Leveraging Variational Autoencoders (VAEs) for Classification of Anthropogenic Aerosols

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My project presents a **low-cost, pragmatic, computational platform** that provides an **accurate classification of raw aerosol signals** through deep unsupervised learning, **without ever requiring human intensive data labeling.**

First, a variational autoencoder (VAE) is trained on large pools of unlabeled aerosol signals clustering similar aerosols together. Next, a new, unseen aerosol signal is passed into the trained VAE, which encodes the signal and extracts its most relevant features. Finally, this latent representation is compared to thousands of previously seen signals to construct an aerosol biodata containing key information about it's properties.

This computational platform **successfully builds aerosol biodatas with 94.6% accuracy on unseen aerosol signals.**

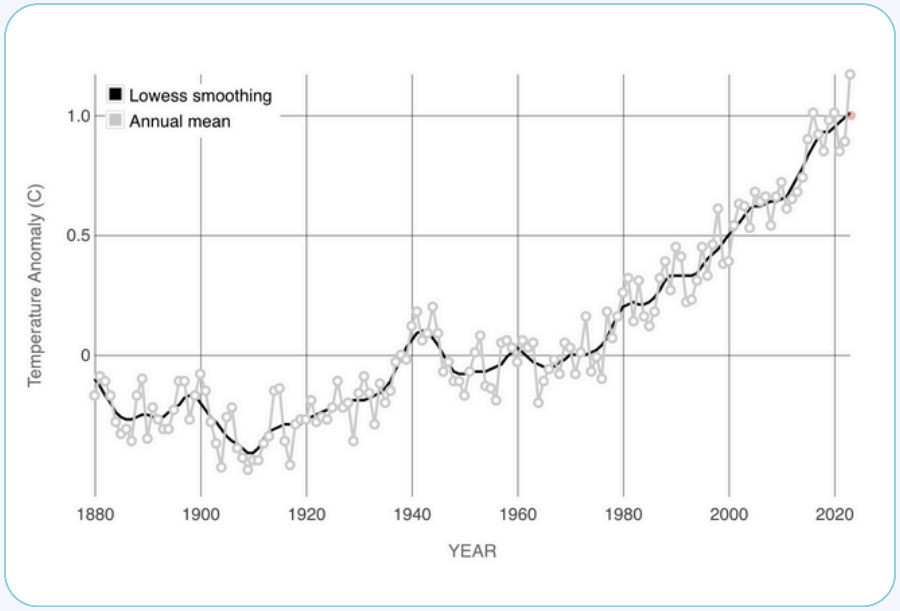
By uncovering key properties like aerosol malignancy, saturation, incandescent intensity, and peak height with high accuracy, **my platform significantly advances aerosol-cloud modeling** which is pivotal for developing effective climate engineering techniques, ultimately **paving the way for more sustainable interventions against global warming.**

Introduction: Project Origin & Key Questions

Project Origin

The Problem: Anthropogenic Global Warming

- Earth's temperatures are the highest since record-keeping began in 1880 [1]
- In the next 20 years, ~250,000 will die from anthropogenic global warming [2]
- Anthropogenic warming will persist for centuries
- **Current climate action is insufficient:** incremental decarbonization efforts will take a long time [3]

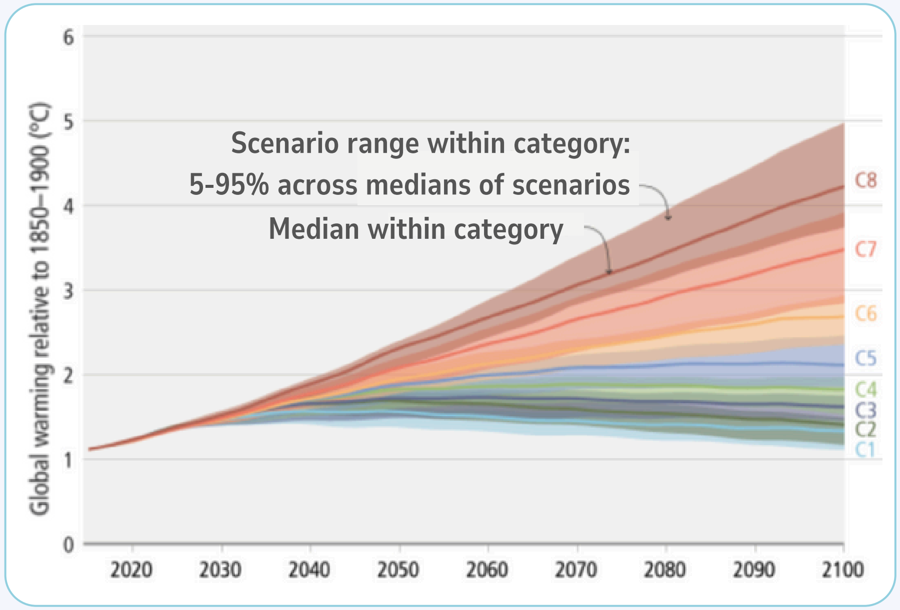


Potential Solution: Stratospheric Aerosol Injection

- The goal of this technique: **inject specifically curated artificial aerosols** into the atmosphere to **offset emissions**

