the so called Hamiltonian,

ic

SYMPLETIC MODEL-REDUCTION WITH A WEIGHTED INNER PRODUCT*

BABAK MABOUDI AFKHAM†, ASHISH BHATT‡, AND JAN S. HESTHAVEN†

Abstract. Abstract to be added...

include abstract to have guide in structure/argumentation!

Key words.

~~bilinear form~~ ?

AMS subject classifications.

1. Introduction.

This is the introduction...

→ introduce other MOR

2. Hamiltonian Systems.

In this section we discuss the basic concepts around the geometry of symplectic linear vector spaces and introduce Hamiltonian and Generalized Hamiltonian systems.

2.1. Generalized Hamiltonian Systems.

Let $(\mathbb{R}^{2n}, \Omega)$ be a symplectic linear vector space, with $\mathbb{R}^{2n}$ the configuration space and $\Omega : \mathbb{R}^{2n} \times \mathbb{R}^{2n} \to \mathbb{R}$ a closed, skew-symmetric and non-degenerate $\boxed{\text{2-form}}$ on $\mathbb{R}^{2n}$. Given a smooth ~~Hamiltonian~~ function $H : \mathbb{R}^{2n} \to \mathbb{R}$, the *generalized Hamiltonian* equation of evolution reads

Q: what is a closed form? continuous?

add "Hamiltonian System"

$$
\begin{cases} \dot{z} = J_{2n} \nabla_z H, \\ z(0) = z_0. \end{cases} \tag{1}
$$

(z)

Here $z \in \mathbb{R}^{2n}$ ~~is~~ are the configuration coordinates and J_{2n} is a full-rank and skew-symmetric $2n \times 2n$ matrix such that $\Omega(x, y) = x^T J_{2n} y$, for all state vectors $x, y \in \mathbb{R}^{2n}$ [11]. Note that one can always find a coordinate transformation $\tilde{z} = Vz$, with $V \in \mathbb{R}^{2n \times 2n}$ such that J_{2n} takes the form $\mathbb{J}_{2n}$ in the new coordinate system [4], and $\mathbb{J}_{2n}$ is the standard symplectic matrix given as

$$
\mathbb{J}_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}. \tag{2}
$$

Here 0_n and I_n are the zero matrix and the identity matrix of size $n \times n$, respectively. A central feature of Hamiltonian systems is the conservation of the Hamiltonian which we summarize in the following theorem.

give Def of ϕ_t (looks like a time-derivative)

THEOREM 2.1. *Consider the flow $\phi_t : \mathbb{R} \times \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ of the Hamiltonian system (1). Then $H \circ \phi_t = H$.*

Under a general coordinate transformation, the equations of evolution of a Hamiltonian system might not take the form (1). It turns out that only transformations which preserve the symplectic form, *symplectic transformations*, also preserve the form of a Hamiltonian system [6]. Suppose that $(\mathbb{R}^{2n}, \Omega)$ and $(\mathbb{R}^{2k}, \Lambda)$ are two symplectic linear vector spaces. A transformation $\alpha : \mathbb{R}^{2n} \to \mathbb{R}^{2k}$ is a symplectic transformation if

$$
\Omega(x, y) = \Lambda(\alpha(x), \alpha(y)), \quad \text{for all } x, y \in \mathbb{R}^{2n}. \tag{3}
$$

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†Institute of Mathematics (MATH), School of Basic Sciences (FSB), Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland (babak.maboudi@epfl.ch, jan.hesthaven@epfl.ch).

‡~~Add your info here~~.

} is affiliation, not funding acknowledgement

German Research Foundation, HA... & SimTech (see earlier papers) of the ~~form~~ $d(x)=Ax$ with

In matrix notation, i.e. when we agree upon a set of basis vectors for $\mathbb{R}^{2n}$ and $\mathbb{R}^{2k}$, a linear symplectic transformation is a matrix $A \in \mathbb{R}^{2n\times 2k}$ that satisfies

$$A^T J_{2n} A = J_{2k}. \tag{4}$$

We are interested in a class of symplectic transformations that transform a symplectic form J_{2n} into the standard symplectic form $\mathbb{J}_{2k}$.

