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Analytical Sensitivities of Principal Components in Time-Series Analysis of Dynamical Systems

D. Todd Griffith*
Sandia National Laboratories, Albuquerque, New Mexico 87185

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Principal components analysis, which is also referred to as proper orthogonal decomposition in the literature, is a useful technique in many fields of engineering, science, and mathematics for analysis of time-series data. The benefit of principal components analysis for dynamical systems comes from its ability to detect and rank the dominant coherent spatial structures of dynamic response, such as operating deflection shapes or mode shapes. In this work, an original method for calculating the analytical sensitivities of the principal components of dynamical systems is developed. Methods for analytical sensitivity calculations are developed for both the singular-value decomposition and eigenanalysis-based approaches for principal component calculation. Sensitivities with respect to state initial conditions and system parameters are enabled by state transition matrix calculations for augmented state and parameter differential equations. A novel approach to compute principal component sensitivities with respect to transient forcing-function parameters is introduced by transforming nonhomogenous differential equations (forced system) into homogenous differential equations (unforced system). These new developments are applied to several example problems in dynamics analysis, with an emphasis on structural dynamics analysis. Analytical sensitivities provide the necessary derivatives for gradient-based optimization algorithms and provide an analytical framework for evaluating structural modifications based on principal components analysis.

Nomenclature

A	=	state matrix
$\hat{\boldsymbol{e}}_i$	=	forcing-function permutation operator for ith forcing component
$\boldsymbol{F}$	=	forcing vector
f_i	=	forcing-function amplitude for ith forcing component
g	=	gravity constant
$\boldsymbol{g}(t)$	=	general forcing-function vector
M,C,K	=	mass, damping, and stiffness matrices
$\boldsymbol{p}$	=	parameter vector
R_U	=	left singular-vector correlation matrix
R_V	=	right singular-vector correlation matrix
$s_i(t)$	=	forcing-function state variable for ith forcing component
t	=	time
U	=	left singular-vector matrix
V	=	right singular-vector matrix
$\boldsymbol{x}(t)$	=	augmented state-parameter variable motion
Z	=	snapshot matrix
$\boldsymbol{z}(t)$	=	state variable motion
α^k_{ji}	=	left singular-vector projection coefficients
β^k_{ji}	=	right singular-vector projection coefficients
$\eta_i(t)$	=	forcing-function state variable for ith forcing component
λ_i	=	ith eigenvalue of Ψ
ξ_i	=	forcing-function decay parameter for ith forcing component
Σ	=	singular-value matrix
$\Phi(t, t_0)$	=	state transition matrix
ϕ_i	=	ith eigenvector of Ψ
Ψ	=	generic matrix
ω_i	=	forcing-function frequency for ith forcing component

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*Senior Member of the Technical Staff, Analytical Structural Dynamics Department, Mail Stop 0557. Senior Member AIAA.

I. Introduction

PRINCIPAL components analysis (PCA), which is also referred to as proper orthogonal decomposition (POD) in the literature, is a useful technique in many fields of engineering, science, and mathematics for analysis of time-series data. The benefit of PCA for dynamical systems comes from its ability to detect and rank the dominant coherent spatial structures of dynamic response [1], such as operating deflection shapes or mode shapes. Structural dynamics is one field in which it is useful, because PCA results in modal-like dynamic properties for linear and nonlinear dynamical systems. Most notable is the use of PCA to generate efficient basis sets for developing reduced-order models for fluid flow dynamics [2] and structural dynamics applications [3]. Similarly, PCA has been investigated for system identification in experimental modal analysis [4]. Additional application of PCA can be found in the image analysis literature; for example, feature recognition of facial characteristics in images of human faces [5]. Additional application in the structural dynamics area is calibration of linear and nonlinear finite element models [6]. These are but a few applications of PCA in the science and engineering literature.

For linear structural dynamics applications, one is interested in natural frequencies, damping ratios, and mode shapes that define a set of dynamic response properties of the system. These dynamic properties can be extracted from experimentally observed responses using one's choice of conventional modal parameter estimation algorithms or they can be computed analytically by solving the eigenproblem associated with the system matrices developed from a finite element analysis. Likewise, PCA provides a set of dynamic properties for the system from time histories of response data, which are generated from either transient dynamics finite element calculations or experimental response measurements.

In the following paragraphs, PCA for analysis of motion time history data is reviewed, and the important properties of PCA that make it valuable for analysis of dynamical systems are considered. Consider the motion response of a system $\boldsymbol{z}(t_k)$, which is the state vector for the system for various times t_k. These time history response data can be placed in a matrix such that

$$z\,(t_k) = Z = \begin{pmatrix} z_1(t_1) & \dots & z_1(t_m) \\ \vdots & \ddots & \vdots \\ z_n(t_1) & \cdots & z_n(t_m) \end{pmatrix} \tag{1}$$

The matrix Z is called a snapshot matrix, because each column of Z contains the state vector at an instant of time, a snapshot from the evolution of the system dynamics. These snapshots are ordered such that the first column corresponds to the initial time with successive columns ordered chronologically until the final time is reached. The first column of the snapshot matrix is the initial condition of the system (all states at the initial time). The first row of the snapshot matrix is the time history for the first degree of freedom, for example.

There are two ways to compute the principal components from motion time series. One can compute the complete set of principal components using a more general method based on the singular-value decomposition (SVD), or they can be computed selectively/economically by eigenanalysis. First, the basic idea of PCA is shown using SVD. The SVD of the snapshot matrix can be written as [7]

$$Z = U\Sigma V^T \tag{2}$$

where U is an orthogonal matrix whose columns contain the left singular vectors, Σ is a pseudodiagonal matrix containing the singular values, and V is an orthogonal matrix whose columns contain the right singular vectors. It is common that U and V are scaled such that they are orthonormal, i.e., $U^T U = I$ and $V^T V = I$. Additionally, the singular values are ordered with descending magnitude (e.g., $\sigma_1 > \sigma_2 > \sigma_3$, and so on). Furthermore, it should be noted that PCA can be applied in the frequency domain as well. One can consider replacing the motion time series in Eq. (1) with frequency-dependent functions, such as frequency response functions, for individual degrees of freedom on the system. Singular-value decomposition is used, as in Eq. (2), to compute the frequency-dependent principal components [8].

Principal components analysis of time-series data based on the SVD results in three matrices that have significance in dynamics. The left singular vectors provide spatial information about the response (similar to mode shapes), the singular values provide information about the amplitude or energy content of the response, and the right singular vectors provide temporal information about the response (similar to modal coordinates). Thus, PCA separates space, time, and amplitude information, which is a useful tool in structural dynamics analysis and dynamics analysis, in general. This work is aimed at making PCA more useful through development of methods for analytical sensitivity calculation. The principal components also have significance in traditional structural dynamics analysis, as noted in [9,10], because under certain conditions the left singular vectors are equivalent to the eigenvectors of a mechanical system. Furthermore, the structure of these matrices is such that the dynamic response can be computed as a sum of contributions from individual principal components; that is, Eq. (2) is analogous to the well-known modal expansion in structural dynamics when only a few principal components are retained. This provides a separation of time and space variables and provides a means to truncate the response into a set of principal components, analogous to truncating into a set of modes. The approximation of the system response can be computed by selecting a small set of principal components. The modal dynamics properties of the principal components and the approximation property are illustrated in Appendix A for a structural dynamics application.

Sensitivity analysis is a standard tool used by analysts and has the potential to impact many applications of PCA. Analytical sensitivities provide the necessary derivatives for gradient-based algorithms, and the principal components have a set of properties similar to modal dynamic properties. Thus, we expect that the sensitivities (derivatives) of the principal components for structural dynamics applications will be useful in a similar fashion as the analogous derivatives of natural frequencies and mode shapes [11,12] have been for structural dynamics applications, which include structural model calibration and optimization problems, system design, as well as damage detection studies. It is often of interest to determine how the dynamic properties of the system will change when system parameters are varied (e.g., mass variation (density change) or stiffness variation (Young's modulus change) or initial condition/loading input change). The focus of this paper is on development and application of original analytical methods for computing the sensitivities of the principal components with respect to these design parameters and conditions. The new methods use developments from existing analytical sensitivity analysis methods based on the SVD [13,14] and eigenanalysis [11,12], although specialization is developed in this work to enable analysis of time-series data for PCA. Here, these sensitivities are applied to dynamics analysis, although this sensitivity analysis method for PCA has general applicability for other time-series analyses (e.g., fluid dynamics).

The two major sections of this paper include a discussion of two original methods for computing the analytical sensitivities of the principal components [15,16] and a presentation of results for several applications of these methods for dynamics analysis. The first major section, Sec. II, is divided into four parts. First, a SVD-based method for PCA sensitivity calculation is presented. Then an eigenbased method is presented. In the third part of the section, a novel method to augment state and parameter differential equations is presented along with state transition matrix calculations for computing state/parameter sensitivities. In the fourth part of the section, several examples that demonstrate augmentation of state and parameter differential equations are presented. These examples include augmentation of system parameter differential equations as well as a novel method to augment differential equations that represent a transient forcing function. The later provides a means to convert a nonhomogenous differential equation (forced system) into a homogenous differential equation (unforced system). In the second major section, Sec. III, four example applications of PCA sensitivities are presented that demonstrate the new methods. These examples include: 1) projectile trajectory analysis, 2) structural modification calculation, 3) model parameter estimation, and 4) sensitivity to force input characteristics.

