The Norm Dependence of Singular Vectors

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ABSTRACT

For a linearized system such as $\partial\boldsymbol{\psi}/\partial t = \mathbf{M}\boldsymbol{\psi}$, singular vector analysis can be used to find patterns that give the largest or smallest ratios between the sizes of $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$. Such analyses have applications to a wide range of atmosphere–ocean problems. The resulting singular vectors, however, depend on the norm used to measure the sizes of $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$, as noted in various applications. This causes complications because the choices of norm are generally nonunique. Based on perturbation theory, a derivation of how singular vectors change with norms typically used in the atmosphere–ocean literature is provided, and it is shown that the norm dependences observed in previous studies can be understood as general properties of singular vectors. This will hopefully clarify the interpretation of these observed norm dependencies, and provide guidance to new studies on how singular vectors would vary for different norms. It is further argued, based on these results, that there may not be as much norm-related ambiguity in problems, such as designing targeted observations or ensemble forecasts, as is often assigned to them.

1. Introduction

Singular vectors are useful tools for a wide range of atmosphere–ocean problems. Singular vectors with rapid growth have been invoked to explain phenomena ranging from extratropical cyclogenesis (Farrell 1989) to El Niño–Southern Oscillation (ENSO; Penland and Sardeshmukh 1995), and have been used to understand the predictability of weather systems (Molteni and Palmer 1993) and coupled atmosphere–ocean systems (Moore and Kleeman 1996), to construct initial perturbations of ensemble weather forecasts (Molteni et al. 1996; Ehrendorfer and Tribbia 1997), as well as to design targeted observations for prediction (Palmer et al. 1998). Singular vectors with small time tendencies, on the other hand, have been used to study, for example, the low-frequency atmospheric variability (Navarra 1993; Goodman and Marshall 2002).

One complication often encountered when using singular vectors is their dependence on the norms used for their derivation. This has been widely noted and discussed (Palmer et al. 1998; Thompson 1998; Errico 2000; Goodman and Marshall 2002; Kim and Morgan 2002). Such dependence casts ambiguity on the determination of singular vectors because choices of norm are in general not unique. This is quite problematic, particularly for targeted observations, because the optimal locations for targeted observations may vary substantially for different, but equally plausible, norm choices.

The goal of this paper is to provide a general understanding of this norm dependence. We shall begin with a brief introduction to singular vectors and their applications (section 2). The various norm dependences, as documented in the atmosphere–ocean literature, are summarized in section 3. In section 4, we derive the general norm dependence of singular vectors based on perturbation theory. Using these results, the norm dependence exhibited by singular vectors in various systems described in section 3 can be understood as general properties of these vectors (section 5). We conclude with a summary of the main results (section 6). Additional discussions for mathematical completeness are included in the appendix.

2. A brief introduction to singular vectors

Consider the linearized problem

$$\frac{\partial}{\partial t}\boldsymbol{\psi} = \mathbf{M}\boldsymbol{\psi}, \tag{1}$$

where $\boldsymbol{\psi}$ is a size N vector describing the state of the system and $\mathbf{M}$ is the $N \times N$ linear tendency matrix. Using singular value decomposition, one may decompose $\mathbf{M}$ as $\mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^*$, where the superscript asterisk denotes the adjoint; $\mathbf{U}$ and $\mathbf{V}$ are unitary matrices and their columns will be referred to as the left and right singular vectors, respectively; $\boldsymbol{\Lambda}$ is diagonal; and the jth diagonal element of $\boldsymbol{\Lambda}$, s_j, is the singular value associated with the jth pair of left and right singular vectors, so that $\mathbf{M}\mathbf{v}_j = s_j\mathbf{u}_j$.

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The singular values are real and nonnegative. Clearly, columns of $\mathbf{U}$ and $\mathbf{V}$ are also the eigenvectors of matrices $\mathbf{A}_u = \mathbf{M}\mathbf{M}^*$ and $\mathbf{A}_v = \mathbf{M}^*\mathbf{M}$, respectively, with the diagonal elements of $\mathbf{\Lambda}^2$ being the eigenvalues of $\mathbf{A}_u$ and $\mathbf{A}_v$. For simplicity, we shall assume that the singular values are distinct (nondistinct cases are discussed in the appendix). And for convenience, we arrange the singular vector pairs so that the associated singular values are in ascending order (i.e., $s_1 < s_2 \cdots < s_N$).

To quantify the growth of a perturbation, that is, to evaluate how the size of the tendency $\partial\boldsymbol{\psi}/\partial t$ relates to the size of $\boldsymbol{\psi}$, one needs to first define a measure of size, that is, the norm. If the Euclidean norm is used, the squared ratio between sizes of $\partial\boldsymbol{\psi}/\partial t$ (or $\mathbf{M}\boldsymbol{\psi}$) and $\boldsymbol{\psi}$, $\|\partial\boldsymbol{\psi}/\partial t\|^2/\|\boldsymbol{\psi}\|^2$ is $\langle\mathbf{M}\boldsymbol{\psi}, \mathbf{M}\boldsymbol{\psi}\rangle/\langle\boldsymbol{\psi}, \boldsymbol{\psi}\rangle$. The inner product of two vectors $\mathbf{x}$, $\mathbf{y}$ is defined as $\langle\mathbf{x}, \mathbf{y}\rangle = \mathbf{y}^*\mathbf{x} = \sum_k x_k\overline{y_k}$, where the overbar denotes the complex conjugate. With this definition of the inner product, we have

$$\frac{\langle\mathbf{M}\boldsymbol{\psi}, \mathbf{M}\boldsymbol{\psi}\rangle}{\langle\boldsymbol{\psi}, \boldsymbol{\psi}\rangle} = \frac{\langle\mathbf{M}^*\mathbf{M}\boldsymbol{\psi}, \boldsymbol{\psi}\rangle}{\langle\boldsymbol{\psi}, \boldsymbol{\psi}\rangle}. \tag{2}$$

