Capturing the diversity of mesoscale trade wind cumuli using complementary approaches from self-supervised deep learning

Dwaipayan Chatterjee¹, Sabrina Schnitt², Paula Bigalke¹, Claudia Acquistapace², and Susanne Crewell¹

¹Institute for Geophysics and Meteorology, University of Cologne
²University of Cologne

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Abstract

At the mesoscale, trade wind clouds organize with a wide variety of spatial arrangements, which influences their effect on Earth’s energy budget. Past studies used high-resolution satellite measurements and clustering/labeling techniques to classify trade wind clouds into distinct classes. However, these methods only capture a part of the observed organization variability. This work proposes an integrated framework using a continuous followed by discrete self-supervised deep learning approach based on cloud optical depth from geostationary satellite measurements. The neural network learns the semantics of cloud system structure and distribution, verified through visualizations of different layers. Our analysis compares classes defined by human labels with machine-identified classes, aiming to address the uncertainties and limitations of both approaches. Additionally, we illustrate a case study of sugar-to-flower transitions, a novel aspect not covered by existing methods.
Capturing the diversity of mesoscale trade wind cumuli using complementary approaches from self-supervised deep learning

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Key Points:
- Mesoscale cloud organization can be taxonomized by a two-step deep learning approach in the feature space continuum
- Comparison with human-annotated labels reveals the need to include uncertainty estimates of the human-derived classification
- Our approach can describe the temporal transition from human-labeled sugar to flower regimes

Corresponding author: Dwaipayan Chatterjee, dchatter@uni-koeln.de
Abstract
At the mesoscale, trade wind clouds organize with a wide variety of spatial arrangements, which influences their effect on Earth’s energy budget. Past studies used high-resolution satellite measurements and clustering/labeling techniques to classify trade wind clouds into distinct classes. However, these methods only capture a part of the observed organization variability. This work proposes an integrated framework using a continuous followed by discrete self-supervised deep learning approach based on cloud optical depth from geostationary satellite measurements. The neural network learns the semantics of cloud system structure and distribution, verified through visualizations of different layers. Our analysis compares classes defined by human labels with machine-identified classes, aiming to address the uncertainties and limitations of both approaches. Additionally, we illustrate a case study of sugar-to-flower transitions, a novel aspect not covered by existing methods.

Plain Language Summary
Clouds are a fundamental player affecting our planet’s energy balance, making their accurate representation crucial in climate models. One open question is how they organize on a scale of a few 100 km (mesoscale) within the trade wind region. Satellite observations can help to categorize these clouds, but previous methods had limitations in capturing the full range of cloud arrangements and transitions between different cloud forms. We have introduced a novel approach that utilizes machine learning and geostationary satellite data to address this issue. Our machine learning model autonomously learns to recognize various cloud patterns and distributions. We conducted a comparative analysis between the categories generated by the machine and those identified by human experts to understand the strengths and weaknesses of both methods. Additionally, we explore a case study where clouds undergo a transformation, changing from a structure resembling sugar to one resembling flowers. This particular transformation was found difficult to capture with numerical simulation before. Our approach successfully captures the transition in the machine-learned feature space. Overall, the new approach can help to better understand cloud evolution, which is crucial for improving climate models and predicting how cloud behavior may change in a changing climate.

1 Introduction
Shallow convective clouds are small in individual extent but cover large areas of the tropical oceans, appearing as distinct cloud fields. Due to their radiative and precipitating properties, their representation in climate models is crucial for understanding the current large inter-model spread in predicted cloud feedback and climate sensitivity (Bony & Dufresne, 2005; Nuijens & Siebesma, 2019; Vogel et al., 2022). The EUREC4A field campaign (Bony et al., 2017; Stevens et al., 2021), which took place in the North Atlantic Trade (NAT) region around Barbados, aimed at investigating the interplay between clouds, convection, and circulation by deploying a large variety of observations between January and February 2020.

While shallow convection was long seen to produce randomly scattered individual clouds, further understanding has been gathered on the importance of cloud field organization for precipitation (Rauber et al., 2007; Radtke et al., 2022) through cold pool formation and rain evaporation (Seifert et al., 2015; Vogel et al., 2021). Among others, open research questions concern a detailed quantification of the role played by shallow mesoscale cloud organizations in controlling cloud amounts and their radiative response in the trades (Bony et al., 2015; Tomassini et al., 2015; Vogel et al., 2020; Vial et al., 2017).

Introducing four shallow convective organizations (Sugar, Gravel, Flower, Fish), with common occurrences on meso-beta (20 to 200 km) and meso-alpha (200 to 2,000...
km) scales, Stevens et al. (2020) rely on human-labeled visible satellite images in the NAT region. Sugar clouds consist of small, scattered clouds with a limited vertical extent, while gravel clouds exhibit organized lines or arcs resembling cell-like patterns. Fish clouds display a network resembling fishbones with distinct cloud-free spaces, and flowers represent larger, stratiform cloud structures forming dispersed closed cells. These patterns vary in net cloud radiative feedback (Bony et al., 2020); and, when classified by a deep neural network trained on human-labeled scenes (Rasp et al., 2020), display fundamental differences in cloud fraction and environmental conditions (Schulz et al., 2021). The four patterns exhibit a daily cycle (Vial et al., 2021) and transitions, e.g., from sugar to flower, have been studied in Large-Eddy-Simulation (LES) to identify the governing processes (Narenpitak et al., 2021, 2023; Dauhut et al., 2023).

Yet, imposing four distinct classes on the diversity of the observed organization does not cover the intermediate cloud patterns or transient states, as highlighted by the LES studies. Hence, some dynamic processes important for climate feedback may be ignored or neglected. Also, to our knowledge, there is no description of one of such transitions among different cloud regimes purely using observations. Furthermore, most of the recent studies trying to quantify the labeled well-organized systems find that these four cloud systems occur only around 50% over NAT (Janssens et al., 2021; Schulz et al., 2021; Vial et al., 2021) and have some ambiguities in agreement from the labelers’ side (Schulz, 2022). Therefore, to handle such complexity, our first objective is to develop simplified, streamlined representations to effectively understand and capture the entire cloud spectrum’s organizational relationships.

There are several different possibilities for ordering the variability of mesoscale cloud systems, such as Janssens et al. (2021) who introduced a set of selected metric spaces for arranging the cloud systems using object-based, scale-based, and retrieved physical-based statistical properties. Utilizing the metric scores and a k-means algorithm, they observe that human-defined classes have better separation starting at seven clusters. Denby (2020) demonstrates that unsupervised neural network models, which involved some human decisions in the learning stage, can be used to distinguish mainly ten different types of cloud organization and their associated radiative properties. In this work, we do not aim to favor any of the presented metrics but rather search for new information purely based on their organizational aspects, minimizing human intervention. Therefore, we aim to identify optimal distinct classes of cloud organizations representing the full spectrum and further compare them with human-identified labels.

