Sensitivity based Proper Orthogonal Decomposition for Nonlinear Parameter Dependent Systems*

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tAbstract—Parameter dependent systems are found in many complex coupled systems. When applying optimization techniques, using full order models for the solution of parameter dependent systems may simply be intractable. Therefore we investigate methods for generating reduced order models that can be applied to nonlinear parameter dependent systems. The development of these reduced order models is made possible by sensitivity analysis of the basis functions. We also introduce a new method using piecewise cubic Hermite interpolating polynomials of the basis functions.

I. INTRODUCTION

In many realistic applications we are interested in the design or optimization of a system that will be used in a range of conditions governed by the parameters. Computing a solution for each set of parameter values may be prohibitively expensive in terms of time or resources. Therefore we are interested in the range of values for which a Reduced Order Model (ROM) can still provide an accurate result while using only a few full order solutions to generate the ROM.

Proper Orthogonal Decomposition (POD) also known as Karhunen-Loève Decomposition or Principal Component Analysis, is a widely used model reduction technique for optimization and control of fluid systems [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12]. Indicative of its applicability and performance, it has been independently rediscovered in many areas of research ranging from image processing to Computational Fluid Dynamics (CFD) [13]. Given data, POD extracts an orthonormal basis that is optimal to represent the data in a mean squared error sense. In the context of model reduction for dynamical systems the POD basis determines the subspace upon which model dynamics are projected on. The POD basis and consequently the subspace is determined by the data used to generate the basis. In many fluid dynamics models the Reynolds number $Re$ is the parameter that describes the balance of viscous and inertial forces of the fluid. When the Reynolds number is small, the flow has a stable steady solution, as the Reynolds number is increased the solution becomes unsteady. If the Reynolds number becomes large, the flow becomes turbulent and special methods are introduced to compute a numerical solution. Thus, the structure of the flow depends on the Reynolds number, and in general, the parameters of the system. We seek to understand how the basis depends on the parameters.

A. POD overview

The POD method is reviewed here since it will facilitate the development of the new material later. For a more thorough introduction see [14], [15], [16].

Let $X$ be a Hilbert space with inner product $(\cdot, \cdot)_X$ and induced norm given by $\|x\|_X = (x, x)^{1/2}$ for $x \in X$.

For an interval $I = (a, b)$, let $L^2(I; X)$ be the Hilbert space of functions $f$ such that for $t \in I$, $f(t) \in X$. Let the inner product on $L^2(I; X)$ be given as

$$
(f, g)_{L^2(I; X)} = \int_I f(t), g(t) \, dx,
$$

then the induced norm of $L^2(I; X)$ is given by

$$
\|f\|_{L^2(I; X)}^2 = (f, f)_{L^2(I; X)}.
$$

Let $I = (0, T)$ and $y \in L^2(I; X)$ be a given solution of a dynamical system. The POD problem is to find an orthonormal basis $\{\phi_i\}_{i=1}^r$ that satisfies the constrained optimization problem

$$
\min_{\{\phi_i\}_{i=1}^r} \|y - P_r y\|_{L^2(I; X)}^2 \\
\text{s.t. } (\phi_j, \phi_i)_X = \delta_{ij}, 1 \leq i, j \leq r
$$

where

$$
P_r y = \sum_{i=1}^r (y(t), \phi_i)_X \phi_i.
$$

By examining the necessary conditions for the existence of the solution of the optimization problem [15] we obtain the eigenvalue problem

$$
\mathcal{R} \phi_i = \lambda_i \phi_i
$$

II. POD FOR PARAMETER DEPENDENT SYSTEMS

As noted above the POD basis directly depends on the data used to generate the basis. In many fluid dynamics models the Reynolds number $Re$ is the parameter that describes the balance of viscous and inertial forces of the fluid. When the Reynolds number is small, the flow has a stable steady solution, as the Reynolds number is increased the solution becomes unsteady. If the Reynolds number becomes large, the flow becomes turbulent and special methods are introduced to compute a numerical solution. Thus, the structure of the flow depends on the Reynolds number, and in general, the parameters of the system. We seek to understand how the basis depends on the parameters.

