Model Reduction for the Spatially Distributed Systems Using the Combined Eigenfunctions and Empirical Eigenfunctions

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Abstract: The selection of spatial basis functions will significantly affect the accuracy and efficiency of modeling for nonlinear spatially distributed processes (SDP). The performance using the general spatial basis functions is not good enough which restricts the applications of the approximated models. The current study compares the model reduction performance of empirical eigenfunctions (EEFs) and a kind of new basis functions for the spatially distributed processes, which are obtained from general spatial basis functions by linear transformation, and the transformation matrix is derived using empirical balanced truncation. The EEFs are assumed the optimal in the sense of the least squares errors for the model reduction of spatially distributed processes, however, the results of the simulations show that the accuracy of the modeling based on the present new basis functions is better than that based on the EEFs derived from the measured spatio-temporal data.

Keywords: Spatially Distributed Process; Basis Functions; Empirical Eigenfunctions; Linear Transformation; Empirical Balanced Truncation

1. Introduction

Many of industrial processes such as convection and diffusion reaction process, thermal process and fluid flow belong to SDPs [1]. Their inputs, outputs, states and parameters vary both temporally and spatially. The first-principle modeling typically leads to various partial differential equations (PDEs), which such models can accurately predict the nonlinear and spatially distributed dynamical behavior. However, Because of the infinite-dimensional nature of these systems, it will does not allow their direct use due to limited computation capacity for numerical implementation and finite actuators/sensors for practical control. Thus, a finite-dimensional modeling is usually required for engineering applications, which makes the model reduction essential to SDP modeling.

The selection of spatial basis functions is important for the accuracy and efficiency of the modeling of nonlinear spatially distributed processes. Under the time–space separation framework[2], different approaches and methods will arise according to the combination proper model reduction approaches and spatial basis functions selection. The popular global basis functions are introduced for model reduction mainly including empirical eigenfunctions (EEFs) [3] and analytical basis functions[4]. However, general analytical basis functions may not be optimal in the sense that the dimension of the reduced model is not the lowest for a given accuracy. Although the model dimension can be further reduced using nonlinear weighted residual method (WRM)[1,5] such as the approximate manifold method[1], the structure of the algorithm is very complex and the computation is significantly large.

As a popular spatial basis functions from the measured data, EEFs are often used for the model reduction of the spatially distributed processes. To obtain the EEFs, a basic assumption is made that the measured data fully represent the temporal progress of a spatially distributed process. Thus, the empirical eigenfunctions also have its limits for the engineering applications. Because the spatio-temporal measured data for the computation of the EEFs depends on the number and locations of the sensors in the spatially distributed processes, the number of the EEFs for the availability of sensors and actuators. Thus, the order and accuracy of the modeling of spatially distributed processes are limited for the only use of the input-output data.

In this note, a kind of new basis functions derived by empirical balanced truncation[6,7,8] is proposed for the modeling of spatially distributed processes. The new spatial basis functions are also obtained by the linear transformation of the general eigenfunctions, and the transformation matrix is derived by empirical balanced truncation for the corresponding high-order nonlinear

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ordinary differential equation (ODE) systems of SDP s, which is derived using spectral method[9] based on a complete family of eigenfunctions of SDPs. This approach combines the ease of use of linear theory with the flexibility required for modeling of nonlinear spatially distributed processes. The modeling performances of the new basis functions are compared with the empirical eigenfunctions. The results of the simulations show that the accuracy of the modeling based on the present new basis functions is better than that based on the empirical eigenfunctions derived from the measured spatio-temporal data.