Based on GOES-16 E cloud optical depth (COD) images (Sec. 2), Section 3 proposes a two-step self-supervised deep learning approach to study shallow convection in a continuous feature space, characterizing the entire diversity of occurring organizations. Further, an optimized discretization of the continuous space is developed to derive a finite set of classes representative of the continuous spectrum. The representations and their characteristics are investigated in Section 4.1, and we conduct a proof-of-concept study in Section 4.2 to explore the extent of agreement between human-annotated cloud organizations and machine-identified classes. Additionally, we investigate in Section 5 how this approach can be used as a tool to study transitions between different organization patterns.

2 Satellite dataset

We use COD retrieved from GOES-16 E Advanced Baseline Imager (Schmit et al., 2005) by the daytime cloud optical and microphysical properties algorithm (DCOMP) (Walther & Heidinger, 2012) at 2 km horizontal resolution and 10 – 15 minutes temporal resolution. Our domain in NAT (5 - 20° N and 40 – 60° W) is similar to domains used in past studies (Bony et al., 2020; Schulz et al., 2021). The regional climate defines December to May as dry and June to November as wet seasons (Stevens et al., 2016). While
most of the studies focus on dry season shallow convections only, we include some contributions from the wet season by selecting the time period from November to April 2017 - 2021. The purpose of choosing convective occurrences from the wet season is to see how they influence our approach.

COD represents the radiative properties of the cloud in the visible range, and its retrieval from DCOMP tackles the aleatoric uncertainties from the atmosphere and surface robustly. For example, the uncertainty associated with COD retrieval remains below 10% for all ranges in water clouds (see Figure 4 in Walther and Heidinger (2012) ). Therefore, we exploit the COD parameter to characterize the cloud system spatio-temporal variability. Note that some fine-scale cloud systems, such as sugar and gravel, also contributing to the variability of mesoscale beta clouds in regional climate systems, may not be fully resolved with the spatial resolution of this product.

Representation learning, also known as feature learning, is a specialized field within machine learning that focuses on extracting meaningful features of a given dataset. To better represent the mesoscale cloud distributions, we use six images per timestamp, including an additional fixed image over the Barbados domain (see S1). Note that the Barbados domain enables comparison with ground-based measurements in future studies. To have an adequate spatial scale of typical occurring cloud fields over NAT (as discussed in Section 1), we use 256 x 256 pixels (roughly 512 square km) as also found in Muller and Held (2012). We exclude crops affected by glint or poor retrieval quality using the respective data flags. Time stamps are limited to 9 am - 3 pm Barbados local time to avoid sun glinting. We utilize land class information to avoid land convection and verify whether 0.98th fraction of random crops belong to the ocean, accepting satellite crops with islands over NAT and excluding those over the northeast South American continent. Finally, to mitigate uncertainties at high COD from DCOMP retrieval, COD values above a threshold of 50, already indicating deep clouds, are clipped to 50. This results in a sample size of 51,000 satellite images.

For further analysis, we make use of hourly ERA-5 (Hersbach et al., 2020) large-scale environmental parameters (horizontal and vertical wind speed, relative humidity) and cloud fraction at a spatial resolution of 0.25°. Hourly cloud amount for four vertical ranges (surface-700 hPa, 700 hPa-500 hPa, 500 hPa-300 hPa, 300 hPa-tropopause) is used from the Clouds and Earth’s Radiant Energy System fourth edition (CERES, Edition - 4A) (Wielicki et al., 1996), characterized by a spatial resolution of 1°.

3 Methods

First, we develop a neural network (N1) that learns to sort the cloud organizations based on the similarity of their visual features, which we call a continuous approach in this work. The purpose is to let the network identify the structural similarities in the cloud systems and map the learned visual features in the 384-dimensional feature space. We use the software package DINO from Facebook Artificial Intelligence Research (FAIR) (Caron et al., 2021) based on PyTorch (Paszke et al., 2019) and the open-source VISSL computer vision library (Goyal et al., 2021) to adapt the network to our requirements. As a backbone neural architecture to process images, we use Vision Transformer (ViT), which has a sequence of self-attention (Vaswani et al., 2023) and feed-forward layers (Bebis & Georgiopoulos, 1994) paralleled with skip connections. This setup helps to identify long-range spatial dependencies by learning relevant information in the image (Khan et al., 2022). To focus on the structural similarities of the cloud system, every epoch, we opt for two random global crops with a 0.75 fraction (192 x 192 pixels) of the parent satellite image. As the largely overlapping global-crop pair has very similar cloud structures, the network learns their essential features and puts the pair closer to each other in the high-dimensional feature space. More details are given in S2.
After obtaining the continuously sorted representation of cloud systems (see Fig. 1.a), we intend to find optimal boundary conditions within the sorted order and, based on it, train a second neural network (N2) to discretize it. As a first step, we reduce the 384-dimension features of the satellite images obtained from N1 to two dimensions using the well-established t-distributed Stochastic Neighbor Embedding (tSNE) algorithm (van der Maaten & Hinton, 2008). tSNE tries to preserve the relative local position between features and the overall global structure of the feature distributions while mapping on a reduced two-dimensional space. On this 2-dimensional representation space, we apply a set of three statistical approaches, namely metric scores of distortion, silhouette (Rousseeuw, 1987), and Calinski-Harabasz (Caliński & Harabasz, 1974) to identify the possible number of optimal classes into which the given features could be clustered. Schubert (2023) suggests taking a collective inference from these three methods to best fit the spherical k-means clustering algorithm used during the training of N2. Supplement 3 illustrates how the three metrics point to an optimal clustering into seven classes.

N2 from Chatterjee et al. (2023) learns to put each satellite image in one of the seven classes as it progressively improves the feature space’s clustering, minimizing the cross entropy between two global random crops (192 x 192) from the parent satellite image. Here, the main difference from N1 is that additional augmented image versions (random flipping and noise addition by random Gaussian blur) of global random crops (see Fig. S2.2.b) are included. Augmentations try to provide auxiliary support to the network’s generalizability and better capture the differences in diversity of the shallow cloud systems (Nie et al., 2021; Paletta et al., 2023). After obtaining the label of each satellite image, we transfer the assigned class to the continuous representation space, which proves helpful because N1 has learned the sorting arrangement of keeping similar cloud systems closer. Therefore, it helps to visualize how each cluster with distinct characteristics can form a separate local region. The N2 feature space is i) more sparse than N1 (see S2 for explanation) and ii) arranged by closeness to the centroids, which, unlike N1, may not be ideal for representing smooth transitions of cloud systems.

4 Results

4.1 Continuous and discrete representations

To investigate how the satellite images arrange themselves in the feature space of N1, we first study the high-dimensional feature space and assess the arrangement of diverse cloud systems inside it. We reduce the feature dimensions to a 2D space to visualize the continuum using the tSNE algorithm (described in Section 3). Different cloud organizations can be identified in different areas of the 2D space (Fig. 1.a). Going anticlockwise from the top, arch-shaped cloud systems lie in the top-left, followed by flower-type distributions on the left side of the 2D feature space. Close to the flowers in the bottom-left are the flowers spreading out into stratocumulus. Note that while modeling studies suffer from capturing the transition of stratocumulus to cumulus (Sarkar et al., 2020), these cloud regimes are adjacent to one another in the 2D representation.

