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Bayesian calibration of the Peng-Robinson fluid model for siloxane MDM vapor flows in the non-ideal regime

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Keywords: Non-ideal Compressible-Fluid Dynamics, parameter calibration, Bayesian Inference, siloxane fluid MDM.

ABSTRACT

Non-Ideal Compressible-Fluid Dynamics (NICFD) investigates the gas dynamics of a special class of fluids, typically (but not limited to) vapors of molecular complex compounds, characterized by a thermodynamic state space containing a *non-ideal* region. In the non-ideal regime, the fluid no longer behaves as an ideal gas with state equation $Pv = RT$ (whereas P is the gas pressure, v the specific volume, R the gas constant and T the temperature) and more complex fluid models are required. Currently, the community is racing to develop reliable and predictive tools to investigate the non-ideal dynamics and to ultimately improve the design of devices involving NICFD flows. A global perspective including experiments, computations, and theory is needed in order to develop sophisticated physical models as well as a systematic and comprehensive treatment of calibration and validation procedures.

This work focuses on the calibration of the polytropic Peng-Robinson (PR) fluid model [Peng and Robinson, 1976] for siloxane MDM (Octamethyltrisiloxane, $C_8H_{24}O_2Si_3$) vapor flows in the non-ideal regime. Specifically, the goal is to calibrate the material-dependent parameters appearing in the equations of state by combining experimental NICFD flows measurements with numerical simulations. The calibration process relies on a standard Bayesian inference framework and it takes advantage of the first-ever experiments on non-ideal expanding flows of siloxane MDM vapor [Spinelli et al., 2018]. The Bayesian framework to infer the polytropic PR model parameters accounts for uncertainties in the test-rig operating conditions (treated as nuisance parameters). Specifically, the inference considers the total pressure P_t and total temperature T_t at the inlet of the test section (uncertain operating conditions) and the fluid critical pressure P_{cr},

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critical temperature T_{cr}, acentric factor ω and specific heat ratio γ (fluid model parameters of interest).

The Bayes' theorem reads

$$\mathcal{P}\left(\mathbf{q} \mid \mathbf{o}\right) \propto \mathcal{P}\left(\mathbf{o} \mid \mathbf{q}\right) \mathcal{P}\left(\mathbf{q}\right), \tag{1}$$

where $\mathbf{q} = (P_t, T_t, P_{cr}, T_{cr}, \omega, \gamma)^T$ is the vector of the unknown parameters and $\mathbf{o}$ is the vector containing the experimental measurements. Uniformly distributed prior distributions $\mathcal{P}\left(\mathbf{q}\right) \sim \mathcal{U}_{\mathbf{q}}[\mathbf{q}_{min}, \mathbf{q}_{max}]$ are considered. The prior bounds for the operating conditions were provided by the experimentalists. For the PR model parameters, the priors were set to largely encompass reference values reported in the literature and to satisfy thermodynamic stability criteria and physical limits. The likelihood $\mathcal{L} \triangleq \mathcal{P}\left(\mathbf{o} \mid \mathbf{q}\right)$ is considered Gaussian. The measurements set compounds N_c experiments at different operating conditions and we explicitly define

$$\mathcal{L} = \Pi_{j=1}^{N_c} \mathcal{L}_j, \quad \mathcal{L}_j = \Pi_{i=1}^{N_{p,j}} \exp\left(-\left(O_{ij} - U_{ij}(\mathbf{q})\right)^2 / 2\sigma_{ij}^2\right), \tag{2}$$

where $N_{p,j}$ is the number of measurements in the j-th experiment, O_{ij} is the measurement of probe i in experiment j, σ_{ij}^2 is the measurement variance and U_{ij} is the measured value predicted by the Computational Fluid Dynamics (CFD) model. SU2 is an open-source suite capable of dealing with non-ideal, fully turbulent, flows and it now embodies the reference among NICFD solvers [Economon et al., 2015, Gori et al., 2017]. The measurement variances were provided by the experimentalists. The resulting posterior distribution is sampled via a Markov-Chain Monte-Carlo (MCMC) approach based on the Metropolis-Hastings (MH) algorithm [Hastings, 1970]. As the sampling requires many model evaluations, we rely here on surrogate models for the $U_{i,j}(\mathbf{q})$.

Results reveal an inherent inconsistency between numerical predictions based on the model and the measurements. Indeed, the sole variation of the PR model parameters does not allow for significant mitigation of the discrepancy between computational results and experimental data. The inconsistency possibly arises from a bias error in the available measurements, from an epistemic uncertainty affecting the PR model, and (or) form using an inadequate computational model to reproduce the experimental flows. We discuss future investigations that could help clarifying the sources of inconsistency.

References

[Peng and Robinson, 1976] Peng, D. Y. and Robinson, D. B. (1976). A New Two-constant Equation of State. *Ind. Eng. Chem. Fundam.*, 15:59–64.

[Spinelli et al., 2018] Spinelli, A. and Cammi, G. and Gallarini, S. and Zocca, M. and Cozzi, F. and Gaetani, P. and Dossena, V. and Guardone, A. (2018). Experimental evidence of non-ideal compressible effects in expanding flow of a high molecular complexity vapour. *Experiments in Fluids*, 59.

[Economon et al., 2015] Economon, T.D. and Palacios, F. and Copeland, S.R. and Lucaczyk, T.W. and Alonso, J.J. (2015). SU2: An Open-Source Suite for Multiphysics Simulation and Design. *AIAA Journal*, 54:828–846.

[Gori et al., 2017] Gori, G. and Zocca, M. and Cammi, G. and Spinelli, A. and Guardone, A. (2017). Experimental assessment of the open-source SU2 CFD suite for ORC applications. *Energy Procedia*, 129:256–263.

[Hastings, 1970] Hastings, W.K. (1970). Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, 57:97–109.

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Accelerated Schwarz Method for Stochastic Elliptic PDEs

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Keywords: Domain decomposition, Stochastic problems, Uncertainty quantification, HPC.

ABSTRACT

This work concerns the resolution of stochastic elliptic equations of the form

$$\nabla \cdot [\kappa(x,\theta)\nabla u(x,\theta)] = -f(x), \quad x \in \Omega, \quad u = u_{\partial\Omega} \text{ on } \partial\Omega, \tag{1}$$

where $\kappa(x,\theta)$ is a random field. We are interested in random fields that cannot be accurately approximated with truncated series, and consider Monte Carlo approaches. In MC approaches, one relies on the multiple resolutions of (1) for different realizations of κ to estimate the statistic of quantities of interest. As millions of samples may be needed to obtain well-converged statistics, efficient solvers are required. We consider a domain decomposition method with a partition of Ω into overlapping subdomains. The additive Schwartz Method (SM) is a fixed-point procedure, where the set of sub-domains' boundary values u_Γ is updated through the parallel resolution of local elliptic problems. The convergence rate of the fixed-point iterations $u_\Gamma^{k+1} = \mathrm{S}(u_\Gamma^k|\kappa)$ reduces with the subdomains size and their overlapping. The convergence can be improved using an affine preconditioner A, resulting in the Accelerated SM (ASM) with iterations: $u_\Gamma^{k+1} = \mathrm{S}(A(u_\Gamma^k)|\kappa)$.

The exact preconditioner A^{ex}, yielding the fixed-point solution in just one iteration, depends on κ and its computation for a single deterministic problem is usually too expensive. Allocating resources to the construction of an effective κ-dependent preconditioners may, however, be interesting in the Monte Carlo context (see for instance [1]). We explore this idea for preconditioners based on low dimensional approximations of the random field involving N random variables: $\kappa(x,\theta) \approx \kappa(x,\boldsymbol{\xi})$ where $\boldsymbol{\xi} = (\xi_1,\ldots,\xi_N)$. The dependencies of the preconditioner $A(\cdot|\boldsymbol{\xi})$ on the random variables are subsequently approximated using Polynomial Chaos expansions [2]: $A(\cdot|\boldsymbol{\xi}) \approx A^{PC}(\cdot|\boldsymbol{\xi}) = \sum_\alpha A_\alpha(\cdot)\Psi_\alpha(\boldsymbol{\xi})$. The expansion coefficients A_α can be determined via a Pseudo-Spectral Projection method [3] requiring the computation of N_p preconditioners, at a cost which is subsequently factorized over the simulated MC samples.

N	2	10	50	100
RMSE $\|\kappa - \hat{\kappa}^N\|$	$3.32\,10^{-1}$	$1.62\,10^{-1}$	$7.17\,10^{-2}$	$5.04\,10^{-2}$
RMSE $\|A^{ex} - A\|_F$	$1.72\,10^{-2}$	$1.44\,10^{-2}$	$5.34\,10^{-3}$	$2.92\,10^{-3}$
RMSE $\|A - A^{PC}\|_F$	$2.83\,10^{-4}$	$1.22\,10^{-3}$	$2.12\,10^{-3}$	$2.18\,10^{-3}$
Size of PC basis (# of PSP nodes)	8 (17)	76 (241)	1,376 (5,201)	5,251 (20,401)
# ASM iterations for $A(\cdot\|\boldsymbol{\xi})$	18.9 ± 5.9	14.6 ± 2.9	8.2 ± 0.9	6.8 ± 0.6
# ASM iterations for $A^{PC}(\cdot\|\boldsymbol{\xi})$	18.9 ± 5.9	14.7 ± 2.9	8.6 ± 0.9	7.4 ± 0.8

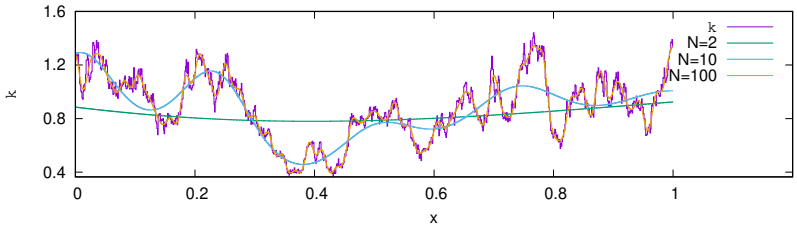

Table 1: *Top: Analysis of performance and complexity of the proposed PC-Accelerated Schwarz method (PC-ASM). Below: Approximations for different N of a realization of κ.*

We demonstrate the PC-ASM approach on a one-dimension problem with domain $\Omega = [0,1]$ and discretized with $\approx 1,000$ finite-elements. The partition consists of 20 uniform subdomains with overlapping of 5 elements. The field κ is log-normal with distribution $\log \kappa \sim N(0, C)$, where $C(x,x') = \sigma^2 \exp(-|x-x'|/L)$. The results use $L = 0.2$ and $\sigma^2 = 0.25$. The approximation of κ is defined as

$$\kappa(x,\theta) \approx \hat{\kappa}^N(x, \boldsymbol{\xi}(\theta)) = \exp\left[\sum_{i=1}^{N} \lambda_i^{1/2} \Phi_i(x) \xi_i(\theta)\right], \quad \xi_i(\theta) = \int \Phi_i(x) \log(\kappa(x,\theta)) dx,$$

where the Φ_i are the dominant eigenfunctions of the covariance C. Table 1 shows for different values of N (top row) the root-mean-squared errors on the field $\hat{\kappa}^N - \kappa$ (second row), on the accelerator $A^{ex} - A$ (in Frobenius norm, third row) and the RMS-error of the PC approximation, $A - A^{PC}$ (fourth row). The fifth row reports the PC basis dimension (for third order expansions) and the number of PSP nodes N_p for the projection. Finally, the number of iterations (averaged value $\pm$ standard deviation) to get $|u_\Gamma^k - u_\Gamma^{k+1}| < 10^{-9}$ is reported in the last two rows for the ASM using A or its PC approximation A^{PC} respectively. For comparison, the Schwartz method without preconditioning requires 14,250 iterations on average to converge. The table indicates that 1) the preconditioning approach is effective, requiring few iterations even for low N, and 2) the PC approximation of the preconditioner has a low impact on the convergence, especially for the smallest N.

References

[1] A. Contreras *et al* (2018). Parallel domain decomposition strategies for stochastic elliptic equations, *SIAM J. Sc. Comp.*.

[2] O. Le Maître and O. Knio (2010). *Spectral Methods for Uncertainty Quantification*, Springer.

[3] J. Winokur *et al* (2016). Sparse Pseudo Spectral Projection Methods with Directional Adaptation for Uncertainty Quantification, *J. Sc. Comp.*.

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Robust Calibration of the Catalytic Properties of Thermal Protection Materials: Application to Plasma Wind Tunnel Experiments

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Keywords: Uncertainty Quantification, Bayesian Inference, Plasma Flows, Catalysis

ABSTRACT

Historically, experiments have been the main source of knowledge since the dawn of scientific pursuit. The invention of computers lead to a raise in computational methods that are widely used in modern engineering to reduce time and costs during the design phase of a complex system, often as an alternative to experiments when our confidence in the models is very high. Another use for computational methods is the capability of solving complex equations which otherwise would remain unsolved or would require a considerable amount of human resources

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[Golemba, 1994]. Since the beginnings of the computational era, experiments and simulations have been used alongside one another to uncover deep physical laws and to understand nature. As our knowledge of the world is never perfect and so far we cannot account for all its different multi-scale details, uncertainties must play a role in the understanding process.

The study of the aerothermal environment surrounding a vehicle during atmospheric entry is extremely complex, as such, experiments and models are put to the test to avoid critical mission failure. In this context, the reliability of our predictions as well as the quality of our models must be assessed. The von Karman Institute (VKI) uses a state-of-the-art Inductively-Coupled Plasma (ICP) torch [Bottin *et al.*, 1999] to collect relevant data to study flow-material interaction phenomena for relevant spacecraft reentry conditions. Depending on the material to be characterized, different testing techniques can be used to assess different aspects of their performance. We focus our interest in reusable materials for which the heat load is partially re-radiated back to the atmosphere. One of the key factors in choosing them is the specified reaction recombination efficiency which measures how much of a chemical species is recombined at the wall compared to its net difussion flux to the wall. The characterization of these surface properties is done in an indirect manner by using several measurement techniques and numerical rebuilding. Uncertainties affecting each part of the rebuilding process must be accounted for, from the measurement errors, to the methodology used to measure, to the model used to perform the rebuilding.

In this work, we address the answer to the following questions: Can the estimation of the recombination efficiency parameter be improved through different experimental methodologies? When doing so, can the Bayesian framework be extended to include new parameters and give accurate posteriors? Is the calibration useful in other testing conditions?

State-of-the-art uncertainty quantification techniques are applied to catalytic thermal protection system characterization using plasma wind tunnel experiments [Viladegut, 2017]. Different testing methodologies are discussed based on their resulting posterior distributions allowing for recommendations regarding the testing. To assess whether or not the calibration of the recombination efficiency parameter can be extrapolated to other testing conditions, a hypothesis testing analysis is also included. The computation of the Bayes factor relates the comparison between two different marginal likelihoods or evidences attached to two alternative hypotheses. The results from this analysis determine the suitability of one hypothesis or the other opening up the discussion about model selection and the influence of the experimental conditions for optimal testing.

From this work, conclusions indicate that a more complex testing methodology must be put in place to obtain more accurate posterior distributions for the recombination efficiency parameter. Choosing two materials of very different catalytic behavior (fully catalytic versus non-catalytic) and having the catalytic behavior of the material we want to characterize somewhere in the middle, gives us a much better estimation of the parameter of interest. Using the calibrated parameter for different testing conditions proves problematic as indicated by the Bayes factor, inviting us to rethink the rebuilding methodology.

In general, this contribution offers a deeper insight to the experiments performed in this domain and how to improve our model upon experimental evidence.

References

[Golemba, 1994] Golemba, B. (1994). Human Computers: The Women in Aeronautical Research. NASA Langley Archives, 1994.

[Bottin *et al.*, 1999] Bottin, B., Chazot, O., Carbonaro M., Van der Haegen V. and Paris S. (1999). The VKI Plasmatron Characteristics and Performance. *Measurement Techniques for High Temperature and Plasma Flows*, RTO-EN 8, pp. 6-1, 6-24.

[Viladegut, 2017] Viladegut A. (2017). Assessment of Gas-Surface Interaction Modelling for Lifting Body Re-Entry Flight Design. PhD thesis VKI/UPC, 2017.

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Different measure approximations for efficient constrained multi-objective optimization under uncertainty

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Keywords: Uncertainty quantification, optimization, robustness, reliability.

ABSTRACT

The SABBa framework has been shown to tackle multi-objective optimization under uncertainty problems efficiently. It deals with robust and reliability-based optimization problems with approximated robustness and reliability measures. The recursive aspect of the Bounding-Box (BB) approach has notably been exploited in [1], [2] and [3] with an increasing number of additional features, allowing for little computational costs. In these contributions, robustness and reliability measures are approximated by a Bounding-Box (or conservative box), which is roughly a uniform-density representation of the unknown objectives and constraints. It is supplemented with a surrogate-assisting strategy, which is very effective to reduce the overall computational cost, notably during the last iterations of the optimization.

In [3], SABBa has been quantitatively compared to more classical approaches with much success both concerning convergence rate and convergence robustness.

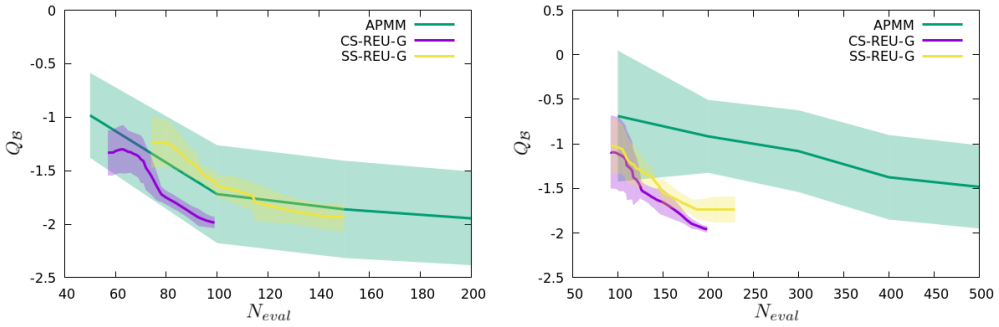
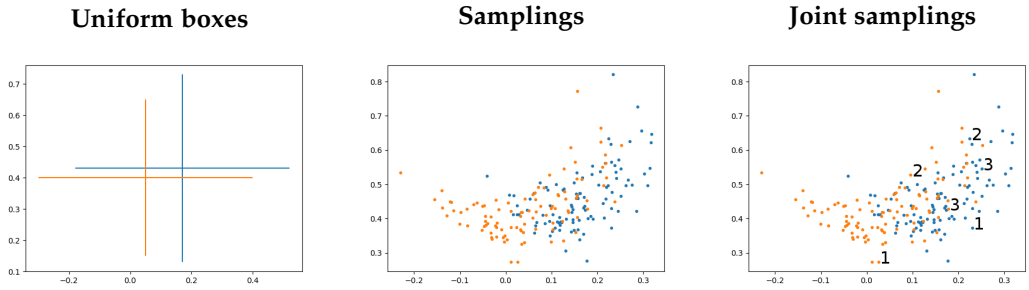


Figure 1: *Cost comparison between APMM and SABBa with a) high-quality or b) low-quality surrogate model.*

Figure 1 shows better mean performance and significantly reduced variability of the SABBa CS-REU-G method w.r.t an A Priori MetaModel strategy. SABBa allows for local refinement, hence higher robustness to low-quality surrogate model.

We propose in this work to further improve the parsimony of the approach with a more general framework, SAMMA (Surrogate-Assisted Multi-fidelity Measure Approximation), allowing for objects other than Bounding-Boxes to be compared in the recursive strategy. Such non-uniform approximations have been proposed in previous works like [4] and [5]. Among others, sampling and Gaussian measure approximations are presented and quantitatively compared in the following. We propose suitable Pareto dominance rules and POP (Pareto Optimal Probability) computations for these new measure approximations. Potential gains in terms of discriminance between boxes of the sampling measure approximation and joint information are depicted in Table 1.



Pareto Optimal Probability			
Design	Uniform	Sampling	Joint
Blue	0.7388	0.4446	0.12
Orange	0.8455	0.868	1

Table 1: *Potential discriminative gains*

To extend the framework applicability to complex industrial cases, and alongside the multi-fidelity between different UQs (Uncertainty Quantification) inherent to the recursive strategy, we propose to plug multi-fidelity approaches within the measure computations. This approach should allow tackling very complex industrial problems in an acceptable timeframe.

References

[1] F. Fusi, P. M. Congedo, An adaptive strategy on the error of the objective functions for uncertainty-based derivative-free optimization, *Journal of Computational Physics*, 309, 241-266.

[2] M. Rivier, P. M. Congedo, Surrogate-Assisted Bounding-Box Approach for Optimization Problems with Approximated Objectives. *[Research Report] RR-9155*, 2018.

[3] M. Rivier, P. M. Congedo, Surrogate-Assisted Bounding-Box Approach Applied to Constrained Multi-Objective Optimisation Under Uncertainty. *[Research Report] RR-9214*, 2018.

[4] R. F. Coelho, Probabilistic Dominance in Multiobjective Reliability-Based Optimization: Theory and Implementation, *IEEE Transactions on Evolutionary Computation*, 2015, 214-224.

[5] F. Khosravi, M. Borst and J. Teich, Probabilistic Dominance in Robust Multi-Objective Optimization, *IEEE Congress on Evolutionary Computation (CEC)*, Rio de Janeiro, 2018, 1-6.

Non-intrusive method to estimate discretization errors on a turbulent single-phase flow

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The computational fluid dynamics frameworks at CEA has been extended to include systematic Verification and Validation (V&V) processes combined with Uncertainty Quantification (UQ) procedures, in order to improve the accuracy and reliability of the simulations. Along this line, we investigate the assessment of the discretization errors by means of non-intrusive methods based on an ensemble of simulations using different discretization levels.

In this work, the discretization errors are assessed using the method proposed by Eça and Hoekstra ["A procedure for the estimation of the numerical uncertainty of CFD calculations based on grid refinement studies", Journal of Computational Physics, Vol. 262, p. 104-130, 2014]. This method requires a minimum of four simulations performed at four different discretization levels. These simulations are subsequently used to estimate the "exact" model solution for the quantity of interest and its error bars, through the resolution of a best-fit problem combined with an error-model selection procedure. The extent of these error bars accounts for the reliability of the error estimation and, therefore, characterizes the confidence in the model prediction.

The main objective of the present work was to investigate the behavior of the method. The simulation of a turbulent single-phase flow in a pipe, presenting a diameter reduction, has been considered for this purpose. The behavior of the method has been analyzed for both integral and local quantities. We focused, in particular, on the error bars estimation and the robustness of the approach with respect to the sequence of discretization parameters (mesh refinements) considered.

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Surrogate-based inversion for first-arrival seismic tomography

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Keywords: Bayesian inference, active tomography, polynomial chaos expansions, uncertainty quantification.

ABSTRACT

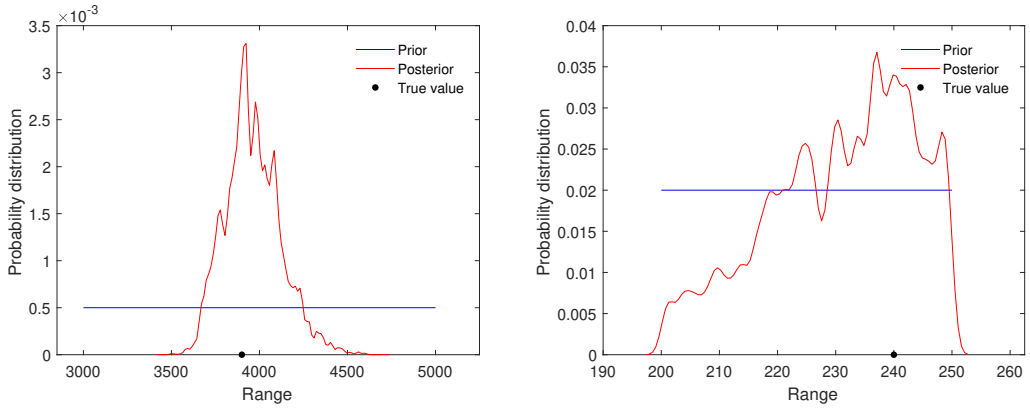
Seismic tomography is used to infer the subsurface seismic structure of a medium from observations of seismic waves. We focus on active tomography where a network of sources generates seismic waves propagating in the subsurface and recorded at seismic stations. The structure of the medium is described by a vector of parameters, denoted $\mathbf{m}$, containing the wave velocities and geometrical informations to be inferred from the observations. Specifically, we consider a Bayesian inversion where a set of first-arrival times, collected in the vector $\mathbf{t}_{\text{obs}}$, is used to infer the parameters using the the Bayes' theorem [Bayes, 1763],

$$p(\mathbf{m}|\mathbf{t}_{\text{obs}}) \propto p(\mathbf{t}_{\text{obs}}|\mathbf{m})p(\mathbf{m}). \tag{1}$$

Here, the vertical bar $\cdot|\cdot$ means "conditional on", and we have denoted $p(\mathbf{m})$ the prior distribution of the parameters, $p(\mathbf{t}_{\text{obs}}|\mathbf{m})$ the likelihood of the arrival times and $p(\mathbf{m}|\mathbf{t}_{\text{obs}})$ the posterior distribution of the parameters.