II. Methods for Analytical PCA Sensitivity Calculation in the Time Domain

The nature of the dynamics response depends on a number of factors including the parameters of the system dynamics model as well as the forcing, boundary, and initial conditions. By computation of the principal component sensitivities, it is determined how the principal components depend on these parameters and conditions. In the following sections, two time-domain methods for computing the PCA sensitivities are introduced. First, a general form based on the SVD is presented, and then a compact form based on eigenanalysis is presented. Next, a novel approach for augmentation of state and parameter differential equations is presented along with state transition matrix calculations that enable the principal component sensitivity calculations. Finally, the approach for augmenting state differential equations of motion with parameter differential equations, which includes system parameter differential equations and forcing-function differential equations, is demonstrated by examples.

A. Principal Components Analysis Analytical Sensitivity Calculations Based on the Singular-Value Decomposition

Suppose that the motion response is dependent upon a vector of parameters $\boldsymbol{p}$. Mathematically, we consider the snapshot matrix to be a function of these parameters given as

$$z\,(t_k) = Z(\boldsymbol{p}) = U\Sigma V^T \tag{3}$$

where $Z(\boldsymbol{p})$ is formed according to Eq. (1).

The objective is to compute the principal component sensitivities, $\partial U/\partial \boldsymbol{p}$, $\partial \Sigma/\partial \boldsymbol{p}$, and $\partial V/\partial \boldsymbol{p}$. General analytical methods for SVD sensitivity calculations have been reported in the literature [13,14]. However, these methods do not consider application to matrices composed of time-series data. A method for calculation of PCA analytical sensitivities is introduced here.

For time-series analysis using PCA, the sensitivity calculations require calculation of state vector partial derivatives that define state departure motions due to system parameter and initial condition changes. A key observation of this work is identification of the derivatives of the state vectors contained in the snapshot matrix as a state transition matrix from dynamical systems theory. The state transition matrices are noted in the development of this section; however, computation of the state transition matrices is discussed later in Sec. II.C.

An expression for the first-order singular-value sensitivity is simply given by [13]

$$\frac{\partial \sigma_i}{\partial p_k} = U_i^T \frac{\partial Z}{\partial p_k} V_i \tag{4}$$

Indicial notation is used in Eq. (4) for the partial derivative of the ith singular value with respect to the kth element of the parameter vector. This equation shows that the singular-value sensitivity is a function of the left and right singular vectors and the snapshot matrix sensitivity (i.e., state transition matrices) and is not a function of the singular-vector sensitivities. The simplicity of Eq. (4) is interesting, and the explanation is given as follows. Consider differentiation of Eq. (3) with respect to the parameter vector, which results in

$$\frac{\partial Z}{\partial \boldsymbol{p}} = \frac{\partial U}{\partial \boldsymbol{p}} \Sigma V^T + U \frac{\partial \Sigma}{\partial \boldsymbol{p}} V^T + U\Sigma \frac{\partial V^T}{\partial \boldsymbol{p}} \tag{5}$$

Now, premultiply both sides of Eq. (5) by U^T and postmultiply by V. The resulting expression is simplified by the orthonormality of U and V to produce

$$U^T \frac{\partial Z}{\partial \boldsymbol{p}} V = U^T \frac{\partial U}{\partial \boldsymbol{p}} \Sigma + \frac{\partial \Sigma}{\partial \boldsymbol{p}} + \Sigma \frac{\partial V^T}{\partial \boldsymbol{p}} V \tag{6}$$

The product of the left singular-vector matrix and its derivative results in a skew-symmetric matrix, which has a zero-valued diagonal. Likewise, this is true for the product of the right singular-vector matrix and its derivative [14]. Because the derivative of the singular-value matrix is diagonal, collection of only the diagonal terms in Eq. (6) results in the simple expression in Eq. (4), because the first and third terms on the right-hand side of Eq. (6) have zero values on the diagonal, due to their skew-symmetric properties.

Continuing with the other principal component sensitivities, assumed forms for computing the left and right singular-vector sensitivities were proposed in [13] and are given as

$$\frac{\partial U_i}{\partial p_k} = \sum_{j=1}^{n} \alpha_{ji}^k U_j \tag{7}$$

$$\frac{\partial V_i}{\partial p_k} = \sum_{j=1}^{n} \beta_{ji}^k V_j \tag{8}$$

The projection coefficients ($\alpha_{ji}^k$and β_{ji}^k) are computed and when multiplied with the corresponding left or right singular vectors [as indicated in Eqs. (7) and (8)] give the desired vector partial derivatives.

Closed form expressions for these projection coefficients for the case when $j \neq i$ (the offdiagonal case) are given by

$$\begin{aligned} \alpha_{ji}^k &= \frac{1}{\sigma_i^2 - \sigma_j^2}\left[\sigma_i\left(U_j^T \frac{\partial Z}{\partial p_k} V_i\right) + \sigma_j\left(U_i^T \frac{\partial Z}{\partial p_k} V_j\right)^T\right] \\ \beta_{ji}^k &= \frac{1}{\sigma_i^2 - \sigma_j^2}\left[\sigma_j\left(U_j^T \frac{\partial Z}{\partial p_k} V_i\right) + \sigma_i\left(U_i^T \frac{\partial Z}{\partial p_k} V_j\right)^T\right] \end{aligned} \tag{9}$$

and, for the diagonal elements, when $j = i$, are given by

$$\begin{aligned} \alpha_{ii}^k - \beta_{ii}^k &= \frac{1}{\sigma_i}\left(U_i^T \frac{\partial Z}{\partial p_k} V_i - \frac{\partial \sigma_i}{\partial p_k}\right) \\ \alpha_{ii}^k - \beta_{ii}^k &= \frac{1}{\sigma_i}\left(-V_i^T \frac{\partial Z^T}{\partial p_k} U_i + \frac{\partial \sigma_i}{\partial p_k}\right) \end{aligned} \tag{10}$$

Thus, the full set of projection coefficients is computed using Eqs. (9) and (10). These projection coefficients depend on the principal components (U, Σ, and V) as well as partial derivatives of the state vector (sensitivities of the snapshot matrix). The desired first-order sensitivities of the left singular vectors are computed using Eq. (7) and first-order sensitivities of the right singular vectors are computed using Eq. (8).

Higher-order sensitivities of the principal components have also been developed. For example, the second-order sensitivities of the singular values are given by

$$\frac{\partial^2 \sigma_i}{\partial p_k \partial p_l} = \frac{\partial U_i^T}{\partial p_l} \frac{\partial Z}{\partial p_k} V_i + U_i^T \frac{\partial^2 Z}{\partial p_k \partial p_l} V_i + U_i^T \frac{\partial Z}{\partial p_k} \frac{\partial V_i}{\partial p_l} \tag{11}$$

which can be derived starting with Eq. (4).

Note that the second-order sensitivities of the singular values depend on the left and right singular vectors, the first- and second-order sensitivities of the snapshot matrix, and only the first-order partials of the left and right singular vectors. First- and higher-order state transition matrix calculations are needed for the second- and higher-order PCA sensitivity calculations.

This SVD-based method has also been extended to the frequency domain. In Appendix A, principal components analysis is applied to frequency response functions and a method to calculate the associated analytical sensitivities is presented [15].

B. Principal Components Analysis Analytical Sensitivity Calculations Based on Eigenanalysis

A second method for computing the PCA sensitivities in the time domain is based on eigenanalysis. As will be shown, this approach offers computational advantages. Recall that the SVD-based PCA is given by

$$z(t_k) = Z(\boldsymbol{p}) = U\Sigma V^T$$

For the eigenbased method, a correlation matrix is formed as the product of the snapshot matrix and its transpose. Depending on the order of this product, two distinct correlation matrices can be defined as

$$R_U = ZZ^T = U\Sigma V^T V \Sigma U^T = U\Sigma^2 U^T \tag{12}$$

and

$$R_V = Z^T Z = V\Sigma U^T U \Sigma V^T = V\Sigma^2 V^T \tag{13}$$

Note that the correlation matrices depend on only the left or right singular vectors after simplification, because the inner products in both Eq. (12) and (13) equal an identity matrix, due to the orthonormal properties of U and V.

Eigenanalysis of these correlation matrices provides another way to compute the left and right singular vectors and the singular values, due to the well-established relationship between SVD and eigenanalysis. The eigenvalues of R_U are the squares of the singular values of Z and the eigenvectors of R_U are the left singular vectors of Z. Likewise, the eigenvalues of R_V are the squares of the singular values of Z and the eigenvectors of R_V are the right singular vectors of Z.

Eigenanalysis not only provides an alternative method for computing the principal components in the time domain, but it also provides another method for principal component analytical sensitivity calculations. This approach is attractive from the standpoint of computational effort when only the left singular vectors and their sensitivities are desired. The length of the state vector is typically much smaller than the number of snapshots; therefore, the associated correlation matrix R_U becomes compact. This is particularly useful for reduced-order model basis selection. Generally, these forms are attractive when one chooses to compute only the left or right singular vectors, or perhaps only a few of them.

In this section, a method for computing the sensitivities of the principal components using eigenanalysis methods is presented [15]. Toward that end, consider a general case applicable to solving the eigenproblem for either R_U or R_V. Note that both matrices are symmetric by construction.

