Applications of Analytical Sensitivities of Principal Components in Structural Dynamics Analysis

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Principal Components Analysis (PCA), which is more recently referred to as Proper Orthogonal Decomposition (POD) in the literature, is a popular 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, such as operating deflection shapes or mode shapes. Structural dynamics is one area 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 dynamics and structural dynamics problems. This is but one application of PCA in the science and engineering literature. The objective of this work is to investigate the applications of principal component sensitivities in structural dynamics analysis to evaluate where opportunities may exist for linear systems and potential new nonlinear analyses. Sensitivity analysis is standard tool used by analysts and has the potential to impact many applications of PCA. In this paper, an analytical approach for sensitivity analysis of PCA, developed and verified in previous work by the authors, is applied to structural dynamics analyses. Analytical sensitivities provide the necessary derivatives for gradient-based algorithms. The proposed applications include an analytical framework for evaluating structural property changes, calibration of linear and nonlinear structural dynamics models, and sensitivity with respect to forcing inputs. Examples applications are considered.

I. Introduction

Principal Components Analysis (PCA), which is more recently referred to as Proper Orthogonal Decomposition (POD) in the literature, is a popular 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, such as operating deflection shapes or mode shapes. Most notable is the use of PCA to generate efficient basis sets for developing reduced order models for fluid flow dynamics and structural dynamics problems. Similarly, PCA has been investigated for system identification in experimental modal analysis. Additional application of PCA can be found in the image analysis literature, for example, feature recognition of facial characteristics in images of human faces. Additional application in the structural dynamics area is calibration of linear and nonlinear finite element models. 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 which 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 eigen problem 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.

We now review how PCA is used for analysis of motion time history data and consider the important properties of PCA that make it valuable for structural dynamics analysis. Consider, the motion response of a

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system \( \mathbf{x}(t_k) \), which is the state vector for the system for various times \( t_k \). We can place this time history response data in a matrix such that

\[
\mathbf{x}(t_k) = \begin{pmatrix}
x_1(t_1) & \cdots & x_i(t_m)
\vdots & \ddots & \vdots 
x_n(t_1) & \cdots & x_n(t_m)
\end{pmatrix}
\]  

(1)

The matrix \( \mathbf{X} \) is called a snapshot matrix because each column of \( \mathbf{X} \) contains a 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 (degree of freedom one at all times), 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 singular value decomposition (SVD), or they can be computed selectively/economically by eigen analysis. First, we illustrate the basic idea of PCA using SVD. The SVD of the snapshot matrix can be written as follows:

\[
\mathbf{X} = \mathbf{U}\Sigma\mathbf{V}^T
\]

(2)

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

PCA of time series data based on SVD results in three matrices which 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. Also, the principal components have significance in dynamics as noted in References 7 and 8, as 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, Equation 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”. For example, the first column of the left singular vector matrix is the shape corresponding to the dominant principal component of the response as it corresponds to the largest singular value (\( \sigma_1 \)). The first column of the right singular vector matrix is the time modulation associated with the first principal component. Furthermore, one can approximate the response of the system 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 \( \Sigma \). Then, these selected partitions are multiplied as indicated in Equation 2 to produce an approximation of the snapshot matrix. This is a restatement of the well-known “optimality” property of SVD, here giving the “best rank-\( k \) approximation” of the snapshot matrix. In linear structural dynamics, this approximation property is analogous to modal truncation.

We now turn our attention to the focus of this paper, the application of analytical methods for sensitivity analysis of the principal components. Sensitivity analysis is a standard tool used by analysts and has the potential to impact many applications of PCA in structural dynamics analysis. 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 are useful as the analogous derivatives of natural frequencies and mode shapes have been for structural dynamics applications including structural model calibration and optimization problems, system design, as well as damage detection studies. One is often interested in determining 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 an analytical method for computing the sensitivities of the principal components with respect to these design parameters and conditions. Here we apply these sensitivities to structural dynamics analysis, although this sensitivity analysis method for PCA has general applicability for other time series analyses, such as fluid dynamics.

The two major sections of this paper include a discussion of two methods for computing the analytical sensitivities of the principal components and a presentation of results for several applications of these methods for structural dynamics analysis. In the first major section, SVD and eigen-based approaches are discussed for PCA sensitivity calculations. Also, we present details regarding the specialization of these sensitivity calculations for PCA with a discussion of necessary state transition matrix sensitivity calculations and development of augmented state-parameter differential equations. The second major section presents three example applications of PCA sensitivities including: 1) structural modification, 2) parameter estimation and 3) sensitivity to forcing input.

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 loading, boundary, and initial conditions. Thus we consider how the principal components depend on these parameters and conditions by computation of the principal component sensitivities. In the following sections, two time domain methods for computing the PCA sensitivities are presented which will be used in examples of proposed structural dynamics analysis applications. First, a general form based on SVD is presented, and then a compact form based on eigen analysis is presented. Next, state transition matrix calculations are described which are needed for the principal component sensitivity calculations. Finally, an approach for augmenting the equations of motion with differential equations describing the system parameters is discussed to enable the desired state transition matrix partial derivative calculations.

