approximation

$$\ell_{\text{assam}}(\boldsymbol{\Psi}, \boldsymbol{\omega}) = \sum_{j=1}^{J} \log \left[\sum_{k=1}^{K} \omega_k \mathcal{N} \left\{ \tilde{\boldsymbol{\theta}}_j | \boldsymbol{\theta}_{jk}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1} \right\} \right]$$

Approximate and scalable SAMs (asSAMs)

- Fast approximate bootstrap for asSAMs
  - ~~Uncertainty due to making the quadratic/normal approximation~~ (goes away with large N?)
  - Uncertainty due to sampling variability given the approximation (dominant source; goes away with large J and N?)

$$\ell_{\text{assam}}(\boldsymbol{\Psi}, \boldsymbol{\omega}) = \sum_{j=1}^{J} \log \left[\sum_{k=1}^{K} \omega_k \mathcal{N} \left\{ \tilde{\boldsymbol{\theta}}_j | \boldsymbol{\theta}_{jk}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1} \right\} \right]$$

Approximate and scalable SAMs (asSAMs)

- Fast approximate bootstrap for asSAMs
  - Bootstrap confidence intervals for parameter estimates, fitted values, predictions follow

Given asSAM estimates $(\hat{\boldsymbol{\Psi}}^\top, \hat{\boldsymbol{\omega}}^\top)^\top$,

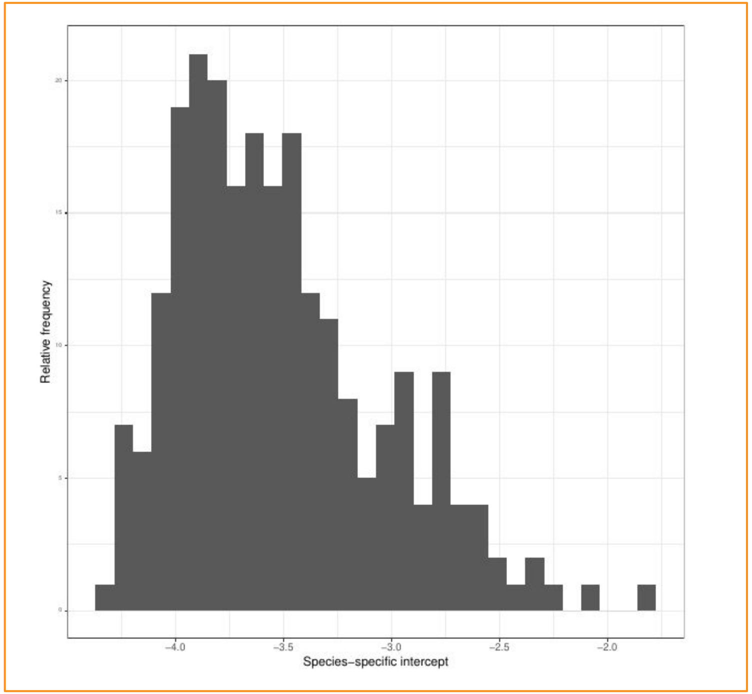
1. For species $j = 1, \ldots, J$, simulate component labels $\boldsymbol{z}_j^* = (z_{j1}^*, \ldots, z_{jK}^*)^\top$ from a multinomial distribution with trial size equal to one and probability vector $\hat{\boldsymbol{\omega}}$;
2. Conditional on $z_{jk}^* = 1$, simulate $\boldsymbol{\theta}_j^* = (\boldsymbol{\alpha}_j^{*\top}, \boldsymbol{\beta}_j^{*\top}, \boldsymbol{\phi}_j^{*\top})^\top$ from a multivariate normal distribution with mean vector $\hat{\boldsymbol{\theta}}_{jk} = (\hat{\boldsymbol{\alpha}}_j^\top, \hat{\boldsymbol{\beta}}_k^\top, \hat{\boldsymbol{\phi}}_j^\top)^\top$ and covariance matrix $\boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1}$;
3. Given bootstrap dataset $\{\boldsymbol{\theta}_j^*; j = 1, \ldots, J\}$, maximize $\ell_{\text{assam}}(\boldsymbol{\Psi}, \boldsymbol{\omega})$ and obtain bootstrap asSAM estimates $(\hat{\boldsymbol{\Psi}}_b^{*\top}, \hat{\boldsymbol{\omega}}_b^{*\top})^\top$.

