Locating an Active Subspace using Gaussian Processes

Dr Robert Milton, Prof. Solomon Brown & Aaron Yeardley, Department of Chemical and Biological Engineering, The University of Sheffield

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Why active subspaces (AS)?

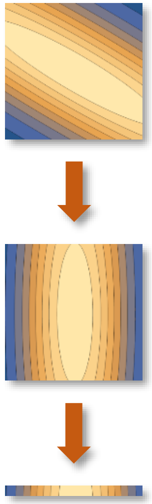
Active subspaces supercharge input screening by exploiting latent possibilities for dimension reduction. The construction by rotates input space before truncating it

$$[z]_{\mathbf{m}} := [\Theta]_{\mathbf{m}\times\mathbf{M}} [x]_{\mathbf{M}} \quad \text{for } m < M$$

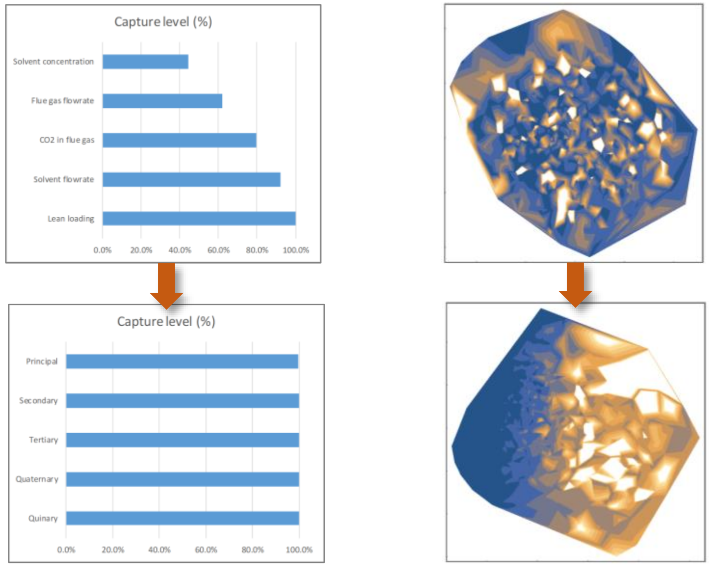
without significantly altering the output $[y]_{\mathbf{L}}$

$$y([\Theta]^{\intercal}_{\mathbf{m}\times\mathbf{M}} [z]_{\mathbf{m}}) \approx y([x]_{\mathbf{M}})$$

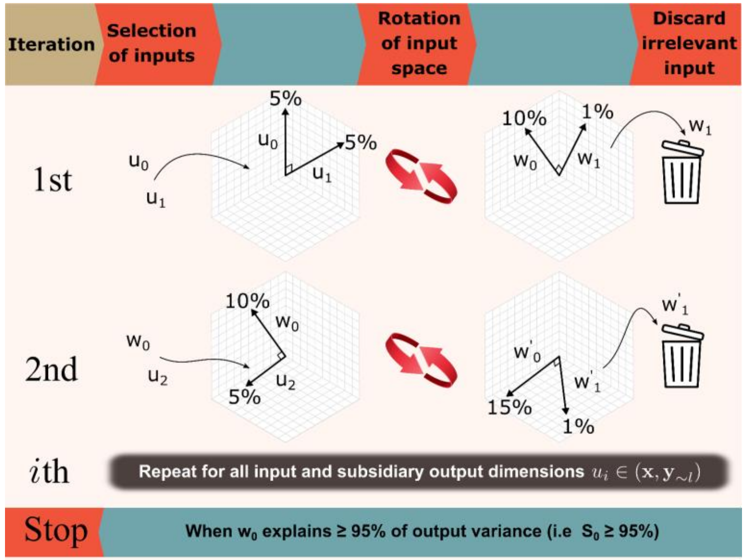
A variety of measures may be used to compare the two sides of this approximation. The measure chosen ultimately determines the rotation Θ and dimension reduction $(M - m)$. This poster describes an implementation of Global Sensitivity Analysis as the similarity measure locating an active subspace.



