

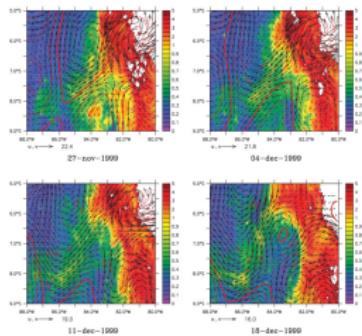
# Empirical Orthogonal Functions and derived methods

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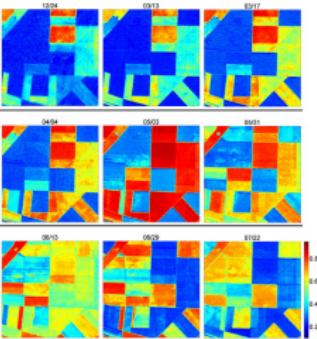
March 2024



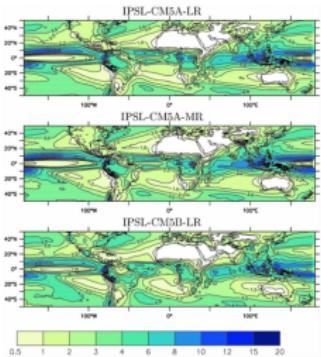
## Oceanography



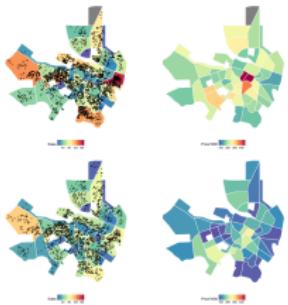
## Agronomy



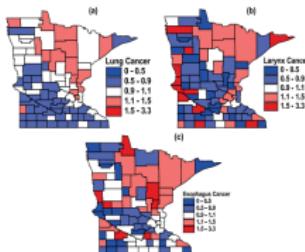
## Climatology



## Economics



## Epidemiology



## Ecology

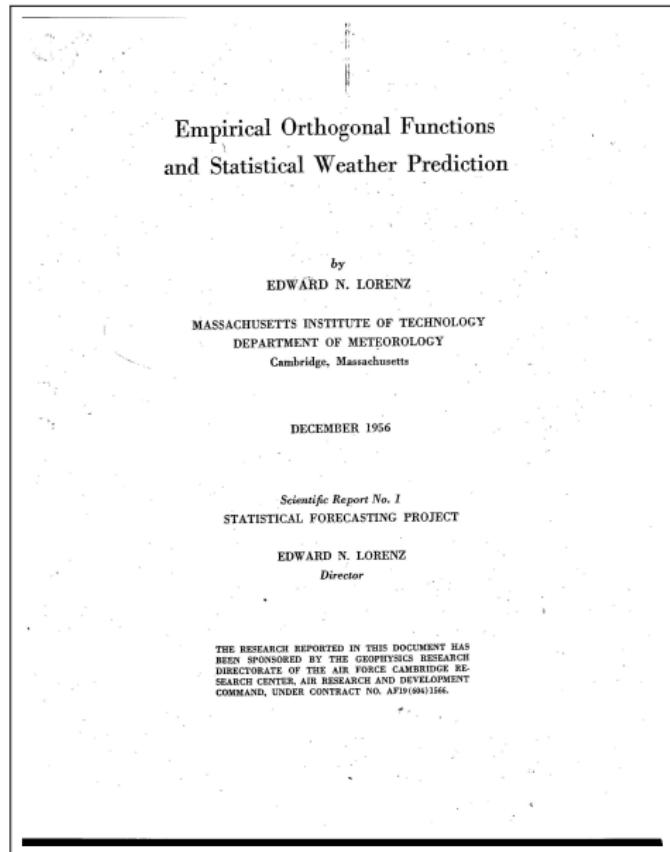
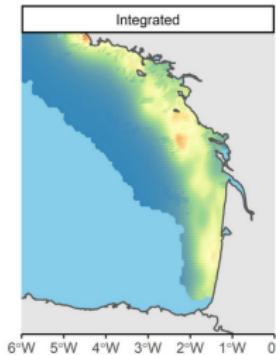