The bottom part of the feature space contains long bony skeletons, i.e., fish-type cloud systems, and the bottom-right corner shows an extended part of fish-type cloud organizations delineated by unusually large cloud-free regions. The top-right region of the 2D space is a collection of deep convective cells. These primarily occur in the month of November. Arc-shaped cloud systems appear on the left and top-left of the 2-D feature space. Vogel et al. (2021) suggest that the horizontal structure of mesoscale arcs is intrinsically linked to gravel, flowers, and fish. In sequence, Figure 1a shows a continuous link in the spatial arrangement of cloud systems rather than the distinct classes. Additionally, in S4, we investigate how N1 is sensitive to different visual features of cloud organizations and find that the network pays attention to specific patterns in cloud or-
Figure 1. a) Visualization of four hundred randomly selected 256 x 256 satellite images arranged in the dimensionally reduced 2D continuous feature space where the closeness of one satellite image to another is learned by N1. b) Optimized classification learned by N2 provides labels overlaid on the continuous feature space to show the clustering performance. Each class shows low, mid-low, mid-high, and high cloud amounts (%) obtained from the CERES hourly data set. c) Centroid COD images belonging to seven clusters as identified by the discrete neural network (N2). The table shows per class mean of cloud fraction (CF, %) from GOES retrieval and integrated water vapor (IWV, kg m$^{-2}$) from ERA-5.
ganization, such as deep convective semantics, adjacent thin convection around deep con-
vection, and clear sky features.

Using N2, each of the images can be attributed to one of the seven classes (refer
to Section 3), revealing distinct spaces within the 2D continuous representation space
(Fig. 1.b). To help investigate how well the seven classes separate, they are evaluated
using cloud amount at four different height levels from CERES data. This analysis, on
the one hand, reflects how each class differs from the others, and on the other hand, it
reasons for the underlying closeness of each class with neighbor classes in the feature space.
The difference between the seven clusters is especially evident when looking at their cen-
troid images (Fig. 1.c).

Deep convective class three has by far the highest cloud fraction of 76% and a third
more water vapor amount (47.0 kgm$^{-2}$) than all other classes (mean = 32.5 kgm$^{-2}$). Neigh-
boring class six (in feature space) includes less frequent higher-level clouds and has a re-
duced CF of 50% compared to class three. All other classes are dominated by low-level
clouds with lower than 50% CF. Classes one and four (neighbor to class six) still have
some mid to high-level cloud amount (below 10%). Class one can be interpreted as rep-
resenting arch-shaped cloud systems, and four resembles the fish class with a more open
sky (also shown by reduction in CF). Classes two, five, and seven, being close in the 2D
feature space, have similar cloud vertical distributions and IWV ranging from 30 to 32
kgm$^{-2}$; however, their organization is very different, as illustrated by the centroids (Fig.
1.c) and mean CFs (43%, 27%, and 33%, respectively). Class two primarily comprises
shallow cloud cover, corresponding to cloud systems resembling fish-type formations. Class
five has the lowest cloud fraction and is an intermediary class type between classes two
and seven. Finally, class seven has a presence of low cloud amounts and negligible mid
to higher cloud amounts, which visually resembles flower-type cloud distributions. There-
fore, discretizing the continuous feature space helps us visually find three main classes
(one, two, and seven) frequently resembling features identified by humans, i.e., sugar,
fish, and flower, respectively. However, it also shows the remaining diversity and their
characteristics in a cohesive approach.

4.2 Machine versus human labels

While we checked for visual correspondence and class-wise characteristics in Sec-
tion 4.1, we now aim to quantify how human labels compare to the machine’s seven clus-
ters. We use the seven previously identified cluster boundaries and cloud system posi-
tions in the continuous feature space (N1 + N2 together defined as “framework” from
now on) and the dataset by Schulz (2022), providing human labels with an agreement
score ranging between 0 and 100%.

For each timestamp where at least one of the four patterns was identified within
our domain, we select a 256 x 256-pixel satellite image centered over the area of high-
est human agreement. In this way, we ensure the best possible intercomparison. Apply-
ing the pre-processing (as in Section 2) leaves us with 52 samples of human-labeled satel-
lite images (fish: 19.3%, gravel: 26.9%, flower: 28.8%, sugar: 25.0%). Note that the best
and worst cloud organization agreements with this procedure are 91% and 7%, respec-
tively. Finally, we get the feature vectors of the images corresponding to the human sam-
ple from N1 and the machine-identified labels from N2.

The framework classifies 40% flower-labeled cloud systems in class seven (see the
hit rate along each class in Fig. 2.a) while sugar-labeled cloud systems are 31% classi-
ﬁed in class one and 20% in class four. For class four, note sugar’s low agreement in Fig.
2.b. Gravel has a total of 44% representation in classes one and five, whereas fish an-
notated labels are allocated 30% in class two and 20% each in classes four and five. Fur-
ther, looking at example images visually (Fig. 2.a), in contrast to images with high hu-
man agreement, it is evident that those with lower agreement significantly deviate from
Figure 2. a) For better visualization and reference purposes of human labels, each column shows 256 x 256 COD images belonging to a certain class marked with the highest and lowest human agreement displayed along the two rows. Below, the images along each column show the proportional machine-predicted class for human labels. b) Continuous feature space colored with different classes (1-7) in the background, along with Human labels (fish, sugar, flower, gravel) in the foreground. The level of human agreement on the identified patterns is indicated by symbol size. c) Relative occurrence of 30 nearest neighbors to human-labeled fish, gravel, flower, and sugar along the seven machine-labeled classes.
the recognized definitions (as given in Stevens et al. (2020)) of sugar, gravel, flower, and fish cloud structures.

Within the 2D feature space (Fig. 2.b), flowers detected with high probability mostly occur in areas of class seven, which was already well reflected in the centroids. Following a similar agreement is sugar (street-type cloud systems), which can be found in areas of class one. However, 38% of sugar samples, with a low agreement, lies in classes four and five, which are extended fish and flower type classes (Section 4.1). Thus, even though these samples reside in those regions of the feature space, their confidence is less than 25%. Rightly, no human-labeled samples are found in class three, which predominantly comprise deep convective cells. For the gravel pattern, 21% samples belong to class six (Fig. 2.b) and exhibit minimal human confidence; in contrast, the rest from the gravel class are positioned between classes one and seven, suggesting that gravel cloud cell sizes fall between sugar and flower. Finally, the fish class exhibits relatively higher confidence in human labels, aligning well with the feature space characteristics, and lies in class two (fish) and four (extended fish).

To compensate for the limited number of human label samples, we analyze the 30 nearest satellite images to each human label as identified by N1 (Fig. 2.c). This analysis aims to show the generalization capacity of our approach and further enhance our understanding of the connection between organizations. The majority of neighbors in human-identified fish-type cloud systems (more than 50%) belong to machine-identified classes two and four, representing fish and extended fish-type cloud structures with large cloud-free regions. The gravel regime includes members of all classes, with notable contributions from classes one, five, and seven, which exhibit cloud cell characteristics similar to gravel systems. One of the reasons for the wider spread of neighbors might be due to the lower human agreement of the images labeled as gravel (75% of gravel-labeled samples had agreement less than 0.25). In contrast, the flower regime mainly belongs to class seven (46%), further aligning with the high confidence of human labels. Regarding sugar-type cloud systems, 37% of the neighbors fall into class one, while those with low human agreement are scattered across the remaining classes. Therefore, we find that machine-labeled classes encompass the human-labeled ones, especially for sugar, flower, and fish, but not so clearly for gravel.