Applications – carbon capture and Li-ion cell thermal runaway



Bottom up AS construction?



Why global sensitivity analysis (GSA)?

GSA is designed to assess model reduction via (closed) Sobol' indices

$$[S_{\mathbf{m}}]_{\mathbf{L}^2} := \frac{\mathbb{V}_{\mathbf{m}}[y_{\mathsf{m}}]}{\mathbb{V}_{\mathbf{M}}[y_{\mathsf{M}}]} = [R^2_{\mathbf{m}}]_{\mathbf{L}^2} =: [1]_{\mathbf{L}^2} - [\mathsf{S}^{\intercal}_{\mathsf{M-m}}]_{\mathbf{L}^2}$$

These are coefficients of determination between full $(\mathbf{M})$ and reduced $(\mathbf{m})$ models. They may be better equipped to capture gross features and gloss over noise than local sensitivity measures.

An active subspace is located by optimizing the rotation to maximize some seminorm of the Sobol' index matrix

$$\Theta = \operatorname{argmax} \|S_{\mathbf{m}}\|_{\mathbf{L}^2}$$

Where the optimization achieves $S_{\mathbf{m}} > 95\%$ say, we may say we have located an active subspace of dimension m.

Why Gaussian processes (GPs)?

Analytic expressions for GSA – with quantified uncertainties (UQ) – have been developed for GPs. Crucially, these furnish $S_{\mathbf{m}}(\Theta)$, telling us the effect of rotation on model comparison which was the one obstacle to using GSA to locate an active subspace. GSA-UQ is entirely a function of the first two moments of the marginalized GP, easily stated in the rotated basis:

$$[\mu_{\mathbf{m}}]_{\mathbf{L}} = \mathbb{E}_{\mathbf{M-m}}\left[k([\mathsf{x}]_{\mathbf{M}}, X)\, K_Y^{-1} Y^{\dagger} \,\middle|\, [\Theta]^{\intercal}_{\mathbf{m}\times\mathbf{M}} [z]_{\mathbf{m}}\right]$$

$$[\mu_{\mathbf{mm'}}]_{\mathbf{L}^2} = [E]_{\mathbf{L}^2} + \mathbb{E}_{\mathbf{M-m}}\mathbb{E}_{\mathbf{M'-m'}}\left[k([\mathsf{x}]_{\mathbf{M}}, [\mathsf{x}]_{\mathbf{M'}}) \,\middle|\, [\Theta]^{\intercal}_{\mathbf{m}\times\mathbf{M}} [z]_{\mathbf{m}}, [\Theta]^{\intercal}_{\mathbf{m}\times\mathbf{M}} [z]_{\mathbf{m'}}\right] - \mathbb{E}_{\mathbf{M-m}}\mathbb{E}_{\mathbf{M'-m'}}\left[k([\mathsf{x}]_{\mathbf{M}}, X)\, K_Y^{-1} k(X, [\mathsf{x}]_{\mathbf{M'}}) \,\middle|\, [\Theta]^{\intercal}_{\mathbf{m}\times\mathbf{M}} [z]_{\mathbf{m}}, [\Theta]^{\intercal}_{\mathbf{m}\times\mathbf{M}} [z]_{\mathbf{m'}}\right]$$

Analytic expressions for $S_{\mathbf{m}}(\Theta)$ are obtained by taking expectations of products of these expressions. For the commonly used RBF/ARD kernel, well suited to smooth outputs, $k(x, x')$ is Gaussian, and this is entirely an exercise in multiplying and marginalizing Gaussian pdfs.

Implementation

The implementation locates an AS for a given GP, then fits a new GP to the rotated inputs. Thus far, convergence has typically required 3-5 iterations through this procedure.

The implementation has thus far optimized Θ one row at a time, re-orthogonalizing between rows. It is not known whether this is necessary or desirable.

Related presentations…

Active subspaces were introduced in Session 1A…

Analytic GSA-UQ using GPs will be described in Session 3A…