It follows that when $\boldsymbol{\psi}$ takes the form of the jth right singular vector, $\partial\boldsymbol{\psi}/\partial t$ (or $\mathbf{M}\boldsymbol{\psi}$) takes the form of the jth left singular vector and the ratio between the sizes of $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$ is simply the jth singular value s_j. Given the initial time t_0 and the time lag τ, instead of Eq. (1), one may also write the system as

$$\boldsymbol{\psi}(t_0 + \tau) = \mathbf{R}(t_0, \tau)\boldsymbol{\psi}(t_0), \tag{3}$$

where $\mathbf{R}(t_0, \tau) = \lim_{\delta t\to 0} \prod_{j=1}^{n-1} e^{\mathbf{M}(t=t_0+j\delta t)\delta t}$ is the propagator matrix ($\delta t = \tau/n$), and examine the ratio between sizes of $\boldsymbol{\psi}(t_0 + \tau)$ and $\boldsymbol{\psi}(t_0)$. The analysis remains the same, except that $\mathbf{M}$ is replaced by the propagator $\mathbf{R}$.

At this point, the connection between singular vectors and the growth of small perturbations over a finite period of time becomes apparent. When one is interested in patterns of $\boldsymbol{\psi}$ that give the highest $\mathbf{M}\boldsymbol{\psi}$-to-$\boldsymbol{\psi}$ ratios (fastest growth) as measured by the selected norm,[1] one seeks to find the pairs of singular vectors associated with the largest singular values, where the right singular vectors of these pairs represent the perturbation (sometimes called the optimal perturbation patterns), and the left ones represent the response. As mentioned in section 1, these singular vectors have been applied to problems ranging from ensemble weather forecasting (Molteni et al. 1996) to ENSO prediction (Thompson 1998; these will be referred to as type I problems).

In another type of problem, instead of perturbation patterns in $\boldsymbol{\psi}$ that give the maximum time tendency, one is interested in patterns of external forcing ($\mathbf{f}$) that for a given size, induce the maximum stationary (or steady state) responses (this will be referred to as the type II problem). Because, for stationary responses, the time tendency term vanishes, one can write this problem as $\mathbf{0} = \mathbf{M}\boldsymbol{\psi} + \mathbf{f}$. [This is not to be confused with the statistically stationary response, in which case it is the ensemble mean statistics that do not change with time (Farrell and Ioannou 1993).] The goal here is therefore to maximize the ratio of the size of the response $\|\boldsymbol{\psi}\|$ to the size of the forcing $\|\mathbf{f}\|$ or equivalently $\|\mathbf{M}\boldsymbol{\psi}\|$, that is, to minimize $\|\mathbf{M}\boldsymbol{\psi}\|/\|\boldsymbol{\psi}\|$. Clearly, patterns from this optimization problem are the pairs of singular vectors associated with the smallest singular values. In this context, the right singular vectors of these pairs represent the response of the system, and the left singular vectors represent the optimal forcing patterns. The right singular vectors here are sometimes called the neutral vectors for their small time tendencies in the corresponding transient problem (Marshall and Molteni 1993), and are linked to the leading empirical orthogonal functions of the system's low-frequency responses to random forcing (Navarra 1993). An example of a type II problem is the climate system's low-frequency variability and its long-term response to external forcing (Navarra 1993; Goodman and Marshall 2002).

[1] Throughout the rest of the paper, $\mathbf{M}$ will be used with the understanding that it will be replaced by $\mathbf{R}$ if Eq. (3) instead of Eq. (1) is used.

3. General aspects of the observed norm dependence of singular vectors

Some rather interesting norm dependences of singular vectors have been documented in the literature on atmosphere–ocean systems, and are briefly summarized here. (The references are not meant to be exhaustive.) In the studies to be summarized, the same norm was used for both $\boldsymbol{\psi}$ and $\mathbf{M}\boldsymbol{\psi}$.

Observation 1: Asymmetric norm sensitivity between left and right singular vectors

In the study of a linearized global quasi-geostrophic atmospheric model, the neutral vectors (the right singular vectors associated with the smallest singular values) are found to be insensitive to different norm selections while their forcing patterns (the corresponding left singular vectors) display a much greater sensitivity (Goodman and Marshall 2002). On the other hand, Palmer et al. (1998) found that the right singular vector associated with the largest singular value is much more norm sensitive than the corresponding left singular vector. Similar behaviors were found for the singular vectors of the Eady model (Kim and Morgan 2002).

Observation 2: When the norm weighs certain components more strongly, these components are more suppressed in the left (right) singular vectors associated with the smallest (largest) singular values

For example, Goodman and Marshall (2002) found that, when the kinetic energy instead of the streamfunction variance is used as the norm, amplitudes of the high-wavenumber components are reduced in the left singular vectors associated with the smallest singular values. A similar result is found for the right singular vector associated with the largest singular value (Palmer et al. 1998). When enstrophy is used as the norm, the right singular vector associated with the largest singular value becomes even broader in scale (Palmer et al. 1998).

