Sequential Factor Separation for the Analysis of Numerical Model Simulations

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ABSTRACT

Models are attractive tools to deepen the understanding of atmospheric and climate processes. In practice, such investigations often involve numerical experiments that switch on or off individual factors (such as latent heating, nonlinear coupling, or some climate forcing). However, as in general many factors can be considered, the analysis of these experiments is far from straightforward. In particular, as pointed out in an influential study on factor separation by Stein and Alpert, the analysis will often require the consideration of nonlinear interaction terms.

In the current paper an alternative factor separation methodology is proposed and analyzed. Unlike the classical method, sequential factor separation (SFS) does not involve the derivation of the interaction terms but, rather, provides some uncertainty measure that addresses the quality of the separation. The main advantage of the proposed methodology is that in the case of \( n \) factors it merely requires \( 2^n \) simulations (rather than \( 2^n \) for the classical analysis). The paper provides an outline of the methodology, a detailed mathematical analysis, and a theoretical intercomparison against the classical methodology. In addition, an example and an intercomparison using regional climate model experiments with \( n = 3 \) factors are presented. The results relate to the Mediterranean amplification and demonstrate that—at least in the particular example considered—the two methodologies yield almost identical results and that the SFS is rather insensitive with respect to design choices.

1. Introduction

During the last decades, the rapid growth of modern supercomputers is seen as a main driver behind the tremendous improvement of numerical weather prediction (e.g., Bauer et al. 2015), has enabled today’s efforts to project climate change into the future (IPCC 2013), and has led to an unseen increase in scientific productivity in these research areas. Indeed, it is sometimes argued that numerical simulations have advanced to become the third methodology of the natural sciences, in addition to the classical use of theory and laboratory experiments.

Since the beginning of numerical models, they have widely been used to disentangle the complexity of nonlinear, multiscale, and chaotic physical systems considered. In numerical models, highly sophisticated experimentation is possible, as individual factors of the modeling systems can be switched on and off at discretion. There are numerous studies that have used this approach and made progress in this way.

While sometimes these numerical experiments are straightforward to undertake, their interpretation involves considerable challenges. In particular, if different factors are investigated, nonlinear interactions between the factors need to be considered. A pioneering study in this area is that of Stein and Alpert (1993). They designed a methodology for factor separation in numerical simulations, which in principle can account for an arbitrary number of factors. A key element of their approach is the derivation of interaction effects. For instance, when consideration is given to two factors, then the joint effect of these is expressed as \( f_1 + f_2 + f_{12} \), where \( f_1 \) and \( f_2 \) denoted the primary (or direct) effects of the factors 1 and 2, respectively, and \( f_{12} \) is an interaction effect that depends on both the factors. We will refer to this methodology as factor separation (FS).

The study of Stein and Alpert (1993) has been highly influential and used in a large number of studies. For instance, it has been used to disentangle global climate feedbacks [e.g., Braconnot et al. 1999; see also the
review of Bony et al. (2006), in the assessment of aerosol microphysical processes (van den Heever et al. 2006), to quantify the relative magnitude of biogeophysical versus biogeochemical processes (Claussen et al. 2001), to separate the effects of changes in climate and emissions on regional air pollution (Hogrefe et al. 2004), to study the impact of different model physical parameterizations and their interactions on mesoscale convective systems (Jankov et al. 2005), and to address uncertainties in regional climate projections (Torma and Giorgi 2014). Additional examples of and background on the factor separation technique can be found in Alpert and Sholokhman (2011a). The wide range of application is testimony of the versatility of the methodology.

One disadvantage of the factor separation methodology is that its complexity grows exponential with the number of factors considered. More specifically, the separation of \( n \) factors requires \( 2^n \) simulations. For instance, in the case of \( n = 4 \) factors a total of 16 simulations are needed, and the analysis yields not only the four direct effects but also a total of 11 interaction terms. As a result of this complexity, most applications of the factor separation technique have addressed merely \( n = 2 \) or \( n = 3 \) factors. Also, a number of studies have used sophisticated sequences of simulations with many different factors but have not conducted a formal factor analysis (Rowell and Jones 2006; Déqué et al. 2007; Boé and Terray 2014; Ceppi and Hartmann 2016). The challenge of analyzing many factors with FS has also been discussed by Alpert and Sholokhman (2011b). They pointed out that the number of required simulations quickly decreases if one restricts the analysis to the leading interaction terms.

In a recent study (Kröner et al. 2016, hereafter KR16), we have explored an alternative factor separation approach with the purpose to identify the key drivers behind the Mediterranean amplification of climate change. This term describes the fact that most climate models project an amplified warming and drying over southern Europe (see section 3 for further details). The alternative factor separation approach will be referred to as sequential factor separation (SFS). It is not as precise and general as the approach of Stein and Alpert (1993), but it has advantages when \( n = 3 \) or more factors are considered, as it requires merely \( 2n \) simulations, rather than \( 2^n \) simulations.

The outline of this paper is as follows. Section 2 introduces the new methodology, provides a detailed mathematical comparison of FS and SFS, and presents an analysis of the two methodologies using operator notation to help their interpretation. Section 3 presents a detailed analysis of an example previously considered in KR16. This includes a full intercomparison of the two methodologies in a case with \( n = 3 \) factors. Section 4 concludes the study.