The likelihood requires a comparison between the measured arrival times and their values predicted by the model for given parameter values in $\mathbf{m}$. An Eikonal solver [Noble *et al*, 2014] can be used to predict the arrival times; however, the computational cost of the Eikonal solvers is too large to permit the extensive sampling of the posterior of $\mathbf{m}$, for instance using a Markov Chain Monte Carlo (MCMC) algorithm [Metropolis *et al*, 1953, Hastings, 1970]. To circumvent this issue, we rely on polynomial chaos expansions [Le Maître and Knio, 2010] as a surrogate of the forward Eikonal solver in the inversion algorithm, therefore saving the computational burden of its computation.

We present results of initial tests using synthetic data. These tests show a satisfactory inference of the parameters, as illustrated in Fig. 1. Plotted are the prior and posterior distributions of two velocity model parameters, namely i) the wave velocity of a geological layer and ii) the location of a geological interface between two layers. The true parameter values used to generate the synthetic data are also reported. We observe that the maximum a posteriori (MAP) values are close to these true values. The narrow velocity posterior means that the observations are very informative for this parameter, when the flatter interface location posterior denotes that it remains more uncertain.



(a) *First layer wave velocity* **(b)** *First interface location*

Figure 1: *Example of Bayesian calibration.*

Our numerical tests also reveal that the location of the sources and recording stations can affect the number of Eikonal model evaluations necessary to build accurate surrogates of the arrival times, in particular by inducing non-smooth dependencies of the arrival times with $\mathbf{m}$. Another challenging question concerns the design of the sources and stations network in order to enhance the parameter calibration.

References

[Bayes, 1763] Bayes, T. (1963). An essay towards solving a problem in the doctrine of chances, *Phil. Trans. of the Royal Soc. of London*, 53, 370-418.

[Noble *et al*, 2014] Noble, M., Gesret, A. and Belayouni, N. (2014). Accurate 3-d finite difference computation of traveltimes in strongly heterogeneous media, *Geophys. J. Int.*, 199, 1572-1585.

[Metropolis *et al*, 1953] Metropolis, N., Rosenbluth, A. W., Rosenbluth, M. N., Teller, A. H. and Teller, E. (1953). Equations of State Calculations by Fast Computing Machines *Journal of Chemical Physics*, 21(6), 1087-1092.

[Hastings, 1970] Hastings, W. K. (1970) Monte Carlo Sampling Methods Using Markov Chains and Their Applications, *Biometrika*, 57(1), 97-109.

[Le Maître and Knio, 2010] Le Maître, O. P. and Knio, O. M. (2010), Spectral Methods for Uncertainty Quantification, *Springer, Scientific Computation*.

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An Imprecise Probabilistic Estimator for the Transition Rate Matrix of a Continuous-Time Markov Chain

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Keywords: Continuous-Time Markov Chain, Statistical Inference, Imprecise Prior, Set of Priors

ABSTRACT

Continuous-time Markov chains (CTMCs) are mathematical models that describe the evolution of dynamical systems under uncertainty [Norris, 1998]. They are pervasive throughout science and engineering, finding applications in areas as disparate as medicine, mathematical finance, epidemiology, queueing theory, and others. We here consider time-homogeneous CTMCs that can only be in a finite number of states.

The dynamics of these models are uniquely characterised by a single *transition rate matrix* Q. This Q describes the (locally) linearised dynamics of the model, and is the generator of the semi-group of transition matrices $T_t = \exp(Qt)$ that determines the conditional probabilities $P(X_t = y \mid X_0 = x) = T_t(x, y)$. In this expression, X_t denotes the uncertain state of the system at time t, and so, for all x, y, the element $T_t(x, y)$ is the probability for the system to move from state x at time zero, to state y at time t.

In this work, we consider the problem of estimating the matrix Q from a single realisation of the system up to some finite point in time. This problem is easily solved in both the classical frequentist and Bayesian frameworks, due to the likelihood of the corresponding CTMC belonging to an exponential family; see e.g. the introductions of [Inamura, 2006, Bladt and Sørensen, 2005]. The novelty of the present work is that we instead consider the estimation of Q in an *imprecise probabilistic* context [Walley, 1991, Augustin *et al.*, 2014].

Specifically, we approach this problem by considering an entire *set* of Bayesian priors on Q, leading to a *set-valued* estimator for this parameter. In order to obtain well-founded hyperparameter settings for this set of priors, we recast the problem by interpreting a continuous-time Markov chain as a limit of *discrete*-time Markov chains. This allows us to consider the imprecise-probabilistic estimators of these discrete-time Markov chains, which are described by the popular Imprecise Dirichlet Model (IDM) [Quaeghebeur, 2009]. The upshot of this approach is that the IDM has well-known prior hyperparameter settings which can be motivated from first principles [Walley, 1996, De Cooman *et al.*, 2015].

This leads us to the two main results of this work. First of all, we show that the limit of these IDM estimators is a set $\mathcal{Q}_s$ of transition rate matrices that can be described in closed-form using a very simple formula. Secondly, we identify the hyperparameters of our imprecise CTMC prior such that the resulting estimator is equivalent to the estimator obtained from this discrete-time limit. The only parameter of the estimator is a scalar $s \in \mathbb{R}_{\geq 0}$ that controls the degree of imprecision. In the special case where $s = 0$ there is no imprecision, and then $\mathcal{Q}_0 = \{Q^{\text{ML}}\}$, where Q^{ML} is the standard maximum likelihood estimate of Q.

The immediate usefulness of our results is two-fold. From a domain-analysis point of view, where we are interested in the parameter values of the process dynamics, our imprecise estimator provides prior-insensitive information about these values based on the data. If we are instead interested in robust inference about the future behaviour of the system, our imprecise estimator can be used as the main parameter of an *imprecise continuous-time Markov chain* [Škulj, 2015, De Bock, 2016, Krak *et al.*, 2017].

The results that we present here have previously been published in [Krak *et al.*, 2018].

References

[Augustin *et al.*, 2014] Augustin, T., Coolen, F.P.A., De Cooman, G., Troffaes, M.C.M. (eds.): *Introduction to Imprecise Probabilities*. John Wiley & Sons (2014)

[Bladt and Sørensen, 2005] Bladt, M., Sørensen, M.: Statistical inference for discretely observed Markov jump processes. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 67(3), 395–410 (2005)

[De Cooman *et al.*, 2015] De Cooman, G., De Bock, J., Diniz, M.A.: Coherent predictive inference under exchangeability with imprecise probabilities. *Journal of Artificial Intelligence Research* 52, 1–95 (2015)

[De Bock, 2016] De Bock, J.: The limit behaviour of imprecise continuous-time markov chains. *Journal of Nonlinear Science* 27(1), 159–196 (2017)

[Inamura, 2006] Inamura, Y.: Estimating continuous time transition matrices from discretely observed data. Bank of Japan (2006)

[Krak *et al.*, 2017] Krak, T., De Bock, J., Siebes, A.: Imprecise continuous-time Markov chains. *International Journal of Approximate Reasoning* 88, 452–528 (2017)

[Krak *et al.*, 2018] Krak, T., Errerygers, A., De Bock, J.: An Imprecise Probabilistic Estimator for the Transition Rate Matrix of a Continuous-Time Markov Chain. *Proceedings of SMPS 2018*, 124–132 (2018)

[Norris, 1998] Norris, J.R.: *Markov chains*. Cambridge university press (1998)

[Quaeghebeur, 2009] Quaeghebeur, E.: *Learning from samples using coherent lower previsions*. Ph.D. thesis

[Škulj, 2015] Škulj, D.: Efficient computation of the bounds of continuous time imprecise Markov chains. *Applied Mathematics and Computation* 250(C), 165–180 (2015)

[Walley, 1991] Walley, P.: *Statistical reasoning with imprecise probabilities*. Chapman and Hall, London (1991)

[Walley, 1996] Walley, P.: Inferences from multinomial data: learning about a bag of marbles. *Journal of the Royal Statistical Society, Series B* 58, 3–57 (1996)

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Airfoil Optimization Using Far-Field Analysis of the Drag Force

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Keywords: Optimization, far-field force prediction, CFD

ABSTRACT

Far-field analysis for drag prediction and decomposition is here explored and applied to aerodynamic shape design problems. This kind of methods, based on formulae derived from the integral momentum equation, gives a *physical* decomposition for the aerodynamic force splitting it in viscous, lift-induced and wave contributions which have a main relevance for the aerodynamic designer. On the contrary, the straightforward computation of the aerodynamic force by stress integration on the body surface (*near-field* method) allows the decomposition of the aerodynamic force in two components: friction and pressure forces. In this work, a far-field method based on entropy variations has been implemented. A detailed description of the method is given in [Paparone and Tognaccini, 2003]. Moreover, this method showed the capability to improve the accuracy in the calculation of total drag from a given CFD solution by removing part of the so-called *spurious* drag implicitly or explicitly introduced by the artificial viscosity of the adopted numerical scheme. Hence, a reliable drag calculation even on very coarse grids is possible. Thus, the aim of the work is the illustration of how the far-field approach may allow substantial reductions of the computational effort which is still a significant concern. Furthermore, the possibility to decompose drag in viscous, wave and lift-induced contributions allows for a selection of the objective function among these three terms. This particular characteristic has already been considered in [Gariepy *et al*, 2015]. In particular, the approach is shown by optimizing the wave drag of a NACA 0012 (466dc) in transonic flow conditions ($M_\infty = 0.85$) at zero angle of attack. Two different set of optimization runs have been performed. The first one used the near-field formulation to evaluate the drag coefficient, while the second one relied upon the far-field method. The near-field method has been applied using three different grid levels, whereas the far-field only the coarsest one. The performance comparison of the optimum airfoils was made using the C_D calculated using the finest grid level.

Table 1: *Drag coefficient,* $C_D \cdot 10^4$ *, using finest grid size*

Optimization using near-field approach	100
Optimization using far-field approach	77

In table 1, the performance of the optimum airfoils obtained by optimizing with the coarsest grid level has been compared. It shows that a higher drag reduction is achieved employing the far-field approach (83.5%) than in the optimization made using the near-field formulation at the same grid level (78.5%). Therefore, it can be concluded that the use of the far-field approach, since only the wave drag is minimized, allows the optimization algorithm to reach to a significantly better solution refinement than that obtainable with the near-field method. Part of this work will be presented at AIAA SciTech Forum 2019.

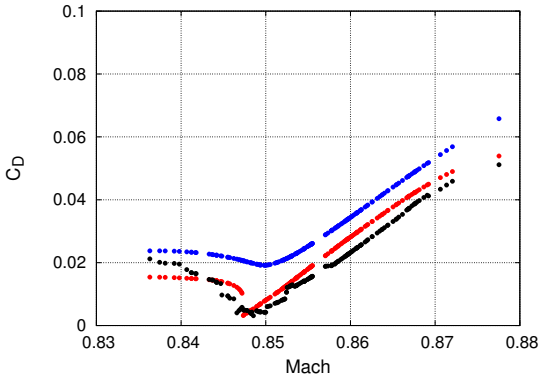

Figure 1: *Drag coefficient obtained using the near-field approach with a fine grid level (●), near-field approach with a coarse grid level (●), far-field approach with a coarse grid level (●) versus the Mach number, M_∞.*

The advantage showed by the far-field method, concerning CPU costs, in the deterministic optimization could be even more evident in robust design problems when the objective function and related constraints are statistical quantities (such as expected values, variances or risk measures [Quagliarella and Iuliano, 2017]). Therefore, a robust optimization problem of the optimum deterministic airfoil obtained with the far-field approach will be performed. The Mach number is considered as an uncertain parameter that may be uniformly located in the interval $[0.83, 0.88]$. Figure 1 illustrates the potential advantage of the far-field method with respect to the near-field one. It can be observed that the C_D obtained at the coarsest grid level using the far-field method gives a much better approximation of the value obtained with the near-field calculation at the finest level with respect to the one found using the near-field approach. Nevertheless, the far-field method still presents problems for a robust design loop as, in some cases, its predictions are not fully validated. This is due to the not yet complete reliability of the shock sensor mechanism that in some cases could lead to a not precise selection of the grid cells to consider in the far-field drag computation. Work is ongoing to improve its reliability and to allow its safe use in a robust design optimization loop.

References

[Paparone and Tognaccini, 2003] Paparone, L., and Tognaccini, R., "Computational Fluid Dynamics-based drag prediction and decomposition", *AIAA Journal*, Vol. 41, No. 9, 2003, pp. 1647 - 1657.

[Gariepy *et al*, 2015] Gariepy, M., Trepanier, J.-Y., Petro, E., Malouin, B., Audet, C., LeDigabel, S., and Tribes, C., "Direct Search Airfoil OptimizationUsing Far-Field Drag Decomposition Results," 53rd AIAA Aerospace Sciences Meeting, AIAA SciTech Forum, AmericanInstitute of Aeronautics and Astronautics, 2015. URL `https://doi.org/10.2514/6.2015-1720`

[Quagliarella and Iuliano, 2017] Quagliarella, D., and Iuliano, E., "Robust Design of a Supersonic Natural Laminar Flow Wing-Body", IEEE Computational Intelligence Magazine, Vol. 12, No. 4, 2017, pp. 14-27. doi:10.1109/MCI.2017.2742718.

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Level Set Methods and Frames for Nonlinear Stochastic Problems

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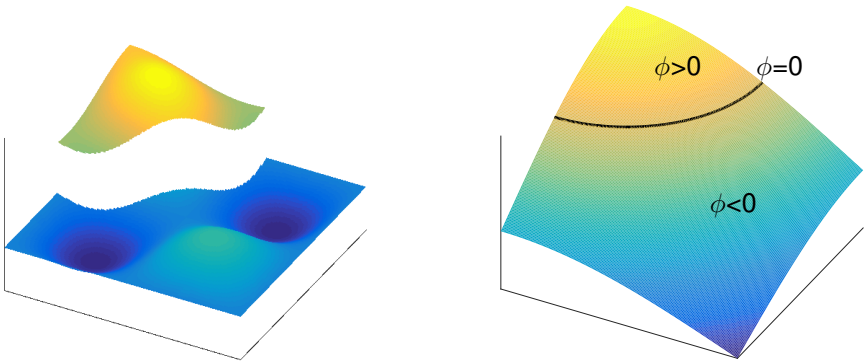
Keywords: level set methods, frames, discontinuity detection, nonlinear problems, conservation laws.

ABSTRACT

The solutions to many engineering problems described by conservation laws exhibit non-smooth dependence on material parameters. In many applications, e.g., large scale CO_2 storage in aquifers [Nordbotten *et al.*, 2012], the material parameters are unknown due to lack of data and inability to accurately resolve small scale variations. The combination of discontinuous dependence on data and uncertainty poses challenging problems when it comes to efficiently estimating quantities of interest. Efficient stochastic representation (e.g., spectral expansions) of quantities of interest requires knowledge of the location of the discontinuities in stochastic space. In this work, we introduce a framework for tracking discontinuities in stochastic space using a level set formulation, followed by reconstruction of quantities of interest with localized basis functions.

Level set methods can be used to track deforming interfaces and are attractive due to the flexibility with respect to the geometry of the regions separated by the interfaces. For instance, they are not restricted to star-convex regions and are therefore of interest in solving complex discontinuous problems with moderate stochastic dimensionality. In this work, we use a level set formulation to identify the location of solution discontinuities. A set of realizations of the nonlinear conservation law of interest is treated as an image, and discontinuities are tracked in pseudo-time by the classical image segmentation techniques introduced in [Malladi *et al.*, 1994].

The zero level set of the steady-state level set function is made to coincide with the discontinuities in stochastic parameter space of the function of interest, as shown in Figure 1. The function of interest (denoted u) is piecewise smooth in regions where the level set function is strictly positive, and strictly negative, respectively.



(a) Discontinuous function $u(\boldsymbol{\xi})$.

(b) Level set function $\phi(\boldsymbol{\xi}; u)$.

Figure 1: *Discontinuous function $u(\boldsymbol{\xi})$ (for fixed space and time) and an associated level set function ϕ with the zero level set being equal to the location of the discontinuity in u. The uncertainty is parameterized by the random vector $\boldsymbol{\xi}$.*

The computed level set solution yields an approximation of the location of conservation law discontinuities. One can see this as a classification problem, where some conservation law realizations may be misclassified due to inexact level set solutions. Because of the irregular shape of the piecewise continuous solution regions, a surrogate for the true solution is constructed using frames, i.e., in this case polynomial functions restricted to each of the different solution regions. Robust computation of the frame coefficients is achieved using the Least Absolute Deviations method [Charnes *et al.*, 1955] to compensate for misclassification of solution realizations, and compared to standard Least Squares Methods.

The performance of the methodology is demonstrated on nonlinear problems from computational fluid dynamics and CO_2 storage, and compared to existing adaptive multi-element generalized polynomial chaos methods [Wan and Karniadakis, 2005]. The proposed method yields a significant speedup in terms of the number of calls to an expensive conservation law solver, at the added cost of solving a level set equation in random space and pseudo-time.

References

[Nordbotten *et al.*, 2012] Nordbotten, J., Flemisch, B., Gasda, S., Nilsen, H., Fan, Y., Pickup, G., Wiese, B., Celia, M., Dahle, H., Eigestad, G., Pruess, K. (2012). Uncertainties in practical simulation of CO2 storage. *Int. J. Greenh. Gas Control*, 9:234–242.

[Malladi *et al.*, 1994] Malladi, R., Sethian, J. A., Vemuri, B. C. (1994). Evolutionary fronts for topology-independent shape modeling and recovery. in *Proceedings of Third European Conference on Computer Vision, Stockholm, Sweden, Lecture Notes in Computer Science 800*, 3–13.

[Charnes *et al.*, 1955] Charnes, A., Cooper, W. W., Ferguson, R. O. (1955). Optimal Estimation of Executive Compensation by Linear Programming. *Management Sci.* 1:138–151.

[Wan and Karniadakis, 2005] Wan, X., and Karniadakis, G. E. (2005). An adaptive multi-element generalized polynomial chaos method for stochastic differential equations. *J. Comput. Phys.* 209:(2):617–642.

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Algebra for a Space Flight Algorithm

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Abstract

We have developed a navigation function for a nanosatellite probe to autonomously fly in deep space. A need is to process uncertainties on-board to select the best accessible measurements to be considered for the autonomous location determination. The main algorithm uses the directions of several celestial objects of the solar system in front of distant stars. A rough position estimate is determined by problem inversion and filtered with a linear Kalman filter, then the process is repeated. Covariances of the measured directions, that are object-dependant, are propagated through the process. We simulated a deep-space cruise from Earth to Mars. The estimated location reaches a 1-σ precision of 200 km. The performance is mainly limited by the strategy of selecting the celestial objects to be measured. Indeed, the ability to gather object directions depends on the sensitivity and agility of the probe and on the availability of objects to be observed. Comparing realistic and purely notional geometries of objects, we expect that an improvement factor up to 10 is still accessible, providing a detailed analysis of the problem's Jacobian. This approach will be further developed into an on-board algorithm to decide on-the-fly the best next object to be measured, as we could take advantage of the many asteroids in all directions of the ecliptic plane.

I. Introduction

As requested by UQOP 2019, only the abstract is provided before 12/2018. The 2-page full paper will be updated in case of selection of the abstract.

II. Methods

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- method 1
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Figure 1: *Example figure*

III. Results

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Table 1: *Example table*

Name		
First name	Last Name	Grade
First name	Last Name	7.5
First name	Last Name	2

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$$e = mc^2 \tag{1}$$

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References

[Segret et al., 2019] Segret, B., Hestroffer, D., Quinsac, G., Agnan, M., Vannitsen, J., Mosser, B. (2019). Optimizations of Autonomous Orbit Determination for a Deep-Space CubeSat. (in press) *18th Australian Aerospace Congress, 24-28 February 2018, Melbourne*, ISSFD 2019.

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A Heuristic Solution to Non-Linear Filtering with Imprecise Probabilities

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Keywords: Non-Linear Filtering, State Estimation, Stochastic Process, Imprecise Probabilities

ABSTRACT

We consider the problem of estimating robust bounds on a functional of the unknown state of a dynamical system, using noisy measurements of the system's historical evolution, and given only partially specified probabilistic descriptions of the system's initial state and measurement (error) models. This problem is a general version of the well-known *filtering* problem, which finds applications throughout science and engineering. The generalisation studied in this work is based on the theory of *imprecise probabilities* [Augustin *et al.*, 2014].

Formally, we consider a dynamical system x_t, $t \geq 0$, taking values in a measurable space $(\mathcal{X}, \mathcal{A}_\mathcal{X})$, with $\mathcal{X} \subset \mathbb{R}^d$ and $d \geq 1$. The system's evolution is governed by the time-homogeneous non-linear vector differential equation

$$\mathrm{d}x_t = f(x_t)\,\mathrm{d}t\,. \tag{1}$$

With P_0, a probability measure on $(\mathcal{X}, \mathcal{A}_\mathcal{X})$, we assume that the initial state x_0 is an unknown realisation of a random variable $X_0 \sim P_0$. Together with (1), this induces random variables X_t, which describe the (uncertainty about the) state of the system at each time t. Explicitly, if for all $t \geq 0$ we define the map $F_t : \mathcal{X} \to \mathcal{X}$ as the point-wise solution to (1), $F_t(x_0) := x_0 + \int_0^t f(x_\tau)\,\mathrm{d}\tau$, then X_t is a random variable governed by the push-forward measure $P_t := P_0 \circ F_t^{-1}$ on $(\mathcal{X}, \mathcal{A}_\mathcal{X})$.

In the setting with *imprecise* probabilities, we additionally deal with (epistemic) uncertainty about the initial distribution P_0. We then say that P_0 is an element of some *set* $\mathcal{P}_0$ of probability measures on $(\mathcal{X}, \mathcal{A}_\mathcal{X})$. Notably, we do not consider any probability distribution over this set $\mathcal{P}_0$.

Finally, it is assumed that the system can only be observed through noisy measurements. The measurement y_t taken at time $t \geq 0$ is a realisation of a random variable Y_t, governed by a (stochastic) measurement model $P(Y_t \mid \cdot)$. We again do not assume full knowledge about $P(Y_t \mid \cdot)$; instead, we only know that $P(Y_t \mid \cdot) \in \mathcal{P}(Y_t \mid x_t)$ for some *set* of probability measures $\mathcal{P}(Y_t \mid x_t)$.

The filtering problem can now in general be described as computing the expected value of some function $h : \mathcal{X} \to \mathbb{R}$ on the uncertain state X_t, given observed measurements $y_{s_1}, \ldots, y_{s_n}$. When using imprecise probabilities, there are multiple precise probability models compatible with our set-valued assessments. The set of these compatible models is denoted $\mathcal{P}$. Any element $P \in \mathcal{P}$ is a probabilistic model, for which we can compute the quantity of interest using Bayes' rule. The aim is now to compute the *lower-* and *upper* expectations,

$$\begin{aligned} \underline{\mathbb{E}}\big[h(X_t) \,\big|\, y_{s_1}, \ldots, y_{s_n}\big] &:= \inf_{P \in \mathcal{P}} \mathbb{E}_P\big[h(X_t) \,\big|\, y_{s_1}, \ldots, y_{s_n}\big] \\ \overline{\mathbb{E}}\big[h(X_t) \,\big|\, y_{s_1}, \ldots, y_{s_n}\big] &:= \sup_{P \in \mathcal{P}} \mathbb{E}_P\big[h(X_t) \,\big|\, y_{s_1}, \ldots, y_{s_n}\big] \end{aligned} \tag{2}$$

which are the tightest possible bounds compatible with our imprecise assessments.

To the best of our knowledge, this is the first time that this filtering problem is considered at this level of generality. A non-exhaustive list of related work includes the imprecise Kalman filter [Benavoli *et al.*, 2011], which assumes the equations of motion to be linear; particle filters based on random set theory [Ristic, 2013], which deals with less general uncertainty structures; and filtering with imprecise hidden Markov chains [Krak *et al.*, 2017], which assumes $\mathcal{X}$ is finite.

In our current work, we take a heuristic approach to computing—approximately—the quantities of interest. To this end, we introduce a novel algorithm based on a problem that is equivalent to solving (2); this form is known as the *generalised Bayes' rule* in the imprecise probability literature. A known recursive decomposition thereof allows us to reduce the problem to computing (i) the n (independent) *lower-* and *upper likelihoods* of the states x_{s_i} given the observations y_{s_i}, (ii) the solution to $\inf_{P_0 \in \mathcal{P}_0} \int_{\mathcal{X}} g(x)\, \mathrm{d}P_0(x)$ for any $g : \mathcal{X} \to \mathbb{R}$, and (iii) the map F_t for any t. We solve problem (i) trivially by parameterising the set $\mathcal{P}(Y \mid X)$ directly in terms of these lower- and upper likelihoods—a more general method would require solving the optimisation explicitly. The problem (ii) is just the lower expectation with respect to the initial model $\mathcal{P}_0$, which although it cannot really be simplified further, is relatively straightforward when compared to the original problem (2). We solve (iii) by replacing the maps F_t with surrogate model approximations that are both local in time (different surrogates for different values of t) and local in space (the approximations are only accurate on certain subsets of $\mathcal{X}$). We build these surrogates on a set of points quasi-randomly sampled from a sequential estimate of an imprecise $(1 - \alpha) \times 100\%$ credible region of X_t, conditional on the sequential observations, and then propagated forward in time.