This behavior was documented more quantitatively in the study of a linearized ENSO model (Thompson 1998). We shall refer to the right singular vector associated with the largest singular value ($\mathbf{v}_N$) as the "dynamic optimal" when it is derived under a norm that puts all weights on the ocean dynamic variables, which include the thermocline depth along with its dynamically consistent upper layer ocean currents, and zero weight on the sea surface temperature (SST). The vector $\mathbf{v}_N$ derived under a norm that puts all weights on the SST and zero weight on the ocean dynamic variables will be referred to as the "SST optimal." Thompson (1998) found that, for a more general norm that weights the ocean variables by w_1 and the SST by w_2, the resulting $\mathbf{v}_N$ can be approximated by a linear combination of the dynamic optimal and SST optimal, and the ratio of the two components is proportional to $(w_2/w_1)^2$, provided that τ is sufficiently large [Eq. (3) was used in Thompson (1998)].

4. Perturbation analysis

The various norms of a vector $\mathbf{x}$ used in previous studies may be expressed as $\|\mathbf{x}\| = \langle \mathbf{Lx}, \mathbf{Lx}\rangle^{1/2}$, with the definition of the inner product unchanged and $\mathbf{L}$ being a weighting matrix that acts on a set of orthogonal bases spanning the linear space of interest. Since these bases constitute the orthogonal eigenvectors of $\mathbf{L}$ with the weights being the real eigenvalues (this can be viewed as the definition of a weighting matrix), $\mathbf{L}$ is self-adjoint (Hermitian). We shall restrict ourselves to these norms, which belong to the so-called Riemannian metric.

We shall use the Euclidean norm in $\boldsymbol{\psi}$ and $\mathbf{M}\boldsymbol{\psi}$ as the reference norm for our perturbation analysis, so that the identity matrix $\mathbf{I}$ is our reference weighting matrix (uniform weighting). No generality is lost because non-Euclidean reference norms can always be transformed to the Euclidean norm through redefinitions of $\mathbf{M}$ and $\boldsymbol{\psi}$.[2] To change from the reference norm to a new norm is therefore to change the weighting from $\mathbf{I}$ to a nonuniform weighting matrix $\mathbf{L}$.

We can always write $\mathbf{L} = \mathbf{I} + \delta\mathbf{L}$, where $\delta\mathbf{L}$ is a perturbation, and examine how singular vectors change when $\mathbf{L}$ instead of $\mathbf{I}$ is used. Following $\mathbf{L}$, $\delta\mathbf{L}$ is also self-adjoint.

[2] For any non-Euclidean reference norms in $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$, $\langle \mathbf{L}_1\mathbf{M}\boldsymbol{\psi}, \mathbf{L}_1\mathbf{M}\boldsymbol{\psi}\rangle$, and $\langle \mathbf{L}_2\boldsymbol{\psi}, \mathbf{L}_2\boldsymbol{\psi}\rangle$, one can always redefine $\mathbf{M}$ as $\mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}$ and $\boldsymbol{\psi}$ as $\mathbf{L}_2\boldsymbol{\psi}$, so that the reference norm is Euclidean in the redefined linear spaces.

We shall allow the norms for $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$ to be different, so that in place of Eq. (2), the squared ratio between the sizes of $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$ is

$$\frac{\langle \mathbf{L}_1\mathbf{M}\boldsymbol{\psi}, \mathbf{L}_1\mathbf{M}\boldsymbol{\psi}\rangle}{\langle \mathbf{L}_2\boldsymbol{\psi}, \mathbf{L}_2\boldsymbol{\psi}\rangle} = \frac{\langle \mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}\boldsymbol{\psi}', \mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}\boldsymbol{\psi}'\rangle}{\langle \boldsymbol{\psi}', \boldsymbol{\psi}'\rangle}, \quad (4)$$

where $\mathbf{L}_{1,2} = \mathbf{I} + \delta\mathbf{L}_{1,2}$ are the nonuniform weighting matrices at the initial and final times, and $\boldsymbol{\psi}' = \mathbf{L}_2\boldsymbol{\psi}$.

By decomposing $\mathbf{M}' \equiv \mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}$ into $\mathbf{U}'\boldsymbol{\Lambda}'\mathbf{V}'^*$, we have

$$\mathbf{M}'\mathbf{v}_j' = s_j'\mathbf{u}_j'. \quad (5)$$

(All primed quantities have meanings analogous to the unprimed ones defined in section 2.) This means that, when $\boldsymbol{\psi}$ is equal to $\mathbf{L}_2^{-1}\mathbf{v}_j'$ (i.e., $\boldsymbol{\psi}'$ is equal to $\mathbf{v}_j'$) multiplied by a nonzero scalar, $\mathbf{M}\boldsymbol{\psi}$ is equal to $\mathbf{L}_1^{-1}\mathbf{u}_j'$ (i.e., $\mathbf{M}'\boldsymbol{\psi}'$ is equal to $\mathbf{u}_j'$) multiplied by the nonzero scalar, and the squared ratio between the sizes of $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$ under the new norms [Eq. (4)] is $(s_j')^2$. Therefore, columns of $\mathbf{L}_2^{-1}\mathbf{V}'$ and $\mathbf{L}_1^{-1}\mathbf{U}'$ are the right and left singular vectors of $\mathbf{M}$ under the new norms.