2. Methodology

a. Factor separation of Stein and Alpert

We first review the main ideas of FS following the study of Stein and Alpert (1993, hereafter SA93). This serves to define the notation and will later be used when providing an intercomparison of the two methodologies.

1) TWO FACTORS

Consider first the case of two factors. In the example presented by SA93 these addressed the role of topography (factor 1) and the role of surface fluxes (factor 2). Simulations are then conducted where these factors are switched on and off, respectively. With \( n = 2 \) factors, a total of four simulations are possible. Let us next consider the results of these simulations in terms of a two-dimensional field \( f(x, y) \) from each of the simulations—for instance, the surface pressure fields. Following SA93, we use a notation where the subscripts denote the factors that are switched on; that is,

\[ f_o: \text{both factors switched off}; \]
\[ f_1: \text{topography on, surface fluxes off}; \]
\[ f_2: \text{topography off, surface fluxes on}; \]
\[ f_{12}: \text{full simulation with topography and surface fluxes switched on}. \]

In the case of a process study as considered by SA93, simulation \( f_o \) can be referred to as the “base” simulation and \( f_{12} \) as the “target” simulation. However, in order to use one single notation throughout this paper, we refer to \( f_o \) as the control simulation (CTRL, all effects are switched off) and to \( f_{12} \) as the scenario simulation (SCEN, all effects are switched on). This terminology is influenced by climate change applications, but it may also be used in other circumstances.

The prime objective of factor separation is then to determine to what extent the total effect SCEN–CTRL is determined by the two factors. To do so, we need to distinguish between the results of the four simulations (denoted by \( f \) terms) and the effects of the factors considered (denoted by \( \hat{f} \) terms). For instance, the fields \( f_1 \) and \( f_2 \) can be expressed as

\[ f_1 = f_o + \hat{f}_1 \quad \text{and} \quad (1a) \]
\[ f_2 = f_o + \hat{f}_2, \quad (1b) \]

where \( \hat{f}_1 \) and \( \hat{f}_2 \) denote the effects of factors 1 and 2, respectively. In the case of simulation \( f_{12} \), the situation is
more complicated, as interactions between the two factors need to be considered; that is,

\[ f_{12} = f_o + \hat{f}_1 + \hat{f}_2 + \hat{f}_{12}. \]  

(1c)

Here \( \hat{f}_{12} \) denotes the interaction effect. The total effect SCEN–CTRL = \( f_{12} - f_o \) can then be expressed as

\[ \text{SCEN–CTRL} = \hat{f}_1 + \hat{f}_2 + \hat{f}_{12}. \]  

(2)

The interaction effect represents the role of non-linearities that depend upon both factors being switched on.

Once all simulations are known, (1) can be solved for the effects to obtain

\[ \hat{f}_1 = f_1 - f_o, \]  

(3a)

\[ \hat{f}_2 = f_2 - f_o, \]  

(3b) and

\[ \hat{f}_{12} = f_{12} + f_o - f_1 - f_2. \]  

(3c)

For the example considered (where \( f \) denotes the resulting pressure field), \( \hat{f}_{12} \) is the pressure drop due to interactions between effects of the underlying topography and the surface fluxes. For instance, in the example of SA93 both the topography and the surface fluxes individually amplify the cyclone and associated precipitation response. In addition, there is a synergistic effect of the two factors that is not represented by the terms \( \hat{f}_1 \) and \( \hat{f}_2 \) but detected with \( \hat{f}_{12} \).

2) THREES AND MORE FACTORS

In the case of three factors the situation is more complicated. Beyond simulation CTRL = \( f_o \), there will be three simulations involving one single factor: that is,

\[ f_1 = f_o + \hat{f}_1, \]  

(4a)

\[ f_2 = f_o + \hat{f}_2, \]  

(4b) and

\[ f_3 = f_o + \hat{f}_3. \]  

(4c)

three simulations involving two factors—that is,

\[ f_{12} = f_o + \hat{f}_1 + \hat{f}_2 + \hat{f}_{12}, \]  

(4d)

\[ f_{13} = f_o + \hat{f}_1 + \hat{f}_3 + \hat{f}_{13}, \]  

(4e) and

\[ f_{23} = f_o + \hat{f}_2 + \hat{f}_3 + \hat{f}_{23}. \]  

(4f)

as well as the simulation involving all three factors—that is,

\[ f_{123} = f_o + \hat{f}_1 + \hat{f}_2 + \hat{f}_3 + \hat{f}_{12} + \hat{f}_{13} + \hat{f}_{23} + \hat{f}_{123}. \]  

(4g)

Despite the rapid increase in the number of simulations and terms, the procedure is in principle the same as with two factors. Equation (4) is a linear system of seven equations for the seven unknown effects. For completeness and later reference we list the solution (see also SA93):

\[ \hat{f}_1 = f_1 - f_o, \]  

(5a)

\[ \hat{f}_2 = f_2 - f_o, \]  

(5b)

\[ \hat{f}_3 = f_3 - f_o, \]  

(5c)

\[ \hat{f}_{12} = f_{12} - (f_1 + f_2) + f_o, \]  

(5d)

\[ \hat{f}_{13} = f_{13} - (f_1 + f_3) + f_o, \]  

(5e) and

\[ \hat{f}_{23} = f_{23} - (f_2 + f_3) + f_o. \]  

(5f)

The total effect of all factors considered—that is, SCEN–CTRL = \( f_{123} - f_o \)—can thus be separated as

\[ \text{SCEN–CTRL} = \hat{f}_1 + \hat{f}_2 + \hat{f}_3 + \hat{f}_{12} + \hat{f}_{13} + \hat{f}_{23} + \hat{f}_{123}. \]  

(6)

Beyond the direct effects of the three factors (\( \hat{f}_1, \hat{f}_2, \hat{f}_3 \)), there are three quadratic interaction terms (\( \hat{f}_{12}, \hat{f}_{13}, \hat{f}_{23} \)) and one cubic interaction term (\( \hat{f}_{123} \)). Thus, a total of seven terms need to be considered.

