Postprint: Design of a Reduced-Order Computational Model for Inverse Problems Based on POD Technology

Authors: Sun Xianhang, Minghai Xu, Jin Shaoyong, Yang Laishun

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Abstract

A reduced-order computational model for inverse problems in engineering is designed based on POD (Proper Orthogonal Decomposition) technology. Using limited collected output results, the model can be solved with only simple nonlinear programming and interpolation methods, substantially reducing both the solution difficulty and computational time for inverse problems in engineering. As the model solution process does not involve the governing equations of the original physical problem, the model exhibits certain universality in practical applications. With forced convective heat transfer in a circular tube as an application example, results demonstrate that based on temperature data measured by several thermocouples, the reduced-order inverse problem computational model can accurately retrieve the unknown fluid inlet temperature and heat flux density on the outer wall of the circular tube, differing from the true values by only approximately 1.0%. Moreover, compared with the classical conjugate gradient method, the reduced-order inverse problem computational model can achieve a computational speedup of over 1200 times.

Full Text

Design of Reduced-Order Computational Model for Inverse Problems Using POD Technology

SUN Xian-Hang, XU Ming-Hai, JIN Shao-Yong, YANG Lai-Shun College of Pipeline and Civil Engineering, China University of Petroleum, Qingdao 266580, China*

Abstract: This paper proposes a reduced-order computational model for inverse problems based on Proper Orthogonal Decomposition (POD). By utilizing limited output data collected in advance, the model can be solved using only simple nonlinear programming and interpolation methods, which substantially reduces both the difficulty and computational time for solving inverse problems in engineering applications. Since the solution process does not involve the governing equations of the original physical problem, the model possesses a certain degree of universality in practice. Using forced convection heat transfer in a circular pipe as an application example, the results demonstrate that the reduced-order inverse problem computational model can accurately determine the unknown fluid inlet temperature and wall heat flux based on temperature data measured by thermocouples, with errors of only about 1.0% compared to the true values. Moreover, the computational speed can be improved by more than 1200 times compared to the classical conjugate gradient method.

Keywords: inverse problem; Proper Orthogonal Decomposition; computational model; forced convection heat transfer in a circular pipe

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Author Introduction: SUN Xian-Hang (1987-), male, Ph.D. candidate, engaged in research on optimal control and inverse problems of fluid flow and heat transfer.

Corresponding Author: YANG Lai-Shun, Ph.D. candidate, Email: sxh19871124@163.com

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Inverse problems in engineering, also known as ill-posed problems, fundamentally aim to determine unknown model parameters based on partial information from output results. The emergence of inverse problems stems from practical engineering needs, particularly in situations where direct measurement of desired parameters is difficult due to various constraints. Examples include predicting material properties, rock properties in oil reservoirs, damage detection in structural engineering, and monitoring boundary temperatures or heat fluxes in heat transfer problems. Among the various methods for solving inverse problems, the conjugate gradient method [?] is the most widely used. This method requires calculating the derivative of the objective function with respect to the parameters to be determined (known as sensitivity coefficients) and gradually approaches the solution by leveraging these sensitivity coefficients. However, since the conjugate gradient method requires solving the governing equations of the original problem repeatedly to obtain sensitivity coefficients, it consumes substantial computational time and storage space, making it unsuitable for applications requiring real-time prediction of unknown parameters. Furthermore, many engineering problems are governed by extremely complex systems of nonlinear partial differential equations, making it difficult or even impossible to solve for sensitivity coefficients.

