ROF routines : Scientific documentation
v1.0

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This short document is intended to provide some technical explanations about the ROF algorithm, and its current implementation.

1 Inputs

1.1 List of inputs

Three inputs are required :
- Y (usually : the observations), a vector of size $n \times 1$,
- X (usually : the response pattern to each external forcing), a matrix of size $n \times I$,
- Z (a sample of realisations of internal climate variability), a matrix of size $n \times n_Z$.

1.2 Pre-processing : Data organisation

The current version of the ROF package is specifically designed for spatio-temporal datasets, with the spatial information corresponding to projection onto spherical harmonics. All input datasets need to be pre-processed as described below.

Let n_T and n_S be, respectively, the temporal and spatial dimensions ($n = n_T n_S$ is the dimension of Y). All input data are assumed to be organised as follows :

$$Y = (Y_{s=1,t=1}, Y_{s=2,t=1}, \ldots, Y_{s=1,t=2}, \ldots, Y_{s=n_S,t=n_T})^T,$$

where s and t denote respectively the spatial and temporal indices.

The spatial information is assumed to be provided via spherical harmonic coefficients. The number of spherical harmonics is given by `Trunc` (triangular truncation is assumed). Note that n_S is a function of `Trunc` :

$$n_S = (\texttt{Trunc} + 1)^2.$$

Then, each s corresponds to a given spherical harmonic. These spherical harmonics need to be sorted in an ascending zonal wave number order, as described in Table 1 (this matters, as a weighting is applied to each spherical harmonic according to its total wave number, following Stott and Tett, 1998).

Table 1 – Correspondence between s and spherical harmonics, as defined by the total wave number l and the zonal wave number m, in the case of a T4-truncation.

$s = 1$	$l = 0$	$m = 0$
$s = 2$	$l = 1$	$m = 0$
$\vdots$	$\vdots$	$\vdots$
$s = 5$	$l = 4$	$m = 0$
$s = 6, 7$	$l = 1$	$m = 1$
$\vdots$	$\vdots$	$\vdots$
$s = 12, 13$	$l = 4$	$m = 1$
$s = 14, 15$	$l = 2$	$m = 2$
$\vdots$	$\vdots$	$\vdots$
$s = 24, 25$	$l = 4$	$m = 4$

1.3 Pre-processing : Temporal centering

The current version of the algorithm assumes that a temporal centering has been applied to the data (previously). Temporal centering means, for Y, that

$$\forall s, \quad \sum_{t=1}^{n_T} Y_{s,t} = 0.$$

Temporal centering can be achieved by removing the mean over the full period. Note that it is required for X and Z as well as for Y.

2 Outputs

The ROF package provides, as the main result, a matrix providing, for each external forcing considered, the scaling factor best-estimate $\widehat{\beta}$, the lower bound of its confidence interval $\widehat{\beta}^{inf}$, and the upper bound of its confidence interval $\widehat{\beta}^{sup}$. In the case of a 2-forcing (ANT+NAT) analysis, this output matrix will be organised as follows :

$$\begin{pmatrix} \widehat{\beta}_{ANT}^{inf} & \widehat{\beta}_{NAT}^{inf} \\ \widehat{\beta}_{ANT} & \widehat{\beta}_{NAT} \\ \widehat{\beta}_{ANT}^{sup} & \widehat{\beta}_{NAT}^{sup} \end{pmatrix}.$$

Note that the bounds of these confidence intervals may vary *very* slightly, as random numbers are used for computing them (see `tls.sci`).

Another useful output is `pv_cons`, which is the p-value of the Residual Consistency Check. Note that this p-value may vary slightly when calculated with the Monte-Carlo algorithm (because the values simulated via the MC algorithm are random).

Other outputs may be useful, eg the reconstructed observations or response patterns (resp. `Y_tilde` and `X_tilde`).

3 Full-ranked covariance matrix and dimension reduction

Let assume here that $n_S = 1$, which means that Y, ε and so on, are time-series. The temporal centering describes above means that $\mathbf{1}^T\varepsilon = 0$, where $\mathbf{1}^T = (1, \ldots, 1)$, so the covariance matrix of ε, C is degenerated : $\mathbf{1}^T C \mathbf{1} = 0$, and $\mathrm{rk}(C) \leq n - 1$.

Is that an issue for estimating C ?
If the sample estimate $\widehat{C}$ is used, then one will have $\mathbf{1}^T \widehat{C} \mathbf{1} = 0$ and $\mathrm{rk}(\widehat{C}) \leq n-1$. This, however, no longer occur with a regularised estimate $\widehat{C}_I$, because regularisation makes that $\mathrm{rk}(\widehat{C}_I) = n$. In such a case, as the *true* matrix C is known to be degenerated, one may want to avoid the use of a full-rank estimate. Moreover, the regularised Ledoit estimate is designed for full-ranked covariance matrices. The estimation of the regularisation coefficients would be deteriorated if this condition is not satisfied.
A solution to this issue is to reduce the dimension of the variables (Y, ε, etc), by projecting onto a subspace of dimension $n-1$, such that $\mathrm{rk}(C) = n-1$ (equivalently, one eliminates the degeneracy). This is done by projecting onto $[\mathbf{1}]_\perp$.

