Kernel-based Active Subspaces with application to CFD problems

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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 correlation matrix of the gradient, evaluate its approximation with Monte Carlo and partition its eigendecomposition,

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

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

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

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

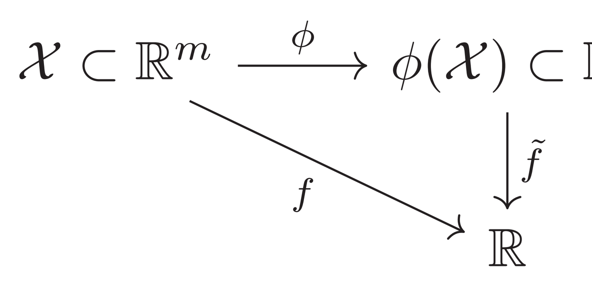
Kernel-based Active Subspaces

We introduce an immersion ϕ from the original domain $\mathcal{X} \subset \mathbb{R}$ to a supposedly infinite-dimensional Hilbert space $\mathbb{H}$

$$\mathbf{z} = \phi(\mathbf{x}) = \sqrt{\frac{2}{D}} \sigma_f \cos(W\mathbf{x} + \mathbf{b}), \qquad \mathbf{x} \in \mathcal{X}, \mathbf{z} \in \mathbb{H}$$

resulting from an approximation of a RBF kernel with Random Fourier Features [3]: $\mathbf{b}$ is a bias term and W is sampled from the spectral measure associated to the kernel.

The kernel-based extension (KAS) of Active Subspaces [2] is obtained applying the usual procedure to the new simulation map $\tilde{f} : \phi(\chi) \subset \mathbb{H} \to \mathbb{R}$.

