UFR de **mathématique** et d'**informatique**
Université de Strasbourg

Inria

Non-linear reduced order models for Hamiltonian systems

Internship presentation

Master 2 Calcul Scientifique et Mathématiques de l'Information

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Notations

Work space : $(\mathbf{R}^{2n}, \omega_{2n})$

Studied system : a parametrised Hamiltonian system for $H_{g \in G} \in \mathcal{C}^1(\mathbf{R}^{2n}, \mathbf{R})$:

$$\begin{cases} \dot{x}_g(t) = X_{H_g}(x_g(t)) \quad \forall t \in [0, T], \\ x_g(0) = x_0(g). \end{cases}$$

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Recall that for $H : \mathbf{R}^{2n} \to \mathbf{R}$:

$$\omega_{2n}(X_H, \cdot) = dH.$$

With $\mathbf{J}_{2n}$ the matrix of ω for the Euclidian scalar product :

$$\omega_{2n}(\cdot, \cdot) = \langle \mathbf{J}_{2n} \cdot, \cdot \rangle, \qquad \mathbf{J}_{2n} = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix},$$

$$X_H = \mathbf{J}_{2n} \nabla H.$$

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Problem :

the system may come from the discretisation of a PDE

$\rightarrow 2n =$ original dimension of the PDE $\times$ nbr of discretisation cells

$\rightarrow$ n can be very large

$\rightarrow$ high cost for the solutions computation

Reduced order models for Hamiltonian systems

Hypothesis : $\{x_g(t)\}_{t\in[0,1],g\in G} \subset \bar{\Sigma} \subset \mathbf{R}^{2n}$, for $\bar{\Sigma}$ a submanifold of dimension $\ll 2n$.

Objective : find a reduce order model in Hamiltonian form, that is :

- a submanifold $\Sigma^{2k} \subset \mathbf{R}^{2n}$, $k \ll n$
- a *decoder* $D : \mathbf{R}^{2k} \to \Sigma^{2k} \subset \mathbf{R}^{2n}$ and an *encoder* $E : \Sigma^{2k} \to \mathbf{R}^{2k}$
- a vector field $f_g : \Sigma^{2k} \to T\Sigma^{2k}$

$$\text{such that} \quad \left\{ D(\hat{x}_g) = x_g \quad \text{where} \quad \begin{cases} \dot{\hat{x}}_g = f_g(\hat{x}_g), \\ \hat{x}(0) = Ex_0(g) \end{cases} \qquad \text{(reduced model)} \right.$$

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Reduced order model : building steps

Step 1. Compute a set of solutions in high dimension $\{x_l\}_l$,
with $x_{l=i*m+j} = (p_l, q_l) = x_{g_i}(t^j)$ for $\{g_i\}_{1\leq i\leq N} \subset G$ and $\{t_j\}_{1\leq j\leq m} \subset [0,1]$.

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Proper Symplectic Decomposition (PSD) : extraction of orthogonal modes (POD) in paired positions and momenta.

$$X = \overbrace{(\underbrace{p_1|\dots|p_{Nm}}_{momenta}\,|\,\underbrace{q_1|\dots|q_{Nm}}_{positions})}^{\in\mathcal{M}_{n,2N}(\mathbf{R})} \overset{SVD}{=} (\underbrace{u_1|\dots|u_k}_{A\in\mathcal{M}_{n,k}(\mathbf{R})}\;|\dots|u_n)\Lambda^t V \quad\longrightarrow\quad \underbrace{D = \begin{pmatrix} A & 0 \\ 0 & A \end{pmatrix}}_{\in\mathcal{M}_{2n,2k}(\mathbf{R})}$$

$\rightarrow$ Set $E = {}^t\mathbf{J}_{2k}{}^tD\mathbf{J}_{2n}$ the *symplectic (left) inverse* of D.