In this work, the developed method is applied to the case of robust state estimation of an Earth satellite orbiting in a strongly perturbed environment, and its performance compared against a traditional filtering approach based on precise probability distributions.

References

[Augustin *et al.*, 2014] Augustin, T., Coolen, F. P. A., De Cooman, G. and Troffaes, M. (2014). *Introduction to Imprecise Probabilities*, John Wiley & Sons.

[Benavoli *et al.*, 2011] Benavoli, A., Zaffalon, M. and Miranda, E. (2011). Robust filtering through coherent lower previsions. *IEEE Transactions on Automatic Control*, 56:1567–1581.

[Krak *et al.*, 2017] Krak, T., De Bock, J. and Siebes, A. (2017). Efficient Computation of Updated Lower Expectations for Imprecise Continuous-Time Hidden Markov Chains. *Proceedings of ISIPTA 2017*, 193–204.

[Ristic, 2013] Ristic, B. (2013). *Particle Filters for Random Set Models*, Springer.

An industry ready approach to characterization and reduction of manufacturing uncertainties

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Significant research and development effort has been dedicated over the past few years to the improvement of uncertainty propagation and robust or reliable optimization techniques. A variety of uncertainty propagation methods spanning from advanced sampling methods like multi-level Monte-Carlo, over various Polynomial chaos based method to perturbation techniques were significantly advanced to address in the order of ten uncertainties in industrial applications [Hirsch *et al.* (2018)]. All these methods, however, rely on the correct characterization of input uncertainties, which in general is a difficult task.

In particular characterizing the manufacturing variability of for example turbomachinery blades remains challenging. One possibility is to measure hundreds of manufactured blades and in this way sample the surface variability resulting from the manufacturing process. This is, on the one hand, expensive and time consuming and, on the other hand, not always applicable, for example for customized designs, which are either unique or comprise of only one or two machines. In this case, insufficient geometry samples are available. Büche *et al.* (2018) show a path to extract an estimation of manufacturing variability from technical norms, which define the allowable manufacturing tolerances typically in clearly defined tolerance classes from coarse to fine.

In the current work, the approach described by Büche *et al.* (2018) forms the basis for the characterization of input uncertainties of a high pressure turbine. Manufacturing tolerances are attributed to engineering design parameters describing the blade shape. In general, such a model or a CAD design will consist of hundreds of lengths, angles and radii. However, a direct treatment of the O(100) uncertainties is still out of reach on industrial scale for state-of-the-art uncertainty propagation techniques. An alternative form design space reduction techniques [Diez *et al.* (2015)], which aim at maintaining the freedom in the geometrical variability, but at a lower computational cost. The number of effective uncertain variables is reduced.

A Latin Hypercube Sampling is performed sampling up to thousands of geometries from uniform- and beta-distributed random variables. On this basis, the covariance of the geometry is calculated and a Principle Component Analysis (PCA) is applied. The resulting Eigen modes for various retained reconstruction accuracies are analyzed and discussed.

In a second step, the uncertainties resulting from the reduction are propagated and compared to the results of the full parametric uncertain problem for the four classes of accuracy defined in the applied technical norm. The uncertainties in the reduced problems correspond to the retained modes and are Gaussian distributed, while the eigenvalues are the variance of these Gaussian distributions.

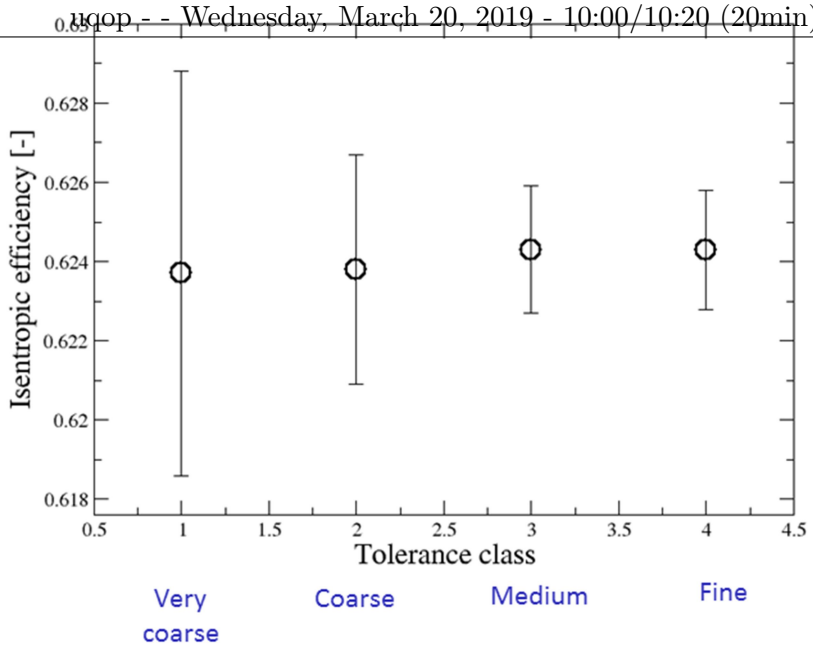

Figure 1: Comparison of mean value and standard deviation of isentropic efficiency for the 4 defined tolerance classes. The bars correspond to ±σ.

The results of the UQ simulations are discussed and compared. Figure 1 shows the evolution of the mean value and standard deviation of the isentropic efficiency for the four tolerance classes defined in the technical norm. As one could expect, the spread of the predicted result reduces with more narrow tolerance classes. It is very interesting to observe that from a practical engineering point of view there is no relevant difference in prediction for the two most narrow tolerance classes 'medium' and 'fine'. This can be exploited in an inverse robust design optimization setting, where the largest allowable tolerance is sought for, while respecting a minimum performance (constraint).

The further, scaled sensitivity derivatives of the various studied problems are compared and the reduced problems are compared with the initial non-reduced problem. This work constitutes an industry ready approach for the characterization and reduction of manufacturing uncertainties.

References

Büche D, Klostermann S, Roge G, Loyatho X, 2018, Uncertainties in Compressor and Aircraft Design, Notes on Numerical Fluid Mechanics and Multidisciplinary Design 140, pp. 35-51

Diez M, Campana EF, Stern F, 2015, Design-Space dimensionality reduction in shape optimization by Karhunen-Loeve expansion, Comput. Methods Appl. Mech. Eng. 283, 1525-1544

Hirsch C, Wunsch D, Szumbarski J, Laniewski-Wolk L, Pons-Prats J, Editors, 2018, *Uncertainty Management for Robust Industrial Design in Aeronautics*, Notes on Numerical Fluid Mechanics and Multidisciplinary Design 140

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An implementation of LASSO using optimization methods for piecewise differentiable functions

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Keywords: LASSO, Sub-gradient, Proximal Gradient Descent, Co-ordinate Descent

ABSTRACT

We present and compare a novel R implementation of *LASSO* using different optimization methods for piecewise differentiable functions. LASSO (or "Least Absolute Shrinkage and Selection Operator") was introduced by Robert Tibshirani [Tibshirani, 1996]. This is one of the popular regularization methods because of its efficient variable selection property. The variable selection is achieved by adding a penalty term to the least square problem. However, this requires in the minimization of a piecewise differentiable objective function. We review three different optimization techniques to tackle this issue: the sub-gradient method, the proximal gradient descent method, and the co-ordinate descent method. The *sub-gradient* method [Shor, 1985] is a simple variant of the gradient descent method which requires a predetermined sequence of step sizes. If these step sizes are not chosen carefully, convergence can be excessively slow.. However, this is not a descent method in general and we must keep track of the best solution to achieve optimality. The *proximal gradient descent* method [Beck *et al.*, 2009] is applicable for a convex function, which is a sum of two convex functions, where one function is differentiable and the other is non-differentiable but has a simple analytical form. The co-ordinate descent method [Sauer *et al.*, 1993] successively minimizes a multivariable function along each co-ordinate. We compare the speed of convergence of these three methods using LASSO. In addition to this, we extend our implementation to the *adaptive LASSO* [Zou, 2006] (or weighted LASSO), as well as cross-validation or boot-strap method for frequentist model validation tools. We split a dataset into K parts for cross validation and then we fit model for $K-1$ part and test it with the remaining

part. We repeat this method for each part so that each data point is used once for model validation. For boot-strap we randomly sample data points from the dataset with replacement for a given number of times and examine the empirical distribution of the modeling parameters.

We introduce the idea of perturbed weights for assessing the sensitivity of regression parameters using the idea of adaptive LASSO. These weights on the penalty term of LASSO force the predictors to shrink earlier than the other depending on the scale of the weights, i.e. higher weight forces a predictor to shrink early whereas lower weight slows down the shrinkage. For the sensitivity of the predictors we use n number of purturbed weights and obtain the LASSO coefficients. We get a behavior of the predictors w.r.t. these weights. We observe that for these purturbed weights the standard deviations of the values of the predictors are often less for the non-important predictors obtained from the regular LASSO than that of the important ones.

References

[Beck *et al.*, 2009] Beck, A. and Teboulle, M. (2009) A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems *SIAM Journal on Imaging Sciences*, 2(1):183-202.

[Sauer *et al.*, 1993] Sauer K. and Bouman C. (1993) A local update strategy for iterative reconstruction from projections *IEEE Transactions on Signal Processing*, 41(2):534-548.

[Shor, 1985] Shor, N. Z. (1985) Minimization Methods for Non-Differentiable Functions *Springer Series in Computational Mathematics*, 3(1):22-47.

[Tibshirani, 1996] Tibshirani, Robert (1996). Regression shrinkage and selection via the lasso *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 58(1):267-288.

[Zou, 2006] Zou, Hui (2006) The Adaptive Lasso and Its Oracle Properties *Journal of the American Statistical Association*, 101(476):1418-1429.

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Evidence-Based Robust and Reliable Optimisation of Dynamic Complex Systems

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Keywords: Evidence Theory, Optimisation, Robustness, Reliability, Complex System, Graph Theory, Evidence Network Model

ABSTRACT

This paper will present a new approach for the Optimisation for Robustness and Reliability of Dynamic Complex Systems when they are affected by epistemic uncertainty.

Commonly, approaches for the design of Complex Systems, like safe margins approach, lack robust procedures for the design, test and redefinition of the system prior to large economical investments. Often, indeed, drawbacks are identified after a lot of money have been already spent for prototyping or after the design has already reached a mature stage. When this happens, engineers has to take a difficult decision: whether to continue and try to minimise the negative impact of this gap, or to abandon part or all of the work for a better design with consequent loss of time and money. Both decisions lead to negative consequences.

There are three main reasons why this occurs with traditional approaches. They don't proper model uncertainty that comes from different sources and manifests itself in different ways. They don't adequately deal with the interaction between sub-systems which form the Complex System and are usually studied by different design teams. Also, they don't consider the evolution in time of the system during its operational life.

About the first point, it is largely accepted to divide uncertainty in in aleatory and epistemic: the former can not be reduced and it is basically due to randomness of nature and it can be captured with a frequentist approach, while the second comes from lack of knowledge and/or subjective probability and it can be reduced to aleatory uncertainty as information increases. Aleatory uncertainty is used, for example for measurement errors; epistemic uncertainty, instead, is always present in the early design phases when experts are used to express their opinions and models are low fidelity; there is epistemic uncertainty also when data is incomplete or has poor quality. To rigorously deal with both types of uncertainty, then, we use Evidence Theory [Shafer, 1976,

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Alicino and Vasile, 2014, Croisard et al., 2010] because it is a promising mathematical tool and it is a generalisation of the classical Probability Theory.

About the second point, we model *Complex Systems* using *Graph Theory* [Boccaletti et al., 2006]: they are represented as networks where each node is a sub-system and each link an information pathway. To each node it is associated a value of the quantity of interest and a measure of uncertainty. Given that we use *Evidence Theory*, the probability measure is generalised by the measures of *Belief* and *Plausibility* and the network is called *Evidence Network Model* (ENM). The graph-structure of the ENM allows also to solve the NP-hard problem - given by the uncertainty propagation with the use of Evidence Theory - drastically reducing the computational cost from exponential to linear with the problem dimention .

The approach of ENM for *Evidence-Based Robust Optimisation* was introduced in [Vasile, et al., 2017, Filippi, et al., WCCI, 2018, Filippi et al., SECESA, (2018), Filippi et al., IAC, (2018)]. Here we are focused in the optimisation for *Robustness* and *Reliability* and in particular the work presents an innovative method for the propagation of uncertainty for the reliability analysis: degradation of the sub-systems' state is modelled, differently from the literature, as a continuous function of time.

Finally an example demonstrates that ENM is a valid tool for the preliminary design of dynamic complex space systems that are affected by epistemic uncertainty: the method is applied to the design of a cube-sat, where the quantity of interest is the overall mass.

References

[Shafer, 1976] Shafer, G. (1976). A mathematical theory of evidence, Princeton University Press. *Princeton University Press*.

[Alicino and Vasile, 2014] Alicino, S. and Vasile, M. (2014). Evidence-based preliminary design of spacecraft. *SECESA*.

[Croisard et al., 2010] Croisard, N., Vasile, M., Kemble, S. and Radice, G. (2010). Preliminary space mission design under uncertainty. *Acta Astronautica*, Volume 66, pages 654-664.

[Vasile, et al., 2017] Vasile, M., Filippi, G., Ortega, C. and Riccardi, A. (2017). Fast Belief Estimation in Evidence Network Models. *EUROGEN*.

[Filippi, et al., WCCI, 2018] Filippi, G., Vasile, M. Marchi, M. and Vercesi, P. (2018). Evidence-Based Robust Optimisation of Space Systems with Evidence Network Models. *WCCI Congress on Evolutionary Computation*.

[Filippi, et al., 2017] Filippi, G., Ortega, C., Riccardi, A. and Vasile, M. (2017). Technical ESA Report, Robust Design Use-Cases. *reference TN-RDO-UC-CDF-v1*.

[Filippi et al., SECESA, (2018)] Filippi, G., Vasile, M., Korondi, Z., Marchi, M., Poloni, C. (2018) Robust Design Optimisation of Dynamical Space System *SECESA*.

[Filippi et al., IAC, (2018)] Filippi, G., Krpelik, D., , Korondi, Z., Vasile, M., Marchi, M., Poloni, C. (2018) Space Systems Resilience Engineering and Global System Reliability Optimisation Under Imprecision and Epistemic Uncertainty *IAC*.

[Holme and Saramaki, 2012] Holme, P. and Saramaki, J. (2012). Temporal networks. *Physics Reports*, vol: 519 (3) pp: 97-125.

[Boccaletti et al., 2006] Boccaletti, S., Latora, V., Moreno, Y., Chavez, M. and Hwang, D. U. (2006). Complex networks: structure and dynamics. *Physics Reports*, 424 (4-5) (2006) 175-308.

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AK-MCS extension for the Efficient Estimation of Extreme Quantiles and Failure Probabilities

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Keywords: Rare Events, Extreme Quantile, Risk Analysis

ABSTRACT

We consider the problem of estimating a probability of failure pf, defined as the volume of the excursion set of a complex (e.g. output of an expensive-to-run finite element model) scalar performance function J below a given threshold, under a probability measure that can be recast as a multivariate standard gaussian law using an isoprobabilistic transformation. We focus on a method able to deal with problems characterized by multiple failure regions, possibly very small failure probability pf (say $\sim 10^{-6}$ - 10^{-9}), and when the number of evaluations of J is limited. The present work is an extension of the popular Kriging-based active learning algorithm known as AK-MCS, as presented in [Schobi et al.]. Similarly, the problem is formulated in such a way that the computation of both very small probabilities of failure and extreme quantiles is unified. The key idea merely consists in replacing the Monte-Carlo sampling, used in the original formulation to propose candidates and evaluate the failure probability, by a centered isotropic Gaussian sampling in the standard space, which standard deviation is iteratively tuned. This extended AK-MCS (eAK-MCS) method inherits its former multi-point enrichment algorithm allowing to add several points in each iteration, and, due to the Gaussian nature of the surrogate, to estimate a failure probability/quantile range at each iteration step. An Importance Sampling procedure allows to accurately estimate a quantile of level as low as 10^{-9}, with a reasonable number of calls to the surrogate ($\sim 10^7$). A batch strategy on the quantile permits to further exploit the parallelization capability of eAK-MCS. Similarly to other Kriging-based methods, the proposed approach suffers from the same limitations, namely the low input dimension and depends strongly on the ability of the surrogate to fit the performance function. We illustrate the performances of the proposed method on several two, six and eight-dimensional benchmark analytical functions, for which the failure probability is very low (pf $\sim 10^{-6}$ - 10^{-9}), including in particular the three test-cases presented in [Bect et al.] (where a Bayesian Subset Simulation approach is proposed). In the context of pure failure probability estimation, there is no clear advantage of eAK-MCS over BSS [Bect et al.]. Its main asset lies in the fact that most AK-MCS based algorithms could be possibly adapted in the context of extreme event, which is illustrated with the proposed extreme quantile estimation tool. In the test-cases studied, small failure probabilities and quantiles are

estimated with a satisfactory accuracy with a moderate number evaluations of the performance function J ($\sim$ 25-140), with a batch strategy.

References

[Schobi et al.] R. Schobi, B. Sudret, S. Marelli (2016). Rare event estimation using polynomial-chaos kriging. *Journal of Risk and Uncertainty in Engineering Systems*

[Bect et al.] J. Bect, L. Li, E. Vazquez (2017). Rare event estimation using polynomial-chaos kriging. *JSIAM/ASA Journal on Uncertainty Quantification*

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A Framework for the Efficient Aerodynamic Shape Optimization Problems under Uncertainty

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Keywords: surrogate models, robust optimization, CFD.

ABSTRACT

The ultimate goal of this work is the development of a framework for Robust Single or Multi-Objective Aerodynamic Design Optimization problems. Robust Optimization allows the obtaining of an optimal design that is less vulnerable with respect to uncertainties in operating conditions (i.e M_∞) and geometric shape (introduced by the tolerances of manufacturing processes). Particularly, the objective function and constraints are statistical quantities, i.e. mean, variances or risk measures [Quagliarella and Iuliano, 2017]). Therefore, there is an increase in the computational cost associated to the Computational Fluid Dynamics (CFD) evaluations in contrast to the classical Deterministic Optimization problems. One of the possible approaches for reducing CPU costs is the use of Surrogate Models. Therefore, the first step for building a efficient framework could be the performance of a benchmarking of surrogate models. So that, comparing different methods with in respect of the number of expensive function evaluations. For that, the DLR Python Library SMARTy has been used.

The test case selected is the RAE 2822 in a transonic inviscid flow, modeled by Euler equations, at $M_\infty = 0.73$ and angle of attack $\alpha = 2$. The reference data has been obtained by Monte Carlo sampling nine uncertain parameters affecting the geometry. In particular, four million CFD simulations has been employed. To build the Surrogate Model the first decision to be taken is the sampling method for the reference data. Quasi Monte Carlo (QMC) based on Latin Hypercube and Sobol sequences were compared, concluding that the best method was QMC based on Sobol Sequences with a normalized sampling to input Distribution. In particular, 33 CFD samples are going to be taken. After that, the different models are built and compared. In Figure 1, the Cumulative Distribution Functions obtained with 33 samples of the real data using Monte Carlo, Kriging, and TPS are compared with respect to the reference data (*orange line*). To assess which Surrogate Model is the most accurate, the Root Mean Square Error of the CDF and the error of the interested statistical quantities (mean, standard deviation or 95% quantile) are calculated. Hence, it was determined that Kriging Surrogate Model with optimized Hyperparameters to MLE was the most suitable SM for the studied test case.

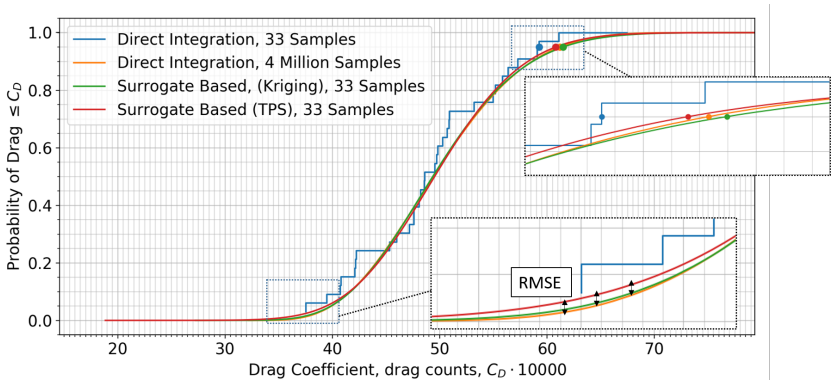

Figure 1: *Comparison of the Cumulative Distribution Function obtained with the different models.*

Once the benchmark of the Surrogate Model has been performed, the subsequent step is the performance of the optimization problem of the before-mentioned test case. Firstly, a deterministic optimization will be done, and, afterwards, a robust one. The airfoil will be parametrized using NURBS representation by means of 10 control points using a python library[1] . For a detailed description refers to [Piegl and Tiller, 2012]. This representation will lead to 14 design variables for the optimization. The optimization design exercise requires to find the airfoil with minimum drag under a geometrical constraint (the area of the optimal airfoil should be greater than the area of the baseline) and a operational condition constraint (the lift coefficient of the optimum configuration must be also greater than the c_l of the RAE 2822 under this conditions). The constraints will be expressed as quadratic penalties. The optimization algorithm that will be used is the Covariance Matrix Adaptation Evolution Strategy (CMA-ES). Moreover, for the robust optimization the design variables will be also the uncertain variables. In particular, the design variables will be uniformly sampled using a Monte Carlo sampling. As mentioned, in robust optimization the objective function or the constraints can be functional. In this case, the optimization will rely on the introduction of the Conditional Value-at-Risk (CVaR) risk-measure [Quagliarella *et al.*, 2015][Quagliarella and Iuliano, 2017] .

References

[Quagliarella and Iuliano, 2017] Quagliarella, D., and Iuliano, E., "Robust Design of a Supersonic Natural Laminar Flow Wing-Body",IEEE Computational Intelligence Magazine, Vol. 12, No. 4, 2017, pp. 14-27. doi:10.1109/MCI.2017.2742718.

[Piegl and Tiller, 2012] Piegl, L., and Tiller, W.,The NURBS book, Springer Science & Business Media, 2012.

[Quagliarella *et al.*, 2015] Domenico Quagliarella, Giovanni Petrone, and Gianluca Iaccarino. Reliability-based design optimization with the generalized inverse distribution function. In David Greiner, Blas Galván, Jacques Périaux, Nicolas Gauger, Kyriakos Giannakoglou, and Gabriel Winter, editors, *Advances in Evolutionary and Deterministic Methods for Design, Optimization and Control in Engineering and Sciences*, volume 36 of *Computational Methods in Applied Sciences*, chapter 5, pages 77-92. Springer International Publishing, 2015. ISBN 978-3-319-11540-5.

[1]NURBS-Python Documentation can be found in `http://nurbs-python.readthedocs.io/en/latest/`

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An adaptive evolutionary surrogate-based approach for single-objective bilevel optimisation

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Keywords: bilevel, optimisation, evolutionary, surrogate assisted.

ABSTRACT

Bilevel optimisation problem refers to a problem where one optimisation problem has another optimisation problem as constraint. The target of this problem is to find the optimum of the upper level problem, taking into consideration the optimality of the corresponding lower level. Despite this basic definition and idea, the problem introduces many challenges, as it is usually not following simplified properties such as convexity or continuity. Moreover, even the simplest case of a linear bilevel optimisation problems has been proved to be NP-hard [Hansen et al., 1992].

The research community so far was concentrated on tackling well-behaved bilevel problems with specific properties in order to be solved with classical methods. In recent years, hybrid and evolutionary approaches have become more popular. Metaheuristic and evolutionary algorithms do not need to make assumptions about the objective functions of the problem and therefore can become really useful for solving bilevel problems. On the other hand these algorithms require a large number of functions evaluations. The nested nature of the bilevel problems contributes even more in transforming the evolutionary approach in bilevel optimisation to a computationally expensive task. The cost worsens when the evaluations of the exact solution of the problems require calling time consuming tasks, e.g. Computation Fluid Dynamics (CFD) for engineering simulations.

Use of meta-modelling or surrogate modelling techniques is one of the ways of dealing with the computational efficiency. Meta-model or surrogate model can be regarded as an approximation function of an actual model, that is simpler and easier to evaluate. This approximation is made by using sampled data of the actual evaluation in the design space.

