

Analytical Sensitivities for Principal Components Analysis of Dynamical Systems

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Abstract

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. 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 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.

The objective of this work is to address the issue of sensitivity analysis for PCA. Sensitivity analysis is standard tool used by analysts and has the potential to impact many applications of PCA. In this paper, analytical approaches for sensitivity analysis of PCA are developed. These analytical approaches are developed in contrast to numerical approaches such as finite differencing. Methods are developed for both time domain and frequency domain implementations of PCA. For the time domain case, both a general complete method and a computationally economical method are developed. Each approach is verified by comparing the analytical sensitivities with numerical finite difference calculations.

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. 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. 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 [2]. Similarly, PCA has been investigated for system identification in experimental modal analysis [3]. Additional application of PCA can be found in the image analysis literature; for example, feature recognition of facial characteristics in images of human faces [4]. Additional application in the structural dynamics area is calibration of linear and nonlinear finite element models [5]. 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

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system matrices developed from a finite element analysis. For the time domain case, PCA results in the extraction of dynamic properties of the system from time histories of response data, which applies to either transient dynamics finite element calculations or experimental response measurements.

Consider, the dynamic response of a system $\mathbf{x}(t)$, which is the state vector for the system for various times t . We can place this response data in a matrix such that

$$\mathbf{x}(t) = X = \begin{pmatrix} x_1(t_1) & \cdots & x_1(t_m) \\ \vdots & \ddots & \vdots \\ x_n(t_1) & \cdots & x_n(t_m) \end{pmatrix} \quad (1)$$

The matrix X is called a snapshot matrix because each column of 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 is at 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).

Principally, there are two ways to compute PCA in the time domain. One can compute the complete PCA using the more general method by singular value decomposition (SVD), or the PCA can be computed selectively/economically by eigen analysis. First, we illustrate the basic idea of PCA in the more general fashion using SVD. In general, the SVD of a matrix can be written as follows [6]:

$$X = U \Sigma V^T \quad (2)$$

where, U is an orthogonal matrix whose columns contain the left singular vectors, Σ is a diagonal 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).

SVD of the snapshot matrix 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, diagonal values of Σ , 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). 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 which provides a separation of time and space variables and a means to truncate the response into a set of “modes”. For example, the first column of the left singular vector matrix is the shape corresponding to the dominant response mode contained in X , and it corresponds to both the largest singular value (the (1,1) element of Σ) and the first column of the right singular vector matrix, which is the “modal coordinate” associated with the first principal component. Furthermore, one can consider in a very general sense how to approximate the matrix X . 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 Equation 2 to compute an approximation of the snapshot matrix. This is a restatement of the well-known property of SVD, here giving the “best rank- k approximation” of a matrix. In linear structural dynamics, this approximation property is analogous to modal truncation.

In order to illustrate the dynamical significance of the principal components and the truncation property, let's consider an example of PCA applied to a cantilever beam with uniform cross-section. An impulse is applied to the tip of the beam, and the resulting motion time histories are placed in a snapshot matrix for various points along the beam and at various times in the motion. The principal components are computed as indicated in Equation 2. In order to evaluate PCA, one can also use Equation 2 to reconstruct an approximation of the snapshot matrix for varying numbers of principal components as described in the previous paragraph. In Figure 1, we plot the resulting approximations for the cases of 1, 2, and 3 principal components along with the original snapshot matrix.

For reference, the original snapshot contains a total of 51 principal components. As one can see in the upper right plot, the dominant motion is described by only 1 principal component. As additional principal components are included, we find the difference to become hardly noticeable when only 3 principal components are used. One can say that the three lowest frequency modes of this system were excited. Furthermore, we note that the vector correlation of the left singular vectors with the eigenvectors (mode shapes) of this system have MAC values of 100, 99.8, and 99.7% which shows they are nearly identical for this example. This indicates the correspondence between the left singular vectors and the eigenvectors. We note that for this example we expect high correlation between the eigenvectors and the left singular vectors. The topic of the correspondence between the left singular vectors and eigenvectors has been reported in previous work [7]. The eigenvectors are orthogonal with respect to the mass matrix, which in this case is diagonal and 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 which is proportional to an identity matrix is needed for correspondence between the eigenvectors and the left singular vectors. As pointed out in Reference 7, this apparent limitation in the interpretation of the left singular vectors can be overcome by use of a coordinate transformation to map the mass matrix into an identity matrix.