Let us now consider $\delta\mathbf{L}_{1,2}$ to be sufficiently small so that second- and higher-order terms can be neglected. Note that columns of $\mathbf{U}'$ and $\mathbf{V}'$ are the eigenvectors of matrices $\mathbf{A}_u' = \mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}(\mathbf{L}_2^{-1})^*\mathbf{M}^*\mathbf{L}_1^*$ and $\mathbf{A}_v' = (\mathbf{L}_2^{-1})^*\mathbf{M}^*\mathbf{L}_1^*\mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}$, while columns of $\mathbf{U}$ and $\mathbf{V}$ are the eigenvectors of $\mathbf{A}_u$ and $\mathbf{A}_v$. Differences between $\mathbf{U}'$, $\mathbf{V}'$ and $\mathbf{U}$, $\mathbf{V}$ can thus be estimated from differences between $\mathbf{A}_u'$, $\mathbf{A}_v'$ and $\mathbf{A}_u$, $\mathbf{A}_v$ using perturbation theory, as described in, for example, Franklin (1968).

Since the departure of $\mathbf{L}_1\mathbf{M}\mathbf{L}_2^{-1}$ from $\mathbf{M}$ is to the first order, $\delta\mathbf{M} = \delta\mathbf{L}_1\mathbf{M} - \mathbf{M}\delta\mathbf{L}_2$($\mathbf{L}_2^{-1}$ is approximated by $\mathbf{I} - \delta\mathbf{L}_2$), the difference between $\mathbf{A}_u'$ and $\mathbf{A}_u$ can be written as

$$\begin{aligned}\delta\mathbf{A}_u &= \delta\mathbf{M}\mathbf{M}^* + \mathbf{M}\delta\mathbf{M}^* \\ &= \delta\mathbf{L}_1\mathbf{U}\boldsymbol{\Lambda}^2\mathbf{U}^* + \mathbf{U}\boldsymbol{\Lambda}^2\mathbf{U}^*\delta\mathbf{L}_1 - 2\mathbf{U}\boldsymbol{\Lambda}\mathbf{V}^*\delta\mathbf{L}_2\mathbf{V}\boldsymbol{\Lambda}\mathbf{U}^*.\end{aligned} \quad (6)$$

We have used the fact that $\delta\mathbf{L}_{1,2}$ are self-adjoint. The deviation of the jth eigenvector $\mathbf{u}_j'$ of $\mathbf{A}_u'$ from that of $\mathbf{A}_u$, $\mathbf{u}_j$, given by perturbation theory is

$$\mathbf{u}_j' - \mathbf{u}_j = \sum_{\substack{k=1 \\ k\neq j}}^{N} \frac{\langle \delta\mathbf{A}_u\mathbf{u}_j, \mathbf{u}_k\rangle}{(s_j^2 - s_k^2)\langle \mathbf{u}_k, \mathbf{u}_k\rangle}\mathbf{u}_k, \quad (7)$$

where $\mathbf{u}_j$, $\mathbf{u}_k$ are the jth and kth columns of $\mathbf{U}$. The derivation of Eq. (7) is given in textbooks in matrix theory such as Franklin (1968), and will not be repeated here.

In order to obtain the jth left singular vector of $\mathbf{M}$ under the new norms $\tilde{\mathbf{u}}_j$, which is in the $\boldsymbol{\psi}$ space, we need to transform $\mathbf{u}_j'$, which is in the $\boldsymbol{\psi}'$ space, to the $\boldsymbol{\psi}$ space, that is, $\tilde{\mathbf{u}}_j = \mathbf{L}_1^{-1}\mathbf{u}_j'$ [also see discussions following Eq. (5)]. Its departure from $\mathbf{u}_j$, the jth left singular vector under the reference norm, is to the first order:

$$\delta \mathbf{u}_j = \tilde{\mathbf{u}}_j - \mathbf{u}_j = -\delta \mathbf{L}_1 \mathbf{u}_j + \sum_{\substack{k=1\\k\neq j}}^{N} \frac{\langle \delta \mathbf{A}_u \mathbf{u}_j, \mathbf{u}_k\rangle}{(s_j^2 - s_k^2)\langle \mathbf{u}_k, \mathbf{u}_k\rangle}\mathbf{u}_k.$$

We shall scale the new singular vectors so that $\delta\mathbf{u}_j$ only contain components that are orthogonal to $\mathbf{u}_j$:

$$\delta \mathbf{u}_j = \sum_{\substack{k=1\\k\neq j}}^{N} \varepsilon_{jk}\mathbf{u}_k, \tag{8}$$

where

$$\varepsilon_{jk} = \frac{\langle \delta \mathbf{A}_u \mathbf{u}_j, \mathbf{u}_k\rangle}{(s_j^2 - s_k^2)} - \langle \delta \mathbf{L}_1 \mathbf{u}_j, \mathbf{u}_k\rangle.$$

High-order terms resulting from the scaling have been neglected.

