Projection-based model order reduction for the estimation of vector-valued variable of interest

Olivier Zahm (zahmo@mit.edu)
Massachusetts Institute of Technology

Groupe de travail problmes inverse et commande,
GIPSA-lab, November 14, 2016

Joint work with Marie Billaud-Friess and Anthony Nouy (École Centrale Nantes)

Context

- **Parameter-dependent equations** are involved in uncertainty quantification, optimization, control...

$$u(\xi) \in V \quad \text{such that} \quad \boxed{A(\xi)u(\xi) = b(\xi)}$$

Computationally intensive model : $\dim(V) \gg 1$.

- **Projection-based model order reduction (PB-MOR)**

$$u(\xi) \approx u_r(\xi) \in V_r$$

where $V_r \subset V$ is a subspace of dimension $r \ll \dim(V)$.

  - **Offline:** Construction of V_r (POD, Reduced Basis,...)
  - **Online:** Galerkin type projection on V_r

- **Among a vast literature...**
  - introduction to PB-MOR [Zahm, Phd thesis 2015]
  - PB-MOR as low-rank methods [Nouy 2015]
  - PB-MOR for control (dynamical) problems [Benner, Gugercin, Willcox 2015]

- **Vector-valued Variable of Interest (VoI):**

$$\boxed{s(\xi) = L(\xi)u(\xi) \ \in Z}$$

For example:

$$s(\xi) = (s_1(\xi), \dots, s_\ell(\xi)) \quad \text{with} \quad Z = \mathbb{R}^\ell$$
$$s(\xi) = u_{|\partial\Omega}(\xi) \quad \text{with} \quad Z = H^{1/2}(\partial\Omega)$$

- For $Z = \mathbb{R}$, the **primal-dual strategy** [Pierce, 2000] yields superconvergent estimate

$$\begin{pmatrix}\text{error in the} \\ \text{VoI } s(\xi)\end{pmatrix} \leq \begin{pmatrix}\text{error in the primal} \\ \text{variable } u(\xi)\end{pmatrix} \begin{pmatrix}\text{error in the dual} \\ \text{variable } q(\xi)\end{pmatrix}$$

where $q(\xi)$ is the solution of a dual (or adjoint) problem.

Plan

1/ **Stability of Galerkin-type projection**

- Petrov-Galerkin projection
- Projection by means of a saddle-point formulation

2/ **Estimation of vector-valued Variable of Interest**

- Generalization of the primal-dual strategy
- Use of the saddle-point formulation

3/ **Construction of the reduced spaces**

- Residual-based error estimator
- Greedy algorithm for the reduced spaces

Stability of Galerkin-type projection

Petrov-Galerkin projection

- Given a reduced space V_r and a test space W_r of **same dimension** r

$$u_r(\xi) \in V_r \qquad \langle A(\xi) u_r(\xi), w_r \rangle = \langle b(\xi), w_r \rangle \qquad \forall w_r \in W_r$$

- Requires the solution of a linear system of size r
- Biased projection : $u_r(\xi) \neq u_r^{\perp}(\xi) = \arg\min_{v_r \in V_r} \|u(\xi) - v_r\|_V$
- **Quasi-optimality result:**

$$\boxed{\|u(\xi) - u_r(\xi)\|_V \leq \frac{1}{\sqrt{1 - C_{\text{PG}}(\xi)^2}} \|u(\xi) - u_r^{\perp}(\xi)\|_V}$$

with

$$C_{\text{PG}}(\xi) = \max_{v_r \in V_r} \min_{w_r \in W_r} \frac{\|v_r - R_V^{-1} A(\xi)^* w_r\|_V}{\|v_r\|_V} \quad \in [0, 1]$$

where R_V denotes the **Riesz map** associated to $\|\cdot\|_V^2 = \langle R_V \cdot, \cdot \rangle$

- if $C_{\text{PG}}(\xi) = 0$, recover the orthogonal projection,
- if $C_{\text{PG}}(\xi) = 1$, no control of the projection error.

