

1 Method 1

Suppose we take time series data points, N (indexed by a) from each of S species.

$$X_i^a \rightarrow X^1 = \begin{bmatrix} x_1^1 \\ x_2^1 \\ \vdots \\ x_S^1 \end{bmatrix}, X^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \vdots \\ x_S^2 \end{bmatrix}, \dots, X^N = \begin{bmatrix} x_1^N \\ x_2^N \\ \vdots \\ x_S^N \end{bmatrix}$$

Goal: Maximizing $P(X|\mu, \sigma^2, d)$

Assumptions:

1). A is a symmetric S by S matrix

2). $A_{ij} = \frac{\mu}{S} + B_{ij}$, where $B_{ij} \sim N(0, \frac{\sigma^2}{S})$, i.e. $A_{ij} \sim N(\frac{\mu}{S}, \frac{\sigma^2}{S})$ 3). $A_{ii} = -d + \frac{\mu}{S}$

4). For A sufficiently large, the determinants of A for different random entries are similar so we use the average determinat of A in place of A. $\langle \det A \rangle = D(\mu, \sigma^2, d)$

Since, x_i are independent, the average probability of observing x_i given μ, σ, d :

$$P(x|\mu, \sigma^2, d) = \int dA \prod (P(x^a|A)P(A|\mu, \sigma^2, d))$$

we can pull the product out and distribute it to each term

$$= \int (\prod_{i<j} (dA_{ij}) \frac{(\det A)^{N/2}}{(2\pi)^{NS/2}} \exp(\frac{1}{2} \sum_{a=1}^N \sum_{ij} x_i^a A_{ij} x_j^a) P(A|\mu, \sigma^2, d))$$

Given our assumptions:

$$= \frac{\langle \det A \rangle^{N/2}}{(2\pi)^{NS/2}} \int (\prod_{i<j} dB_{ij}) \exp(\frac{1}{2} \sum_{a=1}^N (-d \sum (x_i^a)^2 + \frac{\mu}{S} \sum_{ij} x_i^a x_j^a + \sum_{i<j} x_i B_{ij} x_j)) P(B|\sigma^2))$$

pulling out the terms separte from B_{ij}

$$= \frac{\langle \det A \rangle^{N/2}}{(2\pi)^{NS/2}} \exp(\frac{-d}{2} \sum_{a=1}^N \sum_{i=1}^S (x_i^a)^2 + \frac{\mu}{2S} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2) \times \int ((\prod_{ij} dB_{ij}) \exp(\sum_{a=1}^N \sum_{i<j} x_i^a B_{ij} x_j^a) \exp(-\sum_{i<j} \frac{B_{ij}^2}{2\sigma^2/S})) \times (\sqrt{\frac{S}{2\pi}} \frac{1}{\sigma})$$

The first part of the integral becomes

$$\prod_{i<j} dB_{ij} \rightarrow \prod_{i<j} \exp(\frac{\sigma^2}{2S} (\sum_{a=1}^N x_i^a x_j^a)^2) = \exp(\frac{\sigma^2}{4S} \sum_{ij} \sum_a x_i^a x_j^a \sum_b x_i^b x_j^b)$$

Then we can condense the summations and obtain:

$$\exp(\frac{\sigma^2}{4S} \sum_{ab} (\sum_i x_i^a x_i^b)^2)$$

The portion in the exponent becomes

$$\prod_{i < j} \exp(-\frac{B_{ij}^2}{2\sigma^2/S} + \sum_{a=1}^N x_i^a B_{ij} x_j^a) \sqrt{\frac{S}{2\pi}} \frac{1}{\sigma}$$

After rearranging the terms we get

$$\prod_{i < j} dB_{ij} \sqrt{\frac{S}{2\pi}} \frac{1}{\sigma} \exp(-\frac{B_{ij}^2}{2\sigma^2/S} + \sum_{a=1}^N x_i^a B_{ij} x_j^a)$$

$$\text{Let } y = B_{ij}, \tau = \frac{\sigma}{\sqrt{S}}, z = \sum_{a=1}^N x_i^a x_j^a$$

Then our integral becomes :

$$\int dy \sqrt{\frac{1}{2\pi}} \frac{1}{\tau} \exp(\frac{-y^2}{2\tau^2} + yz)$$

Which when solved, simplifies to:

$$\exp(\frac{\tau^2 z^2}{2})$$

Now let us denote $P(x|\mu, \sigma, d)$ as P:

$$P = D \times \exp(\frac{-d}{2} \sum_{a=1}^N \sum_{i=1}^S (x_i^a)^2 + \frac{\mu}{2S} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2 + \frac{\sigma^2}{4S} \sum_{ab} (\sum_i x_i^a x_i^b)^2)$$

$$\frac{2}{N} \log P = \log D - \frac{d}{N} \sum_{a=1}^N \sum_{i=1}^S (x_i^a)^2 - \frac{\mu}{SN} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2 + \frac{\sigma^2}{2SN} \sum_{ab} (\sum_i x_i^a x_i^b)^2$$