Comparing human labels with their nearest neighbors shows that the framework provides more objective freedom and improves our confidence about the feature vectors allocated to images corresponding to human samples. It also shows the uncertainty associated with less agreed-upon human labels. Further, in S5, using ERA-5 large-scale environmental variables and cloud physical properties, we demonstrate that both the neighbors and the human crops share a similar, homogeneous distribution of physical properties.

5 Transitions

To showcase an application that highlights the strengths and weaknesses of the presented framework, we explore the "sugar" to "flower" (S2F) cloud system transition on February 2, 2020. Using LES, Narenpitak et al. (2021) showed a strengthening of large-scale upward wind motion and an increase in total water path and optical depth as the transformation develops towards the flower. Here, we look at how the transition in COD is represented in the feature space. For example, where do the representations of transitions lie in the feature space? How smooth is the transition in the feature space?

Covering the spatio-temporal developments, 47 COD images were collected (after applying quality filter checks (see Section 2)), centered at 12.5° N, 50° W. They cover the time from 10:50 to 19:20 UTC, with a gap between 17:00 to 18:00 UTC likely caused by local sun glint. We ingest the available samples into the trained framework, collect
Figure 3. a) Five COD images covering the transition period between sugar and flower on the second of February 2020. Their position in the 2D feature space is indicated in the center of the bottom row. b) Individual and standard deviation profiles of 1) vertical, 2) horizontal wind speed describing the atmospheric dynamics, and 3) cloud cover showing changes in mesoscale structure of the transition samples. c) Illustration of temporal transition development inside the feature space: cosine distance of the first daytime image feature obtained at 10:50 UTC compared with the cloud system evolution features for the rest of the day (blue). The last obtained image at 19:20 UTC towards the first image (orange) and $\theta_m$ represents the increasing cosine distance.

their features (from N1) and machine labels (from N2), and further dimensionally reduce the features for 2D visualization.
Sugar systems comprise small and shallow clouds with a large spread of individual cloud cells in a domain, as evident in the beginning (10:50, Fig. 3.a). In contrast, flower systems appear in multiple deeper aggregates surrounded by large dry areas and are detected first in the southeast cover at 16:50 before becoming dominated at 19:20 over the full domain. In general, the transition features lie at the border of well-defined clusters one (‘sugar’) and cluster seven (‘flower’) (Fig. 3.a), and the framework is able to capture their intermediary nature as they are neither perfect sugar nor flower type.

We use wind speed (vertical and horizontal) to represent changes in atmospheric dynamics and changes in cloud cover to account for the changes in mesoscale structure from the ERA-5 product. A gradual increase in vertical velocity is observed as the system transitions from sugar to flowers, and consequently, the surface wind speed gradually reduces its strength (Fig. 3.b). In addition, as expected, cloud fraction profiles show a gradual decrease as the transition progresses with time.

Sugar-type mesoscale organizations typically occur during the daytime with shallow boundary layers, while flowers occur at night with deeper boundary layers (Vial et al., 2021). We use cosine distance between the features to show the gradual development of the S2F transition inside the feature space (Fig. 3.c), which quantifies the variation in visual features of the 47 COD images. The transformation appears smooth initially, with relatively more significant changes occurring later (post-18:00 UTC) as the system approaches the flower state. We associate the relatively high changes in cosine distance compared to initial sugar stages to convective developments which are faster once the system starts approaching a well-defined flower state. This example illustrates that the framework can capture the intrinsic characteristics of S2F transitions and can be further exploited as a tool to study cloud system transformations and associated processes with large satellite datasets.

6 Conclusion

In this work, we develop and make use of a two-step self-supervised learning approach to study shallow convective organization properties and their transitions. By analyzing organization in a continuous approach without imposing predefined classes, we include all occurring patterns and transitional states in our analysis. Moreover, the approach shows that mesoscale cloud organizations in NAT can be classified into seven optimal classes for the time period considered. Exploiting the cloud amount at different vertical levels from CERES measurements, we show how the classes are interlinked with each other within the continuous space, and thus, the feature space captures the variability of tropical clouds in more detail.

We compare human-labeled cloud systems (Schulz, 2022) to machine-identified cluster regions. Cloud systems with higher agreement among humans lie in the "correct" region of the feature space, while the ones with less consensus are in the "wrong" regions of the feature space. Two of the seven optimal classes are strongly related to flower and sugar, respectively. Representing the sugar-to-flower transition case study (Narenpitak et al., 2021) for February 2, 2020, in the feature space illustrates the capability to identify and represent the observed transformations smoothly in their clearly interpretable regions. We evaluate the transition’s large-scale environmental parameters and observe a gradual increase in vertical wind speed and a gradual decrease in cloud amount. Finally, we demonstrate the framework’s capability to capture the underlying mesoscale visual transformations, such as the transition approaching mature flower convective stages through quick changes in consecutive cosine distances.

One of the limitations of this study is that we use only the daytime cloud retrievals, and hence, the nocturnal nature of the organizations cannot be captured. Future studies will use infrared satellite measurements for 24-hour coverage. We aim to fine-tune our framework with the ground-based observations of the EUREC4A campaign and fur-
ther extend our analysis to a climate scale. Currently, Destination Earth (Hoffmann et al., 2023) focuses on simulating high-resolution global digital twins at a 1 km grid scale. The developed workflow could be a testing ground for investigating the newly adjusted subgrid parameterization effects on mesoscale cloud systems or atmospheric processes at different scales.

7 Open Research

CERES, Edition-4A, DOI:10.5067/TERRA+AQUA/CERES/SYN1DEG-1HOUR_L3.004A is made available by the NASA CERES group. ERA-5 reanalyses were downloaded from the Copernicus climate change services DOI:10.24381/cds.143582cf.

The code to produce this work and pre-trained weights of N1 and N2 can be accessed at https://doi.org/10.5281/zenodo.8352614

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References From the Supporting Information


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Dwaipayan Chatterjee¹, Sabrina Schnitt¹, Paula Bigalke¹, Claudia
Acquistapace¹, Susanne Crewell¹

¹Institute for Geophysics and Meteorology, University of Cologne, Cologne, Germany

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Corresponding author: Dwaipayan Chatterjee, dchatter@uni-koeln.de
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Plain Language Summary

Clouds are a fundamental player affecting our planet’s energy balance, making their accurate representation crucial in climate models. One open question is how they organize on a scale of a few 100 km (mesoscale) within the trade wind region. Satellite observations can help to categorize these clouds, but previous methods had limitations in capturing the full range of cloud arrangements and transitions between different cloud forms. We have introduced a novel approach that utilizes machine learning and geostationary satellite data to address this issue. Our machine learning model autonomously learns to recognize various cloud patterns and distributions. We conducted a comparative analysis between the categories generated by the machine and those identified by human experts to understand the strengths and weaknesses of both methods. Additionally, we explore a case study where clouds undergo a transformation, changing from a structure resembling sugar to one resembling flowers. This particular transformation was found difficult to capture with numerical simulation before. Our approach successfully captures the transition in the machine-learned feature space. Overall, the new approach can help to better understand cloud evolution, which is crucial for improving climate models and predicting how cloud behavior may change in a changing climate.

