Enhancing ML Models for Solar Weather Forecasting using Clustering and Adversarial Anomaly Detection

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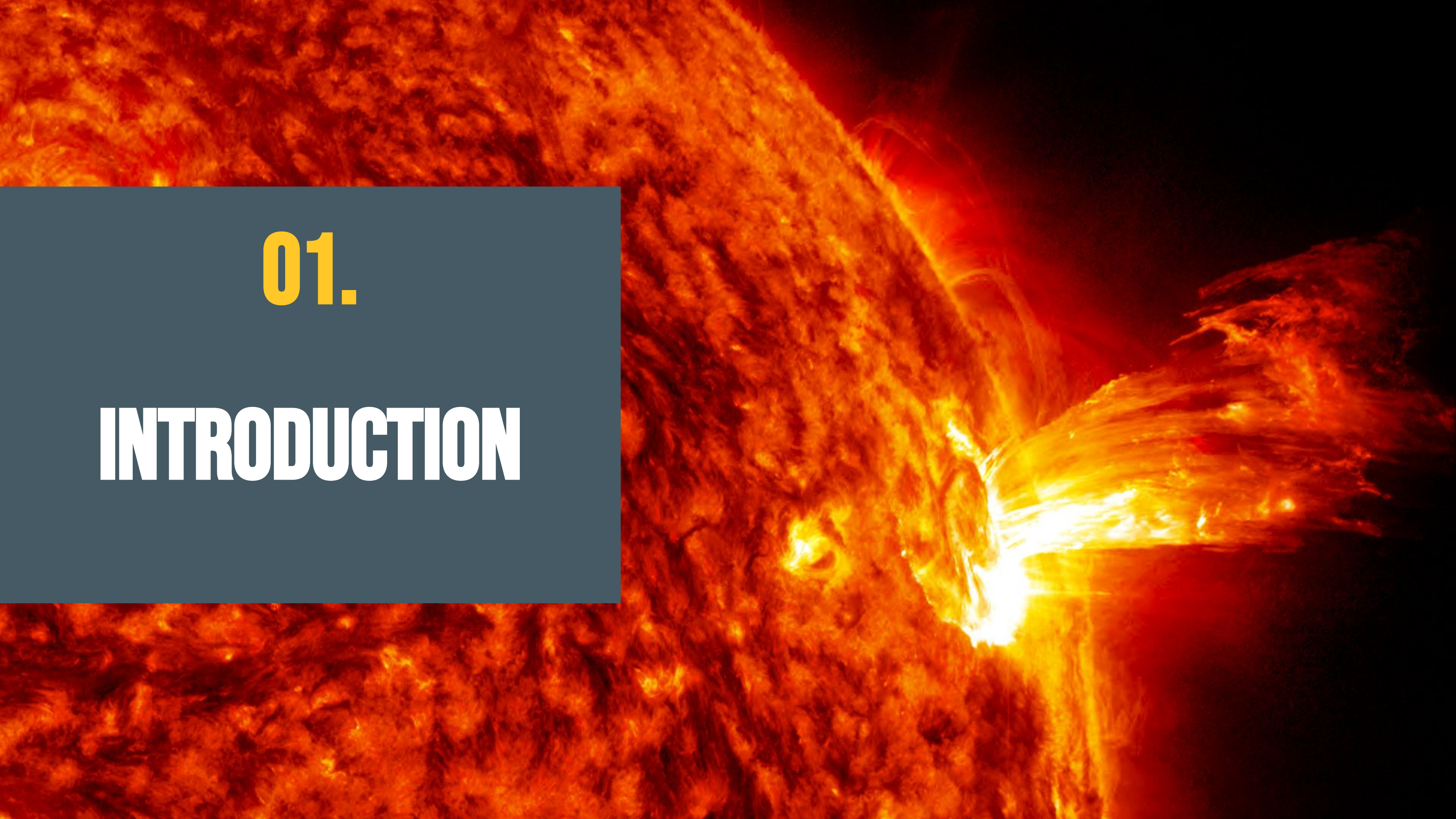


01.