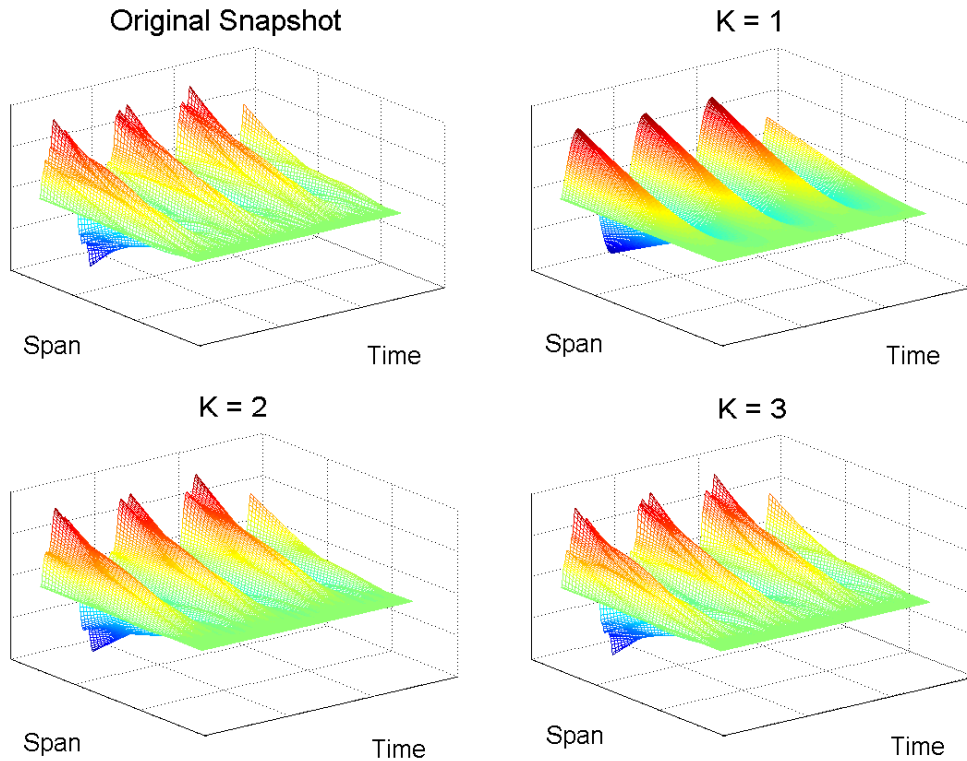


Figure 1. Illustrative Example: Principal Components Analysis of a Cantilever Beam

We now turn our attention to development of analytical methods for sensitivity analysis of the principal components. We have demonstrated that PCA provides a separation of spatial and temporal information of the response and that the principal components have significance in dynamics. Further, we find significance in the sensitivities (derivatives) of the principal components for structural dynamics applications as we do with the analogous derivatives of natural frequencies and mode shapes which have been published previously [8,9] and utilized extensively for structural model calibration and optimization problems, system design, as well as damage detection studies. In particular, one is typically 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 (modulus change) or initial condition/loading input change). The focus of this paper is on development of such an analytical method for computing the sensitivities of PCA due to these factors. However, the method is very general and can be applied to other types of dynamical systems beyond structural dynamics applications.

The objective of this work is to address the issue of sensitivity analysis for PCA. Sensitivity analysis is standard tool used by analysts and has the potential to impact many applications of PCA. In this paper, analytical approaches for sensitivity analysis of PCA are developed. Again, the types of sensitivities considered are those with respect to both state variable and system parameters. Methods are developed for both time domain and frequency domain implementations of PCA. For the time domain case, both a general complete method and a computationally economical method are developed. Each approach is verified by comparing the analytical sensitivities with numerical finite difference calculations.

II. Summary of Methodology: Two Approaches for Sensitivity Analysis in the Time Domain

We note that 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 and boundary conditions. Thus the principal components derived from PCA also depend on these conditions. In the following sections, two time domain methods for computing the PCA sensitivities are developed. First a general form is presented, and then a compact form is presented.