A total of eight simulations are needed for the case of three factors. For later comparison with the sequential factor analysis, the simulations are schematically illustrated in Fig. 1. More generally, the number \( N \) of simulations grows exponentially with the number \( n \) of factors considered; that is

\[ N_s = 2^n, \]  

(7)

as we need simulations with all \( n \) factors on and off. The number of interaction terms to be considered grows as \( 2^n - n - 1 \). The complexity of the problem thus rapidly increases with \( n \). For instance, consideration of four

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**FIG. 1.** Factor separation (FS) following SA93 with \( n = 3 \) factors. Horizontal bars represent individual simulations and the notation lists those factors that are switched on. For instance, \( f_{12} \) denotes the simulation with factors 1 and 2 on but factor 3 off. Simulation \( f_o \) represents the control simulation (CTRL) with all factors off, and \( f_{123} \) the scenarios simulation (SCEN) with all factors on. The arrows point toward increasing number of factors.
factors requires 16 simulations, and consideration of five factors twice that (i.e., 32 simulations). In the latter case, one needs to consider not only the five effects (from \( f_1 \) to \( f_5 \)), but also 10 quadratic interaction terms, 10 cubic interaction terms, five interaction terms of order 4, and one interaction term of order 5, yielding a total of 26 interaction terms.

It is evident that the exponential growth of the complexity is a serious obstacle when using the complete factor separation technique with more than three factors. First, the large number of simulations implies a factor separation technique with more than three factors requires 16 simulations, and consideration of five factors twice that (i.e., 32 simulations). In the latter case, one needs to consider not only the five effects (from \( f_1 \) to \( f_5 \)), but also 10 quadratic interaction terms, 10 cubic interaction terms, five interaction terms of order 4, and one interaction term of order 5, yielding a total of 26 interaction terms.

Third, the presence of noise (which is often present in simulations owing to the chaotic nature of the underlying dynamics) makes the evaluation of the terms like (5g) highly uncertain when a large number of terms appear on the right-hand side. These are the main reasons for seeking a methodology that is simpler to use.

b. Sequential factor separation

1) Basic formulation for three factors

The main simplification behind SFS is the restriction to a particular sequence (or order) of factors. In some cases the order will be arbitrary. For instance, in the example considered in section 2a, one may choose the topology as the first effect, or the surface fluxes. In other cases the investigated problem will determine a natural order of the effects. For instance, consider the case where the effects of climate warming and moistening are investigated. In this particular case, it makes sense to define as the first factor the warming and the associated moistening due to the Clausius–Clapeyron effect (i.e., constant relative humidity), and as the second factor the change in relative humidity. The latter may be viewed as a second-order effect, and it is natural to first consider the overall warming with constant relative humidity.

In discussing SFS in more detail we directly start with the consideration of \( n = 3 \) factors as in KR16. In doing so, we use the same notation as in section 2a to enable a comparison against FS, whereas in KR16 another more problem-oriented notation was used.

The basic layout of SFS simulations for the case with three factors is schematically illustrated in Fig. 2. Consider first the left-hand side of the diagram. Simulation \( f_o \) will serve as the control simulation, representing the case where all factors are switched off. In the SFS methodology, one does not conduct the whole series of simulations, but merely a succession of simulations, where in each simulation one additional factor is switched on. With three factors this yields the simulations \( f_o, f_1, f_{12}, \) and \( f_{123} \). Note that in a later example we will use \( f_o \) and \( f_{123} \) to represent climate simulations for control and future conditions (CTRL and SCEN, respectively).

The simulations on the left-hand side of Fig. 2 do enable some separation of the three factors’ effects, but they do not allow assessing the quality of the separation. To complete this task, an additional set of simulations is needed. It is obtained by successively retracting (switching off) the factors starting from \( f_{123} \), in the same order as they were previously introduced. The resulting sequence of simulations is \( f_{123}, f_{23}, f_3, \) and \( f_o \). The design of the simulations can be interpreted as a circular twin design: the factors are not only sequentially added to \( f_o = \text{CTRL} \), but then also sequentially retracted from \( f_{123} = \text{SCEN} \), so as to end up again at \( f_o = \text{CTRL} \) (see Fig. 2).