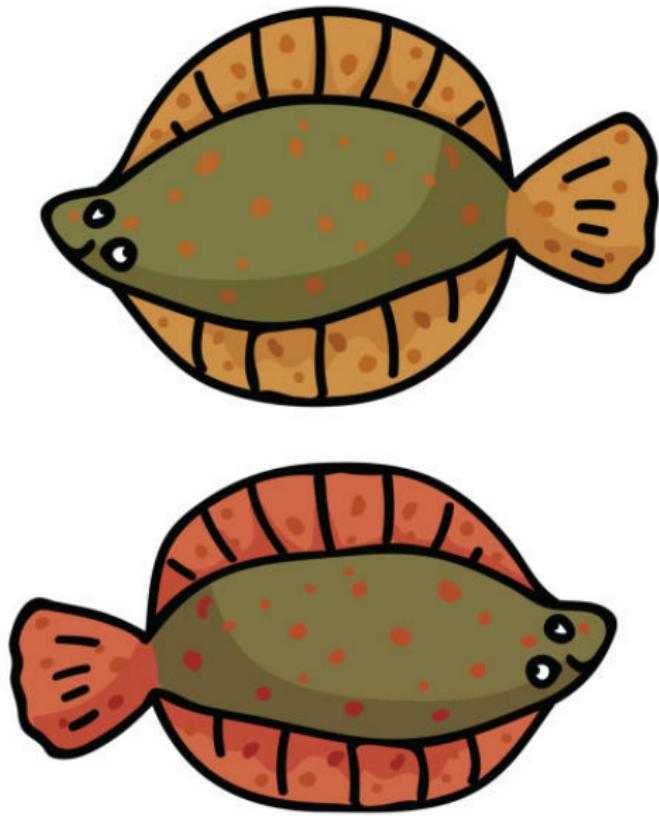
# Empirical Orthogonal Functions

First introduced by Lorenz (1956)

- What is the **best representation** for a spatio-temporal field ?
  - How to perform **dimension-reduction** on a spatio-temporal field ?
  - How to make **projections** ?
- 

Presentation based on a fishery case study.  
Demersal fisheries of the Bay of Biscay.  
Monthly maps from 2008 to 2018 (132 maps)





## Raw data and notations

Let's denote a spatio-temporal process  $S = (S(x, t); x \in \mathbb{R}^2, t \in \{t_1, \dots, t_p\})$ .

The temporal average of  $S$  is denoted:

$$\bar{s}^t(x) = \frac{1}{p} \sum_{k=1}^p S(x, t_k)$$

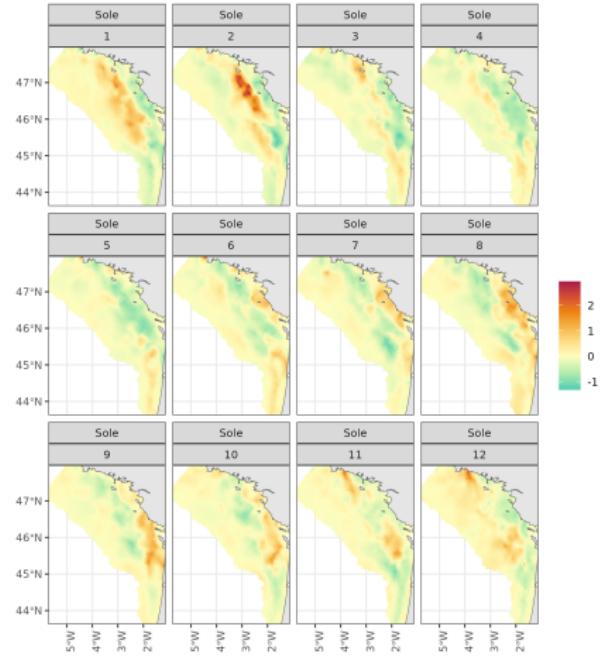
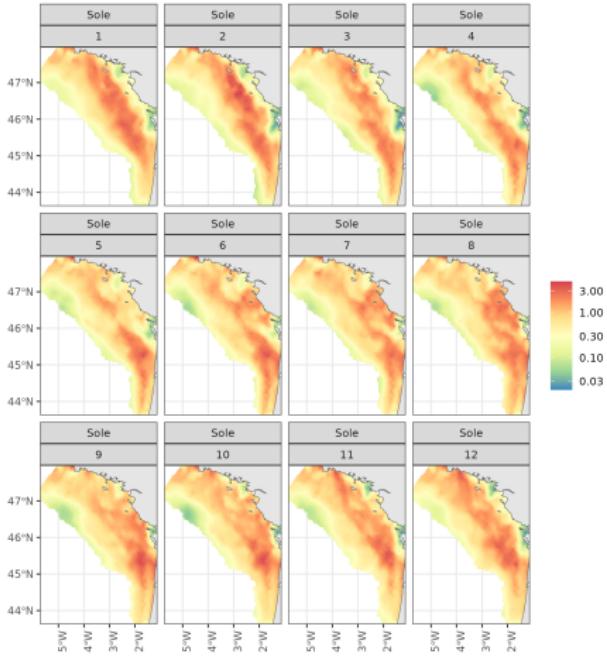
The time-centered space-time field:

$$\mathbf{S}' = (s_{t_1} - \bar{s}^t, \dots, s_{t_p} - \bar{s}^t).$$

Then,  $\mathbf{S}'$  has the form:

$$\mathbf{S}' = \begin{pmatrix} S'(x_1, t_1) & S'(x_1, t_2) & \cdots & S'(x_1, t_p) \\ S'(x_2, t_1) & S'(x_2, t_2) & \cdots & S'(x_2, t_p) \\ \vdots & \ddots & \ddots & \vdots \\ S'(x_n, t_1) & S'(x_n, t_2) & \cdots & S'(x_n, t_p) \end{pmatrix}$$

# Raw data



(left) Monthly spatial log-predictions  $\log S(x, t)$  of the hierarchical model. (right) Monthly anomalies of the spatial predictions  $S^*(x, t)$ . Each panel corresponds to the average distribution of prediction of anomalies for a month over the period 2008 - 2018.

# Basics of EOF

The spatio-temporal field is decomposed so that:

$$S'(x, t) = \sum_{m=1}^r p_m(x) \cdot \alpha_m(t) + \epsilon_m(x, t)$$

with  $r$  the number of dimensions of the EOF ( $r \leq \min(n, p)$ ),  $p_m(x)$  the spatial term of EOF and  $\alpha_m(t)$  the temporal term of EOF for dimension  $m$ .  
 $\epsilon_m(x, t)$  is an error term.

## Constraints:

- minimize  $E = \sum_m \sum_x \sum_y \epsilon_m(x, t)$
- spatial terms and temporal terms are orthogonal

$$\langle p_i(\cdot); p_j(\cdot) \rangle = 0 \quad i \neq j$$

$$\langle \alpha_i(\cdot); \alpha_j(\cdot) \rangle = 0 \quad i \neq j$$

## Basics of EOF

This falls back to a diagonalisation issue through eigen-decomposition:

$$\mathbf{S}'\mathbf{S}'^T = \mathbf{C}_{\mathbf{S}'} = \mathbf{U}\Lambda\mathbf{U}^T$$

or through singular value decomposition:

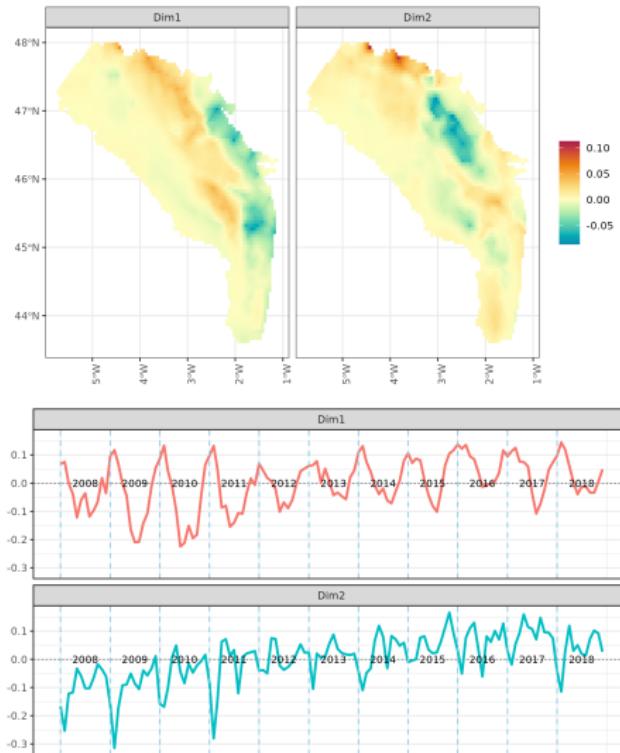
$$\mathbf{S}' = \mathbf{U}\Sigma\mathbf{V}^T \quad (\text{SVD})$$

- $\mathbf{C}_{\mathbf{S}'}$  is the covariance function of  $\mathbf{S}'$
- $\mathbf{U}_{(n \times r)}$  contains the spatial factors ( $p_m(x)$ ),
- $\Lambda_{(r \times r)}$  contains the eigen values and  $\Sigma_{(r \times r)}$  contains the singular values of  $\mathbf{S}'$ .