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where \( R : X \rightarrow X \) is given by
\[
R \eta = \int I(v,y(t)) X y(t) \, dt. \tag{3}
\]
The operator \( R \) is called the continuous POD operator and is compact, self-adjoint and trace class [17]. Since \( R \) is self-adjoint and compact there exist orthonormal eigenvectors with corresponding eigenvalues that decay to zero [18]. Since \( R \) is trace class, the eigenvalues are also summable. Therefore the POD basis of rank \( r \) is defined to be the first \( r \) eigenvectors of the \( R \) operator.

In the case that the data contains solutions of the dynamical system at multiple parameter values the resulting POD basis is referred to as a Global POD (GPOD) basis. Here the basis is still optimal, but only to represent the whole data, not necessarily the solution resulting from a single parameter value. Hence, the GPOD approach can be used to generate a ROM valid for a range of parameters. However, the solution subspaces for any two parameters may be very different. Thus, the GPOD basis may contain vectors that are orthogonal to the solution for some parameter values for which the ROM is being evaluated. Furthermore, an accurate sampling of the parameter space may require many full order solutions to develop an appropriate GPOD basis. Finally, the resulting GPOD ROM may either provide only marginal dimension over the entire parameter range for a fixed dimension, or require the dimension of the reduced order model to be large to meet desired error tolerances across the parameter range of interest.

**B. POD Basis Sensitivity**

To avoid the problem described above, we seek to approximate the optimal basis for any single parameter. If this can be done the advantage is a fixed dimension reduced order model that is also a 'minimal' realization in the sense that the basis is not orthogonal to the solution at the parameter. To accomplish this we use the sensitivity of the basis vectors with respect to the parameter.

Let the solution to the dynamical system depend on a parameter \( q \in \mathbb{R} \), then for each \( t \in I \) and \( q \in \mathbb{R} \), \( y(t,q) \in L^2(X) \). The resulting POD basis also depends on the parameter and we are interested in how the basis will change as the parameter changes. To facilitate the analysis we redefine the continuous POD operator as \( R(q) : \mathbb{R} \rightarrow \mathcal{L}(X) \) given by
\[
[R(q)] \eta = \int_I (v,y(t,q)) X y(t,q) \, dt
\]
where \( \mathcal{L}(X) \) is the space of bounded linear operators on \( X \).

If we assume that the data and resulting operators depend smoothly on the parameter then the derivative of \( R(q) \) at \( \hat{q} \in \mathbb{R} \) in the direction of \( \eta \) is given by
\[
(R'(\hat{q}) \eta) = \eta \left( \int_I (v,y_q(t,\hat{q})) X y(t,\hat{q}) + (v,y(t,\hat{q})) X y_q(t,\hat{q}) \, dt \right).
\]

As is common in the case where the domain is one-dimensional, we abuse notation by writing the gradient in place of the differential in the direction of \( \eta \),
\[
[R_q(q)] = [R'(q) \eta] \big|_{\eta=1} \in \mathcal{L}(X)
\]
where \( [R_q(q)] \) is given by
\[
[R_q(q)] \eta = \int_I (v,y_q(t,q)) X y(t,q) + (v,y(t,q)) X y_q(t,q) \, dt.
\]

and the term \( y_q(\cdot,q) \) is the derivative of the data with respect to the parameter. This can be found by solving the continuous sensitivity equation that corresponds to the dynamical system [19].