1 Introduction

Shallow convective clouds are small in individual extent but cover large areas of the tropical oceans, appearing as distinct cloud fields. Due to their radiative and precipitating properties, their representation in climate models is crucial for understanding the current large inter-model spread in predicted cloud feedback and climate sensitivity (Bony & Dufresne, 2005; Nuijens & Siebesma, 2019; Vogel et al., 2022). The EUREC4A field campaign (Bony et al., 2017; Stevens et al., 2021), which took place in the North Atlantic Trade (NAT) region around Barbados, aimed at investigating the interplay between clouds, convection, and circulation by deploying a large variety of observations between January and February 2020.

While shallow convection was long seen to produce randomly scattered individual clouds, further understanding has been gathered on the importance of cloud field organization for precipitation (Rauber et al., 2007; Radtke et al., 2022) through cold pool formation and rain evaporation (Seifert et al., 2015; Vogel et al., 2021). Among others, open research questions concern a detailed quantification of the role played by shallow mesoscale cloud organizations in controlling cloud amounts and their radiative response in the trades (Bony et al., 2015; Tomassini et al., 2015; Vogel et al., 2020; Vial et al., 2017).

Introducing four shallow convective organizations (Sugar, Gravel, Flower, Fish), with common occurrences on meso-beta (20 to 200 km) and meso-alpha (200 to 2,000
km) scales, Stevens et al. (2020) rely on human-labeled visible satellite images in the NAT region. Sugar clouds consist of small, scattered clouds with a limited vertical extent, while gravel clouds exhibit organized lines or arcs resembling cell-like patterns. Fish clouds display a network resembling fishbones with distinct cloud-free spaces, and flowers represent larger, stratiform cloud structures forming dispersed closed cells. These patterns vary in net cloud radiative feedback (Bony et al., 2020); and, when classified by a deep neural network trained on human-labeled scenes (Rasp et al., 2020), display fundamental differences in cloud fraction and environmental conditions (Schulz et al., 2021). The four patterns exhibit a daily cycle (Vial et al., 2021) and transitions, e.g., from sugar to flower, have been studied in Large-Eddy-Simulation (LES) to identify the governing processes (Narenpitak et al., 2021, 2023; Dauhut et al., 2023).

Yet, imposing four distinct classes on the diversity of the observed organization does not cover the intermediate cloud patterns or transient states, as highlighted by the LES studies. Hence, some dynamic processes important for climate feedback may be ignored or neglected. Also, to our knowledge, there is no description of one of such transitions among different cloud regimes purely using observations. Furthermore, most of the recent studies trying to quantify the labeled well-organized systems find that these four cloud systems occur only around 50% over NAT (Janssens et al., 2021; Schulz et al., 2021; Vial et al., 2021) and have some ambiguities in agreement from the labelers’ side (Schulz, 2022). Therefore, to handle such complexity, our first objective is to develop simplified, streamlined representations to effectively understand and capture the entire cloud spectrum’s organizational relationships.

There are several different possibilities for ordering the variability of mesoscale cloud systems, such as Janssens et al. (2021) who introduced a set of selected metric spaces for arranging the cloud systems using object-based, scale-based, and retrieved physical-based statistical properties. Utilizing the metric scores and a k-means algorithm, they observe that human-defined classes have better separation starting at seven clusters. Denby (2020) demonstrates that unsupervised neural network models, which involved some human decisions in the learning stage, can be used to distinguish mainly ten different types of cloud organization and their associated radiative properties. In this work, we do not aim to favor any of the presented metrics but rather search for new information purely based on their organizational aspects, minimizing human intervention. Therefore, we aim to identify optimal distinct classes of cloud organizations representing the full spectrum and further compare them with human-identified labels.

Based on GOES-16 E cloud optical depth (COD) images (Sec. 2), Section 3 proposes a two-step self-supervised deep learning approach to study shallow convection in a continuous feature space, characterizing the entire diversity of occurring organizations. Further, an optimized discretization of the continuous space is developed to derive a finite set of classes representative of the continuous spectrum. The representations and their characteristics are investigated in Section 4.1, and we conduct a proof-of-concept study in Section 4.2 to explore the extent of agreement between human-annotated cloud organizations and machine-identified classes. Additionally, we investigate in Section 5 how this approach can be used as a tool to study transitions between different organization patterns.

2 Satellite dataset

We use COD retrieved from GOES-16 E Advanced Baseline Imager (Schmit et al., 2005) by the daytime cloud optical and microphysical properties algorithm (DCOMP) (Walther & Heidinger, 2012) at 2 km horizontal resolution and 10 – 15 minutes temporal resolution. Our domain in NAT (5 – 20° N and 40 – 60° W) is similar to domains used in past studies (Bony et al., 2020; Schulz et al., 2021). The regional climate defines December to May as dry and June to November as wet seasons (Stevens et al., 2016). While
most of the studies focus on dry season shallow convections only, we include some contributions from the wet season by selecting the time period from November to April 2017 – 2021. The purpose of choosing convective occurrences from the wet season is to see how they influence our approach.

COD represents the radiative properties of the cloud in the visible range, and its retrieval from DCOMP tackles the aleatoric uncertainties from the atmosphere and surface robustly. For example, the uncertainty associated with COD retrieval remains below 10\% for all ranges in water clouds (see Figure 4 in Walther and Heidinger (2012)). Therefore, we exploit the COD parameter to characterize the cloud system spatio-temporal variability. Note that some fine-scale cloud systems, such as sugar and gravel, also contributing to the variability of mesoscale beta clouds in regional climate systems, may not be fully resolved with the spatial resolution of this product.

Representation learning, also known as feature learning, is a specialized field within machine learning that focuses on extracting meaningful features of a given dataset. To better represent the mesoscale cloud distributions, we use six images per timestamp, including an additional fixed image over the Barbados domain (see S1). Note that the Barbados domain enables comparison with ground-based measurements in future studies. To have an adequate spatial scale of typical occurring cloud fields over NAT (as discussed in Section 1), we use 256 x 256 pixels (roughly 512 square km) as also found in Muller and Held (2012). We exclude crops affected by glint or poor retrieval quality using the respective data flags. Time stamps are limited to 9 am - 3 pm Barbados local time to avoid sun glinting. We utilize land class information to avoid land convection and verify whether 0.98\textsuperscript{th} fraction of random crops belong to the ocean, accepting satellite crops with islands over NAT and excluding those over the northeast South American continent. Finally, to mitigate uncertainties at high COD from DCOMP retrieval, COD values above a threshold of 50, already indicating deep clouds, are clipped to 50. This results in a sample size of 51,000 satellite images.

