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Model Order Reduction for Nonlinear Schrödinger Equation

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Abstract. Proper orthogonal decomposition (POD) is a method for deriving reduced order models of dynamical systems. In this paper, the POD is applied to the nonlinear Schrödinger equation (NLS). The NLS equation is discretized in space by finite differences and is solved in time either by structure preserving symplectic or energy preserving average vector field (AVF) integrators. Numerical results for one dimensional NLS equation with soliton solutions show that the low-dimensional approximations obtained by POD reproduce very well the characteristic dynamics of the system, such as preservation of energy and phase space structure of the NLS equation.
Keywords: Nonlinear Schrödinger equation, model order reduction, periodic solutions .

1 Introduction

The nonlinear Schrödinger (NLS) equation arises as the model equation with second order dispersion and cubic nonlinearity describing the dynamics of slowly varying wave packets in nonlinear optics and fluid dynamics and it appears in Bose-Einstein condensate theory. We consider in this paper the NLS equation

$$\psi_t = i\psi_{xx} + i\gamma \mid \psi \mid^2 \psi \tag{1}$$

with the periodic boundary conditions $\psi(x+L,t) = \psi(x,t)$. Here $\psi = \psi(x,t)$ is a complex valued function, γ is a parameter and $i^2 = -1$. The NLS equation is called focusing if $\gamma > 0$ and defocusing if $\gamma < 0$; for $\gamma = 0$, it reduces to

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the linear Schrödinger equation. In last two decades various numerical methods were applied for solving NLS equation, among them are the well-known symplectic and multisymplectic integrators, discontinuous Galerkin methods.

There is a strong need for model reduction techniques to reduce the computational costs and storage requirements in large scale simulations. They should yield low-dimensional approximations for the full high-dimensional dynamical system, which reproduce the characteristic dynamics of the system. Among the model order reduction techniques the proper orthogonal decomposition (POD) is one of the most widely used method. Surprisingly good approximation properties are reported for POD based model order reduction techniques in the literature. It has been successfully used in different fields including signal analysis and pattern recognition Fukunaga[3], fluid dynamics and coherent structures Berkooz *et al.*[2] and more recently in control theory Kunisch and Volkwein[4]. The POD is applied mostly to linear and nonlinear parabolic equations Kunisch and Volkwein[5]. In this paper, we apply the POD to the NLS equation. To the best of our knowledge, there is only one paper where POD is applied to NLS equation Schlizerman *et al.*[7], where the authors use only one and two modes approximations of the NLS equation. In this paper, the NLS equation is discretized in space and time by preserving the symplectic structure and the energy. Then, from the snapshots of the fully discretized dynamical system, the POD basis are computed using the singular value decomposition (SVD). It turns out that most of the energy of the system can be accurately approximated by using few POD modes. Numerical results for a NLS equation with soliton solutions confirm the energy and phase space preserving properties of the POD.

The paper is organized as follows. Section 2 and Section 3 are devoted to reviewing the POD method and its application to semi-linear dynamical systems. Numerical solution of the semi-discrete NLS equation and the POD reduced form are described in Section 4. In the last section, Section 5, the numerical results for the reduced order models of one-dimensional NLS equation are presented.

2 The Proper Orthogonal Decomposition

Let X be a real Hilbert space endowed with inner product $\langle \cdot, \cdot \rangle_X$ and norm $\|\cdot\|_X$. For $y_1, \ldots, y_n \in X$ we set

$$V = span\{y_1, \cdots, y_n\},$$

and refer to V as the ensemble consisting of the snapshots $\{y_j\}_{j=1}^n$. Let $\{\psi_k\}_{k=1}^d$ denote an orthonormal basis of V with $d = dimV$. Then each member of the ensemble can be expressed as

$$y_j = \sum_{k=1}^{d} \langle y_j, \psi_k \rangle_X \psi_k, \quad j = 1, \ldots, n \tag{2}$$

The POD is constructed by choosing the orthonormal basis such that for every $l \in \{1, \ldots, d\}$ the mean square error between the elements y_j, $1 \leq j \leq n$, and the corresponding $l-th$ partial sum of (2) is minimized on average:

$$\min_{\{\psi_k\}_{k=1}^{l}} \frac{1}{n} \sum_{j=1}^{n} \left\| y_j - \sum_{k=1}^{l} \langle y_j, \psi_k \rangle_X \psi_k \right\|_X^2 \tag{3}$$

$$\langle \psi_i, \psi_j \rangle_X = \delta_{ij}, \quad 1 \leq i \leq l, \quad 1 \leq j \leq i$$