Next we note that the effect of each factor can be estimated as the differences between two pairs of simulations. For instance, the effect of factor 1 can be estimated from the difference \( f_1 - f_o \), but also from \( f_{123} - f_{23} \). In both these differences, factor 1 appears in a switched-on and a switched-off state. Thus the two terms both measure the effect of factor 1, but relative to different states—namely, \( f_o \) and \( f_{23} \), respectively (see also Fig. 2). The availability of two different estimates will later enable us to assess the accuracy of the separation. Based on this procedure, we define the three effects as arithmetic average of the two respective measures. These can directly be read out of Fig. 2:

\[
\begin{align*}
\hat{F}_1 &= \frac{1}{2} [(f_1 - f_o) + (f_{123} - f_{23})], \\
\hat{F}_2 &= \frac{1}{2} [(f_{12} - f_1) + (f_{23} - f_3)], \quad \text{and} \\
\hat{F}_3 &= \frac{1}{2} [(f_{123} - f_{12}) + (f_3 - f_o)].
\end{align*}
\]

In essence, we define the effects as the average of two estimates, one stemming from the set of simulations

![Fig. 2. As in Fig. 1, but for the sequential factor separation (SFS). The methodology considers a sequence of simulations (gray arrows) where factor by factor is switched on (\( f_o, f_1, f_{12}, f_{123} \)), and then factor by factor is switched off (\( f_{123}, f_{23}, f_3, f_o \)) in the same order. In comparison to FS in Fig. 1, two of the experiments (\( f_1, f_2 \)) are not needed for the analysis.](image-url)
f_o \rightarrow f_{123}, the other from the set of simulations f_{123} \rightarrow f_o, which represent the left-hand and right-hand sides of the simulations in Fig. 2, respectively. Note that our notation uses capital $F$ as in general $F_i \neq f_i$.

The approach of estimating some effect as the average of two differences (rather than one single difference) has also been used in some previous studies. In particular, Ceppi and Hartmann (2016) used a related approach when estimating cloud radiative feedbacks in aquaplanet simulations. However, their procedure appears specific to the particular set of simulations considered.

Upon taking the sum of the above three equations [i.e., (8a)–(8c)], most terms disappear, and one obtains the following separation:

$$
\text{SCEN–CTRL} = f_{123} - f_o = \hat{F}_1 + \hat{F}_1 + \hat{F}_1. 
$$

This equation is mathematically exact; that is, the separation itself does not involve any approximation. The separation is also complete—that is, the equation enables the quantification of the percentage contribution of the three factors (e.g., in a pie chart), which is not possible from the separation with (6).

However, whether the three terms on the right-hand side of (9) really represent the factors’ effects, needs to be assessed separately. Here we will use the differences of the two estimates from $f_o \rightarrow f_{123}$ and $f_{123} \rightarrow f_o$ as an error measure and define

$$
\Delta\hat{F}_1 := \frac{1}{2} [(f_1 - f_o) - (f_{123} - f_{23})], \quad (10a) \\
\Delta\hat{F}_2 := \frac{1}{2} [(f_{12} - f_1) - (f_{23} - f_3)], \quad (10b) \\
\Delta\hat{F}_3 := \frac{1}{2} [(f_{123} - f_{12}) - (f_3 - f_o)]. \quad (10c)
$$

Here we have retained the factor $1/2$, as we may then interpret the two terms $\hat{F}_i \pm \Delta\hat{F}_i$ as the two estimates of the respective effect. For instance, $\hat{F}_1 \pm \Delta\hat{F}_1$ corresponds to $f_1 - f_o$ and $f_{123} - f_{23}$, respectively.

The terms defined by (10) do express the degree of dependence between the individual factors. If the factors do not interact, then $f_i = \hat{F}_i$ and the left-hand side of (10) is zero. If the factors are not completely independent, then SFS detects an error, which is estimated by (10). Also, by design the sum of the three terms in (10) disappears; that is, $\Sigma\Delta\hat{F}_i = 0$. We will thus use the root-mean-square average of the $n = 3$ terms

$$
\Delta\hat{F}_o := \left( \frac{1}{n} \sum_{i=1}^{n} \Delta\hat{F}_i^2 \right)^{1/2} \quad (11)
$$

to represent the overall uncertainty of the methodology.

Specifying the sequence of the factors as with SFS greatly reduces the number of required simulations: In the case of $n = 3$ factors, a total of six simulations is needed, which is slightly less than in the case of FS [eight simulations; see section 2a(2)]. However, the important point is that the number of simulations grows linearly (rather than exponentially) with the number of factors $n$, as

$$
N_{\text{sfs}} = 2n. \quad (12)
$$

If consideration is given to a large number of factors, the difference between (7) and (12) quickly becomes very large. From a practical point of view, the advantages of SFS over FS are thus evident in the case of many factors: with $n = 4$ factors, SFS uses 8 rather than 16 simulations, with $n = 5$ factors, 10 rather than 32 simulations; and with $n = 6$ factors, 12 rather than 64. In addition, the results are easier to interpret. With SFS there is no need to consider a large number of interaction terms; rather, for each factor, one deals with an estimate of its effect and one measure relating to the strength of possible interactions; see (9) and (10). The uncertainty term in (11) serves as a measure of the importance of interaction effects. From a theoretical point of view, the advantage of FS over SFS is its mathematically precise formulation. Yet, as will be shown below in section 2c, the SFS estimates can rigorously be interpreted as well.