A. Approach 1: Sensitivity Analysis based on the Singular Value Decomposition

Suppose that the system dynamics response vector $\mathbf{x}(t)$ is dependent upon a vector of parameters \mathbf{p} . This vector of parameters may include system parameters or the state variables. Further, consider this in equivalent terms of the snapshot matrix as a function of these parameters:

$$\mathbf{X} = \mathbf{X}(\mathbf{p}) = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \quad (3)$$

We begin our development by taking the derivative of the snapshot matrix with respect to \mathbf{p} , where the functional dependence of the snapshot matrix and the principal components is assumed notationally henceforth.

$$\frac{\partial \mathbf{X}}{\partial \mathbf{p}} = \frac{\partial \mathbf{U}}{\partial \mathbf{p}} \mathbf{\Sigma} \mathbf{V}^T + \mathbf{U} \frac{\partial \mathbf{\Sigma}}{\partial \mathbf{p}} \mathbf{V}^T + \mathbf{U} \mathbf{\Sigma} \frac{\partial \mathbf{V}^T}{\partial \mathbf{p}} \quad (4)$$

Equation 4 shows that the sensitivity of the system dynamics response depends on the sensitivity of each of the three SVD factors, \mathbf{U} , $\mathbf{\Sigma}$, and \mathbf{V} .

Our goal is to compute $\frac{\partial \mathbf{U}}{\partial \mathbf{p}}$, $\frac{\partial \mathbf{\Sigma}}{\partial \mathbf{p}}$ and $\frac{\partial \mathbf{V}}{\partial \mathbf{p}}$. A general method was developed by Junkins and Kim [10] to compute the partials of the SVD factors. The method is based on a given SVD factorization of a matrix and the derivative of the matrix, i.e. $\frac{\partial \mathbf{X}}{\partial \mathbf{p}}$. The focus of their development was application of singular value sensitivities in gradient-based algorithms to improve stability measures in control law design which use singular value methods.

The key contributions of the developments in this section are identification of the derivative of the snapshot matrix as a state transition matrix from dynamical systems theory, and the application of PCA sensitivities to structural dynamics problems. Computation of the state transition matrix is essential, and is discussed later in this paper.

We continue with the development of the mathematical expressions in a general way. An expression for the first-order singular value sensitivities is simply given by [10]:

$$\frac{\partial \sigma_i}{\partial p_k} = \mathbf{U}_i^T \frac{\partial \mathbf{X}}{\partial p_k} \mathbf{V}_i \quad (5)$$

We now use indicial notation in Equation 5 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 5 is interesting, and the explanation is given as follows. Consider pre-multiplication of both sides of the expression in Equation 4 by U^T and post-multiplication of the expression in Equation 4 by V . The following expression results, again with U and V being orthonormal:

$$U^T \frac{\partial X}{\partial \mathbf{p}} V = U^T \frac{\partial U}{\partial \mathbf{p}} \Sigma + \frac{\partial \Sigma}{\partial \mathbf{p}} + \Sigma \frac{\partial V^T}{\partial \mathbf{p}} V \quad (6)$$

One finds that the product of the left singular vector and its derivative to be a skew symmetric matrix. Likewise, this is true for the right singular vector and its derivative [11]. Because the derivative of the singular value matrix is diagonal, collection of only the diagonal terms in (6) results in the simple expression in (5) because the first and third terms on the right hand side of (6) have zero values on the diagonal.

Junkins and Kim proposed the following method to compute the left and right singular vectors, by beginning with the following assumed forms:

$$\frac{\partial U_i}{\partial p_l} = \sum_{j=1}^n \alpha_{ji}^l U_j \quad (7)$$

$$\frac{\partial V_i}{\partial p_l} = \sum_{j=1}^n \beta_{ji}^l V_j \quad (8)$$

Their approach is to solve for these projection coefficients, which when multiplied with the 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:

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

For the diagonal elements, when $j = i$, they are given by Equation 10:

$$\begin{aligned} \alpha_{ii}^l - \beta_{ii}^l &= \frac{1}{\sigma_i} \left(U_i^T \frac{\partial X}{\partial p_l} V_i - \frac{\partial \sigma_i}{\partial p_l} \right) \\ \alpha_{ii}^l - \beta_{ii}^l &= \frac{1}{\sigma_i} \left(-V_i^T \frac{\partial X^T}{\partial p_l} U_i + \frac{\partial \sigma_i}{\partial p_l} \right) \end{aligned} \quad (10)$$

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.

$$\frac{\partial^2 \sigma_i}{\partial p_k \partial p_l} = \frac{\partial U_i^T}{\partial p_l} \frac{\partial X}{\partial p_k} V_i + U_i^T \frac{\partial^2 X}{\partial p_k \partial p_l} V_i + U_i^T \frac{\partial X}{\partial p_k} \frac{\partial V_i}{\partial p_l} \quad (11)$$

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. These have been developed in previous work by the author and will be discussed later in this paper.