A solution $\{\psi_k\}_{k=1}^{l}$ to (3) is called a POD-basis of rank l. We introduce the correlation matrix $K = \{K_{ij}\} \in \mathbb{R}^{n \times n}$ corresponding to the snapshots $\{y_j\}_{j=1}^{n}$ by

$$K_{ij} = \frac{1}{n} \langle y_j, y_i \rangle_X$$

The matrix K is positive semi-definite and has rank d. Let $\lambda_1 \geq \ldots \geq \lambda_d > 0$ denote the positive eigenvalues of K and $v_1, \ldots, v_d \in \mathbb{R}^n$ the associated eigenvectors. Then a POD basis of rank $l \leq d$ is given by

$$\psi_k = \frac{1}{\sqrt{\lambda_k}} \sum_{j=1}^{n} (v_k)_j y_j$$

where $(v_k)_j$ is the $j-th$ component of the eigenvector v_k. Moreover, we have the error formula

$$\frac{1}{n} \sum_{j=1}^{n} \left\| y_j - \sum_{k=1}^{l} \langle y_j, \psi_k \rangle_X \psi_k \right\|_X^2 = \sum_{j=l+1}^{d} \lambda_j$$

The choice of l is based on heuristic considerations combined with observing the ratio of the modeled to the total energy contained in the system Y which is expressed by

$$\epsilon(l) = \frac{\sum_{i=1}^{l} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$

2.1 POD and SVD

There is a strong connection between POD and singular value decomposition (SVD) for rectangular matrices.

Let Y be a real-valued $m \times n$ matrix of rank $d \leq min\{m, n\}$ with columns $y_j \in \mathbb{R}^m$, $1 \leq j \leq n$. In the context of POD, it will be useful to think of the columns $\{Y_{\cdot,j}\}_{j=1}^{n}$ of Y as the spatial coordinates vectors of a dynamical system at time t_j. Similarly, we consider the rows $\{Y_{i,\cdot}\}_{i=1}^{m}$ of Y as the time trajectories of the dynamical system evaluated at the locations x_i.

SVD guarantees the existence of real numbers $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_d > 0$ and orthogonal matrices $U \in \mathbb{R}^{m \times m}$ with columns $\{u_i\}_{i=1}^{m}$ and $V \in \mathbb{R}^{n \times n}$ with columns $\{v_i\}_{i=1}^{n}$ such that

$$U^T Y V = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} := \Sigma \in \mathbb{R}^{m \times n} \tag{4}$$

where $D = diag(\sigma_1, \sigma_2, \ldots, \sigma_d) \in \mathbb{R}^{d \times d}$ and the zeros in (4) denote the matrices of appropriate dimensions. Moreover, the vectors $\{u_i\}_{i=1}^d$ and $\{v_i\}_{i=1}^d$ satisfy

$$Y v_i = \sigma_i u_i, \quad Y^T u_i = \sigma_i v_i, \quad i = 1, \cdots, d.$$

One of the central issues of POD is the reduction of the data expressing their essential information by means of a few basis vectors. Let us now interpret SVD in terms of POD by the following theorem.

Theorem : (Kunisch and Volkwein[5]) Let $Y = [y_1, \ldots, y_n] \in \mathbb{R}^{m \times n}$ be a given matrix with rank $d \leq min\{m, n\}$. Further, let $Y = U \Sigma V^T$ be the SVD of Y, where $U = [u_1, \ldots, u_m] \in \mathbb{R}^{m \times m}, V = [v_1, \ldots, v_n] \in \mathbb{R}^{n \times n}$ are orthogonal matrices and the matrix $\Sigma \in \mathbb{R}^{m \times n}$ has the form (4). Then, for any $l \in \{1, \ldots, d\}$ the solution to

$$\max_{\widetilde{u}_1, \ldots, \widetilde{u}_l \in \mathbb{R}^m} \sum_{i=1}^{l} \sum_{j=1}^{n} \left| \langle y_j, \widetilde{u}_i \rangle_{\mathbb{R}^m} \right|^2, \quad \langle \widetilde{u}_i, \widetilde{u}_j \rangle_{\mathbb{R}^m} = \delta_{ij}, \quad 1 \leq i, j \leq l \tag{5}$$

is given by the singular vectors $\{u_i\}_{i=1}^l$. A necessary optimality condition for (5) is given by the eigenvalue problem $Y Y^T u_i = \lambda_i u_i$.

