MY-RES Project: Improving Realism of EEMs

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1 Introduction

This project aims to improve the realism of the ensemble ecosystem model (EEM) generation process by incorporating constraints on the steady-state abundances (n^*) of species in a network. To do this, we use a modified version of the Barbier et al. (2021) algorithm for its key strength of being able to sample interaction strengths α characterising feasible ecosystems with 100% acceptance rate. Significantly, this allows for the generation of feasible parameter sets based on supplied values of n^* and r, which in turn, eliminates the need (and the computational cost required) to check the feasibility (and realism) of sampled parameter sets. Achieving this requires adapting the Barbier et al. (2021) algorithm to a system of generalised Lotka-Volterra equations, which was accomplished through the following modifications,

1. Rewriting the algorithm to remove expectation of negative interactions (section 3)
2. Rewriting the algorithm to avoid elimination of α_{ii} from computations (section 4)
3. Rewriting the algorithm to avoid elimination of r from computations (section 5)
4. Amend the algorithm such that interaction strengths α_{ij} may be drawn from normal distributions that differ in their mean and variance between different elements α_{ii} of the matrix α (section 6).
5. Amend the algorithm to allow pre-supposed network structures, such as those with interaction strengths set to zero (section 8)

In addition to these changes, a more streamlined version of this algorithm was derived using the Cong et al. (2017) algorithm - a fast simulation method for sampling multivariate distributions subject to linear constraints. Whilst retaining all the key properties of the original Barbier et al. (2021) algorithm, this new algorithm does not require the usage of a Gram-Schmidt type process to generate a rotation matrix, hence, proves simpler to implement and more efficient to compute.

2 Implementation of Barbier et al. (2021) and Cong et al. (2017) Algorithms

2.1 Problem Statement

Assuming interactions strengths β_{ij} are drawn from randomly from the same Gaussian distribution,

$$\beta_{ij} \sim \mathcal{N}\left(\overline{\beta}, \langle \beta_c^2 \rangle\right) \tag{1}$$

Barbier et al. (2021) defines an exact algorithm for sampling feasible (but not necessarily stable) ecosystems modelled on a specific form of the generalised Lotka-Volterra equations:

$$\frac{d\eta_i}{dt} = r_i \eta_i \left(1 - \eta_i - \sum_{\substack{j=1 \\ j \neq i}}^{S} \beta_{ij} \eta_j \right) \tag{2}$$

Which at a steady-state becomes,

$$1 - \eta_i - \sum_{\substack{j=1 \\ j \neq i}}^{S} \beta_{ij} \eta_j = 0 \tag{3}$$

Besides requiring interactions strengths to be drawn from the same distribution, this model is also subject to the assumptions that:

- The steady state abundances $\boldsymbol{n^*}$ are known
- Interactions strengths are mostly expected to have a negative sign
- No network structure is pre-supposed
- The generalised Lotka-Volterra equations are scaled to eliminate both $\mathbf{r}$ and α_{ii} from computations

In the following sections, modifications to the Barbier et al (2021) algorithm are thus explored in order to overcome the last three context-specific limitations.

2.2 Analytical Formula for Mean and Variance

Wherev

- β_i is a column vector whose elements contain the ith row of the matrix β without β_{ii}
- $\eta_{\setminus i}$ is a column vector whose elements are the relative yields η without η_i

$$\mu_{\beta_i} = \frac{(1-\eta_i)}{|\boldsymbol{\eta_{\setminus i}}|^2} + \overline{\beta}\mathbf{1} - \overline{\beta}\frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\mathbf{1} \tag{4}$$

$$\Sigma_{\beta_i} = \langle \beta_c^2 \rangle \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2} \right] \tag{5}$$