B. Approach 2: Sensitivity Analysis 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:

$$X = X(\mathbf{p}) = U \Sigma V^T$$

Now, let's begin the development of the second method in the time domain which is selective and computationally economical. A correlation matrix can be 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:

$$\begin{aligned} R_U &= X X^T \\ &= U \Sigma V^T V \Sigma U^T \\ &= U \Sigma^2 U^T \end{aligned} \quad (12)$$

and

$$\begin{aligned} R_V &= X^T X \\ &= V \Sigma U^T U \Sigma V^T \\ &= V \Sigma^2 V^T \end{aligned} \quad (13)$$

Note that with U and V being orthonormal, the inner products for each case (both Equation 12 and Equation 13) equal an identity matrix, thus the correlation matrices depend on only the left or right singular vectors after simplification.

Eigen analysis of these correlation matrices provides another way to compute the left and right singular vectors and the singular values: 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_V are the square of the singular values of X and the eigenvectors of R_V are the right singular vectors of X .

Eigen analysis thus provides an alternate method for computing the principal components in the time domain as well as their sensitivities. This approach is particularly economical when only the left singular vectors are to be computed. In this case, the length of the state vector is typically much smaller than the number of snapshots; therefore, the associated correlation matrix becomes compact. Again, these forms are particularly useful when one is only concerned with computing the left or right singular vectors, or perhaps only a few of them.

In this section, our focus is on presenting an alternative method for computing the sensitivities of the principal components using eigen analysis methods. Toward that end, consider a general case applicable to solving the eigen problem for either R_U or R_V . Additionally, at the outset we can identify both matrices as symmetric due to the manner in which they are constructed, thus the solution of the eigen problem and the solution for the sensitivities can be simplified and improved, where applicable, using this property.

In this development, we summarize only the key points of the developments in References 8 and 9, which provide general methods for computing the sensitivities of eigenvalues and eigenvectors. Consider the following where λ_i is the i th eigenvalue and ϕ_i is the i th eigenvector of the matrix A , which symbolically represents R_U or R_V .

$$[A - \lambda_i I] \phi_i = 0 \quad (14)$$

Here, of course, A is a function of some parameters, and the eigenvalue derivative is given by [9]:

$$\frac{\partial \lambda_i}{\partial p_k} = \phi_i^T \left[\frac{\partial A}{\partial p_k} \right] \phi_i \quad (15)$$

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:

$$\begin{aligned} \frac{\partial \sigma_i}{\partial p_k} &= \frac{\frac{\partial \lambda_i}{\partial p_k}}{2\sqrt{\lambda_i}} \\ &= \frac{1}{2\sqrt{\lambda_i}} \left\{ \phi_i^T \left[\frac{\partial A}{\partial p_k} \right] \phi_i \right\} \end{aligned} \quad (16)$$

The eigenvector derivative takes a bit more work to compute, although it is fairly straightforward. First, consider solving the following equation for v_{ik}

$$D_i v_{ik} = b_{ik} \quad (17)$$

where D_i and b_{ik} are given by:

$$D_i = [A - \lambda_i I] \quad (18)$$

$$b_{ik} = \frac{\partial \lambda_i}{\partial p} [I] \phi_i - \left[\frac{\partial A}{\partial p} \right] \phi_i \quad (19)$$

D_i is rank deficient as pointed out in Nelson's solution [8], and the following is proposed to overcome this issue in order to solve (17). The basic idea is to determine the index of the element of highest magnitude in the eigenvector ϕ_i . Then, zero out the corresponding row and the corresponding column of D_i with the exception of the corresponding diagonal entry which is set to one. The corresponding element in b_{ik} is also set to zero. Then, we solve for the vector v_{ik} in Equation 17 based on the modified matrix D_i and the modified vector b_{ik} .

The eigenvector, and this case equivalently the singular vector derivative, is given by

$$\frac{\partial \phi_i}{\partial p_k} = v_{ik} + c_{ik} \phi_i \quad (20)$$

where

$$c_{ik} = -\phi_i^T S v_{ik} - \frac{1}{2} \phi_i^T \frac{\partial S}{\partial p_k} \phi_i \quad (21)$$

S is the eigenvector scaling matrix defined by

$$\phi_i^T S \phi_i = I \quad (22)$$

In some cases, the algorithm used to compute the eigenvectors will result in normalized eigenvectors such that S is an identity matrix. Of course, $\frac{\partial S}{\partial p_k}$ is zero if, for the most common cases, S is constant or independent of p_k .