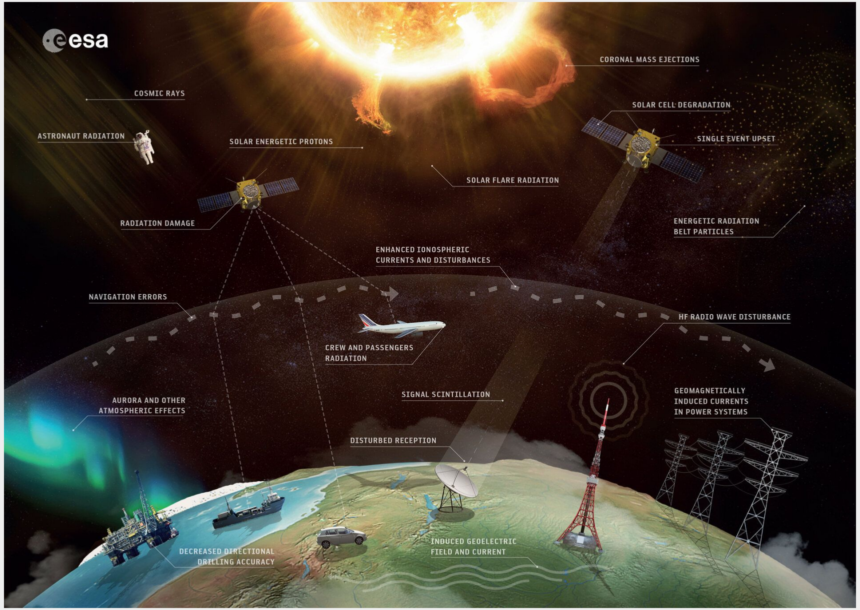
INTRODUCTION

CONTEXT - SOLAR WIND

- **Space Weather Science** is a field of research that aims to understand and predict solar phenomena

- An example of these is the **solar wind**

- **Coronal Mass Ejections** (CMEs) are known to affect:
  - Electrical Grids
  - Geolocation Systems
  - Radio-Communication Systems
  - Spacecraft and human in orbit



Space Weather Effects

Taken from: https://www.esa.int/ESA_Multimedia/Images/2018/01/Space_weather_effects

MOTIVATION

- Most solar phenomena are still not fully understood
  - Prediction remains difficult
- **Magnetohydrodynamic** (MHD) simulators have been developed to extrapolate the conditions that lead to these events
- An example of this is **MULTI-VP** [1]
  - Simulates the 3D structures of solar wind
  - Calculates many 1D solar wind solutions from flux-tube geometries and heating functions

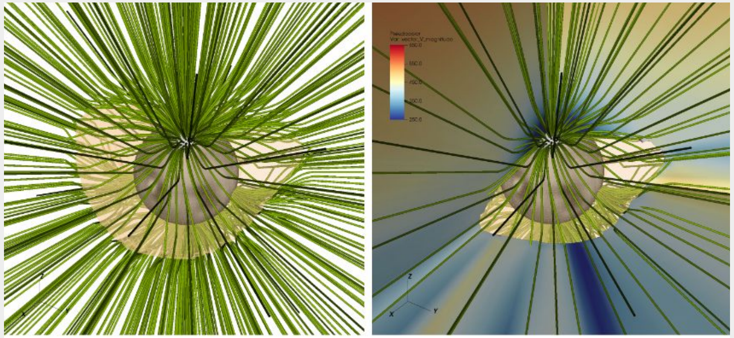
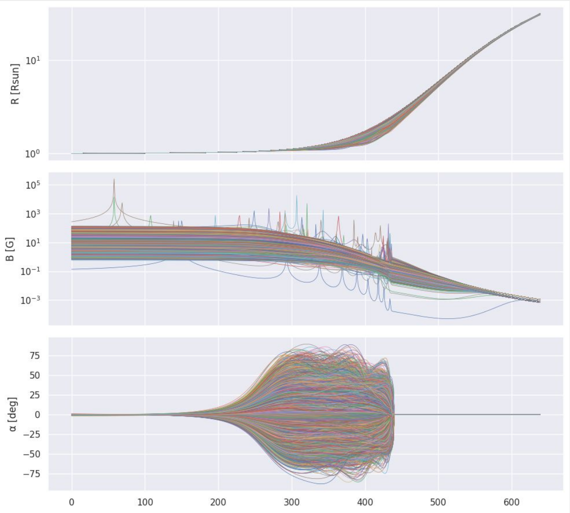


Illustration of the operation of MULTI-VP
Taken from: Rui F. Pinto and Alexis P. Rouillard [1]

MAGNETOGRAM DATA AND PREDICTIONS

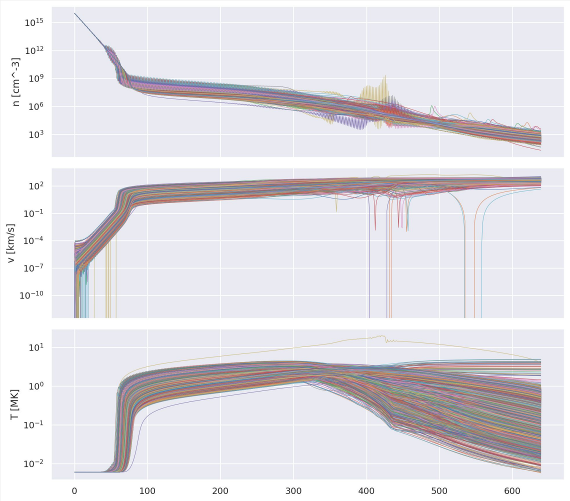
Input (Partial Flows):