These quantifies the percentage of variance captured by each dimension.  
They are diagonal matrices with  $\Lambda = \Sigma^2$

- $\mathbf{V}_{(p \times r)}$  contains the temporal loadings ( $\alpha_m(t)$ )

# Illustration



(Top) Spatial factors for the two first dimensions of the EOF. (Bottom) Loadings for the two first dimensions of the EOF. Blue dashed vertical lines corresponds to the month of January for each year.

## Interpretation:

**U** are spatial factors that capture the variance of  $\mathbf{S}'$ .

**V** are the temporal loadings that relate  $\mathbf{S}'$  to the spatial factors in **U**.

When the loading of dimensions  $j$  denoted  $\mathbf{V}_{j,\cdot}$  are high (resp. low) at time step  $t$  then the process  $\mathbf{s}'_t$  at this time step follows the spatial factor  $\mathbf{U}_{j,\cdot}$  (resp.  $-\mathbf{U}_{j,\cdot}$ ).

# Multivariate EOF

- 1 Empirical Orthogonal Functions
- 2 Multivariate EOF
- 3 Constraining the EOF with an ancillary variable
- 4 Are EOF truly orthogonal?
- 5 Conclusion

# Multivariate EOF

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# Multivariate EOF

Let us denote by  $k \in \{1, \dots, s\}$  the number of variables

$S^{(k)}(x, t)$  is the value of the space time process for the location  $x$ , the time  $t$  and the variable  $k$ .

To build the multivariate spatio-temporal matrix to be diagonalized, there are two options:

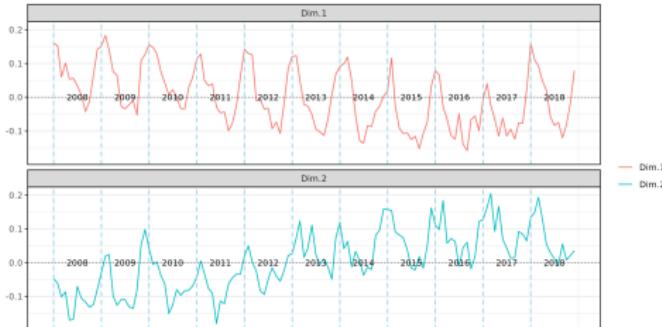
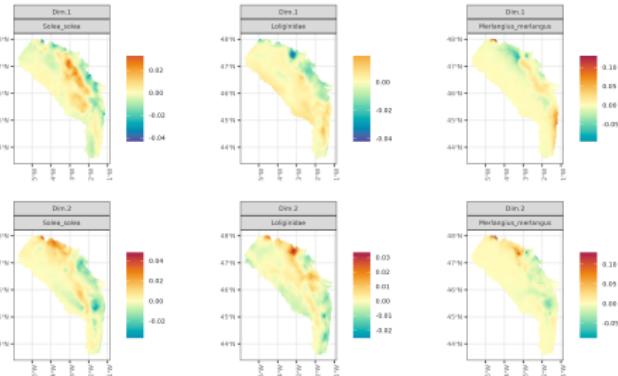
- binding the matrices by rows. The matrix is of dimension  $(n \cdot s) \times p$

$$\mathbf{S}'^{(row)}_{multi} = \begin{pmatrix} \mathbf{S}'^{(1)} \\ \mathbf{S}'^{(2)} \\ \vdots \\ \mathbf{S}'^{(s)} \end{pmatrix}$$

- binding the matrix by columns. The matrix is of dimension  $n \times (p \cdot s)$ .

$$\mathbf{S}'^{(col)}_{multi} = (\mathbf{S}'^{(1)} ; \mathbf{S}'^{(2)} ; \dots ; \mathbf{S}'^{(s)})$$