Possible choice for the test space W_r

$$C_{\mathrm{PG}}(\xi) = \max_{v_r \in V_r} \min_{w_r \in W_r} \frac{\|v_r - R_V^{-1} A(\xi)^* w_r\|_V}{\|v_r\|_V} \quad \in [0,1]$$

- **Standard Galerkin projection**

$$\boxed{W_r = V_r}$$

Optimal test space $C_{\mathrm{PG}}(\xi) = 0$ if $A(\xi)$ symmetric definite positive and if $\|\cdot\|_V$ is the "energy norm" : $R_V(\xi) = A(\xi)$.

- **Minimal residual formulation**

$$\boxed{W_r(\xi) = R_V^{-1} A(\xi) V_r}$$

Ensures stability $C_{\mathrm{PG}}(\xi) < 1$ for general operators.

- **Preconditioned Petrov-Galerkin projection** [Zahm and Nouy, 2016]

$$\boxed{W_r(\xi) = P_m(\xi)^* R_V V_r}$$

where $P_m(\xi)$ is an interpolation of $A(\xi)^{-1}$ at the points $\xi^{(1)}, \dots, \xi^{(m)}$. Then $C_{\mathrm{PG}}(\xi^{(i)}) = 0$ for $1 \le i \le m$.

Projection by Saddle point formulation [Dahmen et al., 2013]

- Given a subspace T_p of dimension p, let $u_{r,p}(\xi) \in V_r$ and $y_{r,p}(\xi) \in T_p$ be the solution of

$$\min_{v \in V_r} \max_{y \in T_p} \frac{\langle A(\xi)v - b(\xi), y\rangle}{\|A(\xi)^* y\|_{V'}}$$

- Requires the solution of a linear system of size $r + p$.

- Same quasi-optimality result as before, but with

$$C_{\mathrm{SP}}(\xi) = \max_{v_r \in V_r} \min_{y_p \in T_p} \frac{\|v_r - R_V^{-1} A(\xi)^* y_p\|_V}{\|v_r\|_V} \quad \in [0, 1]$$

- The saddle point formulation allows T_p to be of **larger dimension** than V_r
  - if $T_p \supset A(\xi)^{-*} R_V V_r$ then $C_{\mathrm{SP}}(\xi) = 0$
  - if $T_p \supset W_r(\xi)$ then $C_{\mathrm{SP}}(\xi) \le C_{\mathrm{PG}}(\xi)$

Estimation of vector-valued Variable of Interest

- Recall that $s(\xi) = L(\xi)u(\xi)$, with $L(\xi) : V \to Z$ a linear operator.
- Define the dual variable $Q(\xi) : Z' \to V$ as a **linear operator** such that

$$A(\xi)^* Q(\xi) = L(\xi)^*$$

- Given $u_r(\xi) \approx u(\xi)$ and $Q_k(\xi) \approx Q(\xi)$, the corrected estimator

$$\widetilde{s}(\xi) = L(\xi)u_r(\xi) - Q_k(\xi)^* \Big(b(\xi) - A(\xi)u_r(\xi) \Big)$$

is such that

$$\boxed{\|s(\xi) - \widetilde{s}(\xi)\|_Z \leq \|u(\xi) - u_r(\xi)\|_V \ \|A(\xi)^* \Big(Q(\xi) - Q_k(\xi) \Big)\|_{Z' \to V'}}$$

where $\| \cdot \|_{Z' \to V'}$ is an **operator norm**.

Projection-based approximation of the primal and dual variables

$$\|s(\xi) - \widetilde{s}(\xi)\|_Z \leq \|u(\xi) - u_r(\xi)\|_V \; \|A(\xi)^* \Big(Q(\xi) - Q_k(\xi) \Big)\|_{Z' \to V'}$$

- **Dual variable:** given $W_k^Q \subset V$, define $Q_k(\xi) : Z' \to W_k^Q$ as a solution of

  $$\min_{Q : Z' \to W_k^Q} \|A(\xi)^* \Big(Q(\xi) - Q \Big)\|_{Z' \to V'}$$

  In practice we only need to compute $Q_k(\xi)^* v$ for some $v \in V'$: this can be done by **solving a linear system of size k =** $\mathbf{dim}(W_k^Q)$.