2.3 Barbier et al. (2021) Sampling Algorithm

1. For a given $\eta_{\setminus i}$, calculate a rotation matrix R whose first row is $a = \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|}$ and all other rows are orthonormal to a and to each other (e.g. through the Gram-Schmidt process)
2. Set $x_1 = \frac{(1-\eta_i)}{|\eta_{\setminus i}|}$
3. Sample $\mathbf{x_{\setminus 1}} \sim \mathcal{N}(\overline{\beta} R_{\setminus 1}\mathbf{1},\, \langle \beta^2 \rangle_c I)$

4. Set $\boldsymbol{x} = \begin{bmatrix} x_1 \\ \mathbf{x_{\setminus 1}} \end{bmatrix}$, and thereafter obtain $\beta_i = R^T \boldsymbol{x}$

5. Repeat steps 1-4 for all rows of β to obtain a sampled matrix β that is drawn from $\beta_{ii} = 1,\ \beta_{ij} \sim \mathcal{N}\left(\overline{\beta}, \langle\beta_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i - \sum_{\substack{j=1 \\ j\neq i}}^{S} \beta_{ij}\eta_j = 0$

2.4 Cong et al. (2017) Sampling Algorithm

1. Sample $y \sim \left(\overline{\beta}, \langle\beta_c^2\rangle\right)$

2. Thereafter obtain $\beta_i = \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right] y + \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|^2}(1 - \eta_i)$

3. Repeat steps 1-2 for all rows of β to obtain a sampled matrix β that is drawn from $\beta_{ii} = 1,\ \beta_{ij} \sim \mathcal{N}\left(\overline{\beta}, \langle\beta_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i - \sum_{\substack{j=1 \\ j\neq i}}^{S} \beta_{ij}\eta_j = 0$

3 Remove Expectation of Negative Interactions ($\beta_{ij} \to -\alpha_{ij}$)

3.1 Problem Statement

Assuming $\alpha_{ii} = -\beta_{ii} = -1$, the steady state equation becomes,

$$\frac{d\eta_i}{dt} = r_i \eta_i \left(1 - \eta_i + \sum_{\substack{j=1 \\ j \neq i}}^{S} \alpha_{ij} \eta_j \right)$$

$$1 - \eta_i + \sum_{\substack{j=1 \\ j \neq i}}^{S} \alpha_{ij} \eta_j = 0 \tag{6}$$

Where,

$$\alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle \alpha_{c}^{2} \rangle\right) \tag{7}$$

We are to develop a new expression for μ_{α_i} and Σ_{α_i}.

3.2 Analytical Formula for Mean and Variance

Where

- α_i is a column vector whose elements contain the ith row of the matrix α without α_{ii}
- $\delta()$ is the Dirac delta function
- $\cdot$ is the vector dot product
- $w = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$
- $R\eta_{\setminus i} = |\eta_{\setminus i}| w$

$$\begin{aligned} p(\boldsymbol{\alpha_i}|\boldsymbol{\eta}) &\propto f(\boldsymbol{\alpha_i};\ \overline{\alpha}\mathbf{1},\ \langle \alpha^2 \rangle_c I) \times \delta(1 - \eta_i + \sum_{\substack{j=1 \\ j \neq i}}^{S} \alpha_{ij}\eta_j) \\ &\propto f(\boldsymbol{\alpha_i};\ \overline{\alpha}\mathbf{1},\ \langle \alpha^2 \rangle_c I) \times \delta(\alpha_i \cdot \eta_{\setminus i} - \eta_i + 1) \\ &\propto f(\boldsymbol{\alpha_i};\ \overline{\alpha}\mathbf{1},\ \langle \alpha^2 \rangle_c I) \times \delta(|\eta_{\setminus i}| x_1 - \eta_i + 1) \end{aligned}$$

Note: the key change as a result of $\beta_{ij} \to -\alpha_{ij}$ appears in the Dirac delta function, and results in,

$$\begin{aligned} 0 &= |\eta_{\setminus i}| x_1 - \eta_i + 1 \\ < x_1 > &= (\eta_i - 1)/|\eta_{\setminus i}| \end{aligned}$$