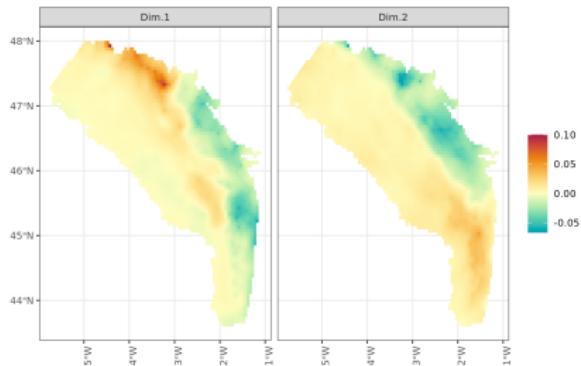
# Bind the matrices by rows



⇒  $\mathbf{U}$  is of dimension  $(n \cdot s) \times r$  and  $\mathbf{V}$  is  $p \times r$

Multivariate EOF on the matrix  $\mathbf{S}'_{multi}^{(row)}$ . (Top) Factor maps for each species and dimensions. (Bottom) Loadings for the two first dimensions.

# Bind the matrices by columns



► **U** is of dimension  $n \times r$  and **V** is  $(p \cdot s) \times r$

Multivariate EOF on the matrix  $S_{multi}^{(col)}$ . (Top) Factor maps for the two first dimensions. (Bottom) Loadings of each species for the two first dimensions.

# Constraining the EOF with an ancillary variable

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# Constraining the EOF with an ancillary variable

**Aim:** “create new variables that are linear combinations of two (multivariate) data sets such that the correlations between these new variables are maximized” (Wickle et al., 2019).

Let's consider two spatio-temporal variables  $S^{(1)}(x, t)$  and  $S^{(2)}(x, t)$ .

Now consider two new variables that are combinations of  $S^{(1)}(x, t)$  and  $S^{(2)}(x, t)$

$$a_k(t_j) = \sum_{i=1}^n \xi_{ik} S^{(1)}(x_i; t_j) = \boldsymbol{\xi}'_k \mathbf{s}_{t_j}^{(1)}$$
$$b_k(t_j) = \sum_{\ell=1}^m \psi_{\ell k} S^{(2)}(r_\ell; t_j) = \boldsymbol{\psi}'_k \mathbf{s}_{t_j}^{(1)}$$

The weights (i.e. the  $k^{\text{th}}$  canonical correlation) are the correlation between  $a_k$  and  $b_k$  with  $k \in \{1, \dots, \min\{n, m\}\}$ :

$$r_k = \text{corr}(\mathbf{a}_k, \mathbf{b}_k) = \frac{\text{cov}(\mathbf{a}_k, \mathbf{b}_k)}{\sqrt{\text{var}(\mathbf{a}_k)} \sqrt{\text{var}(\mathbf{b}_k)}}$$

# Constraining the EOF with an ancillary variable

The correlation takes the form:

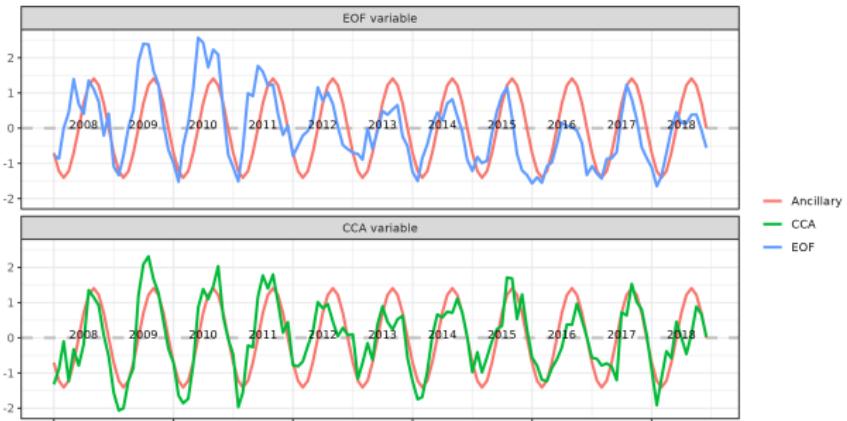
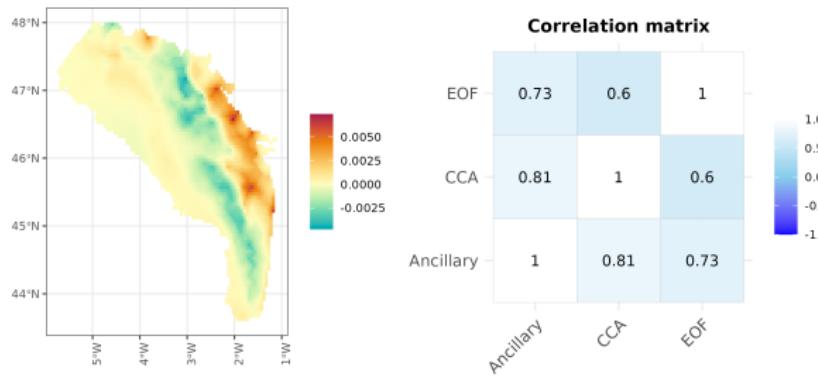
$$r_k = \frac{\xi'_k \mathbf{C}_{S^1 S^2} \psi_k}{(\xi'_k \mathbf{C}_{S^1} \xi_k)^{1/2} (\psi'_k \mathbf{C}_{S^2} \psi_k)^{1/2}}$$