- **R[Rsun]** - radial coordinate radius
- **B[G]** - magnetic field
- **α[degree]** - flux tube inclination

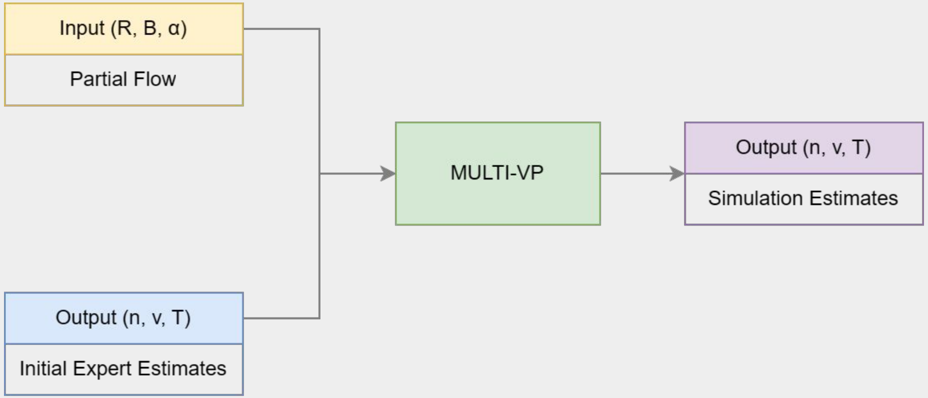


Outputs (Predicted Flows):

- **n[cm^{-3}]** - number of protons per unit volume
- **v[km/s]** - speed-oriented through the line
- **T[MK]** - temperature at a point in space



INITIAL APPROACH: MULTI-VP



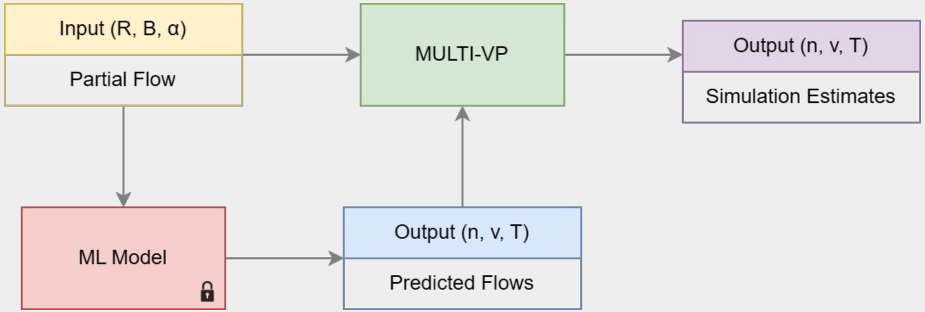
MULTI-VP Methodology

- MHD that simulates 3D structures of the solar wind
- Takes magnetogram data as input
- Predicts solar wind flows based on the initial partial flows and expert estimates

Problems:

- Takes a long time to converge
- Requires expert initial guesses

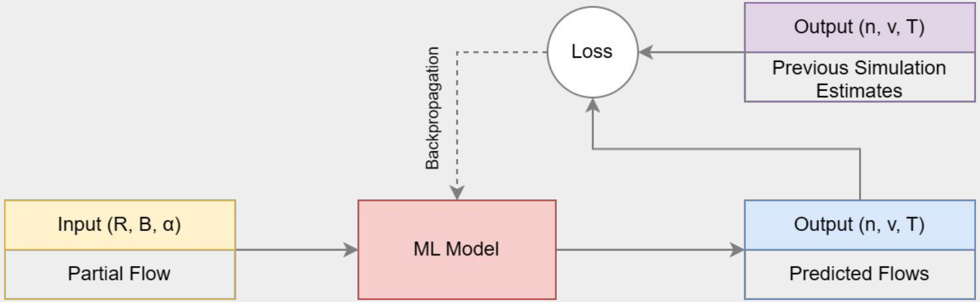
BASELINE APPROACH: ML FOR INITIAL CONDITION ESTIMATION



ML for Initial Condition Estimation Methodology

- Introduces ML model to predict initial flows from partial flows
  - These are passed to MULTI-VP
- Estimations don’t need to be made by hand
- Known to reduce the total simulation time of MULTI-VP

BASELINE APPROACH: ML FOR INITIAL CONDITION ESTIMATION



Training Phase of the ML model

Training:

- Model takes initial flows and produces estimations
- The predictions are compared with initial simulation results from MULTI-VP
- Parameters are updated based on the calculated Loss

Evaluation:

- Comparing MULTI-VP's execution time
- MSE between real estimations and predicted ones

Problem:

- Doesn't capture periphery values
- Sensitive to anomalies in the training dataset

03.