For further analysis, we make use of hourly ERA-5 (Hersbach et al., 2020) large-scale environmental parameters (horizontal and vertical wind speed, relative humidity) and cloud fraction at a spatial resolution of 0.25°. Hourly cloud amount for four vertical ranges (surface-700 hPa, 700 hPa-500 hPa, 500 hPa-300 hPa, 300 hPa-tropopause) is used from the Clouds and Earth’s Radiant Energy System fourth edition (CERES, Edition - 4A) (Wielicki et al., 1996), characterized by a spatial resolution of 1°.

3 Methods

First, we develop a neural network (N1) that learns to sort the cloud organizations based on the similarity of their visual features, which we call a continuous approach in this work. The purpose is to let the network identify the structural similarities in the cloud systems and map the learned visual features in the 384-dimensional feature space. We use the software package DINO from Facebook Artificial Intelligence Research (FAIR) (Caron et al., 2021) based on PyTorch (Paszke et al., 2019) and the open-source VISSL computer vision library (Goyal et al., 2021) to adapt the network to our requirements. As a backbone neural architecture to process images, we use Vision Transformer (ViT), which has a sequence of self-attention (Vaswani et al., 2023) and feed-forward layers (Bebis & Georgiopoulos, 1994) paralleled with skip connections. This setup helps to identify long-range spatial dependencies by learning relevant information in the image (Khan et al., 2022). To focus on the structural similarities of the cloud system, every epoch, we opt for two random global crops with a 0.75 fraction (192 x 192 pixels) of the parent satellite image. As the largely overlapping global-crop pair has very similar cloud structures, the network learns their essential features and puts the pair closer to each other in the high-dimensional feature space. More details are given in S2.
After obtaining the continuously sorted representation of cloud systems (see Fig. 1.a), we intend to find optimal boundary conditions within the sorted order and, based on it, train a second neural network (N2) to discretize it. As a first step, we reduce the 384-dimension features of the satellite images obtained from N1 to two dimensions using the well-established t-distributed Stochastic Neighbor Embedding (tSNE) algorithm (van der Maaten & Hinton, 2008). tSNE tries to preserve the relative local position between features and the overall global structure of the feature distributions while mapping on a reduced two-dimensional space. On this 2-dimensional representation space, we apply a set of three statistical approaches, namely metric scores of distortion, silhouette (Rousseeuw, 1987), and Calinski-Harabasz (Calinski & Harabasz, 1974) to identify the possible number of optimal classes into which the given features could be clustered. Schubert (2023) suggests taking a collective inference from these three methods to best fit the spherical k-means clustering algorithm used during the training of N2. Supplement 3 illustrates how the three metrics point to an optimal clustering into seven classes.

N2 from Chatterjee et al. (2023) learns to put each satellite image in one of the seven classes as it progressively improves the feature space’s clustering, minimizing the cross-entropy between two global random crops (192 x 192) from the parent satellite image. Here, the main difference from N1 is that additional augmented image versions (random flipping and noise addition by random Gaussian blur) of global random crops (see Fig. S2.2.b) are included. Augmentations try to provide auxiliary support to the network’s generalizability and better capture the differences in diversity of the shallow cloud systems (Nie et al., 2021; Paletta et al., 2023). After obtaining the label of each satellite image, we transfer the assigned class to the continuous representation space, which proves helpful because N1 has learned the sorting arrangement of keeping similar cloud systems closer. Therefore, it helps to visualize how each cluster with distinct characteristics can form a separate local region. The N2 feature space is i) more sparse than N1 (see S2 for explanation) and ii) arranged by closeness to the centroids, which, unlike N1, may not be ideal for representing smooth transitions of cloud systems.

4 Results

4.1 Continuous and discrete representations

To investigate how the satellite images arrange themselves in the feature space of N1, we first study the high-dimensional feature space and assess the arrangement of diverse cloud systems inside it. We reduce the feature dimensions to a 2D space to visualize the continuum using the tSNE algorithm (described in Section 3). Different cloud organizations can be identified in different areas of the 2D space (Fig. 1.a). Going anticlockwise from the top, arch-shaped cloud systems lie in the top-left, followed by flower-type distributions on the left side of the 2D feature space. Close to the flowers in the bottom-left are the flowers spreading out into stratocumulus. Note that while modeling studies suffer from capturing the transition of stratocumulus to cumulus (Sarkar et al., 2020), these cloud regimes are adjacent to one another in the 2D representation.

The bottom part of the feature space contains long bony skeletons, i.e., fish-type cloud systems, and the bottom-right corner shows an extended part of fish-type cloud organizations delineated by unusually large cloud-free regions. The top-right region of the 2D space is a collection of deep convective cells. These primarily occur in the month of November. Arc-shaped cloud systems appear on the left and top-left of the 2-D feature space. Vogel et al. (2021) suggest that the horizontal structure of mesoscale arcs is intrinsically linked to gravel, flowers, and fish. In sequence, Figure 1a shows a continuous link in the spatial arrangement of cloud systems rather than the distinct classes. Additionally, in S4, we investigate how N1 is sensitive to different visual features of cloud organizations and find that the network pays attention to specific patterns in cloud or-
Figure 1.  
a) Visualization of four hundred randomly selected 256 x 256 satellite images arranged in the dimensionally reduced 2D continuous feature space where the closeness of one satellite image to another is learned by N1. 
b) Optimized classification learned by N2 provides labels overlaid on the continuous feature space to show the clustering performance. Each class shows low, mid-low, mid-high, and high cloud amounts (%) obtained from the CERES hourly data set. 
c) Centroid COD images belonging to seven clusters as identified by the discrete neural network (N2). The table shows per class mean of cloud fraction (CF, %) from GOES retrieval and integrated water vapor (IWV, kg m$^{-2}$) from ERA-5.
ganization, such as deep convective semantics, adjacent thin convection around deep convection, and clear sky features.

Using N2, each of the images can be attributed to one of the seven classes (refer to Section 3), revealing distinct spaces within the 2D continuous representation space (Fig. 1.b). To help investigate how well the seven classes separate, they are evaluated using cloud amount at four different height levels from CERES data. This analysis, on the one hand, reflects how each class differs from the others, and on the other hand, it reasons for the underlying closeness of each class with neighbor classes in the feature space. The difference between the seven clusters is especially evident when looking at their centroid images (Fig. 1.c).

Deep convective class three has by far the highest cloud fraction of 76% and a third more water vapor amount (47.0 kgm$^{-2}$) than all other classes (mean = 32.5 kgm$^{-2}$). Neighboring class six (in feature space) includes less frequent higher-level clouds and has a reduced CF of 59% compared to class three. All other classes are dominated by low-level clouds with lower than 50% CF. Classes one and four (neighbor to class six) still have some mid to high-level cloud amount (below 10%). Class one can be interpreted as representing arch-shaped cloud systems, and four resembles the fish class with a more open sky (also shown by reduction in CF). Classes two, five, and seven, being close in the 2D feature space, have similar cloud vertical distributions and IWV ranging from 30 to 32 kgm$^{-2}$; however, their organization is very different, as illustrated by the centroids (Fig. 1.c) and mean CFs (43%, 27%, and 33%, respectively). Class two primarily comprises shallow cloud cover, corresponding to cloud systems resembling fish-type formations. Class five has the lowest cloud fraction and is an intermediary class type between classes two and seven. Finally, class seven has a presence of low cloud amounts and negligible mid to higher cloud amounts, which visually resembles flower-type cloud distributions. Therefore, discretizing the continuous feature space helps us visually find three main classes (one, two, and seven) frequently resembling features identified by humans, i.e., sugar, fish, and flower, respectively. However, it also shows the remaining diversity and their characteristics in a cohesive approach.