A. PCA Sensitivity Calculations Based on the Singular Value Decomposition

Suppose that the motion response is dependent upon a vector of parameters \( p \). Mathematically, we consider the snapshot matrix to be a function of these parameters:

\[
X = X(p) = U \Sigma V^T
\]

where \( X \) is formed according to Equation 1.

We desire to compute the principal component sensitivities: \( \frac{\partial U}{\partial p} \), \( \frac{\partial \Sigma}{\partial p} \) and \( \frac{\partial V}{\partial p} \). General analytical methods have been reported in the literature; however, these methods have not been applied to PCA time series data and do not specify how to compute all the necessary terms for PCA sensitivity calculations. A method for calculation of these analytical sensitivities specialized for the principal components was reported in Reference 11 and is reviewed here.

For time series analysis using PCA, the sensitivity calculations require calculation of state transition matrices that define state departure motions due to system parameter and initial condition changes. A key observation of this work is identification of the derivative of 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 this section.

We now review the PCA sensitivity calculations as documented in Reference 11. An expression for the first-order singular value sensitivity is simply given by:

\[
\frac{\partial \sigma_i}{\partial p_k} = U_i^T \frac{\partial X}{\partial p_k} V_i
\]
We use indicial notation in Equation 4 for the partial derivative of the $i^{th}$ singular value with respect to the $k^{th}$ 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, and is not a function of the singular vector sensitivities. The simplicity of Equation 4 is interesting, and the explanation is given as follows. Consider differentiation of Equation 3 with respect to the parameter vector which results in Equation 5.

$$\frac{\partial X}{\partial p} = \frac{\partial U}{\partial p} \Sigma V^T + U \frac{\partial \Sigma}{\partial p} V^T + U \Sigma \frac{\partial V^T}{\partial p}$$  \hspace{1cm} (5)$$

Now, we pre-multiply both sides of Equation 5 by $U^T$ and post-multiply by $V$. The resulting expression is simplified by the orthonormality of $U$ and $V$ to produce:

$$U^T \frac{\partial X}{\partial p} V = U^T \frac{\partial U}{\partial p} \Sigma + \frac{\partial \Sigma}{\partial p} V^T + \Sigma \frac{\partial V^T}{\partial p} V$$  \hspace{1cm} (6)$$

One finds that the product of the left singular vector matrix and its derivative to be a skew symmetric matrix having a zero-valued diagonal. Likewise, this is true for the right singular vector matrix and its derivative\(^{13}\). Because the derivative of the singular value matrix is diagonal, collection of only the diagonal terms in (6) results in the simple expression in (4) because the first and third terms on the right hand side of (6) have zero values on the diagonal.

Continuing with the other principal component sensitivities, the following assumed forms for computing the left and right singular vectors were proposed in Reference 12:

$$\frac{\partial U_i}{\partial p_k} = \sum_{j=1}^{n} \alpha_{ij}^k U_j$$  \hspace{1cm} (7)$$

$$\frac{\partial V_i}{\partial p_k} = \sum_{j=1}^{n} \beta_{ij}^k V_j$$  \hspace{1cm} (8)$$

We solve for the projection coefficients ($\alpha_{ij}^k$ and $\beta_{ij}^k$), which when multiplied with the corresponding left or right singular vectors, as indicated in Equations 7 and 8, give the desired vector partials.

Closed form expressions for these projection coefficients for the off-diagonal case when $j \neq i$ are given by Equation 9:

$$\alpha_{ij}^k = \frac{1}{\sigma_i^2 - \sigma_j^2} \left[ \sigma_j (U_j^T \frac{\partial X}{\partial p_k} V_i) + \sigma_i (U_i^T \frac{\partial X}{\partial p_k} V_j)^T \right]$$

$$\beta_{ij}^k = \frac{1}{\sigma_i^2 - \sigma_j^2} \left[ \sigma_j (U_j^T \frac{\partial X}{\partial p_k} V_i) + \sigma_i (U_i^T \frac{\partial X}{\partial p_k} V_j)^T \right]$$  \hspace{1cm} (9)$$

and, for the diagonal elements, when $j = i$, they are given by Equation 10:
Thus one computes the full set of projection coefficients using (9) and (10). The desired first-order sensitivities of the left singular vectors are computed using (7) and first-order sensitivities of the right singular vectors are computed using (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 Equation 11, which can be simply derived starting with Equation 4.

\[
\frac{\partial^2 \sigma_i}{\partial p_i \partial p_i} = \frac{\partial U_i^T \partial X}{\partial p_i} V_i' + U_i^T \frac{\partial^2 X}{\partial p_i \partial p_i} V_i' + U_i^T \frac{\partial X}{\partial p_i} \frac{\partial V_i}{\partial p_i} \tag{11}
\]

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.