As noted in [15], standard eigensensitivity algorithms can be used to compute PCA sensitivities analytically, although specialized state vector partial derivative expressions must be introduced. Many methods exist to compute derivatives of the matrices R_U and R_V, including [11,12]. These approaches begin by considering an eigenproblem of the form

$$[\Psi - \lambda_i I]\phi_i = 0 \tag{14}$$

where λ_i is the ith eigenvalue and ϕ_i is the corresponding ith eigenvector of the matrix Ψ. Note that Ψ symbolically represents either R_U or R_V, which are the correlation matrices.

Here, of course, Ψ is a function of some parameters, and the eigenvalue derivative is given by [11]

$$\frac{\partial \lambda_i}{\partial p_k} = \phi_i^T \left[\frac{\partial \Psi}{\partial p_k}\right]\phi_i \tag{15}$$

The eigenvalues of Ψ are related to the singular values of Z by

$$\lambda_i = \sigma_i^2$$

Thus, Eq. (15) becomes

$$\frac{\partial \sigma_i}{\partial p_k} = \frac{\frac{\partial \lambda_i}{\partial p_k}}{2\sqrt{\lambda_i}} = \frac{1}{2\sqrt{\lambda_i}}\left\{\phi_i^T\left[\frac{\partial \Psi}{\partial p_k}\right]\phi_i\right\} \tag{16}$$

when rewritten in terms of the singular-value derivative.

The eigenvector derivative is more challenging to compute. The derivation is omitted here, although the process is fairly straightforward. When the eigenvector ϕ_i of R_U or R_V is computed, this produces either the left singular vector or the right singular vector, which corresponds to σ_i. Likewise, $\partial \phi_i / \partial p_k$ produces the analytical sensitivities of the left or right singular vectors.

Clearly, the partial derivative of the matrix Ψ is needed for either case. For the two specific cases, the necessary partial derivative expressions are, for when Ψ represents R_U

$$\frac{\partial R_U}{\partial p_k} = \frac{\partial}{\partial p_k}(ZZ^T) = \frac{\partial Z}{\partial p_k}Z^T + Z\frac{\partial Z^T}{\partial p_k} \tag{17}$$

and for when Ψ represents R_V,

$$\frac{\partial R_V}{\partial p_k} = \frac{\partial}{\partial p_k}(Z^T Z) = \frac{\partial Z^T}{\partial p_k}Z + Z^T\frac{\partial Z}{\partial p_k} \tag{18}$$

Here, the state vector partials (sensitivities of the snapshot matrix) are computed from state transition matrix calculations, which are introduced in the next section.

Additionally, this method is not limited to first-order partials in general as second- and higher-order eigensensitivity analysis has been addressed [12]. The development of higher-order state transition matrix concepts enables the methods developed here to be extended to second and higher order.

C. State Transition Matrix Calculations: Computing the Snapshot Matrix Sensitivity

For both time-domain methods presented in the previous two sections, the partial derivative of the state vector (sensitivity of the snapshot matrix) is identified as a state transition matrix from dynamical systems analysis. [17] provides a good overview of state transition matrix development and their properties. In this section the development of augmented state/parameter differential equations is presented. Computation of the first- and higher-order state transition matrices, which enable the PCA sensitivity calculations, is discussed.

State transition matrices can be used to describe state departure motions from a nominal solution of a set of differential equations, due to changes in system initial conditions, in general. Consider the most general case of a nonlinear dynamical system described by the following state variable differential equations in order to begin development of the state transition matrix

$$\dot{z} = \boldsymbol{f}(z, \boldsymbol{p}, t); \qquad z(t_0) = z_0 \tag{19}$$

where it is seen that the dynamical system is in general a nonlinear function of the states of the system and the system parameters $\boldsymbol{p}$, representing the equations of motion of the system. The objective is to compute sensitivities of the motion of the system due to changes in system parameters in addition to changes in the state initial conditions, $z(t_0)$. For this reason and in the interest of simplicity and notational compactness, the sensitivity to both the state vector and system parameters is considered simultaneously in the development. To achieve this goal, the state vector differential equations are augmented with the parameter vector differential equations to form a set of augmented differential equations given by

$$\dot{\boldsymbol{x}} = \begin{bmatrix} \dot{z} \\ \dot{\boldsymbol{p}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}(z, \boldsymbol{p}, t) \\ \boldsymbol{g}(z, \boldsymbol{p}, t) \end{bmatrix} = \boldsymbol{h}(z, \boldsymbol{p}, t); \qquad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \tag{20}$$

where the augmented state and initial conditions are defined as

$$\boldsymbol{x} = \begin{bmatrix} z \\ \boldsymbol{p} \end{bmatrix}; \qquad \boldsymbol{x}(t_0) = \begin{bmatrix} z(t_0) \\ \boldsymbol{p}(t_0) \end{bmatrix}$$

For now, a general form for the differential equations is considered for the parameter vector. However, for the common case of constant parameters, $\boldsymbol{g}(z, \boldsymbol{p}, t)$ will, of course, equal a zero-valued vector (i.e.$\dot{\boldsymbol{p}} = \boldsymbol{0}$). This augmentation approach enables calculation of $\partial z(t)/\partial z(t_0)$ and $\partial z(t)/\partial \boldsymbol{p}$, state transition matrix sensitivity calculations, which are needed for the principal component sensitivity calculations with respect to initial conditions and system parameters, respectively.

To summarize, the state transition matrix for first-order sensitivity calculations is not new; however, this development is presented in order to provide a means for computing second- and higher-order state transition matrices, which were first reported in [18,19]. The second- and higher-order state transition matrix calculations enable second- and higher-order principal component sensitivity calculations. In integral form, the solution to Eq. (20) is

$$\boldsymbol{x}(t) = \boldsymbol{x}(t_0) + \int_{t_0}^{t} \boldsymbol{h}(\boldsymbol{x}, \tau)\, \mathrm{d}\tau \tag{21}$$

And, upon differentiating Eq. (21) with respect to $\boldsymbol{x}(t_0)$ the result is

$$\frac{\partial \boldsymbol{x}(t)}{\partial \boldsymbol{x}(t_0)} = I + \int_{t_0}^{t}\left(\frac{\partial \boldsymbol{h}(\boldsymbol{x}, \tau)}{\partial \boldsymbol{x}(\tau)}\frac{\partial \boldsymbol{x}(\tau)}{\partial \boldsymbol{x}(t_0)}\right)\mathrm{d}\tau \tag{22}$$

The state transition matrix is defined by $\Phi(t, t_0) = \partial \boldsymbol{x}(t)/\partial \boldsymbol{x}(t_0)$; thus, Eq. (22) can be rewritten as

$$\Phi(t, t_0) = I + \int_{t_0}^{t}\left(\frac{\partial \boldsymbol{h}(\boldsymbol{x}, \tau)}{\partial \boldsymbol{x}(\tau)}\Phi(\tau, t_0)\right)\mathrm{d}\tau \tag{23}$$

Now, upon taking the time derivative of Eq. (23), a state transition matrix differential equation that describes the augmented state variable sensitivity is defined by

$$\dot{\Phi}(t, t_0) = \frac{\partial \boldsymbol{h}(\boldsymbol{x}, t)}{\partial \boldsymbol{x}(t)}\Phi(t, t_0); \qquad \Phi(t_0, t_0) = I \tag{24}$$

where $\Phi(t, t_0)$, again, is the notation for the state transition matrix and I is the identity matrix. The partitions of the state transition matrix are defined as

$$\Phi(t, t_0) = \frac{\partial \boldsymbol{x}(t)}{\partial \boldsymbol{x}(t_0)} = \begin{bmatrix} \frac{\partial z(t)}{\partial z(t_0)} & \frac{\partial z(t)}{\partial \boldsymbol{p}(t_0)} \\ \frac{\partial \boldsymbol{p}(t)}{\partial z(t_0)} & \frac{\partial \boldsymbol{p}(t)}{\partial \boldsymbol{p}(t_0)} \end{bmatrix} \tag{25}$$

For the special case of a linear system, which is often the case in structural dynamics, Eq. (24) becomes

$$\dot{\Phi}(t, t_0) = A\Phi(t, t_0); \qquad \Phi(t_0, t_0) = I \tag{26}$$

where A is the state matrix. Analytical solutions exist for this special case when the state matrix is constant. For example, the matrix exponential solution is given by

$$\Phi(t, t_0) = e^{A(t-t_0)} \tag{27}$$

For the general nonlinear case, Eqs. (20) and (24) must be solved simultaneously by numerical integration. The result is the solution for the motion of the system, $z(t)$, for a nominal set of initial conditions along with a first-order state transition matrix, $\Phi(t, t_0)$. Now, given the motion response $z(t)$, the snapshot matrix is formed and the principal components (U, Σ, V) can be computed. Analytical sensitivities of the principal components are accomplished by either method presented in the previous two sections given the upper partitions of the state transition matrices defined in Eq. (25). The state transition matrix sensitivities in the upper left partition of Eq. (25) are used to compute principal component sensitivities with respect to state vector initial conditions, and those in the upper right partition of Eq. (25) are used to compute the principal component sensitivities with respect to system parameters.