DEFINITION 2.2. *Let $J_{2n} \in \mathbb{R}^{2n\times 2n}$ be a full-rank skew-symmetric matrix. A matrix $A \in \mathbb{R}^{2n\times 2k}$ is J_{2n}-symplectic if*

$$A^T J_{2n} A = \mathbb{J}_{2k}. \tag{5}$$

~~general~~

Note that in the literature [11, 6], symplectic transformations are commonly referred to only $\mathbb{J}_{2n}$-symplectic transformations and not to the cases discussed above.

It is natural to expect a numerical integrator that solves (1) to also satisfy the conservation law expressed in theorem 2.1. Conventional numerical time integrators, e.g. ~~the~~ Runge-Kutta methods, do not generally conserve the symplectic symmetry of Hamiltonian systems and often result in a wrong behaviour of the solution over long time-integration. The class of time-integrators for (1) that preserve the Hamiltonian are called *Poisson integrators* or *symplectic integrators* when $J_{2n} = \mathbb{J}_{2n}$. These methods preserves the symplectic symmetry of Hamiltonian systems that result in the stability of the solution over long time-integration. The implicit midpoint rule

Condition for both notions? What if $J_{2n} \neq \mathbb{J}_{2n}$?

$$z_{n+1} = z_n + \Delta t \cdot J_{2n} \nabla_z H\left(\frac{z_{n+1}+z_n}{2}\right), \tag{6}$$

is an example of a second order Poisson integrator. For more on the construction and the applications of Poisson/symplectic integrators, we refer the reader to [6].

Here Δt indicates a uniform time step-size and $z_n \approx z(n\Delta t)$, $n \in \mathbb{N}_0$ denote approximations of the solution z of (1)

3. Model Order Reduction.

First, we

In this section we summarize basic concepts around ~~model order reduction~~ MOR. We discuss the conventional approach to ~~model order~~ MOR reduction with a weighted inner product. We then outline the main results in [1] regarding symplectic model reduction. In section 4 we shall combine the two concepts to introduce the symplectic model reduction of Hamiltonian systems with respect to a weighted inner product.

from

3.1. Model-Reduction with a Weighted Inner Product.

Consider a dynamical system of the form

$$\begin{cases} \dot{x}(t) = f(t,x), \\ x(0) = x_0. \end{cases} \tag{7}$$

where $x \in \mathbb{R}^m$ and the $f : \mathbb{R}\times\mathbb{R}^m \to \mathbb{R}^m$ is some continuous function. In this paper we may assume that time t is the only parameter that the solution vector x depends on. Nevertheless, it is straight forward to generalize the findings of this paper to the case where x also depends on ~~a set~~ of physical or geometrical parameters that belong to a closed and bounded subset of a Euclidean space.

? of parametric MOR

Suppose that x lies on or very close to a low dimensional linear subspace with the basis $V = [v_1|\dots|v_k]$, $v_i \in \mathbb{R}^m$ for $i = 1,\dots,k$. The approximated solution to (7) in this basis reads

$$x \approx \hat{x} = Vy, \tag{8}$$

$x \neq Vy$!!!

$\in \mathbb{R}^{m\times k}$

(matrix)

[perhaps worth introducing $\mathcal{V} := \cancel{\text{span}}$ colspan(V) as reduced space?]

to be $\quad \mathcal{V} \quad$ ~~states~~

(comments: In RB typically X is a space not a matrix) → K, G more appropriate

where y is the expansion coefficients of x in the basis of V. Note that the method of projecting x onto the span space of V depends on the inner product and the norm that are defined most appropriate to (7). We define the weighted inner product

$$[x, y]_X = x^T X y, \quad \text{for all } x, y \in \mathbb{R}^m, \tag{9}$$

→ perhaps $\langle \cdot, \cdot \rangle_X$?

for some symmetric and positive-definite matrix $X \in \mathbb{R}^{m \times m}$. We also refer to $\| \cdot \|_X$ as the X-norm associated to this inner product. If we choose V to be an ortho-normal basis with respect to the X-norm ($V^T X V = I_k$), then the operator

$$P_{X,V}(x) = V V^T X x, \quad \text{for all } x \in \mathbb{R}^m \tag{10}$$

becomes idempotent. This means that $P_{X,V}$ is a projection operator onto the span space of V.