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Reduced system :

$$
\begin{aligned}
&\text{(init. problem)} & & \dot{x}_g = \mathbf{J}\nabla H_g(x_g)\\
&(x_g = D(\hat{x}_g)) & \iff\ & \frac{d}{dt}D(\hat{x}_g) = \mathbf{J}\nabla H_g(D(\hat{x}_g))\\
&\text{(chain rule)} & \iff\ & \nabla D(\hat{x}_g)\dot{\hat{x}}_g = \mathbf{J}\nabla H_g(D(\hat{x}_g))\\
& & \implies\ & {}^t\mathbf{J}_{2k}{}^t\nabla D(\hat{x}_g)\mathbf{J}_{2n}\nabla D(\hat{x}_g)\dot{\hat{x}}_g = {}^t\mathbf{J}_{2k}{}^t\nabla D(\hat{x}_g)\mathbf{J}_{2n}\mathbf{J}_{2n}\nabla H_g(D(\hat{x}_g)),\\
&(D \text{ is sympl.}) & \iff\ & {}^t\mathbf{J}_{2k}\mathbf{J}_{2k}\dot{\hat{x}}_g = {}^t\mathbf{J}_{2k}{}^t\nabla D(\hat{x}_g)(-I_{2n})\nabla H_g(D(\hat{x}_g)),\\
& & \iff\ & \dot{\hat{x}}_g = \mathbf{J}_{2k}\nabla(H_g\circ D)(\hat{x}_g).
\end{aligned}
$$

Problem 1 : need to come back in high dimension.

Reduced order model : building steps

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Step 2. Find Σ^{2k}, D and E from $\{x_l\}_{l.}$

Step 3. Find $f_g (= X_{\hat{H}_g})$ on Σ^{2k} from $\{x_l\}_{l.}$

Physical system of study

Test case : non-linear piano string model from [Chabassier and Joly, 2010]

$$\begin{cases} H_g(p,q,t) = \displaystyle\int_\Omega \frac{1}{2}|p|^2 + V_g(\partial_z q)dz \\ x_0(g) = z \in \Omega \mapsto (0.1\sin(2\pi z), 0.05\sin(2\pi z)) \end{cases}$$

with

- $\Omega = [0,1]$: the string,
- $x = (p_u, p_v, u, v)$: its deformation in the oscillation plane (u,v) and its speed (p_u, p_v),
- $g \in [0, 0.2]^2$: depends on the characteristics of the string,
- $V_g(u,v) = \frac{1-g}{2}u^2 + \frac{1}{2}v^2 + \frac{g}{2}(u^2 v + \frac{1}{4}u^4)$.

Problem 2 : PSD does not work on the previous system.

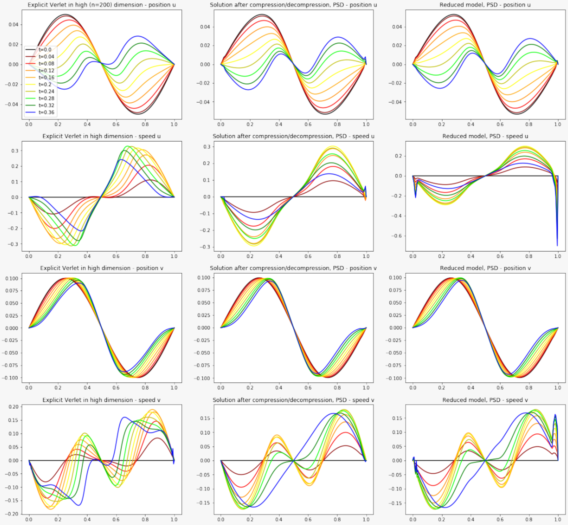

Figure – On each column : (u, p_u, v, p_v). Col 1 : x_g. Col 2 : DEx_g. Col 3 : $\hat{x}_g$.
$g = 0.99$, $D = D_{psd}$, $\hat{H}_g = H_g \circ D$, $N = 10$, $n = 200$, $k = 3$, $dt = 0.0005$, $m = 800$.

How to improve the reduction ?

Keep Σ^{2k} but change the way of solving equation on it.

- **Quadratic correction :** replace D by $D + \phi_\lambda$ (adaptation of [Geelen et al., 2023] in the Hamiltonian case) or $D \circ \phi_\lambda$.

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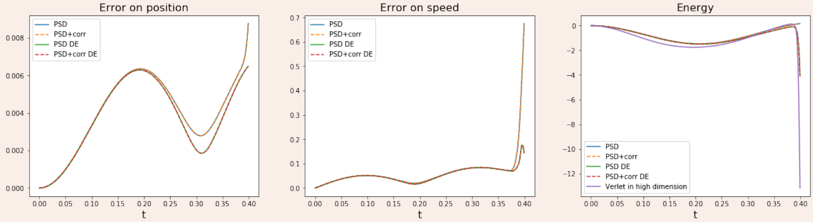

Figure – Errors on trajectories computed with the reduced model, with and without correction and energy along them. ($D_{corr} = D \circ \phi_\lambda, \phi_\lambda = (id - dP, id)$ a shear, $P \in \mathcal{P}^3(\mathbf{R})$).