In the literature so far, there have been developed several bilevel evolutionary algorithms that are surrogate assisted, offering competitive results to bilevel test problems and applications. Some of these algorithms attempt to approximate the mapping of the upper-level variables to the lower level optimal function values. In that way, instead of running the optimisation of lower level

problem for each upper level vector, the value is obtained by the surrogate, reducing the problem to single level.

It is known that the performance of evolutionary algorithms heavily depend on their control parameter settings [Eiben et al., 1999]. Since the (near-)optimal control parameter values may change over the run of an EA, the optimisation process can be used to determine the direction and magnitude of change of the control parameter value [Karafotias et al., 2015]. This process of adapting the control parameters on the fly, is called parameter control. Since in the bilevel problem, the landscape changes dynamically during the optimisation process, such an adaptive approach in parameter control can be very useful.

In this paper, we will attempt to approximate the upper level vector with the lower optimal solutions with Kriging as a surrogate model, an approach tested already in the papers of [Sinha et al., 2018] and [Xia et al., 2018]. The goal is to develop an adaptive Differential Evolution Algorithm (DE) in the upper level, where the parameter control will be done taking into consideration the evaluation of both levels. The population size of the upper level will be updated each time the expected approximation error is not acceptable and the model needs to be retrained. Moreover, a mutation and crossover adaptation strategy will be applied in the upper level optimisation algorithm. For the lower level optimisation, when exact solutions are needed to train the surrogate, a separate evolutionary algorithm (DE or Particle Swarm Optimisation) will be used. The expected outcome is to investigate the improvements that adaptive parameter control can bring to evolutionary surrogate assisted optimisation algorithm by finding good quality bilevel solutions with lower number of functions evaluations in a number of known benchmark test problems.

References

[Xia et al., 2018] , Xia, Yi and Liu, Xiaojie and Du, Gang, (2018). Solving bi-level optimization problems in engineering design using kriging models. *Engineering Optimization*, 50:5, 856–876.

[Sinha et al., 2018] , Sinha, A., Bedi, S., and Deb, K, (2018). Bilevel Optimization Based on Kriging Approximations of Lower Level Optimal Value Function. *IEEE Congress on Evolutionary Computation (CEC)*, 13:5, 1–8.

[Hansen et al., 1992] , Hansen, Pierre and Jaumard, Brigitte and Savard, Gilles, (1992). New Branch-and-bound Rules for Linear Bilevel Programming. *Society for Industrial and Applied Mathematics*, 1194–1217.

[Eiben et al., 1999] , Eiben, Ágoston E., Robert Hinterding, and Zbigniew Michalewicz., (1999). Parameter control in evolutionary algorithms. *IEEE Transactions on evolutionary computation* ,3:2, 124–141.

[Karafotias et al., 2015] , Karafotias, Giorgos, Mark Hoogendoorn, and Ágoston E. Eiben., (2015). Parameter control in evolutionary algorithms: Trends and challenges. *IEEE Transactions on Evolutionary Computation*,19:2, 167–187.

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Approximating Hypervolume Contributions Using Kriging

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Keywords: evolutionary algorithm, hypervolume, metamodel, kriging.

ABSTRACT

Hypervolume is an indicator to assess the quality of an obtained solution-set in multi- and many-objective optimization. Hypervolume-based optimization algorithms are rarely used for solving many-objective optimization problems due to the bottleneck of computing the hypervolume contributions of each solution. The current fastest exact hypervolume-computation algorithm is the incremental method [3]. However, it is not scalable to high dimensional problems because the computation cost grows exponentially with respect to problem's dimension. An alternative method for computing hypervolume-contribution is by using approximations, either approximating the total hypervolume or approximating the (least) contributions.

Examples of hypervolume-approximation algorithms have been proposed by Bringmann and Friedrich [5, 4], Ishibuchi, et al. [6], Bader, et al. [1]. Among these algorithms, only [5] has a guaranteed error bound. In this work we propose a novel approximation method, which incorporates uncertainty quantification techniques, based on *kriging* metamodels. Kriging, or Gaussian Process Regression [7], is a metamodeling approach that approximates outputs over the entire search space, and quantifies the uncertainty of the predictor through the mean square error (MSE), also known as *kriging variance* [10]. Kriging is well-known as an effective predictor because the kriging variance can be exploited to control the accuracy of the approximations.

More formally, let $f(\mathbf{x})$ be a deterministic function that is analytically intractable, where $\mathbf{x} = (x_1, ..., x_d)^T$ is an input vector of decision variables of dimension d. In the interest of fitting a kriging metamodel for the response at n design points, kriging assumes that the unknown response surface can be represented as $f(\mathbf{x}) = \mathbf{f}(\mathbf{x})^T\boldsymbol{\beta} + M(\mathbf{x})$, where $\mathbf{f}(\mathbf{x})$ is a vector of known trend functions (i.e., a prior trend model that can be defined as a smoothly varying deterministic function), $\boldsymbol{\beta}$ is a vector of unknown parameters of compatible dimension and $M(\mathbf{x})$ is a realization of a mean zero covariance-stationary Gaussian random field. It is common to consider a constant β instead of the trend term, as it has shown to more useful in practice [8].

In kriging, some samples are taken from the expensive source as training data to build a cheaper prediction model. We consider several metamodels that are fitted with different predictors (e.g., objective values, R2 and crowding distance). The proposed method works as follows: after

computing the e.g. expensive and exact hypervolume contributions of the points in the current front, we fit a kriging metamodel to the response surface of the hypervolume contribution. We exploit the kriging information to search for new points in view of improving the current front. Since for higher dimensions (i.e., more than 10 objectives), even computing the exact hypervolume contribution of each point in the current front is expensive, we also use other indicators with less computational complexity as predictors.

The consistency and correctness rate of the metamodels, as well as the computational cost, are compared against the exact hypervolume contributions and the newly proposed approximation method of Shang, et al.[9]. Preliminary results show that the method has potential. By exploiting both the kriging predictor and its uncertainty, the approximations can be used to sample points in e.g., sequential algorithms such as SMS-EMOA [2], as the computational cost is reduced significantly. Furthermore, we observe that the estimation of the kriging hyperparameters (via maximum likelihood) and the choice of kernel play a crucial role in training the metamodel in order to achieve accurate approximations. Additional experiments will provide valuable information in this regard.

References

[1] Johannes Bader, Kalyanmoy Deb, and Eckart Zitzler. Faster hypervolume-based search using monte carlo sampling. volume 634 of *Lecture notes in economics and mathematical systems*, pages 313 – 326. Springer, 2010.

[2] Nicola Beume, Boris Naujoks, and Michael Emmerich. SMS-EMOA: Multiobjective selection based on dominated hypervolume. *Eur. J. Oper. Res.*, 181(3):1653 – 1669, 2007.

[3] L. Bradstreet, L. While, and L. Barone. A fast incremental hypervolume algorithm. *IEEE Transactions on Evolutionary Computation*, 12(6):714–723, Dec 2008.

[4] Karl Bringmann and Tobias Friedrich. Approximating the volume of unions and intersections of high-dimensional geometric objects. *Comput. Geom.*, 43(6):601–610, 2010.

[5] Karl Bringmann and Tobias Friedrich. Approximating the least hypervolume contributor: Np-hard in general, but fast in practice. *Theor. Comput. Sci.*, 425:104 – 116, 2012.

[6] Hisao Ishibuchi, Noritaka Tsukamoto, Yuji Sakane, and Yusuke Nojima. Indicator-based evolutionary algorithm with hypervolume approximation by achievement scalarizing functions. In *Genetic and Evolutionary Computation (GECCO)*, pages 527–534, New York, NY, 2010. ACM.

[7] Carl Edward Rasmussen. *Gaussian processes for machine learning*. Citeseer, 2006.

[8] Thomas J Santner, Brian J Williams, and William I Notz. *The design and analysis of computer experiments*. Springer Science & Business Media, 2013.

[9] Ke Shang, Hisao Ishibuchi, and Xi Ni. R2-based hypervolume contribution approximation, 2018.

[10] Wim CM Van Beers and Jack Kleijnen. Kriging for interpolation in random simulation. *Journal of the Operational Research Society*, 54(3):255–262, 2003.

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Change of Probability Measure in Weighted Empirical Cumulative Distribution Function

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Keywords: Change of Probability Measure, Weighted Empirical Cumulative Distribution Function, Radon-Nikodym derivative, Girsanov theorem.

ABSTRACT

Change of probability measure is a fundamental and intensely treated concept in measure theory, and it has important implications and applications in probability theory, financial modeling and engineering and the theory of stochastic processes. Indeed, the capability of changing the probability measure that defines a probability space can be handy in any situation in which a risk measure should be estimated, and variance reduction or importance sampling techniques are used to reduce the computational cost of risk function estimation. In these cases, the data samples available to estimate the risk function value are not computed according to the actual statistical distribution that models the uncertain input parameters, and a change of probability measure should be introduced to recover the correct estimation of the quantity of interest.

The approach here illustrated for changing the probability measure derives directly from the methodology illustrated in [Amaral et al., 2016], and it relies on the introduction of a Weighted Empirical Cumulative Distribution Function (WECDF). The main difference is in the approach used to change the weights, that relies on empirical density function ratios rather than cumulative distributions and, consequently, in the numerical algorithms used to compute the weights.

The development of new efficient approaches to robust or reliability-based optimization problems requires the ability to obtain reasonable estimates of the risk function during the optimization process even when the samples are few and have not been generated according to the actual distribution of the input random variables. In most cases only a small finite number of evaluations obtained by discrete sampling of the input parameters is available, and this can be a problem if a good estimation of the risk measure governing the problem is required. The methods commonly used in these cases either rely on response surfaces [Crestaux et al., 2009], or sophisticated quadrature laws [Witteveen and Iaccarino, 2012, Congedo et al., 2013], or, finally, on multi-level sampling methods [Giles, 2015]. Appropriate use of importance sampling and, consequently, of change of probability measure, alone or in conjunction with the previously

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mentioned methods, could help to drastically reduce the number of costly evaluations of the objective function required.

The change of probability measure is obtained through a constrained optimization process aimed to assign suitable values to the weights of the WECDF:

$$\begin{aligned} \mathbf{w} = \arg\min_{\mathbf{w}} \quad & \omega^2(\mathbf{w}) \\ \text{s. to:} \quad & w_i \geq 0,\ i = 1, \ldots, n \\ & \sum_{i=1}^{n} w_i = 1 \end{aligned} \tag{1}$$

with ω^2 a suitable objective function that will be described in the full work. The problem can be solved using a non-negative least squares algorithm, like the Lawson and Hanson algorithm [Lawson and Hanson, 1995], or transforming it into a convex quadratic programming problem [Amaral, 2015]. Figure 1 reports the result obtained to restore the proper CDF related to the function $f = \frac{1}{n}\sum_{i=1}^{n}(2\pi - u_i)\cos(u_i - d_i)$ with $\mathbf{u} \in [0,3]^n$, $\mathbf{d} \in [0, 2\pi]^n$ and $n = 6$. The probability measure was changed to let the random vector $\mathbf{u}$ have components with a uniform distribution function.

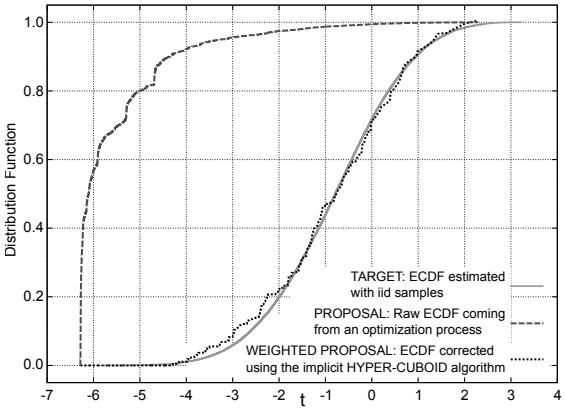

Figure 1: *Change of probability measure example.*

The approach will be illustrated using various examples of a multi-dimensional proposal and target distribution with different correlation levels, and a robust optimization problem.

References

[Amaral, 2015] Amaral, S. (2015). *A Decomposition-Based Approach to Uncertainty Quantification of Multicomponent Systems*. Phd thesis, MIT, Cambridge, MA.

[Amaral et al., 2016] Amaral, S., Allaire, D., and Willcox, K. (2016). Optimal L_2-norm empirical importance weights for the change of probability measure. *Statistics and Computing*, pages 1–19.

[Congedo et al., 2013] Congedo, P. M., Witteveen, J., and Iaccarino, G. (2013). A simplex-based numerical framework for simple and efficient robust design optimization. *Computational Optimization and Applications*, 56(1):231–251.

[Crestaux et al., 2009] Crestaux, T., Le Maître, O., and Martinez, J.-M. (2009). Polynomial chaos expansion for sensitivity analysis. *Reliability Engineering & System Safety*, 94(7):1161 – 1172. Special Issue on Sensitivity Analysis.

[Giles, 2015] Giles, M. B. (2015). Multilevel monte carlo methods. *Acta Numerica*, 24:259–328.

[Lawson and Hanson, 1995] Lawson, C. L. and Hanson, R. J. (1995). *Solving Least Squares Problems*, chapter 23. Linear Least Squares with Linear Inequality Constraints, pages 158–173. Classics in Applied Mathematics. SIAM — Society for Industrial and Applied Mathematics, Philadelphia. ISBN: 978-0-89871-356-5.

[Witteveen and Iaccarino, 2012] Witteveen, J. A. and Iaccarino, G. (2012). Simplex stochastic collocation with random sampling and extrapolation for nonhypercube probability spaces. *SIAM Journal on Scientific Computing*, 34(2):A814–A838.

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Aerodynamic shape optimization of 2D and 3D wings under uncertainties

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Keywords: Robust Optimization, Uncertainties, Non-intrusive, Polynomial Chaos, Adjoints, CFD.

ABSTRACT

In this work, an algorithm for shape optimization under uncertainties is presented and applied to 2D and 3D wings using gradient based optimization. A polynomial chaos based uncertainty quantification method is combined with adjoints for optimization under uncertainties (or robust optimization). The uncertain design objective is characterized by its mean and its variance using polynomial chaos expansion. The gradient based optimization requires the overall gradient, i.e. the gradient of both quantities. These gradients are obtained from the polynomial chaos expansion of the gradient of the objective. The proposed approach is applied to the optimal shape design of the RAE2822 airfoil and the ONERA M6 wing under operational uncertainties where the objective is to minimize the mean and the standard deviation of the drag coefficient simultaneously with a constraint in the mean lift coefficient. It is observed that the convergence is achieved within few iterations (an order of 10). The coefficients of variance are reduced significantly when the uncertainties are introduced in the optimization process, thus making the wings robust against the uncertainties.

METHODOLOGY

Robust optimization is an extension of conventional optimization where uncertainties are also included in the design procedure [1, 2, 3, 4, 5]. The presence of uncertainties brings several difficulties to the optimization process. Due to the uncertainties in a design process, the objective becomes non-deterministic and can be characterized by its mean and standard deviation, i.e. in a robust design the optimization becomes multi-objective. Gradient based optimization of the mean objective and of the standard deviation of the objective therefore requires the gradient of both quantities.

In stochastic applications, the stochastic objective function is usually written as the weighted sum of its statistical moments. A new objective function can be defined as a linear combination of the mean and the standard deviation of the original objective function. A detailed flowchart for the proposed robust optimization model is depicted in Figure 1.

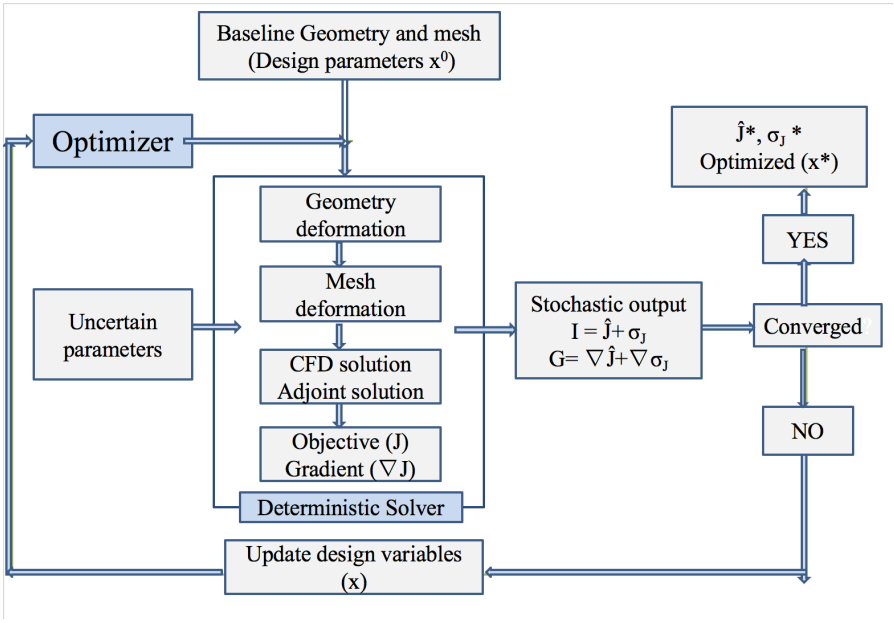

Figure 1: *Flowchart: Robust optimization*

To validate the developed methodology, the robust optimization approach is applied to one of the basic test cases of the UMRIDA project, the RAE2822 airfoil in transonic viscous flow and a 3D wing, the ONERA M6 in Euler flow. For both test cases, the Mach number and the angle of attack are considered as uniformly distributed uncertain parameters.

References

[1] Zhang W. and Kang Z., Robust shape and topology optimization considering geometric uncertainties with stochastic level set perturbation, *Int. J. Numer. Meth. Engng* 110:31-56, 2017.

[2] Georgioudakis M, Lagaros N. D. and Papadrakakis M., Probabilistic shape design optimization of structural components under fatigue, *Computers and Structures*, 182, 252-266, 2017.

[3] Takalloozadeh M. and Yoon G. H., Development of Pareto topology optimization considering thermal loads, *Comput. Methods Appl. Mech. Engrg.*, 317, 554-579, 2017.

[4] Thore C.-J., Holmberb E., Klarbring A., A general framework for robust topology optimization under load-uncertainty including stress constraints, *Comput. Methods Appl. Mech. Engrg.* 319, 1-18, 2017.

[5] Palar S. P., Takeshi T. and Geoff P., Decomposition-based Evolutionary Aerodynamic Robust Optimization with Multi-fidelity Point Collocation Non-intrusive Polynomial Chaos, *17th AIAA Non-Deterministic Approaches Conference, AIAA SciTech*, AIAA paper 2015-1377, 2015.

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A Surrogate-Assisted Multiple Shooting Approach for Optimal Control Problems under Severe Uncertainty

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Keywords: Optimal Control under Uncertainty; Robust Control; Imprecise Probabilities; Intrusive Polynomial Algebra; Low-thrust Trajectory Optimisation.

ABSTRACT

This paper presents an approach to the solution of optimal control problems under epistemic uncertainty. Traditional approaches for deterministic optimal control problems compute a nominal control policy $\mathbf{u}(t)$ to steer the state $\mathbf{x}(t)$ of a dynamical system to satisfy imposed constraints while optimising a performance index. However, in real-life applications, perfect compliance to the nominal trajectory is very hard, if possible, to achieve as uncertainty always affects any real system. Examples of this uncertainty can be imperfect state knowledge, dynamical parameters $\mathbf{d}$ known up to a certain degree, or missed realisation of the control. To improve the solution robustness, usually design margins are considered to account for possible deviations from the reference scenario. On the other hand, an optimal control problem under uncertainty deals with this uncertainty directly from its problem statement, such that the computed control policy would have enhanced robustness and reliability from the very first design iteration.

In most real applications, the specification of a single probability measure is non-trivial, and usually a specific choice is the result of simplifying assumptions. Hence, to enlarge the model validity, in this paper we generalise a previous work on optimal control problem under precise epistemic uncertainty [Greco *et al.*, 2018] to handle imprecise random variables as described by the theory of *imprecise probability* [Augustin *et al.*, 2014]. Specifically, now the random variables $\boldsymbol{\xi} \in \Omega_{\boldsymbol{\xi}}$ have a probability distribution within a parametrised set $P(\boldsymbol{\xi}) \in \mathcal{P}(\boldsymbol{\xi})$, on which no priority rule is imposed. Although replacing a single probability measure with a set results in increased level of uncertainty, we consider this case of severe uncertainty to be a more realistic representation of reality in a large number of practical applications. In this work, the uncertain variables considered are the state initial conditions $\mathbf{X}_0 \sim P(\mathbf{X}_0) \in \mathcal{P}(\mathbf{X}_0)$ and the model parameters $\mathbf{D} \sim P(\mathbf{D}) \in \mathcal{P}(\mathbf{D})$.

From here, the optimal control under imprecision addressed in this work is formulated as

$$\min_{\mathbf{u}(t)\in U} \overline{\mathbb{E}}\left[\phi_J\right] \tag{1}$$

$$\text{s.t.} \quad \dot{\mathbf{x}} = f(t, \mathbf{x}, \mathbf{u}, \mathbf{d}) \tag{2}$$

$$\underline{\mathbb{E}}\left[\phi_{\mathbf{g}}(t, \mathbf{x}, \mathbf{u}, \mathbf{d})\right] \in \mathbf{\Phi_g}, \quad \overline{\mathbb{E}}\left[\phi_{\mathbf{g}}(t, \mathbf{x}, \mathbf{u}, \mathbf{d})\right] \in \mathbf{\Phi_g} \tag{3}$$

where $\mathbf{x}$ is an unknown outcome of the random variable $\mathbf{X}(t)$, resulting from $\mathbf{X}_0$ and $\mathbf{D}_0$ and induced by equation (2), which describes how a point-wise trajectory realisation evolves in time. Being the state and parameter uncertain, they induce the auxiliary objective ϕ_J and constraint function $\phi_{\mathbf{g}}$ to be random variables themselves. Since the probability measure is set-valued by definition, lower- and upper-expectations are defined as

$$\underline{\mathbb{E}}\left[\phi\right] = \inf_{P\in\mathcal{P}} \mathbb{E}_P\left[\phi\right] \qquad \overline{\mathbb{E}}\left[\phi\right] = \sup_{P\in\mathcal{P}} \mathbb{E}_P\left[\phi\right] . \tag{4}$$

Therefore, the optimisation is formulated to minimise the upper bound (worst-case) of the expectation operator on the objective (1), while the constraints (3) impose all the range of expected values to lay within the convex set $\mathbf{\Phi_g}$. It is worth underlining how the expectation formulation encloses common cases of constraints (or objective) in *expected value*, e.g. $\phi_{\boldsymbol{\psi}}(t_f, \mathbf{x}_f) = \mathbf{x}_f$, or in *probability*, e.g. $\phi_{\boldsymbol{\psi}}(t_f, \mathbf{x}_f) = \mathbb{I}_A(\mathbf{x}_f)$.

In general, the optimal control problem under imprecision is infinite-dimensional with no closed-form solution. Hence, the dynamical optimal control problem is converted into a static constrained optimisation, which is then possible to solve with black-box numerical routines, e.g. local NLP solvers. This finite dimensional conversion is realised by means of a transcription scheme. In this paper, we present a novel transcription for optimal control problems under uncertainty that extends the classical direct multiple shooting transcription to account for random variables defined on extended sets. The proposed approach employs a Generalised Intrusive Polynomial Expansion to model and propagate uncertainty within each sub-segment of the multiple shooting, resulting in a chain of polynomial surrogates $\widetilde{F}_{\bar{t}} : \Omega_{\boldsymbol{\xi}} \to \mathbb{R}^{n_s}$ that maps the uncertain initial conditions and parameters to the state vector at a future time $\bar{t}$.

This inexpensive surrogate is then used to reduce the computational complexity in the computation of the expectations in (1)-(3) , which require a further inner loop of optimisation on the set of probability measures to find the requested bounds. In particular, for the generic density function $p(\boldsymbol{\xi})$, the expectation in (4) is approximated with a quadrature scheme as

$$\mathbb{E}_p\left[\phi\right] = \int_{\Omega_{\boldsymbol{\xi}}} \phi(\boldsymbol{\xi}) p(\boldsymbol{\xi}) d\boldsymbol{\xi} \approx \sum_{j=1}^{N} w_j \phi(\boldsymbol{\xi}_j) p(\boldsymbol{\xi}_j) . \tag{5}$$

This approach requires the computation of $\phi(\boldsymbol{\xi}_j)$ only once for an inner optimisation, reducing considerably its computational burden to the cheap evaluation of the different densities $p(\boldsymbol{\xi})$ within the imprecise set $\mathcal{P}(\boldsymbol{\xi})$.

In this paper, the developed approach is then applied to the design of a full 3D robust low-thrust trajectory with uncertain initial conditions.

References

[Augustin *et al.*, 2014] Augustin, T., Coolen, F. P. A., De Cooman, G. and Troffaes, M. (2014). *Introduction to Imprecise Probabilities*, John Wiley & Sons.