3 Application to Semi-linear Time Dependent Systems

We consider the semi-linear initial value problem

$$\dot{y}(t) = Ay(t) + f(t, y(t)), \quad t \in [0, T], \quad y(0) = y_0, \tag{6}$$

where $f : [0, T] \times \mathbb{R}^m \to \mathbb{R}^m$ is continuous in both arguments and locally Lipschitz-continuous with respect to the second argument. The NLS equation (1) is a semi-linear equation, where the cubic nonlinear part is locally Lipschitz continuous.

Suppose that we have determined a POD basis $\{u_j\}_{j=1}^l$ of rank $l \in \{1, \ldots, m\}$ in $\mathbb{R}^m$. Then we make the ansatz

$$y^l(t) = \sum_{j=1}^{l} \underbrace{\langle y^l(t), u_j \rangle}_{=: y_j^l(t)} u_j, \quad t \in [0, T], \tag{7}$$

where the Fourier coefficients y_j^l, $1 \leq j \leq l$, are functions mapping $[0, T]$ into $\mathbb{R}^m$, and the inner product $\langle \cdot, \cdot \rangle$ represents the Euclidean inner product $\langle \cdot, \cdot \rangle_{\mathbb{R}^m}$ to make the notation simple. Since

$$y(t) = \sum_{j=1}^{m} \langle y(t), u_j \rangle u_j, \quad t \in [0, T]$$

holds, $y^l(t)$ is an approximation for $y(t)$ provided $l < m$. Inserting (7) into (6) yields

$$\sum_{j=1}^{l} \dot{y}_j^l(t)u_j = \sum_{j=1}^{l} y_j^l(t)Au_j + f(t, y^l(t)), \quad t \in [0,T], \quad \sum_{j=1}^{l} y_j^l(0)u_j = y_0 \tag{8}$$

Note that (8) is an initial-value problem in $\mathbb{R}^m$ for $l \leq m$ coefficient functions $y_j^l(t), \quad 1 \leq j \leq l$ and $t \in [0,T]$, so that the coefficients are overdetermined. Therefore, we assume that (8) holds after projection on the l dimensional subspace $V^l = span\,\{u_j\}_{j=1}^l$. From (8) and $\langle u_j, u_i \rangle = \delta_{ij}$ we infer that

$$\dot{y}_i^l(t) = \sum_{j=1}^{l} y_j^l(t) \langle Au_j, u_i \rangle + \left\langle f(t, y^l(t)), u_i \right\rangle \tag{9}$$

for $1 \leq i \leq l$ and $t \in (0,T]$. Let us introduce the matrix

$$B = \{b_{ij}\} \in \mathbb{R}^{l \times l}, \quad b_{ij} = \langle Au_j, u_i \rangle$$

and the non-linearity $F = (F_1, \cdots, F_l)^T : [0,T] \times \mathbb{R}^l \to \mathbb{R}^l$ by

$$F_i(t,y) = \left\langle f(t, \sum_{j=1}^{l} y_j u_j), u_i \right\rangle, \quad t \in [0,T], \quad y = (y_1, \cdots, y_l) \in \mathbb{R}^l$$

Then, (9) can be expressed as

$$\dot{y}^l(t) = By^l(t) + F(t, y^l(t)), \quad t \in (0,T] \tag{10}$$

For initial condition, we derive $y^l(0) = y_0$ where

$$y_0 = \left(\langle y_0, u_1 \rangle, \ldots, \langle y_0, u_l \rangle \right)^T \in \mathbb{R}^l$$

This system is called the POD-Galerkin projection for (6). In case of $l << m$ the $l-$dimensional system is a low-dimensional approximation for (6). Therefore, it is the reduced-order model for (6).