2. Eigenfunctions for the Modeling of SDPs

Assume that a nonlinear SDP is governed by a PDE with following state description:

$$\frac{\partial X}{\partial t} = \mathrm{A}X + \mathrm{B}U + F\left(X, \mathbf{L}, U, \mathbf{L}\right) \quad (1)$$

In Eq.(1), $t \in [0, \infty)$ is time variable, $z \in \Omega$ is the spatial coordinate, and only one spatial-dimension is considered. A and B are two linear operators that involve linear spatial derivatives for X and U, where $X = X(z,t)$ denotes the vector of state variable and $U = U(z,t) = \sum_{i=1}^{p} u_i(t) h_i(z)$ denotes the vector of manipulated spatio-temporal input. $F(X, \partial X/\partial z, \mathbf{L}, U, \partial U/\partial z, \mathbf{L})$ is a nonlinear function containing spatial derivatives for $X(z,t)$ and $U(z,t)$. Eq.(1) is considered on a bounded spatial domain Ω and subjects to a number of boundary and initial conditions. The phase space of (1) is on the infinite-dimensional Hilbert space $H(\Omega)$ of sufficiently smooth functions from Ω into real numbers. A scalar products is introduced in $H(\Omega)$, which is usually given by $[g,h] = \int_{\Omega} g(z) h(z) dz$ for two arbitrary functions $g(z), h(z) \in H(\Omega)$.

A family denotes the infinite set of the eigenfunctions of linear operator A for PDE (1) is first derived by the following equation:

$$\mathrm{A} f_i(z) = l_i f_i(z), \quad i = 1, 2, \mathbf{L} \quad (2)$$

This family is a complete family of smooth global spatial orthogonal basis functions $\{f_1(z), f_2(z), \mathbf{L}, \mathbf{L}\}$. The spatio-temporal variable of PDE (1) can be expanded onto the infinite number of eigenfunctions with the corresponding temporal coefficients.

Suppose that the system is controlled by p actuators with implemental temporal signal $u(t)$, $u(t) = [u_1(t), u_2(t), \mathbf{L}, u_p(t)]^T$ and certain spatial distributions. The spatiai-temporal output $Y(z,t)$ is measured at M locations. Due to the orthogonal of the eigenfunctions, an infinite-dimensional ODE system can be obtained by the Galerkin method as follows.

To reduce the infinite-dimensional nonlinear ODE system in to a finite set of nonlinear ODE equations, the fast modes are excluded according to the eigenvalues, and the retained finite-dimensional nonlinear ODE system can be rewritten in a general form as follows:

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t) + f\left(x(t), u(t)\right) \\ y(t) &= Cx(t) \end{aligned} \quad (3)$$

Where $x(t) = [x_1, x_2, \mathbf{L}, x_N]^T$,

$y(t) = \left[Y(z_1,t), Y(z_2,t), \mathbf{L}, Y(z_M,t)\right]^T$,

$A = diag\left(l_1, l_2, \mathbf{L}, l_N\right)$,

$B = \left[b_{ij}\right]_{N\times p}, b_{ij} = \int_{\Omega} \mathrm{B}(h_j(z)) f_i(z) dz$,

$C = \left[c_{ij}\right]_{L\times N}, c_{ij} = j_j(z_i)$, $z_l, l = 1, 2, \mathbf{L}, L$ in the lth of L measured spatial locations.

$f(x(t), u(t)) = \left[f_1(x(t), u(t)), f_2(x(t), u(t)), \mathbf{L}, f_N(x(t), u(t))\right]^T$

and

$f_i(\hat{x}(t), u(t)) = \int_{\Omega} F(X, \partial X/\partial z, \mathbf{L}, U, \partial U/\partial z, \mathbf{L}) f_i(z) dz$

3. New Basis Functions Derived by Balancing of Empirical Gramians

Let each new spatial basis function be a linear combination of the first N eigenfunctions corresponding to finite-dimensional nonlinear ODE system (3) of nonlinear spatially distributed processes. Define a basis function transformation matrix S, we have

$$\{j_1(z), j_2(z), \mathbf{L}, j_K(z)\} = \{f_1(z), f_2(z), \mathbf{L}, f_N(z)\} S \quad (4)$$

where $K < N$, $\{f_1(z), f_2(z), \mathbf{L}, f_K(z)\}$ and $\{j_1(z), j_2(z), \mathbf{L}, j_N(z)\}$ denote new spatial basis functions and eigenfunctions, respectively.