From (2) for each \( i = 1, ..., r \), \( \phi_i(q) \) solves the eigenvalue problem given by
\[
R(q) \phi_i(q) = \lambda_i(q) \phi_i(q).
\]

Differentiating the eigenvalue problem with respect to the parameter yields
\[
(R(q) - \lambda_i(q)) \phi_{i,q}(q) = (-R(q) + \lambda_{i,q}(q)) \phi_i(q).
\]

Taking the inner product of both sides with \( \phi_i(q) \) we have
\[
\left((R(q) - \lambda_i(q)) \phi_{i,q}(q), \phi_{i,q}(q)\right)_X
= \left(\phi_i(q), (-R(q) + \lambda_{i,q}(q)) \phi_i(q)\right)_X
\]
where the self-adjoint property of \( R(q) - \lambda_i(q) \) has been used. On the left hand side, \( \phi_i(q) \) is the eigenvector that satisfies the eigenvalue problem, hence the equation reduces to
\[
\lambda_{i,q}(q) = \left(\phi_i(q), R(q) \phi_i(q)\right)_X.
\]

Since \( \phi_i(q) \) is in the null space of \( R(q) - \lambda_i(q) \) for any \( \alpha \in \mathbb{R} \), \( \psi = \alpha \phi_i(q) + \phi_{i,q}(q) \) is a solution to (4). To find a suitable solution recall the constraint of the POD problem was that the POD vectors should be orthonormal i.e.
\[
\left(\phi_i(q), \phi_j(q)\right)_X = \delta_{ij}.
\]

Differentiating this condition respect to the parameter, for \( j = i \) yields
\[
\left(\phi_{i,q}(q), \phi_i(q)\right)_X + \left(\phi_i(q), \phi_{i,q}(q)\right)_X = 0.
\]

Due to the symmetric nature of the inner product, the proper choice for the \( \phi_{i,q}(q) \) should be orthogonal to \( \phi_i(q) \). To achieve this, the least squares solution is found and then orthogonalized against \( \phi_i(q) \).

**C. Sensitivity based POD ROMs**

The sensitivity of the POD basis functions can be used to estimate the optimal POD basis as the parameter changes. This has the obvious benefits of keeping the reduced order model dimension low. There are several methods to estimate the optimal basis for new parameter from an existing basis and sensitivities. The methods covered include extrapolation, interpolation and expansion of the basis.
1) Extrapolation: Given a single POD basis and respective sensitivities the optimal POD basis can be estimated using a first order Taylor series expansion of the basis functions. Therefore for a nominal parameter \( \tilde{q} \in \mathbb{R} \), the optimal POD basis functions can be written as
\[
\phi_i(q) = \phi_i(\tilde{q}) + \phi_{i,q}(\tilde{q}) (q - \tilde{q}) + \text{HOT}.
\]
Using the first order approximation we can then estimate \( \phi_i(q) \approx \phi_i(\tilde{q}) + \phi_{i,q}(\tilde{q}) (q - \tilde{q}) \). This approximation is valid when \( q \) is in a local neighborhood of \( \tilde{q} \) where the higher order terms can be neglected.

2) Interpolation: Given a POD basis and respective sensitivities for several points in the parameter space, the optimal POD basis can be estimated by interpolating the known optimal bases and respective sensitivities. Here we use a Piecewise Cubic Hermite Polynomial. Given a set of parameter sample points, \( q_1,...,q_n \in \mathbb{R} \) where the POD basis functions \( \phi_i(q_j) \) and respective sensitivities \( \phi_{i,q}(q_j) \) are known for each \( j = 1,...,n \). We construct the piecewise cubic Hermite interpolating polynomial \( H_i(q) \) of the basis functions \( \phi_i(q) \) that satisfies for all \( i = 1,...,r, j = 1,...,n \)
\[
H_i(q) = \begin{cases} 
H_i(q_j) &= \phi_i(q_j) \\
H_{i,q}(q_j) &= \phi_{i,q}(q_j). 
\end{cases}
\]

Care should be exercised when interpolating bases. The interpolation methods here interplate between the vectors of the POD bases by index. Since the basis vectors are ranked according to their POD energy which depends on the parameters, in different regimes similar vectors can have different rankings within their respective basis. Additionally, the solution of the eigenvalue problem (2) is not unique in the sense that multiple vectors associated with the same eigenvalue may come in any order. Moreover, the negative of an eigenvector is also an eigenvector. To overcome the ambiguity, a congruence transformation is used [20]. The congruence transformation problem seeks to find a common coordinate system in which to represent the bases. When the parameters affect the domain, or the parameter space has higher dimension manifold interpolation techniques can be used to appropriately interpolate between bases. [21].