Now suppose that $\{x(t_i)\}_{i=1}^N$ is a collection of N samples of the solution to (7) at time instances $t_1, \ldots, t_N$. We would like to find V such that it minimizes the collective projection error of the samples onto the span space of V. This corresponds to the minimization problem

This is the so called proper orthogonal decomposition (POD) [Volkwein Book Chapter in "Model reduction & approx." SIAM 2017]

$\mathcal{V}$ = colspan(V)

(nicer as smooth)

$$\begin{aligned} &\underset{V \in \mathbb{R}^{m \times k}}{\text{minimize}} && \sum_{i=1}^N \| x_i - P_{X,V}(x_i) \|_X^2, \\ &\text{subject to} && V^T X V = I_k. \end{aligned} \tag{11}$$

Following the derivations in [14] the above minimization is equivalent to

$$\begin{aligned} &\underset{V \in \mathbb{R}^{m \times k}}{\text{minimize}} && \| \tilde{S} - \tilde{V} \tilde{V}^T \tilde{S} \|_2^2, \\ &\text{subject to} && \tilde{V}^T \tilde{V} = I_k. \end{aligned} \tag{12}$$

where $\tilde{V} = X^{1/2} V$, $\tilde{S} = X^{1/2} S$, S is the matrix that contains samples $\{x(t_i)\}_{i=1}^N$ in its columns referred to as the *snapshot matrix*, and $X^{1/2}$ is the matrix square root of X. According to Schmidt-Mirsky-Eckart-Young theorem [10] the solution $\tilde{V}$ to the minimization (12) is the truncated singular value decomposition (SVD) of $\tilde{S}$. The basis V ~~can~~ is then ~~be computed from~~ $V = X^{-1/2} \tilde{V}$. The reduced system to (7) corresponding to the basis V and the projection $P_{X,V}$ then is

is. Note that (12) & this computation strategy is not generally practical as ~~[illegible]~~ computing $X^{1/2}$ involves Cholesky decomposition which may be prohibitive. Instead, ~~one computes~~ ~~[illegible]~~ one computes an Eigenvalue decomposition of a Gramian matrix, see Remark... in [Haasdonk, RB Tutorial, book chapter in Model Red. & Appl., SIAM 2017]

$$\begin{cases} \dot{y}(t) = V^T X f(t, V y), \\ y(0) = V^T X x_0. \end{cases} \tag{13}$$

If k can be chosen such that $k \ll m$, then the reduced system (13) can potentially be evaluated significantly faster than the full order system (7). We refer the reader to [7, 14] for further information regarding the development and the efficiency of reduced order models.

~~It is worthwhile to note that the proper orthogonal decomposition (POD) method [7] corresponds to taking $X = I_m$. In this case, the projection $P_{I_m,V}$ constructed from the solution to (11) becomes the POD-Galerkin projection [7].~~

3.2. Symplectic Model-Reduction. Conventional model reduction methods, e.g. those introduced in Section 3.1, do no generally preserve the conservation law expressed in Theorem 2.1. This often results in the lack of robustness in the reduced system over long time-integration. In this section we summarize the main findings

As mentioned earlier,

+[Haasdonk, RB tutorial]

In particular there exist many other ways of basis generation, e.g. greedy strategies, Krylov subspace methods, Balanced Truncation, etc. [Antoulas 2005, Book SIAM]

(POD is always in a functional space, i.e. weighted. See Volkwein) of [1] regarding symplectic model reduction of Hamiltonian systems with respect to the standard Euclidean inner product. Symplectic model reduction aims to construct a reduced system that conserves the geometric symmetry expressed in ~~theorem~~ T 2.1 which helps with the stability of the reduced system. Consider a Hamiltonian system of the form

(Why now specialized H?)

$$\begin{cases} \dot{z}(t) = \mathbb{J}_{2n} L z(t) + \mathbb{J}_{2n} \nabla_z f(z), \\ z(0) = z_0. \end{cases} \tag{14}$$