Proper Orthogonal Decomposition (POD) [?] is a technique that extracts a set of orthogonal basis functions dependent only on spatial variables from known physical field samples (obtained through numerical simulation or experiments) corresponding to several parameters (control parameters or physical properties). These basis functions represent the dynamic characteristics of the original physical system. When combined with the Galerkin projection method [?], POD can achieve reduction of the governing equations of the original physical system, i.e., establish a reduced-order model. Here, "order" refers to the number of variables to be solved at each time step. Such reduced-order models can rapidly compute the physical field corresponding to any parameter within the variable range. This represents the mainstream reduced-order method using POD as the reduction tool and is its most typical application. Through this approach, POD has been successfully applied in many scientific and engineering fields, including signal analysis [?], fluid flow and heat transfer [?], structural dynamics [?], optimal control [?], and inverse problems [?]. For inverse problems, references [?] and [?] introduced reduced-order models into inverse problems of laminar convection heat transfer in circular pipes and saturated groundwater flow, respectively. The main solution method remained the conjugate gradient method, with POD serving to reduce the order of the governing equations that needed to be solved during each sensitivity coefficient calculation, thereby reducing computational time. Although the final computational time was reduced by dozens of times, this still belongs to the mainstream reduction category, where POD' s role in reducing computational time is only realized in the step of solving the governing equations, and its implementation difficulty increases with the complexity of the governing equations. For instance, the reduced-order model in reference [?] is only applicable to laminar flow and cannot handle turbulent flow.

In view of the aforementioned issues, this paper employs an alternative POD-based approach, namely POD interpolation, to design a new computational model for inverse problems—the reduced-order inverse problem computational model. Using forced convection heat transfer in a circular pipe as an application example, the accuracy and computational efficiency of this method are examined.

1. Introduction to POD Technology

Let $\mathbf{w}$ represent the parameter vector, where N is the number of vector components, and $\theta(\mathbf{x}, \mathbf{w})$ represents a state parameter sample at steady state under parameter $\mathbf{w}$, where $\mathbf{x}$ represents spatial variables. A set of orthogonal basis functions $\phi_m(\mathbf{x})$ dependent only on spatial variables can be extracted from N state parameter samples corresponding to parameters $\mathbf{w}_n$ $(n = 1, 2, \cdots, N)$. After obtaining these basis functions, the state parameter $\theta(\mathbf{x}, \mathbf{w})$ can be reconstructed through:

$$\theta(\mathbf{x}, \mathbf{w}) \approx \sum_{m=1}^{M} \alpha_m(\mathbf{w}) \phi_m(\mathbf{x}) \quad (1)$$

where M is the truncation order, i.e., the number of basis functions employed; $\alpha_m(\mathbf{w})$ are coefficients corresponding to each basis function, representing the contribution of the m-th POD basis function $\phi_m(\mathbf{x})$ to reconstructing $\theta(\mathbf{x}, \mathbf{w})$. For steady-state conditions, these coefficients depend only on the parameter $\mathbf{w}$.

1.1 "Snapshot" Method

The POD basis functions can be obtained using the "snapshot" method proposed by Sirovich [?]. Sirovich expressed POD basis functions as linear combinations of the samples:

$$\phi_m(\mathbf{x}) = \sum_{n=1}^{N} b_{mn}\theta(\mathbf{x}, \mathbf{w}_n) \quad (4)$$

where the coefficients b_{mn} represent the contribution of the n-th sample corresponding to parameter $\mathbf{w}_n$ in constructing the m-th POD basis function. These coefficients can be obtained by solving the following eigenvalue problem:

$$\mathbf{C}\mathbf{b}_n = \lambda_n \mathbf{b}_n \quad (3)$$

where $\mathbf{C}$ is an N-dimensional symmetric matrix; λ_n is the n-th eigenvalue of $\mathbf{C}$, and $\mathbf{b}_n$ is the corresponding eigenvector whose elements are the coefficients b_{mn} in equation (4). The elements of matrix $\mathbf{C}$ are:

$$C_{ij} = \frac{1}{N}\int_{\Omega} \theta(\mathbf{x}, \mathbf{w}_i)\theta(\mathbf{x}, \mathbf{w}_j) d\mathbf{x} \quad (5)$$

1.2 Energy Optimality

The magnitude of eigenvalues λ_n in equation (3) represents the amount of energy captured by the corresponding POD basis functions in the original physical field. Define the parameter:

$$\xi_M = \frac{\sum_{n=1}^{M} \lambda_n}{\sum_{n=1}^{N} \lambda_n} \quad (5)$$

It is evident that parameter ξ_M represents the contribution of the first M POD basis functions to the total energy. According to the "energy optimality" principle of POD basis functions [?], when eigenvalues are arranged in descending order, only the first M ($M \ll N$) eigenvalues are needed to make ξ_M approach 1. Due to this energy optimality property of POD basis functions, the reconstruction formula (1) can reconstruct the original state parameter with high accuracy using only a very small number of POD basis functions.

