CSD-CMAD: Coupling Similarity and Diversity for Clustering Multivariate Astrophysics Data

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ABSTRACT

Traditionally, clustering of multivariate data aims at grouping objects described with multiple heterogeneous attributes based on a suitable *similarity* (conversely, *distance*) function. One of the main challenges is due to the fact that it is not straightforward to directly apply mathematical operations (e.g., sum, average) to the feature values, as they stem from heterogeneous contexts.

In this work we take the challenge a step further and tackle the problem of clustering multivariate datasets based on jointly considering: (a) *similarity* among a subset of the attributes; and (b) distance-based *diversity* among another subset of the attributes. Specifically, we focus on astrophysics data, where the snapshots of the stellar evolution for different stars contain over 40 distinct attributes corresponding to various physical and categorical (e.g., `'black hole'`) attributes. We present CSD-CAMD – a prototype system for Coupling Similarity and Diversity for Clustering Astrophysics Multivariate Datasets. It provides a flexibility for the users to select their preferred subsets of attributes; assign weight (to reflect their relative importance on the clustering); and select whether the impact should be in terms of proximity or distance. In addition, CSD-CAMD allows for selecting a clustring algorithm and enables visualization of the outcome of clustering.

CCS CONCEPTS

• **Information systems** → **Data management systems**; • **Computing methodologies** → *Modeling and simulation.*

KEYWORDS

Stellar Evolution, Clustering, Diversity

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1 INTRODUCTION AND MOTIVATION

Clustering is considered a canonical problem in data analysis and its main objective is to partition a given set into subsets, in a manner that will ensure that the objects in given subset are "more similar" (modulo certain distance function) to each other than to the objects in the rest of the subsets [10].

In its rich history, many variants to the basic approaches (e.g., K-means [6]; DBSCAN [3]) have been considered. Shortly after tackling the issues due to the high dimensionality of the data were recognized [5], researchers have addressed settings in which peculiar challenges arise due to the *heterogeneity* of the data. Namely, the elements of the set in question may not only have > 1 dimension, but those dimensions may be incompatible due to their physical properties (i.e., the domain of the attributes) [1, 2]. Another complementary extension was incorporating the *diversity* in the clustering process, which was more recently considered for improving ranking in recommendation systems [4].

Complementary to this, the scientific discipline of astrophysics studies the properties (and relationships) of various astronomical objects, such as stars, galaxies, interstellar medium, etc. [7]. The advances in optical and other sensing technologies along with the increase of computational and storage capabilities have enabled the creation of large repositories of observational data like, for example, Sloan Digital Sky Survey[1]. Often times, to evaluate the proposed theoretical models against observational data, astrophysicists resort

[1] https://www.sdss.org

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to simulation models, relying on tools such as MESA (Modules for Experiments in Stellar Astrophysics) [8].

Our POSYDON[2] project also relies on MESA based data and has generated large datasets (5 ∼ 10 GB) of stellar evolution. As part of the project, we have already developed a database for storing and querying the stars' trajectories via web-based User Interface (UI). In addition to the sheer volume, the data (which can be perceived as multivariate time series) is also characterized by a large number of attributes pertaining to different physical phenomena, such as mass, luminosity, He-concentration, temperature, etc.

What motivates this work is the observation that, for the purpose of testing models and hypotheses, the domain scientists may be interested in clustering the instances of the stellar evolution trajectories in a manner that would:

- Favor certain attributes more than the others (i.e., their impact on clustering is stronger).
- Insist on diversity for the values of other attributes (i.e., stars within a particular cluster should differ in each of those attributes by a predefined threshold).

As an example, one may want to cluster all the stars that end up in black holes with a stronger influence of mass and temperature (than the other attributes) *and* with at least 30% of a difference between the corresponding metalicity values.

Towards that end, the main contribution of the CSD-CMAD system prototype is that it enables scientists to focus on a targeted dataset and, once uploaded in the database, provide them with the opportunity to select the corresponding parameters for both classes of preferred attributes (i.e., stronger proximity as well as diversity via separability) – and visualize the outcome of applying a clustering algorithm. In the rest of this paper, in Section 2 we describe the basic architecture of CSD-CMAD and the way we modify the traditionally used distance functions to cater to the two complementary requests for the subsets of attributes. Section 3 lists the steps of the actual demo scenario that the attendees will be able to experience, and Section 4 offers concluding remarks.