[Greco *et al.*, 2018] Greco, C., Di Carlo, M., Vasile, M. and Epenoy, R. (2018). *An Intrusive Polynomial Algebra Multiple Shooting Approach to the Solution of Optimal Control Problems*, *69th IAC 2018*.

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Near-optimal smoothing in derivative-free stochastic optimization

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Abstract

SNOWPAC (Stochastic Nonlinear Optimization With Path-Augmented Constraints) solves optimization under uncertainty (OUU) problems where the underlying problem is only available as black box, using a derivative-free trust region approach. Monte Carlo estimators are used to evaluate the objective and constraint functions of the OUU formulation. Fully linear models for noisy functions and Gaussian process surrogate models smooth these noisy function evaluations. We use these ingredients to develop near-optimal noise correction schemes for SNOWPAC. We also describe the use of multifidelity Monte Carlo estimators, and their error estimates, to reduce the overall computation cost of optimization. We report results on benchmark problems and demonstrate the entire framework in the computationally challenging design of a scramjet combustor.

I. Introduction

The stochastic optimization method SNOWPAC [Augustin & Marzouk, 2017] extends the deterministic derivative-free trust region method NOWPAC [Augustin & Marzouk, 2014], which proposes a new way of handling nonlinear constraints via an "inner boundary path" that guarantees feasibility. In particular, NOWPAC employs an additive function to convexify nonlinear constraints that are known only through pointwise evaluations, thus yielding feasible trial steps and global convergence to a local first-order minimum.

SNOWPAC tackles OUU problems formulated as follows:

$$\begin{aligned} &\min \mathcal{R}^f_\pi(\mathbf{x},\theta), \\ \text{s.t.} \quad &\mathcal{R}^{c_i}_\pi(\mathbf{x},\theta) \leq 0,\ i = 1,\dots,r. \end{aligned} \tag{1}$$

with design parameters $\mathbf{x} \in \mathbb{R}^d$ and uncertain parameters $\theta \sim \pi$, where π is a probability distribution over $\Theta \subseteq \mathbb{R}^k$. Here $\mathcal{R}^f_\pi$ and $\mathcal{R}^c_\pi$ are measures of robustness or risk derived from the objective function $f : \mathbb{R}^d \times \Theta \to \mathbb{R}$ and nonlinear inequality constraints $c_i : \mathbb{R}^d \times \Theta \to \mathbb{R}$, $i = 1 \dots r$, respectively. An example robustness measure is a linear combination of mean $\mathbb{E}_\pi[\,\cdot\,]$

and variance $\mathbb{V}_\pi[\,\cdot\,]$, which accounts for the average and spread of possible realizations. Other options include event probabilities (yielding chance constraints) or conditional value-at-risk.

II. Methods

To evaluate the measures $\mathcal{R}_\pi^b$ given in (1), we use Monte Carlo estimators R^b (where b is f or c_i). Doing so introduces an error that depends on the number of samples N, i.e., $\mathcal{R}^b = R^b + \varepsilon_N^b$ for some random variable ε_N^b. A first step to mitigating the impact of this error is to employ the minimum Frobenius norm surrogate models m_k^b introduced in [Kannan and Wild, 2012], in a neighborhood (called the trust region) of size ρ_k around the current design $\mathbf{x}_k$. The maximum magnitude of the noise yields a lower bound on the trust region radius, $\rho_k \geq \lambda\sqrt{\varepsilon_{\max,k}} = \max_i \lambda\sqrt{\varepsilon_N(\mathbf{x}_{k,i})}$, for $\lambda \in (0,\infty)$ and evaluation points $\{\mathbf{x}_{k,i}\}_{i=1}^M$ at each optimization step k.

To allow the trust region radius to shrink, SNOWPAC uses Gaussian process (GP) surrogates to gradually *smooth* the noisy function evaluations $R_{k,i}^b := R^b(\mathbf{x}_{k,i})$, replacing them with

$$\widetilde{R}_{k,i}^b = \gamma_{k,i}\mu_{k,i}^{GP} + (1-\gamma_{k,i})R_{k,i}^b, \tag{2}$$

where $\mu_{k,i}^{GP} := \mu^{GP}(\mathbf{x}_{k,i}; \{R_i^b\}_{i=1}^M)$ denotes mean of a GP trained on all available evaluations $\{R_i^b\}_{i=1}^M$, and $\gamma_{k,i} \in [0,1]$ is a mixing weight. We show that an optimal weight can be found by calculating

$$\gamma_{k,i} = \frac{\mathbb{V}[R_{k,i}^b] - \mathbb{C}\mathrm{ov}[\mu_{k,i}^{GP}, R_{k,i}^b]}{(\mathbb{E}[\mu_{k,i}^{GP}] - \mathcal{R}_{k,i}^b)^2 + \mathbb{V}[\mu_{k,i}^{GP} - R_{k,i}^b]}. \tag{3}$$

This choice minimizes the magnitude of the noise $\varepsilon_{k,i}$, i.e., the mean squared error (MSE) of our estimator

$$\mathrm{MSE}(\widetilde{R}_{k,i}^b) = [\gamma_{k,i}(\mathbb{E}[\mu_{k,i}^{GP}] - \mathcal{R}_{k,i}^b)]^2 + \mathbb{V}[\gamma_{k,i}\mu_{k,i}^{GP} + (1-\gamma_{k,i})R_{k,i}^b]. \tag{4}$$

We present approximations of (3) that provide near-optimal reduction of the MSE in each step.

III. Results

We validate our smoothing approach using OUU problems derived from the CUTEst benchmark suite showing improved results compared to other optimization methods. Additionally, we demonstrate the use of multilevel Monte Carlo estimators of the robustness measures, and their recently developed error estimators (see [Menhorn et al., 2018]), for an artificial turbulent flow scenario and a realistic scramjet design optimization problem.

References

[Augustin & Marzouk, 2014] Augustin, F. and Marzouk, Y. M. (2014), A Path-Augmented Constraint Handling Approach for Nonlinear Derivative-Free Optimization, *arXiv*, 1403.1931v3

[Augustin & Marzouk, 2017] Augustin, F. and Marzouk, Y. M. (2017), A Trust-Region Method for Derivative-Free Nonlinear Constrained Stochastic Optimization, *arXiv*, 1703.04156

[Kannan and Wild, 2012] Kannan, A and Wild, S.M. (2012), Obtaining Quadratic Models of Noisy Functions, *Technical Report ANL/MCS-P1975-1111*, Argonne National Laboratory, USA

[Menhorn et al., 2018] Menhorn, F., Geraci G., Eldred M.S. and Marzouk Y.M. (2018), Multifidelity OUU for a Scramjet-Inspired Problem, *ECCM-ECFD 2018*, Glasgow, UK

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Recursive Polynomial Chaos Co-Kriging for Reliability-based Design Optimisation

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Keywords: Co-Kriging, Reliability-based Design Optimisation, Polynomial Chaos, Multi-fidelity

ABSTRACT

This work proposes to combine multi-fidelity Co-Kriging with Polynomial Chaos regression for reliability-based design optimisation. In many engineering fields, complex design optimisation problems are tackled by multi-fidelity optimisation. Simple models are built to understand the landscape of the design space. This approximate landscape is then refined by running high-fidelity simulations in the most promising regions. Various approaches exist to propagate the information from the low-fidelity simulations to the high-fidelity models. Recently, Co-Kriging has obtained increased attention to fuse together the information from many computationally-cheap simulations and a limited number of high-accuracy simulations [Forrester et al.]. In essence, Co-Kriging builds a Kriging (or Gaussian process regression) model based on the low-fidelity observations. This low-fidelity surrogate model is used to construct an accurate high-fidelity surrogate by considering the covariances of both low- and high-fidelity observations. This multi-fidelity model can provide a sufficiently accurate surrogate model at a relatively-low computational cost. Two recent advancements of Co-Kriging have made the surrogate technique appealing for solving computationally expensive problems under uncertainty. On the one hand, Co-Kriging was extended to fuse the information of arbitrary number of hierarchical fidelity levels and rewritten into a recursive formulation [Le Gratiet, L. and Garnier, J.]. On the other hand, Polynomial Chaos was integrated into the Kriging technique to provide and efficient quantile estimation of a problem under uncertainty [Schöbi et al.]. These two advancement are combined in this work to solve complex reliability-based design optimisation problems under uncertainty. The recursive formulation facilitates the information fusion of an arbitrary number of fidelity levels. The integration of Polynomial Chaos combines the advantages of Polynomial Chaos and Kriging. The

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global trend is efficiently approximated by Polynomial Chaos while Kriging captures the local variations of the landscape. Moreover, Polynomial Chaos enables the fast estimation of quantile values which are used as reliability measures of the optimisation problem under uncertainty [Schöbi, R. and Sudret, B.]. Therefore, the recursive Polynomial Chaos Co-Kriging (RePCoK) provides an efficient manner to build an accurate surrogate model by utilising the information from observations of various fidelity. The technique reduces the number of required high-fidelity computations; however, the computational effort required for the training of the surrogate model is increased. Thus, RePCoK is proposed for problems where the computational cost of the high-fidelity observations are many orders of magnitude higher than the computational cost of the surrogate model training. The performance and characteristics of the proposed technique are presented through the optimisation of common test functions as well as a reliability-based design optimisation of a simplified aerospace problem.

References

[Forrester et al.] Forrester, A. I. and Sóbester, A. and Keane, A. J. (2007). Multi-fidelity optimization via surrogate modelling. *In Proceedings of the royal society of london a: mathematical, physical and engineering sciences*, Vol. 463, No. 2088, pp. 3251-3269.

[Le Gratiet, L. and Garnier, J.] Le Gratiet, L. and Garnier, J. (2014). Recursive co-kriging model for design of computer experiments with multiple levels of fidelity. *International Journal for Uncertainty Quantification*, 4(5).

[Schöbi et al.] Schöbi, R. and Sudret, B. and Wiart, J. (2015). Polynomial-chaos-based Kriging. *International Journal for Uncertainty Quantification*, 5(2).

[Schöbi, R. and Sudret, B.] Schöbi, R. and Sudret, B. (2014). PC-Kriging: A new meta-modelling method and its application to quantile estimation. *In The 17th Working Conference of the IFIP Working Group 7.5 on Reliability and Optimization of Structural Systems (IFIP2014)*.

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Quantifying the Uncertainty on Ab-Initio Rate Coefficients by means of Bayesian Machine Learning

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Keywords: Uncertainty Quantification, Stochastic Modeling, Bayesian Machine Learning, Hypersonic Flows, Potential Energy Surfaces, Quasi Classical Trajectory Method, Rate Coefficients.

ABSTRACT

Reaction rate coefficients are cornerstones in modeling hypersonic flows, as they quantify the rates at which the quantum states of the mixture components get populated, or depleted, as a result of collisional processes; they play a fundamental role in the identification of the energy-conversion mechanisms and, thus, in the final prediction of the heat fluxes experienced by the surfaces of hypersonic vehicles. Thanks to the exponential increase in computational power, in the last 15 years rapid progress has been made in computing state-to-state rate coefficients starting from the first principles of quantum chemistry, by taking advantage of Potential Energy Surfaces (PESs) for characterizing the interactions between atoms. However, the reaction rates obtained following such ab-initio procedure are heavily influenced by the choices that are made at the moment of deciding the geometric configurations at which the electronic SchrÃűdinger equation is solved, of selecting the techniques to use in order to obtain the electronic energies (i.e., electron correlation effects and atomic orbital basis set expansion), and of electing the functional form for fitting the points Fig. 1. Consequently, one of the priorities for the hypersonic community is the development of a systematic approach for assessing the impacts that such choices have on the flow-filed quantities of interest. We propose the construction of a non-deterministic PES, by extending in a stochastic manner the Permutation Invariant Polynomials Neural Networks proposed by Jiang and Guo. Bayesian Inference through the Automatic Differentiation Variational Inference algorithm by Kucukelbir *et al.* is applied in order to compute the posterior distributions of network's weights and biases. The stochastic PES, Fig. 2, is then sampled, and the gradients of the resulting surfaces are used as source terms of the Hamiltonian Equations, based on the Quasi Classical Trajectory method (QCT). By repeating these collisions for a number of initial atomic

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distances and velocities, it is finally possible to quantify the impact of the PES and trajectory dynamics uncertainties on the state-specific rate coefficients, Fig. 3.

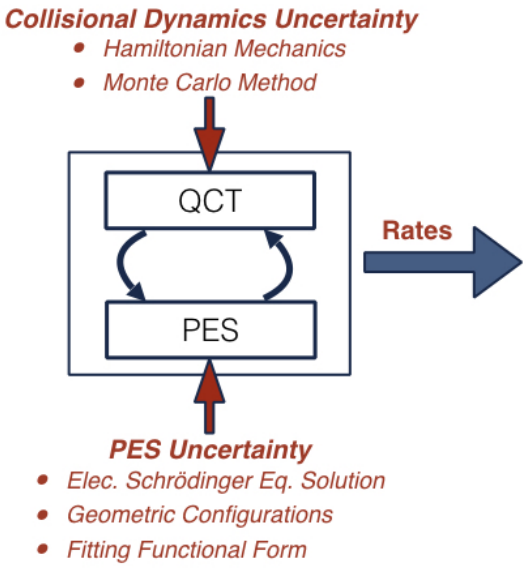

Figure 1: *Main sources of uncertainties in the ab-initio computation of rate coefficients.*

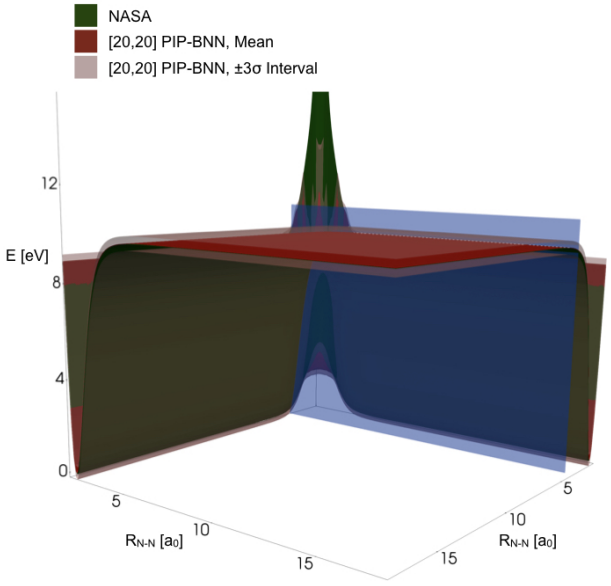

Figure 2: *Comparison between the Permutation Invariant Polynomial Neural Network (in red) and the N3 NASA Ames (in green) PESs.*

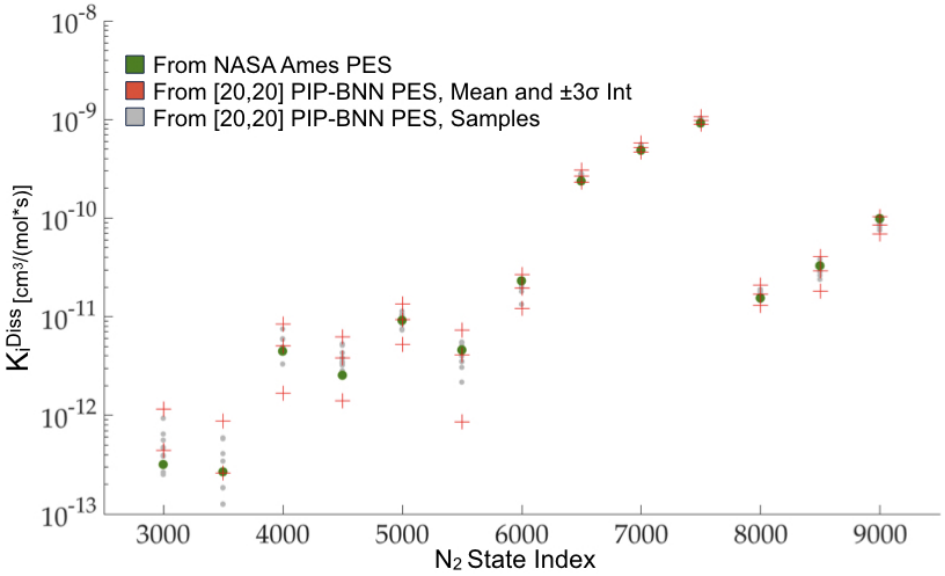

Figure 3: *Propagation of potential energy surface and collision dynamics uncertainties to some N_2 state-specific dissociation rates.*

References

[Venturi et al., 2019] Venturi, S., Sharma, M., and Panesi, M. (2019). A Machine Learning Framework for the Quantification of the Uncertainties Associated with Ab-Initio Based Modeling of Non-Equilibrium Flows. *AIAA SciTech Forum*, January 2019, AIAA 2019-0788.

[Jaffe et al., 2018] Jaffe, R. L., Schwenke, D. W., Grover, M., Valentini, P., Schwartzentruber, T. E., Venturi, S., and Panesi, M. (2018). Comparison of quantum mechanical and empirical potential energy surfaces and computed rate coefficients for N2 dissociation. *Journal of Thermophysics and Heat Transfer*, Vol. 32, No. 4.

[Kolb et al., 2016] Kolb, B., Zhao, B., Li, J., Jiang, B., and Guo, H. (2016). Permutation invariant potential energy surfaces for polyatomic reactions using atomistic neural networks. *The Journal of Chemical Physics*, Vol. 144, No. 22, 2016, pp. 224103.

[Neil, 1995] Neil, R. (1995). Bayesian Learning for Neural Networks *Doctoral Dissertation*, University of Toronto Toronto, Ont., Canada, Canada.

[Kucukelbir et al., 2017] Kucukelbir, A., Tran, D., Ranganath, R., Gelman, A., and Blei, D. M. (2017). Automatic Differentiation Variational Inference *J. Mach. Learn. Res.*, Vol. 18, No. 1, pp. 430-474.

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Calibration of TACOT Material Database and PATO Through Bayesian Inference and Surrogate Modeling

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Keywords: multidisciplinary, aerospace engineering, ablation, calibration, uncertainty quantification, surrogate modeling, bayesian inference, polynomial chaos, msl, TACOT, PATO

ABSTRACT

On August 6, 2012 the Mars Science Lab (MSL) vehicle entered the atmosphere of Mars following its launch on November 26, 2011. During its hypersonic entry through the planetary atmosphere, the heatshield of the vehicle that was composed of individual Phenolic Impregnated Carbon Ablator (PICA) tiles protected it from the excessive heat generated by the surrounding flow field. The design of the heatshield included a full range of instrumentation designed to capture among others material temperature history throughout the atmospheric entry phase. The availability of these data allow for calibration and uncertainty quantification to be undertaken on existing material response computational frameworks such as NASA's Porous Material Analysis Toolbox (PATO) and the TACOT material database [Meurisse et. al.]. The present study will be carried out through Bayesian inference [Tarantola] and is aimed at improving the ability of the framework to predict future flight performance and to be able to accurately capture prediction uncertainty. Because Bayesian inference methodology can incur heavy computational costs due to the reliance on sampling algorithms, polynomial chaos surrogate model is used here to approximate the response of the original model [Blatman].

The calibration data set in the present analysis consists of material temperature history profiles from the 3 deepest thermocouples (TCs) located inside of MISP-4 plug on the vehicle heat shield.

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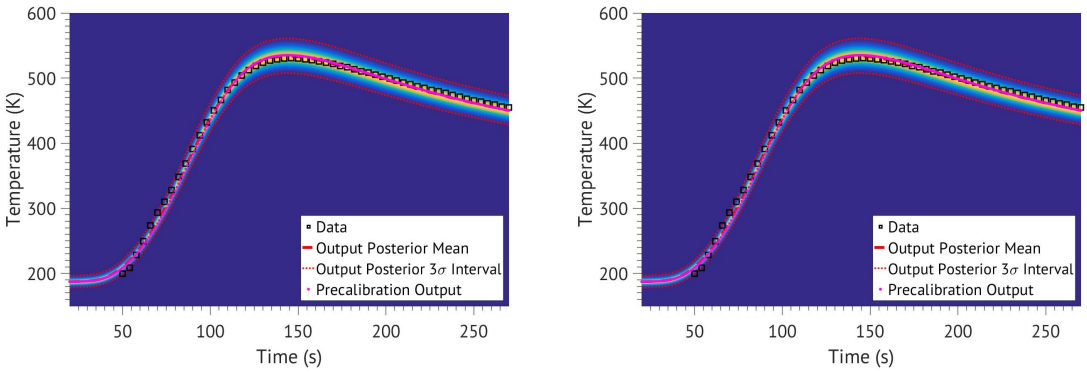

Figure 1: *Output distribution from the forward propagation of posterior distributions for TC2 (left) and TC3 (right)*

The uncertain parameter space consists of temperature dependent thermal conductivity parameters of virgin and char states of the PICA ablator. In addition, uncertainty due to modeling and data error sources will be quantified per thermocouple basis. It is important to note that the material model was calibrated using a deterministic method prior to the present study.

Bayesian inference was carried out by sampling posterior distributions using a Markov Chain Monte Carlo (MCMC) sampling scheme. For the MSL scenario being studied, the intercept parameters for the virgin and char thermal conductivity parameters exhibit the largest influence over output. Differences, although minuscule, are also present between the Maximum A Posteriori (MAP) and pre-calibrated parameter values, and their respective posterior distributions exhibit moderate uncertainty. Following, quantified uncertainty due to parametric, modeling, and data error sources were forward propagated through the model which yielded probabilistic calibrated output in Figure 1. The MAP calibrated outputs in general exhibit minor improvements in overall agreement with the majority of the thermocouples with the exception of the third thermocouple under study. Above all else, the total uncertainty due to parametric, modeling, and data error sources has been captured in the calibrated output across all thermocouple locations. These uncertainty bounds have the potential of reducing safety factors in future vehicle designs.

References

[Meurisse et. al.] J. B.E. Meurisse, J. Lachaud, F. Panerai, C. Tang and N. N. Mansour (2018). Multidimensional material response simulations of a full-scale tiled ablative heatshield. *Aerospace Science and Technology*, 76:497–511

[Tarantola] A. Tarantola (2009). Adaptive sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis. Philadelphia, PA:SIAM

[Blatman] G. Blatman (2005). Inverse Problem Theory and Methods for Model Parameter Estimation. Université Blaise Pascal, Clermont-Ferrand, France

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Reliability of reliability assessments

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Keywords: reliability, confidence, valid inference, uncertainty propagation, fiducial inference.

ABSTRACT

Reliability of a system denotes the chance that it will complete its mission successfully. System is a collection of interacting components and the evaluation of its reliability depends on the knowledge of laws governing the evolution of states of the components -their failure laws-, and a relation describing how particular combinations of system states influence the state of the system -the structure function, in case when this relation is deterministic. In the classical reliability theory, only two possible states are considered for both components and the system, them being functional or failed. System reliability is then the chance that the system is functional over the whole course of its mission. Once the component failure laws are known, assessing the system reliability is simply a technical matter, but they are often not and have to be inferred by statistical methods. Our interest in this contribution lies upon investigating how we can conduct such inference on each component separately and how to integrate them into the assessment of system reliability whilst ensuring that the resulting assessment will posses proper frequency properties in the sense of type I and II errors.

Despite the success of Bayesian inference, whose resulting posterior probabilities can be straightforwardly propagated into distribution for any derived assessment, they assure proper frequency properties only asymptotically and are sensitive to the choice of prior measure in cases when only little amount of observations is available. To overcome this disadvantage, we will employ inferential methods derived from Fisher's fiducial inference. Lately, the notion of *valid* inference has been introduced in this branch of statistics to ensure proper frequency properties even for small number of observations. *Validity* represents that the inference will *unlikely* lead to incorrect results. Exactly stated, for a parameter inference in a parametric model $X \sim f_\theta$, where X represents the random observation and θ model parameters, an inference is *valid* iff

$$P_X(Bel_X(\theta \in A) \geq 1 - \alpha) \leq \alpha$$

for each $\theta \notin A$, and

$$P_X(Bel_X(\theta \in A) \leq \alpha) \leq \alpha$$

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for each $\theta \in A$.
Bel_x represents a set function describing the *belief* in statements about θ given an observation x. It is the result of the conducted inference. High values of $Bel_x(\theta \in A)$ means that observed x support statement $\theta \in A$. We use the term *belief* to emphasise that the *Bel* function need not to be an additive measure as is the case in the Bayesian inference where *Bel* would be exactly the posterior distribution. Validity criterion then states that the chance that we will draw an observation x, the $P_X(.)$, which would overestimate the *belief* in incorrect statements or underestimate the same for the correct ones, is properly bounded.
The theory underlying valid inferences was described in [Martin et al., 2010], [Martin and Liu, 2013], and, more extensively, in the book [Martin and Liu, 2015]. Nevertheless, the emphasis is usually put on assuring the validity property on assertions about the model parameter. In our contribution, we will demonstrate how the same property can be achieved also for assertions about derived quantities, specifically for one sided assertions about the system reliability. We will show what are the general conditions sufficient for *valid* inference and how they manifest in specific scenarios.