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

$$\begin{aligned} \frac{\partial R_U}{\partial p_k} &= \frac{\partial}{\partial p_k} (X X^T) \\ &= \frac{\partial X}{\partial p_k} X^T + X \frac{\partial X^T}{\partial p_k} \end{aligned} \quad (23)$$

and when A represents R_V ,

$$\begin{aligned} \frac{\partial R_V}{\partial p_k} &= \frac{\partial}{\partial p_k} (X^T X) \\ &= \frac{\partial X^T}{\partial p_k} X + X^T \frac{\partial X}{\partial p_k} \end{aligned} \quad (24)$$

Here, once again the partials of the snapshot matrix will be 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 for dynamical systems. State transition matrix calculations are addressed in the following section.

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

For the time domain methods, we identify the partial derivative of the snapshot matrix as a state transition matrix from dynamical systems analysis [12]. This matrix is needed in both methods of computing the PCA sensitivities, whether it be the general SVD form or the economical correlation matrix form. In this section we discuss methods for computing 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 to a set of differential equations due to changes in system initial conditions, in general. Let's consider the 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

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}, \mathbf{p}, t); \quad \mathbf{z}(t_0) = \mathbf{z}_0 \quad (25)$$

where in Equation 25 we see that the dynamical system is in general a nonlinear function of the states of the system and system parameters \mathbf{p} . Equation 25 represents 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, $\mathbf{z}(t_0)$. 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 arrive at the following set of augmented differential equations:

$$\begin{aligned} \dot{\mathbf{x}} = \begin{bmatrix} \dot{\mathbf{z}} \\ \dot{\mathbf{p}} \end{bmatrix} &= \begin{bmatrix} \mathbf{f}(\mathbf{z}, \mathbf{p}, t) \\ \mathbf{g}(\mathbf{z}, \mathbf{p}, t) \end{bmatrix}; \quad \mathbf{x}(t_0) = \mathbf{x}_0 \\ &= \mathbf{h}(\mathbf{z}, \mathbf{p}, t) \end{aligned} \quad (26)$$

where the augmented state is defined as

$$\mathbf{x} = \begin{bmatrix} \mathbf{z} \\ \mathbf{p} \end{bmatrix}$$

Here we have assumed a general form for the differential equations for the parameter vector. For the likely case of constant parameters, $\mathbf{g}(\mathbf{z}, \mathbf{p}, t)$ will, of course, equal a zero-valued vector.

We now summarize the development of the state transition matrix differential equation. In integral form, the solution to Equation 26 is

$$\mathbf{x}(t) = \mathbf{x}(t_0) + \int_{t_0}^t \mathbf{h}(\mathbf{x}, \tau) d\tau \quad (27)$$

And, upon differentiating (27) with respect to $\mathbf{x}(t_0)$ we arrive at the following expression:

$$\frac{\partial \mathbf{x}(t)}{\partial \mathbf{x}(t_0)} = \mathbf{I} + \int_{t_0}^t \left(\frac{\partial \mathbf{h}(\mathbf{x}, \tau)}{\partial \mathbf{x}(\tau)} \frac{\partial \mathbf{x}(\tau)}{\partial \mathbf{x}(t_0)} \right) d\tau \quad (28)$$

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 (28) can be re-written as:

$$\Phi(t, t_0) = \mathbf{I} + \int_{t_0}^t \left(\frac{\partial \mathbf{h}(\mathbf{x}, \tau)}{\partial \mathbf{x}(\tau)} \Phi(\tau, t_0) \right) d\tau \quad (29)$$

Now, we take the time derivative of (29) 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:

$$\dot{\Phi}(t, t_0) = \frac{\partial \mathbf{h}(\mathbf{x}, t)}{\partial \mathbf{x}(t)} \Phi(t, t_0); \quad \Phi(t_0, t_0) = I \quad (30)$$

where $\Phi(t, t_0)$, again, is our notation for the state transition matrix.

For the special case of a linear system, which is typically the case in structural dynamics, Equation 30 becomes:

$$\dot{\Phi}(t, t_0) = \mathbf{A}\Phi(t, t_0); \quad \Phi(t_0, t_0) = I \quad (31)$$

\mathbf{A} is the “state matrix”. Analytical solutions exist for this special case including the condition that the state matrix is constant. For example, the matrix exponential solution is given by:

$$\Phi(t, t_0) = e^{\mathbf{A}(t-t_0)} \quad (32)$$

For the general nonlinear case, one must solve Equations 26 and 30 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 reviewed in this section. Differential equations for the second- and higher-order state transition matrices were developed in Reference 13, and can be used to implement the higher-order methods developed in this work.