The Gap: Accurate Classification of Raw Aerosol Signals

- Predictable outcomes from target climate engineering techniques **like SAI depend on accurate determination of chemio-physical properties of aerosols** (i.e. their malignance, saturation, height)



Key Questions

- What is involved in determining chemio-physical properties of aerosols?
- What are the **challenges** encountered in **accurate classification of raw aerosol signals**?

1. https://climate.nasa.gov/vital-signs/
2. https://www.who.int/health-climate-change
3. https://www.ipcc.ch/sr15/chapter/spm/

Introduction: Previous Work, Engineering Goal and Hypothesis

Previous Work - Drawbacks

- Use supervised learning which requires **tedious, human intensive labeling** of aerosol data
- Trains algorithms on lab proxies thereby **lacking adaptability for real-time data**
- **Approach not practical in real world** where aerosol data is constantly changing and has to be assessed in time and in place for effective climate intervention
- **Unable to generalize** to **ambient atmospheric aerosols**

Engineering Goal

- Design a **pragmatic**, **effective** & **accurate** aerosol classification system

Hypothesis

Hypothesis 1: Increase Practicality via New Technique
Leverage unsupervised deep learning models that do not require prior, human-intensive, manual, labeling of data sets Enhanced suitability to discern aerosols in real-time in their natural state

Hypothesis 2: Increase Accuracy
Improve the detection accuracy by integrating the output of unsupervised deep learning models with SP2 data Assess the model's ability to generalize to different environmental conditions

Hypothesis 3: Increase Effectiveness
Effective Separation between at least 3 of the Aerosol Classes. Ensure that the average inter-class distance is maximized, indicating clear separation between the three classes.

Methods: Data Collection

Aerosol Dataset

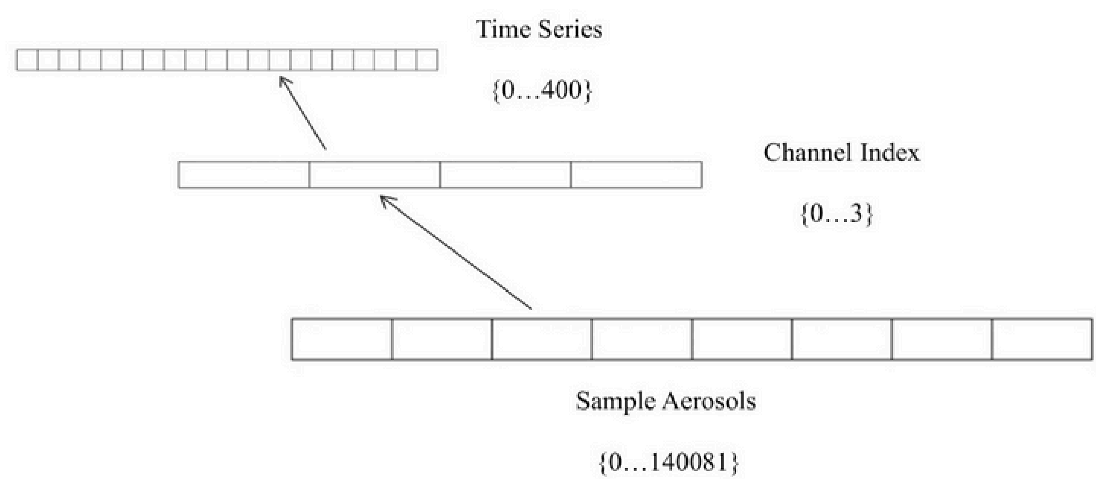
- Dataset composed of aerosols from the following 7 classes that are laboratory proxies for aerosols typically found in the atmosphere.
- The data was structured in the following tuple **(sample particle #, time series, # channels)**. In particular, the number of particles **(p)** was **140081**, the time series **(t)** ranged from **0 < t < 400**, and the number of channels from **(c) 0 < c < 4**.
- Due to the relatively minimal impact of the second and third channels on the vaporization of the aerosol, we focus on the scattering and blue incandescent channel to classify absorbing aerosols.