Only the first-order state transition matrix differential equation was developed in this section, although the development lays the groundwork for the higher-order methods. Differential equations for the second- and higher-order state transition matrices can be developed by, first, differentiating Eq. (22) with respect to the augmented state variable initial condition and then taking the time derivative of the resulting expression as was done to produce Eq. (24). This process can be repeatedly used to derive the second- and higher-order state transition matrix concepts [18,19].

The following section provides examples of augmented state-parameter differential equations for structural dynamic systems.

D. Differential Equation Augmentation for State Transition Matrix Sensitivity Calculations

In this section, the approach for augmenting equations of motion and parameter differential equations is demonstrated to produce augmented state-parameter differential equations for example applications considered later in this work. The first considers augmentation of system parameters for a structural dynamic system, and the second considers augmentation of forcing-function parameters with the state variables.

The motivation for augmentation of system parameters, obviously, is to enable important design sensitivities to be computed. On the other hand, the motivation for calculation of analytical sensitivities with respect to forcing-function parameters may not be obvious. These sensitivities are explored because the principal components are dependent upon the characteristics of the loading conditions unlike the eigenvectors of mechanical systems, which are inherent properties of a structural dynamic system.

1. *Augmentation of System Parameters for a Linear Structural Dynamic System*

Recall from Eq. (20) that the system equations of motion and parameter differential equations can be augmented as

$$\dot{\boldsymbol{x}} = \begin{bmatrix} \dot{z} \\ \dot{\boldsymbol{p}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}(z, \boldsymbol{p}, t) \\ \boldsymbol{g}(z, \boldsymbol{p}, t) \end{bmatrix}; \qquad \boldsymbol{x}(t_0) = \boldsymbol{x}_0$$

For a linear structural dynamic system the equations of motion are

$$M\ddot{\boldsymbol{y}} + C\dot{\boldsymbol{y}} + K\boldsymbol{y} = \boldsymbol{F} \tag{28}$$

or, in first-order form

$$\dot{z} = \begin{bmatrix} \dot{\boldsymbol{y}} \\ \ddot{\boldsymbol{y}} \end{bmatrix} = \begin{bmatrix} 0 & I \\ -M^{-1}K & -M^{-1}C \end{bmatrix}\begin{bmatrix} \boldsymbol{y} \\ \dot{\boldsymbol{y}} \end{bmatrix} + \begin{bmatrix} \boldsymbol{0} \\ M^{-1}F \end{bmatrix} \tag{29}$$

and with the parameter vector defined as

$$\boldsymbol{p} = [m_1 \cdots m_n \quad c_1 \cdots c_n \quad k_1 \cdots k_n]^T \tag{30}$$

with

$$\dot{\boldsymbol{p}} = \boldsymbol{0} \tag{31}$$

The augmented set of differential equations becomes

$$\dot{\boldsymbol{x}} = \begin{bmatrix} \dot{\boldsymbol{y}} \\ \ddot{\boldsymbol{y}} \\ \dot{\boldsymbol{p}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} & I & \boldsymbol{0} \\ -M^{-1}K & -M^{-1}C & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}\begin{bmatrix} \boldsymbol{y} \\ \dot{\boldsymbol{y}} \\ \boldsymbol{p} \end{bmatrix} + \begin{bmatrix} \boldsymbol{0} \\ M^{-1}F \\ \boldsymbol{0} \end{bmatrix} \tag{32}$$

State transition matrix calculations can be performed numerically or analytically for this problem. Furthermore, this procedure can be used for a nonlinear model by including nonlinear terms in Eq. (32); of course, the state transition matrices would need to be computed numerically.

2. *Augmentation of Transient Forcing-Function Parameters*

Now consider formation of augmented state-parameter differential equations including the parameters of a transient forcing function. The sensitivities can be calculated with respect to any variable that is included in the state vector; therefore, this requires the forcing function to be parameterized analytically in this case. A few common loading cases are considered that are useful in structural dynamics analysis.

The development begins by considering a multiple-degree-of-freedom system forced with a general forcing function given by

$$M\ddot{\boldsymbol{y}} + C\dot{\boldsymbol{y}} + K\boldsymbol{y} = \boldsymbol{g}(t) \tag{33}$$

Consider $\boldsymbol{g}(t)$ written in two ways: 1) a forcing function as a sum of sinusoids and 2) a forcing function as a sum of decaying sinusoids defined as

Case 1:

$$\boldsymbol{g}(t) = \sum_{i=1}^{n} \boldsymbol{f}_i \sin(\omega_i t)$$

Case 2:

$$\boldsymbol{g}(t) = \sum_{i=1}^{n} \boldsymbol{f}_i e^{-\xi_i t} \sin(\omega_i t)$$

.

Case 2 is very similar to the way in which acceleration time history inputs are defined for input to structural dynamics codes for transient dynamics analysis to simulate environmental loads. Additionally, note that case 2 is very general and could approximate many general forcing inputs in the sense of a Fourier approximation.

a. Case 1: Forcing as Summation of Sinusoidal Inputs. First, consider the case of forcing at a single frequency ($n = 1$), given by

$$\boldsymbol{g}(t) = \boldsymbol{f} \sin(\omega t) \tag{34}$$

A new variable can be defined to describe the time modulation of the forcing input as

$$s = \sin(\omega t) \tag{35}$$

such that Eq. (33) becomes

$$M\ddot{\boldsymbol{y}} + C\dot{\boldsymbol{y}} + K\boldsymbol{y} = \boldsymbol{f}s \tag{36}$$

Now, a differential equation that governs the time modulation of the forcing input with solution given by Eq. (35) is defined as

$$\ddot{s} + \omega^2 s = 0 \tag{37}$$

Augmented state-parameter differential equations based on Eqs. (36) and (37) can be written as

$$\begin{bmatrix} M & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{bmatrix}\begin{bmatrix} \ddot{\boldsymbol{y}} \\ \ddot{s} \end{bmatrix} + \begin{bmatrix} C & \boldsymbol{0} \\ \boldsymbol{0} & 0 \end{bmatrix}\begin{bmatrix} \dot{\boldsymbol{y}} \\ \dot{s} \end{bmatrix} + \begin{bmatrix} K & -\boldsymbol{f} \\ \boldsymbol{0} & \omega^2 \end{bmatrix}\begin{bmatrix} \boldsymbol{y} \\ s \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \\ 0 \end{bmatrix} \tag{38}$$

where the parameter vector is simply

$$\boldsymbol{p} = s \tag{39}$$

Note that Eq. (38) is written in second-order form here to simplify the notation in order to demonstrate augmentation with forcing parameters. Note that the new augmented system is a homogenous differential equation with one additional degree of freedom to account for the forcing function. Here, the forcing amplitude, f, was not included in the parameter vector. In the next example, forcing amplitude is included in the parameter vector, which permits PCA sensitivity calculation with respect to forcing amplitude.

The key to implementing this approach is that a differential equation (i.e., $\dot{\boldsymbol{p}} = \boldsymbol{g}(z, \boldsymbol{p}, t)$) must be carefully selected to describe the parameters that represent the forcing function for augmentation with the state equations of motion. In this first example, dependence on the forcing frequency is implicitly defined with respect to the new variable s. Further, the augmented structure of Eq. (38) can be continued as the number of desired terms in the forcing function gets larger ($n > 1$).

b. Case 2: Forcing as Summation of Decaying Sinusoids. For the more general case of a sum of decaying sinusoids, a differential equation to describe the time modulation of the forcing input must be determined. It can be shown that for $n = 1$,

$$\eta_1(t) = e^{-\xi_1 t}\sin(\omega_1 t) \tag{40}$$

where the forcing function is defined as

$$g(t) = f_1\eta_1(t) \tag{41}$$

The expression in Eq. (40) is the solution to the differential equation defined as

$$\ddot{\eta}_1 + 2\xi_1\dot{\eta}_1 + (\xi_1^2 + \omega_1^2)\eta_1 = 0 \tag{42}$$

which can be verified by substitution.

As an example, the augmented set of differential equations, for $n = 1$, becomes

$$\begin{bmatrix} M & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 1 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 1 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} \ddot{\boldsymbol{y}} \\ \ddot{\eta}_1 \\ \ddot{f}_1 \\ \ddot{\omega}_1 \\ \ddot{\xi}_1 \end{bmatrix} + \begin{bmatrix} C & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 2\xi_1 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \dot{\boldsymbol{y}} \\ \dot{\eta}_1 \\ \dot{f}_1 \\ \dot{\omega}_1 \\ \dot{\xi}_1 \end{bmatrix}$$
$$+ \begin{bmatrix} K & -f_1\hat{\boldsymbol{e}}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \xi_1^2 + \omega_1^2 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 0 \\ \mathbf{0} & 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} \boldsymbol{y} \\ \eta_1 \\ f_1 \\ \omega_1 \\ \xi_1 \end{bmatrix} = \mathbf{0} \tag{43}$$

by augmenting Eq. (42) and differential equations for the constant parameters of the forcing function with the system dynamics model, again in second-order form for clarity, where the parameter vector is defined as

$$\boldsymbol{p} = [\eta_1 \quad f_1 \quad \omega_1 \quad \xi_1]^T \tag{44}$$

Again, this formulation generalizes to higher dimension with additional decaying sinusoidal terms used to parameterize the forcing function ($n > 1$). Here, f_1 is defined explicitly in the parameter vector. If principal component sensitivity calculations with respect to forcing input level are not of interest, then the prior form can be used with these parameters not appearing explicitly in the parameter vector.