III. Methodology Extended to the Frequency Domain

We now consider sensitivity analysis applied to PCA in the frequency domain. One frequency domain method for computing the principal components is the so-called Frequency Domain Decomposition. As described in Reference 14, the Singular Value Decomposition (SVD) method was applied to power spectral density (PSD) functions of the response to identify modes of output-only systems. Here, we consider a similar approach; however, it is applied to frequency response functions (FRFs).

Let’s begin by considering the following definition of a FRF matrix written in terms of the system matrices:

$$H_{ij}(\omega, \mathbf{p}) = \left[-\omega^2 \mathbf{M}(\mathbf{p}) + j\omega \mathbf{C}(\mathbf{p}) + \mathbf{K}(\mathbf{p}) \right]^{-1} \quad (33)$$

Here, i represents the response degree of freedom and j represents the input degree of freedom; and ω represents the frequency lines. From Equation 33, we can compute FRFs 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 \mathbf{p} .

To begin the development of the sensitivity analysis, we take the derivative of Equation 33 with respect to one parameter p_k , where the dependence of the system matrices on the parameters \mathbf{p} is assumed notationally:

$$\begin{aligned} \frac{\partial H_{ij}}{\partial p_k} &= -H_{ij}(\omega, \mathbf{p}) \frac{\partial \left[-\omega^2 \mathbf{M} + j\omega \mathbf{C} + \mathbf{K} \right]}{\partial p_k} H_{ij}(\omega, \mathbf{p}) \\ &= H_{ij}(\omega, \mathbf{p}) \left[\omega^2 \frac{\partial \mathbf{M}}{\partial p_k} - j\omega \frac{\partial \mathbf{C}}{\partial p_k} - \frac{\partial \mathbf{K}}{\partial p_k} \right] H_{ij}(\omega, \mathbf{p}) \end{aligned} \quad (34)$$

Using Equation 34, one can compute the derivatives of the FRF matrix needed for the PCA sensitivity analysis 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 Equation 33:

$$H_{is}(\omega) = \begin{pmatrix} h_1(\omega_1) & \dots & h_1(\omega_m) \\ \vdots & \ddots & \vdots \\ h_n(\omega_1) & \dots & h_n(\omega_m) \end{pmatrix} \quad (35)$$

Note that Equation 35 is the frequency domain analog of Equation 1. The rows of (35) represent the response degrees of freedom while the columns of (35) are “snapshots” of the FRFs at different frequency lines.

As with the time domain analog, we can consider this FRF matrix to be a function of some parameters, and consider computation of its principal components using the SVD:

$$H_{is}(\omega, \mathbf{p}) = \Psi \Theta \Omega^T \quad (36)$$

where Ψ 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). Here, we see that in a fashion similar to the time domain analog, PCA as indicated in (36) results in separation of spatial and frequency dependent information.

The sensitivities of the principal components described by (36) can also be computed using the formulas developed earlier. For example, using the SVD method, the singular value sensitivities are computed from Equations 5 and 11; and the left and right singular vectors sensitivities are computed from Equations 7 through 10. First, one computes the SVD of the matrix of FRFs in Equation 35 for the set of responses and the chosen input location. Then, the partial derivatives of Equation 35 are determined using Equation 34. For a particular input, only a subset of the derivatives in 34 is needed. Keep in mind that the system matrices are implicitly assumed to be a function of the parameter vector in Equation 34.

Alternatively, one can consider assembling a data matrix of PSDs as is done in Reference 14. There appears to be no reason why this sensitivity analysis could not also be applied to PSDs 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.

IV. Verification of the Methods for Calculating PCA Sensitivities

A. Time Domain Methodology Verification

Both 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.

