Gradient-enhanced least-square Polynomial Chaos expansions in uncertainty quantification and robust optimization

T. Ghisu\textsuperscript{a}, D. I. Lopez\textsuperscript{a}, P. Seshadri\textsuperscript{b}, S. Shahpar\textsuperscript{c}

\textsuperscript{a}University of Cagliari (Italy) \textsuperscript{b}Imperial College, London (UK) \textsuperscript{c}Rolls-Royce plc., Derby (UK)

AIAA AVIATION Forum and Exposition, 2-6 August 2021

Copyright © by Rolls-Royce plc.
Published by the American Institute of Aeronautics and Astronautics, Inc., with permission.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grand agreement N. 769025 (MADELEINE)
Contents

- Polynomial Chaos Expansions
  - General Introduction
  - Estimation of Coefficients
  - Gradient Enhancement
- Verification
- Application
Polynomial Chaos Expansion – General Introduction

\[ f(\mathbf{x}) \approx \sum_{j=1}^{n} k_j \psi_j(\mathbf{x}) \]

- **f** quantity of interest (qoi)
- **x** vector of uncertain variables with given probability density functions (pdfs)
- **\psi_j** orthogonal (or orthonormal) polynomials
- **k_j** coefficients of the expansion

**KNOWN**

**TO BE ESTIMATED**
How can we calculate the coefficients of the expansion?

1) QUADRATURE

2) REGRESSION

\[ \hat{k} = \arg\min_k \|Ak - b\|_2. \]

where

\[ A_\mathcal{F}(i, j) = \omega_i \psi_j(x_i), \quad j \in \mathcal{J}, \quad i = 1, \ldots, r, \]

\[ b_\mathcal{F}(i) = \omega_i f(x_i), \quad i = 1, \ldots, r, \]

\(A\) and \(b\) are obtained from \(A_\mathcal{F}\) and \(b_\mathcal{F}\) with some appropriate methodology.
What if we have gradient information (i.e. coming from an adjoint solver)?

**APPROACH 1:** We can increment our least square approximation using the derivative information

\[
\tilde{k} = \text{argmin}_k \left\| \begin{pmatrix} A & b \end{pmatrix} k - \begin{pmatrix} b \end{pmatrix} \right\|_2^2,
\]

\[
C_{\mathcal{F}}^{(k)}(i, j) = \frac{\partial \psi(x_i)}{\partial x^{(k)}}, \quad j \in \mathcal{J}, \quad i = 1, \ldots, r,
\]

\[
C_{\mathcal{F}} = \begin{pmatrix} C_{\mathcal{F}}^{(1)} \\ \vdots \\ C_{\mathcal{F}}^{(d)} \end{pmatrix} \quad \text{and} \quad d_{\mathcal{F}} = \begin{pmatrix} d_{\mathcal{F}}^{(1)} \\ \vdots \\ d_{\mathcal{F}}^{(d)} \end{pmatrix},
\]

\[
d_{\mathcal{F}}^{(k)}(i) = \frac{\partial f(x_i)}{\partial x^{(k)}}, \quad i = 1, \ldots, r,
\]

Similarly to \(A\) and \(b\), \(C\) and \(d\) can be determined from \(C_{\mathcal{F}}\) and \(d_{\mathcal{F}}\) by subsampling the quadrature points, following a given heuristic.
Polynomial Chaos Expansion – Gradient Enhancement

What if we have gradient information (i.e. coming from an adjoint solver)?

**APPROACH 2: NULL-SPACE**

We can approach the task of determining the coefficient of the expansion as an equality constrained optimization problem:

\[
\tilde{k} = \arg\min_k \|Ck - d\|_2.
\]

subject to \(Ak = b\).

With this approach, we assume that the qoi information (coming from the direct solver) is more reliable than the gradient information (coming from the adjoint solver) as this often contains a larger degree of noise. The above mathematical problem can be solved using the null-space method from Bjork ("Numerical methods in matrix computations", Springer 2015).
Verification – Simple test case

\[ f(x_1, x_2) = \exp(2x_1 + x_2) \]

\[ \nabla f = \begin{pmatrix} 2\exp(2x_1 + x_2) + \kappa \\ \exp(2x_1 + x_2) + \kappa \end{pmatrix}. \]

\[ x_1 = U[-1 : 1], \ x_2 = U[-1 : 1]. \kappa \text{ is random (white) noise of different levels. We use a 15th order Polynomial Chaos expansion.} \]