B. PCA Analytical Sensitivity Calculations Based on Eigen Analysis

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

\[
X = X(p) = U\Sigma V^T
\]

For the eigen-based method, we begin by forming a correlation matrix which is formed by the product of the snapshot matrix and its transpose. Depending on the order of this product, two distinct correlation matrices can be formed:

\[
R_U = XX^T = U\Sigma V^T V \Sigma U^T = U\Sigma^2 U^T \tag{12}
\]

and

\[
R_V = X^T X = V \Sigma U^T U \Sigma V^T = V\Sigma^2 V^T \tag{13}
\]

Owing to the orthonormal properties of \(U\) and \(V\), the inner products in both Equation 12 and Equation 13 equal an identity matrix, thus the correlation matrices depend only on the left or right singular vectors after this simplification.

Eigen analysis 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 eigen analysis. The eigenvalues of \(R_U\) are the square of the singular values of \(X\) and the eigenvectors of \(R_U\) are the left singular vectors of \(X\).
Likewise, the eigenvalues of \( R_y \) are the square of the singular values of \( X \) and the eigenvectors of \( R_y \) are the right singular vectors of \( X \).

Eigen analysis not only provides an alternative method for computing the principal components in the time domain, but it also provides another method for principal component 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, the focus is on reviewing a method for computing the sensitivities of the principal components using eigen analysis methods\(^{11}\). Toward that end, consider a general case applicable to solving the eigen problem for either \( U_R \) or \( V_R \). Note that both matrices are symmetric due to the manner in which they are constructed.

As noted in Reference 11, standard eigen sensitivity algorithms can be used to compute PCA sensitivities analytically. Many methods exist to compute derivatives of \( U_R \) and \( V_R \), including References 9 and 10. These approaches begin by considering an eigen problem of the form of Equation 14.

\[
\begin{bmatrix} A - \lambda_i I \end{bmatrix} \phi_i = 0
\]

where \( \lambda_i \) is the \( i \)th eigenvalue and \( \phi_i \) is the corresponding \( i \)th eigenvector of the matrix \( A \). We again note that \( A \) symbolically represents either \( R_U \) or \( R_V \), which are the correlation matrices.

Here, of course, \( A \) is a function of some parameters, and the eigenvalue derivative is given by\(^9\):

\[
\frac{\partial \lambda_i}{\partial p_k} = \phi_i^T \begin{bmatrix} \frac{\partial A}{\partial p_k} \end{bmatrix} \phi_i
\]

(15)

The eigenvalues of \( A \) are related to the singular values of \( X \) by the following relationship:

\[
\lambda_i = \sigma_i^2
\]

Thus (15) becomes the following when rewritten in terms of the singular value derivative:

\[
\frac{\partial \sigma_i}{\partial p_k} = \frac{\frac{\partial \lambda_i}{\partial p_k}}{2\sqrt{\lambda_i}} = \frac{1}{2\sqrt{\lambda_i}} \left\{ \phi_i^T \begin{bmatrix} \frac{\partial A}{\partial p_k} \end{bmatrix} \phi_i \right\}
\]

(16)

The eigenvector derivative takes a bit more work to compute. It is omitted here, although the process is well-established and is fairly straightforward. When the eigenvector \( \phi_i \) is computed, one is computing either the columns of the left singular vector matrix or the columns of the right singular vector matrix which correspond to \( \sigma_i \).

Clearly, one needs the partial derivative of the matrix \( A \) for either case. For the two specific cases, we present the necessary partial derivative expressions as follows. When \( A \) represents \( R_U \),

\[
\frac{\partial A}{\partial p_k} = \begin{bmatrix} \frac{\partial A}{\partial p_k} \end{bmatrix}
\]

\[
\frac{\partial \sigma_i}{\partial p_k} = \frac{1}{2\sqrt{\lambda_i}} \left\{ \phi_i^T \begin{bmatrix} \frac{\partial A}{\partial p_k} \end{bmatrix} \phi_i \right\}
\]

(16)
\[
\frac{\partial R_k}{\partial \theta_k} = \frac{\partial}{\partial \theta_k} \left( XX^T \right)
= \frac{\partial X}{\partial \theta_k} X^T + X \frac{\partial X^T}{\partial \theta_k}
\tag{17}
\]

and when \( A \) represents \( R_k \),

\[
\frac{\partial R_k}{\partial \theta_k} = \frac{\partial}{\partial \theta_k} \left( X^T X \right)
= \frac{\partial X^T}{\partial \theta_k} X + X^T \frac{\partial X}{\partial \theta_k}
\tag{18}
\]

Here, once again the partials of the snapshot matrix are computed from state transition matrix calculations.