The spatio-temporal variable of the PDE (1) can be expanded onto the new spatial basis functions $f_i(z)$ with the corresponding temporal coefficients $\overline{x}_i(t)$ as follows.

$$X(z,t) \approx \sum_{i=1}^{K} \overline{x}_i(t) f_i(z) \quad (5)$$

Using the basis functions expansions and Galerkin method will transform Eq.(1) into

$$D\dot{\overline{x}}(t) = \overline{A}\overline{x}(t) + \overline{B}u(t) + g\left(\overline{x}(t), u(t)\right) \quad (6)$$

Let the D^{-1} denotes the inverse matrix of D, S_i denotes the i th column of the matrix S then a nonlinear ODE system with fewer modes of nonlinear PDE (1) can be derived as follows.

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$$\dot{\bar{x}}(t) = D^{-1}\bar{A}\bar{x}(t) + D^{-1}\bar{B}u(t) + D^{-1}g(\bar{x}(t),u(t))$$
$$y(t) = \bar{C}\bar{x}(t) \quad (7)$$

Where $\bar{x}(t) = [\bar{x}_1(t), \bar{x}_2(t), \ldots, \bar{x}_K(t)]^T$,

$u(t) = [u_1(t), u_2(t), \ldots, u_p(t)]^T$,

$g(\bar{x}(t),u(t)) = [g_1(\bar{x}(t),u(t)), g_2(\bar{x}(t),u(t)), \ldots, g_K(\bar{x}(t),u(t))]^T$

and

$$D_{ij} = \int_\Omega \varphi_i(z)\varphi_j(z)dz = \sum_{k=1}^{N} S_{ki}S_{kj}\int_\Omega \phi_i(z)\phi_j(z)dz = S_i^T S_j$$

$$\bar{A}_{ij} = \int_\Omega \mathcal{A}(\varphi_j(z))\varphi_i(z)dz = \int_\Omega \mathcal{A}\left(\sum_{k=1}^{N} S_{kj}\phi_k(z)\right)\left(\sum_{k=1}^{N} S_{ki}\phi_k(z)\right)dz = S_i^T \mathcal{A} S_j$$

$$\bar{B}_{ij} = \int_\Omega \mathcal{B}(h_j(z))\varphi_i(z)dz = \int_\Omega \mathcal{B}(h_j(z))\left(\sum_{k=1}^{N} S_{ki}\phi_k(z)\right)dz = S_i^T \mathcal{B}_j$$

$$\bar{C}_{ij} = \varphi_j(z_i) = [c_{i1} \quad c_{i2} \quad \ldots \quad c_{iN}]S_j,$$

$$g_i(\bar{x}(t),u(t)) = \int_\Omega F\left(\sum_{i=1}^{K}\bar{x}_i(t)\varphi_i(z), \frac{\partial\left(\sum_{i=1}^{K}\bar{x}_i(t)\varphi_i(z)\right)}{\partial z}, \ldots, \sum_{i=1}^{p}u_i(t)h_i(z), \frac{\partial\left(\sum_{i=1}^{p}u_i(t)h_i(z)\right)}{\partial z}, \ldots\right)\varphi_j(z)dz.$$

In this section, an algorithm to obtain the spatial basis functions transformation matrix by empirical balanced truncation[6-8] is present for the nonlinear ODE system (3), taking explicit account of the input-output connection of the system. For the nonlinear system (3), the following sets need to be defined for empirical gramians. Let $T^N = \{T_1, T_2, \ldots, T_r\}$ be a set of r orthogonal $N \times N$ matrices, where r denotes the number of matrices for excitation/perturbation directions. Let $M^s = \{c_1, c_2, \ldots, c_s\}$ be a set of s positive constants, where s denotes the number of different excitation/perturbation sizes for each direction. Let $E^p = \{e_1, e_2, \ldots, e_p\}$ be p standard unit vectors in $\Re^p$, where p denotes the number of inputs to the system (3). Given a function $x(t)$, define the mean by $\langle x(t)\rangle = \lim_{T\to\infty}\int_0^T x(t)dt / T$. For system (3), define the empirical controllability gramian by

$$\hat{W}_C = \sum_{l=1}^{r}\sum_{m=1}^{s}\sum_{i=1}^{p}\frac{1}{rsc_m^2}\int_0^\infty \Phi^{ilm}(t)dt \quad (8)$$