2 SYSTEM ASPECTS

We now describe the system architecture of CSD-CMAD and discuss the details of our distance function implementation.

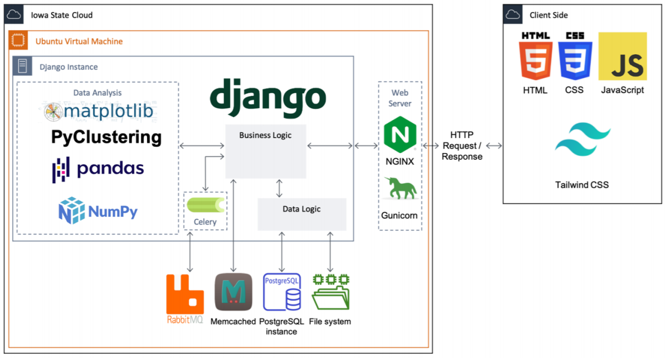


Figure 1: Overview of system architecture

2.1 System Architecture

From a broad perspective, the architecture of CSD-CMAD is the one of a client-server type[3]. An illustration of the main components is provided in Figure 1.

2.1.1 Backend. As shown, we have a web server in the backend, running on an Ubuntu VM, hosted on Iowa State Cloud. In the VM, the primary systems are `nginx`, `Gunicorn`, `PostgreSQL`, and `Memcached`.

1. `nginx` is our primary web server, and is our initial interaction to incoming requests on port 80.
2. `Gunicorn` reacts whenever `nginx` spawns new processes, to run a `WSGI` server for the `Django` instance.
3. The `Django` instance houses the logic and functionality of our project, as well as the algorithms that interpret the data. It also interacts with a `PostgreSQL` database for data storage, as well as a `Memcached` cache for caching of data to speed up response times.

Since an adjustable metric for the distance function (as well as diversity) was required, we relied on the `PyClustering` package for implementation of the clustering algorithms. In addition, in order to provide a better user experience with the large files for datasets, the asynchronous package `Celery` was used, along with it's asynchronous service provider `RabbitMQ`. Lastly, we note that the job of rendering the graphs to be displayed to the users shifted from the client to the backend to reduce data transmission, and we used `Matplotlib`.

2.1.2 Frontend. Our client side consists of a website that provides the following main categories of functionalities for the users:

- Select a dataset – either an existing one from the database, or a datasets generated by a new simulation (in .csv format) which will firstly be pre-processed with the corresponding scripts to become a new database table (cf. Figure 2). An existing dataset can also be removed.
- Display the attributes of the dataset, and select the ones desired for proximity as well as diversity (cf. Figure 3).
- View the graphs displaying the outcome of the clustering algorithm.

For the sake of the visual appeal of the UI, we set up and styled the wireframe, and the corresponding `Django` forms and `JS`-controlled forms. The UI was built with three main parts in mind: a data view/selection part; a distance function selection and an attributes weight section; and the visualization of the clustering outcome – corresponding to the main functionalities. We provide a more detailed description of the UI parts in Section 3.

We close this section with a remark that one of our aims during the design of the CSD-CMAD system was to enable easy extensions in terms of augmenting its functionality with other clustering algorithms – which was part of the reason for selecting `PyClustering`. Also, we note that the code of our implementation is publicly available at https://github.com/sdmay21-31.

[2] https://www.POSYDON.org

[3] For more detailed discussion, including design-decisions, technology consideration, testing (user/integration/acceptance) etc. – please see the publicly available report at https://sdmay21-31.sd.ece.iastate.edu/docs/DesignDocumentFinal.pdf

2.2 Distance Functions

Since at the core of every clustering algorithm is a calculation of a *distance function*, and we are attempting at providing clustering capabilities for data with (multiple) heterogeneous attributes, we applied the following pre-processing steps.