The original nonhomogeneous differential equation with forcing input on the right-hand side has been rewritten as a homogeneous differential equation with increased dimension, due to the new forcing parameters. The augmented state-parameter differential equations can be solved as an initial condition problem.

This augmentation approach is verified by considering the equation given by

$$M\ddot{\boldsymbol{y}} + C\dot{\boldsymbol{y}} + K\boldsymbol{y} = \boldsymbol{f}_1 e^{-\xi_1 t}\sin(\omega_1 t) \tag{45}$$

A 20-degree-of-freedom mass-damper-spring system was chosen; each mass had a value of 1 kg and each spring had a constant of 50 N/m. C was chosen such that $C = 0.05^* M$. The following parameters were chosen for the forcing function: $[f_1; \omega_1; \xi_1] = [10; 0.7; 0.1]$ with the input only applied to the tip mass. Equation (45) was solved using a fourth-order Runge–Kutta numerical integration scheme with the initial position and velocity conditions equaling zero. Note that Eq. (45), in second-order form, has a dimension of 20.

Next, Eq. (43) was solved using the same fourth-order Runge–Kutta numerical integration scheme using the same forcing-function parameters and initial conditions. In this case, in second-order form, Eq. (43) has a dimension of 24, with four additional initial conditions for the four forcing-function parameters. Of course, $f_1, \omega_1, and\, \xi_1$ are constants, and $\eta_1(t_0)$ and $\dot{\eta}_1(t_0)$ are defined by Eq. (40) and its time derivative.

The solutions for the motion for both forms are identical. Further, the force input as reconstructed by post processing the forcing parameters resulting from solving Eq. (43) is equivalent to the desired input force given on the right-hand side of Eq. (45). Thus, the homogenous augmented form was verified to be equivalent to the original nonhomogeneous form.

Now, the sensitivities of the principal components (U, Σ, V) can be computed based on the forms presented here, e.g., $\partial U/\partial f_i$, $\partial U/\partial \omega_i$, and $\partial U/\partial \xi_i$, with respect to forcing-function parameters given the following state vector partials $\partial \boldsymbol{y}(t)/\partial f_i$, $\partial \boldsymbol{y}(t)/\partial \omega_i$, and $\partial \boldsymbol{y}(t)/\partial \xi_i$ [i.e., from $\partial z(t)/\partial \boldsymbol{p}_0$ in Eq. (25)] computed from state transition matrix calculations.

III. Applications of Principal Component Sensitivities to Dynamics Analysis

The methods described in the preceding section are applied to a number of applications in dynamics analysis including projectile dynamics and structural dynamics. Examples considered include 1) projectile trajectory analysis, 2) structural modification (e.g., evaluating the effect of mass/stiffness changes), 3) model calibration or parameter estimation, and 4) calculation of the sensitivities with respect to forcing-function parameters.

A. Example 1: Projectile Trajectory Analysis and Verification

Both the SVD-based and eigenbased approaches for calculating the PCA sensitivities in the time domain were verified by considering, as an example, the motion of a projectile in a constant-gravity field. This example provides a case in which the partial derivative of the snapshot matrix (i.e., the state transition matrix) is known analytically. Additionally, this example is considered to demonstrate interpretations of the principal components and their sensitivities for trajectory analysis.

The equations of motion for a projectile in a constant-gravity field are given simply by

$$\ddot{x} = 0 \qquad \ddot{y} = 0 \qquad \ddot{z} = -g \tag{46}$$

This problem is chosen because analytical expressions exist for its solution: namely,

$$x(t) = x_0 + \dot{x}_0(t - t_0) \qquad y(t) = y_0 + \dot{y}_0(t - t_0)$$
$$z(t) = z_0 + \dot{z}_0(t - t_0) - \tfrac{1}{2}g(t - t_0)^2 \tag{47}$$

Furthermore, in order to also consider sensitivity to the gravity constant, a parameter differential equation can be written as

$$\dot{g} = 0 \tag{48}$$

An augmented system such as done in Eq. (20) can be formed. In matrix form, the analytical expression for the motion solution to Eq. (46) can be written, where the first three rows are a restatement of Eq. (47), the next three rows describe the velocity solution, and the final row defines the gravity parameter as a constant. The result is

$$\begin{bmatrix} x(t) \\ y(t) \\ z(t) \\ \dot{x}(t) \\ \dot{y}(t) \\ \dot{z}(t) \\ g \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & (t-t_0) & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & (t-t_0) & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & (t-t_0) & -\frac{1}{2}(t-t_0)^2 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -(t-t_0) \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x(t_0) \\ y(t_0) \\ z(t_0) \\ \dot{x}(t_0) \\ \dot{y}(t_0) \\ \dot{z}(t_0) \\ g \end{bmatrix}$$

$$\text{or} \quad z(t) = \Phi(t, t_0) z(t_0) \tag{49}$$

The 7×7 matrix is an analytical expression for the state transition matrix, $\Phi(t, t_0)$. Recall, that this state transition matrix is the complete array of snapshot matrix sensitivities that are needed to compute the PCA sensitivities.

Analytical sensitivity calculations for the time-domain methods were verified using the analytical state transition matrix. The state transition matrix in Eq. (49) was computed for times from 0 to 4 s with a time interval of 0.1 s. The initial conditions for the problem are used along with the state transition matrix calculations to compute the full seven-dimension state vector at each instant in time. The selected initial conditions are

$$[x(t_0); y(t_0); z(t_0)] = [1.0; 2.0; 3.0] \text{ m}$$

and

$$[\dot{x}(t_0); \dot{y}(t_0); \dot{z}(t_0)] = [20.0; 20.0; 20.0] \text{ m/s}$$

The gravitational parameter is constant with a value of 9.81 m/s^2. The principal components are computed based on the time histories of the position coordinates only; thus, the snapshot matrix has dimension 3 by 41.

Using an analytical state transition matrix removes numerical error from this verification exercise. Sensitivity of the principal components to the three initial position coordinates, the three initial velocities, and the gravitational constant are calculated using the SVD-based and eigenbased methods, and when compared to forward finite difference calculations show that these methods compute the desired partials to a high degree of accuracy. The finite difference calculations were performed with a precision of six significant figures.

Selected verification results are given in Table 1. For example, the partial derivative of the first principal component left singular vector, $\boldsymbol{U}_1$, with respect to the gravitation parameter is tabulated. The first column provides the finite difference result, while the second column lists the analytical result using the general/complete SVD-based approach and the third column lists the analytical result using the selective/economical eigenbased approach. The two analytical methods produce identical results and agree with finite difference calculations to the precision of its calculation. The partial derivatives of the largest (principal) singular value and the corresponding right singular vector with respect to the initial conditions $x(t_0)$ and $\dot{x}(t_0)$ and the gravity parameter are also listed in Table 1. Again, the analytical calculations were verified. Note that due to the dimension of the right singular vector, only the 2-norm value is tabulated.

One advantage of the analytical approach over finite difference methods is that all desired partials are computed at once for all parameters in the parameter space. Finite differencing requires isolation of each individual parameter. To illustrate this point, consider the solution of a differential equation with initial condition changes. The finite difference method requires this differential equation to be solved for each individual initial condition perturbation. For this projectile problem this required solving the differential equations seven times in addition to the solution for the nominal initial conditions to perform forward finite difference calculations. If a central difference finite difference approach had been used, 14 additional solutions of the differential equations would be needed in addition to the nominal case solution. The analytical approach developed in this work requires only one solution of the differential equations, although the state transition matrix must either be computed analytically or its associated differential equations must also be solved numerically.

Furthermore, consider the significance of the principal components in the analysis of the projectile motion. Recall that principal components analysis results in the separation of spatial, amplitude, and time information. When analyzing the motion time series of the projectile, the left singular vectors (U) can be interpreted as spatial configurations of the response, while the singular values provide the amplitudes for the corresponding spatial configurations and the right singular vectors provide the time modulations of these configurations. This can be considered as a coordinate transformation where the new coordinates are defined as the configurations of the left singular vectors. The singular-value decomposition attempts to crowd the energy of the response into a small set of coordinates and orders the configurations by amplitude. PCA can also be used to identify coordinates in the response that are unnecessary, which is the case of over-parameterized dynamical systems.