Additionally, this method is not limited to first-order partials in general as second- and higher-order eigen sensitivity analysis has been addressed\(^9\). 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 the time domain methods, we identify the partial derivative of the snapshot matrix as a state transition matrix from dynamical systems analysis\(^{14}\). These matrices are needed in both methods previously described for computing the principal component sensitivities. In this section we discuss computation of the first- and higher-order state transition matrices which enable the PCA sensitivity calculations.

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. Let’s consider the most general case of a nonlinear dynamical system in order to begin development of the state transition matrix. Consider the following dynamical system described by the following set of differential equations and initial conditions

\[
\dot{z} = f(z, p, t); \quad z(t_0) = z_0
\tag{19}
\]

where in Equation 19 we see that the dynamical system is in general a nonlinear function of the states of the system and the system parameters \( p \), representing the equations of motion of the system. Our 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, we consider sensitivity to both the state vector and system parameters simultaneously in our development. To achieve this goal, we augment the state vector differential equations with the parameter vector differential equations to form a set of augmented differential equations:

\[
\begin{align*}
\dot{x} &= \begin{bmatrix} \dot{z} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} f(z, p, t) \\ g(z, p, t) \end{bmatrix}; \quad x(t_0) = x_0 \\
 &= h(z, p, t)
\end{align*}
\tag{20}
\]

where the augmented state and initial conditions are defined as

\[
x = \begin{bmatrix} z \\ p \end{bmatrix}; \quad x(t_0) = \begin{bmatrix} z(t_0) \\ p(t_0) \end{bmatrix}
\]
For now, we consider a general form for the differential equations for the parameter vector. However, for the common case of constant parameters, \( \mathbf{g}(\mathbf{z}, \mathbf{p}, t) \) will, of course, equal a zero-valued vector (i.e. \( \dot{\mathbf{p}} = \mathbf{0} \)). This augmentation approach enables calculation of \( \frac{\partial \mathbf{z}(t)}{\partial \mathbf{z}(t_0)} \) and \( \frac{\partial \mathbf{z}(t)}{\partial \mathbf{p}} \), state transition matrix sensitivity calculations, which are needed for the principal component sensitivity calculations with respect to initial conditions and system parameters, respectively.

We now summarize the development of the state transition matrix differential equation. The state transition matrix for first-order sensitivity calculations is not new; however, we present this development in order to provide a means for computing second- and higher order state transition matrices for the second- and higher-order principal component sensitivity calculations. In integral form, the solution to Equation 20 is

\[
\mathbf{x}(t) = \mathbf{x}(t_0) + \int_{t_0}^{t} \mathbf{h}(\mathbf{x}, \tau) d\tau
\]  

(21)

And, upon differentiating (21) with respect to \( \mathbf{x}(t_0) \) we arrive at the following expression:

\[
\frac{\partial \mathbf{x}(t)}{\partial \mathbf{x}(t_0)} = I + \int_{t_0}^{t} \left( \frac{\partial \mathbf{h}(\mathbf{x}, \tau)}{\partial \mathbf{x}(\tau)} \right) d\tau
\]  

(22)

We define the state transition matrix using the following notation: \( \Phi(t, t_0) = \frac{\partial \mathbf{x}(t)}{\partial \mathbf{x}(t_0)} \), thus (22) can be re-written as:

\[
\Phi(t, t_0) = I + \int_{t_0}^{t} \left( \frac{\partial \mathbf{h}(\mathbf{x}, \tau)}{\partial \mathbf{x}(\tau)} \right) \Phi(\tau, t_0) d\tau
\]  

(23)

Now, we take the time derivative of (23) to arrive at a differential equation which describes the augmented state variable sensitivity. The differential equation for the state transition matrix and its initial condition are given by:

\[
\dot{\Phi}(t, t_0) = \frac{\partial \mathbf{h}(\mathbf{x}, t)}{\partial \mathbf{x}(t)} \Phi(t, t_0); \quad \Phi(t_0, t_0) = I
\]  

(24)

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

\[
\Phi(t, t_0) = \frac{\partial \mathbf{x}(t)}{\partial \mathbf{x}(t_0)} = \begin{bmatrix}
\frac{\partial \mathbf{z}(t)}{\partial \mathbf{z}(t_0)} & \frac{\partial \mathbf{z}(t)}{\partial \mathbf{p}(t_0)} \\
\frac{\partial \mathbf{p}(t)}{\partial \mathbf{z}(t_0)} & \frac{\partial \mathbf{p}(t)}{\partial \mathbf{p}(t_0)}
\end{bmatrix}
\]  

(25)

For the special case of a linear system, which is often the case in structural dynamics, Equation 24 becomes:

\[
\dot{\Phi}(t, t_0) = A\Phi(t, t_0); \quad \Phi(t_0, t_0) = I
\]  

(26)
\( A \) 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:

\[
\Phi(t, t_0) = e^{A(t-t_0)}
\] (27)

For the general nonlinear case, one must solve Equations 20 and 24 simultaneously by numerical integration. The result is the solution for the motion of the system for a nominal set of initial conditions along with a first-order state transition matrix which can be used to compute perturbations from the nominal motion solution due to changes in the initial conditions (again, these initial conditions include state and parameter initial conditions for the augmented system).