Data Sample Characteristics

- Each sample initially represented as a raw time series signal. T
- The time (t) demonstrates the incandescence of the aerosol particle over a period of time as the interaction between the laser light and particle ensues.

Material	Abbreviations
Iron (II) Oxide	Fe_3O_4
Iron (III) Oxide	Fe_2O_3
Volcanic Ash	VA
Arizona Test Dust	ATD
Clifty-F Fly Ash	CFA
Fullerene Soot + glycerol	Fs_{glyc}
Fullerene Soot	FS

The Seven Different Aerosol Classes Utilized in this project



A visualization of the dataset structure. 140081 aerosols each of which has 4 channels and a 400 pt time series associated with it: (140081, 400, 4)

Methods: Preprocessing

Preprocessing Techniques

- Explored four different types of preprocessing strategies for the different channels from the SP2 L-II signal time series:

$$X_{train}[:, :, i] = \frac{X_{train}[:, :, i]}{s_0}$$

$$X_{val}[:, :, i] = \frac{X_{val}[:, :, i]}{s_0}$$

$$X_{test}[:, :, i] = \frac{X_{test}[:, :, i]}{s_0}$$

- The first data processing technique attempted was the division by maximum per channel for the training dataset:
  - The process initiates a loop that iterates over each sample's time series and computes the max value of the i-th channel (where $0 < i < 4$ and each i represents a different detector) individually. Within each iteration, the maximum values for the i-th channel are calculated as follows
    - max(X_train[:, :,i])
  - Subsequently, each element in the i-th channel of all datasets is divided by the normalization factor s0

$$X[p_{idx}, :, c_{idx}] = \frac{X[p_{idx}, :, c_{idx}] - min_{c_{idx}}}{max_{c_{idx}} - min_{c_{idx}}}$$

- The second technique was channel normlization by min & max values computed across the training, validation, and test datasets
  - Calculated the global minimum and maximum values for each feature across this concatenated datasets & applied normalization using these values

$$particle\_relative\_scaling[p_{idx}][c_{idx}] = log(train\_max\_heights[p_{idx}][c_{idx}])$$

$$sum[p_{idx}][c_{idx}] = \sum (X_{train}[p_{idx}, :, c_{idx}])$$

$$X_{train}[p_{idx}, :, c_{idx}] = \frac{X_{train}[p_{idx}, :, c_{idx}]}{sum[p_{idx}][c_{idx}]} \; x \; particle\_relative\_scaling[p_{idx}][c_{idx}]$$

- The third technique was relative scaling using logarithmic normalization
  - For each sample, the logarithm of the max height found in the time series per channel is taken (Lamb et. al 2023). The result is stored in a matrix that is later used in the normalization process.

$$channel_{min} = min(X_{train}[p_{idx}, :, c_{idx}])$$

$$channel_{max} = max(X_{train}[p_{idx}, :, c_{idx}])$$

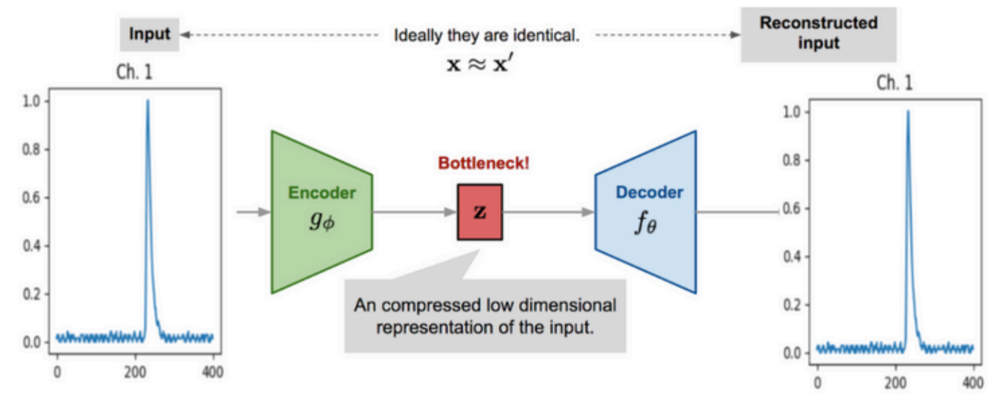
$$X_{train}[p_{idx}, :, c_{idx}] = \frac{X_{train}[p_{idx}, :, c_{idx}] - channel_{min}[p_{idx}][c_{idx}]}{channel_{max}[p_{idx}][c_{idx}] - channel_{min}[p_{idx}][c_{idx}]}$$

