Design of a POD-Based Low-Order Computational Model for Inverse Problems (Postprint)

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Abstract

A low-order computational model for inverse problems in engineering is developed based on Proper Orthogonal Decomposition (POD) technology. By employing limited collected output results, the model can be solved using only simple nonlinear programming and interpolation methods, substantially reducing both the solution difficulty and computational time for inverse problems in engineering. Since the solution process does not involve the governing equations of the original physical problem, the model exhibits a certain degree of universality in practical applications. Using forced convection heat transfer in a circular tube as an application example, the results demonstrate that based on temperature data measured by several thermocouples, the low-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, with only approximately 1.0% deviation from the true values. Moreover, compared with the classical conjugate gradient method, the low-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

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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 computational difficulty and time required for engineering inverse problems. Since the solution process does not involve the governing equations of the original physical problem, the model exhibits a certain degree of universality in practical applications. 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 unknown fluid inlet temperature and wall heat flux based on temperature data measured by thermocouples, with errors of only about 1.0% compared to true values. Moreover, the computational speed is 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

Introduction

Inverse problems in engineering aim to determine unknown model parameters based on partial information from output results. Such problems arise from practical engineering needs, particularly in situations where direct measurement of desired parameters is limited by conditions. Examples include predicting material properties, rock properties in oil reservoirs, damage detection in structural engineering, and monitoring boundary temperatures or heat flux in heat transfer problems. Among solution methods for inverse problems, the conjugate gradient method is most widely applied. This method requires calculating derivatives of the objective function with respect to the parameters (called sensitivity coefficients) and gradually approaches the solution using these coefficients. However, solving for sensitivity coefficients using the conjugate gradient method requires repeatedly solving the governing equations of the original problem, consuming substantial computational time and storage space, making it unsuitable for real-time parameter prediction applications. Furthermore, many engineering problems are governed by extremely complex systems of nonlinear partial differential equations, making sensitivity coefficients difficult or even impossible to obtain.

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 or physical parameters). These basis functions represent the dynamic characteristics of the original physical system. When combined with the Galerkin projection method, POD can reduce the order of the governing equations, establishing a low-order model where "order" represents the number of variables solved at each time step. Such low-order models can rapidly compute physical fields for any parameter within the variable range. This represents the mainstream reduced-order method using POD as a tool and its most typical application. Through this approach, POD has been successfully applied in numerous scientific and engineering fields, including signal analysis, fluid flow and heat transfer, structural dynamics, optimal control, and inverse problems. For inverse problems, references [12] and [13] introduced low-order models into inverse problems of laminar convection heat transfer in circular pipes and saturated groundwater flow, respectively, with the conjugate gradient method still serving as the main solution approach. POD achieved order reduction for the governing equations during each sensitivity coefficient calculation, thereby reducing computational time. Although the final computational time was reduced by several dozen times, this still belongs to the mainstream reduction category where POD' s time-saving effect is only realized during the equation-solving step, and implementation difficulty increases with the complexity of the governing equations. For instance, the low-order model in reference [12] is only applicable to laminar flow and cannot handle turbulent flow.

Given these limitations, this paper employs an alternative POD approach—POD interpolation—to design a novel inverse problem computational model: 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 $\mathbf{x}$ denotes spatial variables. From N state parameter samples corresponding to parameters $\mathbf{w}_n$ $(n = 1, 2, \ldots, N)$, a set of orthogonal basis functions $\phi_m(\mathbf{x})$ dependent only on spatial variables can be extracted. The state parameter $\theta(\mathbf{x}, \mathbf{w})$ can then 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 (number of basis functions used), and $\alpha_m(\mathbf{w})$ 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 parameter $\mathbf{w}$.