1.1 Optimization

To optimize P we take the partial derivatives wrt μ, σ , and d and set them all equal to 0

- 1). $\frac{2}{N} \frac{\partial \log P}{\partial d} = \frac{1}{D} \frac{\partial D}{\partial d} - \frac{1}{N} \sum_{a=1}^N \sum_{i=1}^S (x_i^a)^2 = 0$
- 2). $\frac{2}{N} \frac{\partial \log P}{\partial \sigma^2} = \frac{1}{D} \frac{\partial D}{\partial \sigma^2} + \frac{1}{2SN} \sum_{ab} (\sum_i x_i^a x_i^b)^2 = 0$
- 3). $\frac{2}{N} \frac{\partial \log P}{\partial \mu} = \frac{1}{D} \frac{\partial D}{\partial \mu} - \frac{1}{SN} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2 = 0$

1.2 Determinant of A

The average determinant as given to us by the semicircular law in Random Matrix Theory-Robert Wiegner

$$\langle \log D \rangle = \sum_i \log(\lambda_i) = \log(d + \mu) + (S - 1) \int d\lambda \frac{\sqrt{4\sigma^2 - (\lambda + d)^2}}{2\pi\sigma} \log(\lambda)$$

We evaluate this integral from $-d - 2\sigma$ to $-d + 2\sigma$ as that is the radius in which all of our eigenvalues lie according to the semicircular law. Let $z = \frac{\lambda - d}{2\sigma}$, $b = \frac{2d}{\sigma}$ so $\lambda \rightarrow 2\sigma z + d$, $d\lambda \rightarrow 2\sigma dz$. Now we divide everything by 2σ and the integral:

$$\int_{-d/2\sigma-1}^{-d/2\sigma+1} d\lambda \frac{\sqrt{1 - (\frac{\lambda - d}{2\sigma})^2}}{2\pi\sigma} \log(\frac{\lambda}{2\sigma}) + \log(2\sigma)$$

becomes:

$$I = \frac{2\sigma}{\pi} [\log(2\sigma) \int_{-b-1}^{-b+1} dz \sqrt{1 - z^2} + \int_{-b-1}^{-b+1} dz \log(z + b) \sqrt{1 - z^2}]$$

By using mathematica we solve the integral, where $F_{3,1}$ is the Hypergeometric function $HypergeometricPFQ[(1, 1, \frac{3}{2}), (2, 3), \frac{1}{b^2}]$:

$$I = \log(d) - \frac{\sigma^2}{2d^2} [F_{3,1}(\frac{4\sigma^2}{d^2})]$$

Now we can rewrite the average log determinant as:

$$\frac{1}{S} \langle \log D \rangle = \frac{1}{S} \log(d + \mu) + (1 - \frac{1}{S}) I$$

1.3 Solving the Optimization Equations

Now that we have the $\langle \log D \rangle$ we can solve optimization equations 1)., 2). and 3).

So first let $g(x) = \frac{1}{2} x F_{3,1}(4x)$, Then $g'(x) = \frac{1}{1 + \sqrt{1 - 4x - 2x}}$

Optimization equation 3). becomes

$$\frac{2}{N} \frac{\partial \log P}{\partial \mu} = \frac{1}{d + \mu} - \frac{1}{SN} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2 = 0$$

If we solve optimization equation 3). for $d + \mu$ we get $d + \mu = \frac{SN}{\sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2}$.

We replace $d + \mu$ in optimization equation 1). with this.

Optimization equation 1). becomes:

$$\begin{aligned}\frac{2}{N} \frac{\partial \log P}{\partial d} &= \frac{1}{d} + \frac{2\sigma^2}{d^3} g'(\frac{\sigma^2}{d^2}) - \frac{1}{SN} \sum_{a=1}^N \sum_{i=1}^S (x_i^a)^2 + \frac{1}{S^2 N} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2 = 0 \\ &\rightarrow \frac{1}{d} + \frac{2\sigma^2}{d^3} g'(\frac{\sigma^2}{d^2}) = \frac{1}{SN} \sum_{a=1}^N \sum_{i=1}^S (x_i^a)^2 - \frac{1}{S^2 N} \sum_{a=1}^N (\sum_{i=1}^S x_i^a)^2\end{aligned}$$

Optimization equation 2). becomes:

$$\begin{aligned}\frac{2}{N} \frac{\partial \log P}{\partial \mu} &= -\frac{1}{d^2} g'(\frac{\sigma^2}{d^2}) + \frac{1}{2SN} \sum_{ab} (\sum_i x_i^a x_i^b)^2 = 0 \\ &\rightarrow \frac{1}{S} \frac{1}{2SN} \sum_{ab} (\sum_i x_i^a x_i^b)^2 = \frac{1}{d^2} g'(\frac{\sigma^2}{d^2})\end{aligned}$$

To solve for μ, σ and d we use rootsolvers in R...