References

[Martin et al., 2010] Martin, R., Zhang, J., and Liu, Ch. (2010). Dempster–Shafer Theory and Statistical Inference with Weak Beliefs *Statistical Science*, Vol. 25, Number 1, pp. 72-87

[Martin and Liu, 2013] Martin, R. and Liu, Ch. (2013). Inferential models: A framework for prior-free posterior probabilistic inference *Journal of the American Statistical Association*, Vol. 108, Number 501, pp. 301-13

[Martin and Liu, 2015] Martin, R. and Liu, Ch. (2015). Inferential Models: Reasoning with Uncertainty. *Chapman & Hall/CRC Monographs on Statistics and Applied Probability*, ISBN: 9781439886489

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Investigating Uncertainties with a Game-Benchmark

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Keywords: benchmarking, uncertainty analysis, games, evolutionary algorithms.

ABSTRACT

Most real-world problems cannot be fully specified, and thus contain uncertainties such as noise or modelling bias. As these uncertainties can have a considerable impact on optimisation results, investigating these uncertainties in more depth is becoming increasingly popular in multiple research communities. However, conducting large-scale and in-depth investigations of real-world problems is often difficult, because the corresponding problems are often expensive to evaluate (in terms of costs and computational resources etc.). Furthermore, benchmarks consisting of artificial problems, even when enhanced with simulated uncertainties, have not been shown to possess characteristics of real-world problems. As a result, these benchmarks cannot be used exclusively to investigate algorithm behaviour in the presence of uncertainties.

We identify the following requirements for a benchmark that would be suitable to investigate uncertainties in the context of real-world problem optimisation:

I: Problem characteristics Problems should not be artificial in nature. The benchmark should contain a diverse set of fitness functions which are expected to make sense within their real-world context. Fitness functions should be of considerable complexity and involve different types of uncertainties.

II: Practicality The execution of the benchmark should still be possible within a reasonable time frame. Therefore, it should be easy to parallelise the benchmark and the evaluation of a single solution should result in practical execution speeds on standard machines.

III: Analysis of Uncertainties The benchmark should allow an analysis of all or some of the uncertainties that occur in optimisation problems. It should also include features that allow an analysis of non-symmetric biases.

IV: Statistical significance As evolutionary algorithms are stochastic, the statistics obtained via the benchmark should be statistically justified and thus interpretable.

V: Investigation of scaling behaviour Functions should be scalable in search space dimension, so that scaling behaviour can be analysed.

The game-benchmark for evolutionary algorithms (GBEA)[1] fulfils all of the above requirements

[1]`http://norvig.eecs.qmul.ac.uk/gbea/gamesbench.html`

(see below) and we thus propose it as a means to investigate uncertainty. The GBEA currently features two game-based function suites both taken from research on procedural content generation for well-known games (Top Trumps and Super Mario Bros.). The actual functions in each suites are described in more detail in corresponding publications [2, 3]. The function suites are implemented so that they are compatible with a well-known benchmarking framework[2].

I: Problem characteristics The GBEA contains more than 80 single-objective problems, and even more multi-objective ones, ranging from non-simulation based functions to ones that depend on playthroughs with different AI agents. Preliminary experiments show that the problems in the GBEA are suitably complex and contain a variety of uncertainties. Similar problems are faced in the game industry regularly.

II: Practicality Game-based problems obviously do not pose safety concerns, but they are also mostly reasonably fast to compute. GBEA functions range between 1-300 seconds, and are usually faster than comparable real-world benchmarks [1]. The benchmark includes a batch mode.

III: Analysis of Uncertainties Games engines are often stochastic, and so are may state-of-the-art game AIs. This often creates vastly differing behaviour in playthroughs for different generated levels, thus resulting in very complex problems and non-symmetric uncertainties. Additional uncertainties typical for search-based procedural content generation are due to modelling errors, as often AI players or other measures are used to approximate human behaviour or perception.

IV: Statistical significance Statistical significance is ensured by the implementation of multiple instances of the same function. In the GBEA, instances are obtained by varying the initiation settings for training processes of the different content generators.

V: Investigation of scaling behaviour In cases where generated content is directly encoded in the solution (see Top Trumps suite), it is possible to scale the search space of the problem by just specifying different targets for the generated content. Otherwise, the representation itself often already contains a corresponding parameter (see Mario suite).

A set of first baseline results has already been obtained using the GBEA. We tested several state-of-the-art evolutionary algorithms (CMA-ES, SMS-EMOA, MO-CMA-ES), as well as surrogate-assisted versions of these optimisers. We were able to uncover multiple weaknesses in the aforementioned algorithms. Results for algorithms designed for noisy and uncertain optimisation (SAPEO) should be produced in the future. Besides that, the obtained data on modelling errors suggests that for some of the analysed algorithms, model validation is absolutely crucial.

We expect results and insights received for uncertainty handling and analysis from the GBEA to be easily transferable to other domains, such as aeronautical engineering.

References

[1] S. J. Daniels et al. "A Suite of Computationally Expensive Shape Optimisation Problems Using Computational Fluid Dynamics". In: *Parallel Problem Solving from Nature (PPSN XV)*. Springer Nature, Switzerland, 2018, pp. 296–308.

[2] V. Volz, G. Rudolph, and B. Naujoks. "Demonstrating the Feasibility of Automatic Game Balancing". In: *Genetic and Evolutionary Computation Conference (GECCO)*. ACM Press, New York, 2016, pp. 269–276.

[3] V. Volz et al. "Evolving Mario Levels in the Latent Space of a Deep Convolutional Generative Adversarial Network". In: *Genetic and Evolutionary Computation Conference (GECCO)*. ACM Press, New York, 2018, pp. 221–228.

[2] http://numbbo.github.io/coco-doc/

Uncertainty propagation in multiphysics systems of solvers: application to robust space object reentry predictions

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January 20, 2019

Since the beginning of space exploration, the number of orbiting space objects is dramatically increasing and critical Earth orbits, such as the Geostationary Orbit (GEO), are saturated with non functioning satellites. The "Loi relative aux Oprations Spatiales" (LOS, Law of Space Operation) legally obliges space companies like ArianeGroup to deorbit end-of-life objects and to ensure that the reentry in the Earth atmosphere of these objects presents no risk for human assets.

To assess the risk associated with a reentry event, ArianeGroup (AG) needs to numerically quantify the human risk caused by one of their space objects. The numerical tool in use at AG to simulate the reentry of space object is a system of solvers (SoS) consisting of a set of interdependent solvers coupled together. It includes a trajectory solver coupled with an aerodynamic solver, a probabilistic fragmentation model and an ablation solver. These physical models involve many unknown parameters and dedicated uncertainty quantification methods are needed to assess the reliability of the simulation-based predictions. Propagating uncertainties in a system of solvers can be challenging, due to the coupling effects on the dependences of the trajectory with respect to the uncertain input and the computational cost arising from the sequential evaluation of multiple solvers. In these situations, standard uncertainty propagation methods are too costly and alternative methods dedicated to SoS have to be derived. In this work, we propose an original method for constructing a system of Gaussian Processes (SoGP) to form a surrogate model of a system of solvers. The SoGP is composed of a set of Gaussian Processes (GP) that reproduce the structure of the SoS under study. Each solver of the SoS is associated with a GP in the SoGP which is trained to approximate its corresponding solver. The prediction of the SoGP is not Gaussian as it is generally the composition of GP models.

The advantages of the SoGP, compared to constructing a single GP for the whole system at once, are essentially the following. First, the SoGP has a richer structure and offer more flexibility, and therefore it can fit a larger range of functions. Second, training the SoGP requires learning multiple but usually simpler individual solvers, possibly adapting the training efforts. On

the contrary, a global GP model needs to learn the (generally) more complex mapping between the SoS inputs and its outputs and requires the simulation of the whole system. Finally, SoGPs have the ability to propose a predictive error estimate that can be used in active learning strategies. In this work we propose an original active learning strategy to efficiently increase the accuracy of SoGPs. We are able to identify new training samples for each GP and select a subset of GPs to be trained. To do so, we derive a predictive variance decomposition of the SoGP into contributions from individual GP. The SoGP framework is validated on analytical functions and applied to construct a surrogate of the space objects reentry system of solvers used at ArianeGroup and predict the ground impact point. Using SoGP brings major improvements, in terms of precision, compared to using single GP model.

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A particle filtering method for the opportunistic update of a space debris catalogue

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Keywords: space debris, particle filtering, uncertainty propagation, orbit prediction.

ABSTRACT

The large increase in the amount of debris orbiting our planet has become a problem for present and future space missions. Space debris is mainly composed of inactive satellites, rocket bodies and pieces of both detached by collisions. The number of spacecrafts has grown in a sustained manner since the 1950s and, as a consequence, debris created by fragmentation of large satellites has increased at a very fast rate. Currently, the number of objects resulting from fragmentation duplicates the number of inactive satellites and rockets. Approximately 20,000 pieces of debris larger than a softball ($\approx$ 10 cm) have been catalogued and it is believed that more than 2 million objects with a diameter larger than 2 cm orbit the Earth. Actively tracking all these objects is a very expensive task in terms of time and resources. A method to propagate uncertainties into the future up to a new programmed or expected observation in a reliable way is needed to compensate the lack of continuous tracking.

In recent years, several attempts have been made at incorporating probabilistic tools for propagating uncertainties in orbital mechanics [1, 5, 4]. Among the latter, particle filters (PFs) [3, 2] stand out because of their flexibility and generality. PFs are sequential Monte Carlo methods used for Bayesian statistical inference in dynamical models. To be specific, they aim at constructing empirical (sample based) approximations of the probability distribution of the dynamic state variables conditional on the available observations. PFs consist of two stages: a *prediction* step, where the dynamical model is employed to generate candidate state values (often termed *particles*), and an *update* step where the observed data are used to weight these particles according to their likelihood. PFs are well suited for nonlinear tracking problems and, in particular, they appear as very promising tools for tracking space debris.

We introduce a PF-based methodology that allows, on the one hand, to update the orbital parameters of pieces of space debris when they are sparsely observed and, on the other hand, to reveal previously uncatalogued objects orbiting the Earth. The dynamics of each piece is represented in terms of six (time-varying) orbital elements, namely its angular momentum (h),

	500 particles	10^4 particles
FAR	0.048	0.048
MDR	0.085	0.057

Table 1: *False alarm rates (FAR) and missed detection rates (MDR) for a computer experiment with synthetic data generated from the TLE catalogue.*

eccentricity (e), true anomaly (ν), ascending node (Ω), inclination (i) and perigee (ω). The proposed method starts from a catalogue of objects and it takes advantage of opportunistic (and possibly heterogeneous) celestial observations in order to

(a) identify new objects to be added to the catalogue and

(b) to compute and update a probability distribution for the orbital elements $(h, e, \nu, \Omega, i, \omega)$ associated to each catalogued object.

The scheme is designed to maintain and update a large-scale catalogue of objects, as the computational algorithms needed are easily parallelisable. We employ efficient PF-based techniques to perform data association (i.e., to link each celestial observation to a subset of pieces of debris), to detect new objects, and to generate and update empirical probability distributions for the orbital elements of the catalogued objects. The latter enable us to estimate and predict the complete orbit around Earth of an object at any given time. The estimates can be endowed with expected errors of various types (covariances, collision risks, prediction errors, ...) which are easily computed from the empirical distributions generated by PFs.

We have assessed the validity of the method in a set of numerical experiments using both synthetic and real (publicly available) data. As a preview of our numerical results, Table 1 shows the false alarm rate (FAR) and the missed detection rate (MDR) for a computer experiment involving the assimilation of 126 observations synthetically generated from a set of 40 objects (30 of them catalogued). The attained FAR is $\approx 5\%$ and the MDR is $\approx 8.5\%$ (when using 500 particles in the PFs) but can be reduced to $\approx 5.7\%$ by increasing the computational effort (by generating 10,000 particles per PF).

References

[1] Kyle J DeMars, Robert H Bishop, and Moriba K Jan. A splitting Gaussian mixture method for the propagation of uncertainty in orbital mechanics. *Spaceflight Mechanics*, 140, 2011.

[2] P. M. Djurić, J. H. Kotecha, J. Zhang, Y. Huang, T. Ghirmai, M. F. Bugallo, and J. Míguez. Particle filtering. *IEEE Signal Processing Magazine*, 20(5):19–38, September 2003.

[3] J. S. Liu and R. Chen. Sequential Monte Carlo methods for dynamic systems. *Journal of the American Statistical Association*, 93(443):1032–1044, September 1998.

[4] Alinda Mashiku, James Garrison, and J Russell Carpenter. Statistical orbit determination using the particle filter for incorporating non-Gaussian uncertainties. In *AIAA/AAS Astrodynamics Specialist Conference*, page 5063, 2012.

[5] James Woodburn and Sergei Tanygin. Detection of non-linearity effects during orbit estimation. *Paper AAS*, pages 10–239, 2010.

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Searching for an optimal and reliable design under epistemic modelling uncertainty

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Keywords: robust optimisation, system reliability, imprecise probability, multi-objective optimisation, complex system engineering, risk measures, dempster-shafer theory of evidence

ABSTRACT

Complex systems, like satellites, require a deliberate process to develop from an idea to the actual product. Commonly, such a development process is divided to multiple phases where in each phase we consider multiple design configurations. But in the early phases of this process, we usually suffer from a lack of knowledge about models of the expected system behaviour, which will be more accurately addressed only in later design phases by refining the mathematical models and collecting experimental data. Nevertheless, in order to choose the studies which are supposed to eventually predict the system behaviour with reasonable accuracy, and also to plan for other actions necessary for the final system deployment, we need to be able to predict, to some extent, which of the possible designs from the initial design space might lead to desirable solutions and, more importantly, which will not. The issue with answering these questions lies in impossibility to construct a *reliable* precise predictive model from the information available at the initial design phase. Such an attempt usually requires us to rely on several strong and unjustifiable assumptions, like that of precise stochastic models describing the system or component responses. In our approach, we, instead, base our assessments on genuinely imprecise models which allow to better model our initial lack of knowledge.
A reasonable *optimal* design would need to satisfy two basic criteria. First, we would like it to perform better that adversarial designs based on whatever performance criteria we deem desirable. Secondly, we would like the system to perform at all. When a system becomes more complex, the amount of possible failure modes (events which would render the system in-operational) generally

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increases. It is therefore crucial to also address such possibility in our models and choose the design which would conclude in a reasonably *reliable* system. Reliability of a system can also be increased based on our design choices, for example by using more robust components or backing up some of the crucial sub-systems, and, similarly as with the performance, we can construct mathematical models for its prediction.
Our main concern in this contribution therefore lies in how to formulate a mathematical problem of finding a reliable system design when the system performance is subjected to uncertainty, and how to do the same in case when our models can give us only imprecise answers which results in loosing the total ordering of the designs based on their quality.
Optimisation under uncertainty may be addressed in several ways. One is to make decisions, choosing an optimal design, based on the expected (mean) performance of the system [deFinetti]. Such an approach also allows us to reduce the problem of performance-based-design into a problem of optimising a real function in the case when uncertainties are described by precise stochastic models. It also allows us to naturally include the reliability because the state of a system, functional or failed, directly influences its performance and therefore its expected performance. But the expected value approach is unable to properly capture the variation of performance indices. In case when we would be constructing a large amount of identical *in-mean-optimal* systems, they would perform optimally as a group, but in the case of a *one-of-a-kind* system, like a satellite, we would like to 'ensure' that it would perform as well as possible *itself*. Other formulations of the optimisation problem try to address the issue with performance variability. In order to properly ensure that the designed system will perform within some specified bounds, we can instead choose a system with the best *worst-case-scenario* performance. But such a choice is usually overly conservative so several optimisation methodologies based on the quantile function of the distribution of system performance were developed. Among them, we will focus on the risk measure approach [ITIP, Chapter 12], which, again, would allow us to reduce the problem of performance-based-design into an optimisation of a real function in the case of precisely specified stochastic models. There are multiple ways how to include also the reliability in such problem specification.
When an imprecision is present in the mathematical models or when the reliability cannot be naturally included in the performance index, the problem turns into a multi-objective optimisation with objective functions being the lower and upper performance and reliability. In our talk, we will demonstrate the main features of such problem formulations, discuss the interpretation of the results, and numerical algorithms needed to obtain a solution.

References

[ITIP] Augustin, T., Coolen, P.A.F., de Cooman, G. and Troffaes, C.M.M. (2014). Introduction to Imprecise Probabilities. *Wiley series in Probability and Statistics*, ISBN: 978-0-470-97381-3.

[deFinetti] de Finetti, B. (2017). Theory of Probability, A critical introductory treatment. *Wiley series in Probability and Statistics*, ISBN: 978-1-119-28637-0

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Recycling Krylov subspace strategies to solve stochastic elliptic equations

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Keywords: Stochastic PDEs, Iterative solvers, Deflation, Monte Carlo, MCMC.

ABSTRACT

This work addresses the iterative resolution of linear systems which arise upon sampling discretized stochastic PDEs of the form

$$\nabla \cdot [\kappa(\mathbf{x},\theta)\nabla u(\mathbf{x},\theta)] = -f(\mathbf{x}),\ \mathbf{x} \in \Omega,\ \theta \in \Theta \tag{1}$$

with random coefficient field $\kappa(\mathbf{x},\theta)$. Following a Monte Carlo (MC) approach, each realization of $\kappa(\mathbf{x},\theta)$ leads to a linear system whose solution is used to compute statistics of the random solution $u(\mathbf{x},\theta)$. To reduce the error of those statistics, a large number of realizations needs to be drawn resulting in a long sequence of linear systems whose resolution dominates the overall computational cost and time of uncertainty analyses.

When solving those systems with Krylov-based iterative techniques, it is possible to extract spectral information of previous systems to accelerate the convergence of subsequent resolutions. For instance, the deflation method constrains the search of solution to iterates with residuals in the orthogonal complement of an invariant subspace. Realistically, this deflation subspace (DS) is spanned by eigenvector approximations of the sampled operator associated with the eigenvalues which most hinder convergence. As a system is resolved, a basis of the augmented Krylov subspace is stored and used to approximate relevant eigenvectors of the next sampled operator, see [1]. These two steps (deflated resolution followed by approximate spectral reduction) are repeated throughout the sequence of sampled systems. In practice, the deflation is applied to preconditioned systems where the preconditioner can be (i) the same for all systems, or (ii)

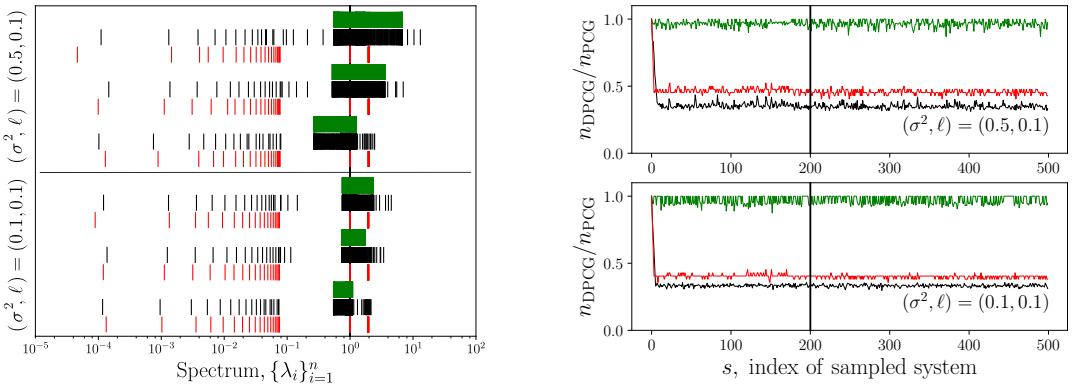

Figure 1: *Left: Spectra of preconditioned operators. Right: Relative decrease of iterations of DPCG over PCG.*

system-dependent. While the former may reduce the cost of setting up and computing potential factorizations, it will statistically not act as efficiently as a system dependent approach.

This work investigates the effect of the preconditioner and sampling strategy on the performance of the deflated method. We consider the 1D case of Eq. (1) over a domain of unit length with stationary log-normal coefficient field, such that $\log \kappa(\mathbf{x}, \theta)$ has a squared exponential covariance with variance σ^2 and correlation length ℓ. All sampled problems are discretized on the same finite element mesh, resulting in symmetric positive definite systems. Truncated Karhunen-Loève (KL) expansions of $\log \kappa$ are used to sample the coefficient field. The random variables in the KL expansion are sampled (i) by MC, or (ii) by Markov chains MC (MCMC), leading to sequences of independent or correlated realizations of κ, respectively. The rationale behind the MCMC sampling is to improve the relevance of the computed DS by using a correlated sequence of operators.

We consider two constant and one system-dependent preconditioners, namely, the median system, the block-Jacobi (BJ) of the median system, and the BJ of each system. Fig. 1 compares the spectra of preconditioned systems for 3 independent samples of κ at two variance values (left plot). Preconditioning with each system-BJ (in red) shows efficient clustering of the eigenvalues around unity with a number (related to the number of blocks) of eigenvalues isolated away from one. Median-BJ (in black) exhibits similar spectra, but with less effective clustering around one. System-BJ leads to faster PCG resolutions than median-BJ, and increasingly so as the variance is increased. Preconditioning with the median (in green) clusters efficiently all the eigenvalues around one, leads to fastest PCG resolutions, but is not a viable option for high-dimensional problems. Fig. 1 shows the acceleration measured by the ratio $n_{\mathrm{DPCG}}/n_{\mathrm{PCG}}$ of iterations needed to converge with or without deflation (right plot). For the median preconditioner (in green), DPCG yields no significant improvement; in contrast, deflating with median-BJ (in black) exhibits a sharp drop in the iteration numbers, asymptotically more than halved compared to PCG. This suggests a convergence to an almost system-independent DS which can be exploited to save computational resources, ceasing to update the DS after it has converged. For instance, reusing the DS of the 200-th system for all subsequent computations induced here no deterioration of the performance. Although not plotted here, MCMC sampling of κ results in similar accelerations as MC, so that MC should be preferred for its higher sampling efficiency.

References

[1] Y. Saad *et al* (2000). A deflated version of the conjugate gradient algorithm, *SIAM J. Sc. Comp.*.

Robust multi-disciplinary ship design optimisation under uncertainty

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Abstract:

The present paper deals with the parametric design and multi-objective optimisation of ships. The methodology includes a complete parametric model of a ship's external and internal geometry, along with the development of all tools required to determine the design constraints and the optimisation objectives used to evaluate the parametrically generated designs. A parametric hull model is generated in CAESES® and then imported to NAPA® to continue with the internal compartmentation. A ship model is developed, including the estimation of lightweight, deadweight and the generation of the examined loading conditions. Uncertainties are identified throughout the methodology and taken into consideration during the optimisation process. Effort is made to limit the effect of uncertainty in the conceptual design phase by selecting the most robust design variants during the optimisation procedure. Multi-fidelity methods are used for the calculation of the calm water resistance, including empirical methods and CFD tools. Processes which require high computational power are represented by use of surrogate models to reduce the overall computational time. The proposed methodology is demonstrated by a case study, where a Ro-Pax ship is optimised in the concept design phase with regard to the minimisation of the total resistance, required freight rate and steel weight.

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Multilevel Monte Carlo estimation of Sobol' indices for sensitivity analysis

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Keywords: Monte Carlo, Multilevel Monte Carlo, Covariance estimation, Sensitivity analysis, Sobol' indices.

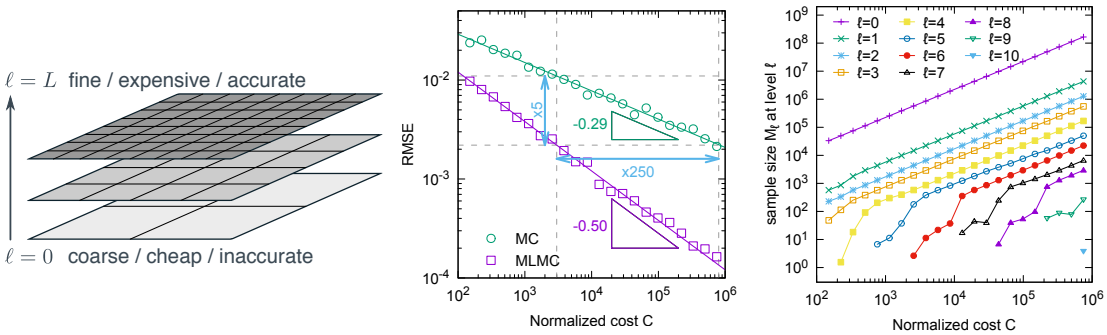
ABSTRACT

We consider an abstract numerical simulator described by the function:

$$\begin{aligned} f\colon \mathcal{X} &\to \mathbb{R} \\ \mathbf{x} &\mapsto f(\mathbf{x}) \equiv y, \end{aligned} \tag{1}$$

whose scalar input parameters $(x_1, \ldots, x_d) = \mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d$ are uncertain, leading to an uncertainty in the output value y. In a probabilistic uncertainty quantification (UQ) framework, these uncertain input parameters are commonly described by random variables defined on a probability space $(\Omega, \mathcal{A}, \mathbb{P})$. The input vector $\mathbf{x}$ is then replaced by a $\mathcal{X}$-valued random vector $\mathbf{X}\colon \Omega \to \mathcal{X}$ whose components X_i are independent random variables with probability distributions given by expert knowledge; as a consequence, $Y \equiv f(\mathbf{X})$ is a random variable whose distribution is unknown. In UQ studies, we are often interested in the first central moments of Y. Moreover, sensitivity measures such as Sobol' indices are commonly computed to quantify the shares of output variability attributable to the different input parameters.

