Reduction in parameter space with non-linear Active Subspaces

Francesco Romor, Marco Tezzele, Andrea Lario, Gianluigi Rozza
Mathematics Area, mathLab, SISSA, Trieste, Italy
Department of Mathematics and Geosciences, University of Trieste, Italy

Introduction

The Active Subspace property (AS) proposed by Trent Russi and developed by Paul Constantine [1] is employed in supervised dimensional reduction techniques. Dimension reduction in parameter studies confers benefits in a great number of engineering applications [4]. One of the main reasons behind it, is that parameter studies and scientific computing tasks are affected by the curse of dimensionality: the methods involved scale exponentially with the dimension of the parameters space making it unfeasible to be applied unless increasing the computational budget.

Random Fourier Features

Thanks to Bochner theorem and Monte Carlo method we can approximate the RBF-ARD kernel

$$k(\mathbf{x},\mathbf{x}') = \sigma_f \ \exp - \frac{(\mathbf{x}-\mathbf{x}')\Lambda(\mathbf{x}-\mathbf{x}')}{2}$$

with Random Fourier features [3]

$$k(\mathbf{x},\mathbf{x}') = \int_{\mathbb{R}^m} e^{i\mathbf{w}^T(\mathbf{x}-\mathbf{x}')}\lambda(\mathbf{w})\,\mathrm{d}\mathbf{w} \approx \langle z(\mathbf{x}), z(\mathbf{x}')\rangle$$

$$z(\mathbf{x}) = \sqrt{\frac{2}{n}}\sigma_f \ \cos(\mathbf{W}\mathbf{x}+\mathbf{b})$$

where n is the number of random Fourier features, $\mathbf{b} \in \mathbb{R}^n$ is a uniform sampled bias and $\mathbf{W} \in \mathbb{R}^{n\times m}$ is the projection matrix sampled from the spectral measure λ obtained from the Bochner theorem

$$\lambda(\mathbf{w}) = \mathcal{N}(0,\ \Lambda^{-1})$$

The feature map $\phi : \chi \subset \mathbb{R}^m \to \mathcal{H}$ from the input space to the Reproducing Kernel Hilbert Space can be approximated with $z(\mathbf{x})$.

The Active Subspace Property

Consider a Lipschitz continuous, differentiable and square-integrable function, its gradient vector and a sampling density

$$f : \chi \subset \mathbb{R}^m \to \mathbb{R} \quad \nabla f(\mathbf{x}) \in \mathbb{R}^m, \quad \rho : \mathbb{R}^m \to \mathbb{R}_+$$

Take the uncentered covariance matrix of the gradient, evaluate its approximation with Monte Carlo and partition its eigendecomposition,

$$\mathbf{C} = \int (\nabla_{\mathbf{x}} f)(\nabla_{\mathbf{x}} f)^T \rho\, d\mathbf{x} \approx \frac{1}{M}\sum_{i=1}^{M} (\nabla_{\mathbf{x}} f)(\nabla_{\mathbf{x}} f)^T = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$$

$$\mathbf{\Lambda} = \begin{bmatrix} \mathbf{\Lambda}_1 & \\ & \mathbf{\Lambda}_2 \end{bmatrix}, \qquad \mathbf{W} = [\mathbf{W}_1 \quad \mathbf{W}_2], \qquad \mathbf{W}_1 \in \mathbb{R}^{m\times l}$$

where l is the dimension of the Active Subspace. Then the input data can be decomposed as

$$\mathbf{x} = \mathbf{W}\mathbf{W}^T\mathbf{x} = \mathbf{W}_1\mathbf{W}_1^T\mathbf{x} + \mathbf{W}_2\mathbf{W}_2^T\mathbf{x} = \mathbf{W}_1\mathbf{y} + \mathbf{W}_2\mathbf{z}.$$

Non-linear Active Subspaces

The nonlinear extension (NAS) of Active Subspaces [2] is obtained applying the usual procedure to the new simulation map $\tilde{f} : \phi(\chi) \subset \mathcal{H} \to \mathbb{R}$. The gradient is approximated with the chain rule as solution of the over-determined system