$$\ell_{\text{assam}}(\boldsymbol{\Psi}, \boldsymbol{\omega}) = \sum_{j=1}^{J} \log \left[\sum_{k=1}^{K} \omega_k \mathcal{N} \left\{ \tilde{\boldsymbol{\theta}}_j | \boldsymbol{\theta}_{jk}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1} \right\} \right]$$

Application to Great Barrier Reef dataset

- Example: Great Barrier Seabed biodiversity project

- asSAMs application
  - K = 14 species archetypes chosen
  - All covariates important
  - Environment-agnostic archetype
  - Most species classified with relatively high probability; this is typical of (as)SAMs
  - The rarity of most species is clear!



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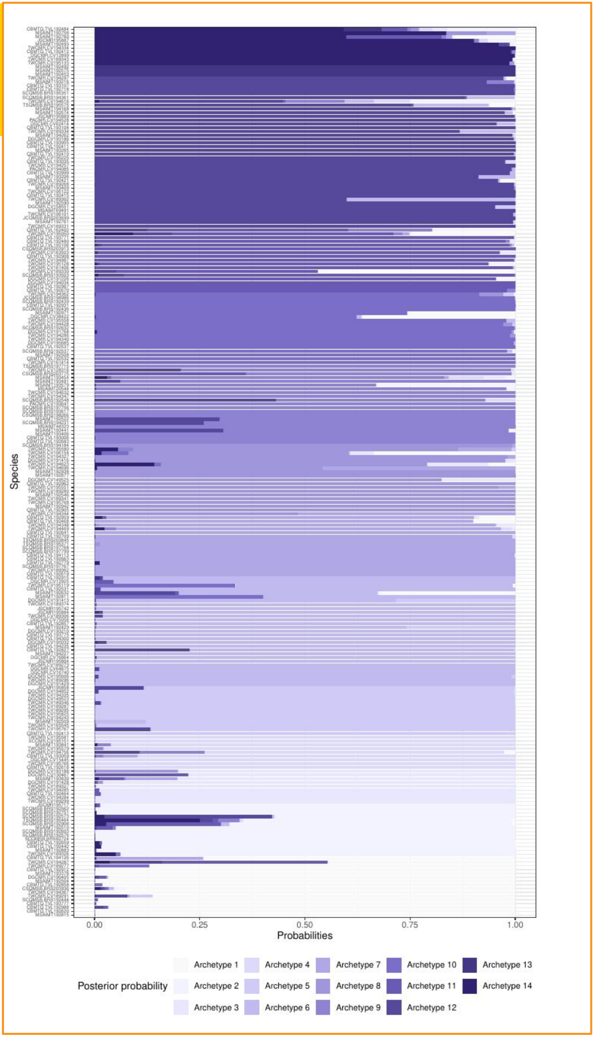

Concluding remarks

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- The package allows:
    - A number of response types
    - Specific-specific effects besides intercepts e.g., sampling effort, survey effect
    - Specific-specific spatial fields

- Extensions to semi-parametric/ML-based archetypa
    - Careful consideration of how to perform the quadratic
      issue here)
    - Spatially-varying effects/spatio-temporal asSAMs foll

- Hierarchical asSAMs?
    - Fit a finite mixture on the species-specific slopes rather than on the responses
    - Allows for heterogeneity within an archetype

Appendix

Algorithm 1 Computing asSAM estimates

Require: Multivariate abundance data $\{(y_{ij}, \boldsymbol{x}_i); i = 1, \ldots, N; j = 1, \ldots, J\}$; number of archetypes set to K; mapping matrix $\boldsymbol{M}$; tolerance value e.g., $\epsilon = 10^{-4}$.