4 Numerical solution of NLS equation

One dimensional NLS equation (1) can be written by decomposing $\psi = p + iq$ in real and imaginary components

$$p_t = -q_{xx} - \gamma(p^2 + q^2)q, \quad q_t = p_{xx} + \gamma(p^2 + q^2)p \tag{11}$$

as an infinite dimensional Hamiltonian pde in the phase space $u = (p,q)^T$

$$\dot{u} = \mathcal{D}\frac{\delta \mathcal{H}}{\delta u}, \quad \mathcal{H} = \int \frac{1}{2}\left(p_x^2 + q_x^2 - \frac{\gamma}{2}(p^2+q^2)^2\right) dx, \quad \mathcal{D} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

After discretizing the Hamiltonian in space

$$H = \frac{1}{2\Delta x^2}\sum_{j=1}^{n}((p_{j+1}-p_j)^2+(q_{j+1}-q_j)^2) - \frac{\gamma}{4}\sum_{j=1}^{n}(p_j^2+q_j^2)^2.$$

we obtain the semi-discretized Hamiltonian ode's

$$p_t = -Aq - \gamma q(p^2+q^2), \quad q_t = Ap + \gamma p(p^2+q^2), \tag{12}$$

where A is a circulant matrix.

To solve (12) we apply the second order Strang split-step method by adapting the linear, non-linear splitting

$$u_t = \mathcal{N}u + \mathcal{L}u, \quad \mathcal{L}u = iu_{xx}, \quad \mathcal{N}u = i\gamma|u|^2u.$$

4.1 POD Basis for NLS equation

Suppose that we have determined POD bases $\{u_j\}_{j=1}^{l}$ and $\{v_j\}_{j=1}^{l}$ of rank $l = \{1,\dots,m\}$ in $\mathbb{R}^m$. Then we make the ansatz

$$p^l = \sum_{j=1}^{l}\alpha_j u_j(x), \quad q^l = \sum_{j=1}^{l}\beta_j v_j(x) \tag{13}$$

where $\alpha_j =< p^l, u_j >, \quad \beta_j =< q^l, v_j >$ and $p^l,\ q^l$ are approximations for p and q, respectively. Inserting (13) into (12), and using that $\langle u_i, u_j\rangle = \delta_{ij}$ and $\langle v_i, v_j\rangle = \delta_{ij}, \quad i,j = 1,\cdots,l$, we obtain

$$\dot{\alpha}_i = -\sum_{j=1}^{l}\beta_j\langle Av_j, u_i\rangle - \gamma\left\langle\left(\sum_{j=1}^{l}\beta_j v_j\right)\left(\sum_{j=1}^{l}\alpha_j u_j\right)^2, u_i\right\rangle - \gamma\left\langle\left(\sum_{j=1}^{l}\beta_j v_j\right)^3, u_i\right\rangle$$

$$\dot{\beta}_i = \sum_{j=1}^{l}\alpha_j\langle Au_j, v_i\rangle + \gamma\left\langle\left(\sum_{j=1}^{l}\alpha_j u_j\right)\left(\sum_{j=1}^{l}\beta_j v_j\right)^2, v_i\right\rangle + \gamma\left\langle\left(\sum_{j=1}^{l}\alpha_j u_j\right)^3, v_i\right\rangle$$

As defining $V = [v_1, v_2, \cdots, v_l] \in \mathbb{R}^{m\times l}, \quad \beta \in \mathbb{R}^l, \quad U = [u_1, u_2, \cdots, u_l] \in \mathbb{R}^{m\times l}, \quad \alpha \in \mathbb{R}^l, \quad B = \{b_{ij}\}, \quad b_{ij} = \langle Av_j, u_i\rangle, \quad B^T = \{c_{ij}\}, \quad c_{ij} = \langle Au_j, v_i\rangle$, we obtain

$$\begin{aligned}\dot{\alpha} &= -B\beta - \gamma U^T\left((V\beta)\cdot(U\alpha)^2\right) - \gamma U^T\left((V\beta)^3\right)\\ \dot{\beta} &= B^T\alpha + \gamma V^T\left((U\alpha)\cdot(V\beta)^2\right) + \gamma V^T\left((U\alpha)^3\right)\end{aligned} \tag{14}$$

with both the operation '$\cdot$' and the powers are hold elementwise.

The reduced order system (14) is solved, as the unreduced one (1), with the energy preserving AVF method and symplectic midpoint method applying

linear-nonlinear Strang spliting Weideman and Herbst[8]. The nonlinear parts of the equations are solved by Newton-Raphson method. For solving the linear system of equations, we have used the Matlab toolbox **smt** Redivo-Zaglia and Rodriguez[6], which is designed for solving linear systems with a structured coefficient matrix like the circulant and Toepltiz matrices. It reduces the number of floating point operations for matrix factorization to $O\,(n \log n)$.