Where $\Phi^{ilm}(t) \in \Re$ is given by $\Phi^{ilm}(t) = (x^{ilm}(t) - \bar{x}^{ilm})(x^{ilm}(t) - \bar{x}^{ilm})^T$, and $x^{ilm}(t)$ is the state of system(3) corresponding to the impulsive input $u(t) = c_m T_l e_i d(t)$.

For system (3), define the empirical observability gramian by

$$\hat{W}_O = \sum_{l=1}^{r}\sum_{m=1}^{s}\frac{1}{rsc_m^2}\int_0^\infty T_l \Psi^{lm}(t) T_l^T dt \quad (9)$$

Where $\Psi^{ilm}(t) \in \Re^{N\times N}$ is given by $\Psi_{ij}^{lm}(t) = (y^{ilm}(t) - \bar{y}^{ilm})^T(y^{ilm}(t) - \bar{y}^{ilm})$, and $y^{ilm}(t)$ is the output of system(3) corresponding to the initial condition $x_0 = c_m T_l e_i$ with the $u(t) = 0$.

The empirical controllability gramian and empirical observability gramian are computable generalization of controllability gramian and observability gramian to nonlinear systems. It therefore led to a methodology for model reduction of nonlinear ODE system (3) motivated by a standard idea from realization theory. Because the empirical gramians are by the nature based upon discrete measured of system properties, like states and outputs, it is advantageous to reformulate them in a discrete form for numerically calculation. A simple numerical technique for balancing the empirical gramians $\hat{W}_c$ and $\hat{W}_O$ is shown as follows. First, apply the Cholesky factorization[10] to $\hat{W}_O$ so that $\hat{W}_O = ZZ^T$, where Z is a lower triangular matrix with non-negative diagonal entries. Let $U\Sigma^2U^T$ be a eigenvalue decomposition of $Z^T\hat{W}cZ$. Thus, $\bar{S} = \Sigma^{1/2}U^TZ^{-1}$, and the transformed empirical gramians $\bar{W}c = \bar{S}\hat{W}c\bar{S}^T$; $\bar{W}o = (\bar{S}^{-1})^T\hat{W}o\bar{S}^{-1}$.

The nonlinear ODE system (3) that is balanced has the following form, which empirical controllability gramian $\bar{W}c$ and empirical observability gramian $\bar{W}o$ are equal to $\Sigma = diag(s_1, s_2, \ldots, s_N)$. $s_1 \geq s_2 \geq s_3 \geq \ldots s_N \geq 0$ and the s_i's are the Hankel singular values. The columns of $\bar{S}$ may be thought of as giving the modes of the system associated with the Hankel singular values in Σ. To derive a superior set of new spatial basis functions, the first K columns of matrix $\bar{S}$ of balancing of the empirical gramians is selected to be a $N \times K$ spatial basis functions transformation matrix. Using the MATLAB style colon notation, transformation matrix $S = \bar{S}(:,1:K)$. The performance of the new spatial

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basis functions from this transformation matrix is illustrated by a numerical example.

4. Comparisons of the Performance with Empirical Eigenfunctions

In order to compare the modeling performance with empirical eigenfunctions for nonlinear spatially distributed processes, a long thin rod[11] in a reactor as is studied which is a typical transport-reaction process in the chemical industry. The reactor is fed with pure species A and a zeroth order exothermic catalytic reaction of the form A→B takes place in the rod. Since the reaction is exothermic, a cooling medium that is in contact with the road is used for cooling.