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  - did not give satisfying results
  - still have to come back in high dimension to compute $\hat{H}_g$
- **Hyperreduction :** keep D but replace $H_g \circ D$ by a Hamiltonian function $\hat{H}_g$ in $\mathbf{R}^{2k}$ which gives good trajectories : $D\hat{x}_g \approx x_g$.
  - here, we take an optimal control approach

Hyperreduction via optimal control

Take $F = \{f_i\}_{1 \leq i \leq K} \subset \mathcal{C}^2(\mathbf{R}^{2k}, \mathbf{R})$.

Optimisation problem :

$$\mathcal{L}_\alpha(\theta) = \int_{g \in G} \| D\hat{x}_{g,\theta}(t) - x_g(t) \|_{L^2}^2 \, dt + \alpha \|\theta\|_1,$$

- $\hat{H}_{g,\theta} := \sum_{i=1}^K \theta_i f_i$ for $\theta \in \mathbf{R}^K$,
- $\hat{x}_{g,\theta} : [0,1] \to \mathbf{R}^{2k}$: solution of the reduced model with $\hat{H}_{g,\theta}$ as Hamiltonian,
- $\alpha \geq 0$: sparsity coefficient.

In practise : use a gradient descent

implies to have an explicit expression for $\nabla \mathcal{L}$

$\to$ find it with an adjoint method

Hyperreduction : adjoint method

Step 1. Note $\mathcal{F} : \theta \mapsto \hat{x}_\theta$. Developing $\mathcal{L}_\alpha(\theta + h)$, we find

$$d_\theta \mathcal{L}_g \cdot h = 2\langle d_\theta \mathcal{F}(h), \mathcal{F}(\theta) - {}^t D x_g \rangle_{L^2}.$$

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Step 2. $d_\theta \mathcal{F}(h)$ is solution of

$$\begin{cases} \dot{z}(t) = d_{\mathcal{F}(\theta)(t)} X_{\hat{H}_\theta}(z(t)) + X_{\hat{H}_h}(\mathcal{F}(\theta)(t)) \quad \forall t \in [0,1], \\ z(0) = 0_{\mathbf{R}^{2k}}. \end{cases}$$

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Adjoint problem

$$\begin{cases} \dot{a}(t) = d_{\mathcal{F}(\theta)(t)} X^*_{\hat{H}_\theta}(a(t)) + \Big(\mathcal{F}(\theta)(t) - {}^t D x_g(t)\Big) \quad \forall t \in [0, 1], \\ a(T) = 0_{\mathbf{R}^{2k}}. \end{cases}$$

Hyperreduction : adjoint method

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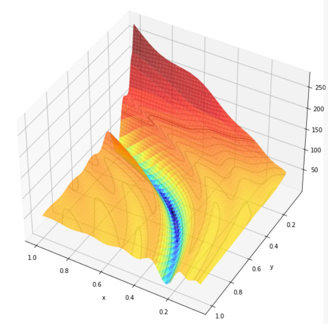
Step 3. Insert a in the expression of $d_\theta \mathcal{L}_g \cdot h$ and integer by parts.

$$d_\theta \mathcal{L}_g(h) = \langle -2 \int_0^1 \mathbf{X}\Big(\mathcal{F}(\theta)(t)\Big) a(t) dt, h \rangle_{\mathbf{R}^K}$$

where $\mathbf{X} \in \mathcal{M}_{K,2k}(\mathcal{C}^0(\mathbf{R}^{2k}, \mathbf{R}))$ depends on F.