4.2 Machine versus human labels

While we checked for visual correspondence and class-wise characteristics in Section 4.1, we now aim to quantify how human labels compare to the machine’s seven clusters. We use the seven previously identified cluster boundaries and cloud system positions in the continuous feature space (N1 + N2 together defined as “framework” from now on) and the dataset by Schulz (2022), providing human labels with an agreement score ranging between 0 and 100%.

For each timestamp where at least one of the four patterns was identified within our domain, we select a 256 x 256-pixel satellite image centered over the area of highest human agreement. In this way, we ensure the best possible intercomparison. Applying the pre-processing (as in Section 2) leaves us with 52 samples of human-labeled satellite images (fish: 19.3%, gravel: 26.9%, flower: 28.8%, sugar: 25.0%). Note that the best and worst cloud organization agreements with this procedure are 91% and 7%, respectively. Finally, we get the feature vectors of the images corresponding to the human samples from N1 and the machine-identified labels from N2.

The framework classifies 40% flower-labeled cloud systems in class seven (see the hit rate along each class in Fig. 2.a) while sugar-labeled cloud systems are 31% classified in class one and 20% in class four. For class four, note sugar’s low agreement in Fig. 2.b. Gravel has a total of 44% representation in classes one and five, whereas fish annotated labels are allocated 30% in class two and 20% each in classes four and five. Further, looking at example images visually (Fig. 2.a), in contrast to images with high human agreement, it is evident that those with lower agreement significantly deviate from
Figure 2. a) For better visualization and reference purposes of human labels, each column shows 256 x 256 COD images belonging to a certain class marked with the highest and lowest human agreement displayed along the two rows. Below, the images along each column show the proportional machine-predicted class for human labels. b) Continuous feature space colored with different classes (1-7) in the background, along with Human labels (fish, sugar, flower, gravel) in the foreground. The level of human agreement on the identified patterns is indicated by symbol size. c) Relative occurrence of 30 nearest neighbors to human-labeled fish, gravel, flower, and sugar along the seven machine-labeled classes.
the recognized definitions (as given in Stevens et al. (2020)) of sugar, gravel, flower, and fish cloud structures.

Within the 2D feature space (Fig. 2.b), flowers detected with high probability mostly occur in areas of class seven, which was already well reflected in the centroids. Following a similar agreement is sugar (street-type cloud systems), which can be found in areas of class one. However, 38% of sugar samples, with a low agreement, lies in classes four and five, which are extended fish and flower type classes (Section 4.1). Thus, even though these samples reside in those regions of the feature space, their confidence is less than 25%. Rightly, no human-labeled samples are found in class three, which predominantly comprise deep convective cells. For the gravel pattern, 21% samples belong to class six (Fig. 2.b)) and exhibit minimal human confidence; in contrast, the rest from the gravel class are positioned between classes one and seven, suggesting that gravel cloud cell sizes fall between sugar and flower. Finally, the fish class exhibits relatively higher confidence in human labels, aligning well with the feature space characteristics, and lies in class two (fish) and four (extended fish).

To compensate for the limited number of human label samples, we analyze the 30 nearest satellite images to each human label as identified by N1 (Fig. 2.c). This analysis aims to show the generalization capacity of our approach and further enhance our understanding of the connection between organizations. The majority of neighbors in human-identified fish-type cloud systems (more than 50%) belong to machine-identified classes two and four, representing fish and extended fish-type cloud structures with large cloud-free regions. The gravel regime includes members of all classes, with notable contributions from classes one, five, and seven, which exhibit cloud cell characteristics similar to gravel systems. One of the reasons for the wider spread of neighbors might be due to the lower human agreement of the images labeled as gravel (75% of gravel-labeled samples had agreement less than 0.25). In contrast, the flower regime mainly belongs to class seven (46 %), further aligning with the high confidence of human labels. Regarding sugar-type cloud systems, 37 % of the neighbors fall into class one, while those with low human agreement are scattered across the remaining classes. Therefore, we find that machine-labeled classes encompass the human-labeled ones, especially for sugar, flower, and fish, but not so clearly for gravel.

Comparing human labels with their nearest neighbors shows that the framework provides more objective freedom and improves our confidence about the feature vectors allocated to images corresponding to human samples. It also shows the uncertainty associated with less agreed-upon human labels. Further, in S5, using ERA-5 large-scale environmental variables and cloud physical properties, we demonstrate that both the neighbors and the human crops share a similar, homogeneous distribution of physical properties.

5 Transitions

To showcase an application that highlights the strengths and weaknesses of the presented framework, we explore the "sugar" to "flower" (S2F) cloud system transition on February 2, 2020. Using LES, Narenpitak et al. (2021) showed a strengthening of large-scale upward wind motion and an increase in total water path and optical depth as the transformation develops towards the flower. Here, we look at how the transition in COD is represented in the feature space. For example, where do the representations of transitions lie in the feature space? How smooth is the transition in the feature space?

Covering the spatio-temporal developments, 47 COD images were collected (after applying quality filter checks (see Section 2)), centered at 12.5° N, 50° W. They cover the time from 10:50 to 19:20 UTC, with a gap between 17:00 to 18:00 UTC likely caused by local sun glint. We ingest the available samples into the trained framework, collect
Figure 3. a) Five COD images covering the transition period between sugar and flower on the second of February 2020. Their position in the 2D feature space is indicated in the center of the bottom row. b) Individual and standard deviation profiles of 1) vertical, 2) horizontal wind speed describing the atmospheric dynamics, and 3) cloud cover showing changes in mesoscale structure of the transition samples. c) Illustration of temporal transition development inside the feature space: cosine distance of the first daytime image feature obtained at 10:50 UTC compared with the cloud system evolution features for the rest of the day (blue). The last obtained image at 19:20 UTC towards the first image (orange) and $\theta_m$ represents the increasing cosine distance.

their features (from N1) and machine labels (from N2), and further dimensionally reduce the features for 2D visualization.
Sugar systems comprise small and shallow clouds with a large spread of individual cloud cells in a domain, as evident in the beginning (10:50, Fig. 3.a). In contrast, flower systems appear in multiple deeper aggregates surrounded by large dry areas and are detected first in the southeast cover at 16:50 before becoming dominated at 19:20 over the full domain. In general, the transition features lie at the border of well-defined clusters one (‘sugar’) and cluster seven (‘flower’) (Fig. 3.a), and the framework is able to capture their intermediary nature as they are neither perfect sugar nor flower type. We use wind speed (vertical and horizontal) to represent changes in atmospheric dynamics and changes in cloud cover to account for the changes in mesoscale structure from the ERA-5 product. A gradual increase in vertical velocity is observed as the system transitions from sugar to flowers, and consequently, the surface wind speed gradually reduces its strength (Fig. 3.b). In addition, as expected, cloud fraction profiles show a gradual decrease as the transition progresses with time.