Monte Carlo (MC) methods are popular and powerful approaches for the estimation of statistical parameters (expectations, variances, covariances). However, it is well-known that the root mean square error ε of the MC estimator of the expectation converges slowly as a function of the sample size M, specifically $\varepsilon = \mathcal{O}(1/\sqrt{M})$ for the sample mean estimator of the expectation. Reducing this error by a factor of r thus implies increasing the sample size by a factor of r^2. In practice, for the quantity of interest $Y = f(\mathbf{X})$, obtaining a realization of the expectation estimator $E_M[Y]$ requires M calls to the numerical simulator f. This slow convergence may thus become a critical issue, especially if sampling involves computationally expensive operations, such as solving a (discretized) partial differential equation.



(a) *Illustrative MLMC mesh hierarchy* **(b)** *MLMC vs MC convergence* **(c)** *Sample size per level*

Figure 1

Multilevel Monte Carlo (MLMC) methods [1] were developed to improve the overall computational cost of MC sampling by introducing a sequence of so-called levels ℓ, usually corresponding to a hierarchy of numerical simulators $\{f_\ell\}_{\ell \geq 0}$ with increasing accuracy and corresponding cost of individual simulations (see Fig. 1(a)). Typically, an efficient MLMC estimation will require a large number of samples on the coarsest (cheapest) levels and fewer samples on finer (more expensive) levels. Originally designed for the estimation of expectations, MLMC was recently extended to the estimation of higher-order statistical moments such as variances [2]. We focus here on the MLMC estimation of covariances, which are particularly interesting for the computation of Sobol' indices in the context of sensitivity analysis [3]. Indeed, the first-order Sobol' index S_i associated to the i-th random input X_i can be written in "pick-and-freeze" formulation as

$$S_i \equiv \frac{\mathbb{V}[\mathbb{E}[f(\mathbf{X})|X_i]]}{\mathbb{V}[f(\mathbf{X})]} = \frac{\mathbb{C}[f(\mathbf{X}), f(\mathbf{X}^{[i]})]}{\mathbb{V}[f(\mathbf{X})]}, \quad \mathbf{X}^{[i]} \equiv (X'_1, \ldots, X'_{i-1}, X_i, X'_{i+1}, \ldots, X'_d), \tag{2}$$

where $\mathbf{X}^{[i]}$ denotes the random vector whose i-th component is X_i ("frozen"), while its j-th component ($j \neq i$) is X'_j, where X'_j is an i.i.d. copy of X_j.

We applied the MLMC methodology to the estimation of the covariance term in the numerator of S_i, for the output of a discretized ordinary differential equation with random parameters. Fig. 1(b) shows that MLMC has a better convergence rate compared to standard MC, specifically $\varepsilon_{\text{ML}} = \mathcal{O}(C^{-1/2})$ and $\varepsilon_{\text{MC}} = \mathcal{O}(C^{-1/3})$, leading to a significant reduction of the overall estimation cost. Indeed, using standard MC sampling to obtain an RMSE of 2×10^{-3} is about 250 times more expensive than using MLMC. Fig. 1(c) confirms that more samples are required on cheaper levels. Moreover, as we increase the computational budget, finer (more expensive) levels are considered.

References

[1] M. Giles (2008). Multilevel Monte Carlo path simulation, *Operations Research*.

[2] C. Bierig & A. Chernov (2015). Convergence analysis of multilevel Monte Carlo variance estimators and application for random obstacle problems, *Numerische Mathematik*.

[3] P. Mycek & M. De Lozzo (2019). Multilevel Monte Carlo covariance estimation for the computation of Sobol' indices, *SIAM/ASA Journal on Uncertainty Quantification* (in revision). https://cerfacs.fr/wp-content/uploads/2018/09/TR-PA-18-128-.pdf

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Robust design optimization of a hydrogen-based solar energy storage system using an efficient stepwise regression method for sparse polynomial chaos expansions

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Keywords: Regression-based sparse polynomial chaos expansion, robust design optimization, photovoltaic-electrolyzer system, levelized cost of hydrogen.

ABSTRACT

To tackle the dual challenge of complying with increasing energy demand and reducing fossil-based energy supply, power-to-H_2 is a viable solution. In this framework, the design of a directly coupled photovoltaic-electrolyzer system is widely studied [Maroufmashat, 2014, García-Valverde, 2011]. In these studies, the main focus lies on designing the number of electrolyzers in series and parallel with deterministic model parameters (i.e. perfectly known and fixed parameters) to optimize the system performance. However, by considering deterministic model parameters, the inherent uncertainty of the system performance during real-life operation is disregarded (e.g. unexpected costs). This limitation can lead to suboptimal design decisions.

To address the limitation of deterministic model parameters and to validate the use of a directly coupled photovoltaic-electrolyzer system as the foundation for a seasonal energy storage solution, we performed a techno-economic-environmental design optimization under parameter uncertainties (i.e. robust design optimization), including the addition of a fuel cell and energy demand to the photovoltaic-electrolyzer system. This work provides the hydrogen-based energy

system robust designs which are least sensitive to the inherent parameter variations and illustrates the contribution of each system parameter to the total variation of the levelized cost of hydrogen and levelized cost of emissions.

To perform the uncertainty quantification in the robust design optimization process, we used a robust, efficient stepwise regression method for building the sparse Polynomial Chaos (PC) expansions [Abraham, 2017]. In this method, an automated search procedure is applied to determine the most significant PC contributions. In previous work at our research group [Abraham, 2017], the efficiency and robustness of the method was proven by illustrating its superior performance compared to the method based on Least Angle Regression (LAR) for sparse PC expansions [Blatman, 2009]. To further improve the computational efficiency of the robust design optimization algorithm, we applied a stochastic dimension reduction method based on Sobol' indices, where the stochastic parameters with negligible contribution to the objective variance are highlighted and further considered as deterministic [Turati, 2017].

The robust designs for the levelized cost of hydrogen and levelized cost of emissions ensure the highest cross-field performance quality over the system lifetime. If a trade-off exists between optimizing the mean objective and minimizing the objective standard deviation, the gain in robustness comes at the expense of a loss in mean performance. Therefore, an optimal design under uncertainty is determined out of the Pareto set of design solutions. Moreover, by considering various locations, several uncertainty ranges are applied (e.g. difference in uncertainty on the electricity price from the grid for various locations). As a result, different scenarios are evaluated, resulting in specific robust designs according to the location characteristics.

Next to that, by performing a global sensitivity analysis through PC-based Sobol' indices for each stochastic model parameter, the most significant contributors to the objective variance are highlighted. Consequently, guidelines are provided for further enhancement of the system robustness and therefore its performance quality (e.g. bulk manufacturing of the system technologies when the variance of the levelized cost is dominated by CAPEX, or more demonstration projects and continuous high-quality system maintenance for a dominating OPEX uncertainty).

Future works will investigate the integration of imprecise probabilities in the robust design optimization framework.

References

[Abraham, 2017] Abraham S. ,Raisee M. ,Ghorbaniasl G. ,Contino F. , Lacor C. (2017), A robust and efficient stepwise regression method for building sparse polynomial chaos expansions. *Journal of Computational Physics*, 332:461–474.

[Blatman, 2009] Blatman G. (2017), Adaptive sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis. *Ph.D. thesis, Université Blaise Pascal, Clermont Ferrand*.

[García-Valverde, 2011] Garciía-Valverde R., Espinosa N., Urbina A. (2011), Optimized method for photovoltaic-water electrolyser direct coupling. *International Journal of Hydrogen Energy*, 36:10574–10586.

[Maroufmashat, 2014] Maroufmashat, A.,Sayedin F., Khavas S. S. (2014), An imperialist competitive algorithm approach for multi-objective optimization of direct coupling photovoltaic-electrolyzer systems. *International Journal of Hydrogen Energy*, 39:18743–18757.

[Turati, 2017] Turati P., Pedroni N., Zio E. (2017), Simulation-based exploration of high-dimensional system models for identifying unexpected events. *Reliability Engineering and System Safety* 165:317–330.

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Damage tolerance reliability assessment combining adaptive kriging and support vector machine

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Keywords: reliability, subset simulation, adaptive kriging, support vector machine, damage tolerance, aerospace engineering.

ABSTRACT

In the aerospace sector, the design approach follows the damage tolerance rules considering fracture mechanics numerical models subjected to uncertainties about geometry, material properties, loads or presence of defects. The conventional approach to treat the uncertainties is to perform deterministic evaluation setting the properties in worst conditions. Even if they ensure the strength of the component, conservative hypotheses may generate an unquantifiable over-sizing. A more rigorous way to consider uncertainties is to assess the probability of failure by setting stochastic models as input. Here, a specific procedure is defined to assess the probability of failure for damage tolerance, combining several criteria.

In the reliability context, the uncertainties are modelled by random variables X_i mapped into the standard space where all variables are defined according to an uncorrelated normal distribution law such as $u_i \sim \mathcal{N}(0;1)$. The reliability is quantified by the probability of failure p_f.

The aim of the damage tolerance approach is to ensure the component safety during its lifetime N_{target}. At each step of the crack propagation, the outputs are post-processed considering the Failure Assessment Diagram (FAD) according to R6-rule [Milne *et al.*, 1988]. The FAD margin M_{FAD} is set to qualify the state of the component at each increment of the crack. If $M_{\text{FAD}} \leq 0$, the process is stopped and the component is rejected. Otherwise, it is accepted if $N_{life} = N_{target}$. Note that, the use of linear elastic fracture mechanics hypothesis leads to obtain a qualitative information when $M_{\text{FAD}} \leq 0$. In the damage tolerance reliability assessment, FAD margin is considered as the performance function $g(\mathbf{U})$. Our goal is to assess the probability of failure limiting the damage

*Thanks to Rudy Chocat who worked as a PhD student on this topic

tolerance model evaluations considering a performance function which provides quantitative information for a safe component and qualitative information for a failed one.

The reliability problem may be considered as a classification one because the standard space is divided into a failure region where the performance function $g(\mathbf{u}) < 0$, a safe region $g(\mathbf{u}) > 0$, and the limit state $g(\mathbf{u}) = 0$. The kriging regression [Echard *et al.*, 2011] or Support Vector Machine (SVM) classification [Hurtado, 2013] may be applied according to the allowable dataset. On the one hand, kriging allows taking into account the trends of the model. On the other hand, the SVM classification can treat all kinds of dataset information without any condition about the continuity of the performance function.

The idea of the proposed method is to combine kriging and SVM to take advantages of both approaches. They are associated with the Subset Simulation [Au and Beck, 2001] based on a sequence of subset steps relaxing the limit state threshold. For the first subset steps, when dataset contains positive, i.e., quantitative values only, a kriging model is built with the Adaptive Kriging (AK) [Echard *et al.*, 2011] enrichment strategy to improve the accuracy. For the last subset step, when the Design Of Experiments (DOE) is composed of both qualitative ($g(\mathbf{u}) \leq 0$) and quantitative data points ($g(\mathbf{u}) > 0$), a SVM separator is coupled with an Adaptive SVM (ASVM) [Pan and Dias, 2017] to accurately describe the limit state. The transition between the kriging and SVM phases is ensured if one of the following criteria is satisfied:

- The subset threshold is less or equal to zero, inspired by Subset Simulation,
- the DOE is composed of 2 x number of random variables failed experiments, it must prevent a deterioration of the current threshold using kriging.

This method, combining kriging and SVM by Subset Simulation, is custom-built for the damage tolerance application due to the specificity of dataset, composed of both qualitative and quantitative information. The results for low probability estimations are attractive when compared to those obtained with existing reference methods. This approach has also been successfully extended to high dimensional cases in an industrial context, with CPU-demanding finite element simulations of crack propagation.

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References

[Au and Beck, 2001] Au, S.K. and Beck, J.L. (2001). Estimation of small failure probabilities in high dimensions by subset simulation. *Probabilistic Engineering Mechanics*, 16(4):207–217.

[Echard *et al.*, 2011] Echard, B., Gayton, N. and Lemaire, M. (2011). AK-MCS: an active learning reliability method combining Kriging and Monte Carlo simulation. *Structural Safety*, 33(2):145–154.

[Hurtado, 2013] Hurtado, J.E. (2013). Structural reliability: statistical learning perspectives. *Springer Science & Business Media*, 17.

[Milne *et al.*, 1988] Milne, I., Ainsworth, R.A., Dowling, A.R. and Stewart, A.T. (1988). Assessment of the integrity of structures containing defects. *Structural Safety*, 32(1):3–104.

[Pan and Dias, 2017] Pan, Q. and Dias, D. (2017). An efficient reliability method combining adaptive Support Vector Machine and Monte Carlo Simulation. *Structural Safety*, 67:85–95.

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Bayesian parameter calibration using surrogate models

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Keywords: Bayesian inference, surrogate model, polynomial chaos, optimization

ABSTRACT

This talk discusses the inference of physical parameters using model surrogates. Attention is focused on the use of sampling schemes to build suitable representations of the dependence of the model response on uncertain input data. Non-intrusive regularized regressions are used for this purpose. A Bayesian inference formalism is then applied to update the uncertain inputs based on available measurements or observations. To perform the update, we consider two alternative approaches, based on the application of Markov Chain Monte Carlo methods or of adjoint-based optimization techniques. We illustrate the implementation of these techniques to calibrate wind drag parametrization in an ocean general circulation model, and to infer chemical rate parameters in shock tube experiments.

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Optimization under Uncertainty of High Dimensional Problems using Quantile Bayesian Regression

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Keywords: Bayesian Optimization, Quantile Regression, Optimization under Uncertainty.

ABSTRACT

The use of robust optimization techniques is increasing in popularity in order to come up with configurations less sensitive to aleatory uncertainties. Instead of optimizing the Quantity of Interest, QoI, an statistic of the QoI is sought. The quantile is a flexible statistic to be chosen as objective function in engineering problems. For example a high quantile can be minimized to reduce extreme events. If the median is chosen, day to day events are minimized.

Traditionally, an uncoupled approach can be used, in which at each iteration of the optimization process a complete uncertainty quantification is performed to obtain the statistic of the QoI. To reduce the computational cost, the stochastic space can be characterized through surrogate models. Then, a large number of Quasi Monte Carlo samples can be cheaply evaluated in the surrogate.

However, when dealing with a large number of uncertainties, the required number of training samples to construct an accurate surrogate increases exponentially. Also, surrogate models are not suitable to model non-parametric uncertainties. Another disadvantage is that the uncoupled approach does not fully explore the intrinsic relationship between uncertainties and design parameters. Samples used to construct the surrogate at each optimization are not reused. The combination of uncertainties with design parameters is expected to improve the efficiency of the optimization. The objective of this paper is to develop coupled framework for optimization under uncertainty that is insensitive to the number of uncertainties by means of a Bayesian approach.

A global Design of Experiments, DoE, is selected, covering both the design and uncertainty space. This initial sampling is chosen by Quasi Monte Carlo because of its good capability of filling the design space. All the realizations are then projected into a single plane, in order to obtain the response of all the realizations only as a function of the design parameters, X.

Then, quantile regression is applied to the initial DoE sampling [1]. The objective is to obtain an explicit relation between the quantile and the design parameters. This relation is parametrized through a Thin Plane Spline, TPS, [2] that is characterized through the X and Y coordinates of its control points. These control points are uniformly spaced in X, the design space. The Y coordinates

are selected according to the minimization of a loss function (maximization of the likelihood) following quantile regression. As a result the TPS provides an initial predictor of the quantile as a function of the design parameters.

Due to the trade-off between model complexity and model accuracy, there is an optimum number of control points to define the TPS. By increasing the number of control points, the loss function would be minimized more and more. However, risk of overfitting could occur and additional sampling points would not be properly predicted. The initial number of control is then selected by k-fold cross validation on the loss function of quantile regression.

In addition, it is desired to have an estimation of the error of the quantile predicted by the TPS at any given point. The formulation of quantile regression can be considered from a Bayesian point of view through the Asymmetric Laplace Distribution and the assumption of an improper uniform prior [3]. The posterior distribution of the Y coordinates of the control points is obtained by sampling the likelihood function through Markov Chain Monte Carlo. In particular, an adaptive Metropolis-Hastings algorithm is used. The covariance of the step function is adapted according to the covariance of the chain. From the MCMC sampling it is possible to obtain the posterior distribution of the Y coordinate of each control point of the TPS.

The addition of infill samples should balance exploration in areas with large uncertainty in the estimation of the quantile with exploitation in locations close to the minimum. Once the model is built, several realizations from the MCMC chain are randomly chosen. New samples are placed in the minimum location of each realization (in the design space), at a random location in the stochastic space. After the infill, the predictor is recomputed again until convergence occurs in either the optimum location of the design parameter or in the optimum quantile value.

In addition, it is possible to increase the model complexity by adding additional control points to build the TPS in locations closer to the local minima. This should be done as far as the increase in model accuracy does not penalize the model complexity.

The framework has been validated in a one dimensional test function with two local minima for the optimization of the 80% quantile. The use of cross validation results in an optimum number of 21 points to define the TPS. Bayesian quantile regression is a powerful tool to globally estimate the quantile and its error as a function of the design parameters. The predicted quantile converges globally to the real one as the number of samples increases. The infill criteria can be used improve the accuracy in the region of the local minima and accelerate the optimization process.

In conclusion, an optimization under uncertainty framework insensitive to the number of uncertainties has been presented. The application of Bayesian Quantile Regression makes possible the estimation of the quantile and its prediction error at any given design point. This can be used for sequential optimization under uncertainty. In the future, the framework will be applied to an engineering problem with a large number of manufacturing tolerances

References

[1] Brian S. Cade and Barry R. Noon. A gentle introduction to quantile regression for ecologists. *Frontiers in Ecology and the Environment*, 1(8):412–420, oct 2003.

[2] Jean Duchon. Splines minimizing rotation-invariant semi-norms in sobolev spaces. In *Constructive Theory of Functions of Several Variables*, pages 85–100. Springer Berlin Heidelberg, 1977.

[3] Keming Yu and Rana A. Moyeed. Bayesian quantile regression. *Statistics & Probability Letters*, 54(4):437–447, oct 2001.

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A bi-level energy management strategy for HEVs under traffic conditions.

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Keywords: Hybrid electric vehicles, Traffic, Bi-level Optimization

ABSTRACT

In 2015, according to data from the European Environement Agency, road transportation contributed to 21% of total EU-28 greenhouse gas emissions [Eur]. Traffic congestion has a major impact on driving behaviors, and therefore plays a key role in the level of fuel consumption [VKK00]. Hybridization technologies allow for a better overall energy management between the two propulsion systems, and are able to recover energy during deceleration phases, making hybrid electric vehicle (HEV) less fuel demanding. Several approaches have been developed during the last decades [Mal14] to determine the optimal electric motor power P_m.

We propose here an energy management system taking advantage of the knowledge of the global traffic in order to reduce the consumption. A bi-level method is applied to optimize the consumption over a trip under traffic constraints. Based on [LBD18], the traffic constraint is represented as a joint probability distribution μ of speed and acceleration. The speed $\mathbf{V}$ and the acceleration $\mathbf{A}$ of the vehicle are then modeled as random variables following this distribution.

The first stage of the method ('micro') determines the electric torque T minimizing the mean consumption on a small road segment, given its traffic data and a final constraint on the state of charge (SoC_f). The method used to solve the problem is a stochastic dynamic programming (SDP).

$$\min_{T} \quad \mathbb{E}_\mu \left[\sum_{t=0}^{\mathcal{T}} C(T_t, \mathbf{V}_t, \mathbf{A}_t)\Delta t + (SoC_f - SoC(\mathcal{T}))^+ \right] \tag{1}$$

$$s.t\ \forall t, \quad T_t \in [T_{min}, T_{max}] \tag{2}$$

$$SoC_t \in [0,1] \tag{3}$$

$$SoC_{t+1} = SoC_t + \frac{1}{C_{max}} P_m(\mathbf{V}_t, \mathbf{A}_t, T_t)\Delta t \tag{4}$$

$$D_{t+1} = D_t + \mathbf{V}_t \Delta t \tag{5}$$

$$SoC(0) = SoC_{init},\ D(0) = 0 \tag{6}$$

$$\mathcal{T} = \inf\{t | D_t > L\} \tag{7}$$

$$\tag{8}$$

Below is a comparison of this SDP solution with the deterministic solution of the optimization with exact trafic information. The simulations use real data from the platform GECO air [Geco] and indicate a good relevance of the SDP micro approach.

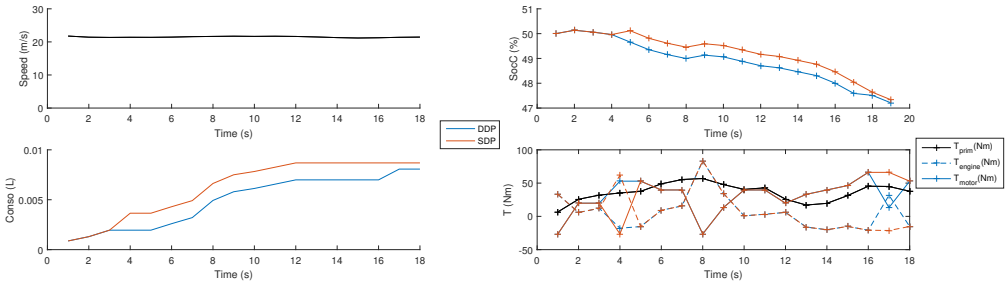

Figure 1: *Comparison between the deterministic and the stochastic solution.*

This 'micro' stage is solved for different values of SoC_f, which provides an estimate of the consumption function VF_s over the segment s depending on the traffic state, initial SoC and final SoC.

Then in the second stage ('macro'), we optimize the whole trip with the SoC increment over each segment as contol variable.

$$\min_{SoC_s} \quad \sum_{s=1}^{N} VF_s(SoC_{s-1}, SoC_s, \mu) \tag{9}$$

$$s.c \quad SoC_0 = SoC_{init} \tag{10}$$

$$SoC_N = SoC_{final} \tag{11}$$

This stage is solved by deterministic dynamic programming (DDP). Simulations based on real traffic data are currently in progress.

References

[Eur] European Strategies - White Paper 2011. [Online]. Available: https://goo.gl/GoSWcf

[VKK00] I. D. Vlieger, D. D. Keukeleere, and J. Kretzschmar (2000). Environmental effects of driving behaviour and congestion related to passenger cars, *Atmospheric Environment*, vol. 34, no. 27, pp. 4649 – 4655.

[Mal14] A. A. Malikopoulos (2014). Supervisory Power Management Control Algorithms for Hybrid Electric Vehicles: A Survey, *IEEE Transactions on Intelligent Transportation Systems*, vol. 15, no. 5, pp. 1869–1885.

[LBD18] Arthur Le Rhun, Frédéric Bonnans, Giovanni De Nunzio, Thomas Leroy, Pierre Martinon (2018), A stochastic data-based traffic model applied to vehicles energy consumption estimation, *preprint*, HAL: hal.inria.fr/hal-01774621.

[Geco] Geco air, URL: www.gecoair.fr.

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Robust Optimisation using Voronoi-Based Archive Sampling

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Keywords: Robust optimisation, Voronoi, Fitness approximation, Uncertainty.

ABSTRACT

A key issue in tackling robust problems is the appropriate selection of solutions from the uncertainty set associated with a putative design, in order to estimate its robust quality and therefore guide the search process. We consider here problems where the variation of performance is due to some variability in the actual design realised (due to *e.g.* engineering tolerances), and the uncertainty set is therefore some disturbance neighbourhood around a design. We outline a framework, first reported in [Doherty et al., 2018], for online estimation solution quality in a robust optimisation setting by exploiting samples from the search history and using Monte Carlo sampling to approximate a Voronoi tessellation of the design space. Voronoi tessellations (and their Euclidean dual graphs, Delaunay triangulations) have a wide range of applications across the natural sciences [Aurenhammer, 1991]. The Voronoi tessellation of a set of discrete points in a continuous space divides the space into a set of *cells*, one for each point, so that for each point, its corresponding cell contains the volume of space that is closest to it. A useful feature of the Voronoi tessellation is that the point that is furthest from all of the points used to generate the tessellation will be a vertex of one of the cells. Therefore, a Voronoi tessellation provides us with a finite set of candidate points for the farthest point from all others. This is used to determine a new point in the disturbance neighbourhood of a given solution such that — along with the relevant archived points — they form a well-spread distribution. This approach is integrated within the widely used Covariance Matrix Adaptation–Evolution Strategy (CMA-ES) [Hansen & Ostermeier, 2001]. It is also used to weight the archive points to mitigate any selection bias in the neighbourhood history.