3) Expansion: By construction, the POD basis sensitivity functions are orthogonal to the corresponding basis functions and therefore span different subspaces. In the basis extrapolation method for a nearby parameter, a precise linear combination of the nominal POD basis functions and sensitivities are used to estimate the optimal POD basis according to the Taylor series expansion. In the expanded basis approach the POD basis dimension is increased by inclusion of the sensitivity functions. Then any linear combination of the nominal POD basis and respective sensitivity vectors can be used to approximate the optimal basis. For the nominal parameter the overall performance increase from doubling the basis may be minimal, since even though the POD basis and sensitivity vectors are orthogonal, the sensitivity vectors may not be ‘next’ set of POD basis functions. However the expanded POD basis performance should be better than the extrapolated basis method for off nominal parameters since it allows for any linear combination of the basis and sensitivity vectors to estimate the optimal POD basis.

### III. Numerical Experiments

In this section the POD model reduction techniques are applied to 1D Burgers’ equation which is given by
\[
u_t(t,x,q) + u(t,x,q)u_x(t,x,q) - qu_{xx}(t,x,q) = 0
\]
for \( x \in (0,1) \), \( t > 0 \), with homogeneous Dirichlet boundary conditions
\[
u(t,0,q) = 0 = u(t,1,q)
\]
and initial condition given by
\[
u(0,x,q) = u_0(x,q) \in L^2(0,1).
\]
Here the parameter represents the viscosity of the fluid and in a normalized setting we have \( q = 1/Re \), where \( Re \) plays the role of the non-dimensional Reynolds number.

Using the finite element method the PDE is discretized into an ODE system of the form
\[
M\dot{u}(t,q) + C(u(t,q))u(t,q) + qKu(t,q) = 0
\]
where \( M \) is the mass matrix, \( K \) is the stiffness matrix and \( C \) is the nonlinear convective matrix. The system of nonlinear ODEs is then solved using a trapezoidal time stepping method with Picard iteration.

To obtain the solution sensitivity with respect to the parameter we differentiate the Burgers’ equation with respect to the parameter to obtain the sensitivity equation. Using \( s(t,x,q) = u_q(t,x,q) \) the sensitivity equation is given by
\[
s_t(t,x,q) + s(t,x,q)u_x(t,x,q) + u(t,x,q)s_x(t,x,q)
\]
\[
- u_{xx}(t,x,q) - qu_{xx}(t,x,q) = 0
\]
for \( x \in (0,1) \), \( t > 0 \) with homogeneous Dirichlet boundary conditions
\[
s(t,0,q) = 0 = s(t,1,q)
\]
and initial condition given by
\[
s(0,x,q) = \frac{\partial}{\partial q}u_0(x,q) \in L^2(0,1).
\]
We note that the sensitivity equation uses the same bilinear and trilinear forms as the weak form of Burgers’ equation [22]. However, in this case the PDE is linear in \( s(t,x,q) \).

Using the finite element method the sensitivity ODE system is given as
\[
M\dot{s}(t,q) + \left(C(u(t,q)) + \tilde{C}(u(t,q))\right)s(t,q)
\]
\[
+ Ku(t,q) + qKs(t,q) = 0.
\]
Here \( \tilde{C}(u(t,q)) \) represents the weak derivative of the convection term and is used in the Newton iteration step for Burgers’ equation.