2) RELATIONSHIP BETWEEN COMPLETE AND SEQUENTIAL FACTOR ANALYSIS

As already alluded to above, the FS and SFS estimates are not identical; that is, $\hat{F}_i \neq f_i$. In addition, by design,

$$
\Sigma\hat{F}_i = \text{SCEN–CTRL}, \quad (13)
$$

which is not the case for $\Sigma f_i$. The link between the two methodologies can quantitatively be established as follows: We express all terms on the right-hand side of (8) and (10) using the relations listed in (4). Introducing this into (8) yields

\[ \begin{array}{c}
\text{SCEN} = f_{234} \\
\text{CTRL} = f_o
\end{array} \]

\[ \begin{array}{c}
\hat{f}_{234} \quad \hat{f}_{234} \\
\hat{f}_{123} \quad \hat{f}_{123} \\
\hat{f}_{12} \quad \hat{f}_{12} \\
\hat{f}_1 \quad \hat{f}_1 \\
\hat{f}_4 \quad \hat{f}_4 \\
\hat{f}_3 \quad \hat{f}_3 \\
\hat{f}_2 \quad \hat{f}_2 \\
\hat{f}_0 \quad \hat{f}_0
\end{array} \]

FIG. 3. As in Figs. 1 and 2, but for $n = 4$ factors. Black bars indicate the simulations required for the SFS and gray bars the additional simulations needed for the complete FS.
Further discussion and interpretation of these relations alluded to in (13).

The result of this analysis is consistent in the sense that the leading terms of the SFS effects \( \hat{F} \) are identical to the corresponding FS effects \( \hat{f} \). It is also evident that the FS interaction terms are implicitly distributed to the three SFS effects. Each of the FS interaction terms appears with a factor 1/2 in two of the SFS effects. Taking the sum of all three effects in (14) gives

\[
\hat{F}_1 + \hat{F}_2 + \hat{F}_3 = \hat{f}_1 + \hat{f}_2 + \hat{f}_3 + \hat{f}_{12} + \hat{f}_{13} + \hat{f}_{23} + \hat{f}_{123}.
\]

(15)

This is consistent with (9) and demonstrates one of the fundamental differences between the two methodologies alluded to in (13).

While the above analysis provides the full mathematical relationship between the two factor separation approaches, and demonstrates that the two analyses are consistent, its further interpretation is not straightforward. In particular, the analysis assigns the interaction terms of FS to individual SFS factors, but it does not reveal the details of this assignment.

3) FORMULATION FOR \( n > 3 \)

For completeness we here also provide the general methodology for \( n \) factors. Based on Fig. 2, the effect of factor \( k \) (with \( 1 \leq k \leq n \)) and its error measure can be expressed as

\[
\hat{F}_k = \hat{f}_k + \frac{1}{2}(\hat{f}_{12} + \hat{f}_{13} + \hat{f}_{123}), \quad \text{(14a)}
\]

\[
\hat{F}_2 = \hat{f}_2 + \frac{1}{2}(\hat{f}_{12} + \hat{f}_{23}), \quad \text{and} \quad \text{(14b)}
\]

\[
\hat{F}_3 = \hat{f}_3 + \frac{1}{2}(\hat{f}_{13} + \hat{f}_{23} + \hat{f}_{123}). \quad \text{(14c)}
\]

The result of this analysis is consistent in the sense that the leading terms of the SFS effects \( \hat{F} \) are identical to the corresponding FS effects \( \hat{f} \). It is also evident that the FS interaction terms are implicitly distributed to the three SFS effects. Each of the FS interaction terms appears with a factor 1/2 in two of the SFS effects. Taking the sum of all three effects in (14) gives

\[
\hat{F}_1 + \hat{F}_2 + \hat{F}_3 = \hat{f}_1 + \hat{f}_2 + \hat{f}_3 + \hat{f}_{12} + \hat{f}_{13} + \hat{f}_{23} + \hat{f}_{123}.
\]

While the fields \( f \) will explicitly be handled with when doing the analysis, the model simulations \( \phi \) will in general not be stored in full as part of the analysis. Depending upon the simulation strategy considered, they could encompass a huge amount of data. For instance, in the case of climate simulation, \( \phi \) would in general need to include all prognostic model variables with full spatial and high temporal resolution and would need to contain all information to conduct the respective simulation (including for instance the lateral boundary conditions).

Next let us define operators that represent the different factors. For instance, let us introduce operator \( A_1 \) to denote factor 1. More specifically, we may express the simulation \( \phi \) as

\[
\phi = A_1 \phi_o,
\]

(18)

where \( \phi_o \) represents the control simulation. This notation is attractive as it separates the factors from the specific model simulations. In the above example, one could define operator \( A_1 \) by a recipe-like description that tells how to switch on factor 1. For example, in the example provided in section 2a, it would include all information needed to switch on the topography. The operators \( A_1 \) may thus be thought of as a piece of code (or more specifically as the model in a specific setup).

We can also use the inverse operator \( A_1^{-1} \) to denote switching-off some factor (e.g., this could correspond to switching off the topography). The existence of inverse operators is implicit in the notation of “switching on and off” the factors. The existence of an inverse operator then implies

\[
A_1^{-1} A_1 = I,
\]

(19)

where \( I \) denotes the identity operator. The inverse operators can also be used to expand the sequence of the set of \( f_{123} \rightarrow f_o \) simulations. For instance, in the case of \( n = 3 \) factors, one may write

\[
\phi_{23} = A_1^{-1} \phi_{123}.
\]

(20)

To express more complex simulations, we will invoke the sequential application of operators. For instance \( \phi_{12} \) may be expressed as

\[
f_i = B(\phi_i).
\]

(17)
\[ \phi_{12} = A_2 A_1 \phi_o. \]  

(21)

As all factors can individually be switched on and off, the two operators representing the factors 1 and 2 will commute; that is,

\[ [A_1, A_2] = A_1 A_2 - A_2 A_1 = 0. \]  

(22)

In essence, it does not matter which of the two factors has been switched on first.