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 (22) with respect to the state variable initial condition and then taking the time derivative of the resulting expression as was done to produce (24). This process can be repeatedly used and was first reported in References 15 and 16 to derive the second- and higher-order state transition matrix concepts.

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

D. Examples of 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 two of the example applications considered later in the paper. The first considers augmentation of system parameters for a linear structural dynamics problem, and the second considers augmentation of forcing function parameters with the state variables.

1) Augmentation of System Parameters for a Linear Structural Dynamics Problem

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

\[
\dot{x} = \begin{bmatrix} \dot{z} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} f(z, p, t) \\ g(z, p, t) \end{bmatrix}; \quad x(t_0) = x_0
\]

For a linear structural dynamics problem we have

\[
M\ddot{y} + C\dot{y} + Ky = F
\] (28)

or, in first-order form

\[
\dot{z} = \begin{bmatrix} \dot{y} \\ \dot{\dot{y}} \end{bmatrix} = \begin{bmatrix} 0 & I \\ -M^{-1}K & -M^{-1}C \end{bmatrix}\begin{bmatrix} y \\ \dot{y} \end{bmatrix} + \begin{bmatrix} 0 \\ M^{-1}F \end{bmatrix}
\] (29)

and

\[
p = \begin{bmatrix} m_1 \cdots m_n \\ c_1 \cdots c_n \\ k_1 \cdots k_n \end{bmatrix}^T
\] (30)

with

\[
\dot{p} = 0
\] (31)

thus the augmented set of equation becomes
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 (32); of course, the state transition matrices would need to be computed numerically.

2) Augmentation of Forcing Function Parameters

We now consider forming a set of augmented state-parameter differential equations including the parameters of the forcing function. Here we only consider forcing parameters for simplicity. The sensitivities can be calculated with respect to any variable which is included in the state vector, and this requires the forcing function to be parameterized analytically. We consider a few common loading cases useful in structural dynamics analysis.

We begin the development by considering a MDOF system forced with a general forcing function:

\[ M\ddot{y} + C\dot{y} + Ky = g(t) \]  

First, we consider the case of forcing at a single frequency, such that:

\[ g(t) = f \sin(\omega t) \]  

One can define a new variable to describe the time modulation of the forcing input:

\[ s = \sin(\omega t) \]  

Such that (33) becomes:

\[ M\ddot{y} + C\dot{y} + Ky = f \cdot s \]  

Now, the following differential equation, which governs the time modulation of the forcing input and has solution given by (35) can be augmented with the equations of motion:

\[ \ddot{s} + \omega^2 s = 0 \]  

An augmented state-parameter differential equations can be written as:

\[
\begin{bmatrix}
M & 0 \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
\dot{y} \\
\dot{s}
\end{bmatrix}
+
\begin{bmatrix}
C & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\dot{y} \\
\dot{s}
\end{bmatrix}
+
\begin{bmatrix}
K & -f \\
0 & \omega^2
\end{bmatrix}
\begin{bmatrix}
y \\
s
\end{bmatrix}
=
\begin{bmatrix}
0 \\
0
\end{bmatrix}
\]  

where the parameter vector is simply

\[ p = s \]  

Note that (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.

The key to implementing this approach is that a differential equation (i.e. \( \dot{p} = g(z, p, t) \)) must be carefully selected to describe the parameters chosen to 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 $s$.

Now we extend the idea to demonstrate that more general forcing functions can be considered for augmentation. Consider $g(t)$ written in two ways: 1) a forcing function as a sum of sinusoids, and 2) a forcing function as a sum of decaying sinusoids:

Case 1) $g(t) = \sum_{i=1}^{n} f_i \sin(\omega_i t)$

Case 2) $g(t) = \sum_{i=1}^{n} f_i e^{-\xi t} \sin(\omega_i t)$

Case 2 is very similar to the manner in which acceleration time history inputs are defined for input to structural dynamics codes for transient dynamics analysis to simulate environmental loads.