Does the choice of the projection have some impact ?
Yes. Under a transformation $Z \mapsto AZ$, $\widehat{C} \mapsto A^T \widehat{C} A$, but this no longer occurs with $\widehat{C}_I$. As mentioned in Ribes et al (2013), however, it is found to have little impact on the final results.

4 TLS implementation

4.1 Use of non-independent predictors $\widetilde{x}_i$

In many cases, sets of simulations are not available for each wished combination of external forcings.

Illustration : one wants to decompose the observed changes as ANT + NAT contributions, while only ALL and NAT simulations are available (ANT : anthropogenic only, NAT : natural only, ALL : all historical). Equivalently, one wants to infer $\beta = (\beta_{ANT}, \beta_{NAT})$, from the input $X = [x_{ALL}, x_{NAT}]$.

Solution in OLS (following Tett et al, 1999, Supplementary Material, Section 9).
In OLS, a first step could be to define $x_{ANT} = x_{ALL} - x_{NAT}$, using the additivity assumption (widespread in D&A). Then, the OF algorithm could be applied with $X^* = [x_{ANT}, x_{NAT}]$.
In such a case (C is assumed to be known here),

$$\widehat{\beta} = (X^{*\prime} C^{-1} X^*)^{-1} X^{*\prime} C^{-1} Y.$$

As X^* has been derived from X with

$$X = X^* P, \quad \text{or} \quad X^* = X P^{-1},$$

where $P = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$, and $P^{-1} = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$, one has

$$\begin{aligned} \widehat{\beta} &= \left((XP^{-1})'C^{-1}XP^{-1}\right)^{-1}(XP^{-1})'C^{-1}Y \\ &= P(X'C^{-1}X)^{-1}X'C^{-1}Y, \\ &= P[\widehat{\beta}_{ALL}, \widehat{\beta}_{NAT}]. \end{aligned}$$

This results means that the algorithm may be performed with X instead of X^*, if the obtained estimates $[\widehat{\beta}_{ALL}, \widehat{\beta}_{NAT}]$ are properly transformed (by applying matrix P).

What is P ? (variable `Proj` in `main.sci`)
The matrix P is very easy to understand, and provide the information about what forcing is taken into account in each simulation. More precisely :

- the columns of P are the sets of simulations available ; here : ALL, NAT,
- the rows of P are the external forcings studied ; here : ANT, NAT.

The entry $p_{i,j}$ of P tells whether forcing i is included in simulation j (basically : 1 means *included*, 0 means *not included*).

Solution in TLS.
This issue is even more problematic in TLS, because each response pattern is then assumed to be noised. Following notations used in (Ribes et al, 2013), X is not known in such a case, and what is observed instead is (still in the same example) :

$$\widetilde{X} = [\widetilde{x}_{ALL}, \widetilde{x}_{NAT}] = [x_{ALL}, x_{NAT}] + [\varepsilon_{x_{ALL}}, \varepsilon_{x_{NAT}}].$$

Because $\widetilde{x}_{ALL}$ and $\widetilde{x}_{NAT}$ are derived from different sets of simulations, one may assume $\varepsilon_{x_{ALL}}$ and $\varepsilon_{x_{NAT}}$ to be independent. However, if one computes $\widetilde{x}_{ANT} = \widetilde{x}_{ALL} - \widetilde{x}_{NAT}$, the corresponding noise will be $\varepsilon_{x_{ANT}} = \varepsilon_{x_{ALL}} - \varepsilon_{x_{NAT}}$, which is no longer independent from $\varepsilon_{x_{NAT}}$. Then, the columns of $\widetilde{X}^* = [\widetilde{x}_{ANT}, \widetilde{x}_{NAT}]$ cannot be assumed to be independent. As a consequence, the TLS fit has to be based on $\widetilde{X}$ and not $\widetilde{X}^*$. Then, the outputs are corrected (matrix P is applied) to provide the wished scaling factors. Note that this issue also makes the computation of confidence intervals more complicated in TLS.

4.2 TLS confidence intervals

Note : Details about the algorithm used to compute confidence intervals should be added to this section.

In the case of a TLS fit, the results in terms of scaling factor confidence intervals may be surprising, as $\pm\infty$ may be included in the confidence interval. For that reason, the coefficients provided for a given forcing, say $[\widehat{\beta}^{inf}, \widehat{\beta}, \widehat{\beta}^{sup}]$, may be :

- $\widehat{\beta}^{inf} \leq \widehat{\beta} \leq \widehat{\beta}^{sup}$, eg $[-1, 0, 1]$ (most common case).
- $\widehat{\beta} \leq \widehat{\beta}^{sup} \leq \widehat{\beta}^{inf}$, eg $[10, 0, 1]$; in such a case, the confidence interval may be written as $[10, +\infty[\cup] - \infty, 1]$, and it does include $\beta = 0$.
- $\widehat{\beta}^{sup} \leq \widehat{\beta}^{inf} \leq \widehat{\beta}$, eg $[-1, 0, -10]$; in such a case, the confidence interval may be written as $[-1, +\infty[\cup] - \infty, -10]$, and it does include $\beta = 0$.

However, if you find another case (eg $\widehat{\beta}^{sup} \leq \widehat{\beta} \leq \widehat{\beta}^{inf}$,...), then my script is bugged. You should tell me !

Références

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