Here $z \in \mathbb{R}^{2n}$ is the state vector, $L \in \mathbb{R}^{2n\times 2n}$ is a symmetric and positive-definite matrix and $f : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is some function. Note that the Hamiltonian for system (14) is given by $H(z) = z^T L z + f(z)$. Suppose that the solution to (14) lies on a low dimensional symplectic subspace. Let $A \in \mathbb{R}^{2n\times 2k}$ be a $\mathbb{J}_{2n}$-symplectic basis containing the basis vectors $A = [e_1|\dots|e_k|f_1|\dots|f_k]$ such that $z = Ay$ with y the expansion coefficients of $\hat{z}$ in this basis. Using the symplectic inverse $A^+ = \mathbb{J}_{2k}^T A^T \mathbb{J}_{2n}$ we can construct the reduced system

$\frac{1}{2}$

or is close to

$z \approx \hat{z} = Ay$

$$\dot{y} = A^+ \mathbb{J}_{2n} (A^+)^T A^T L A y + A^+ \mathbb{J}_{2n} (A^+)^T \nabla_y f(Ay). \tag{15}$$

We refer the reader to [1] for the details of the derivation. It is shown in [13] that $(A^+)^T$ is also $\mathbb{J}_{2n}$-symplectic, therefore $A^+ \mathbb{J}_{2n} (A^+)^T = \mathbb{J}_{2k}$ and (15) reduces to

$\in \mathbb{R}^{n\times r}$

$$\dot{y}(t) = \mathbb{J}_{2k} A^T L A y + \mathbb{J}_{2k} \nabla_y f(Ay). \tag{16}$$

This system is a Hamiltonian system with the Hamiltonian $\tilde{H}(y) = y^T A^T L A y + f(Ay)$. To reduce the complexity of evaluating the nonlinear term in (16), we may apply the discrete empirical interpolation method (DEIM) [2, 3]. Assuming that $\nabla_z f(z)$ lies on a low dimensional subspace with a basis U, the DEIM approximation reads

$\frac{1}{2}$

or close to

[Wirtz/Sorensen/Haasdonk SISC 2014]

$$\nabla_z f(z) \approx U(P^T U)^{-1} P^T \nabla_z f(z). \tag{17}$$

Here P is the interpolating index matrix [3]. For a general choice of U the approximation in (17) destroys the Hamiltonian structure in (14). It is shown in [1] that by taking $U = (A^+)^T$ we can recover the Hamiltonian structure in (16). Therefore, the reduced system to (14) becomes

is inserted in

$$\begin{cases} \dot{y}(t) = \mathbb{J}_{2k} A^T L A y + \mathbb{J}_{2k} (P^T (A^+)^T)^{-1} P^T \nabla_z f(Ay), \\ y(0) = A^+ z_0. \end{cases} \tag{18}$$

y

Note that the Hamiltonian formulation of (18) allows us to integrate it using a symplectic integrator. This conserves the symmetry expressed in ~~theorem~~ T 2.1 at the level of the reduced system. It is also shown in [1, 13] that the stability of the critical points of (14) is preserved in the reduced system. Therefore, the overall behavior (18) is close to the full order Hamiltonian system (14). In the next subsection we discuss methods for generating a $\mathbb{J}_{2n}$-symplectic basis A.

3.3. The Greedy Generation of a $\mathbb{J}_{2n}$-Symplectic Basis. Suppose that S is the snapshot matrix containing the time instances $\{z(t_i)\}_{i=1}^N$ of the solution to (14). We would like to find the $\mathbb{J}_{2n}$-symplectic basis A such that the collective symplectic projection error of samples in S onto the span space of A is minimized.

worth introducing $\mathcal{A} = \mathrm{colspan}(A)$

$$\begin{aligned} &\underset{A\in\mathbb{R}^{n\times k}}{\text{minimize}} && \|S - P^{\text{symp}}_{I,A}(S)\|_F^2, \\ &\text{subject to} && A^T \mathbb{J}_{2n} A = I_{2k}. \end{aligned} \tag{19}$$

$2n\times 2k$

$\mathbb{J}_{2k}$

Experiments:
use example with non
equispaced spatial
discretization

product ~~projection~~

Here $P_{I,A}^{\text{symp}} = AA^+$ is the symplectic projection operator with respect to the standard Euclidean inner ~~production~~ onto the span space of A. Note that $P_{I,A}^{\text{symp}} \circ P_{I,A}^{\text{symp}} = P_{I,A}^{\text{symp}}$ [13, 1].