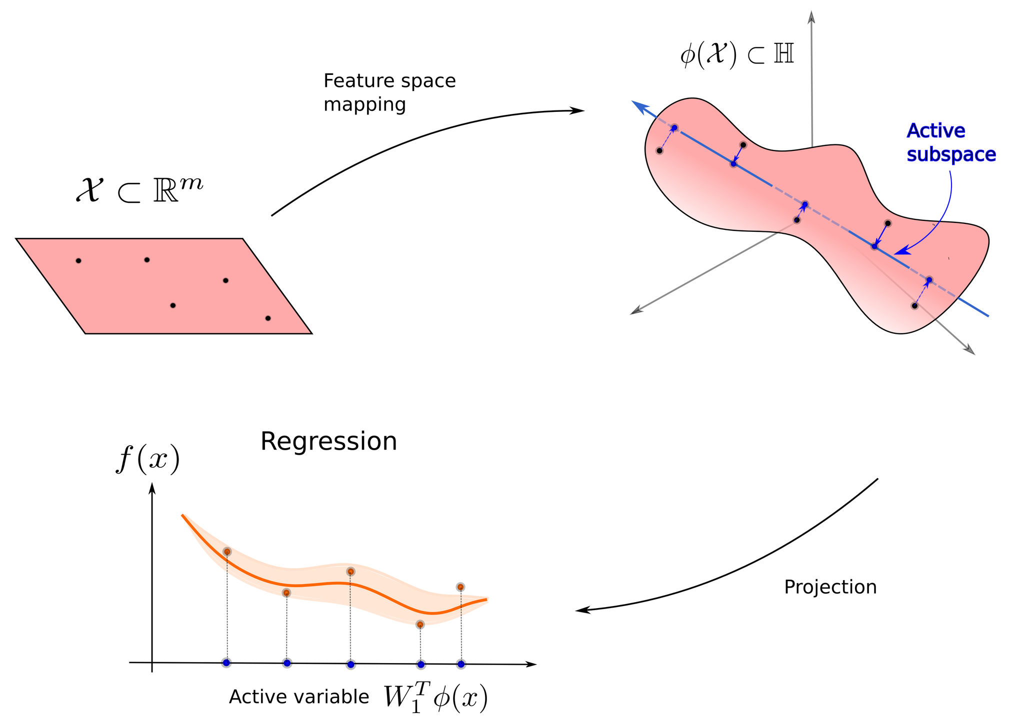


In this case the correlation matrix is

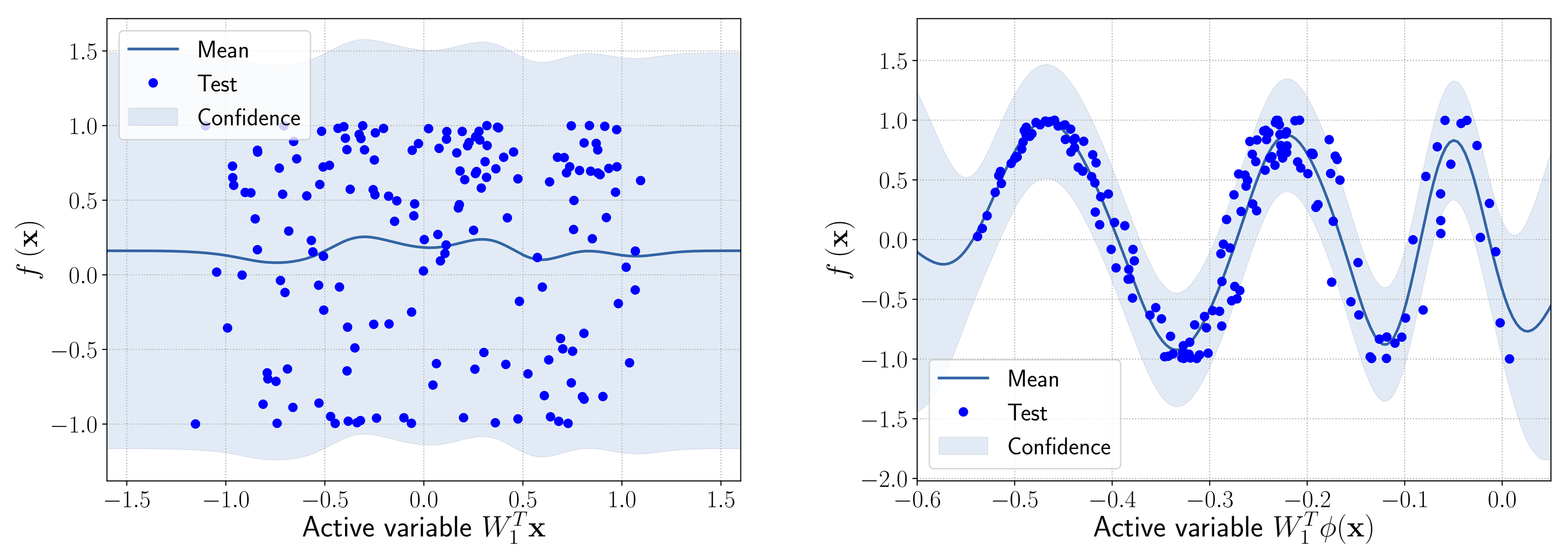
$$\tilde{\mathbf{C}} = \int_{\phi(\mathcal{X})} (\nabla_{\mathbf{z}} \tilde{f})(\mathbf{z})(\nabla_{\mathbf{z}} \tilde{f}(\mathbf{z}))^T \, d\mu(\mathbf{z}) \approx \frac{1}{M} \sum_{i=1}^{M} (\nabla_{\mathbf{z}} \tilde{f})(\nabla_{\mathbf{z}} \tilde{f})^T = \tilde{\mathbf{W}}\tilde{\mathbf{\Lambda}}\tilde{\mathbf{W}}^T$$

Response surfaces with Gaussian process regression

The term response surface refers to the general procedure of finding the values of a model function f for new inputs without directly computing it but exploiting regression or interpolation from a training set $\{\mathbf{x}_i, \ f(\mathbf{x}_i)\}$.



The code is implemented in the library ATHENA (Advanced Techniques for High dimensional parameter spaces to Enhance Numerical Analysis) at https://github.com/mathLab/ATHENA.