2) TWO FACTORS

In the case of FS, the two effects are given by (3a) and (3b). Using the aforementioned operator notation, (3a) can be expressed as

\[ \dot{\phi}_1 = (A_1 - I)\phi_o. \]  

(23a)

Here the operator \( (A_1 - I) \) “measures” the effect of factor 1 when applied to some model simulation, in this case the control simulation \( \phi_o \). Similarly, (3b) can be expressed as

\[ \dot{\phi}_2 = (A_2 - I)\phi_o. \]  

(23b)

This can be expressed as

\[ \dot{\phi}_k = (A_k - I)\phi_o. \]  

(24a)

Note the high degree of symmetry with (24a).

3) ARBITRARY NUMBER OF FACTORS

Here we consider the general case with \( n \) factors. Following (16a), the contribution of factor \( k \) is

\[ \dot{\phi}_k = \frac{1}{2}[(A_k - I)A_{k-1} \cdots A_1 \phi_o + (A_k - I)A_{k+1} \cdots A_n \phi_o]. \]  

(25)

This can be expressed as

\[ \dot{\phi}_k = (A_k - I)\phi_o. \]  

(26a)

For completeness and clarity we here also list the result for \( k = 1 \) and \( n \):

\[ \dot{\phi}_1 = (A_1 - I)\frac{1}{2}(I + A_2 \cdots A_n)\phi_o \]  

(26b)

\[ \dot{\phi}_n = (A_n - I)\frac{1}{2}(A_{n-1} \cdots A_1 + I)\phi_o. \]  

(26c)

Similar as the derivation of (26a) above, it can also be shown that the error estimate can be expressed as

\[ \Delta \dot{\phi}_k = (A_k - I)\frac{1}{2}(A_{k-1} \cdots A_1 - A_{k+1} \cdots A_n)\phi_o. \]  

(27)

4) DISCUSSION

The main results of this section are as follows: The complete FS defines its effects relative to the control simulation. Effects that depend upon two or more factors are classified as interaction effects and pinpoint the nonlinearities of the system relative to the control simulation. In a perfectly linear system the interaction effects would disappear. However, it is not always clear whether the nonlinearities relative to CTRL are the target of the factor analysis. In many potential applications, one would rather like to know how the factors affect the results “in average” between the control and the scenario simulation. This goal is not addressed with FS, as the separation is relative to the control simulation by design.
In the framework of the SFS methodology, the total effect (SCEN–CTRL) is separated into $n$ effects. These effects are not defined relative to the control state but, rather, relative to intermediate states between CTRL and SCEN. The separation into $n$ effects is mathematically exact, but the identification of these effects with the respective factors requires some a posteriori assessment. Above we suggest using the uncertainty measure (11) for this purpose. It provides an estimate of nonlinearity and also of the sensitivity of the SFS methodology with respect to the define sequence of factors.

### 3. Example using a regional climate model

In this section we apply the methodology introduced in section 2 to investigate the origin of the Mediterranean amplification in climate change projects. The term Mediterranean amplification describes the common signal seen in most European climate change scenarios for the summer season, encompassing an enhanced warming and drying over the Mediterranean region. The example was previously investigated by KR16. They designed a set of RCM simulations to disentangle and quantify the influences of three key large-scale drivers (or factors). The factors are 1) the thermodynamic effect, 2) the lapse-rate effect, and 3) the combined effect of the remaining changes including circulation changes and land–sea contrast. Below we use this example to systematically investigate the differences between the two factor separation methodologies (FS and SFS). The three factors and their sequence are presented in Table 1.

#### a. Setup of numerical experiments

The analysis will restrict attention to the 2-m temperature for the summer season (JJA), but the consideration of precipitation leads to the same overall conclusions. The full climate change signal is taken from a model chain consisting of a global and a regional climate model (GCM and RCM). The GCM is the MPI-ESM-LR member of the CMIP5 global climate ensemble, using a T67 (200 km) spectral resolution (Stevens et al. 2013). The RCM is the COSMO model in Climate Mode (CCLM) in the Coordinated Regional Climate Downscaling Experiment (CORDEX) setup (Kotlarski et al. 2014; Keuler et al. 2016) with a horizontal resolution of 50 km. We use the transient climate simulation driven by the RCP8.5 emissions scenario and consider the control and scenario periods 1971–2000 (CTRL) and 2070–99 (SCEN), respectively. The simulated surface warming as projected by this model chain is shown in Fig. 4. It exhibits the characteristic signature of the Mediterranean amplification—that is, an amplified warming over the Mediterranean in comparison to mean European conditions. A more detailed analysis also shows an enhanced drying (see KR16).

Following the analysis of KR16 we separate the warming seen in Fig. 4 into the three factors presented in Table 1. Consistent with the notation introduced in section 2, the CTRL and SCEN simulations will also be referred to as $f_0$ and $f_{123}$. To separate the different factors, we use an extended version of the surrogate climate change methodology introduced by Schär et al. (1996). In this approach, the lateral boundary conditions of the RCM experiments CTRL and SCEN are suitably modified such as to reflect the desired changes for each of the factors. One important extension of KR16 is that the specific climate change factors (e.g., the mean warming/moistening) are not only added to CTRL, but also subtracted from SCEN. This twin design allows performing all simulations needed for the two factor separation approaches considered.

