ATHENA: Advanced Techniques for High Dimensional Parameter Spaces to Enhance Numerical Analysis

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Abstract

ATHENA is an open source Python package for reduction in parameter space. It implements several advanced numerical analysis techniques such as Active Subspaces (AS), Kernel-based Active Subspaces (KAS), and Nonlinear Level-set Learning (NLL) method. It is intended as a tool for regression, sensitivity analysis, and in general to enhance existing numerical simulations’ pipelines tackling the curse of dimensionality.

Keywords: Parameter space reduction, Active subspaces, Kernel-based active subspaces, Nonlinear level-set learning, Python

1. The ATHENA package

Parameter space reduction techniques are particularly suited to tackle the curse of dimensionality affecting high dimensional problems for many-queries and outer-loop applications such as optimization, uncertainty propagation, and statistical inference. The increased capabilities in simulating every day more and more complex phenomena with many input design parameters need to be compensated by a proper handling of the dimension of such parameters. This is due to the fact that the amount of samples needed scales superlinearly with respect to the input dimension. Possible strategies to mitigate this issue could be sparse grid sampling, adaptive sampling, and model order reduction [1, 2].

In this package we focus on techniques which use linear and nonlinear transformations to align the input space along the directions of maximum variation of the function of interest. In particular in the ATHENA open

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source Python package are implemented the interfaces to easily employ Active Subspaces [3], Kernel-based Active Subspaces [4], and the Nonlinear Level-set Learning [5] method. Figure 1 depicts a simple application of AS and NLL.

These techniques are purely data driven, since they necessitate only input-output couples. We emphasize that even if the methods are gradient-based, it is possible to approximate the gradients of the target function with respect to the parameters using only input-output data. Thus they are particularly suited to enhance existing numerical simulations’ pipelines such as optimization procedures, possibly including commercial softwares. Moreover it is possible to couple parameter space reduction with reduced order methods, enabling higher speedup computations with controlled accuracy, especially for the solution of parametric PDEs, both in academia and in industry.

The package is multi-purpose and intended for practitioners, engineers, data scientists, and researchers.

2. The impact to research fields

The package made possibile the creation of several new methods for optimization, regression, and classification tasks. The interface for Active Subspaces studies of ATHENA is used in [6] to enhance genetic algorithms when
optimizing complex and high-dimensional functions. The reduction affects the dimension of the population of the genetic algorithm at each step. The same interface for Active Subspaces is used in [7] to improve the approximation of Gaussian process regression of scalar functions with low intrinsic dimensionality. The information regarding the presence of an Active Subspace is delivered to a nonlinear multi-fidelity model thus able to reach a higher accuracy. In some cases the Active Subspace is not present due to its linear nature, an extension is introduced in [4] with Kernel-based Active Subspaces. In this case the inputs are projected to a high-dimensional space and then reduced, mimicking the framework of reduction in Reproducing Kernel Hilbert Spaces. Figure 2 shows a sketch to understand how the KAS method works. In the context of a computational fluid dynamic benchmark, ATHENA’s Kernel-based Active Subspaces interface is tested on the design of a response surface showing an improvement of the accuracy with respect to Active Subspaces. In [8] a local approach to parameter space reduction is presented to improve the accuracy of regression and classification.

3. The impact to industrial collaborations

ATHENA has been created thanks to an industrial collaboration with Fincantieri S.p.A., matching the demand of an intuitive, easily integrable tool
for parameter space reduction in the framework of structural optimization of modern passenger ship hulls. In an ongoing industrial Ph.D. grant sponsored by Electrolux Professional, the package is used to reduce the dimensionality of convolutional artificial neural networks for image recognition.

ATHENA is also utilized in [9] to reduce the dimensionality of a response surface resulting from the shape optimization of an airfoil. The proposed pipeline couples Dynamic Mode Decomposition with Dynamic Active Subspaces to reduce the overall computational resources. The methods are used also in [10] to optimize the shape of a benchmark hull using advanced geometrical morphing.

4. Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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References

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Illustrative Examples

Optional: you may include one explanatory video that will appear next to your article, in the right hand side panel. (Please upload any video as a single
supplementary file with your article. Only one MP4 formatted, with 50MB maximum size, video is possible per article. Recommended video dimensions are 640 x 480 at a maximum of 30 frames / second. Prior to submission please test and validate your .mp4 file at http://elsevier-apps.sciverse.com/GadgetVideoPodcastPlayerWeb/verification. This tool will display your video exactly in the same way as it will appear on ScienceDirect.

**Required Metadata**

**Current code version**

Ancillary data table required for subversion of the codebase. Kindly replace examples in right column with the correct information about your current code, and leave the left column as it is.

| Nr. | Code metadata description                               | Please fill in this column                          |
|-----|--------------------------------------------------------|-----------------------------------------------------|
| C1  | Current code version                                   | v0.1.2                                              |
| C2  | Permanent link to code/repository used for this code version | https://github.com/mathLab/ATHENA                     |
| C3  | Permanent link to Reproducible Capsule                 | Add repr capsule                                    |
| C4  | Legal Code License                                     | MIT License (MIT)                                   |
| C5  | Code versioning system used                            | git                                                 |
| C6  | Software code languages, tools, and services used      | Python                                              |
| C7  | Compilation requirements, operating environments & dependencies | ATHENA requires numpy, matplotliblib, scipy, torch, GPy, GPyOpt, scikit-learn, sphinx (for the documentation) and nose (for local test) |
| C8  | If available Link to developer documentation/manual    | https://mathlab.github.io/ATHENA/                   |
| C9  | Support email for questions                            | marco.tezzele@sissa.it (francesco.romor@sissa.it)    |

Table 1: Code metadata (mandatory)

**Current executable software version**

Ancillary data table required for sub version of the executable software: (x.1, x.2 etc.) kindly replace examples in right column with the correct information about your executables, and leave the left column as it is.
| Nr. | (Executable) software metadata description | Please fill in this column |
|-----|------------------------------------------|---------------------------|
| S1  | Current software version | v0.1.2 |
| S2  | Permanent link to executables of this version | [https://github.com/mathLab/ATHENA/releases/tag/v0.1.2](https://github.com/mathLab/ATHENA/releases/tag/v0.1.2) |
| S3  | Permanent link to Reproducible Capsule | Add capsule |
| S4  | Legal Software License | MIT License (MIT) |
| S5  | Computing platforms/Operating Systems | Linux, OS X, Unix-like |
| S6  | Installation requirements & dependencies | ATHENA requires **numpy**, **matplotlib**, **scipy**, **torch**, **GPy**, **GPyOpt**, **scikit-learn**, **sphinx** (for the documentation) and **nose** (for local test) |
| S7  | If available, link to user manual - if formally published include a reference to the publication in the reference list | [https://mathlab.github.io/ATHENA/](https://mathlab.github.io/ATHENA/) |
| S8  | Support email for questions | marco.tezzele@sissa.it francesco.romor@sissa.it |

Table 2: Software metadata (optional)