After choosing spatial orthogonal basis functions for time/space separation, the set of new spatial basis functions and empirical eigenfunctions are used for modeling of the nonlinear spatially distributed processes respectively.

Suppose that $Y(z,t)$ and $\overline{Y}(z,t)$ are the measured output and the prediction output at M spatial locations $z_1, z_2, \ldots, z_M$ and some sampling times $t_1, t_2, \ldots, t_{Ntim}$, respectively. The root of mean square error (RMSE) between the real dynamical process and the approximation model is defined as the performance index as follows:

$$RSME = \sqrt{\sum_{i=1}^{M}\sum_{j=1}^{Ntim}\left(Y(z_i,t_j)-\hat{Y}(z_i,t_j)\right)^2 \Big/ M \cdot Ntim} \qquad (10)$$

Under the assumption of constant density and heat capacity of the rod, constant conductivity of the rod, and constant temperature at both sides of the rod, and excess of species A in the furnace, the mathematical model that describes the spatio-temporal evolution of the rod temperature consists of the following parabolic PDE:

$$\frac{\partial X(z,t)}{\partial t} = \frac{\partial^2 X(z,t)}{\partial z^2} + b_T\left(e^{-g/(1+T)} - e^{-g}\right) + b_u\left(h(z)^T u(t) - X(z,t)\right)$$
(11)

In this study, (11) subject to the following Dirichlet boundary and initial conditions:

$$X(0,t)=0,\ X(p,t)=0,\ X(z,0)=X_0(z) \qquad (12)$$

Where $X(z,t)$, $u(t)$, $h(z)$, b_T, b_u, g denote the temperature in the reactor, the manipulated input (temperature of the cooling medium), the actuator distribution, the heat of reaction , the heat transfer coefficient, and the activation energy, respectively. The process parameters are set to be $b_T = 50, b_u = 2, g = 4$. There are four actuators $u(t) = [u_1(t), u_2(t), \ldots u_4(t)]^T$ available with the spatial distribution functions $h(z) = [h_1(z), h_2(z), \ldots h_4(z)]^T$, where $h_i(z) = H(z-(i-1)p/4) - H(z-ip/4),\ i = 1,2,3,4$ and $H(\cdot)$ is the standard Heaviside function. The input signals are selected as $u_i(t) = 1.1 + 4\sin(t/10 + i/10),\ i = 1, 2, 3, 4$. Suppose that nineteen sensors uniformly distributed in the space are used for measurement. Four hundred data for each sensor location is collected from (11). The sampling interval Δt is 0.01s and the simulation time is 4s. The initial condition $X_0(z)$ is set to be $\sin(z)$.

To compare the modeling performance based on the new basis functions and EEFs with the same order, the same input signals are used. Nineteen sensors that have been uniformly distributed in the space are used for measurements. The random process noise is bounded by 0.3 with zero mean. The EEFs used for time/space separation and dimension reduction are selected from Karhunen-Loeve (KL) decomposition. In the Galerkin method, obtaining an exact analytical description of the low-dimensional ODE systems is difficult because of the nonlinearities in the system. Therefore, the neural networks are used to identify the long-term dynamics from the inputs and temporal coefficients. As the energy percentage of the first three EEFs has reached larger than 99%, the RMSEs of the approximated models based on two kinds of basis functions on testing data are compared in Table S1 in support information. As shown in Table 1, the values of the RMSE using the new spatial basis functions are little smaller than when using the same number of EEFs.