More specifically, the thermodynamic effect (represented in simulation $f_1$) is isolated by repeating the 30-yr RCM CTRL experiment, after raising the temperatures of the lateral boundary conditions by a homogenous warming $\Delta T$, while keeping the relative humidity constant. The experiment thus includes an increase in absolute humidity consistent with the Clausius–Clapeyron effect. Such a change is dynamically consistent with the governing equations (Schär et al. 1996). Likewise, simulation $f_{23}$, which represents the effects of factors 2 and 3 (see Table 1), can be obtained by repeating the SCEN experiment, but with the corresponding cooling and drying applied to the SCEN lateral boundary conditions. The resulting simulation uses the SCEN circulation but

### Table 1. Factors considered in the example investigated in section 3. The second column refers to the name used in KR16.

<table>
<thead>
<tr>
<th>Number</th>
<th>Name</th>
<th>Factor</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>TD</td>
<td>Thermodynamic effects</td>
<td>Effects of domain-mean changes in temperature and associated moistening, and changes in greenhouse gas concentrations. The warming is taken from the 850-hPa level of SCEN–CTRL.</td>
</tr>
<tr>
<td>2</td>
<td>LR</td>
<td>Lapse-rate effect</td>
<td>Effects of domain-mean changes in lapse rate, representing the projected increase in stratification in the troposphere (and decrease in the stratosphere).</td>
</tr>
<tr>
<td>3</td>
<td>CO</td>
<td>Circulation and other effects</td>
<td>Effects of changes in large-scale circulation, storm track, and land–sea contrast.</td>
</tr>
</tbody>
</table>
at a temperature and humidity level corresponding to CTRL. The complete technical details of these surrogate experiments can be found in KR16.

KR16 considered a set of \(2n = 6\) numerical experiments required for SFS with \(n = 3\) factors. For the complete FS, we require all \(2^n = 8\) simulations. We thus performed the two additional simulations to enable a full comparison between the FS and SFS methodologies. In these two simulations only the lapse-rate change (without mean warming) was applied, once it was added to CTRL (simulation \(f_2\)), and once subtracted from SCEN (simulation \(f_{13}\)). The setup of these simulations is otherwise similar as for the other simulations (see KR16). Each of the eight RCM simulations has a length of 31 yr, with the first year being discarded as spinup.

b. Comparison of FS and SFS methodologies

For the comparison of the two separation methodologies we use the simulation strategy and the terminology as introduced in section 2. In particular, \(f_o\) will denote the CTRL (current climate) experiment and \(f_{123}\) the SCEN (future climate) experiment. The additional experiments denote simulations where some of the three factors are switched on or off. For instance, \(f_1\) denotes an experiment where factor 1 (the thermodynamic effect; see Table 1) is switched on in CTRL. Similarly, experiment \(f_{23}\) denotes an experiment where factor 1 is switched off in the SCEN experiments. The intercomparison of the two separation methodologies then uses the equations as defined in section 2.

First, we discuss the SFS approach presented in Fig. 5. The three direct effects \(F_1, F_2,\) and \(F_3\) are shown in the left-hand column, and the corresponding error measures \(\Delta F_i\) in the right-hand column. They are computed using (8) and (10), respectively. One can see that the error terms \(\Delta F_i\) are much smaller than the effects \(F_i\). As already discussed, the three error terms add up to zero by design (see bottom-left panel). The right-hand bottom panel shows the overall uncertainty estimate according to (11).

The separation is of physical interest and discussed in more detail in KR16. In short, one can see that the Mediterranean amplification is due to the lapse-rate effect \(F_2\) and the circulation effect \(F_3\), while the thermodynamic effect yields a much weaker spatial pattern.

Figure 6 shows the corresponding results for the full FS methodology computed from (5). The top three left-hand panels show the three direct effects and the right-hand column the four interaction terms. Comparing the results for the three direct effects in Figs. 5 and 6, one can see that SFS and FS yield almost identical results. There are some small differences—for example, over the Iberian Peninsula between effects \(F_1\) and \(f_3\)—but these differences are likely too small to be statistically significant.

In comparison to SFS, the SF methodology yields the interaction terms. In the current case (see right-hand side of Fig. 6), it can be seen that the largest signal is due to the interaction term \(f_{123}\) in northern Africa. However, there are opposing signals in \(f_{12}\) and \(f_{13}\), which leaves only a small net signal in the sum of the interaction terms (see bottom-left panel of Fig. 6). As this paper is not primarily about the physical mechanisms behind the Mediterranean amplification, we do not attempt a thorough interpretation of the interaction terms. However, in general, the interaction terms of FS look similar as the delta terms of the SFS methodology, and their mathematical relationship can be gained using the same methodology as when deriving (14).