1.1 Snapshot Method

POD basis functions can be obtained using the "snapshot" method proposed by Sirovich. This method expresses 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 coefficients b_{mn} represent the contribution of the n-th parameter sample $\mathbf{w}_n$ to constructing the m-th POD basis function. These coefficients are 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 eigenvalues λ_n in equation (3) represent the energy content of the corresponding POD basis functions in the original physical field. Define the parameter:

$$\xi_M = \frac{\sum_{m=1}^{M} \lambda_m}{\sum_{n=1}^{N} \lambda_n} \quad (6)$$

This 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 eigenvalues (where $M \ll N$) can make ξ_M approach 1. Due to this energy optimality, the reconstruction formula (1) can accurately reconstruct the original state parameter 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 projection formula:

$$\alpha_m(\mathbf{w}_n) = \int_{\Omega} \theta(\mathbf{x}, \mathbf{w}_n)\phi_m(\mathbf{x})d\mathbf{x} \quad (7)$$

For non-design parameters $\mathbf{w}$, the coefficients $\alpha_m(\mathbf{w})$ can be determined through interpolation of the coefficients $\alpha_m(\mathbf{w}_n)$ from design parameters:

$$\alpha_m(\mathbf{w}) = f(\alpha_m(\mathbf{w}_1), \alpha_m(\mathbf{w}_2), \ldots, \alpha_m(\mathbf{w}_N)) \quad (8)$$

where the function f depends on 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: given measured physical field information θ_0 at steady state, solve for its corresponding POD coefficients α_m^* $(m = 1, 2, \ldots, M)$, then determine the optimal parameter $\mathbf{w}^*$ from a series of design parameters. The mathematical model can be expressed as:

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

$$\|\theta_0 - \sum_{m=1}^{M} \alpha_m \phi_m(\mathbf{x})\|_2 \quad (9)$$

subject to:

$$\alpha_m^{\min} \leq \alpha_m \leq \alpha_m^{\max} \quad (10)$$

where $\|\cdot\|_2$ represents the vector 2-norm. Equations (9) and (10) are used to compute the optimal POD coefficients α_m^* corresponding to the known physical field θ_0, where $\alpha_m^{\min}$ and $\alpha_m^{\max}$ are the lower and upper bounds of POD coefficients, determined by the ranges of POD coefficients corresponding to a series of design parameters $\mathbf{w}_n$. The process of solving for α_m^* is essentially a simple nonlinear programming problem.

Equations (11) and (12) 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 $\alpha_m(\mathbf{w})$ satisfies the required solution accuracy in equation (11), that parameter is identified as the optimal parameter $\mathbf{w}^*$.

2.2 Computational Procedure

The computational procedure for the reduced-order inverse problem 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 to obtain N samples.

2. Apply POD technology to the samples to extract a set of orthogonal basis functions $\phi_m(\mathbf{x})$ $(m = 1, 2, \ldots, M)$.

3. Calculate the POD coefficients $\alpha_m(\mathbf{w}_n)$ for all design parameters using equation (7), and determine the minimum values $\alpha_m^{\min}$ and maximum values $\alpha_m^{\max}$.
4. Use the nonlinear programming model in equations (9) and (10) to compute the optimal POD coefficients α_m^* corresponding to θ_0.
5. Determine the optimal parameter $\mathbf{w}^*$ from the series of design parameters $\mathbf{w}_n$ using the interpolation formula in equation (12) such that equation (11) meets a specified accuracy. The specific solution steps are:
   - Set solution accuracy ε for equation (11).
   - Double the number of parameter values within the computational domain to $2N$.
   - Use equation (12) to sequentially compute POD coefficients for the newly added parameter values.
   - Substitute POD coefficients for each parameter into equation (11). If equation (11) satisfies accuracy ε, the computation converges and the parameter corresponding to the POD coefficients $\alpha_m(\mathbf{w})$ is the optimal parameter $\mathbf{w}^*$. If not, restart from step until equation (11) satisfies accuracy ε.

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

From the above solution procedure, compared with the mainstream POD reduction methods in references [12] and [13], 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 order reduction for the inverse problem. This substantially reduces both the solution difficulty and computational time for inverse problems. Moreover, since the solution process does not involve governing equations (i.e., it is independent of problem complexity), the proposed method exhibits certain universality in practical engineering applications. Additionally, it should be noted that the reduced-order inverse problem computational model is only applicable to problems where the parameters to be solved are constant (i.e., 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 [12] 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 pipe wall are the parameters to be determined, both constant. The pipe has a radius of $r = 0.025$ m and length $l = 1$ m, with pipe wall thermal resistance neglected. Fluid properties are: thermal conductivity $\lambda = 0.599$ W/(m · K), density $\rho = 1000$ kg/m³, specific heat capacity $c_p = 4.183$ kJ/(kg · K), and kinematic viscosity $\nu = 1.0 \times 10^{-6}$ m²/s. The radial velocity distribution at the fluid inlet is:

$$u(r) = 2u_m \left[1 - \left(\frac{r}{R}\right)^2\right] \quad (13)$$

where $u_m = 0.05$ m/s is the average velocity.