- $\mathbf{C}_{S^1}$  and  $\mathbf{C}_{S^2}$  are covariance matrices of dimension  $m \times m$  and  $n \times n$
- $\mathbf{C}_{S^1 S^2}$  is the covariance matrix between  $\mathbf{S}^{(1)}$  and  $\mathbf{S}^{(2)}$  with dimension  $m \times n$ .
- The first pair of canonical variable corresponds to the weights  $\xi_1$  and  $\psi_1$  that maximize  $r_1$ .

## interpretation:

The time series of the first few canonical variables ( $\mathbf{a}_1$  and  $\mathbf{b}_1$ ) typically match up fairly closely (they maximize correlation  $r_1$ )

The spatial patterns (the weights  $\xi_1$  and  $\psi_1$ ) show the areas in space that are most responsible for the high correlations.



Results of the canonical correlation analysis. (Top left) Canonical vectors  $\xi_1$  that maximise correlation between  $a_k$  and  $b_k$ . (Top right) Correlation matrix between the first time series of the EOF  $U_{\cdot,1}$ , the EOF time series in the CCA  $a_1$  and the ancillary variable. (Bottom) Comparison of the EOF variables with the ancillary variable and the CCA variables with the ancillary variable. These time series are standardized.

# Are EOF truly orthogonal?

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## Are EOF truly orthogonal?

EOFs are statistically orthogonal i.e. for  $i \neq j$ ,  $\{\mathbf{u}_i, \mathbf{u}_j\} = 0$

But they are not spatially orthogonal i.e. the cross-covariance of the different EOF maps is not necessarily 0.

EOM consist in a two step analysis:

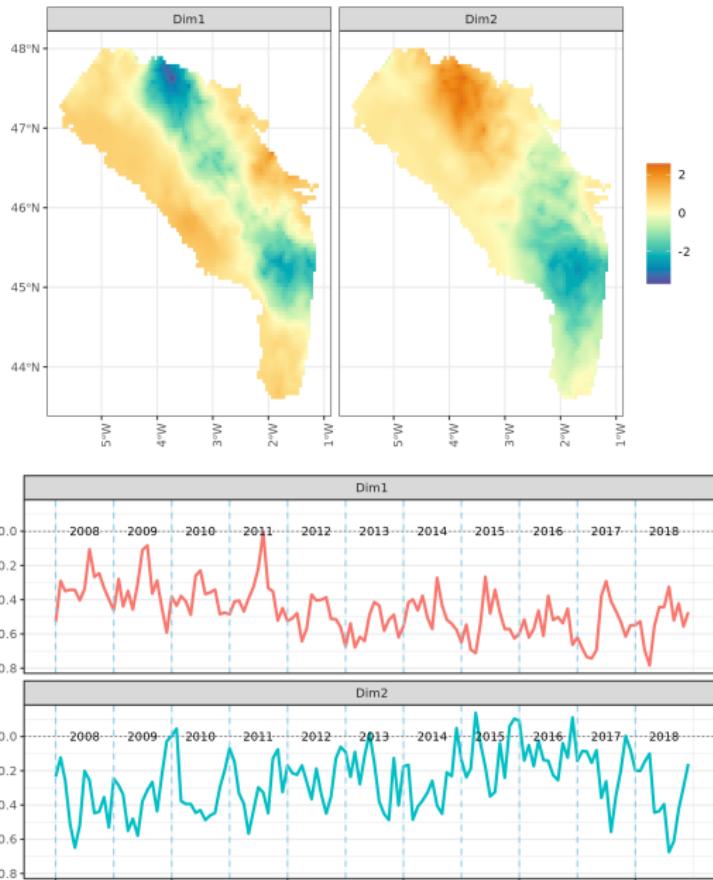
- perform an EOF on  $\mathbf{S}' \rightarrow$  obtain statistically decorrelated plans
- compute the variogram and the cross-variogram of  $\mathbf{U}$  for a specific distance  $r$  that we denote  $\boldsymbol{\Gamma}_r$  of dimension  $(p \times p)$ .