a) Case 1: Forcing Due to Summation of Sinusoidal Inputs

Case 1 is a generalization of the first example. Equation 38 can be extended for the case when multiple harmonics are required to approximate the forcing function, for example, with $n=2$, and again in second-order form with the damping matrix omitted for clarity we have:

\[
\begin{bmatrix}
M & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
\ddot{y} \\
\dot{s}_1 \\
\dot{s}_2 \\
\dot{f}_1 \\
\dot{f}_2 \\
\omega_1 \\
\end{bmatrix}
= \begin{bmatrix}
K & -f_1 \hat{e}_1 & -f_2 \hat{e}_2 & 0 & 0 & 0 & 0 \\
0 & \omega_1^2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \omega_2^2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
y \\
s_1 \\
s_2 \\
f_1 \\
f_2 \\
\omega_1 \\
\end{bmatrix}
\]

where $f_1$ and $f_2$ are the magnitude (scalar quantities) and $\hat{e}_1$ and $\hat{e}_2$ are vectors of ones and zeros that define the degrees of freedom to which the force is applied; and $\omega_1$ and $\omega_2$ are frequencies of the input force terms. The parameters $f_1$, $f_2$, $\omega_1$, and $\omega_2$ are constant parameters as noted by their differential equations in (40) and $s_1$ and $s_2$ are defined similarly to (37).

Here, we have chosen to define $f_1$ and $f_2$ explicitly in the parameter vector. If one is not concerned with principal component sensitivity calculations with respect to forcing input level, then the prior form can be used with these parameters not appearing explicitly in the parameter vector. In the case of (40), the parameter vector is defined as

\[
p = [s_1 \ s_2 \ f_1 \ f_2 \ \omega_1 \ \omega_2]^T
\]

And, the trend continues as the number of desired terms in the forcing function gets larger.

b) Case 2: Forcing Due to Summation of Decaying Sinusoids

For the more general case of a sum of decaying sinusoids, one must again determine a differential equation to describe the time modulation of the forcing input. One can show that for $n=1$

\[
\alpha_i(t) = e^{-\xi t} \sin(\omega_i t)
\]
where the forcing function is

$$g(t) = f(t)\alpha_1(t) \tag{43}$$

The expression in (42) is the solution to the following differential equation:

$$\ddot{\alpha}_1 + 2\xi_1\dot{\alpha}_1 + (\xi_1^2 + \omega_1^2)\alpha_1 = 0 \tag{44}$$

which can be verified by substitution.

As an example, the augmented set of differential equations, for n=1, becomes the following by augmenting (44) and the constant parameter differential equations with the system dynamics model, again in second-order form for clarity:

$$\begin{bmatrix} M & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \ddot{y} \\ \dot{\alpha}_1 \\ \dot{f}_1 \\ \dot{\xi}_1 \end{bmatrix} + \begin{bmatrix} C & 0 & 0 & 0 & 0 \\ 0 & 2\xi_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{y} \\ \dot{\alpha}_1 \\ \dot{f}_1 \\ \dot{\xi}_1 \end{bmatrix} + \begin{bmatrix} K & -f_1\dot{\alpha}_1 & 0 & 0 & 0 \\ 0 & \omega_1^2 + \xi_1^2 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} y \\ \alpha_1 \end{bmatrix} = \mathbf{0} \tag{45}$$

where the parameter vector is defined

$$\mathbf{p} = [\alpha_1 \quad f_1 \quad \omega_1 \quad \xi_1]^T \tag{46}$$

Again, this formulation generalizes to higher dimension with additional decaying sinusoidal terms used to parameterize the forcing function (n>1).

Essentially, we are re-writing the differential equation with forcing input 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.

We verified this approach by considering the following example:

$$M\ddot{y} + C\dot{y} + Ky = f_1 e^{-\xi t} \sin(\omega_1 t) \tag{47}$$

We chose a 20 degree of freedom mass-damper-spring system, 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 (47) was solved using a 4th order Runge Kutta numerical integration scheme with the initial position and velocity conditions equaling zero. Note that Equation (47), in second-order form, has a dimension of 20.

Next, Equation (45) was solved using the same 4th order Runge Kutta numerical integration scheme using the same forcing function parameters and initial conditions. In this case, in second-order form, Equation (45) 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 $\alpha_1(t_0)$ and $\dot{\alpha}_1(t_0)$ are defined by Equation (42) 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 (45) is equivalent to the desired input force given on the right hand side of (47). Thus the homogenous augmented form was verified to be equivalent to the forced system.
Now, one can compute the sensitivities of the principal components \((U, \Sigma, V)\) based on the forms presented here, e.g. \(\frac{\partial U}{\partial f_i}, \frac{\partial U}{\partial \omega_i},\) and \(\frac{\partial U}{\partial \xi_i}\) with respect to forcing function parameters given the following state vector partials \(\frac{\partial y(t)}{\partial f_i}, \frac{\partial y(t)}{\partial \omega_i},\) and \(\frac{\partial y(t)}{\partial \xi_i}\) computed from state transition matrix calculations.

**IV. Applications of PCA Sensitivities to Structural Dynamics Analysis**

We now apply the methods described in previous sections to structural dynamics analyses. Examples considered include 1) structural modification (e.g. evaluating the effect of mass/stiffness changes), 2) calibration or parameter estimation (i.e. use sensitivities to compute parameter changes) and 3) demonstration of the effect of forcing input characteristics on the principal components for a forced system.