Solving the sensitivity equation as above provides an efficient approach with very little additional computational cost. Usually the matrices required for the sensitivity equation are built as part of a Newton method stepping solution to
the nonlinear equation, thus the sensitivity solution requires only a single extra linear solve per time step. In the case of existing software that cannot be easily modified, Automatic Differentiation (AD) programs can provide a non-intrusive method to obtain the solution sensitivity. One code that has been tested in this application is AD Deriv [23]. The results using AD Deriv agree very well with the sensitivity equation implementation. Furthermore, coupling the solution and solution sensitivity using AD Deriv provides a robust method to compute the POD basis and corresponding sensitivities concurrently using existing code for computing the POD basis.

The reduced order models are now tested for a variety of bases. First, a fixed basis is used where an optimal POD basis is computed for a single nominal parameter \( \hat{q} \). Next, the extrapolation and interpolation methods are used to obtain an estimate of the optimal POD basis at the new parameters. Finally, we compare the error against the optimal POD error estimate for a basis generated solely from data at the tested parameter.

The models are solved using \( N = 1024 \) elements on the time interval of \([0, 1]\) with a time step of \( \Delta t = 0.0005 \) and no forcing. The initial condition for all models is

\[
\bar{u}_0(x) = \begin{cases} 
\sin(4\pi x) & 0 \leq x \leq \frac{1}{4} \\
0 & x > \frac{1}{4}.
\end{cases}
\]

The nominal parameter is chosen to be \( \nu = 1/100 \), and the parameter range is chosen such that the endpoints of the parameter range represent a 30% difference from the nominal parameter. This equates to a parameter range of \( \nu \in [1/142.86, 1/76.92] \). Two sets for results are shown below, in each set we show the results for \( r = 6 \), \( r = 10 \) and \( r = 16 \).

In Figures 1, 2 and 3, a single full order solution is used to generate the POD basis and sensitivities for the fixed, extrapolated and expanded bases. The nominal parameter for the fixed basis and extrapolation method is \( \hat{q} = 1/100 \). Here, the expanded basis has \( r/2 \) POD basis vectors with their corresponding sensitivity vectors so that the fixed dimension of the ROM is \( r \).

In Figures 4, 5 and 6, three full order solutions are used to generate the POD basis and sensitivities for the GPOD, Linear Interpolation (LI) and Piecewise Cubic Hermite Interpolating Polynomial (PCHIP) method. The parameter points used are \( \nu \in \{1/142.86, 1/100, 1/76.92\} \). The resulting relative errors for each case are compared to the optimal POD errors.

In the first set of figures, the results show that fixed basis is indeed optimal for the nominal parameter, however as the ROM is evaluated at parameters that are not near the nominal parameter the error increases greatly, up to two full orders of magnitude in the case of \( r = 16 \). Similarly, the extrapolation technique which estimates the optimal POD basis using the POD basis and corresponding sensitivities at the nominal parameter is able to extend the region for which the basis is valid. However, eventually this basis may also no longer be accurate away from the nominal parameter. Next, we see that the expanded basis approach provides a basis that is not optimal for the nominal parameter but can provide more performance in other parts of the parameter range.
it is seen that since that linear and Hermite interpolation methods do not match the optimal basis at the parameter test points, and can provide a better approximation than the GPOD method over the interpolation intervals. In addition, the PCHIP method which uses the sensitivity of the basis functions provides more performance overall than the linear interpolation and provides optimal or near optimal performance for nearby parameters.

IV. CONCLUSIONS

In this paper we have demonstrated how to use the sensitivities of the POD basis to improve the standard POD methods. Specifically, using the extrapolation approach the optimal POD basis is estimated by a first order approximation. Next, the PCHIP POD was introduced by combining the optimal basis and corresponding sensitivities using a piecewise cubic Hermite interpolation. By incorporating the sensitivity information this provided better performance over the parameter range than a standard linear interpolation of the basis. We remark here that the cost of generating the sensitivity information in with the full order solutions is small since the sensitivity equation is linear and has the same structure as the full order equations and thereby can be solved efficiently with the full order solution.

REFERENCES