Substituting Eq. (6) into $\langle \delta \mathbf{A}_u \mathbf{u}_j, \mathbf{u}_k\rangle$ and recognizing that $\mathbf{U}$ and $\mathbf{V}$ are unitary and $\boldsymbol{\Lambda}$ is diagonal, we have (intermediate steps are presented in the appendix)

$$\langle \delta \mathbf{A}_u \mathbf{u}_j, \mathbf{u}_k\rangle = (s_j^2 + s_k^2)\langle \delta \mathbf{L}_1 \mathbf{u}_j, \mathbf{u}_k\rangle - 2 s_j s_k \langle \delta \mathbf{L}_2 \mathbf{v}_j, \mathbf{v}_k\rangle. \tag{9}$$

Substituting this into Eq. (8) and combining terms gives

$$\varepsilon_{jk} = s_k\left(\frac{2s_k\langle \delta \mathbf{L}_1 \mathbf{u}_j, \mathbf{u}_k\rangle - 2s_j\langle \delta \mathbf{L}_2 \mathbf{v}_j, \mathbf{v}_k\rangle}{s_j^2 - s_k^2}\right). \tag{10}$$

Applying the same analysis to $\mathbf{A}_v$ leads to

$$\delta \mathbf{v}_j = \sum_{\substack{k=1\\k\neq j}}^{N} \sigma_{jk}\mathbf{v}_k,$$

with

$$\sigma_{jk} = s_j\left(\frac{2s_k\langle \delta \mathbf{L}_1 \mathbf{u}_j, \mathbf{u}_k\rangle - 2s_j\langle \delta \mathbf{L}_2 \mathbf{v}_j, \mathbf{v}_k\rangle}{s_j^2 - s_k^2}\right). \tag{11}$$

Note that terms in the square bracket are identical for both the right and left singular vectors [Eqs. (10) and (11)], which will be referred to as Ω_{jk}. The sizes of the changes in the singular vectors are therefore[3]

$$\Delta^2_{\mathbf{u}_j} = \sum_{\substack{k=1\\k\neq j}}^{N} s_k^2\Omega_{jk}^2, \quad \text{and} \tag{12}$$

$$\Delta^2_{\mathbf{v}_j} = \sum_{\substack{k=1\\k\neq j}}^{N} s_j^2\Omega_{jk}^2. \tag{13}$$

[3] We have used the reference norm (which is Euclidean in this case) to measure sizes of the changes. We could also measure them using the new norms. The size difference from the two measures involves only second- or higher-order terms of $\delta\mathbf{L}_{1,2}$ and may be neglected.

5. Observed norm dependences as general properties of singular vectors

For each j, let us define weights w_k^2 as $s_j^2\Omega_{jk}^2$. From Eqs. (12) and (13), it is clear that

$$\frac{\Delta^2_{\mathbf{u}_j}}{\Delta^2_{\mathbf{v}_j}} = \frac{\sum_{k\neq j} w_k^2(s_k/s_j)^2}{\sum_{k\neq j} w_k^2}, \tag{14}$$

that is, the weighted average of s_k^2/s_j^2. For $j = 1$, the maximum of s_k^2/s_j^2 is s_N^2/s_1^2 and the minimum is s_2^2/s_1^2, as we have assumed $s_1 < s_2 \cdots < s_N$. Because all weights are positive and every individual term is bounded by s_N^2/s_1^2 and s_2^2/s_1^2, the weighted average must obey

$$1 < s_2/s_1 \leq \Delta_{\mathbf{u}_1}/\Delta_{\mathbf{v}_1} \leq s_N/s_1. \tag{15}$$

Alternatively, one may think of $\Delta^2_{\mathbf{v}_j}/\Delta^2_{u_j}$ as the weighted averaged of s_j^2/s_k^2 with the weights being $s_k^2\Omega_{jk}^2$. (Cases where $\Delta_{\mathbf{u}_j} = \Delta_{\mathbf{v}_j} = 0$ are discussed in the appendix.) By the same argument, we have

$$1 < s_N/s_{N-1} \leq \Delta_{\mathbf{v}_N}/\Delta_{\mathbf{u}_N} \leq s_N/s_1. \tag{16}$$

We have therefore shown that for the smallest singular value, the associated right singular vector has lower norm sensitivity than the left singular vector, and the reverse is true for the largest singular value. Matrix $\mathbf{M}$ being singular (i.e., $s_1 = 0$) may be considered as a special case, where $\Delta_{\mathbf{u}_N} = \Delta_{\mathbf{v}_1} = 0$. This asymmetric norm sensitivity holds regardless of the form of $\mathbf{M}$. The asymmetry is strictly true for singular vectors associated with the largest or the smallest singular value. For intermediate singular values (i.e., $1 < j < N$), whether $\Delta_{\mathbf{u}_j}/\Delta_{\mathbf{v}_j}$ is greater or less than 1 depends on the problem. However, for N sufficiently large, one expects the asymmetry shown for $j = 1$ (and $j = N$) to extend to the smallest (and largest) singular values as well.

For properties that do not depend on the specific forms of $\mathbf{M}$, analogous behaviors of the singular vectors associated with the largest and the smallest singular values, with left and right reversed, should come as no surprise. This is because the singular vectors associated with the largest singular values for $\mathbf{M}$ are the singular vectors associated with the smallest singular values for $\mathbf{M}^{-1}$ (assuming $\mathbf{M}$ is not singular), with right and left reversed. Recall that we are interested in singular vectors associated with the smallest singular values in type II problems and those associated with the largest singular values in type I problems. Also note that the response and forcing/perturbation fields are reversed in terms of right and left in the two types of problems. Properties that are independent of the forms of $\mathbf{M}$ are therefore shared by singular vectors of the response field in both types of problems. The same is true for general properties of singular vectors of the forcing/perturbation field. For example, singular vectors of the response field are less norm sensitive than singular vectors of the forcing field in both types of problems [Eqs. (15) and (16)].