Toy example : classical gradient descent

Test case 1 : $n = k = 1, D = Id, (p_0, q_0) = (1, 0)$
$H : (p, q) \in \mathbf{R}^2 \mapsto \frac{1}{2}p^2 + \frac{1}{2}q^2$
$F = \{(p, q) \mapsto p^2, (p, q) \mapsto q^2\}$



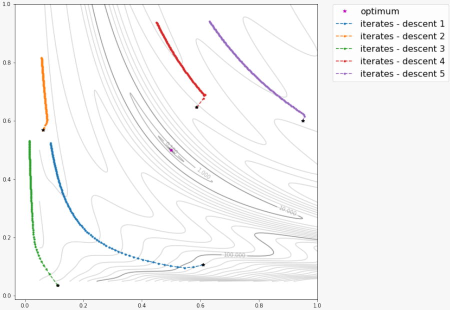


Figure – Graph of $\mathcal{L}$ (left) and iterates of a classical gradient descent starting from different points in the parameter space on level sets of $\mathcal{L}$ (right).

Variation on the classical gradient descent

Algorithm 1 Progressive gradient descent

Require: $\theta_0 \in \mathbf{R}^K, \alpha, \eta, \rho > 0$, $G = \{g_i\}_{1_leqi \leq N}, x_G := \{x_{g_i}\}_i, w \in [\![1, m]\!], \Delta t, \mathbf{X}$

$\theta \leftarrow \theta_0$
while $\frac{\|\nabla \mathcal{L}(\theta)\|}{\|\nabla \mathcal{L}(\theta_0)\|} > \eta$ **do**
    $\nabla \leftarrow \frac{\alpha\theta}{\sqrt{\theta^2+\epsilon}}$
    for $i = 0, ..., \lfloor \frac{m}{w} \rfloor$ **do**
        $b \leftarrow iw$
        $c \leftarrow b + w$
        for all $g \in G$ **do**
            compute primal solution $x_{\theta,g}$ starting at $x_0 = x_g(b\Delta t)$ on $[b\Delta t, c\Delta t]$.
            compute dual solution $a_{\theta,g}$ from $x_{\theta,g}$ ending at $a(c\Delta t) = 0$ on $[b\Delta t, c\Delta t]$.
            compute $\nabla \mathcal{L}_g(\theta)$ with a_θ and x_θ on the interval $[b\Delta t, c\Delta t]$.
            $\nabla \leftarrow \nabla + \nabla \mathcal{L}_g(\theta)$
        end for
        $\theta \leftarrow \theta - \rho\nabla$
    end for
end while

Toy example : modified gradient descent

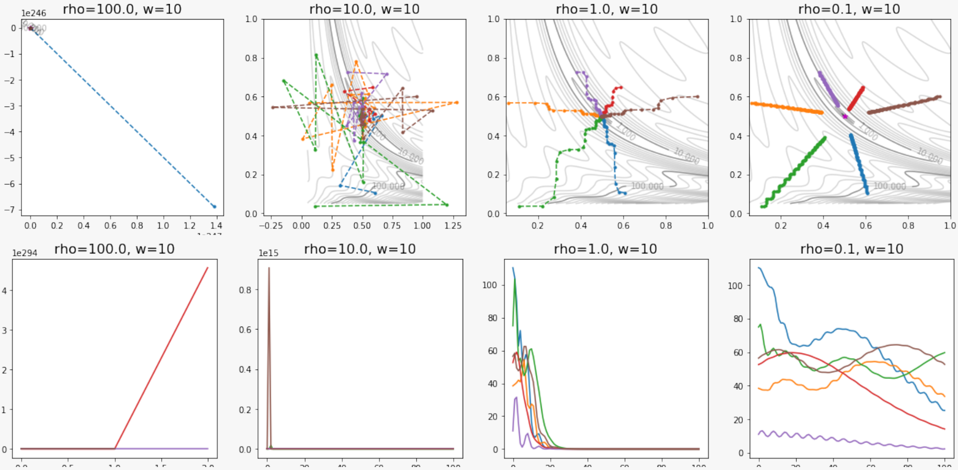


Figure – Iterates of a modified gradient descent starting from different points in the parameter space on level sets of $\mathcal{L}$.