c. Sensitivity of SFS factor separation with respect to sequence of factors

As introduced in section 2b, the SFS methodology requires specifying the sequence (or order), with which the factors are considered. To explore the role of this—to some extent arbitrary—choice, we here provide a sensitivity analysis. In Fig. 5 we used the sequence \(f_o \rightarrow f_1 \rightarrow f_{12} \rightarrow f_{123}\) and \(f_{123} \rightarrow f_{23} \rightarrow f_3 \rightarrow f_o\) of simulations. We next compare Fig. 5 against an alternative analysis where we use the sequence \(f_o \rightarrow f_2 \rightarrow f_{23} \rightarrow f_{123}\)
FIG. 5. SFS. (left) The three main effects $\hat{F}_i$ and (right) their respective error measures $\Delta F_i$. (bottom) The overall uncertainty is further analyzed, which show (left) the sum $\Sigma \Delta F_i$ of all uncertainty terms (which is zero by definition for SFS) and (right) the RMS average of all error terms $\Delta F_i$. The three effects relate to 1) thermodynamic changes, 2) lapse-rate changes, and 3) circulation and other changes.
FIG. 6. As in Fig. 5, but for the complete FS methodology of SA03. (left) The three effects $f_1, f_2$, and $f_3$ and (right) the interaction terms $f_{12}, f_{13}, f_{23}$, and $f_{123}$. (bottom left) The sum of all interaction terms.
and \( f_{13} \rightarrow f_{1} \rightarrow f_{0} \). To arrive at a valid intercomparison, both orders satisfy the elementary design criteria introduced in section 2b; that is, the second sequence retracts the factor in the same order as they were first introduced.

Figure 7 shows the results for the latter sequence. The different panels show the same effects as in Fig. 5, but they are calculated with the new sequence. First of all, one can easily recognize that the three factors \( \tilde{F}_{1} \) look very similar and show almost no change. For \( \tilde{F}_{1} \) this is no surprise, because it is calculated in the exact same way for both sequences, but the similarity is also evident for the other two factors. The differences are difficult to detect. This similarity is surprising, as the two sequences are rather different. In Fig. 5 the thermodynamic effect (factor 1) was applied first with a synoptic-scale forcing that corresponds to CTRL, while in Fig. 7 it is applied last with a synoptic-scale forcing that corresponds to SCEN. The error measures of the factors are again much smaller than the factors themselves (see bottom-right panels of the figures). However, the RMS uncertainty in Fig. 7 has a slightly different pattern and is somewhat stronger than that in Fig. 5. Again, by design the sum of the \( \Delta \tilde{F}_{1} \) terms is zero independent of the sequence used in the SFS.

Overall, the analysis in section 3b shows that SFS and FS yield very similar results, and the analysis above demonstrates that SFS is barely sensitive to the sequence of factors. This indicates that the SFS method gives a good estimate of the three main factors, at least in the case considered.

However, this conclusion likely depends on the case and factors under investigation. For instance, Alpert et al. (1995) considered the pressure drop in a specific Alpine lee cyclogenesis event. In their case, the results depend significantly upon the number (and likely the sequence) of the factors considered. On the other hand, Bony et al. (2006) reviewed the analysis of climate feedbacks in global simulations. For modest climate changes, they found that there are “relatively small nonlinearities at the global scale, and a high degree of separability between the different radiative feedbacks” (p. 3476). In any case, we expect that pronounced sensitivities to the sequence of factors would be revealed by the uncertainty term (11).

### 4. Conclusions

In this paper we have proposed a sequential factor separation (SFS) technique and have tested it using a comprehensive set of regional climate model simulations. In comparison to the classical factor separation (FS) methodology of Stein and Alpert (1993), the main characteristics of SFS are as follows:

- The SFS methodology relies on a specified sequence (order) of the factors, and the required numerical experiments involve switching on and off the factors in this particular order (see Fig. 2). Strictly speaking, the results pertain only to this order, but in practice the order may often be of secondary importance.
- The FS methodology allows computing the interaction effects and thus provides quantitative measures of nonlinearity. The total effect of the factors is expressed as the sum of the \( n \) effects and the \( 2^{n} - n - 1 \) interaction terms. With the SFS methodology, the interaction effects are not computed and the total effect can be expressed as the sum of the \( n \) effects.
- Although SFS does not provide the interaction effects, it enables the computation of an uncertainty measure that is suited to addresses the quality of the factor separation. This uncertainty term [see (11)] is a measure of the interactions between the factors considered.
- While with FS the direct and interaction effects are defined relative to the control simulation, the SFS defines its effects relative to some intermediate states, intermediate in the sense that these states are somewhere in between the control and the scenario simulation.

To test the suitability of the SFS methodology, we also considered an example that involved sophisticated regional climate model experiments with \( n = 3 \) factors following KR16. The analysis has addressed a detailed intercomparison between SFS and FS, as well as the sensitivity of SFS with respect to the specified sequence of factors. The results demonstrate that—at least in the particular example considered—the two methodologies yield almost identical results and that the SFS is rather insensitive with respect to design choices. Although this result cannot be generalized to an arbitrary case of factor separation, the results indicate that SFS may often be successful in highly complex factor separation tasks.

Overall, the main strength of FS is the explicit consideration of the nonlinear interaction effects. We think that FS should always be used when considering merely two factors, as it provides an explicit quantification of the interaction effects. On the other hand, SFS has strengths regarding its simplicity and is recommended for situations with \( n \geq 3 \) factors: it requires less computational resources (i.e., fewer numerical experiments), the results are easier to interpret, and the uncertainty measure provides a mean for an a posteriori assessment of the SFS’s validity. In cases where the uncertainty measure questions the validity of the results, one can still expand SFS toward FS, as the simulations required for SFS are a subset of those needed for the full FS analysis.
FIG. 7. As in Fig. 5, but with another sequence of factors. Here the sequence of factors is \( f_0 \rightarrow f_2 \rightarrow f_{33} \rightarrow f_{123} \) and \( f_{123} \rightarrow f_{33} \rightarrow f_1 \rightarrow f_0 \); that is, the thermodynamic effect is considered as the last factor in the sequence of simulations, whereas it is the first factor in Fig. 5.
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