From Eqs. (10) and (11), we also see that if $\langle \delta \mathbf{L}_1 \mathbf{u}_1,$

$\mathbf{u}_k\rangle$ and $\langle \delta \mathbf{L}_2\mathbf{v}_1, \mathbf{v}_k\rangle$ are of similar magnitude, $\mathbf{L}_1$ (or $\mathbf{L}_2$) tends to have greater effects on the singular vectors associated with the smallest (or largest) singular values. Again, this means that changes in the norm of the forcing field have greater influence on the singular vectors than changes in the norm of the response field in both types of problems.

We shall now make use of the fact that for many atmosphere–ocean systems of interest, the largest (or smallest) singular values are substantially larger (or smaller) than the rest of the singular values. For example, Fig. 10 of Palmer et al. (1998) shows the rapid decrease of singular values from the high end downward in the global atmospheric system that they studied. Similar behavior is found in the ENSO model used by Thompson (1998). On the other hand, singular values for the neutral vectors of Goodman and Marshall (2002) show a rapid increase from the low end upward (J. Goodman 2003, personal communication), and so do those in an earlier study based on a global barotropic model (Navarra 1993). Satisfaction of this condition in these systems is not coincidental, and is in fact linked to the usefulness of the singular vector analysis in these types of problems: when singular vector analyses are used to identify patterns that, for a forcing of certain size, give larger responses than other patterns, their results are most meaningful when the largest (or smallest, depending on whether the problem is of type I or type II) singular values are sufficiently larger (or smaller) than the others.

Given the above arguments, let us now consider $s_1 \ll s_2$. We shall base our discussion on singular vectors associated with the smallest singular value, that is, on type II problems. The results, being independent of the forms of $\mathbf{M}$, remain valid for type I problems when they are cast in terms of the response and forcing/perturbation fields. For the studies summarized in section 3, the same norm was used for both $\mathbf{M}\boldsymbol{\psi}$ and $\boldsymbol{\psi}$; that is, $\mathbf{L}_1 = \mathbf{L}_2 = \mathbf{L}$. However, it is easy to see from Eq. (10) that, so long as $\langle \delta \mathbf{L}_1\mathbf{u}_1, \mathbf{u}_k\rangle$ and $\langle \delta \mathbf{L}_2\mathbf{v}_1, \mathbf{v}_k\rangle$ are of similar magnitude, $\mathbf{L}_2$ has little effect on $\mathbf{u}_1$ and $\mathbf{v}_1$ when $s_1 \ll s_2$. Equation (10) can thus be simplified to $\varepsilon_{1k} = -2\langle \delta \mathbf{L}_1\mathbf{u}_1, \mathbf{u}_k\rangle$, or

$$\delta \mathbf{u}_1 \approx -2\delta \mathbf{L}_1\mathbf{u}_1. \tag{17}$$

Note that the size of the change in $\mathbf{u}_1$ is about $|2\delta \mathbf{L}_1\mathbf{u}_1|$. Therefore, the difference in the norm sensitivities of $\mathbf{v}_1$ and $\mathbf{u}_1$ arises from reduced norm sensitivity in the singular vector of the response field $\mathbf{v}_1$ rather than from enhanced sensitivity in the singular vector of the forcing field $\mathbf{u}_1$. From Eq. (15), it is clear that when $s_1 \ll s_2$, the response pattern $\mathbf{v}_1$ would be rather insensitive to norm changes. A similar statement can of course be made for $\mathbf{u}_N$. The asymmetric norm sensitivity between left and right singular vectors stated in observation 1 can therefore be understood as a general property of singular vectors.

Equation (17) and an analogous equation for $\mathbf{u}_N$ and $\mathbf{v}_N$ are also, to the limit of the perturbation analysis, the mathematical equivalents of observation 2, which states that when the norm weights certain components more strongly, these components are more suppressed in the left (right) singular vector associated with the smallest (largest) singular value. Again, for N sufficiently large, the properties shown for $j = 1$ (and $j = N$) are expected to extend to the smallest (and largest) singular values as well.

Neglecting higher-order terms, Eq. (17) can also be written as

$$\tilde{\mathbf{u}}_1 \approx \mathbf{L}_1^{-2}\mathbf{u}_1, \tag{18}$$

where $\tilde{\mathbf{u}}_1$ is the first left singular vector (the optimal forcing pattern) under the new norms. This gives a simple formula that describes how optimal forcing patterns change with norm. While Eq. (18) is derived from a perturbation analysis, the same equation can be shown to hold for finite norm changes by regarding Eq. (18) as the ''differential'' form and integrating it to give the response to finite norm changes (appendix). The results from Thompson (1998) as described in observations 2 directly follow from these results.

Here, as an example, we apply Eq. (18) to the neutral vectors derived under different norms for a global three-layer quasigeostrophic atmospheric model (Goodman and Marshall 2002). In Figs. 1a and 1b, we show the first left singular vectors associated with the smallest singular value (the optimal forcing patterns, as this is a type II problem) in terms of the streamfunction under the kinetic energy norm (KE norm) and the squared streamfunction norm (psi norm), respectively. When spherical harmonics are chosen to be the coordinates, the KE norm may be viewed as weighting each harmonic prior to the inner product by the square root of the coefficient that represents the Laplace operator (Ehrendorfer 2000). Equation (18) in this case states that applying the Laplace operator to the first left singular vector derived under the KE norm (the result is shown in Fig. 1c) should give approximately the first left singular vector under the psi norm (Fig. 1b). This statement is confirmed to a remarkable precision. The cosine of the angle formed by the two vectors, $\cos\theta$, is 0.998. Note that the difference between the KE norm and the psi norm is quite substantial. Equation (18) also works well for the second left singular vector ($\cos\theta = 0.94$), although the error becomes large for the third left singular vector ($\cos\theta = 0.60$).