Table 1. Comparisons for RMSEs with empirical eigenfunctions

RMSE	$K=1$	$K=2$	$K=3$
EEFs	0.3023	0.1987	0.0930
New spatial basis functions	0.2879	0.1652	0.0822

From the Table 1, the RMSEs for the predicted temperature distributions of approximate models based on the proposed new spatial basis functions of kind two and EEFs are 0.0822 and 0.0930, respectively. In many cases, EEFs are frequently used in Galerkin projections to obtain low-dimensional models of DPSs. However, the optimality of the KL decomposition lies in a posteriori data reconstruction, and there are no guarantees of optimality in modeling. In order to illustrate the details of the comparisons for the two kinds of spatial basis functions, the first three EEFs and the first new spatial basis functions are shown in Figure 1 and Figure 2 respectively.

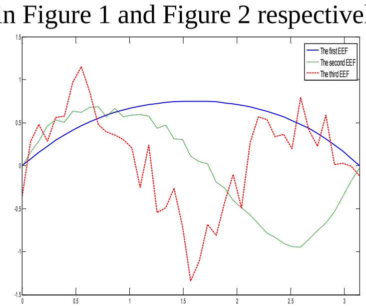

Figure 1. The first three empirical eigenfunctions

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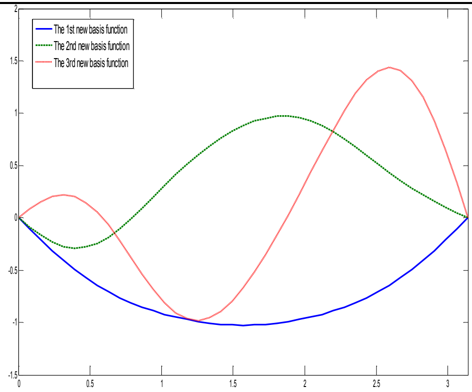

Figure 2. The first three new spatial basis functions

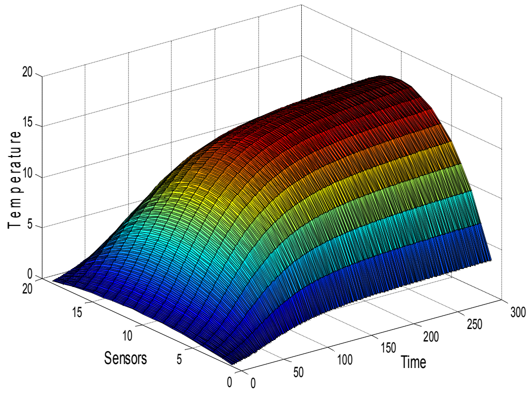

Figure 3. Temperature distributions with a three-order approximate model based on new basis functions

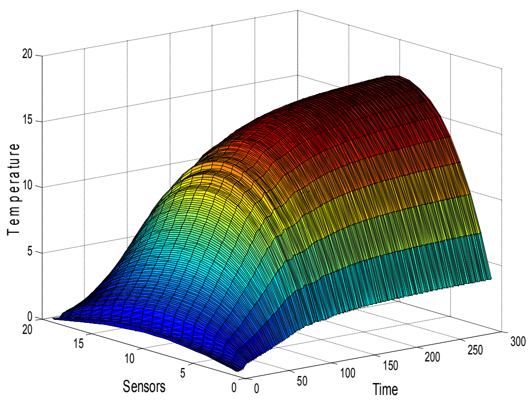

Figure 4. Temperature distributions with a three-order approximate model based on empirical eigenfunctions

The approximate temperature distributions of the catalytic rod based on a three-order dynamical model and a three-order dynamical model based on EEFs are shown in Figure 3 and 4, respectively. Apparently, the performance of temperature distribution with a three-order approximate model based on new basis functions in Figure 3 is better than that based on three EEFs in Figure 4.

Conclusion

The current study compares the model reduction performance of empirical eigenfunctions (EEFs) and a kind of new basis functions for the spatially distributed processes, which are obtained from general spatial basis functions by linear transformation, and the transformation matrix is derived using empirical balanced truncation. The proposed new basis functions were calculated using the linear theory of matrix computation for nonlinear processes. The results of the simulations showed that the accuracy of the modeling based on the present new basis functions was better than that based on the empirical eigenfunctions derived from the measured spatio-temporal data.

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