1.3 POD Interpolation

For design parameters $\mathbf{w}_n$, the coefficients $\alpha_m(\mathbf{w}_n)$ can be obtained through the following projection formula:

$$\alpha_m(\mathbf{w}_n) = \int_\Omega \theta(\mathbf{x}, \mathbf{w}_n)\phi_m(\mathbf{x})d\mathbf{x} \quad (6)$$

For non-design parameters $\mathbf{w}$, the coefficients $\alpha_m(\mathbf{w})$ can be obtained by interpolating the coefficients $\alpha_m(\mathbf{w}_n)$ corresponding to design parameters $\mathbf{w}_n$ [?]:

$$\alpha_m(\mathbf{w}) = f(\mathbf{w}, \mathbf{w}_n, \alpha_m(\mathbf{w}_n)) \quad (7)$$

where the function f is determined by the interpolation method employed.

2. Low-Order Inverse Problem Computational Model

2.1 Mathematical Model

Based on the POD interpolation method, the fundamental concept of the reduced-order inverse problem computational model proposed in this paper is as follows: according to the physical field information θ_0 measured at steady state, solve for the corresponding POD coefficients α_m^* $(m = 1, 2, \cdots, M)$, and then determine the optimal parameter $\mathbf{w}^*$ from a series of design parameters. The mathematical model can be expressed as:

Find α_m $(m = 1, 2, \cdots, M)$ that minimizes:

$$\|\theta_0 - \sum_{m=1}^{M} \alpha_m \phi_m(\mathbf{x})\|_2 \quad (8)$$

subject to:

$$\alpha_m^{\min} \le \alpha_m \le \alpha_m^{\max} \quad (9)$$

where $\|\cdot\|_2$ represents the vector 2-norm. Equations (8) and (9) are used to calculate the optimal POD coefficients α_m^* $(m = 1, 2, \cdots, M)$ corresponding to the known physical field θ_0, where $\alpha_m^{\min}$ and $\alpha_m^{\max}$ are the lower and upper bounds of the POD coefficients, respectively, determined by the ranges of POD coefficients corresponding to a series of design parameters $\mathbf{w}_n$. It is evident that the process of solving for α_m $(m = 1, 2, \cdots, M)$ is simply a straightforward nonlinear programming problem. Equations (10) and (11) constitute the computational model for determining the optimal parameter $\mathbf{w}^*$ from a series of design parameters $\mathbf{w}_n$ using interpolation. In the calculation, as long as the parameter $\mathbf{w}$ corresponding to the POD coefficients $\alpha_m(\mathbf{w})$ satisfies a certain accuracy requirement in equation (10), that parameter is the optimal parameter being sought.

2.2 Computational Steps

The computational steps of the reduced-order inverse problem computational model based on POD technology can be summarized as follows:

1. Uniformly select N design parameters $\mathbf{w}_n$ within the parameter range, compute the state parameters $\theta(\mathbf{x}, \mathbf{w}_n)$ at certain measurement points at steady state for each parameter value, and obtain N samples.
2. Apply POD technology to the samples to obtain a set of orthogonal basis functions $\phi_m(\mathbf{x})$ $(m = 1, 2, \cdots, M)$.
3. Calculate the POD coefficients $\alpha_m(\mathbf{w}_n)$ for all design parameters using equation (6), and determine the minimum values $\alpha_m^{\min}$ and maximum values $\alpha_m^{\max}$.
4. Use the nonlinear programming model of equations (8) and (9) to compute the optimal POD coefficients α_m^* $(m = 1, 2, \cdots, M)$ corresponding to θ_0.
5. From a series of design parameters $\mathbf{w}_n$, use the interpolation formula of equation (11) to find the optimal parameter $\mathbf{w}^*$ that satisfies a certain accuracy requirement in equation (10). The specific solution steps are:
   - Set the solution accuracy ε for equation (10);
   - Double the number of parameter values $\mathbf{w}$ within the computational domain, i.e., $\mathbf{w}_n$ $(n = 1, 2, \cdots, 2N)$;
   - Use equation (11) to compute the POD coefficients corresponding to each newly added parameter value;
   - Substitute the POD coefficients corresponding to each parameter into equation (10) one by one. If equation (10) satisfies the accuracy ε, the computation converges, and the parameter corresponding to the POD coefficients $\alpha_m(\mathbf{w})$ at this point is the optimal parameter $\mathbf{w}^*$ being sought. If not, restart the calculation from step until equation (10) satisfies the accuracy ε.