RESEARCH STATEMENT

HYPOTHESIS

"By integrating clustering and adversarial anomaly detection techniques, the initial conditions predicted by RNNs for the MULTI-VP simulator will be closer to the final simulation results and contribute to faster executions."

RESEARCH QUESTIONS

RQ1 - Are clustering methods capable of detecting characteristics in the dataset that were overlooked by the original RNN and would help with the prediction task?

RQ2 - Do the estimates obtained with clustering-based training significantly improve the simulation's performance?

RQ3 - Can adversarial learning methods detect anomalies in solar wind profiles?

RQ4 - Does the resulting dataset significantly improve the predictive ability of the RNN?

RQ5 - Does the improved predictive ability of the RNN result in a reduction of execution time for MULTI-VP?

03.

CLUSTERING

STATE-OF-THE-ART

Focus: Clustering techniques to enhance ML models
Platforms: Scopus, Google Scholar

Paper	Year	Type	Topic	Dimensionality Reduction
JAIN[3]	2010	Survey	KMeans Analysis	No
FAHAD EA.[4]	2014	Survey	Large Data Clustering	Yes
FAHIMAN EA.[5]	2017	Primary	Improving ML	No

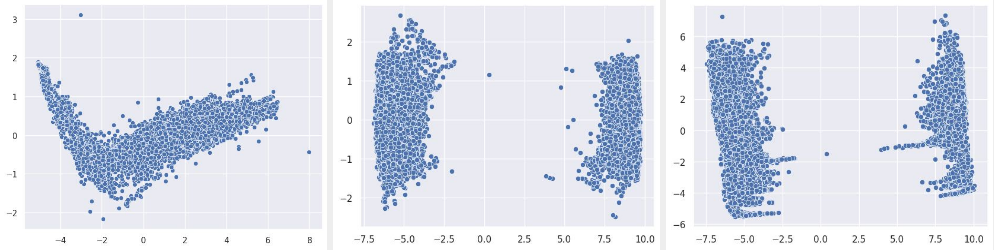
EXPERIMENTS

Methods:
- TimeSeriesKMeans
- SOM
- KMeans
- AgglomerativeClustering
- DBSCAN

Validity:
- Elbow Test (KMeans)
- Silhouette Score
- Calinski-Harabasz Index
- Davies-Bouldin Index

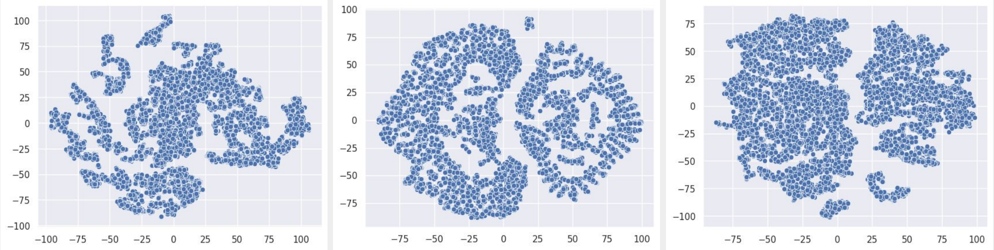
ML Evaluation:
- Train a model for each cluster
- Measure Predictions' MSE

Principal Component Analysis



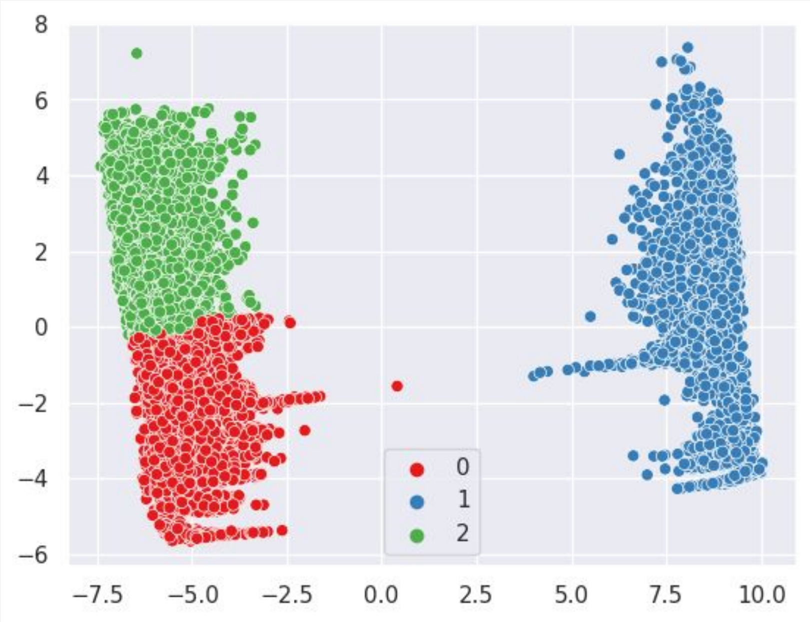
B [G] | α [degree] | Joint Inputs

t-distributed Stochastic Neighbor Embedding



B [G] | α [degree] | Joint Inputs

EXPERIMENTAL RESULTS



KMeans of the PCA of the joint input variables

Selection Criteria:

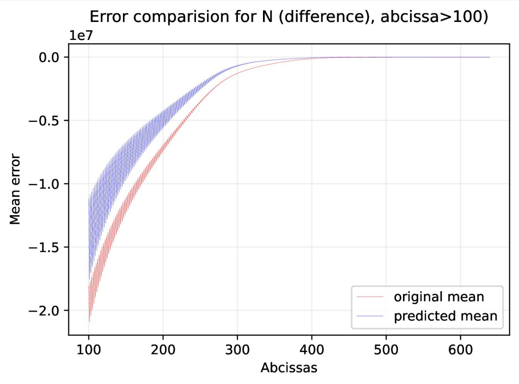
- Predictions' MSE (after model training with clustering approach)
- Validity metrics
- Cluster Distribution

Chosen methodology:

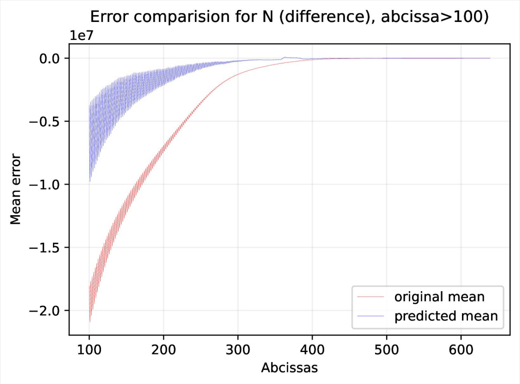
1. Apply **PCA** on the **joint input** variables
2. **KMeans** clustering of the representation
3. Train prediction model for each cluster
4. Generate **validation predictions** and use them as **initial conditions** to MULTI-VP

MULTI-VP EVALUATION: N [CM^{-3}]

Baseline Results



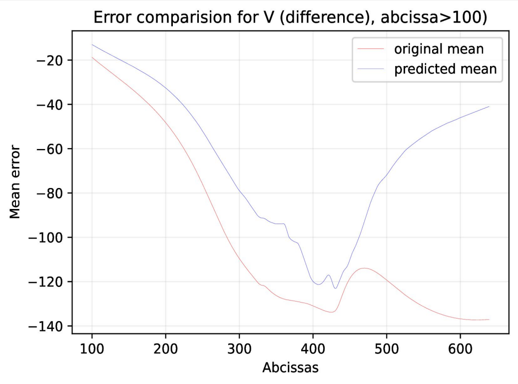
Clustering RNN Results



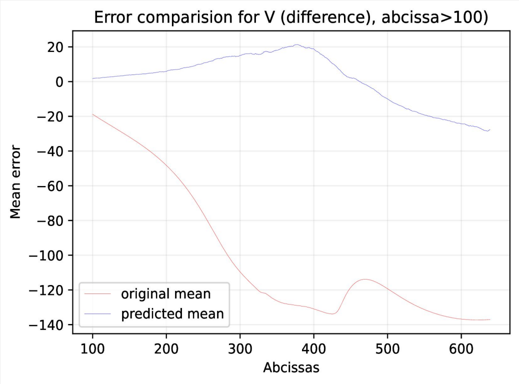
- MSE between the initial conditions and simulation outputs for the *n [cm^{-3}]* variable
- Significant reduction in the distance between initial conditions and final outputs in the clustering approach

MULTI-VP EVALUATION: V [KM/S]