6. Discussion and summary

In this paper, we derived some general results of the norm dependence of singular vectors using perturbation theory. We have done so for the norms (of a vector $\mathbf{x}$) that may be expressed as $\|\mathbf{x}\| = \langle \mathbf{L}\mathbf{x}, \mathbf{L}\mathbf{x}\rangle^{1/2}$, with $\mathbf{L}$ being a weighting matrix that acts on a set of orthogonal bases spanning the linear space of interest. These are the norms typically used in the atmospheric–ocean literature

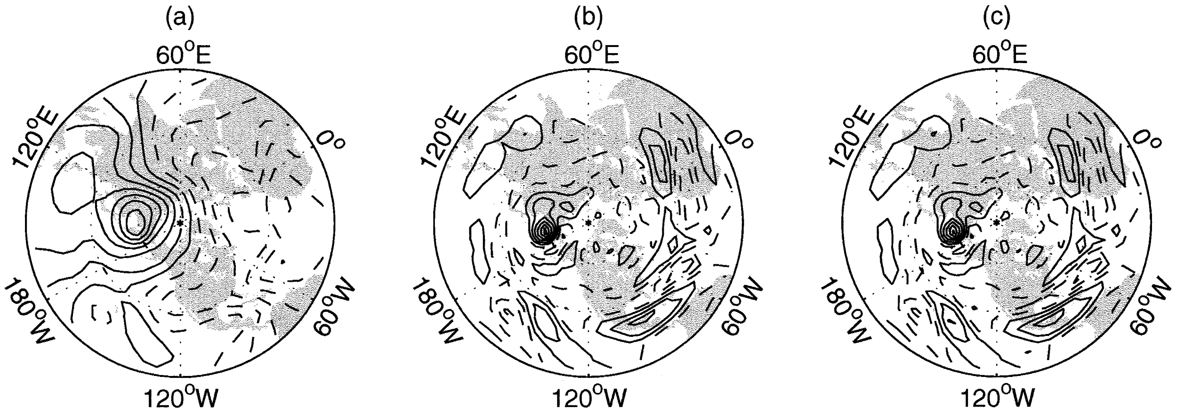

FIG. 1. The optimal forcing patterns in terms of streamfunction of a three-layer global quasi-geostrophic atmospheric model (Goodman and Marshall 2002) derived under (a) the KE norm, (b) the psi norm, and (c) by applying Eq. (18) on (a). While the model contains three levels, only the 800-mb level is shown.

on singular vectors. We are interested in singular vectors associated with the smallest singular values in type II problems (e.g., low-frequency climate variability), and those associated with the largest singular values in type I problems (weather forecasting, ENSO prediction, targeted observations, etc.). We found that, as general properties of singular vectors, those of the response field ($\mathbf{v}_N$ for type I problems and $\mathbf{u}_1$ for type II problems) have reduced norm sensitivity compared to those of the forcing/perturbation field ($\mathbf{u}_N$ for type I problems and $\mathbf{v}_1$ for type II problems). This is true regardless of the specific forms of the linear tendency matrix (or the propagator). Moreover, norm changes of the response field tend to have greater influences on singular vectors than those of the forcing/perturbation field. We further observe that for singular vector analyses to be useful, the singular value spectrum should be sufficiently sharp in the portion that is of interest (the lower end for type II problems and the higher end for type I problems). Satisfaction of this condition is confirmed in many atmosphere–ocean systems where singular vector analyses were found useful. Under this condition, singular vectors of the response field become norm insensitive, as observed in many studies. Moreover, norm changes of the response field become ineffective in changing the singular vectors, and the effect of norm changes on singular vectors tends to be dominated by that of the forcing/perturbation field. A formula was derived that describes how singular vectors of the forcing field should change with the norm of the forcing field [Eq. (18) and its equivalent for $\mathbf{v}_N$]. Although Eq. (18) was derived from a perturbation analysis, it can be extended quite well to finite norm changes.

As argued by Palmer et al. (1998), for targeted (or adaptive) observations, the appropriate norm for the forcing field should be uniquely determined by the one for which all unit amplitude forcing patterns are equally likely a priori. This requirement would eliminate the ambiguity in the norm of the forcing/perturbation field. In this case, the optimal forcing/perturbation patterns also become norm insensitive, because norm uncertainties of the response field are not effective in changing the singular vectors. This implies that it is possible for targeted observations to obtain optimal forcing patterns that are insensitive to different norm choices for the response field (so long as they are Riemannian metrics). The same argument applies to other problems such as designing ensemble forecasts. These results therefore suggest that there may not be as much norm-related ambiguity in these types of problems as is often assigned to them.

In summary, we derived in this paper some general results that explain the norm dependencies of singular vectors as observed in many previous studies. It is hoped that these results would help clarify the interpretations of these observed norm dependences, and provide guidance to new studies on how singular vectors would differ for different norms. In addition, our results suggest that there may not be as much norm-related ambiguity in problems such as designing targeted observations or ensemble forecasts as is often assigned to them.

