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

\[ u(\xi) \in V \text{ such that } A(\xi)u(\xi) = b(\xi) \]

Computationally intensive model: \( \text{dim}(V) \gg 1 \).

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 \( r \ll \text{dim}(V) \).

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

Among a vast literature...

- Introduction to PB-MOR
- PB-MOR as low-rank methods
- PB-MOR for control (dynamical) problems

\[ \text{Zahm, Phd thesis 2015} \]
\[ \text{Nouy 2015} \]
\[ \text{Benner, Gugercin, Willcox 2015} \]
• **Vector-valued Variable of Interest (VoI):**

\[ s(\xi) = L(\xi)u(\xi) \in Z \]

For example:

\[ s(\xi) = (s_1(\xi), \ldots, s_\ell(\xi)) \quad \text{with} \quad Z = \mathbb{R}^\ell \]

\[ s(\xi) = u_{|\partial\Omega}(\xi) \quad \text{with} \quad Z = H^{1/2}(\partial\Omega) \]

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

\[
\left( \text{error in the} \right)_{\text{VoI } s(\xi)} \leq \left( \text{error in the primal variable } u(\xi) \right) \left( \text{error in the dual variable } q(\xi) \right)
\]

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

- 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:**

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

with

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

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

- if $C_{PG}(\xi) = 0$, recover the orthogonal projection,
- if $C_{PG}(\xi) = 1$, no control of the projection error.
Possible choice for the test space $W_r$

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

- **Standard Galerkin projection**

  $$W_r = V_r$$

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

- **Minimal residual formulation**

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

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

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

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

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

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

- The saddle point formulation allows $T_p$ to be of larger dimension than $V_r$

  - if $T_p \supset A(\xi)^*R_VV_r$ then $C_{SP}(\xi) = 0$
  - if $T_p \supset W_r(\xi)$ then $C_{SP}(\xi) \leq C_{PG}(\xi)$
Estimation of vector-valued Variable of Interest
Extension of the primal-dual strategy

• 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
  \[
  \tilde{s}(\xi) = L(\xi)u_r(\xi) - Q_k(\xi)^* \left( b(\xi) - A(\xi)u_r(\xi) \right)
  \]
  is such that
  \[
  \|s(\xi) - \tilde{s}(\xi)\|_Z \leq \|u(\xi) - u_r(\xi)\|_V \|A(\xi)^* \left( Q(\xi) - Q_k(\xi) \right)\|_{Z' \to V'}
  \]
  where \( \| \cdot \|_{Z' \to V'} \) is an operator norm.
Projection-based approximation of the primal and dual variables

\[ \|s(\xi) - \tilde{s}(\xi)\|_Z \leq \|u(\xi) - u_r(\xi)\|_V \|A(\xi)^* \left( Q(\xi) - Q_k(\xi) \right)\|_{Z' \rightarrow V'} \]

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

  \[
  \min_{Q : Z' \rightarrow W_k^Q} \|A(\xi)^* \left( Q(\xi) - Q \right)\|_{Z' \rightarrow V'}
  \]

  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** \( k = \dim(W_k^Q) \).

- **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 Vol 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 Vol

$$\tilde{s}(\xi) = L(\xi) \left( u_{r,p}(\xi) + R_{V}^{-1} A(\xi)^* y_{r,p}(\xi) \right)$$

is such that:

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

• We can choose

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

  ○ $T_p(\xi) \supset W_r(\xi)$ : 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

\[-\nabla \cdot (\kappa \nabla u) + Dv \cdot \nabla u = f\]

- \(\xi_1 = \kappa_{IC}\) diffusion coefficient in \(\Omega_{IC}\)
- \(\xi_2 = r\) thermal contact conductance on \(\Gamma_C\)
- \(\xi_3 = D\) advection term
- \(\xi_4 = e\) geometrical parameter

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

\[s_i(\xi) = \frac{1}{\text{mes}(\Omega_{IC_i})} \int_{\Omega_{IC_i}} u(\xi) d\Omega, \quad i \in \{1, 2\}\]

Figure: Five samples of the solution \(u(\xi)\). Finite element approximation \((\text{dim}(V) = 12000, \text{SUPG})\)
Reduced spaces: span of snapshots selected at random

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

Test spaces

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

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

\[
\sup_{\xi} \|s(\xi) - \bar{s}(\xi)\|_Z
\]
Illustration (linear elasticity problem)

$$\text{div}(K(\xi) : \varepsilon(u(\xi))) = 0$$ \quad \text{with} \quad 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 $\eta = 0.3$.

- **Vol**: vertical displacement over $\Gamma$:

  $$s(\xi) = u_{|\Gamma}(\xi) \in Z \equiv \mathbb{R}^{44}$$

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)

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

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

- **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)
  - \( T_p = V_r + W_k^Q \)

\[
\sup_{\xi} \| s(\xi) - \tilde{s}(\xi) \|_Z = \begin{cases} 
  2.60 & \text{(primal-dual)} \\
  0.356 & \text{(saddle point)} 
\end{cases}
\]
Greedy construction of the reduced spaces
Residual-based error indicator for the Vol

- Let $\alpha(\xi) > 0$ such that
  \[
  \alpha(\xi) \| \cdot \|_V \leq \| A(\xi) \cdot \|_{\mathcal{V}'}
  \]
  - 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 Vol**
  \[
  \| s(\xi) - \tilde{s}(\xi) \|_Z \leq \Delta(\xi) := \frac{1}{\alpha(\xi)} \| A(\xi) \tilde{u}(\xi) - b(\xi) \|_{\mathcal{V}'} \| A(\xi)^* \tilde{Q}(\xi) - L(\xi)^* \|_{Z' \to \mathcal{V}'}
  \]

  - Primal-dual
    \[
    \begin{align*}
    \tilde{u}(\xi) &= u_r(\xi) \\
    \tilde{Q}(\xi) &= Q_k(\xi)
    \end{align*}
    \]

  - Saddle point
    \[
    \begin{align*}
    \tilde{u}(\xi) &= u_{r,p}(\xi) + R_{\mathcal{V}}^{-1} A(\xi)^* y_{r,p}(\xi) \\
    \tilde{Q}(\xi) &= Q_p(\xi)
    \end{align*}
    \]

  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 $\Delta(\xi)$:

$$\hat{\xi} \in \text{arg max}_\xi \Delta(\xi)$$

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

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

Partial enrichment strategy:

$$W_{k+1}^Q = W_k^Q + \text{span}\{Q(\hat{\xi})z\}$$

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

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

\[
\max_{\xi} \Delta(\xi) = fct(\text{Offline complexity})
\]

\[
\max_{\xi} \Delta(\xi) = fct(\text{Online complexity})
\]

\[r = \text{number of operator factorizations computed during the greedy algorithm}\]

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

- 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 Vol 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.

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

O. Zahm and A. Nouy

Interpolation of inverse operators for preconditioning parameter-dependent equations.