Applying a rotation transformation on $\boldsymbol{\alpha_i}$ with the rotation matrix R,

$$x = R\boldsymbol{\alpha_i}$$

The equation above transforms into,

$$\begin{aligned} p(\boldsymbol{x}|\boldsymbol{\eta}) &\propto f(\boldsymbol{x};\ \overline{\alpha}R\mathbf{1},\ \langle \alpha^2 \rangle_c I) \times \delta(|\eta_{\setminus i}| x_1 - \eta_i + 1) \\ &= f(\boldsymbol{x};\ \boldsymbol{w}(\eta_i - 1)/|\eta_{\setminus i}|) + (I - \boldsymbol{w}\boldsymbol{w}^T)\overline{\alpha}R\mathbf{1}, \langle \alpha_c^2 \rangle (I - \boldsymbol{w}\boldsymbol{w}^T)) \end{aligned}$$

3.2.1 Mean

Transforming back,

$$\begin{aligned}
\boldsymbol{\mu}_{\boldsymbol{\alpha_i}} &= R^T \boldsymbol{\mu}_{\boldsymbol{x}} \\
&= R^T [\boldsymbol{w}(\eta_i - 1)/|\eta_{\setminus i}|) + (I - \boldsymbol{w}\boldsymbol{w}^T)\overline{\alpha} R \mathbf{1}] \\
&= (\eta_i - 1)/|\eta_{\setminus i}|) \times R^T \boldsymbol{w} + \overline{\alpha}[R^T I R - R^T \boldsymbol{w}\boldsymbol{w}^T R]\mathbf{1} \\
&= (\eta_i - 1)/|\eta_{\setminus i}|) \times R^T \boldsymbol{w} + \overline{\alpha}[I - R^T \boldsymbol{w}(R\boldsymbol{w}^T)^T]\mathbf{1} \\
&= (\eta_i - 1)/|\eta_{\setminus i}|) \times R^T \boldsymbol{w} + \overline{\alpha}\mathbf{1} - \overline{\alpha} R^T \boldsymbol{w}(R\boldsymbol{w}^T)^T]\mathbf{1} \\
&= \frac{(\eta_i - 1)\eta_{\setminus i}}{|\boldsymbol{\eta_{\setminus i}}|^2} + \overline{\alpha}\mathbf{1} - \overline{\alpha}\frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\mathbf{1}
\end{aligned}$$

Note: $R\boldsymbol{w}^T = \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|}$

3.2.2 Variance

$$\Sigma_{\alpha_i} = \langle \alpha_c^2 \rangle \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2} \right] \tag{8}$$

3.3 Barbier et al. Sampling Algorithm

1. For a given $\eta_{\setminus i}$, calculate a rotation matrix R whose first row is $a = \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|}$ and all other rows are orthonormal to a and to each other (e.g. through the Gram-Schmidt process)
2. Set $x_1 = \frac{(\eta_i - 1)}{|\eta_{\setminus i}|}$
3. Sample $\boldsymbol{x_{\setminus 1}} \sim \mathcal{N}(\overline{\alpha} R_{\setminus 1}\mathbf{1},\, \langle \alpha^2 \rangle_c I)$
4. Set $\boldsymbol{x} = \begin{bmatrix} x_1 \\ \boldsymbol{x_{\setminus 1}} \end{bmatrix}$, and thereafter obtain $\alpha_i = R^T \boldsymbol{x}$
5. Repeat steps 1-4 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle \alpha_c^2 \rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1 \\ j \neq i}}^{S} \alpha_{ij}\eta_j = 0$

3.4 Cong et al. Sampling Algorithm

1. Sample $y \sim \left(\overline{\alpha}, \langle \alpha_c^2 \rangle\right)$
2. Thereafter obtain $\alpha_i = \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2} \right] y + \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|^2}(\eta_i - 1)$
3. Repeat steps 1-2 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle \alpha_c^2 \rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1 \\ j \neq i}}^{S} \alpha_{ij}\eta_j = 0$