- The fourth technique was normalization of data by particle min/max rather than across the dataset
  - Found this data pre-processing technique to be empirically the best and used this for all final results

Methods: Variational Autoencoder Architecture (VAE)

Variational Autoencoder

- A VAE has two main parts that are essential to its structure: the **encoder** and the **decoder**. The encoder part of the network takes an input and encodes it into a latent representation.
- From a **mathematical perspective**, it can then be represented as follows: $q_{\phi}(z|x)$, where the x is the input and z is the latent representation. (Naeem et. al 2023).
- The **encoder outputs parameter to a probability distribution**, typically Gaussian which are the mean **u** and variance **log**(σ^2).Meanwhile the **decoder** takes a point z in the latent space and **aims to reconstruct the input x**.
- The decoder defines a probability distribution over the possible outputs given a latent point. The decoder tries to reconstruct the original input as best as possible -- as a method of assessing how good this latent representation is.
- In the context of this project, the **problem is then how to optimize the mapping from the decoder** $p_{\phi}(x|z)$ **to the latent space z.**



A visualization of the variational autoencoder as it compresses the L-II signals into a bottle neck representation and does a reconstruction to achieve a similar input, thus reducing dimensionality. In the topmost, the input is channel 0, which provides information about the optical size of the particle. The autoencoder reconstructs the input using the decoder. In the bottom image the input is a signal from channel 1, which provides information about the chemio-physical properties of the aerosol. (Figure Adapted from Weng 2018)

Kullbeck-Leibler Divergence Algorithm

- **Optimization Algorithm** for the encoder and decoder framework. D_KL is the Kullback-Leibler divergence and the KL divergence loss ensures that the distribution of latent variables is close to a normal distribution. The total loss accounts for both the reconstruction loss and KL divergence loss.

$$L_{\text{reconstruction}} = -q(z|x)\,[\log p(x|z)]$$

$$L_{\text{KL}} = D_{\text{KL}}(q(z|x)\,||\,p(z))$$

$$D_{\text{KL}}(p(x)\,||\,q(x)) = \int -p(x)\ln\left(\frac{p(x)}{q(x)}\right)dx$$

$$L_{\text{total}} = L_{\text{reconstruction}} + L_{\text{KL}}$$

The training of a VAE involves optimizing the parameters of both the encoder and decoder. The loss function for a VAE is the sum of the reconstruction loss and KL divergence loss.

Methods: End-to-End Architecture

Training Procedure:

Step 1: Raw aerosol signals from the atmosphere are captured using the SP2

Step 2: These raw aerosol signals are fed into a VAE. From these signals, the model learns a robust latent representation based on patterns that make each aerosol unique, clustering similar aerosols together.

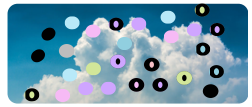
Step 3: Then, a new, unseen signal can be passed into the trained VAE, which encodes the signal into its latent representation. This latent has now learned to extract the most relevant features of the aerosol from this signal

Step 4: This latent representation is compared to thousands of previous data to construct a signal biodata, containing key information about the aerosol's properties based on aerosols with similar latent representations

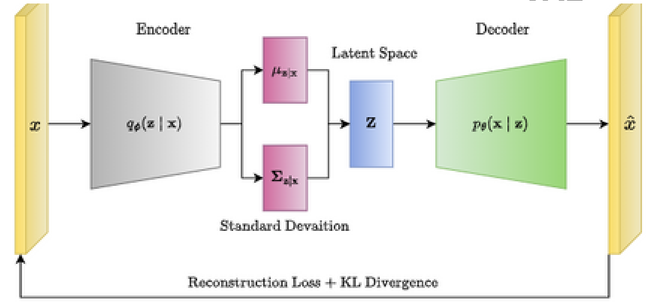
Step 5: This biodata can be used to enable techniques such as stratospheric aerosol injection (SAI) to reduce emissions globally

Steps 3 - 5 can be repeated for new, completely unseen aerosol types, allowing for unprecedented generalizability to new environments.