Baseline Results



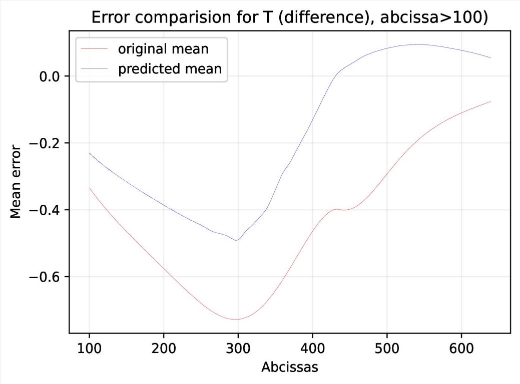
Clustering RNN Results



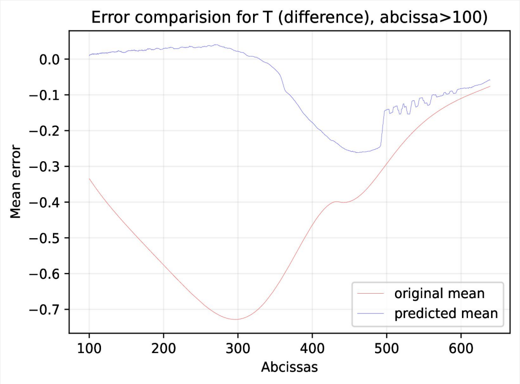
- MSE between the initial conditions and simulation outputs for the *v [Km/s]* variable
- Significant reduction in the distance between initial conditions and final outputs in the clustering approach

MULTI-VP EVALUATION: T [MK]

Baseline Results



Clustering RNN Results



- MSE between the initial conditions and simulation outputs for the *T [MK]* variable
- Significant reduction in the distance between initial conditions and final outputs in the clustering approach

MULTI-VP EVALUATION: MEAN SPEED-UP

1.06 → 1.05

Baseline — Clustering Models

03.

ADVERSARIAL ANOMALY DETECTION

STATE-OF-THE-ART

Focus: Adversarial anomaly detection in tabular data
Platform: Scopus

Paper	Year	Training Method	Anomaly Detection	Architecture	Application
MAD-GAN[6]	2019	Normal	Reconstruction and D Loss	Vanilla	Time Series
TANO-GAN[7]	2020	Normal	Reconstruction	Vanilla	N/A
FGAN[8]	2019	Normal and Division Boundary	Adapted G and D Loss	Vanilla	Time Series

EXPERIMENTS

Architectures:

- Linear GAN
- MAD-GAN (adapted from [4])
- Adversarial AE

Anomaly Scores (AS):

- Discriminator Score
- MSE Reconstruction (Generator)
- MSE-Discriminator Reconstruction (Generator and Discriminator)

General Approach:

1. Learn the normal distribution of the data in the training phase
2. Use either/both generator and discriminator to determine anomaly score for each profile
3. Filter profiles with anomaly scores above a predefined threshold (hyperparameter)

(Each architecture was designed and optimized around the input variables and later applied to the output variables from MULTI-VP)

EXPERIMENTS: ARCHITECTURE SELECTION

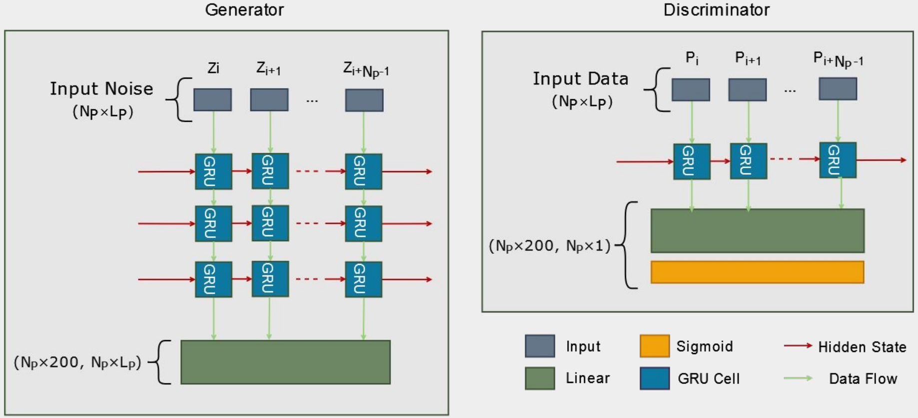
- Select best AS for each architecture (based on visual inspection of the datasets after filtering)
- Compare architecture+AS performances and select best

		Inputs		Outputs	
Architecture	**Function**	**Thresh (%)**	**#Profiles**	**Thresh (%)**	**#Profiles**
LINEAR GAN	Rerr	10	1177	10	1177
MAD-GAN	**Rerr**	**3**	**352**	**3**	**352**
AAE	RDerr	10	1177	10	1177