Sparse Identification of Non-linear Dynamics

SINDy method : proposed in [Brunton et al., 2016]

Train set : $G =$ set of IC, $G_{train} = \{x_0^i\}_{1 \leq i \leq 5}$ uniformly sampled in $[0, 10]^2$

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$$F = \bigcup_{1 \leq n \leq 4} \left\{ x \mapsto \cos(\frac{2\pi}{n} p), x \mapsto \cos(\frac{2\pi}{n} q), x \mapsto \sin(\frac{2\pi}{n} p), x \mapsto \sin(\frac{2\pi}{n} q) \right\}$$

$$H : (p, q) \mapsto \sum_{i=1}^{16} \theta_i^* f_i, \quad \theta^* = (0, 0, 0, -0.9, 0.1, 2.1, 4.3, 0, 0, 0, 0, 3.0, 0, 0, 0, 0)$$

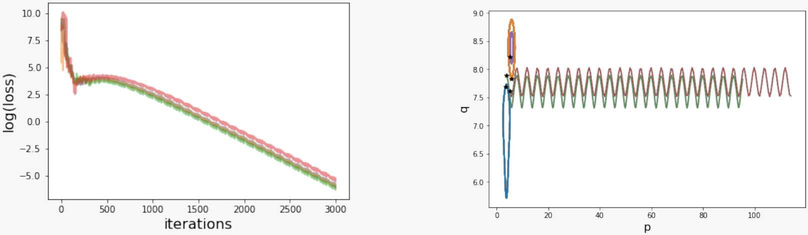

Figure – Decreasing of the loss during optimisation with the modified gradient descent (left) and trajectories obtained with final theta starting from 5 initial conditions outside G_{train} (coloured) compared to targetted trajectories (in gray) (right). $w = \Delta t$

Sparse Identification of Non-linear Dynamics

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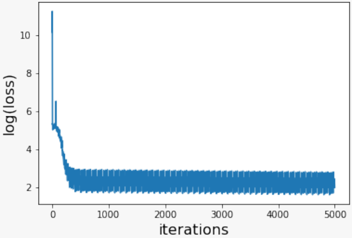
Train set : G = set of IC, $G_{train} = \{x_0^i\}_{1 \leq i \leq 5}$ uniformly sampled in $[0, 10]^2$

$$F = \{x \mapsto 1\} \cup \left(\bigcup_{1 \leq n \leq 24} \left\{ x \mapsto \cos(\frac{2\pi}{n} p), x \mapsto \cos(\frac{2\pi}{n} q) \right\} \right)$$

$$H : (p, q) \mapsto \frac{1}{2} p^2 + \frac{1}{2} q^2$$



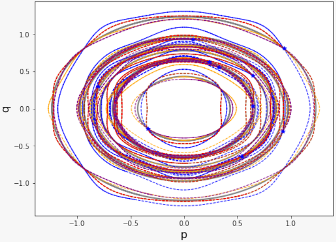


Figure – Decreasing of the loss during one optimisation process with the modified gradient descent (left) and trajectories obtained with final theta starting from 5 initial conditions outside G_{train} for 5 optimisation processes (right). $w = \Delta t$

Hyperreduction : discussion

- **On the modified gradient descent :**
  - could we use the additional hyperparameter w to improve the descent ?
  - how could we prove the convergence ?
    $\rightarrow$ idea : use policy-gradient theory

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  - how could we prove the convergence ?
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- **On SINDy application :**
  - the choice of F seems to be important
    $\rightarrow$ could we find an intelligent way to make this choice ?
    $\rightarrow$ idea : use several layers
- **On the reduced order model :**
  - for the moment, no satisfying results on this test case
    $\rightarrow$ problem in the choice of the family ?
    $\rightarrow$ further tests needed
  - theoretical guarantees ?
    $\rightarrow$ can we achieve a good reduction if we made an error on Σ^{2k} ?
    $\rightarrow$ what kind of error are admissible ?

Discussion : geometric guarantees for Hamiltonian reduced models

Conjecture

Let $n, k \in \mathbf{N}$ such that $k \ll n$. Consider two k-dimensional manifolds Σ^k and $\tilde{\Sigma}^k$ embedded in $\mathbf{R}^{2n}$ endowed with its usual symplectic structure. Denote by $i : \Sigma^k \to \mathbf{R}^{2n}$ and $\tilde{i} : \tilde{\Sigma}^k \to \mathbf{R}^{2n}$ the corresponding inclusions.
If k is sufficiently small in front of n, then there exists a symplectic homeomorphism

$$h : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$$

such that $h(\Sigma^k) = \tilde{\Sigma}^k$. Moreover, if i and $\tilde{i}$ are $\mathcal{C}^0$-close, then h is $\mathcal{C}^0$-close from the identity.

Objectives of the geometric part :

- Understand h-principle and its application in symplectic geometry (ref. [Eliashberg and Mishachev, 2002]).
- (medium term objective) Use it to prove the conjecture.

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