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

It should be noted that although the solution process of the proposed reduced-order inverse problem computational model does not involve governing equations (making it applicable to both laminar and turbulent flows for this example), laminar flow is adopted in this paper primarily to enable comparison of computational efficiency with the classical conjugate gradient method. Reference [15] provides detailed implementation of the conjugate gradient method for this example. For turbulent flows, due to the extreme complexity of governing equations, the conjugate gradient method is almost impossible to implement, and no relevant literature has been reported.

3.2 Solution of POD Basis Functions

The ranges and values of the two parameters to be determined are shown in . Arbitrary combinations of these parameter values yield 48 parameter sets. Temperature values at the thermocouple locations on the axis ($r = 0$) at steady state are collected for each parameter combination, resulting in 48 samples. POD technology is applied to these samples, and presents the first five eigenvalues and their corresponding energy distributions.

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

3.3 Accuracy Verification of POD Basis Functions

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

$$E = \frac{\|\theta - \theta_M\|_2}{\|\theta\|_2} \times 100\% \quad (14)$$

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 (7)). In figure (a), samples within each variation period are arranged with constant inlet temperature while outer wall heat flux density increases continuously; in figure (b), outer wall heat flux density is constant while inlet temperature increases continuously. The sample POD coefficients vary almost linearly with parameters, and similar relationships exist for the other three groups of POD coefficients (not shown here). Therefore, linear interpolation is adopted in this paper to compute POD coefficients for non-design parameters.

To verify the accuracy of POD basis functions for interpolation results at non-design parameters, [Figure 5: see original paper] compares linear interpolation results with direct numerical solution results on the axis ($r = 0$) for partial non-design parameters, using the first five POD basis functions. The lines represent numerical solution results, while 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. The interpolation results are essentially consistent with numerical solution results, with average error E of 0.367% for [FIGURE:5(a)] and 0.413% for [FIGURE:5(b)], demonstrating that the obtained POD basis functions span the solution space across a wide parameter range 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] show several sets of temperature data measured by thermocouples at axial locations $r = 0$, $r = 0.0125$ m, and $r = 0.024$ m, respectively. compares the computational results from the reduced-order inverse problem model with actual results, where the solution accuracy is $\varepsilon = 0.1\%$. The results are close to true values, with average relative error e of only 1.069%, where e is calculated as:

$$e = \frac{1}{2}\sum_{i=1}^{2} \frac{|\omega_i^r - \omega_i|}{\omega_i^r} \times 100\% \quad (15)$$

where ω_i^r represents true results and ω_i represents computational results.

To compare computational efficiency, the classical conjugate gradient method was also used to solve the inverse problem. Since the focus of this paper is the reduced-order inverse problem computational model, only the computational results of the conjugate gradient method are presented here; detailed implementation can be found in reference [15]. shows the iterative solution results of the conjugate gradient method, where convergence accuracy is $c = 0.1\%$ (i.e., results converge when the difference between current and previous iteration results is less than c).

The computational time comparison between the conjugate gradient method and the reduced-order inverse problem computational model is also provided in . The advantages of the reduced-order model are evident: despite a slight loss in accuracy, the reduced-order inverse problem computational model saves more than 1200 times the computational time compared to the conjugate gradient method. It should be noted that the reported computational time excludes sample collection and POD basis function solution processes. Although these processes consume considerable time, they are performed only once when measured data changes require rapid parameter calculation and can thus be considered preprocessing steps.

Conclusion

This paper develops 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, instead using only a small number of POD coefficients as intermediate solution variables. This significantly simplifies the computational process while demonstrating the method' s universality. Using forced convection heat transfer in a circular pipe as an application example, computational results show that the average relative error between the reduced-order model results and true values is approximately 1.0%, with computational speed more than 1200 times faster than the classical conjugate gradient method. These results verify the correctness and feasibility of the method, providing 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.