To demonstrate these properties, consider the following example. Consider a 2-D projectile example with $[x(t_0); z(t_0)] = [1.0; 1.0]$ m and $[\dot{x}(t_0); \dot{z}(t_0)] = [20.0; 40.0]$ m/s simulated for a total of 6 s. This 2-D problem was chosen in order to demonstrate some interesting geometric features that result from PCA. First, consider the motion in phase space in Fig. 1. Using the SVD-based method, an estimate of the state motion history based on each individual principal component was constructed. That is, $U_1 \sigma_1 V_1^T$, and $U_2 \sigma_2 V_2^T$ were

Table 1 Verification of analytical PCA sensitivity calculations: time domain

Analytical PCA sensitivity	Numerical (finite difference)	Analytical SVD method	Analytical eigenbased method
$\partial \boldsymbol{U}_1 / \partial g$	−0.007505206	−0.007505207	−0.007505207
	−0.007623310	−0.007623311	−0.007623311
	0.04859494	0.04859494	0.04859494
$\partial \sigma_1 / \partial x_0$	3.856470	3.856470	3.856470
$\partial \sigma_1 / \partial \dot{x}_0$	10.17011	10.17011	10.17011
$\partial \sigma_1 / \partial g$	−4.799836	−4.799836	−4.799836
$\lvert \partial \boldsymbol{V}_1 / \partial x_0 \rvert$	0.004495183	0.004495183	0.004495183
$\lvert \partial \boldsymbol{V}_1 / \partial \dot{x}_0 \rvert$	0.001862972	0.001862972	0.001862972
$\lvert \partial \boldsymbol{V}_1 / \partial g \rvert$	0.003680486	0.003680485	0.003680485

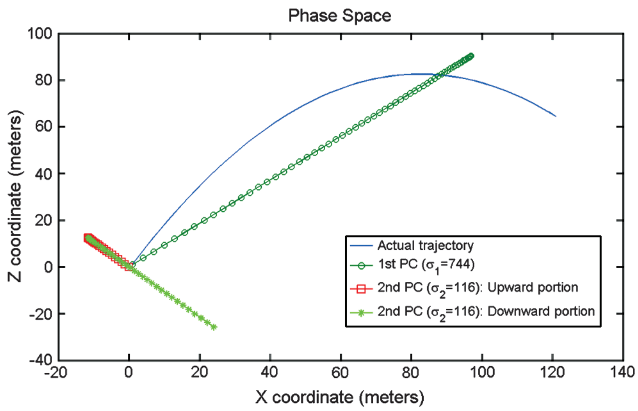

Fig. 1 Two-dimensional projectile motion in phase space.

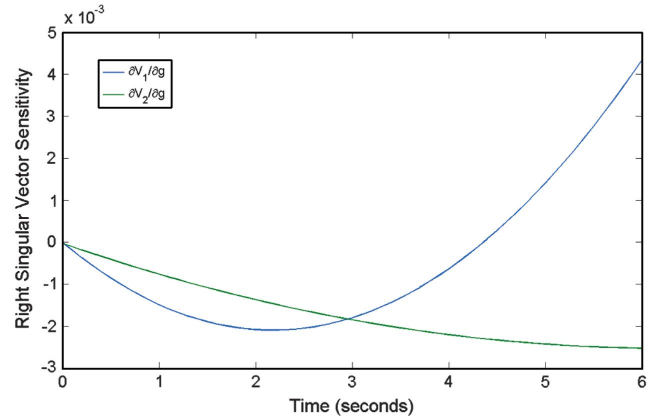

Fig. 2 Two-dimensional projectile right singular vector sensitivities.

calculated where their sum equals the actual motion response $[x(t); z(t)]$. For this case, only two principal components are needed to completely describe this 2-D problem, which are plotted in phase space in Fig. 1 along with the actual trajectory. Again, note that the summation of the first and second principal component reconstructions will sum to equal the actual trajectory. The first, or dominant, principal component captures motion in the global sense similar to a linear least-squares-type approximation. On the other hand, the second principal component produces the necessary additions (and subtractions) to the first principal component reconstruction, at each instant of time, necessary to reconstruct the actual trajectory. These principal components provide a new set of coordinates in which to describe the motion of projectile or rigid body dynamics.

In addition to the interpretation of principal components for analysis of dynamical systems, their sensitivities can be used to investigate motion changes due to initial condition or parameter variations. Sensitivities of the left singular vectors describe how the spatial configurations of the response are affected by initial condition and parameter changes. The sensitivities of the singular values demonstrate how the amplitudes of the PCs are affected and sensitivities of the right singular vectors demonstrate how the time response is affected. As an example, consider the sensitivities of the PCs with respect to the gravitational constant in the 2-D projectile example. Table 2 lists the left singular-vector and singular-value sensitivities. In Fig. 2, the right singular-vector sensitivities are shown. These sensitivities demonstrate the manner in which individual principal components change when the gravity constant is changed. These methods could be useful for rigid body dynamics analysis, in addition to identification of over-parameterized dynamical systems.

B. Example 2: Structural Modification

Consider a 20-degree-of-freedom mass-damper-spring system with equations of motion and initial conditions given by

$$M\ddot{\boldsymbol{y}} + C\dot{\boldsymbol{y}} + K\boldsymbol{y} = \boldsymbol{F} = \boldsymbol{0}; \qquad \boldsymbol{y}(t_0) = \boldsymbol{y}_0; \qquad \dot{\boldsymbol{y}}(t_0) = \dot{\boldsymbol{y}}_0 \quad (50)$$

with system parameters defined by

$$m_i = 1; \qquad c_i = 0; \qquad k_i = 50; \qquad i = 1, 2, \ldots, 20 \quad (51)$$

Table 2 Two-dimensional projectile sensitivities

Sensitivity	Value
$\partial \boldsymbol{U}_1/\partial g$	0.0378
	−0.0406
$\partial \boldsymbol{U}_2/\partial g$	0.0406
	0.0378
$\partial \sigma_1/\partial g$	39.9280
$\partial \sigma_2/\partial g$	−18.2119

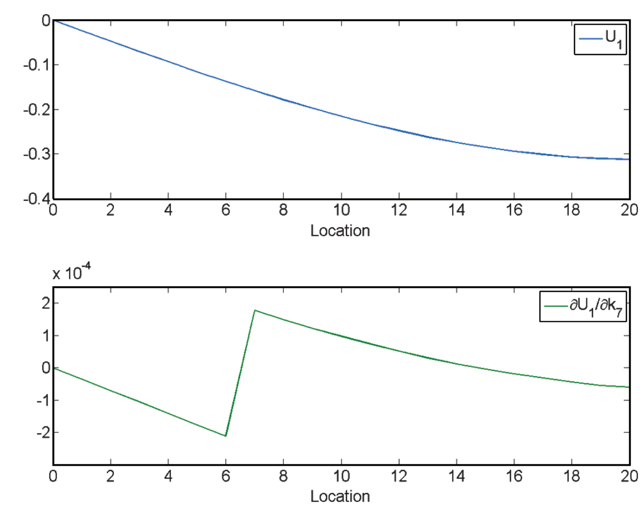

Fig. 3 Left singular vector (shape) and left singular vector sensitivity of first principal component with respect to k_7.

and the initial condition is such that the system is at rest and the end mass is initially displaced from equilibrium. It is desired to compute $\partial U_i/\partial p_k$, $\partial \sigma_i/\partial p_k$, and $\partial V_i/\partial p_k$ for $i = 1, 2, \ldots, 20$ and $\boldsymbol{p} = [k_1 \quad k_2 \quad \cdots \quad k_{20}]$.

In the following, a few selected sensitivities are presented to graphically demonstrate the nature of the principal component sensitivities for this structural dynamics problem. The use of these sensitivities for parameter estimation is also examined in the next example. First, in Fig. 3, the first principal component shape (U_1) and its sensitivity with respect to k_7, the stiffness at the location of the seventh spring, are plotted. U_1 resembles the first eigenmode of the system and $\partial U_1/\partial k_7$ has a discontinuity at the location of k_7. These can be compared to the first eigenmode and the first eigenmode sensitivity to demonstrate that they are nearly identical for this example.

Table 3 provides a list of the singular values and their sensitivities with respect to k_7. Only the first four of the 20 total singular values and sensitivities are tabulated. Note that σ_1 accounts for most of the energy of the response. The singular-value sensitivities are multiplied by 1000 as entered in Table 3. In analyzing the effect of the parameter k_7, we find that the largest effect is with the third principal component singular value.

Figure 4 shows the time modulation associated with the first principal component (V_1) and its sensitivity ($\partial V_1/\partial k_7$). By comparing the two plots, it can be seen that an increase in k_7 shifts the peaks of V_1 to the left according to the modification resulting from $\partial V_1/\partial k_7$. As expected, an increase in k_7 shifts the frequency to a higher value.

In summary, these calculations indicate in different ways how principal components for a structural dynamic system change due to

Table 3 Singular values and their sensitivities

Principal component number	Singular values (σ_i)	$(\partial\sigma_i/\partial k_7) \times 1e3$
1	12.1255	−1.8443
2	1.3192	−0.6273
3	0.4739	−2.9421
4	0.2393	1.9597

system parameter changes. The principal component sensitivities provide a means to evaluate structural modifications. The shape sensitivity, $\partial U_1/\partial k_7$, for example, indicates where a stiffness change has occurred. And, $\partial V_1/\partial k_7$ indicates how the frequency changes, while $\partial\sigma_1/\partial k_7$ indicates how the amplitude of the principal component changes. Again, the use of these sensitivities for parameter estimation is examined in the next example.