The equations of motion are given simply by:

$$\begin{aligned} \ddot{x} &= 0 \\ \ddot{y} &= 0 \\ \ddot{z} &= -g \end{aligned} \quad (37)$$

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

$$\begin{aligned}
x(t) &= x_0 + \dot{x}_0(t-t_0) \\
y(t) &= y_0 + \dot{y}_0(t-t_0) \\
z(t) &= z_0 + \dot{z}_0(t-t_0) - \frac{1}{2}g(t-t_0)^2
\end{aligned} \tag{38}$$

Furthermore, in order to also consider sensitivity to the gravity constant, we may write a parameter differential equation:

$$\dot{g} = 0 \tag{39}$$

and proceed to form an augmented system such as we do in Equation 26. In matrix form, we can write the analytical expression for the solution to Equation 37, where the first three rows are a restatement of Equation 38, the next three rows describe the velocity solution, and the final row states that the state defining the gravity parameter is a constant:

$$\begin{bmatrix} x(t) \\ y(t) \\ z(t) \\ \dot{x}(t) \\ \dot{y}(t) \\ \dot{z}(t) \\ g \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & (t-t_0) & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & (t-t_0) & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & (t-t_0) & -\frac{1}{2}(t-t_0)^2 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -(t-t_0) \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x(t_0) \\ y(t_0) \\ z(t_0) \\ \dot{x}(t_0) \\ \dot{y}(t_0) \\ \dot{z}(t_0) \\ g \end{bmatrix} \tag{40}$$

$$z(t) = \Phi(t, t_0)z(t_0)$$

The 7x7 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. Equation 40 illustrates augmentation of state motion variables with system parameters as is accomplished in Equation 26.

Analytical sensitivity calculations for the time domain methods are verified using the following approach. The state transition matrix in Equation 40 is computed for times from 0 to 4 seconds with a time interval of 0.1 seconds. The initial conditions for the problem are utilized along with the state transition matrix calculations to compute the full 7 dimension state vector at each instant in time. The selected initial conditions are $[x(t_0); y(t_0); z(t_0)] = [1.0; 2.0; 3.0]$ meters and $[\dot{x}(t_0); \dot{y}(t_0); \dot{z}(t_0)] = [20.0; 20.0; 20.0]$ meters/second. The gravitational parameter is constant with a value of 9.81 meters/second². 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 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 two methods developed for the time domain, and when compared to forward finite difference calculations show that these methods accurately compute the desired partials. The finite difference calculations were performed with a precision of 6 significant figures.

A selection of these verification results are given in Table 1. For example, the partial derivative of the first principal component left singular vector, 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 eigen analysis 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 principal 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 are verified. Note that due to the dimension of the right singular vector, only the 2-norm value is provided.

Table 1. Verification of Analytical PCA Sensitivity Calculations: Time Domain

	Numerical (finite difference)	Analytical SVD method	Analytical Correlation Method
$\partial U_1 / \partial g$	-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
$ \partial V_1 / \partial x_0 $	0.004495183	0.004495183	0.004495183
$ \partial V_1 / \partial \dot{x}_0 $	0.001862972	0.001862972	0.001862972
$ \partial V_1 / \partial g $	0.003680486	0.003680485	0.003680485

We note one advantage of the analytical approach over finite difference methods. All desired partials are computed at once using these analytical methods. 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 7 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 requires only one solution of the differential equations, although the state transition matrix must either be computed analytically or its differential equations must also be solved.

B. Frequency Domain Methodology Verification

In order to verify the method for sensitivity analysis of PCA in the frequency domain, we consider a linear structural dynamics problem of a spring-mass-damper system with 20 degrees of freedom. The system is composed of 20 masses and 20 spring elements with a fixed boundary condition on the free node of the first spring. The mass and stiffness matrices are formed for the case of each mass having a value of 1 kg and each spring having a spring constant of 50 N/m. The damping matrix is chosen to be 0.01 times the mass matrix, which provides about 0.9% critical damping at the first natural frequency with diminishing magnitude as frequency increases. Frequency lines are selected from 0 to 2 rad/sec in intervals of 0.005 rad/sec. With the system matrices and the chosen frequency range, the FRF matrix is computing using Equation 33 for a single input at the location of the 20th mass degree of freedom. To illustrate the analytical sensitivity calculations, the partials of the system matrices with respect to system parameters (required for Equation 34) are selected such that $\partial M / \partial p_k$ and $\partial C / \partial p_k$ equal zero and $\partial K / \partial p_k = \partial K / \partial k_7$. In other words, we desire partial derivatives of the principal components with

respect to the value of the 7th spring constant. In Table 2, we list the first three singular value sensitivities. The comparison of the analytical results and numerical finite difference calculations demonstrate the accuracy of the analytical approach.