1: Fit J separate generalized linear models, via parallel computing if possible. That is, for $j = 1, \ldots, J$, compute

$$\tilde{\boldsymbol{\theta}}_j = (\tilde{\boldsymbol{\alpha}}_j, \tilde{\boldsymbol{\beta}}_j, \tilde{\boldsymbol{\phi}}_j) = \arg \max_{\boldsymbol{\alpha}_j, \boldsymbol{\beta}_k, \boldsymbol{\phi}_j} \log\{L_{jk}(\boldsymbol{\theta}_{jk})\},$$

and also $\boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j) = -\nabla^2 \log\{L_{jk}(\tilde{\boldsymbol{\theta}}_j)\}$.

2: Construct a set of initial values $(\hat{\boldsymbol{\Psi}}^{(0)\top}, \hat{\boldsymbol{\omega}}^{(0)\top})^\top$ from step 1 e.g., apply a K-medoids algorithm to the estimates $\{\tilde{\boldsymbol{\beta}}_j; j = 1, \ldots, J\}$ to obtain $(\hat{\boldsymbol{\beta}}_1^{(0)\top}, \ldots, \hat{\boldsymbol{\beta}}_K^{(0)\top})^\top$.

3: **for** $t = 1, 2 \ldots$ **do**

- *E-step:* Construct $\hat{\boldsymbol{\theta}}_{jk}^{(t)} = (\hat{\boldsymbol{\alpha}}_j^{(t)}, \hat{\boldsymbol{\beta}}_k^{(t)\top}, \hat{\boldsymbol{\phi}}_j^{(t)\top})^\top$, and compute the posterior probabilities

$$\hat{\tau}_{jk}^{(t+1)} = \frac{\hat{\omega}_k^{(t)} \mathcal{N}\{\tilde{\boldsymbol{\theta}}_j | \hat{\boldsymbol{\theta}}_{jk}^{(t)}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1}\}}{\sum_{k'=1}^K \hat{\omega}_{k'}^{(t)} \mathcal{N}\{\tilde{\boldsymbol{\theta}}_j | \hat{\boldsymbol{\theta}}_{jk'}^{(t)}, \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)^{-1}\}}; \; j = 1 \ldots, J, k = 1, \ldots, K$$

- *M-step:* Update the mixing proportions as $\hat{\omega}_k^{(t+1)} = J^{-1} \sum_{j=1}^J \hat{\tau}_{jk}^{(t+1)}$, and the remaining parameters as

$$\hat{\boldsymbol{\Psi}}^{(t+1)} = \left(\boldsymbol{M}^\top \boldsymbol{W}^{(t+1)} \boldsymbol{M}\right)^{-1} \boldsymbol{M}^\top \boldsymbol{W}^{(t+1)} \tilde{\boldsymbol{\Theta}},$$

where $\tilde{\boldsymbol{\Theta}} = (\boldsymbol{1}_K^\top \otimes \tilde{\boldsymbol{\theta}}_1^\top, \ldots, \boldsymbol{1}_K^\top \otimes \tilde{\boldsymbol{\theta}}_J^\top)^\top$ and $\boldsymbol{W}^{(t+1)}$ is a block-diagonal matrix where block $j = 1, \ldots, J$ equals $\text{Diag}(\hat{\boldsymbol{\tau}}_j^{(t+1)}) \otimes \boldsymbol{I}(\tilde{\boldsymbol{\theta}}_j)$.

until $|\ell_{\text{assam}}(\hat{\boldsymbol{\Psi}}^{(t+1)}, \hat{\boldsymbol{\omega}}^{(t+1)}) - \ell_{\text{assam}}(\hat{\boldsymbol{\Psi}}^{(t)}, \hat{\boldsymbol{\omega}}^{(t)})| < \epsilon$.

4: **end for**

5: **return** Estimates $(\hat{\boldsymbol{\Psi}}^\top, \hat{\boldsymbol{\omega}}^\top)^\top$ and posterior probabilities $\{\hat{\tau}_{jk}; j = 1, \ldots, j; k = 1, \ldots, K\}$.