$$\boldsymbol{\Gamma}_r = \mathbf{U}_{\text{eom}} \boldsymbol{\Sigma}_{\text{eom}} \mathbf{V}_{\text{eom}}^T$$

Plans are ordered by increasing variance explained in  $\mathbf{S}'$

$$p_k = \frac{\text{tr}(\mathbf{C}_{\hat{\mathbf{S}}_k})}{\text{tr}(\mathbf{C}_{\mathbf{S}})}$$

where  $p_k$  is the proportion of variance explained by factor  $k$  and  $\hat{\mathbf{S}}_k$  is the projection of  $\mathbf{S}$  in the space of the EOM.



(Top) Spatial factors obtained by EOM for the two first dimensions. (Bottom) Temporal loadings for the first two dimensions.

# Conclusion

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# Conclusion: some bibliographic metrics

sources	articles
JOURNAL OF CLIMATE	391
CLIMATE DYNAMICS	271
JOURNAL OF GEOPHYSICAL RESEARCH: OCEANS	257
INTERNATIONAL JOURNAL OF CLIMATOLOGY	256
GEOPHYSICAL RESEARCH LETTERS	142
JOURNAL OF THE ATMOSPHERIC SCIENCES	126
MONTHLY WEATHER REVIEW	103
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JOURNAL OF GEOPHYSICAL RESEARCH ATMOSPHERES	97
THEORETICAL AND APPLIED CLIMATOLOGY	85
PROCEEDINGS OF SPIE - THE INTERNATIONAL SOCIETY FOR OPTICAL ENGINEERING	75
ATMOSPHERE	72
CONTINENTAL SHELF RESEARCH	72
JOURNAL OF PHYSICAL OCEANOGRAPHY	72
QUARTERLY JOURNAL OF THE ROYAL METEOROLOGICAL SOCIETY	68

# Infering loading factors from sparse data

- EOF are mainly applied in climate science . . .
- but progressively being transferred to other fields of applications
- ⇒ In **ecology**, EOF must be computed from sparse data (VAST, Jim Thorson)

For instance, we could consider a **hierarchical model** where the **latent field** take the form:

$$\log(S(x, t)) = \beta(t) + \omega(x) + \sum_{f=1}^{N_f} \lambda(t, f) \epsilon(x, f)$$

where  $f$  are the dimension of the EOF with  $N_f$  dimensions,  $\omega \sim \mathcal{MG}(O, \Sigma_\omega)$  and  $\epsilon \sim \mathcal{MG}(O, \Sigma_\epsilon)$ .  $\lambda(t, f)$  are the loadings and  $\epsilon(x, g)$  are the EOF.

---

and **the observations** are zero-inflated and takes the form:

$$\Pr(y_i = Y) = \begin{cases} 1 - p_i & \text{if } y_i = 0 \\ p_i \times \mathcal{L}(y_i; \log S(x_i, t_i); \sigma^2) & \text{if } y_i > 0 \end{cases}$$

Where  $Y$  is an observations as random variable and  $y_i$  is the realized observation.  $p_i$  is the probability to obtain a positive observation.  $\mathcal{L}$  is the probability of the positive observations.

## Take home message

- EOF and EOM provide patterns that capture variance of a spatio-temporal dataset while being orthogonal.
- EOF can be extended to several variables.
- EOF can be constrained with an ancillary variable through CCA.
- EOF maps are only statistically orthogonal.
- EOM maps are spatially orthogonal ➔ loadings are also harder to interpret.
- EOM could be realized on time steps, not on locations → but not both at the same time.

## Open questions:

- How to perform dimension-reduction and take into account both spatial and temporal correlation?
- How to perform dimension reduction without the need if svd?



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