\[ \kappa = 0 \]
Verification – Simple test case

\[ f(x_1, x_2) = \exp(2x_1 + x_2) \]

\[ \nabla f = \begin{pmatrix} 2\exp(2x_1 + x_2) + \kappa \\ \exp(2x_1 + x_2) + \kappa \end{pmatrix} . \]

\[ x_1 = U[-1 : 1], \ x_2 = U[-1 : 1]. \ \kappa \text{ is random (white) noise of different levels. We use a 15th order Polynomial Chaos expansion.} \]

\[ \kappa = N(0, 0.01) \]
Verification – Simple test case

\[ f(x_1, x_2) = \exp(2x_1 + x_2) \]

\[ \nabla f = \begin{pmatrix} 2\exp(2x_1 + x_2) + \kappa \\ \exp(2x_1 + x_2) + \kappa \end{pmatrix}. \]

\[ x_1 = \mathcal{U}[-1:1], \ x_2 = \mathcal{U}[-1:1]. \ \kappa \text{ is random (white) noise of different levels. We use a 15th order Polynomial Chaos expansion.} \]

\[ \kappa = \mathcal{N}(0, 0.01) \]

**COEFFICIENTS**

**WEIGHTED**

**NULL-SPACE**

**MEAN**

**STD**
Verification – Real Case (Rotor37)

- qoi: adiabatic efficiency
- 5 uncertain variables (tangential stacking)

4 METHODS
- SGNI (sparse grid numerical integration) 2\textsuperscript{nd} order
- SGNI-G (SGNI, with gradient) 1\textsuperscript{st} o.
- LSA-G (least-square approx. with gradient, stacked) 2\textsuperscript{nd} o.
- LSA-G-NS (least-square approx with gradient, null-space) 2\textsuperscript{nd} o.

Example of typical noisy gradients:
Fig. 9  Polynomial Chaos expansion coefficients comparison using different methodologies. LSA approaches are tested with different levels of oversampling (o-s)
Verification – Real Case (Rotor37)

(a) 2nd-order SGNI without gradients vs 1st- (b) 2nd-order SGNI without gradients vs 2nd- (c) 2nd-order SGNI without gradients vs 2nd-order LSA with gradients

Fig. 10  Sobol indices comparison using different methodologies. LSA approaches uare tested with different levels of oversampling (o-s)
Fig. 11  Gradient of the mean: comparison using different methodologies. LSA approaches were tested with different levels of oversampling (o-s)
Verification – Real Case (Rotor37)

(a) 2nd-order SGNI without gradients vs 1st-
(b) 2nd-order SGNI without gradients vs 2nd-
order SGNI with gradients

(c) 2nd-order SGNI without gradients vs 2nd-
order LSA with gradients

(c) 2nd-order SGNI without gradients vs 2nd-
order LSA-NS with gradients

Fig. 12  Gradient of the standard deviation: comparison using different methodologies. LSA approaches are tested with different levels of oversampling (o-s)
Application – Robust Optimisation of Vital Fan

**Mean Efficiency**

\[
\min_x \{ -\mu(\eta(x, \omega)) \cdot \sigma(\eta(x, \omega)) \}
\]

*Design Variables*

\[ x \in \chi \subseteq \mathbb{R}^m \]

*Uncertainties*

\[ \omega \in \Omega \subseteq \mathbb{R}^k \]

subject to

\[ 0.99 \ P_R^{\text{datum}} \leq P_R(x) \leq 1.05 \ P_R^{\text{datum}} \]

**35 design variables**

**25 uncertainties**
Application – Robust Optimisation of Vital Fan

DGO = DETERMINISTIC GLOBAL OPTIMUM
Application – Robust Optimisation of Vital Fan

(a) Meridional View
(b) Isometric View
(c) View From the Top

EFFICIENCY

IS. MACH NUMBER 80% SPAN
Application – Robust Optimisation of Vital Fan
We have presented an approach for constructing Polynomial Chaos approximations using gradient information.

The approach is more robust to noise in the gradients.

Its applicability has been demonstrated through test-cases of increasing complexity.

... and it has been applied to the robust optimisation of a high-efficiency research fan blade.
Acknowledgments

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 769025 (MADELEINE)

The authors would like to express their gratitude to Rolls-Royce plc. For their support and permission to publish the work

t.ghisu@unica.it