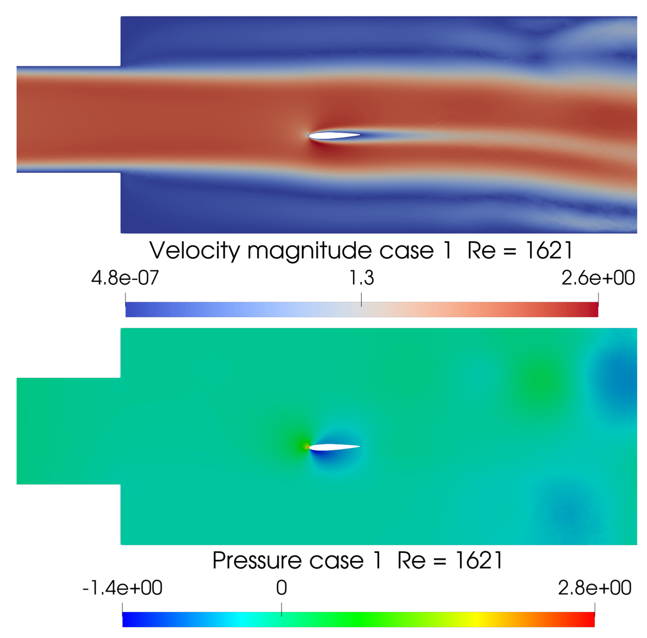


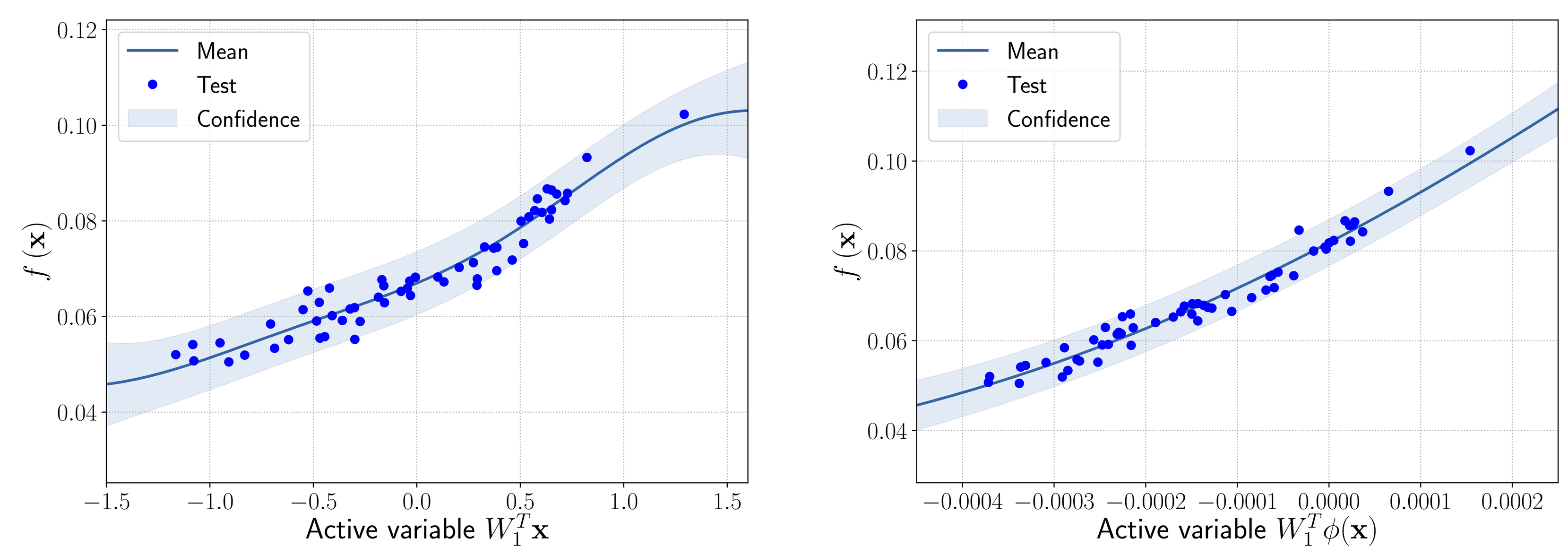
Comparison between the sufficiency summary plots obtained from the application of AS and KAS methods for the surface of revolution model function with domain $[-3, 3]^2$ and generatrix the sine function. The left plot refers to AS, the right plot to KAS.

A CFD application of KAS using Discontinuous Galerkin method

Lift (C_L) and drag (C_D) coefficients of a NACA 0012 airfoil are considered as model functions. We consider physical and geometrical parameters and build a response surface: the first component of the initial velocity, the kinematic viscosity, the vertical and horizontal displacements of the airfoil and its angle of attack, the vertical displacements of the upper and lower side of the initial conduct. Reynolds number ranges from 400 to 2000.

$$\begin{cases} \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu \Delta \mathbf{u} & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \mathbf{x} \in \Omega, \\ \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0, \quad p(\mathbf{x}, 0) = 0 & \mathbf{x} \in \Omega, \\ \mathbf{u}(\mathbf{x}, t) = \mathbf{u}_0, \quad \mathbf{n} \cdot \nabla p(\mathbf{x}, t) = 0 & \mathbf{x} \in \partial\Omega_I, \\ \mathbf{u}(\mathbf{x}, t) = 0, \quad \mathbf{n} \cdot \nabla p(\mathbf{x}, t) = 0 & \mathbf{x} \in \partial\Omega_W, \\ \mathbf{n} \cdot \nabla \mathbf{u}(\mathbf{x}, t) = 0, \quad p(\mathbf{x}, t) = 1 & \mathbf{x} \in \partial\Omega_O, \end{cases}$$





Comparison between the sufficiency summary plots obtained from the application of AS and KAS methods for the drag coefficient C_D. The left plot refers to AS, the right plot to KAS. With the blue solid line we depict the mean of the GP regression, with the shadow area the confidence intervals, and with the blue dots the testing points.

References

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