Direct approaches to solve (19) are often inefficient. Some SVD-type solutions to (19) are proposed by [13]. However, these solutions are only suited for the standard Euclidean inner product and cannot be generalized to be compatible with a weighted inner product.

(why not?)

The greedy generation of a $\mathbb{J}_{2n}$-symplectic basis aims to find a near optimal solution to (19) in an iterative procedure. This method enhances the overall accuracy of the basis by adding the best possible basis vectors at each iteration. Suppose that $A_{2k} = [e_1|\dots|e_k|f_1|\dots|f_k]$ is a $\mathbb{J}_{2n}$-symplectic basis. We may assume that A_{2k} is also an ortho-normal basis [1]. The first step of the greedy methods is to find the snapshot $\cancel{z(t^{k+1})}$), that is worst approximated by the basis A_{2k}.

$z_{k+1} \in \{z(t_i)\}_{i=1}^{N}$

$$z_{k+1} \; \cancel{t^{k+1}} := \underset{z \in \{z(t_i)\}_{i=1}^{N}}{\operatorname{argmax}} \|z(\cancel{t}) - P_{I,A}^{\text{symp}}(z(\cancel{t}))\|_2. \tag{20}$$

If e_{k+1} is the vector obtained by $\mathbb{J}_{2n}$-orthogonalize(ing) $\cancel{z(t^{k+1})}$ z_{k+1} with respect to A_{2k} [1], then the enriched basis A_{2k+2} reads

give formula for e_{k+1}

$$A_{2k+2} = [e_1|\dots|e_k|e_{k+1}|f_1|\dots|f_k|\mathbb{J}_{2n}^T e_{k+1}]. \tag{21}$$

Q: why $e_{k+1} \neq 0$?
Q: why $\mathbb{J}_{2n}^T e_{k+1}$ linearly indep. of e_{k+1}?

It is easily checked that A_{2k+2} is $\mathbb{J}_{2n}$-symplectic and ortho-normal. We point out that the choice of orthogonalization routine generally depends on the application. In this paper we use the symplectic Gram-Schmidt (GS) process as the orthogonalization routine.

Evaluation of the projection error is impractical for parametric problems. The loss in the Hamiltonian function can be used as a cheap surrogate to the projection error.

$$\omega^{k+1} = \underset{\omega \in \Omega}{\operatorname{argmax}} \, |H(z(\omega)) - H(P_{I,A}^{\text{symp}}(z(\omega)))|. \tag{22}$$

Here $\Omega \subset \mathbb{R}^d$ is a closed and bounded set of parameters that the original Hamiltonian system depends on. It is shown in [1] that the loss in the Hamiltonian is constant in time. Therefore, ω^{k+1} can be identified prior to time integration.

We summarize the greedy algorithm for generating a $\mathbb{J}_{2n}$-symplectic basis in Algorithm 1. The first loop constructs a $\mathbb{J}_{2n}$-symplectic (basis) for the Hamiltonian system (14), and the second loop adds the nonlinear snapshots to the basis. We refer the reader to [1] for more detail ~~on the generation and properties of a symplectic basis~~. In Section ?? we will show how this algorithm can be generalized to support any weighted inner product.

4. Symplect(ic) Model-Redcution with a Weighted Inner Product. In this section we will combine the concept of model reduction with a weighted inner product in section 3.1 with the symplectic model model reduction discussed in section 3.2. We will discuss how the new method can be viewed as a natural extension to the original symplectic method. Finally we generalize the greedy method for the symplectic basis generation, and the symplectic model reduction of nonlinear terms to be compatible with any weighted inner product.