Anomalies for each of the architecture+AS combination

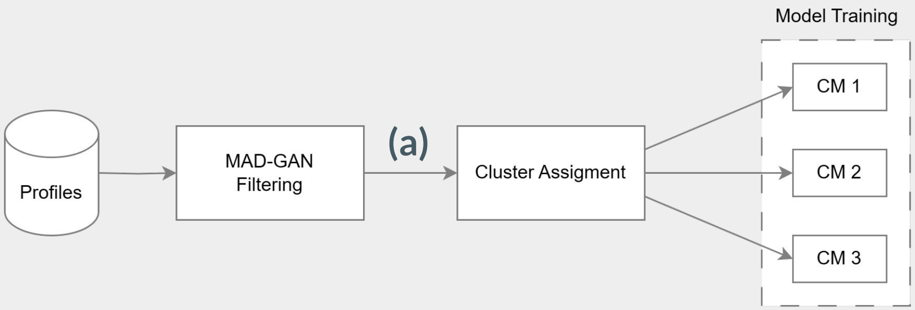
MAD-GAN

- Takes dataset windows of consecutive observations
- Determines anomaly score based on the abnormality of samples within the window and the entire dataset
- Adapted to accept consecutive profiles instead of time-series:
  - Dimensionality reduction of the data features
  - Anomaly detection in the magnetic field for the input model
  - Anomaly detection in all the output variables for the output model



MAD-GAN Architecture

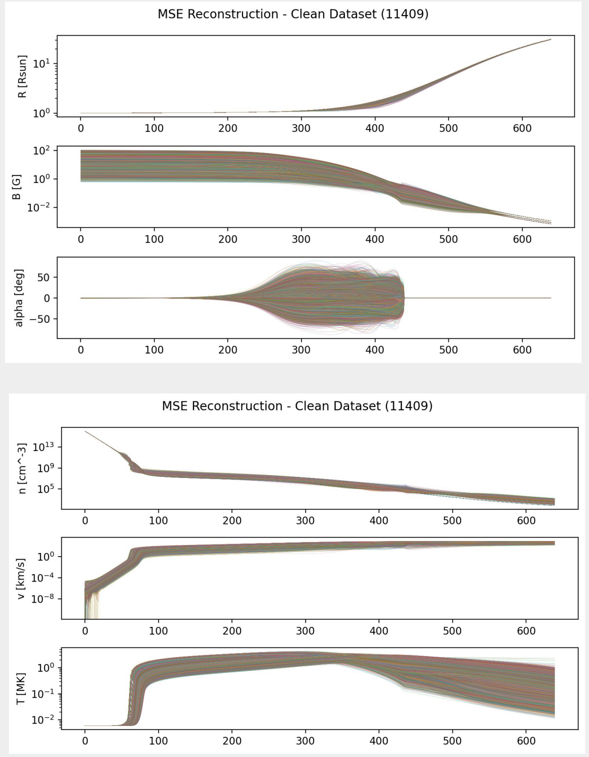
MULTI-VP EXPERIMENTS - SETUP



Anomaly Detection Clustering Dataflow

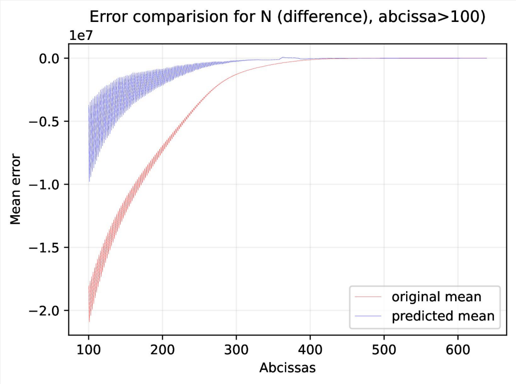
1. Detect and filter profiles with **anomalous input** or **output variables**
2. Separate the dataset into clusters
3. Retrain the clustering models from the previous experiments with the new datasets
4. Generate **validation predictions** and use them as **initial conditions to MULTI-VP**

(a) Filtered Dataset

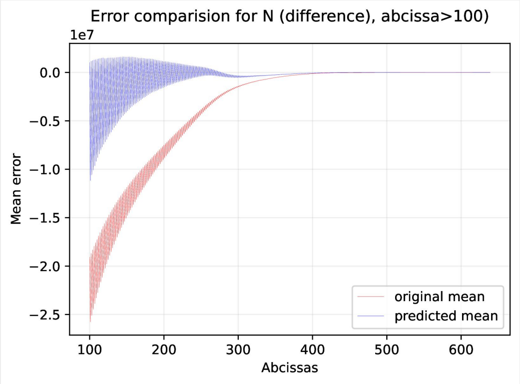


MULTI-VP EVALUATION: N [CM^{-3}]