Table 2. Verification of Analytical PCA Sensitivity Calculations: Frequency Domain

	Numerical Finite Difference	Analytical Frequency Domain
$\partial\theta_1/\partial k_7$	-0.144613	-0.144614
$\partial\theta_2/\partial k_7$	-0.004412	-0.004411
$\partial\theta_3/\partial k_7$	-0.000838404	-0.000838407

In Figure 2, we plot the sensitivity of the first principal component left singular vector with respect to the spring constant of the 7th spring by three methods including a numerical finite difference calculation, an analytical calculation by the method developed in this paper, and one using a previously published method. The analytical result is compared with the numerical finite difference calculation to indicate the accuracy of the analytical method. The derivative of the eigenvector corresponding to the lowest frequency mode of this system is also calculated using the method of Reference 9. The intent here is to show that when there is equivalence between a left singular vector and an eigenvector, or to put it another way, when a principal component corresponds to a mode of the system, the derivative of the left singular vector is also equivalent to the derivative of the corresponding eigenvector. The plot shows that the analytical sensitivity of the principal left singular vector and the eigenvector derivative are equal. Thus, the method developed in this paper provides a new method to compute eigenvector derivatives of second-order mechanical systems. However, the method developed here also works in general for other applications of PCA beyond structural dynamics applications.

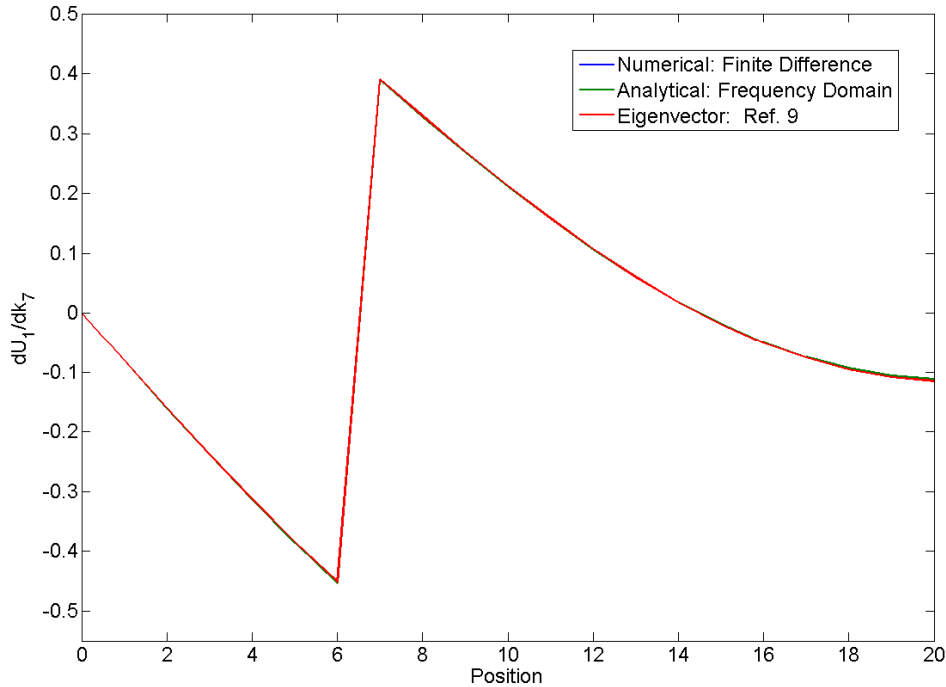


Figure 2. Comparison of First Principal Component Left Singular Vector Sensitivities

Sensitivities of the right singular vectors have also been computed analytically and compared with numerical finite difference calculations. It has been found for this example, that the analytically computed right singular vector

sensitivities are somewhat noisy between resonant peaks. Otherwise, the calculations agree quite accurate near the peaks of the analytically computed vectors and near the peaks of finite difference calculations.

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 -- two approaches were developed for the time domain and one approach was developed for the frequency domain. These analytical methods were verified by numerical finite difference calculations. These results demonstrate promise for the use of analytical principal components sensitivities in the broad application space in which PCA is utilized. For example, these sensitivities can be used in gradient-based optimization algorithms or for error estimation. Specifically for structural dynamics applications, these results indicate that the time and frequency domain methods provide new means for computing the derivatives of the eigenvectors of second-order mechanical systems. Perhaps an even more promising result lies with one benefit of PCA in that it does not suffer from the limited applicability of traditional linear analysis methods. Additionally, 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. Future work includes application of these methods to problems in structural dynamics.

VI. References

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