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APPENDIX

Additional Discussion for Mathematical Completeness

a. Nondistinct singular values

For simplicity, I have assumed the singular values to be distinct. If a singular value is repeated for *m* times, then the right or left singular vectors can be any arbitrary orthogonal base of the m-dimensional subspace spanned by the right or left singular vectors that share this singular value. Variations in the singular vectors should thus be generalized into variations in this subspace. The results will still hold with this generalization when the singular values are not distinct.

b. Derivation of Eq. (9)

To derive Eq. (9), we substitute Eq. (6) into $\langle \delta \mathbf{A}_u \mathbf{u}_j, \mathbf{u}_k \rangle$ and use the fact that $\mathbf{U}$ and $\mathbf{V}$ are unitary and $\mathbf{\Lambda}$ is diagonal. This gives us

$$\begin{aligned}\langle \delta \mathbf{A}_u \mathbf{u}_j, \mathbf{u}_k \rangle &= \mathbf{u}_k^* \delta \mathbf{A}_u \mathbf{u}_j \\ &= \mathbf{u}_k^* \delta \mathbf{L}_1 \mathbf{U} \mathbf{\Lambda}^2 \mathbf{U}^* \mathbf{u}_j + \mathbf{u}_k^* \mathbf{U} \mathbf{\Lambda}^2 \mathbf{U}^* \delta \mathbf{L}_1 \mathbf{u}_j \\ &\quad - 2\mathbf{u}_k^* \mathbf{U} \mathbf{\Lambda} \mathbf{V}^* \delta \mathbf{L}_2 \mathbf{V} \mathbf{\Lambda} \mathbf{U}^* \mathbf{u}_j \\ &= s_j^2 \mathbf{u}_k^* \delta \mathbf{L}_1 \mathbf{u}_j + s_k^2 \mathbf{u}_k^* \delta \mathbf{L}_1 \mathbf{u}_j - 2 s_j s_k \mathbf{v}_k^* \delta \mathbf{L}_2 \mathbf{v}_j \\ &= (s_j^2 + s_k^2) \langle \delta \mathbf{L}_1 \mathbf{u}_j, \mathbf{u}_k \rangle - 2 s_j s_k \langle \delta \mathbf{L}_2 \mathbf{v}_j, \mathbf{v}_k \rangle.\end{aligned}$$

c. The case where $\Delta_{\mathbf{u}_j} = \Delta_{\mathbf{v}_j} = 0$

In Eqs. (12) and (13), it is possible that $\Delta_{\mathbf{u}_j} = \Delta_{\mathbf{v}_j} = 0$ when $\delta \mathbf{L}_1 \mathbf{u}_j \propto \mathbf{u}_j$ and $\delta \mathbf{L}_2 \mathbf{v}_j \propto \mathbf{v}_j$. (It is not possible for $\langle \delta \mathbf{L}_1 \mathbf{u}_j, \mathbf{u}_k \rangle / \langle \delta \mathbf{L}_2 \mathbf{v}_j, \mathbf{v}_k \rangle = s_j / s_k$ because the left-hand side stays the same when j and k are exchanged, as $\delta \mathbf{L}_1$ and $\delta \mathbf{L}_2$ are self-adjoint, while the right-hand side does not as $s_j \neq s_k$.) In this case, the ratio between the two is undefined. Since these pairs of singular vectors also have no effect on changes in the other singular vectors, we can eliminate these pairs from the list of singular vectors.

d. Extending Eq. (18) to finite norm changes

Now let us take a look at how Eq. (18) may be extended to finite norm changes by regarding it as the differential form. Let us consider a weighting matrix $\mathbf{L}_w$ that deviates from the identity matrix substantially. For simplicity, we consider $\mathbf{L}_w$ to be real and diagonal (No generality is lost because $\mathbf{L}_w$ is self-adjoint so that it can be transformed to a real diagonal one by a similarity transformation, which does not change the singular vectors.) One can always write $\mathbf{L}_w$ as $\mathbf{L}^m = (\mathbf{I} + \delta \mathbf{L})^m$. For a sufficiently large m, $\mathbf{L}$ becomes sufficiently close to the identity matrix to warrant the perturbation analysis. The effect of $\mathbf{L}_w$ can be viewed as applying $\mathbf{L}$ for m times. Now let us again consider $s_1 \ll s_2$ so that

$$\mathbf{u}_1(i+1) = \{\mathbf{L}^{-2} + O[(\delta \mathbf{L})^2]\} \mathbf{u}_1(i), \qquad \text{(A1)}$$

where $\mathbf{u}_1(i)$ is the first left singular vector after applying $\mathbf{L}$ i times. If the norm change does not disrupt the general singular value structure of the system so that $s_1 \ll s_2$ always holds, we have

$$\mathbf{u}_1(m) = \{\mathbf{L}^{-2} + O[(\delta \mathbf{L})^2]\}^m \mathbf{u}_1(0). \qquad \text{(A2)}$$

When the departure of $\mathbf{L}$ from $\mathbf{I}$ is of order 1, it can be shown that, for large m, Eq. (A2) can be written as

$$\mathbf{u}_1(m) \approx \mathbf{L}^{-2m} \mathbf{u}_1(0) = \mathbf{L}^{-2} \mathbf{u}_1(0) \qquad \text{(A3)}$$

to an excellent degree of approximation. Equation (18), therefore, can be applied to weighting matrices that are substantially nonuniform. A similar extension can, of course, be made for $\mathbf{v}_N$.

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