It should be noted that within a certain neighborhood of the minimum point of $\mathbf{w}$, there may be multiple parameters whose corresponding POD coefficients satisfy the accuracy ε. In this case, simply select the parameter that yields the minimum value of the objective function.

From the above solution steps, it can be seen that compared with the mainstream POD reduction methods in references [**?**] and [**?**], the reduced-order inverse problem computational model does not involve governing equations. Instead, it uses only a small number of POD coefficients as intermediate variables and solves for the desired parameters using simple nonlinear programming and interpolation methods, achieving direct reduction of the inverse problem. This can significantly reduce both the difficulty and computational time for solving inverse problems. Moreover, since the solution process does not involve governing equations—that is, it is independent of the complexity of the problem under investigation—the proposed method possesses a certain degree of universality in practical engineering applications. Additionally, it is worth noting that the reduced-order inverse problem computational model proposed in this paper is only applicable to problems where the parameters to be solved are constant values, i.e., they do not vary with time or space.

3. Application Example

3.1 Problem Description

This paper uses the steady-state forced convection heat transfer problem in a circular pipe from reference [?] as an application example to illustrate the implementation process of the reduced-order inverse problem computational model. The physical model is shown in [Figure 1: see original paper]. The fluid inlet temperature T_{in} and the heat flux density q on the outer wall of the circular pipe are the parameters to be determined, and they are constant values. The pipe has a radius of $r = 0.025$ m, length $l = 1$ m, and wall conduction thermal resistance is neglected. The fluid properties are: thermal conductivity $k = 0.599$ W/(m · K), density $\rho = 1000$ kg/m^3, specific heat capacity $c_p = 4.183$ kJ/(kg · K), and dynamic viscosity $\mu = 1.0 \times 10^{-3}$ Pa · s. The radial distribution of fluid inlet velocity is:

$$u(r) = 2u_m \left[1 - \left(\frac{r}{R}\right)^2\right] \quad (12)$$

where u_m is the average flow velocity, 0.05 m/s.

The black dots in the circular pipe represent thermocouples. Assuming 25 thermocouples are uniformly arranged along the axial direction to measure the fluid temperature at steady state, r_m is the radial distance from the measurement point to the wall, and measurement errors are neglected. The goal is to determine the fluid inlet temperature T_{in} and the heat flux density q on the outer wall of the circular pipe using the reduced-order inverse problem computational model based on temperature measurements from the thermocouples. Gravity effects are neglected, and the computational mesh is 2000×50.

It should be noted that although the solution process of the reduced-order inverse problem computational model proposed in this paper does not involve governing equations—meaning it is applicable to both laminar and turbulent flows for this application example—laminar flow is adopted in this paper primarily for the purpose of comparing the computational efficiency of the proposed method with the classical conjugate gradient method. Reference [?] provides a detailed implementation of the conjugate gradient method for solving this application example. For turbulent flow, due to the extreme complexity of the governing equations, the conjugate gradient method is almost impossible to implement, and no relevant literature has been reported to date.

3.2 Solution of POD Basis Functions

The ranges and values of the two parameters to be determined are shown in . By arbitrarily combining the parameter values, a total of 48 parameter combinations are obtained. The temperature values at the grid points where the thermocouples are located on the axis $r = 0$ at steady state are collected for each parameter combination, yielding 48 samples. POD technology is applied to these samples. presents the first five eigenvalues and their corresponding energy distributions.

As shown in , the first five basis functions capture almost the entire energy fraction of the samples.

3.3 Accuracy Verification of POD Basis Functions

[Figure 2: see original paper] shows the reconstruction errors for partial samples. It can be observed that the reconstruction error E decreases rapidly with increasing truncation order M and approaches a constant value. When $M = 5$, the value of E has already dropped to approximately 0.05%. The definition of E is:

$$E = \frac{\|\theta - \theta_M\|_2}{\|\theta\|_2} \times 100\% \quad (13)$$

where θ is the numerical solution result and θ_M is the reconstructed result.