- **Primal variable:** given $V_r \subset V$, define $u_r(\xi)$ as a Galerkin-type projection of $u(\xi)$ on V_r

Estimation of the VoI using the saddle point formulation

- Recall that $u_{r,p}(\xi) \in V_r$ and $y_{r,p}(\xi) \in T_p$ is the solution of

$$\min_{v \in V_r} \max_{y \in T_p} \frac{\langle A(\xi)v - b(\xi), y \rangle}{\|A(\xi)^* y\|_{V'}}$$

- Using $y_{r,p}(\xi) \in T_p$, the corrected estimate of the VoI

$$\widetilde{s}(\xi) = L(\xi)\Big(u_{r,p}(\xi) + R_V^{-1} A(\xi)^* y_{r,p}(\xi)\Big)$$

is such that:

$$\|s(\xi) - \widetilde{s}(\xi)\|_Z \leq \left(\frac{1}{\sqrt{1 - C_{\mathrm{SP}}(\xi)^2}} \min_{v \in V_r} \|u(\xi) - v\|_V \right) \left(\min_{Q : Z' \to T_p} \|A(\xi)^* (Q(\xi) - Q)\|_{Z' \to V'} \right)$$

- We can choose

$$T_p(\xi) = W_r(\xi) + W_k^Q \qquad (p \leq r + k)$$

  - $T_p(\xi) \supset W_r(\xi)$: improve the **projection** of the primal variable
  - $T_p(\xi) \supset W_k^Q$: improve the **approximation** of the dual variable
  - Don't need to solve the dual problem anymore !

Numerical illustration

Illustration (benchmark OPUS)

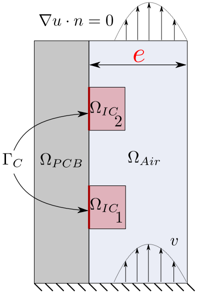
- Cooling of electronic components

$$\boxed{-\nabla \cdot \left(\kappa \nabla u\right) + D v \cdot \nabla u = f}$$

  - $\xi_1 = \kappa_{IC}$ diffusion coefficient in Ω_{IC} $[2\ 10^{-1}, 1.5\ 10^{2}]$
  - $\xi_2 = r$ thermal contact conductance on Γ_C $[10^{-1}, 10^{2}]$
  - $\xi_3 = D$ advection term $[5\ 10^{-4}, 10^{-2}]$
  - $\xi_4 = e$ geometrical parameter $[2.5\ 10^{-3}, 5\ 10^{-2}]$

- **VoI:** mean temperature of the two components ($Z = \mathbb{R}^2$)

$$s_i(\xi) = \frac{1}{\mathrm{mes}(\Omega_{IC_i})} \int_{\Omega_{IC_i}} u(\xi) \mathrm{d}\Omega, \qquad i \in \{1, 2\}$$



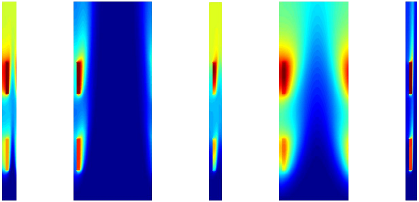


Figure: Five samples of the solution $u(\xi)$. Finite element approximation ($\dim(V) = 12000$, SUPG)

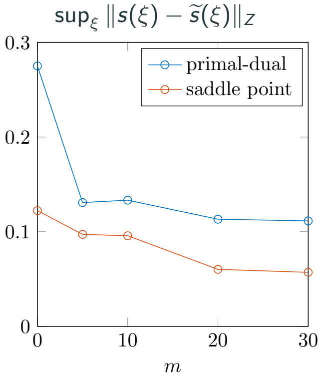
Reduced spaces: span of snapshots selected at random