Atmospheric aerosols

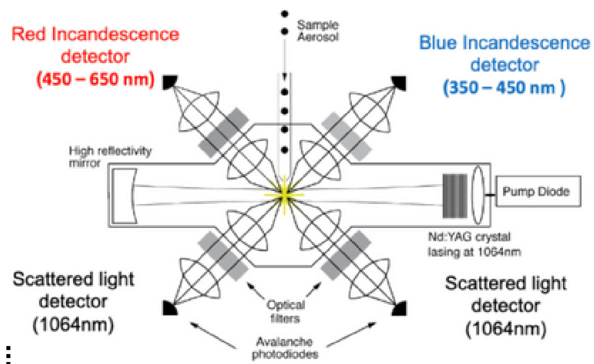


Step 1



Step 3

Single Particle Soot Photometer

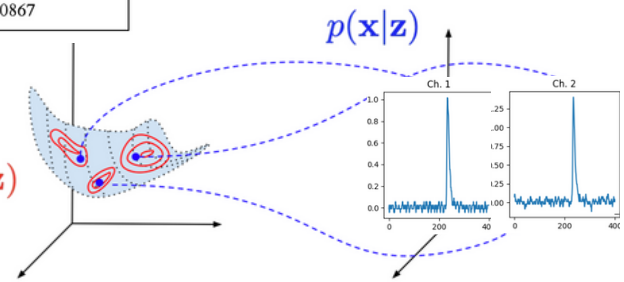


Raw Aerosol Signals

Red Incandescent Detector (Scaled) (nm) (Channel 0)	Blue Incandescent Detector (Scaled) (nm) (Channel 1)	Scattering Light Detector 1 (Scaled) (nm) (Channel 2)	Scattering Light Detector 2 (Scaled) (nm) (Channel 3)
0.2109975	0.0231634	0.012409	2.48937423
0.2089529	0.0082767	0.016545	2.52218092
0.2570632	0.0140635	0.011581	2.51818463
0.0429058	0.1174718	0.172898	0.00384139
0.2741635	0.0132362	0.015718	0.27400867

Step 2

Aerosol Biodata



Step 4 & 5

Results & Discussion (1/2)