4 Reintroducing α_{ii} $(-1 \rightarrow \alpha_{ii})$

4.1 Problem Statement

Assuming $-1 \rightarrow \alpha_{ii}$, the steady state equation becomes,

$$\frac{d\eta_i}{dt} = r_i\eta_i \left(1 + \alpha_{ii}\eta_i + \sum_{\substack{j=1\\ j\neq i}}^{S} \alpha_{ij}\eta_j\right)$$

$$= r_i\eta_i \left(1 + \sum_{j=1}^{S} \alpha_{ij}\eta_j\right)$$

$$1 + \sum_{j=1}^{S} \alpha_{ij}\eta_j = 0 \tag{9}$$

Where,

$$\alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right) \tag{10}$$

We are to develop a new expression for μ_{α_i} and Σ_{α_i}.

4.2 Analytical Formula for Mean and Variance

$$\mu_{\alpha_i} = \frac{(-\alpha_{ii}\eta_i - 1)\eta_i}{|\boldsymbol{\eta_{\setminus i}}|^2} + \overline{\alpha}\mathbf{1} - \overline{\alpha}\frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\mathbf{1} \tag{11}$$

$$\Sigma_{\alpha_i} = \langle\alpha_c^2\rangle \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right] \tag{12}$$

4.3 Barbier et al. Sampling Algorithm

1. For a given $\eta_{\setminus i}$, calculate a rotation matrix R whose first row is $a = \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|}$ and all other rows are orthonormal to a and to each other (e.g. through the Gram-Schmidt process)

2. Set $x_1 = \frac{(-\alpha_{ii}\eta_i - 1)}{|\eta_{\setminus i}|}$

3. Sample $\boldsymbol{x_{\setminus 1}} \sim \mathcal{N}(\overline{\alpha}R_{\setminus 1}\mathbf{1},\ \langle\alpha^2\rangle_c I)$

4. Set $\boldsymbol{x} = \begin{bmatrix} x_1 \\ \boldsymbol{x_{\setminus 1}} \end{bmatrix}$

5. Repeat steps 1-4 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1\\ j\neq i}}^{S} \alpha_{ij}\eta_j = 0$

4.4 Cong et al. Sampling Algorithm

1. Sample $y \sim \left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$

2. Thereafter obtain $\alpha_i = \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right] y - \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|^2}(\alpha_{ii}\eta_i + 1)$

3. Repeat steps 1-2 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1\\ j\neq i}}^{S} \alpha_{ij}\eta_j = 0$

5 Reintroducing r $(r_i\alpha_{ij} \to \alpha_{ij})$

5.1 Problem Statement

Assuming $r_i\alpha_{ij} \to \alpha_{ij}$, the steady state equation becomes,

$$\frac{d\eta_i}{dt} = r_i\eta_i\left(1 + \sum_{j=1}^{S}\alpha_{ij}\eta_j\right)$$

$$r_i\eta_i + \sum_{j=1}^{S}\alpha_{ij}\eta_i\eta_j = 0 \tag{13}$$

Where,

$$\alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right) \tag{14}$$

We are to develop a new expression for μ_{α_i} and Σ_{α_i}.

5.2 Analytical Formula for Mean and Variance

$$\mu_{\alpha_i} = \frac{(-\alpha_{ii}\eta_i - r_i)\eta_i}{|\boldsymbol{\eta_{\setminus i}}|^2} + \overline{\alpha}\mathbf{1} - \overline{\alpha}\frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\mathbf{1} \tag{15}$$

$$\Sigma_{\alpha_i} = \langle\alpha_c^2\rangle\left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right] \tag{16}$$

5.3 Barbier et al. Sampling Algorithm

1. For a given $\eta_{\setminus i}$, calculate a rotation matrix R whose first row is $a = \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|}$ and all other rows are orthonormal to a and to each other (e.g. through the Gram-Schmidt process)
2. Set $x_1 = \frac{(-\alpha_{ii}\eta_i - r_i)}{|\eta_{\setminus i}|}$
3. Sample $\boldsymbol{x}_{\setminus\mathbf{1}} \sim \mathcal{N}(\overline{\alpha}R_{\setminus 1}\mathbf{1},\ \langle\alpha^2\rangle_c I)$
4. Set $\boldsymbol{x} = \begin{bmatrix} x_1 \\ \boldsymbol{x}_{\setminus\mathbf{1}} \end{bmatrix}$
5. Repeat steps 1-4 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1 \\ j\neq i}}^{S}\alpha_{ij}\eta_j = 0$