Some potential applications not demonstrated here include 1) computation of PCA sensitivities based on experimental data, 2) computation of second- and higher-order sensitivities for nonlinear analysis, 3) camera calibration, and 4) enrichment of reduced order models by improved domain of validity.

We now look at several examples.

**A. Example 1: Structural Modification**

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

\[
M\ddot{y} + C\dot{y} + Ky = F = 0; \quad y(t_0) = y_0; \quad \dot{y}(t_0) = \dot{y}_0
\]  

(48)

with parameters defined by

\[
m_i = 1; c_i = 0; k_i = 50; \quad i = 1, 2, \ldots, 20
\]  

(49)

and the initial condition is such that the system is at rest and end mass is initially displaced from equilibrium. We compute \(\frac{\partial U_i}{\partial p_k}, \frac{\partial \sigma_i}{\partial p_k},\) and \(\frac{\partial V_i}{\partial p_k}\) for \(i = 1, 2, \ldots, 20\) and \(p = [k_1, k_2, \ldots, k_{20}]\).

In the following, a few selected sensitivities are presented to graphically demonstrate the nature of the principal component sensitivities. First, in Figure 1, we plot the first principal component shape \((U_1)\) and its sensitivity with respect to \(k_7\), the stiffness at the location of the 7th spring. \(U_1\) resembles the first eigen mode of the system and \(\frac{\partial U_1}{\partial k_7}\) has a discontinuity at the location of \(k_7\). These can be compared to the first eigen mode and the first eigen mode sensitivity to demonstrate that they are nearly identical for this example.
Figure 1. Left Singular Vector (Shape) and Left Singular Vector Sensitivity of
First Principal Component with Respect to $k_7$

Table 1 provides a comparison of the singular values and their sensitivities with respect to $k_7$. Only the first 4 of the 20 total singular values and sensitivities are provided. Note that $\sigma_1$ accounts for most of the “energy” of the response. The singular values are, of course, in descending order. The singular value sensitivities are multiplied by 1000 as entered in Table 1. If one was doing an analysis of the effect of the parameter $k_7$, we would find that the largest effect is with the third principal component singular value.

<table>
<thead>
<tr>
<th>Principal Component Number</th>
<th>Singular Values ($\sigma_i$)</th>
<th>$\frac{\partial \sigma_i}{\partial k_7} \times 10^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.1255</td>
<td>-1.8443</td>
</tr>
<tr>
<td>2</td>
<td>1.3192</td>
<td>-0.6273</td>
</tr>
<tr>
<td>3</td>
<td>0.4739</td>
<td>-2.9421</td>
</tr>
<tr>
<td>4</td>
<td>0.2393</td>
<td>1.9597</td>
</tr>
</tbody>
</table>
Figure 2 shows the time modulation associated with the first principal component ($V_1$) and its sensitivity ($\frac{\partial V_1}{\partial k_7}$). By comparing the two plots, one can see that an increase in $k_7$ shifts $V_1$ peaks to the left, according to the modification resulting from $\frac{\partial V_1}{\partial k_7}$, to a higher frequency as one would expect.

![Figure 2. Right Singular Vector (Time Modulation) and Right Singular Vector Sensitivity for First Principal Components with Respect to $k_7$](image)

In summary, these calculations indicate in different ways how principal components change due to system parameter changes. The principal component sensitivities could provide a means to evaluate structural modifications. The shape sensitivity, $\frac{\partial U_1}{\partial k_7}$, for example, indicates where a stiffness change has occurred. And, $\frac{\partial V_1}{\partial k_7}$ indicates how the frequency changes, while $\frac{\partial \sigma_1}{\partial k_7}$ indicates how the amplitude of the principal component changes. The use of these for parameter estimation is examined in the next example.

**B. Example 2: Parameter Estimation**

In this section, we consider using principal component sensitivity calculations to locate and estimate the value of parameter changes. Use of principal components for calibration has been considered by other researchers\textsuperscript{5,17} using non-gradient based approaches. Here, a simple least-squares gradient-based approach was taken to evaluate these different strategies for computing the unknown $\Delta p_k$ using analytical principal component sensitivities. The least-squares problem is posed as:
\[
\begin{align*}
\begin{bmatrix}
\Delta U_i \\
\Delta \sigma_i \\
\Delta V_i
\end{bmatrix} &=
\begin{bmatrix}
\frac{\partial U_i}{\partial p_k} & \frac{\partial \sigma_i}{\partial p_k} & \frac{\partial V_i}{\partial p_k}
\end{bmatrix}
\Delta p_k
\end{align*}
\]