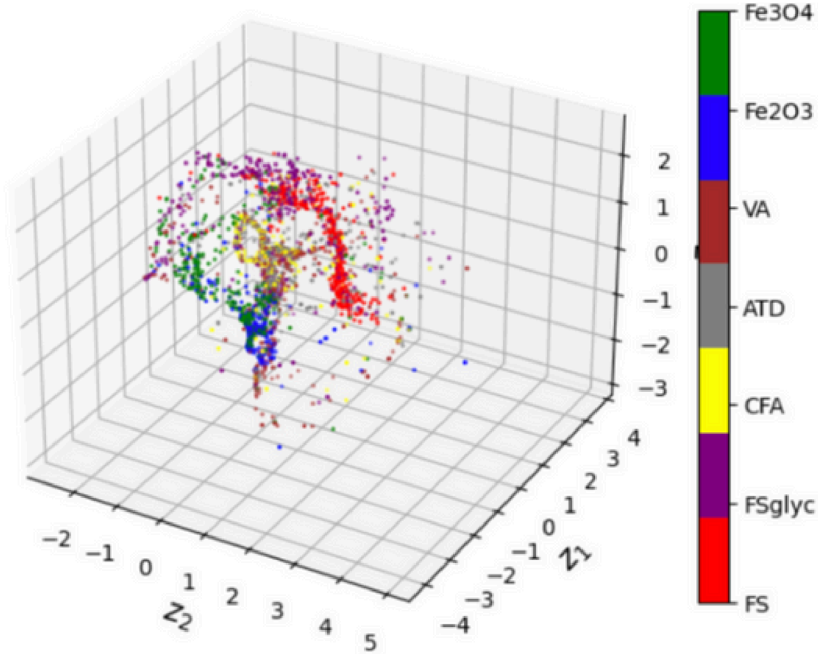


Figure 1a: Channel 0 3D High N_Latent Space Visualization

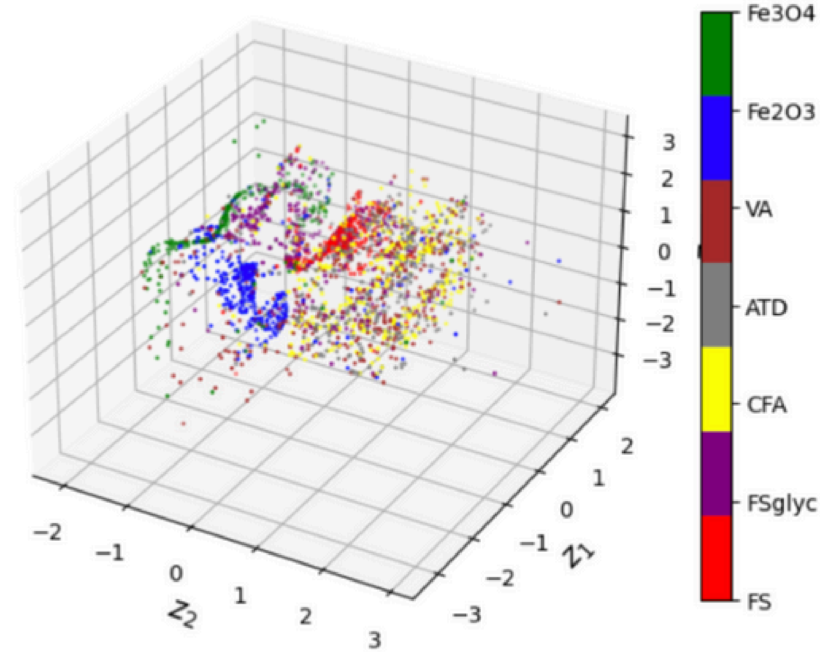


Figure 1b: Channel 1 3D High N_Latent Space Visualization

Figure 1a - Latent Space Dimension = 3, Channel = 0:
The autoencoder **achieves a high separability between aerosol classes** for this latent space and scattering channel. Iron oxide aerosols in particular are grouped together well. Classes such as Fe3O4 and Fe2O3 are easily distinguishable – as is FSglyc and FS.

Figure 1b - Latent Space Dimension = 3, Channel = 1:
Similarly to channel 0, **the clustering is evident for the incandescent channel** as classes such as Fe3O4, Fe2O3, FS, and FSglyc as particles are concentrated in certain sections.

This **demonstrates the success of the latent space in compressing the raw aerosol signals into their distinctive qualities**, overcoming noise in the raw data.

Results & Discussion (2/2)

Figure 2a - Latent Space Dimension 2, Channel = 0:
The **two classes of iron oxide aerosols** Fe3O4 and Fe2O3 **achieve clear separation** despite similar chemical composition.

Figure 2b - Latent Manifold Channel 0 Interpretability:
Saturation of signals shows flatness at peaks that is more common for larger particles like ATD, CFA, and VA. Additionally, particles like Fe2O3 and Fe3O4 have more symmetrical scattering signals like those shown in the first two rows. We also see that more **saturated signals** like iron oxide **have greater incandescent intensity**.

Figure 3a - Latent Space Dimension = 2, Channel = 1:
This time for the blue incandescent channel, the iron oxide aerosols **once again achieve high separability**. A qualitative **analysis for these results highlights that variational autoencoder performed very promisingly** when separating the latent representations.

Figure 3b - Latent Manifold Channel 1 Intepretability:
FS and coated FS have **more skewed incandescent signals** (middle rows) compared to Fe2O3 and Fe3O4 which **have symmetrical signals** (top rows). The skewed representations of signals for particles like FS generally have low saturation.