Clustering Models' Results



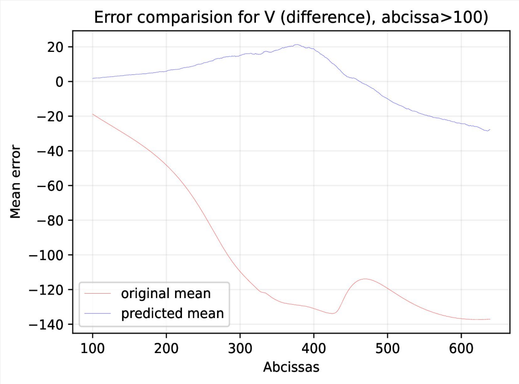
Anomaly+Clustering Models' Results



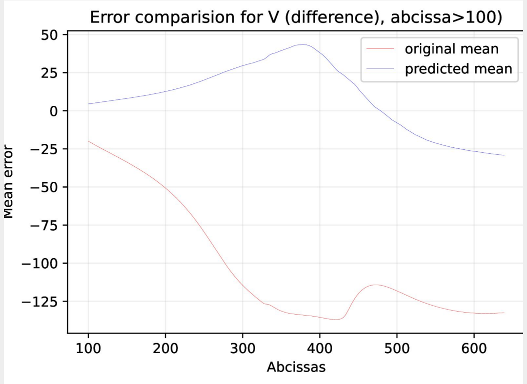
- MSE between the initial conditions and simulation outputs for the *n* [cm^{-3}] variable
- Slight improvement in some of the initial abscissas when compared to the method without anomaly detection

MULTI-VP EVALUATION: V [KM/S]

Clustering Models' Results



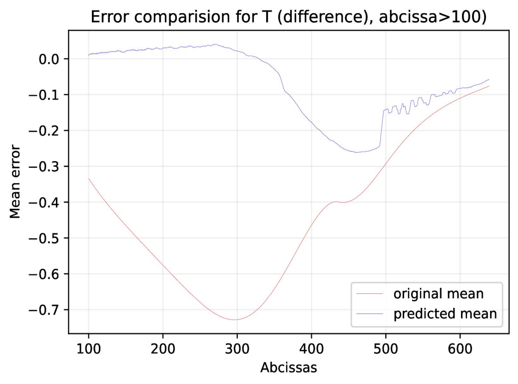
Anomaly+Clustering Models' Results



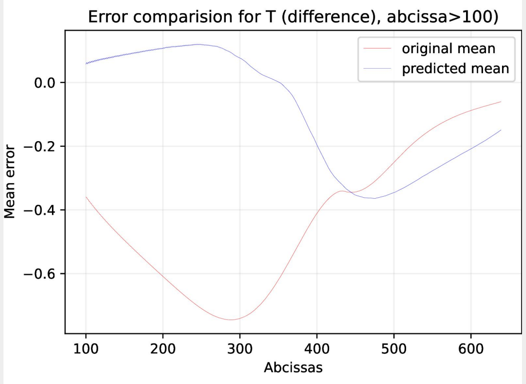
- MSE between the initial conditions and simulation outputs for the *v [Km/s]* variable
- Significant increase in the abscissa distance in comparison with the previous results

MULTI-VP EVALUATION: T [MK]

Clustering Models' Results



Anomaly+Clustering Models' Results



- MSE between the initial conditions and simulation outputs for the *T [MK]* variable
- Worse distance to the simulation predictions when compared to the initial expert estimates and the previous experiments

MULTI-VP EVALUATION: MEAN SPEED-UP

1.06	→	1.05	→	1.06
Baseline		Clustering Models		Anomaly + Clustering Models

RESEARCH QUESTION ANALYSIS I

RQ1 - ***Are clustering methods capable of detecting characteristics in the dataset that were overlooked by the original RNN and would help with the prediction task?*** Yes. We managed to produce closer initial conditions to the final simulation outputs. Dividing the data into clusters of approximately the same size, made it possible for the RNN to capture previously unseen/ignored features.

RQ2 - Do the estimates obtained with clustering-based training significantly improve the simulation's performance? No. The overall computation time didn't improve over the baseline model. A mean speedup of 1.05 was obtained with the clustering method, in contrast to the 1.06 speedup from the baseline.

RESEARCH QUESTION ANALYSIS II

RQ3 - Can adversarial learning methods detect anomalies in solar wind profiles? Yes. Every implemented architecture was able to detect anomalous profiles in the dataset, with MAD-GAN outperforming the others. We managed to produce an apparently cleaner version of the original dataset.

RQ4 - Does the resulting dataset significantly improve the predictive ability of the RNN? No. The removal of anomalous profiles hindered the quality of the predictions from the RNN model. By excluding entire profiles from training, we might have removed important features.

RQ5 - Does the improved predictive ability of the RNN result in a further reduction of execution time for MULTI-VP? Even with worse initial conditions, the simulation took less time to reach a viable solution. This might indicate that the computation time is not directly linked to the proximity of the initial conditions to the simulation outputs.

CONCLUSIONS

- Managed to produce initial conditions closer to simulation outputs
- Didn’t reduce computation time of the simulation

Future Work:

- Explore if the speedup is being well calculated
- Test the physical validity of the estimates
- Surrogate model
- Test on other MHD simulators

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