C. Example 3: Parameter Estimation

In this section, the use of analytical principal component sensitivities to *locate and estimate* the value of parameter changes is considered. Use of principal components for calibration has been considered by other researchers [6,20] using non-gradient-based approaches. Here, a simple least-squares gradient-based approach is proposed to evaluate different strategies for computing the unknown Δp_k using analytical principal component sensitivities. The least-squares problem is posed as

$$\begin{Bmatrix} \Delta U_i \\ \Delta\sigma_i \\ \Delta V_i \end{Bmatrix} = \begin{bmatrix} \frac{\partial U_i}{\partial p_k} \\ \frac{\partial \sigma_i}{\partial p_k} \\ \frac{\partial V_i}{\partial p_k} \end{bmatrix} \Delta p_k \tag{52}$$

which is solved for the unknowns as

$$\Delta p_k = \begin{bmatrix} \frac{\partial U_i}{\partial p_k} \\ \frac{\partial \sigma_i}{\partial p_k} \\ \frac{\partial V_i}{\partial p_k} \end{bmatrix}^{\dagger} \begin{Bmatrix} \Delta U_i \\ \Delta\sigma_i \\ \Delta V_i \end{Bmatrix} \tag{53}$$

where † represents the pseudoinverse operation. The change in the observation parameter is given by the difference in a reference principal component and a new, modified principal component given by

$$\Delta U_i = U_i^{\text{modified}} - U_i^{\text{reference}} \tag{54}$$

$$\Delta\sigma_i = \sigma_i^{\text{modified}} - \sigma_i^{\text{reference}} \tag{55}$$

$$\Delta V_i = V_i^{\text{modified}} - V_i^{\text{reference}} \tag{56}$$

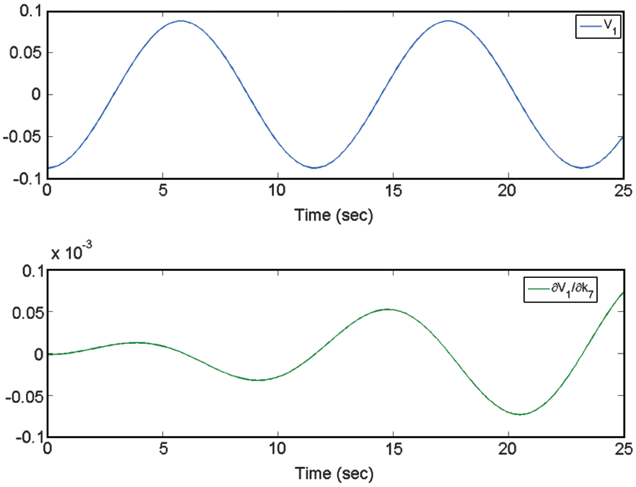

Fig. 4 Right singular vector (time modulation) and right singular vector sensitivity for first principal components with respect to k_7.

and the unknown is defined as the change in the parameter values

$$\Delta p_k = p_k^{\text{modified}} - p_k^{\text{reference}} \tag{57}$$

Thus, this can be applied to two types of problems: 1) calibration or test-analysis reconciliation where test observations would represent the reference and analysis predictions would represent the modified or 2) structural modification assessment (damage detection) with a baseline measurement as the reference and the new evaluation of the principal components representing the modified. In either case, Δp_k is the change in parameter values needed to describe the differences in the principal components, and for the calibration case an updated estimate of the calibrated system parameters can be computed as $p_k^{\text{new}} = p_k^{\text{old}} + \Delta p_k$.

Possible strategies to estimate the unknowns include using only the left singular vectors (shape information) as observations by solving partitions of the problem in Eq. (53); however, the singular values or the right singular vectors can also be included. Furthermore, combinations of this information can be considered to evaluate the use of principal component sensitivities to estimate and locate system parameter changes.

To test these ideas, a truth model was chosen with unknown parameter changes having values of $\Delta p_7 = \Delta k_7 = 0.1$ and $\Delta p_{11} = \Delta k_{11} = 0.2$, for the 20-degree-of-freedom model described in the previous section.

First, only the left singular vectors are considered in the parameter estimation to produce estimates for all 20 unknown stiffness parameter changes assuming no prior knowledge of any parameter values. The results are generally accurate, as estimates for the two nonzero parameters are in error by about 10% (as noted in Fig. 5) when only one iteration solved by Eq. (53) is performed. The parameters were estimated on a principal component by principal component basis; that is, only one principal component shape was used in each of the four estimates.

Next, the use of the left singular vectors and singular values together was examined, and the result is nearly perfect identification, as shown in Fig. 6, again with only one iteration. The nonzero and zero-valued parameters are both correctly identified.

Results for use of the right singular-vector sensitivities are not reported because they were found to result in ill-conditioning. They are ineffective for this example, because the right singular-vector sensitivities are nearly linearly dependent.

D. Example 4: Sensitivity to Forcing Input Parameters

Here, calculation of principal component sensitivities with respect to forcing input parameters is considered. Unlike the normal modes of a structural dynamic system, the dynamic properties described by the principal components are dependent upon loading input characteristics. The lack of dependence of the normal modes on forcing input is taken advantage of for a number of applications in

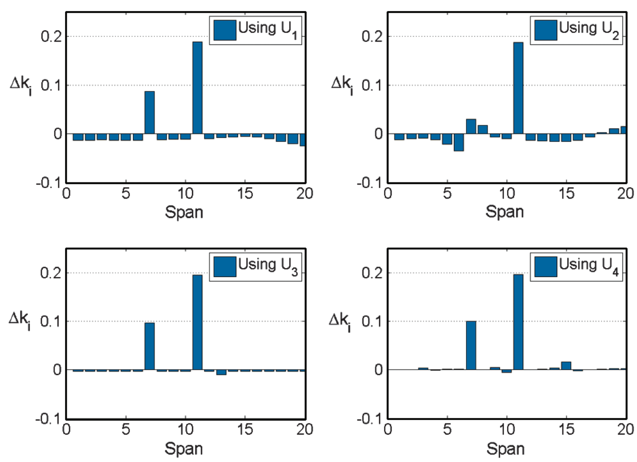

Fig. 5 Estimates of stiffness change using left singular vector sensitivities.

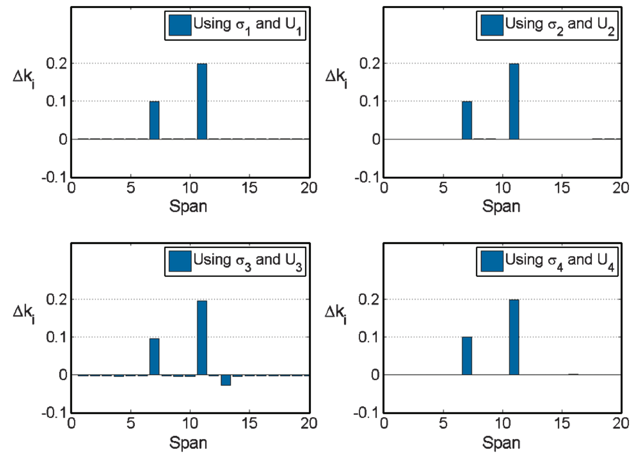

Fig. 6 Estimates of stiffness change using left singular vector and singular-value sensitivities.

structural dynamics analysis including model calibration. Although this dependence for the principal components adds complexity, an opportunity for these methods lies with nonlinear systems analysis. As one example of an opportunity enabled by this method, consider that for a nonlinear problem drastic simplifications may need to be made; for example, linearization to enable use of well-established linear analysis methods or the need to resort to methods with applicability to low-order models to account for the nonlinear effects. In this section, the dependence of the principal components on the characteristics of the forcing input is demonstrated by calculation of analytical sensitivities. Results for calculation and use of principal component sensitivities with respect to loading input parameters are presented.

Of interest is how the left singular vectors (shapes), singular values (amplitudes), and right singular vectors (time modulations) of the principal components are affected by the parameters of the forcing input. Consider as an example a 10-degree-of-freedom problem driven at degree of freedom number 6 by a forcing input given by

$$g(t) = f_1 e^{-\xi_1 t} \sin(\omega_1 t) = e^{-0.1t} \sin(0.7t) \tag{58}$$

In Fig. 7, the first four left singular vectors and the corresponding sensitivities with respect to the forcing frequency are plotted. The data plotted in Fig. 7 was verified by numerical finite difference calculations.

These sensitivities could be useful to predict a new solution in dynamics analysis for a new forcing input solely based on a set of principal components. This has been of interest in recent work [21]. These could also be used to enrich a PCA basis to overcome one difficulty of PCA based reduced-order models, their domain of validity for new forcing inputs.

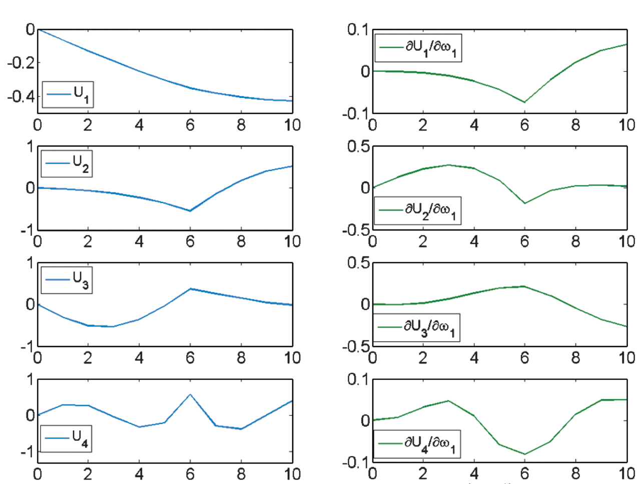

Fig. 7 Sensitivities with respect to forcing frequency.

