Active Subspaces via Monte Carlo Sampling

Jordan R. Hall

Department of Mathematical and Statistical Sciences
University of Colorado Denver

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Dimension Reduction and the Active Subspace

Active Subspaces via Monte Carlo

Quick Example!

References

- We consider functions $f : \Lambda \to \mathcal{D}$ where $\dim(\Lambda) = N$ is large and $\dim(\mathcal{D}) = M$ is such that $M < N$ or $M << N$.
  - Functions of interest may represent postprocessed quantities from the solution of complex physical models.
- It is not often that every parameter has equal impact on function values – usually some parameters matter more than others.
- The dimension reduction techniques considered seek to explain outputs $f(\Lambda)$ in an *active subspace* $\mathcal{A} \subset \Lambda$ for which $\dim(\mathcal{A}) < N$.
  - A lower-dimensional representation of f can save computational costs.

- $\nabla f(\lambda) \in \Lambda$ is a column vector with rows containing the N partial derivatives of f, which for this discussion we assume exist, and are square integrable in Λ equipped with some probability density that is positive everywhere in Λ and 0 otherwise.
  - We consider $\pi_\Lambda^{\text{prior}}(\lambda)$, the density describing our prior state of knowledge, which we abbreviate as π_Λ.
- One transforms inputs λ to the origin with some fixed variance, typically so that $\lambda \in [-1, 1]^N$. We define

Covariance in Gradient Space [1]

$$W = \int_\Lambda \nabla f(\lambda) \nabla f(\lambda)^\top \pi_\Lambda(\lambda) d\lambda, \tag{1}$$

which is an $N \times N$ symmetric positive semi-definite matrix.

[1] Constantine

- Interpreting W as a certain covariance structure over Λ leads one to the idea of computing the Singular Value Decomposition of W,

Singular Value Decomposition (SVD) of W

$$W = U\Sigma V^*, \tag{2}$$

where U is $N \times N$ unitary, Σ is $N \times N$ diagonal with the singular values of W along its diagonal, and V^* is $N \times N$ unitary.

- We plot the singular values, $\{\sigma_i\}_{i=1}^n$ and seek a drop-off in magnitude between some pair of singular values, σ_j and σ_{j+1}. The active subspace is the span of $u_1, \ldots, u_j$, which are the first j columns of U, the left singular vectors of W.

- For a point $\lambda \in \Lambda$, we define

Projection into $\mathcal{A}$, *active variables*

$$\mathcal{P}_{\mathcal{A}}(\lambda) = \sum_{i=1}^{j} \left(u_i^T \lambda\right) u_i \in \mathcal{A}, \tag{3}$$

which is the projection of λ in the active directions of f.

- We have arrived at the property that

Resolution of f in $\mathcal{A}$

$$f\left(\mathcal{P}_{\mathcal{A}}(\lambda)\right) \approx f(\lambda). \tag{4}$$

- Finding an active subspace requires forming an approximation to W via Monte Carlo. Here we consider techniques in [1] [2].
- We let $D_S = \{(\lambda_i, f(\lambda_i))\}_{i=1}^S$, which is a set of S pairs of samples $\lambda_i \in \Lambda$ and their function values. One may use D_S to approximate ∇f. We denote each estimation to $\nabla f(\lambda_i)$ with $\widehat{\nabla f}(\lambda_i)$.
- We form the $N \times S$ matrix $\tilde{W}$ (which we present as $\tilde{W}^\top$)

Monte Carlo Approximation to W [1]

$$\tilde{W}^\top := \left[\widehat{\nabla f}(\lambda_1) \cdots \widehat{\nabla f}(\lambda_S) \right]. \tag{5}$$

[1] Russi, T.M.
[2] Constantine, Eftekkari, Wakin

- Forming the SVD of $\tilde{W}$, $\tilde{W} = \tilde{U}\tilde{\Sigma}\tilde{V}^*$, we search for a drop off in the magnitude of the singular values $\{\tilde{\sigma}_i\}_{i=1}^S$. Assuming such a drop off occurs for an index $j : 1 < j < S$, we have the j corresponding left singular vectors,$\tilde{u}, \ldots, \tilde{u}_j$.
- Then we define

Monte Carlo approximation to $\mathcal{A}$

$$\mathcal{A}\left(f; D_S\right) := \text{span}\{\tilde{u}, \ldots, \tilde{u}_j\},$$

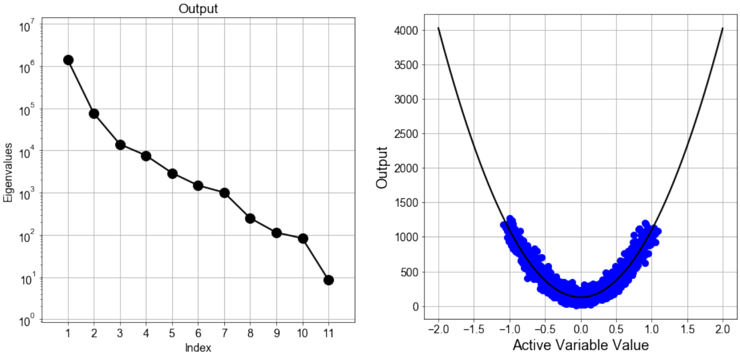
the active subspace of f with respect to the samples D_S.

- We check the extent to which the active subspace accounts for functions values $f(\lambda)$ by checking for resolution in a *sufficient summary plot*, where we plot active variables against function values.

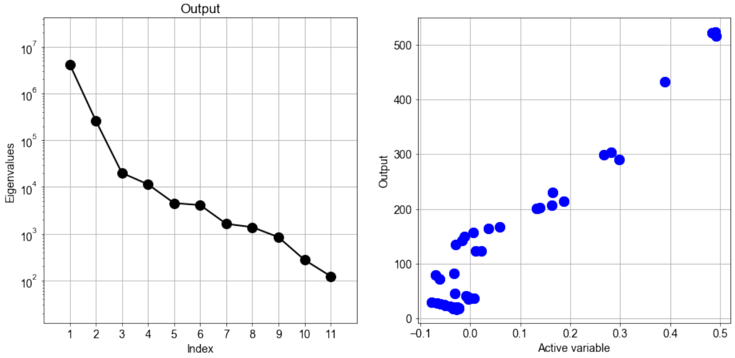
Example 1. Let $\Lambda = [-1, 1]^{11}$ and define

$$f(\lambda) = \sum_{i=0}^{10} 2^{(-1)^i i} \lambda_i^2 + \epsilon(\lambda),$$

where $\epsilon(\lambda)$ is a draw of additive noise corresponding to the input λ; here, we take draws of ϵ of order 10^{-4}. We see that $\mathcal{D} = [0, 2^{10}]$ and $N = 11$, $M = 1$. Note that the minimum of f is given by $0 \in \Lambda$. Here, as i increases, terms in f become either more important or less important, depending on whether i is even or odd.



Left: A plot of the eigenvalues of the matrix $\hat{W}$ formed from 1000 Monte Carlo samples in Λ. We see one dominant eigenvalue on the order of 10^6. Right: A sufficient summary plot where all 1000 samples are projected into $\mathcal{A}$ and plotted against their function values; a quadratic surrogate fits the projected data with $R^2 \approx 0.9$.



Left: A plot of the eigenvalues of the matrix $\hat{W}$ formed from using 100 DFO iterates as samples in Λ. We again see one dominant eigenvalue between orders 10^6 and 10^7. Right: A sufficient summary plot where all 100 samples are projected into $\mathcal{A}$ and plotted against their function values.

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