- $V_r = \text{span}\{u(\xi^{(1)}), \dots, u(\xi^{(50)})\}$ $\qquad r = 50$
- $W_k^Q = \text{range}\{Q(\xi^{(1)})\} + \dots + \text{range}\{Q(\xi^{(25)})\}$ $\qquad k = 50$

Test spaces

- $W_r(\xi) = P_m^*(\xi) R_V V_r$
- $T_p(\xi) = W_r(\xi) + W_k^Q$ (saddle point)

Here, $P_m(\xi)$ is an interpolation of $A(\xi)^{-1}$ using m interpolation points selected in a greedy way ($P_0(\xi) = R_V^{-1}$).



$$\boxed{\operatorname{div}\big(K(\xi) : \varepsilon\big(u(\xi)\big)\big) = 0} \quad \text{with } K(\xi) = K_0\left(1_{\Omega_0} + \sum_{i=1}^{6} \xi_i 1_{\Omega_i}\right), \quad \xi_i \in [10^{-1}, 10^{1}]$$

- K_0 is the Hooke's tensor with Young modulus $E = 1$ and Poisson coefficient $\eta = 0.3$.
- **VoI:** vertical displacement over Γ: $\boxed{s(\xi) = u_{|\Gamma}(\xi) \ \in Z \equiv \mathbb{R}^{44}}$

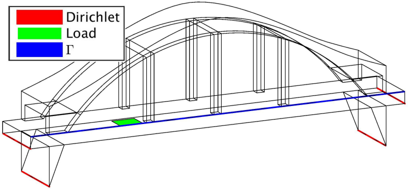


Figure: Geometry, boundary conditions, and variable of interest

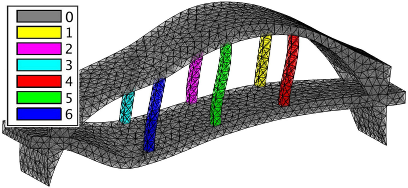


Figure: One realization of the solution $u(\xi)$. Finite element approximation ($n = 8916$)

Illustration (linear elasticity problem)

$$\boxed{\mathrm{div}\big(K(\xi) : \varepsilon\big(u(\xi)\big)\big) = 0} \quad \text{with } K(\xi) = K_0\left(1_{\Omega_0} + \sum_{i=1}^{6} \xi_i 1_{\Omega_i}\right), \quad \xi_i \in [10^{-1}, 10^{1}]$$

- K_0 is the Hooke's tensor with Young modulus $E = 1$ and Poisson coefficient $\eta = 0.3$.
- **VoI:** vertical displacement over Γ: $\boxed{s(\xi) = u_{|\Gamma}(\xi) \ \in Z \equiv \mathbb{R}^{44}}$

- **Reduced spaces:**
  - 20 snapshots for V_r : $r = 20$
  - 2 snapshots for W_k^Q : $k = 88$
- **Test spaces:**
  - $W_r = V_r$ (standard Galerkin)
  - $T_p = V_r + W_k^Q$

$$\sup_{\xi} \|s(\xi) - \widetilde{s}(\xi)\|_Z = \begin{cases} 2.60 & \text{(primal-dual)} \\ 0.356 & \text{(saddle point)} \end{cases}$$

Greedy construction of the reduced spaces

Residual-based error indicator for the VoI

- Let $\alpha(\xi) > 0$ such that

$$\alpha(\xi)\|\cdot\|_V \leq \|A(\xi)\cdot\|_{V'}$$

  - inf-sup constant or coercivity constant (using the theta-method)
  - a lower bound of the inf-sup constant (using SCM)

- **Upper bound of the error on the VoI**

$$\|s(\xi) - \widetilde{s}(\xi)\|_Z \leq \Delta(\xi) := \frac{1}{\alpha(\xi)}\|A(\xi)\widetilde{u}(\xi) - b(\xi)\|_{V'} \; \|A(\xi)^*\widetilde{Q}(\xi) - L(\xi)^*\|_{Z' \to V'}$$

  - Primal-dual $\begin{cases} \widetilde{u}(\xi) & = & u_r(\xi) \\ \widetilde{Q}(\xi) & = & Q_k(\xi) \end{cases}$