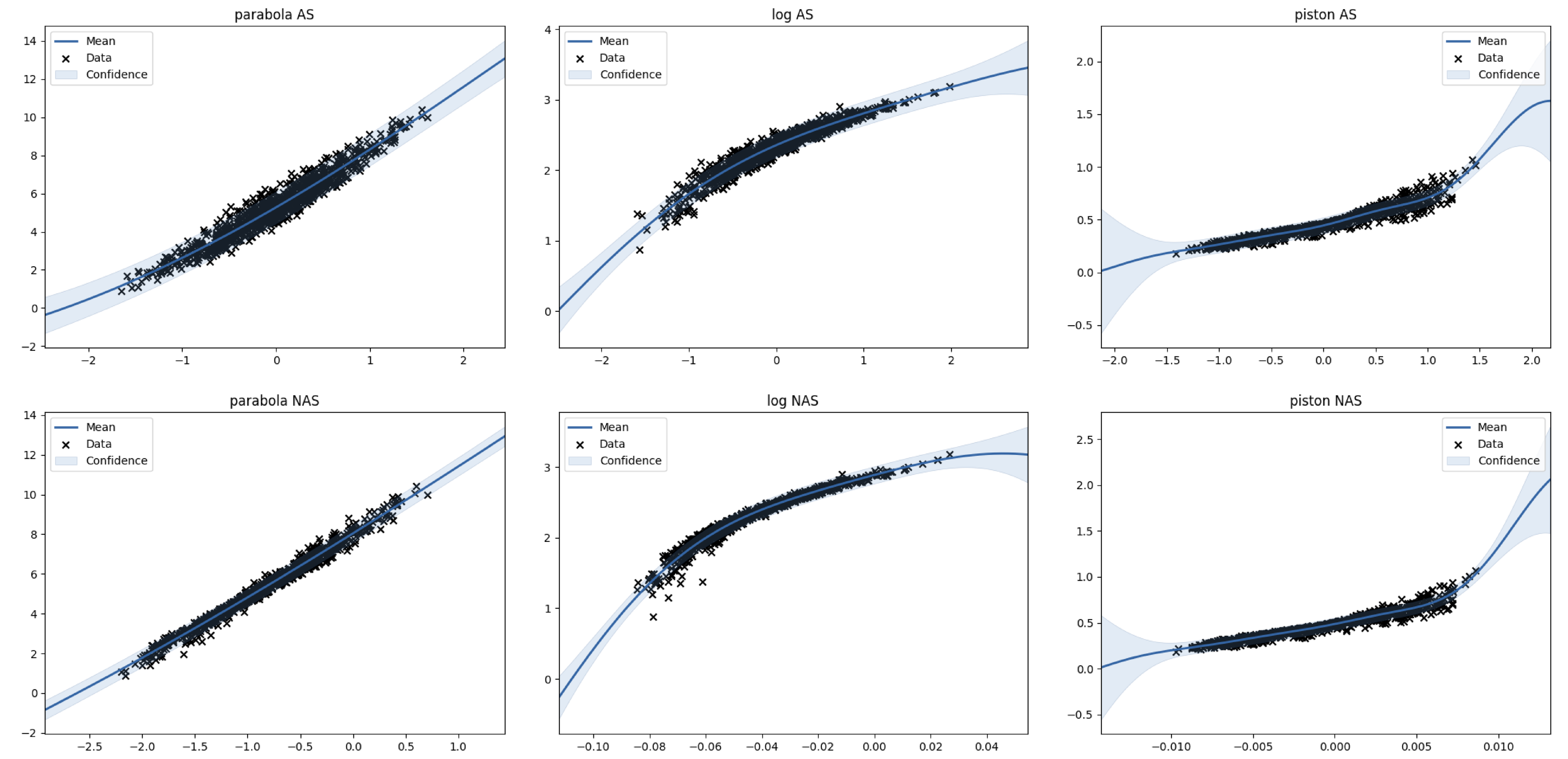
$$\frac{\partial \tilde{f}}{\partial \mathbf{z}} = \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}^T\right)^{\dagger} \frac{\partial \tilde{f}}{\partial \mathbf{x}}$$

$$\frac{\partial z_i}{\partial x_d} = -\sqrt{\frac{2}{n}}\ \sigma_f \sin\left(\sum_{j=1}^{m} W_{ij}x_j + b_i\right) W_{id}$$

where $\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}^T\right)^{\dagger} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}}\left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}}^T \frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right)^{-1}$ is the pseudo inverse matrix.

Application to Gaussian Process regression

The following Gaussian Process regressions (GPR) are the result of AS and NAS procedures applied to test cases with simulation functions given by the piston function from the benchmarks of Constantine work and some hypersurfaces of revolution in $\mathbb{R}^9$ with different generatrices and input space $[0,2]^8$.



The piston function C models the cycle time of a piston within a cylinder

$$C = 2\pi\sqrt{\frac{W}{k + S^2 \frac{P_0 V_0}{T_0}\frac{T_a}{V^2}}}$$

The parameters involved are the Piston Weight(W), the piston Surface Area(S), the initial Gas Volume(V_0), the spring Coefficient(k), the atmospheric Pressure(P_0), the ambient Temperature(T_a) and the filling Gas Temperature(T_0). They have different ranges and are sampled uniformly.

	AS RRMSE	NAS RRMSE	var NAS
parabola	0.076314	**0.037359**	0.003268
log	0.038513	**0.031320**	0.008919
piston	0.080755	**0.076236**	0.011082

M=1500 n=1000, the chosen dimension of the Active Subspace for the GPR is $l = 1$, the relative root mean square error (RRMSE) of NAS is estimated over 10 runs, the associated variance is reported.

References

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