5 Numerical Results

For the one dimensional NLS equation we have taken the example in Celledoni *et al.*[1] with $\gamma = 1$, and the periodic boundary conditions in the interval $[-20, 20]$. The initial conditions are given as $p(x,0) = \exp(-(x-1)^2/2)$, $q(x,0) = \exp(-x^2/2)$. As mesh sizes in space and time we have used $dx = 40/20$ and $dt = 0.1$, respectively.

We compare the energy error and the norm error with ROM-AVF and ROM-MID using with and without difference quotients in Table 1. With increasing number of POD basis l, the errors in the energy and discrete solutions of the fully discretized NLS equation and the reduced order model decreases. The singular values of the snapshot matrix are rapidly decaying (Figure 4) so that the only few POD modes would be sufficient to approximate the fully discetized NLS equation. For POD basis with $l = 3$ (Figure 3), hence, the energy is well preserved as for the fully discretized form (Figure 2) and more accurate solutions are obtained with increasing number of POD modes (Figure 4).

Table 1. L_∞-errors of the energy and solutions

POD	Energy (ROM-AVF)	Energy (ROM-MID)	Solution (ROM-AVF)	Solution (ROM-MID)
2	6.125e-002	6.107e-002	2.164e-001	2.159e-001
3	5.529e-002	5.528e-002	2.010e-001	2.011e-001
4	4.612e-002	4.609e-002	1.847e-001	1.835e-001
5	4.100e-002	4.095e-002	1.838e-001	1.817e-001

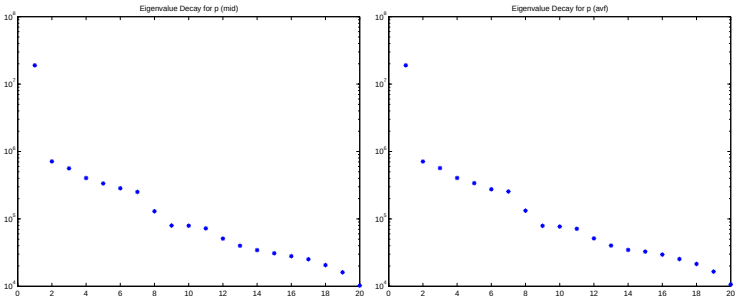

Fig. 1. Singular values: left: mid-point, right: AVF

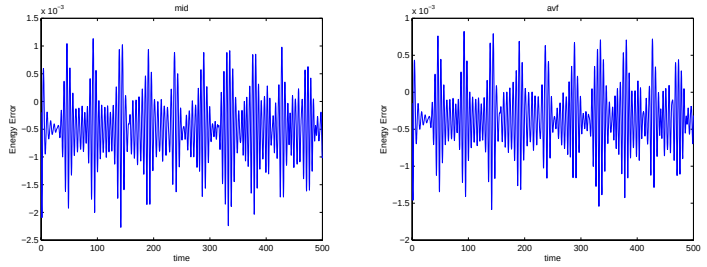

Fig. 2. Energy (full discretization): left: mid-point, right: AVF

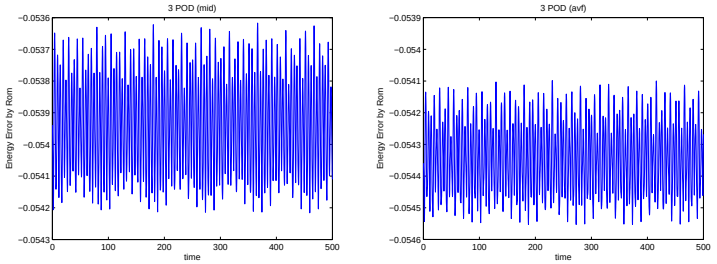

Fig. 3. Energy (POD, l=3) : left: mid-point, right: AVF

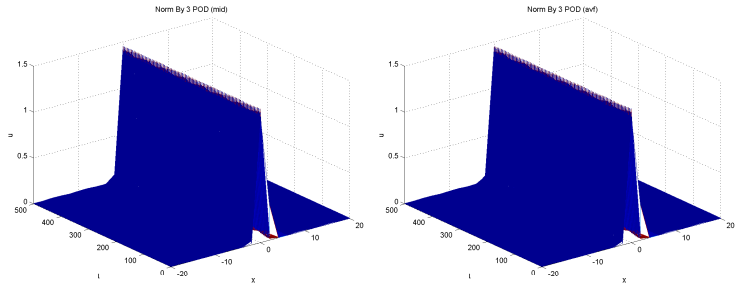

Fig. 4. ROM solutions with 3 POD modes: left: mid-point, right: AVF

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