We consider three robustness quality measures: the expected fitness with a uniform disturbance (UD); the expected fitness with a Gaussian disturbance (GD); and the 95th percentile of fitness values, with a uniform disturbance (PC). We assess the performance of our framework on benchmark problems with different properties and design dimensionality [Paenke et al., 2006, Branke & Fei, 2016] and compare the results with existing frameworks that incorporate the search history in the estimation of solution robustness [Tsutsui & Ghosh, 1997, Branke, 1998, Tsutsui, 1999, Tsutsui & Ghosh, 2003, Kruisselbrink et al., 2010, Branke & Fei, 2016, Fei et al., 2018]. Our method performs competitively with these, and may be considered a new state-of-the-art approach for optimising such problem types.

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References

[Aurenhammer, 1991] Aurenhammer, F (1991). Voronoi Diagrams — A Survey of a Fundamental Geometric Data Structure *ACM Computing Surveys (CSUR)*, 23:3 345–405.

[Branke, 1998] Branke, J. (1998). Creating robust solutions by means of evolutionary algorithms *Parallel Problem Solving from Nature — PPSN V: 5th International Conference*, 119–128.

[Branke & Fei, 2016] Branke, J. and Fei, X. (2016). Efficient Sampling When Searching for Robust Solutions *Parallel Problem Solving from Nature – PPSN XIV: 14th International Conference*, 237–246.

[Doherty et al., 2018] Doherty, K and Alyahya, K and Fieldsend, J E and Akman, O E (2018). Voronoi-based archive sampling for robust optimisation *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, 249–250.

[Hansen & Ostermeier, 2001] Hansen, N. and Ostermeier, A. (2001). Completely Derandomized Self-Adaptation in Evolution Strategies *Evolutionary Computation*, 9:2 159–195

[Fei et al., 2018] Fei, X. and Branke, J. and Gülpınar, N. (2018). New Sampling Strategies when Searching for Robust Solutions *IEEE Transactions on Evolutionary Computation*, doi: 10.1109/TEVC.2018.2849331.

[Kruisselbrink et al., 2010] Kruisselbrink, J. and Emmerich, M. and Bäck, T. (2010). An Archive Maintenance Scheme for Finding Robust Solutions *Parallel Problem Solving from Nature, PPSN XI: 11th International Conference*, 214–223.

[Paenke et al., 2006] Paenke, I. and Branke, J. and Jin, Y. (2006). Efficient search for robust solutions by means of evolutionary algorithms and fitness approximation *IEEE Transactions on Evolutionary Computation*, 10:4 405–420.

[Tsutsui & Ghosh, 1997] Tsutsui, S. and Ghosh, A. (1997). Genetic Algorithms with a Robust Solution Searching Scheme *IEEE Transactions on Evolutionary Computation*, 1:3 201–208.

[Tsutsui, 1999] Tsutsui, S. (1999). A comparative study on the effects of adding perturbations to phenotypic parameters in genetic algorithms with a robust solution searching scheme *Systems, Man, and Cybernetics, 1999. IEEE SMC '99 Conference Proceedings. 1999 IEEE International Conference on*, 3 585–591.

[Tsutsui & Ghosh, 2003] Tsutsui, S. and Ghosh, A. (2003). Effects of Adding Perturbations to Phenotypic Parameters in Genetic Algorithms for Searching Robust Solutions *Advances in evolutionary computing*, 203–365.

Opening chemical reaction paths in a plasma global model: an uncertainty quantification approach

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Keywords: Iodine, Global Model, UQ, Monte-Carlo

As iodine is establishing itself as an alternative to xenon for electric propulsion in space, different global models are published to characterize the plasma formed by molecular iodine [2, 3]. The model by Grondein et al. [2] is derived from the xenon version by Chabert et al. [1]. This model is constructed around a particle balance and a power balance. A differential system is composed of an equation of temporal evolution per chemical species (2 for the xenon model [1] and 6 for the iodine model [2]), an equation for the temporal evolution of the electron energy (or electron temperature) and one for the neutral energy (or neutral gas temperature). This differential system is solved until a steady state is reached.

Ten volume or surface reactions are considered by Grondein et al. [2], with I, I_2, I^+, I_2^+ or I^- in reactants or products. Some of these reactions are poorly characterized due to lack of data, and many reactions are missing because assumed negligible. The uncertainty quantification is used to answer two questions:

- How does the poor understanding of some reactions affect the error of the code output?
- Among the reactions currently in the code and others that could be added, where should the effort to better characterize the reactions be focused?

The first question is addressed using a Monte-Carlo approach, generating one hundred thousand configurations with reaction coefficients drawn from a log-normal distribution around their usual value and solving the differential system each time. This gives an absolute uncertainty on the outputs, and we also calculate Sobol indices to determine the sensitivity to each parameters. This allowed to determine that for the xenon model, the electron density and temperature are additive functions of the uncertain parameters, and can be modeled using a polynomial regression on these coefficients, greatly reducing the computation time required to compute the uncertainties.

The second question is answered by opening reaction paths in the code with a 'guessed' reaction rate associated to a large uncertainty. It is then observed 1) if the reaction has an effect on the final output and 2) if the uncertainty of the reaction has an effect on the uncertainty of the final output. If the reaction changes the results without increasing the uncertainty too much, it can be added to the reaction scheme with no further effort. If it also affects the uncertainty, this reaction can be listed as prioritary in the list of reactions to investigate.

References

[1] P. Chabert et al. “Global model of a gridded-ion thruster powered by a radiofrequency inductive coil”. In: *Physics of Plasmas* 19.7 (July 2012), p. 073512. ISSN: 1070-664X, 1089-7674. DOI: 10.1063/1.4737114. URL: http://aip.scitation.org/doi/10.1063/1.4737114.

[2] P. Grondein et al. “Global model of an iodine gridded plasma thruster”. In: *Physics of Plasmas* 23.3 (Mar. 2016), p. 033514. ISSN: 1070-664X, 1089-7674. DOI: 10.1063/1.4944882. URL: http://aip.scitation.org/doi/10.1063/1.4944882.

[3] Konstantinos Katsonis and Chloe Berenguer. “A Detailed Global Model of Iodine Plasma for Optimization and Diagnostics of Electric Thrusters”. In: *Imperial Journal of Interdisciplinary Research (IJIR)* 2.12 (2016), p. 10.

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Decay and Re-Entry Analysis of Space Debris

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Keywords: Re-entry analysis, design for demise, casualty risk, sensitivity analysis, uncertainty quantification, space debris.

ABSTRACT

This contribution gives an overview of some activities and results obtained within the framework of several research projects on the analysis of space debris propagation and decay, and atmospheric re-entry. Different approaches have been applied to perform sensitivity analyses and quantify the uncertainties related to the re-entry time (decay analysis), as well as the impact point and the associated casualty risk (atmospheric re-entry analysis).

Within the framework of the decay analysis, the work to characterize and propagate the uncertainties on the atmospheric re-entry time of the GOCE (Gravity field and steady-state Ocean Circulation Explorer) satellite, done with the framework of an ESA ITT project, is presented [1, 2]. Non-intrusive techniques based on Chebyshev polynomial approximation, and the Adaptive High Dimensional Model Representation multi-surrogate adaptive sampling have been used to perform uncertainty propagation and multivariate sensitivity analyses when both 3 and 6 degrees-of-freedom models where considered, considering uncertain-ties on initial conditions, and atmospheric and shape parameters. Two different uncertainty quantification/characterization approaches have been also proposed. In this case, the same surrogate approaches previously used for uncertainty propagation allowed the development of the Boundary Set Approach and the Inverse Uncertainty Quantification. Moreover, the use of meta-modelling techniques to obtain a very fast characterisation of the probability density function of the atmospheric re-e-entry time of satellites and space debris, when a range of initial conditions and model uncertainties, as well as characteristics of the object are considered, has been investigated [3]. Two meta-modelling approaches have been considered and preliminarily tested. The first approach directly maps the initial and model uncertainties, as well as the characteristics of the considered object and the characteristics of the atmosphere, into the parameters of the skew-normal distribution that characterises the re-entry time windows. The second approach maps the initial conditions, the atmospheric and object characteristics into the re-entry time and a probability density function of the re-entry time is built via Monte Carlo sampling of the achieved meta-model.

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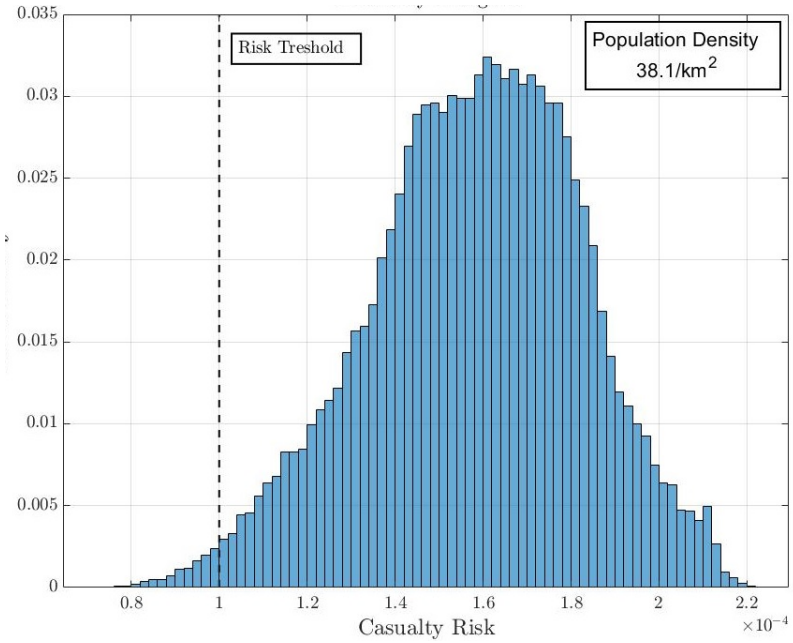

Figure 1: *Histogram of the averaged population density casualty risk*

Within the framework of the atmospheric re-entry analysis, since well-known tools developed for satellite and debris re-entry perform break-up and trajectory simulations in a deterministic sense and do not perform any uncertainty treatment, we have developed and proposed surrogate based methods for the efficient probabilistic analysis of atmospheric re-entry cases. Both aleatory and epistemic uncertainties that affect the trajectory and ground impact location are considered [4, 5]. The method is applicable to both controlled and uncontrolled re-entry scenarios, and the results show that the resulting ground impact distributions, both with and without fragmentation, are far from the typically used Gaussian or ellipsoid distributions. The approach, when combined with information such us the population density, can directly give the statistical analysis of the re-entry casualty risk as defined by the guidelines proposed by the IADC, NASA, and ESA (see Figure 1) [6].

References

[1] E. Minisci, R. Serra, M. Vasile, A. Riccardi, S. Grey, and S. Lemmens, “Uncertainty Treatment in the Goce Re-Entry," 1st IAA Conference on Space Situational Awareness (ICSSA), Orlando, FL, USA, 2017.

[2] A. Falchi, E. Minisci, M. Kubicek, M. Vasile, and S. Lemmens, “HDMR-based sensitivity analysis and uncertainty quantification of GOCE aerodynamics using DSMC," Stardust Final Conference: Advances in Asteroids and Space Debris Engineering and Science. Vasile, M., Minisci, E., Summerer, L. Mcginty, P. (eds.). Cham: Springer Netherlands, p. 301-323 23 p., Feb 2018.

[3] E. Minisci, R. Serra, M. Vasile, and A. Riccardi, “Meta-model Approach for the Quantification of the Reentry Distributions," 14th International Workshop on Space Debris Re-entry, ESA ESOC, Darmstadt, Germany, 28 February 01 March 2018.

[4] P.M. Mehta, M. Kubicek, E. Minisci, and M. Vasile, “Sensitivity Analysis and Probabilistic Re-entry Modeling for Debris using High Dimensional Model Representation based Uncertainty Treatment," Advances in Space Research, Vol.59, Issue 1, pp 193-211, January 2017.

[5] A. Falchi, E. Minisci, M. Vasile, and M. Kubicek, “Aero-Thermal Re-Entry Sensitivity Analysis Using DSMC and a High Dimensional Model Representation-Based Approach," 7th European Conference on Space Debris, ESA ESOC, Darmstadt, Germany, 18-21 April 2017.

[6] A. Falchi, “Atmospheric Re-entry Analysis of Space Objects," PhD Thesis, to be submitted.

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The simulation of complex fluid flows is an ongoing challenge in the scientific community. The computational cost of Direct Numerical Simulation (DNS) or Large Eddy Simulation (LES) of turbulent flows quickly becomes imperative when one is interested in control, design, optimization and uncertainty quantification. For these purposes, simplified models are typically used, such as reduced order models, surrogate models, low-fidelity models, etc.

In this work we will study reduced order models (ROMs) that are obtained by projecting the fluid flow equations onto a lower-dimensional space. Classically, this is performed by using a POD-Galerkin method, where the basis for the projection is built from a proper orthogonal decomposition of the snapshot matrix of a set of high-fidelity simulations. Ongoing issues of this approach are, amongst others, the stability of the ROM, handling turbulent flows, and conservation properties [1,2].

We will address the stability of the ROM for the particular case of the incompressible Navier-Stokes equations. We propose to use an energy-conserving finite volume discretization of the Navier-Stokes equations [3] as full-order model (FOM), which has the important property that it is energy conserving in the limit of vanishing viscosity and thus possesses non-linear stability. We project this FOM on a lower-dimensional space in such a way that the resulting ROM inherits the energy conservation property of the FOM, and consequently its non-linear stability properties. The stability of this new energy-conserving ROM is demonstrated for various test cases, and its accuracy as a function of time step, Reynolds number, number of modes, and amount of snapshot data is assessed.

[1] K. Carlberg, Y. Choi, and S. Sargsyan. Conservative model reduction for finite-volume models. Journal of Computational Physics, 371:280-314, 2018.
[2] L. Fick, Y. Maday, A.T. Patera, and T. Taddei. A stabilized POD model for turbulent flows over a range of Reynolds numbers: Optimal parameter sampling and constrained projection, Journal of Computational Physics, 371:214-243, 2018.
[3] B. Sanderse. Energy-conserving Runge-Kutta methods for the incompressible Navier-Stokes equations, Journal of Computational Physics, 233:100-131, 2013.

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Probabilistic learning on manifolds for the small-data challenge in Uncertainty Quantification

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Keywords: Probabilistic learning on manifolds, Optimization under uncertainties, Design optimization under uncertainties, Model-form uncertainties.

ABSTRACT

This work is devoted to a novel approach concerning a probabilistic learning on manifolds [1] from small datasets with applications to Uncertainty Quantification. This new tool of the computational statistics can be viewed as a useful method in scientific machine learning based on the probability theory. We first explain the concept/method of this probabilistic learning on manifolds by discussing a challenging problem of nonconvex optimization under uncertainties (OUU). We will then present the mathematical formulation and the main steps of the method based on the construction of a diffusion-maps basis and the projection on it of a nonlinear Itô stochastic differential equation. After having presented two simple illustrations, fours applications will be presented:

1. Optimization under uncertainties using a limited number of function evaluations [2].
2. Design optimization under uncertainties of a mesoscale implant in biological tissues using probabilistic learning [3].
3. Enhancing model predictability for a scramjet using probabilistic learning on manifolds [4].
4. Probabilistic learning on manifolds for nonparametric probabilistic approach of model-form uncertainties in nonlinear computational mechanics [5].

References

[1] C. Soize and R. Ghanem (2016). Parallel domain decomposition strategies for stochastic elliptic equations, *Journal of Computational Physics*.

[2] R. Ghanem and C. Soize (2018). Probabilistic nonconvex constrained optimization with fixed number of function evaluations, *International Journal for Numerical Methods in Engineering*.

[3] C. Soize (2018). Design optimization under uncertainties of a mesoscale implant in biological tissues using a probabilistic learning algorithm, *Computational Mechanics*.

[4] C. Soize, R. Ghanem, C. Safta, *et al*(2019). Enhancing model predictability for a scramjet using probabilistic learning on manifold, *AIAA Journal*.

[5] C. Soize, C. Farhat (2019). Probabilistic learning for model-form uncertainties in nonlinear computational mechanics, *International Journal for Numerical Methods in Engineering*.

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Application of Machine Learning Techniques for the Prediction of Free Plasma Jet Oscillatory Phenomena and Cloud Classification for In-flight Icing from Experimental Data

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Keywords: Machine Learning, Plasma Jet Instabilities, High Speed Camera Data, Cloud Classification, In-flight Icing, Uncertainty Quantification.

ABSTRACT

This paper presents the application of Machine Learning (ML) techniques to two different experimental data sets.

The first set concerns experiments carried out using the Plasmatron facility, a plasma wind tunnel located at the von Karman Institute for Fluid Dynamics in Belgium [1]. The experiments aim at reproducing the complex flow developing around a spacecraft during atmospheric entry. Prediction of the heating rate which is experienced by the Thermal Protection System (TPS) of the spacecraft remains an imperfect art, consequently, leading to very large safety margins for the vehicle design. On the other hand, failing to correctly predict the heat loads and associated material response of the TPS during the design phase can lead to catastrophic mission failure. To address this problem, experimental facilities are developed to study different aspects of atmospheric entry flows [2]. The facilities are capable of generating high speed flows of plasma which is discharged over testing probes, to characterise and investigate the response of different TPS materials.

Unfortunately, on ground facilities are often subject to spurious physical phenomena, that do not occur in real flights, due to the particular design of the facility itself. In this regard, we investigate the oscillations of the plasma jet generated using the Plasmatron. These oscillations are related to the experimental set up and they do not extrapolate from the reproduced flight. Such instabilities are due to a ripple originating from the power supply system and to the entrapment of cold gas within the hot plasma stream expanding in the chamber. Traditionally, the experimental

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investigation of plasma jet instabilities is performed by analysing the frequency spectrum obtained by applying the Fast Fourier Transforms (FFT) to stacks of high speed camera pictures. The proposed work looks into the application of ML algorithm to determine the main frequency of the oscillations. This frequency can be used for code validation or input for stability studies [3].

Introducing ML in this scenario will allow us to go one step further in the determination of the main frequency from the testing conditions as well as reduce the overall computational cost. Additionally, pictures uncertainty (intensity scale and width of pixels) can be considered and included into the ML framework, generating more robust predictions.

The second data set includes the properties of a large number of atmospheric clouds collected at different geographical locations. Clouds are visible arrays of tiny water droplets which are generated by uplift air motions. As the air raises, its temperature decreases. As soon as the dew point is reached, the air saturates and vapour condensates around cloud condensation nuclei (CCN). CCN are particulate matter found in the air and their origin can be anthropogenic or natural. Examples of anthropogenic and natural CCN sources are soot and salt particles, respectively.

Cloud properties vary according to the number and type of CCN suspended in the air mass. A large number of CCN entails large numbers of cloud particles for the same liquid water content. Generally, the atmospheric concentration of anthropogenic CCN is larger then the one related to natural CCN. Therefore, it is expected that clouds located in continental regions, namely close to large cities and industrial regions, present larger numbers of droplets than those found in oceanic regions.

The study of the micro-physical properties is relevant because it is directly related to the radiative properties of clouds. Furthermore, the knowledge of such properties helps with the estimation of the precipitation efficiency or the study of clouds dynamics. In addition, the industry is interested in this research field because of its potential w.r.t. to in-flight aircraft icing applications. One of the objective is to foresee the most severe ice accretion scenario, to help preventing aircraft flying in hazardous conditions.

In literature, clouds have been divided into two groups: Continental and Maritime/Oceanic [4]. Some other authors claim that maritime clouds can be polluted due to environmental phenomena such as air currents which redistribute the pollution in the atmosphere [5]. Therefore, the fine line between the two cloud types still remains undefined. Furthermore, it remains unclear whether there is any other possible grouping.

To investigate this, we rely on published data set [4], where clouds have been classified as maritime and continental. The set contains cloud properties measurements collected at very diverse geographical locations. The application of ML algorithms could support the division of the data set into clouds of different types, either Maritime/Continental or a third type.

References

[1] B. Bottin, O. Chazot, M. Carbonaro, V. Van der Haegen and S. Paris, Measurement Techniques for High Temperature and Plasma Flows, RTO-EN-8: The VKI Plasmatron Characteristics and Performance, 1999

[2] O. Chazot and F. Panerai, High enthalpy facilities and plasma wind tunnels for aerothermodynamics ground testing. *Nonequilibrium Hypersonic flows*, Ed. Eswar Josyula ARLF.

[3] A. Cipullo, Ground Testing Methodologies Improvement in Plasma Wind Tunnels using Optical Diagnostics. *PhD thesis defended at Seconda Università degli Studi di Napoli*, 2012

[4] N. L. Miles, J. Verlinde et al, Cloud droplet size distributions in low-level stratiform clouds. *Journal of the atmospheric sciences, 57(2), 295-311*, 2000

[5] A. A. Costa, C. J. Oliveira et al, Microphysical observations of warm cumulus clouds in Ceará, Brazil. *Atmospheric Research, 54(2-3), 167-199*, 2000

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Structured-Chromosome GA Optimisation for satellite tracking

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Keywords: Genetic Algorithms, variable-size optimisation, satellite Observation Scheduling, aerospace engineering.

ABSTRACT

This research addresses the problem of autonomous scheduling of space objects' observations from a network of tracking ground stations to enhance the knowledge of their orbit while respecting allocated resources. The presented approach aims at supporting the space sector by tracking both operational satellites and non-collaborative space debris. As for the former, it is crucial to accurately know the satellite state to precisely calibrate the instruments, interpret scientific data, and communicate with ground stations. For the latter, the debris position and velocity is mainly employed to predict and avoid impacts with other objects, as well as monitor the decay and predict the possible re-entry. However, in the last years, the number of space objects to be tracked has been increasing strongly and now most of them are tracked infrequently and with low accuracy.

An optimisation routine has been used for minimising the uncertainty on the final state of an orbiting object scheduling the observations from a network of ground stations. The performance index and objective function is a measure of the uncertainty that is evaluated by means a sequential filtering approach based on unscented Kalman Filter [1] that estimates the satellite state distribution conditional on received indirect measurements.

The free variables describing the observation schedules are 1) the number of times a specific ground station is used, 2) in which satellite pass over the station this has to measure and 3) the number of observation to perform. Consequently, without simplifying assumptions, the number of design variables is not constant among different solutions, and the observation scheduling optimisation falls under the area of the variable-size mixed-discrete global optimisation. To deal with dynamically varying search spaces, a number of additional challenges, harden dramatically the complexity of the search algorithm. Among the different algorithms, genetic algorithms

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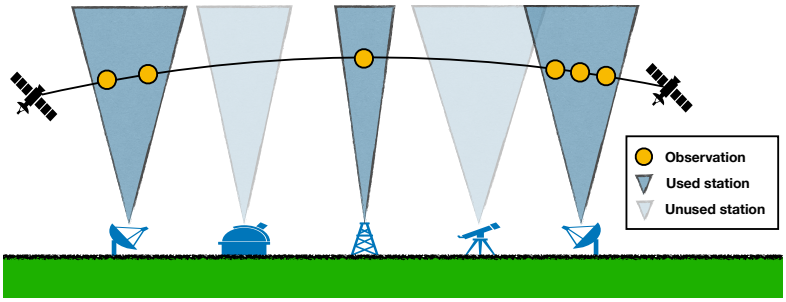

Figure 1: *Graphical 2D representation of satellite single passage over network of ground stations. The dark shaded blue field-of-view indicates that a station is used to take measurement, whereas the light shaded blue indicates that the station is not operated.*

(GAs) are recognise as the most suited to face this kind of problem [2]. For handling the optimisation of satellite tracking observation campaigns we propose the Structured-Chromosome Genetic Algorithm (SCGA) [3]. This bases its strategy on revised genetic operators that have been reformulated for handling hierarchical search spaces. Furthermore, the performances of presented tool are compared to an implementation of the "hidden-genes" Genetic Algorithm [4], standard Genetic Algorithm and Random Search.

The potential of the presented methodology is shown by solving the optimisation of a tracking window schedule for a very low Earth satellite operating in a highly perturbed dynamical environment.

References

[1] R. Van Der Merwe, and E. A. Wan, “The square-root unscented Kalman filter for state and parameter-estimation," Proceedings of IEEE International Conference on Acoustics, Speech, and Signal Processing, vol. 6, 2001.

[2] J. Pelamatti, L. Brevault, M. Balesdent, E. Talbi, and Y. Guerin, “How to deal with mixed-variable optimization problems: An overview of algorithms and formulations," in World Congress of Structural and Multidisciplinary Optimisation, p. 64–82, Springer, 2017.

[3] H. M. Nyew, O. Abdelkhalik, and N. Onder, “Autonomous interplanetary trajectory planning using structured-chromosome evolutionary algorithms," AIAA/AAS Astrodynamics Specialist Conference, 2012.

[4] S. A. Darani and O. Abdelkhalik, “Space trajectory optimization using hidden genes genetic algorithms," Journal of Spacecraft and Rockets, 55(3):764–774, 2017.

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