IV. Conclusions

Principal components analysis (PCA) is useful for a number of applications in the fields of science, engineering, and mathematics. Structural dynamics is one area in which it is useful, because PCA results in modal-like dynamic properties for linear and nonlinear dynamical systems. The key contributions of this paper are the development of two original methods for analytically computing sensitivities of principal components of time-series data based on the singular-value decomposition and eigenanalysis. An approach was introduced to augment state differential equations of motion with differential equations describing system parameters. State transition matrix calculations of the augmented differential equations were introduced to compute state vector sensitivities required to implement the methods. A novel approach to augment differential equations representing dynamic forcing functions was introduced, which transformed the nonhomogenous differential equations (forced system) into homogeneous differential equations (unforced system). It was shown that these methods result in the calculation of principal component sensitivities for all variables in the parameter space, including state variables, system parameters, and forcing input parameters. These results demonstrate promise for the use of analytical principal components sensitivities in the broad application space in which PCA is used. Several example problems in dynamics and structural dynamics analysis were studied. Trajectory analysis for projectile motion was considered for verification and also in interpretation of principal components for dynamics analysis. It was found that principal components analysis is useful for identifying over-parameterized dynamical systems. For structural dynamics applications, sensitivities were used to evaluate the effect of structural modifications analytically, were applied in gradient-based optimization to estimate system parameters, and demonstrated for calculation of sensitivities with respect to forcing input parameters. A promising opportunity lies with one benefit of PCA in that it does not appear to suffer the limited applicability of traditional linear analysis methods.

These examples demonstrate a number of new insights. This general sensitivity method would appear to have potential for other applications, including 1) computation of PCA sensitivities based on experimental data, 2) PCA sensitivity calculation for fluid dynamics analysis, 3) image analysis and camera calibration, 4) basis enrichment of reduced-order models, and 5) assessment of errors in reduced-order models based on principal components.

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Appendix A: Illustrative Example of Principal Components Analysis for a Structural Dynamic System

An approximation of the system response can be computed by selecting a small set of principal components. This is accomplished by choosing, for example, the first k columns of the left and right singular-vector matrices and choosing the corresponding k by k partition of Σ. Then these selected partitions are multiplied as indicated in Eq. (2) to produce an approximation of the snapshot matrix. The resulting approximation is optimal, due to the well-known optimality property of the SVD, which results in the best rank-k approximation of a matrix. In linear structural dynamics, this approximation property is analogous to modal truncation.

To illustrate the dynamical significance of the principal components and the truncation property, consider an example of PCA applied to a cantilever beam with uniform cross section. An

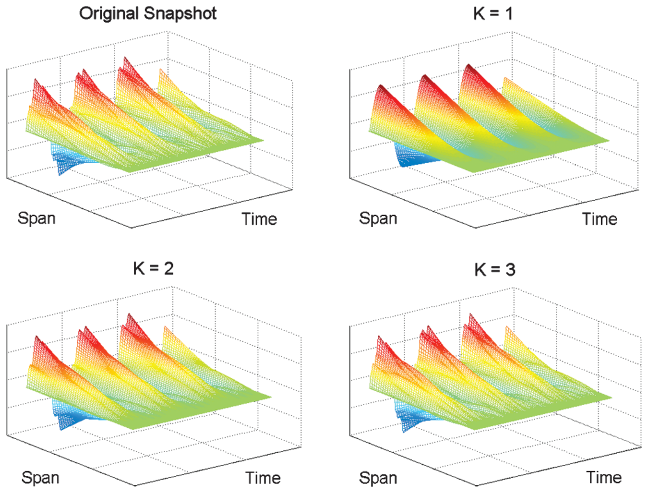

Fig. A1 Illustrative example: principal components analysis of a cantilever beam.

impulse is applied to the tip of the beam, and the resulting motion time histories for a number of spanwise locations along the beam are computed and used to construct the snapshot matrix. The principal components are computed as indicated in Eq. (2). To evaluate the truncation property of PCA, Eq. (2) is used to reconstruct an approximation of the snapshot matrix based on a limited set of principal components. In Fig. A1, the resulting approximations for the cases of one, two, and three principal components are shown along with the original snapshot matrix. For reference, the original snapshot contains a total of 51 principal components. As can be seen in the upper right plot, the dominant motion is described by only one principal component. As additional principal components are included, the difference becomes hardly noticeable as only three principal components are used. The three lowest-frequency modes of this system were excited. Furthermore, note that the vector correlation of the left singular vectors with the eigenvectors (mode shapes) of this system have modal assurance criterion values of 100, 99.8, and 99.7%, which shows that they are nearly identical for this example. This indicates the correspondence between the left singular vectors and the eigenvectors. Note that for this example, a high correlation between the eigenvectors and the left singular vectors is expected [9]. The eigenvectors are orthogonal with respect to the mass matrix, which in this case is diagonal and nearly proportional to an identity matrix. The equivalence can then be expected considering that the left singular vectors are orthogonal with respect to the identity matrix (i.e., $U^T U = I$). Thus, a mass matrix that is proportional to an identity matrix is needed for correspondence between the eigenvectors and the left singular vectors. As pointed out in [9], this apparent limitation in the interpretation of the left singular vectors for a nonidentity proportional mass matrix can be overcome by use of a coordinate transformation to map the mass matrix into an identity matrix.

Appendix B: Sensitivity Analysis Extended to the Frequency Domain

Analytical sensitivity analysis applied to PCA in the frequency domain is now considered. In a manner similar to time-domain-based PCA, the left singular vectors provide shape information and the singular values provide amplitude information. However, the right singular vectors describe the modulations of the principal components in the frequency domain. Thus, in the frequency domain, PCA provides separation of spatial, amplitude, and frequency information. One frequency-domain method for computing the principal components is the so-called frequency-domain decomposition. As described in [8], the SVD method was applied to PSD functions of the response to identify modal parameters from response-only measurements. Here, a similar approach is considered; however, it is applied to frequency response functions (FRFs).

Consider the following definition of a FRF matrix written in terms of the system matrices given by

$$H_{ij}(\omega, \boldsymbol{p}) = [-\omega^2 M(\boldsymbol{p}) + j\omega C(\boldsymbol{p}) + K(\boldsymbol{p})]^{-1} \tag{B1}$$

Here, i represents the response degree of freedom and j represents the input degree of freedom; and ω represents the frequency lines. From Eq. (B1), the FRFs are computed for all responses and all inputs described by the degrees of freedom in the system matrices. Also note that the system matrices are considered to be a function of some parameters $\boldsymbol{p}$.

To begin the development of the sensitivity analysis, the derivative of Eq. (B1) with respect to one parameter p_k is computed, where the dependence of the system matrices on the parameters $\boldsymbol{p}$ is assumed notationally and is given by

$$\begin{aligned}\frac{\partial H_{ij}}{\partial p_k} &= -H_{ij}(\omega, \boldsymbol{p})\frac{\partial[-\omega^2 M + j\omega C + K]}{\partial p_k}H_{ij}(\omega, \boldsymbol{p})\\ &= H_{ij}(\omega, \boldsymbol{p})[\omega^2 \partial M/\partial p_k - j\omega \partial C/\partial p_k - \partial K/\partial p_k]H_{ij}(\omega, \boldsymbol{p})\end{aligned} \tag{B2}$$

Using Eq. (B2), the derivatives of the FRF matrix needed for the PCA sensitivity analysis are computed given the partial derivatives of the system matrices.

Now, consider the following equation, which is a matrix of FRFs for a single input at location s. This matrix is a subset of the FRFs contained in Eq. (B1) and is defined by

$$H_{is}(\omega) = \begin{pmatrix} h_1(\omega_1) & \dots & h_1(\omega_m) \\ \vdots & \ddots & \vdots \\ h_n(\omega_1) & \cdots & h_n(\omega_m) \end{pmatrix} \tag{B3}$$

Note that Eq. (B3) is the frequency-domain analog of Eq. (1). The rows of Eq. (B3) represent the response degrees of freedom while the columns of are snapshots of the FRFs at different frequency lines.

As with the time-domain analog, the FRF matrix is considered to be a function of some parameters, and computation of its principal components using the SVD is given by

$$H_{is}(\omega, \boldsymbol{p}) = \Upsilon\Theta\Omega^T \tag{B4}$$

where Υ are the left singular vectors (spatial information), Θ is a diagonal matrix of singular values (scaling parameters), and Ω are the right singular vectors (modulation functions dependent on frequency). Again, PCA as indicated in Eq. (B4) results in separation of spatial, amplitude, and frequency-dependent information.

The sensitivities of the principal components described by Eq. (B4) can also be computed using the formulas developed earlier. For example, using the SVD-based method, the singular-value sensitivities are computed from Eqs. (4) and (11); and the left and right singular-vector sensitivities are computed from Eqs. (7–10). First, compute the SVD of the matrix of FRFs in Eq. (B3) for the set of responses and the chosen input location. Then the partial derivatives of Eq. (B3) are determined using Eq. (B2). For a particular input, only a subset of the derivatives in Eq. (B2) is needed. Note that the system matrices are implicitly assumed to be a function of the parameter vector in Eq. (B2).

Alternatively, it can be considered to assemble a data matrix of PSDs as is done in [8]. Thus, this sensitivity analysis could also be applied to PSDs, or other frequency-dependent functions, as well. The major difference will be the interpretation of the right singular vectors and their sensitivities. The left singular vectors should be nearly identical for structural dynamics applications as considered here, because they relate to spatial configurations of the response (e.g., eigenvectors or mode shapes).

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A. Sinha
Associate Editor