  - Saddle point $\begin{cases} \widetilde{u}(\xi) & = & u_{r,p}(\xi) + R_V^{-1}A(\xi)^* y_{r,p}(\xi) \\ \widetilde{Q}(\xi) & = & Q_p(\xi) \end{cases}$

  where $Q_p(\xi) : Z' \to T_p(\xi)$ a minimizer of the dual residual norm

Reduced Basis approach for constructing the reduced spaces

Loop over the following steps:

1/ Find the maximum of $\Delta(\xi)$:

$$\hat{\xi} \in \arg\max_{\xi} \Delta(\xi)$$

2/ Compute a factorization of $A(\hat{\xi})$ and solve:

$$u(\hat{\xi}) = A(\hat{\xi})^{-1} b(\hat{\xi}) \quad \text{and} \quad Q(\hat{\xi}) = A(\hat{\xi})^{-*} L(\hat{\xi})$$

3/ Enrich the reduced spaces

$$V_{r+1} = V_r + \text{span}\{u(\hat{\xi})\} \quad \text{and} \quad W^Q_{k+\dim(Z)} = W^Q_k + \text{range}\{Q(\hat{\xi})\}$$

Partial enrichment strategy:

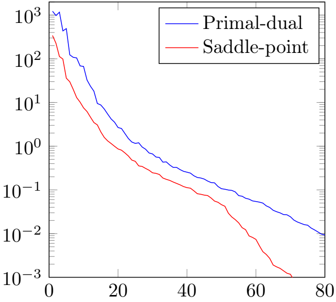
$$W^Q_{k+1} = W^Q_k + \text{span}\{Q(\hat{\xi})z\}$$

where $z \in Z'$ is the solution of

$$\max_{z \in Z'} \frac{\|A(\hat{\xi})^* \left(Q(\hat{\xi}) - \widetilde{Q}(\hat{\xi})\right) z\|_{V'}}{\|z\|_{Z'}} = \|A(\hat{\xi})^* \left(Q(\hat{\xi}) - \widetilde{Q}(\hat{\xi})\right)\|_{Z' \to V'}$$

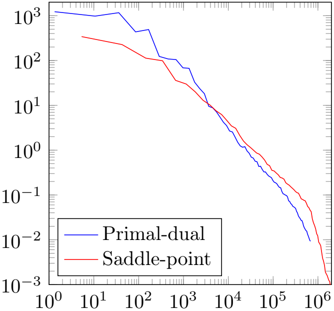
Illustration (linear elasticity problem)

$\max_{\xi} \Delta(\xi) = fct\big($**Offline complexity**$\big)$



r = number of operator factorizations computed during the greedy algorithm

$\max_{\xi} \Delta(\xi) = fct\big($**Online complexity**$\big)$



Cost for solving one reduced problem:

- Primal-dual: $C(r^3 + k^3) = 2Cr^3$
- Saddle-point: $C(p + r)^3 = 27Cr^3$

Conclusion

Summary

- Projection-based model order reduction methods for vector-valued VoI.
- Quality of the test space (Petrov-Galerkin projection) can be improved using preconditioners.
- For fixed reduced spaces, the saddle point formulation always improves the approximation of the VoI compared to the primal-dual strategy,
- but it may present higher online computational costs.

Perspectives

- Dedicated solver for the saddle point formulation,
- Balance the enrichment of V_r and W_k^Q to optimize the convergence rate.

Save the date : November 24, LJK seminar

Reduction of the input parameter space
for high-dimensional Bayesian inverse problem

Thank you for your attention.

About this presentation:

O. Zahm, M. Billaud-Friess and A. Nouy
Projection-based model order reduction methods for the estimation of vector-valued variables of interest.
ArXiv e-prints, March 2016.

About preconditioner $P_m(\xi) \approx A(\xi)^{-1}$:

O. Zahm and A. Nouy
Interpolation of inverse operators for preconditioning parameter-dependent equations.
SIAM Journal on Scientific Computing, 38(2), A1044–A1074, 2016.