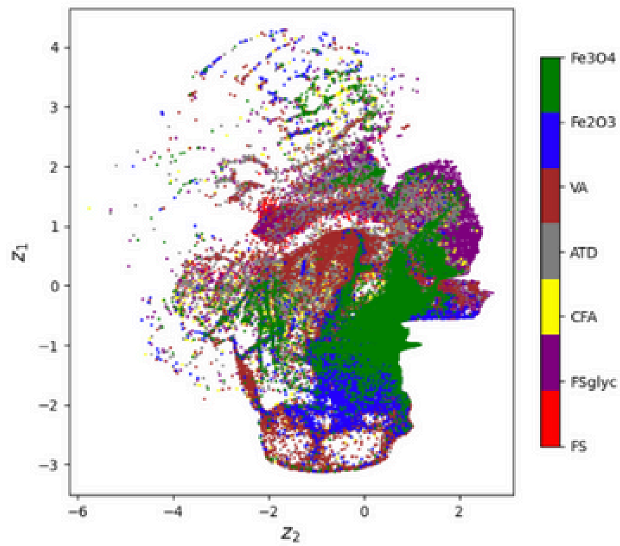


Figure 2a: Channel 0 2D latent Space Visualization Clustering

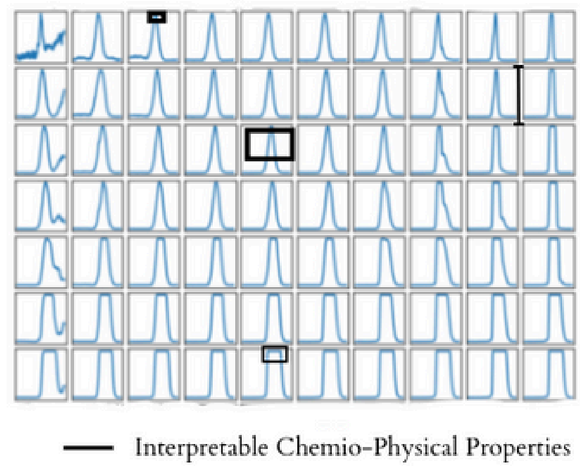


Figure 2b: Latent Manifold Channel 0 Chemio-Physical Properties Insight

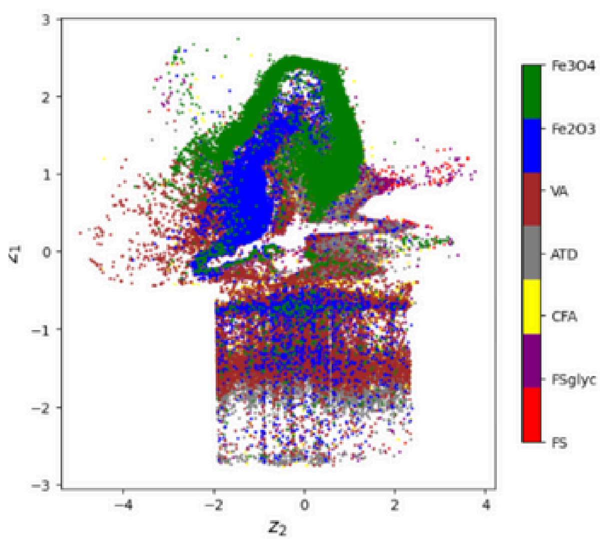


Figure 3a: Channel 1 2D Latent Space Visualization Clustering

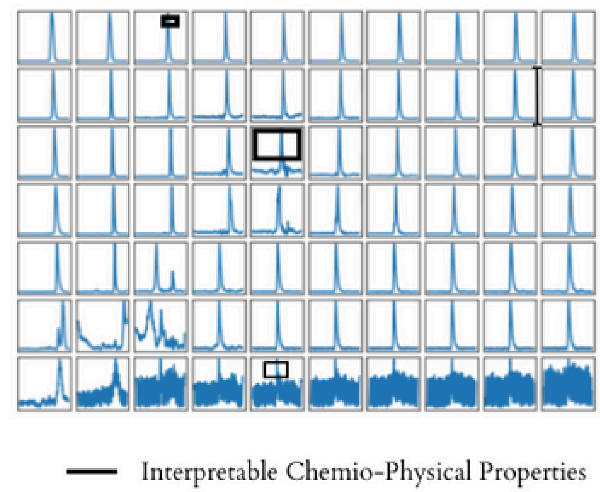


Figure 3b: Latent Manifold Channel 1 Chemio-Physical Properties Insight

Conclusions - Objectives Achieved and Research Impact

All three research objectives achieved

Pragmatic Cost-Effective Foundation for aerosol Classification

- Unsupervised machine learning algorithms used in this research successfully bypass both limitations of current research (tedious data labeling and inability to generalize) by harnessing an unlabelled dataset and classifying data points through pattern matching and identification resulting in a **flexible, pragmatic, cost-effective** foundation, especially for **classification ambient aerosols (which are unseen during training) in real-time**.

Enhanced effectiveness of aerosol classification

- By compressing the input into a bottleneck latent representation, the variational autoencoder creates an intrinsic manifold that capitalizes on the most relevant features for clustering, and illustrates the chemio-physical properties of aerosols with **higher degree of detail** thereby **improving upon the effectiveness of aerosol classification**.

Aerosol classification achieves high degree of accuracy

- The framework yields an **accuracy** of **94.6%** when comparing the results to labeled samples, further highlighting the **effectiveness** of this as an approach to **shed light on the unknown characteristics of aerosols in the atmosphere**

Impact - generalizable, rapid, scalable approach for climate engineering

- **First generalizable method** for rapid aerosol classification including identification of anomalies or harmful variants
- **Facilitates rapid identification** of atmospheric anomalies resulting from new, harmful and anthropogenic aerosols.
- **Enables dramatic increase** in new training samples by using cluster-based label propagation without needing any complex instrumentation to collect it thereby overcoming the inherent imitations of supervised learning and offering a scalable and efficient pathway to gain critical insights into the emission contributing atmospheric aerosols.
- **Amplifies benefits from climate engineering efforts** (SRM, SAI) to tailor their cooling aerosols using the detected chemio-physical properties thereby their **increasing effectiveness and minimizing unintended consequences**.