[Figure 3: see original paper] and [Figure 4: see original paper] respectively show the first and second groups of POD coefficients for each sample calculated using the projection formula (equation (6)). In figure (a), samples within each variation period are arranged with increasing outer wall heat flux density while keeping the inlet temperature constant, whereas in figure (b), the outer wall heat flux density remains constant while the inlet temperature increases continuously. It can be seen that the POD coefficients of the samples vary almost linearly with the parameters. The other three groups of POD coefficients exhibit similar variation relationships, which are not presented here for brevity. Therefore, this paper adopts linear interpolation to compute the POD coefficients corresponding to non-design parameters.

To verify the accuracy of interpolation results using POD basis functions for non-design parameters, [Figure 5: see original paper] compares the linear interpolation results with direct numerical solution results on the axis $r = 0$ for partial non-design parameters, where the first five POD basis functions are selected. The lines in the figures represent numerical solution results, while the geometric symbols represent interpolation results. For [FIGURE:5(a)], the heat flux density is 7500 W/m^2; for [FIGURE:5(b)], the fluid inlet temperature is 305 K.

As shown in [Figure 5: see original paper], the interpolation results are essentially consistent with the numerical solution results. For [FIGURE:5(a)], the average error E is 0.367%; for [FIGURE:5(b)], E is 0.413%. This indicates that the obtained POD basis functions span the solution space across a wide range of parameters in the original problem and can be repeatedly used through interpolation within the allowable parameter variation range.

3.4 Computational Results

[Figure 6: see original paper] through [Figure 8: see original paper] respectively show several sets of temperature data measured by thermocouples located at $r = 0$ m, $r = 0.0125$ m, and $r = 0.024$ m on the axis. presents a comparison between the computational results of the reduced-order inverse problem model and the true results, where the solution accuracy is $\varepsilon = 0.1\%$.

As shown in , the computational results are relatively close to the true values, with an average relative error e of only 1.069%. The formula for calculating the average relative error e is:

$$e = \frac{1}{2}\left(\frac{|q_r - q|}{q_r} + \frac{|T_{in,r} - T_{in}|}{T_{in,r}}\right) \times 100\% \quad (14)$$

where q_r and $T_{in,r}$ are the true results, and q and T_{in} are the computational results.

To compare the computational efficiency of the reduced-order inverse problem computational model, this paper also solved the aforementioned inverse problem using the classical conjugate gradient method. Since the focus of this paper is on the reduced-order inverse problem computational model, only the computational results of the conjugate gradient method are presented here; the specific implementation process can be found in reference [?]. shows the iterative solution results of the conjugate gradient method, where the convergence accuracy is $c = 0.1\%$, meaning that convergence is achieved when the difference between the current iteration result and the previous iteration result is less than c.

The computational time comparison between the conjugate gradient method and the reduced-order inverse problem computational model is also presented in . The CPU frequency of the computer used for computation is 3.30 GHz with 8.00 GB of memory. The advantages of the reduced-order inverse problem model are evident: although there is a slight loss in computational accuracy, the reduced-order inverse problem computational model can save more than 1200 times the computational time compared to the conjugate gradient method. It should be noted that the computational time here does not include the sample collection and POD basis function solution processes. Although these processes consume considerable time, they are performed only once when rapid calculation of the parameters to be determined is required due to changes in measured data, and can therefore be categorized as preprocessing work.

Conclusion

This paper proposes a reduced-order computational model for general engineering inverse problems using POD technology. Compared with the classical conjugate gradient method, the reduced-order inverse problem computational model does not involve the governing equations of the original physical problem during the solution process. Instead, it uses only a small number of POD coefficients as intermediate solution variables, which greatly simplifies the computational process and demonstrates the universality of the method. Using forced convection heat transfer in a circular pipe as an application example, the computational results show that the average relative error between the results of the reduced-order inverse problem computational model and the true results is approximately 1.0%, and the computational speed is more than 1200 times faster than the classical conjugate gradient method. This proves the correctness and feasibility of the method and provides theoretical support for developing rapid unknown parameter prediction technology in engineering applications.

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Note: Figure translations are in progress. See original paper for figures.