1. For each attribute a_j in the database, we detected the maximal (a_j^{max}) and minimal (a_j^{min}) values across the entire dataset of stars (at corresponding time instant).
2. For an attribute a_j corresponding to a particular star S_i, we relativized its value $S_i.a$ by scaling it with respect to a_j^{max} and a_j^{min}, obtaining $S_i'.a_j = (S_i.a_j - a_j^{min})/(a_j^{max} - a_j^{min})$.
3. In addition to the numerical scaling (which generates values in the range [0,1]), the ratio also eliminated the different physical dimensions and therefore we can now proceed with using the traditional Euclidean-based calculation of the distances between two points (i.e., stars). Assuming a total of n attributes, the distance between two stars S_i and S_k becomes a numerical quantity:

$$dist(S_i, S_k) = \sqrt{\sum_{j=1}^{n} (S_i'.a_j - S_k'.a_j)^2}$$

If more weight is desired for a particular attribute a_m (i.e., increase the impact of a_m on the clustering result), the user is allowed to select a desired weight value w_m. In the current implementation of CSD-CMAD , the values are integers. However, in terms of above equation for distances, the implication is that its reciprocal is used to multiply the respective attribute (i.e., $(1/w_m) \times (S_i'.a_j - S_k'.a_j)^2$) when calculating the sum. This has the effect to to decrease the impact on the distance for the chosen attribute – i.e., to "bring" the objects closer in the dimension of that particular attributes. The selection of values for w_m's is part of the UI.

Now, to incorporate diversity with respect to a desired attribute a_d, in CSD-CMAD we take the following approach:

1. We let the user select a percentage portion (i.e., a value between 0 and 1) α.
2. If the difference $|S_i.a_d - S_k.a_d|$ is smaller then $\alpha \times (a_d^{max} - a_d^{min})$, we set the value of that difference to a large constant (e.g., 100). That way, since all the other addends in the sum in the equation for $dist(S_j, S_k)$ are ≤ 1, the pair (S_j, S_k) is guaranteed to have a large enough value of $dist(S_j, S_k)$ so that it is not considered close enough for the respective clustering algorithm.

3 DEMONSTRATION SCENARIO

We now present the details of the demonstration scenarios that the attendees can experience, essentially providing a step-by-step illustration of the functionalities of CSD-CMAD .

We note that in addition to the publicly available source code of the implementation of CSD-CMAD , we also have a video illustrating the functionalities, publicly available at:
https://sdmay21-31.sd.ece.iastate.edu/med/demo.mp4.

1. **Opening Menu** As shown in Figure 2, the landing page offers the option to add a new dataset, or use one of the existing ones (or even edit it). In addition, the opening menu has the option to provide the "User Manual" type of help, as well as administrative privileges (e.g., add a new user) – provided the user currently logged on is a designated administrator. We will show how to create a new dataset.

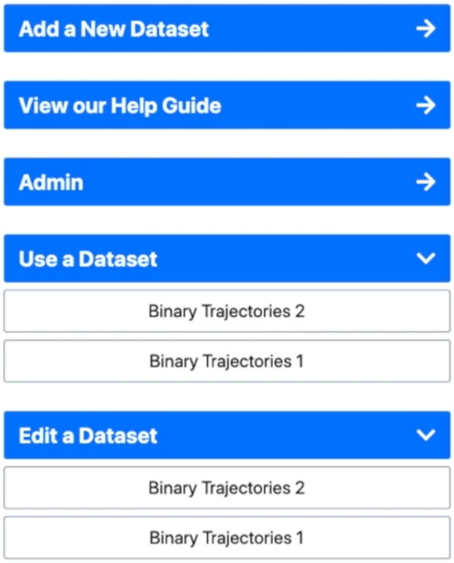
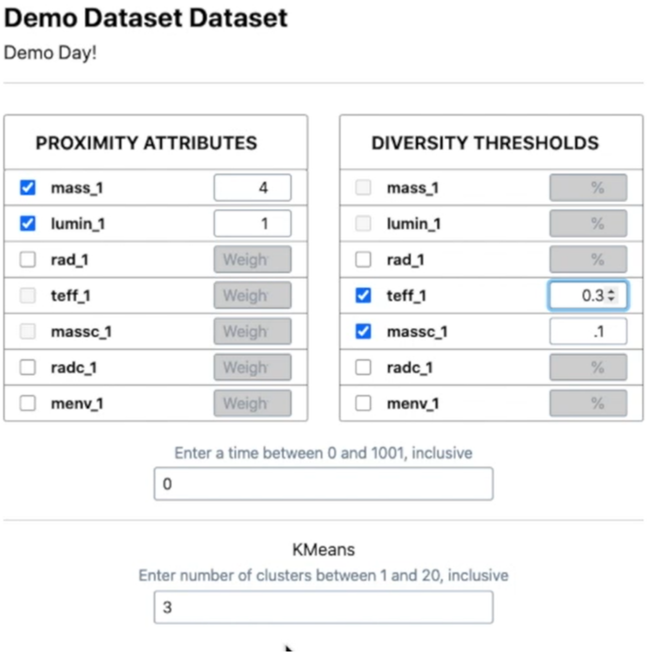


Figure 2: Opening menu of CSD-CMAD



Demo Dataset Dataset

Demo Day!