Conclusions - Further Work

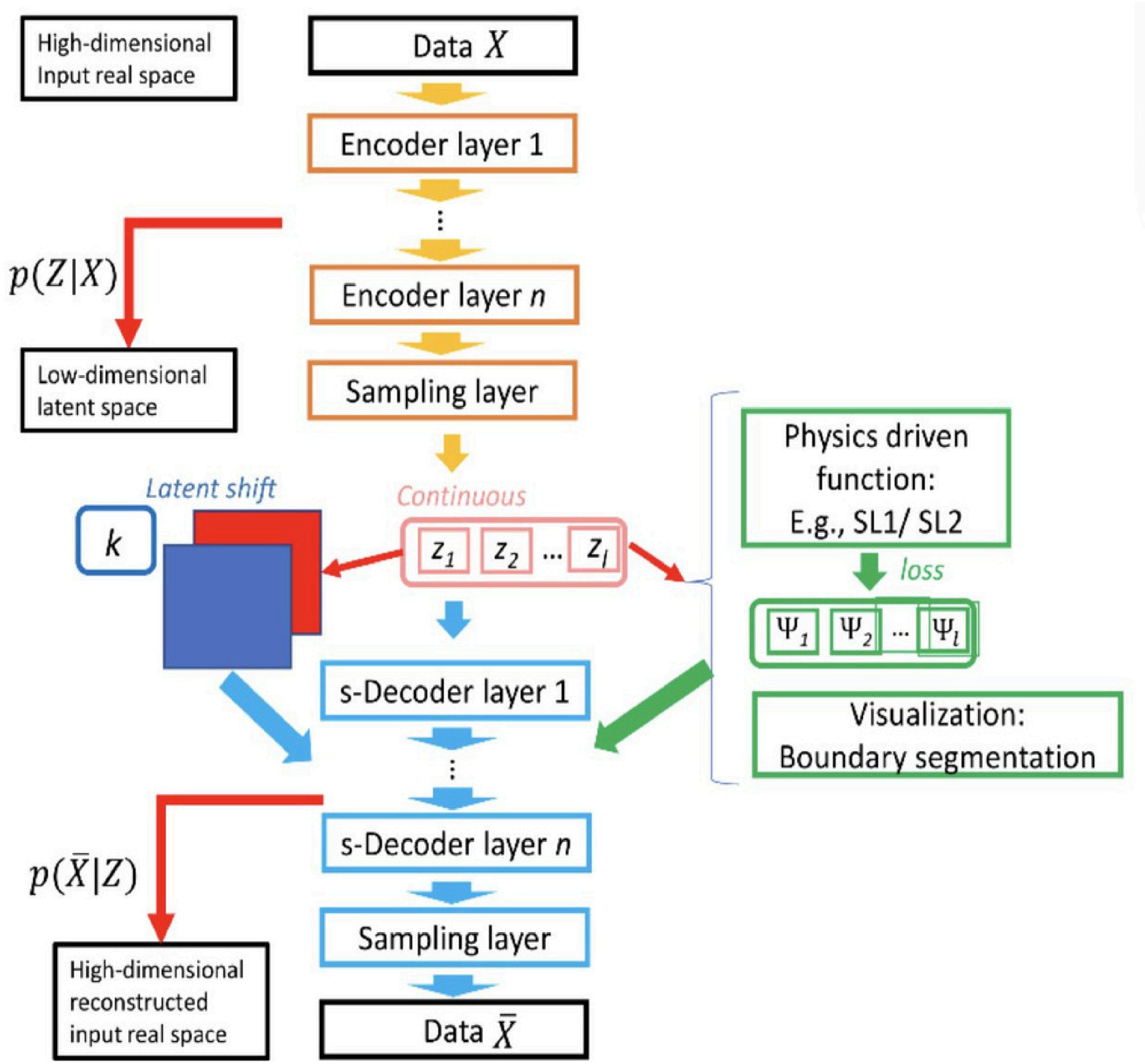


Figure 8: Shift Variance Autoencoder model (Ziatdinov et. al 2021)

- **Enhance the foundation to leverage a shift-invariance model** to more robustly in handle positional and random variations in signal locations from the SP2 (Single Particle Soot Photometer).
- **Integrate our approach with SRM and SAI techniques** to significantly enhance the accuracy and effectiveness of climate-engineering to combat anthropogenic warming
- Leverage this approach to **generate new, larger aerosol data samples** without complex instrumentation that can feed into climate-models. resulting in **significant enhanced predication, accuracy, and projection of climate-change**

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