4.1. Generalization of the Symplectic Projection. As discussed in section 3.1, proper error analysis of methods for solving partial differential equations often

? more comments for parameter set.
make more clear that you now comment on an extension for parametric problems: need to select new parameter, then run greedy extension for this parameter, then repeat parameter selection, greedy, starting from previous basis not start with 0.

z_{k+1} $\quad Z \quad z \in \{z(t_i)\}_{i=1}^N$

$\mathcal{G} :=$ and $\{\nabla f(z(t_i))\}_{i=1}^N$

Algorithm 1 The greedy algorithm for generation of a $\mathbb{J}_{2n}$-symplectic basis

Input: Tolerated projection error δ, initial condition z_0

1. $t^1 \leftarrow t = 0$
2. $e_1 \leftarrow z_0$
3. $A \leftarrow [e_1|\mathbb{J}_{2n}^T e_1]$
4. $k \leftarrow 1$
5. **while** $\|z(t) - P_{I,A}^{\text{symp}}(z(t))\|_2 > \delta$ for all $t \in [0,T]$ $\quad z \in Z$
6. $\quad t^{k+1} := \underset{t\in[0,T]}{\text{argmax}} \|z(t) - P_{I,A}^{\text{symp}}(z(t))\|_2$
7. $\quad \mathbb{J}_{2n}$-orthogonalize $z(t^{k+1})$ to obtain e_{k+1}
8. $\quad A \leftarrow [e_1|\dots|e_{k+1}|\mathbb{J}_{2n}^T e_1|\dots,\mathbb{J}_{2n}^T e_{k+1}]$
9. $\quad k \leftarrow k+1$
10. **end while**
11. compute $(A^+)^T = [e_1'|\dots|e_k'|\mathbb{J}_{2n}^T e_1'|\dots|\mathbb{J}_{2n}^T e_k']$
12. **while** $\|\nabla f(z(t)) - P_{I,(A^+)^T}^{\text{symp}}(\nabla f(z(t)))\|_2 > \delta$ for all $t \in [0,T]$ $\quad g \in \mathcal{G}$
13. $\quad t^{k+1} := \underset{t\in[0,T]}{\text{argmax}} \|\nabla f(z(t)) - P_{I,(A^+)^T}^{\text{symp}}(\nabla f(z(t)))\|_2$ $\quad g_{k+1}$
14. $\quad \mathbb{J}_{2n}$-orthogonalize $\nabla f(z(t^{k+1}))$ to obtain e_{k+1}'
15. $\quad (A^+)^T \leftarrow [e_1'|\dots|e_{k+1}'|\mathbb{J}_{2n}^T e_1'|\dots|\mathbb{J}_{2n}^T e_{k+1}']$
16. $\quad k \leftarrow k+1$
17. **end while**
18. $A \leftarrow \left(\left((A^+)^T\right)^+\right)^T$

Output: $\mathbb{J}_{2n}$-symplectic basis A.

rather input $\{z(t_i)\}_{i=1}^N$ then select from this.

Z

Currently sounds like repeated solving for $z(t)$ is required.

Q: why second loop required??

why $(A^+)^T$ instead of A?

require using a weighted inner product. This is particularly important when dealing with Hamiltonian systems where the system energy can induce a norm that is fundamental to the dynamics of the system.

Consider a Hamiltonian system of the form (14) together with the weighted inner product defined in (9) with $m = 2n$. Also suppose that the solution z (14) lies on a $2k$ dimensional symplectic subspace with the basis A. We would like to construct a projection operator that minimizes the projection error with respect to the X-norm while preserving the symplectic dynamics of (14) in the projected space. Consider the operator $P : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ defined as

$$P = A\mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X. \tag{23}$$

It is easy to show that P is idempotent if and only if

$$\mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X A = I_{2k}. \tag{24}$$

This means that P is a projection operator onto the span space of A. Suppose that S is the snapshot matrix containing time samples $\{z(t_i)\}_{i=1}^N$ of the solution to (14). We like to find the basis A that minimizes the projection error of the samples in S with respect to $P_{X,A}^{\text{symp}}$.

$$\begin{aligned} &\underset{A\in\mathbb{R}^{2n\times 2k}}{\text{minimize}} && \|S - P(S)\|_X, \\ &\text{subject to} && \mathbb{J}_{2k}^T A^T X \mathbb{J}_{2n} X A = I_{2k}. \end{aligned} \tag{25}$$

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