PROXIMITY ATTRIBUTES	
☑ mass_1	4
☑ lumin_1	1
□ rad_1	Weigh
□ teff_1	Weigh
□ massc_1	Weigh
□ radc_1	Weigh
□ menv_1	Weigh

DIVERSITY THRESHOLDS	
□ mass_1	%
□ lumin_1	%
□ rad_1	%
☑ teff_1	0.3
☑ massc_1	.1
□ radc_1	%
□ menv_1	%

Enter a time between 0 and 1001, inclusive

0

KMeans

Enter number of clusters between 1 and 20, inclusive

3

Figure 3: Weights Selection

2. **Attributes Selection** Subsequently (i.e., after selecting an existing one, or creating a new dataset), the user will be able to select (via check-box) the attributes that should be considered for the chosen clustering algorithm (at this version, CSD-CMAD only has K-means and DBSCAN).

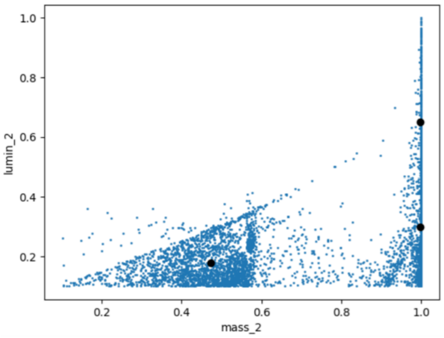


Figure 4: 2D Visualization of Clustering

(3) **Weights Selection** Once the attributes to participate in the calculation of distance have been selected, as shown in Figure 3, the user can (cf. Section 2.2):
   - Select the values for the weight for the attributes that should have heavier impact.
   - Select the threshold for exclusion of a particular pair from clustering, on the grounds of not being diverse enough in the values of selected attribute(s).

(4) **Visualization** The user is expected to provide a time instant (from the interval of the evolution of the stars) and, upon clicking the "*Process*" button, CSD-CMAD will start the execution of the processing algorithm. When the algorithm is completed, the 2D or 3D graph will be displayed, showing the clusters (and their centroids), as illustrated in Figures 4 and 5.

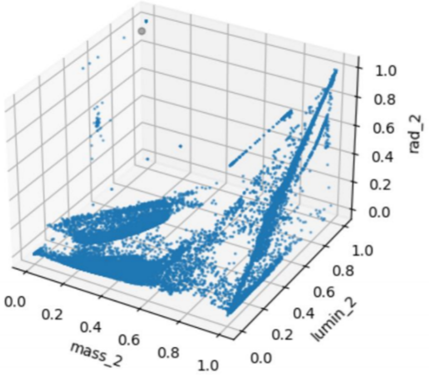


Figure 5: 3D Visualization of Clustering

Duration: We expect that completing a run of the scenario in an interactive demonstration of the features of CSD-CMAD should be completed within 4 ~ 5 minutes, with additional 2 minutes to illustrate the help/user manual aspects, as well as the administrative features of the main menu.

4 CONCLUSION AND FUTURE WORK

We presented CSD-CMAD , a system for context-aware clustering of multivariate astrophysics data of stellar evolution tracks. The heterogeneity of the data stems from the fact that the attributes correspond to different physical phenomena. The context awareness comes into play because we allow to select: (1) *favorite* attributes – i.e., the ones for which the proximity should have greater impact (compared to the rest of the attributes); and *diversity* attributes – i.e., the ones for which it is of interest that the pair of stars has a distance larger than a certain threshold. As mentioned, the code for implementing CSD-CMAD and extended documentation are publicly available.

There are several extensions to CSD-CMAD that we plan to address in our future work. Firstly, we plan to incorporate additional clustering algorithms and provide a context-aware quality assessment (i.e., which algorithms are better suited for which subsets of attributes). We would also like to add a "spatio"-temporal aspect – i.e., consider the coupling of similarity and diversity over the entire trajectory of stellar evolution[9]. From a broader perspective, we will also work on developing an implementation of CSD-CMAD in distributed environments, that will cater to even larger datasets.

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