5.4 Cong et al. Sampling Algorithm

1. Sample $y \sim \left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$
2. Thereafter obtain $\alpha_i = \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right]y - \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|^2}(\alpha_{ii}\eta_i + r_i)$
3. Repeat steps 1-2 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1 \\ j\neq i}}^{S}\alpha_{ij}\eta_j = 0$

6 Sampling Interactions Strengths from Individual Distributions

6.1 Problem Statement

Instead of sampling interaction strengths from a single mean and variance,

$$\alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right) \tag{17}$$

We want to sample from individual means and variances,

$$\alpha_{ij} \sim N\left(\overline{\alpha_{ij}}, \langle\alpha_{ij}^2\rangle_c\right) \tag{18}$$

The following modifications enable this - allowing interaction strength mean and variance matrices as inputs (excluding diagonal elements).

6.2 Analytical Formula for Mean and Variance

Where

$\overline{\boldsymbol{\alpha_i}}$ is the ith row of the alpha mean matrix excluding $\overline{\alpha_{ii}}$

$\langle\alpha_i^2\rangle_c$ is the ith row of the alpha covariance matrix excluding $\langle\alpha_{ii}^2\rangle_c$

$$\mu_{\alpha_i} = \frac{(-\alpha_{ii}\eta_i - r_i)\eta_i}{|\boldsymbol{\eta_{\setminus i}}|^2} + \overline{\alpha_i} - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\overline{\alpha_{\mathbf{i}}} \tag{19}$$

$$\Sigma_{\alpha_i} = \langle\alpha_i^2\rangle_c\left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right] \tag{20}$$

6.3 Barbier et al. Sampling Algorithm

1. For a given $\eta_{\setminus i}$, calculate the rotation matrix R whose first row is $a = \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|}$ and all other rows are orthonormal to a and to each other (e.g. through Gram-Schmidt process)
2. Set $x_1 = \frac{(-\alpha_{ii}\eta_i - r_i)}{|\eta_{\setminus i}|}$
3. Sample $x_{\setminus 1} \sim \mathcal{N}(R_{\setminus 1}\overline{\alpha_i},\ \langle\alpha_i^2\rangle_c)$
4. Set $\boldsymbol{x} = \begin{bmatrix} x_1 \\ \boldsymbol{x_{\setminus 1}} \end{bmatrix}$
5. Repeat steps 1-4 for all rows of α to obtain a sampled matrix α that is drawn from $\alpha_{ii} = 1,\ \alpha_{ij} \sim \mathcal{N}\left(\overline{\alpha}, \langle\alpha_c^2\rangle\right)$ for all $i \neq j$ conditional on $1 - \eta_i + \sum_{\substack{j=1 \\ j\neq i}}^{S} \alpha_{ij}\eta_j = 0$

6.4 Cong et al. Sampling Algorithm

1. Sample $y \sim \mathcal{N}(\overline{\alpha_i},\ \langle\alpha_i^2\rangle_c)$
2. Thereafter obtain $\alpha_i = \left[I - \frac{\eta_{\setminus i}\eta_{\setminus i}^T}{|\eta_{\setminus i}|^2}\right] y - \frac{\eta_{\setminus i}}{|\eta_{\setminus i}|^2}(\alpha_{ii}\eta_i + r_i)$
3. Repeat steps 1-2 for all rows of α to obtain a sampled matrix α

7 Appendix

Tom's Notes

- A conversion from relative yields to species abundances can be performed as:

$$n_i = -\frac{\eta_i \alpha_{ii}}{r_i}$$

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