(50)

which is solved for the unknown as follows:

\[
\Delta p_k =
\begin{bmatrix}
\frac{\partial U_i}{\partial p_k} & \frac{\partial \sigma_i}{\partial p_k} & \frac{\partial V_i}{\partial p_k}
\end{bmatrix}^t
\begin{bmatrix}
\Delta U_i \\
\Delta \sigma_i \\
\Delta V_i
\end{bmatrix}
\]

(51)

Where “\(^t\)” represents the pseudo-inverse operation. The change in the “observation” parameter is given by the difference in a “reference” principal component and a new, “modified” principal component:

\[
\Delta U_i = U_i^{\text{modified}} - U_i^{\text{reference}}
\]

(52)

\[
\Delta \sigma_i = \sigma_i^{\text{modified}} - \sigma_i^{\text{reference}}
\]

(53)

\[
\Delta V_i = V_i^{\text{modified}} - V_i^{\text{reference}}
\]

(54)

and the unknown is defined as the change in a set of parameter values:

\[
\Delta p_k = p_k^{\text{modified}} - p_k^{\text{reference}}
\]

(55)

Thus, one can consider application of this 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 with a baseline measurement as the “reference” and the new evaluation of the principal components representing the “modified”. In either case, \(\Delta p_k\) is the difference 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) by solving partitions of the problem in (51); however, one can also use the singular values or the right singular vectors. Furthermore, one can consider using combinations of this information to evaluate the use of principal component sensitivities to estimate and locate system parameter changes.

To test these ideas, a truth model with unknown parameter changes were chosen with 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, we consider only the left singular vectors in the parameter estimation and produce estimates for all 20 unknown stiffness parameter changes. We find that the results are generally accurate as estimates for the two non-zero parameters although they are in error by about 10% as noted in Figure 3 when only one iteration solved by (51)
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, we examined using left singular vectors and singular values together, and found nearly perfect results as shown in Figure 4, again with only one iteration. The non-zero and zero-valued parameters are both correctly identified.
We found that use of the right singular vectors to be ill-conditioned and ineffective because the right singular vector sensitivities are nearly linearly dependent.

**C. Example 3: Sensitivity to Forcing Input Parameters**

Here, we demonstrate calculation of principal component sensitivities with respect to forcing input parameters. Unlike the normal modes of a structural dynamics 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 of structural dynamics analysis including model calibration. Depending on the point of view, one can consider the dependence of the principal components on the loading input to be limiting to their potential uses or one could consider this to be an opportunity. As one example of an opportunity, consider that for a nonlinear problem one is forced to make drastic simplifications; for example, linearization to enable use of well-established linear analysis methods or to resort to methods with applicability to low-order models to account for the nonlinear effects. In this section, we aim to demonstrate the dependence of the principal components on the characteristics of the forcing input. We present preliminary results for calculation and use of principal component sensitivities with respect to loading input parameters.

We are interested in 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. We consider as an example a 10 degree of freedom problem driven at degree of freedom 6 by the following forcing input:

\[
g(t) = f_t e^{-\zeta t} \sin(\omega t) = e^{-0.1t} \sin(0.7t)
\]  

In Figure 5, we plot the first four left singular vectors and the corresponding sensitivities with respect to the forcing frequency. The data plotted in Figure 5 was verified by numerical finite difference calculations. Additionally, sensitivities with respect to the damping parameter of the forcing input were successfully verified for the left singular vectors.

![Figure 5. Sensitivities with Respect to Forcing Frequency](image)
For sensitivity with respect to forcing input level, we find that for this linear system the left and right singular vector sensitivities are zero. This is expected because for a linear system, changes in input level only change the magnitude of the response according to the principle of linear superposition, and only the singular values should be sensitive to forcing level. The singular value sensitivities with respect to forcing input level were verified by numerical finite difference calculations. On the other hand, all of the right singular vector sensitivities could not be verified with respect to either the forcing frequency or damping parameter, although the few that did not agree with numerical finite difference calculations trended generally with finite difference calculations and modulated at the same frequencies of the principal components. Further, the singular value sensitivities with respect to the forcing and damping parameters are only verified for the 3rd through 10th singular values. They were in error for the 1st and 2nd singular values. It is not yet understood why some of the analytical sensitivities and the numerical finite difference calculations did not agree. The left singular vector sensitivities were verified for all forcing input parameters, while the singular value and right singular vector sensitivities were completely verified with respect to only the forcing input level.

These sensitivities could be useful to reconstruct a new solution for a dynamics model solely based on a set of principal components for a new forcing input. This has been of interest in some recent work\textsuperscript{18}. Also, these could 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.

V. 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 methods for computing sensitivities of principal components based on time series data, and application of these sensitivities to structural dynamics analysis. It was shown that these methods result in the calculation of principal component sensitivities for all variables in the parameter space, including state variables and system parameters such as system properties 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 utilized. For structural dynamics applications, these sensitivities were used to evaluate the effect of structural modifications analytically, were used in gradient-based optimization to estimate system parameters, and were 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

VI. References