Sugar-type mesoscale organizations typically occur during the daytime with shallow boundary layers, while flowers occur at night with deeper boundary layers (Vial et al., 2021). We use cosine distance between the features to show the gradual development of the S2F transition inside the feature space (Fig. 3.c), which quantifies the variation in visual features of the 47 COD images. The transformation appears smooth initially, with relatively more significant changes occurring later (post-18:00 UTC) as the system approaches the flower state. We associate the relatively high changes in cosine distance compared to initial sugar stages to convective developments which are faster once the system starts approaching a well-defined flower state. This example illustrates that the framework can capture the intrinsic characteristics of S2F transitions and can be further exploited as a tool to study cloud system transformations and associated processes with large satellite datasets.

6 Conclusion

In this work, we develop and make use of a two-step self-supervised learning approach to study shallow convective organization properties and their transitions. By analyzing organization in a continuous approach without imposing predefined classes, we include all occurring patterns and transitional states in our analysis. Moreover, the approach shows that mesoscale cloud organizations in NAT can be classified into seven optimal classes for the time period considered. Exploiting the cloud amount at different vertical levels from CERES measurements, we show how the classes are interlinked with each other within the continuous space, and thus, the feature space captures the variability of tropical clouds in more detail.

We compare human-labeled cloud systems (Schulz, 2022) to machine-identified cluster regions. Cloud systems with higher agreement among humans lie in the "correct" region of the feature space, while the ones with less consensus are in the "wrong" regions of the feature space. Two of the seven optimal classes are strongly related to flower and sugar, respectively. Representing the sugar-to-flower transition case study (Narenpitak et al., 2021) for February 2, 2020, in the feature space illustrates the capability to identify and represent the observed transformations smoothly in their clearly interpretable regions. We evaluate the transition’s large-scale environmental parameters and observe a gradual increase in vertical wind speed and a gradual decrease in cloud amount. Finally, we demonstrate the framework’s capability to capture the underlying mesoscale visual transformations, such as the transition approaching mature flower convective stages through quick changes in consecutive cosine distances.

One of the limitations of this study is that we use only the daytime cloud retrievals, and hence, the nocturnal nature of the organizations cannot be captured. Future studies will use infrared satellite measurements for 24-hour coverage. We aim to fine-tune our framework with the ground-based observations of the EUREC4A campaign and fur-
ther extend our analysis to a climate scale. Currently, Destination Earth (Hoffmann et al., 2023) focuses on simulating high-resolution global digital twins at a 1 km grid scale. The developed workflow could be a testing ground for investigating the newly adjusted subgrid parameterization effects on mesoscale cloud systems or atmospheric processes at different scales.

7 Open Research

CERES, Edition-4A, DOI:10.5067/TERRA+AQUA/CERES/SYN1DEG-1HOUR_L3.004A) is made available by the NASA CERES group. ERA-5 reanalyses were downloaded from the Copernicus climate change services DOI:10.24381/cds.143582cf.

The code to produce this work and pre-trained weights of N1 and N2 can be accessed at https://doi.org/10.5281/zenodo.8352614

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References From the Supporting Information


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Capturing the diversity of mesoscale trade wind cumuli using complementary approaches from self-supervision

Dwaipayan Chatterjee\textsuperscript{1}, Sabrina Schnitt\textsuperscript{1}, Paula Bigalke\textsuperscript{1}, Claudia Acquistapace\textsuperscript{1}, Susanne Crewell\textsuperscript{1}

\textsuperscript{1}Institute for Geophysics and Meteorology, University of Cologne, Cologne, Germany
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Corresponding author: D. Chatterjee, Institute for Geophysics and Meteorology, University of Cologne, Cologne, Germany. (dchatter@uni-koeln.de)
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S1 Domain description

Figure S1 (Domain). GOES’s COD image on February 2, 2020, at 13:00 UTC with coastal boundaries (thick yellow) and Barbados Cloud Observatory (red dot). One (out of five) random and a fixed (Barbados domain) 256 x 256-pixel crop over EUREC4A domain are shown. During the learning process, each crop is twice randomly sub-cropped (pink and green dashed lines) by the network, leading to a spatial dimension of 75% (192 x 192 pixels) of the original crop. The Barbados domain enables comparison with ground-based measurements in future studies.
**S2 Network architectures** Here, N1 and N2 (Chatterjee et al., 2023) architectures are described in detail.

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**Figure S2.1 (Schematic diagram of N1).** This work adopts a deep learning architecture from Caron et al. (2021), where $x_1$ and $x_2$ are 75% random crops of the parent satellite image $x$. The student and teacher vision transformers ($g_{\theta_s/t}$) have the same number of trainable parameters (weights and biases) $\theta$. The feature output $h_{xi}$ from $g_{xi}$ subsequently connects to $\text{Proj}(h_{xi})$, a 3-layer multilayer perceptron activated by Gaussian error linear units (GELU, with the last layer, $l_2$ normalized). Softmax (Bridle, 1989) normalizes MLP’s raw activation ($z_{s/t}$), and centering maintains teacher activations ($z_t$) near batch mean properties. $P_s$ and $P_t$ represent normalized student distribution of $z_s$ and centered and normalized distribution of teacher activation $z_t$. The student network optimizes its parameters through stochastic gradient descent (SGD), minimizing cross-entropy between $P_t$ and $P_s$. Teacher parameters ($g_{\theta t}$) are exponential moving averages of students ($g_{\theta s}$), aligning the networks. This interaction forms the architecture’s backbone, enhancing performance and knowledge transfer in the deep learning framework.
1. Continuous network (N1)

1.1. Definition of the network input

$N$ satellite images of COD built the input training data set $X = \{x_1, x_2, x_3, \ldots, x_N\}$ of the deep learning architecture illustrated in Fig. S2.1 (Schematic diagram of N1). The only intuitive augmentation we opt for here is global random cropping for learning continuous representations. For random cropping, we opt for two global crops $(x_1, x_2)$ with a random 0.75 fraction (192 x 192 pixels) of the parent satellite image to focus on the global distribution of the cloud system. Figure S2.1 (Schematic diagram of N1) shows each random crop fed into different branches of the network, and from the learning aspect of the neural network, it becomes challenging for one side of the network to know what part of the parent satellite image the other is being fed with; therefore, it focuses on learning the critical semantics of global cloud distribution.

1.2. General network architecture

The neural network’s task is to learn visual features from each satellite image. A function $g$ represents the transformations performed by the network’s vision Transformer (ViT) as $g(x_i) = h_j$ with $i = 1, \ldots, N, j = 1, \ldots, M$ that maps the image $x_i$ into the array of features $h = \{h_1, h_2, h_3, \ldots, h_M\}$, where $M$ is the output dimension of ViT feature arrays. The selected dimension of $M$ is equal to 384, which means the information contained in the
192 x 192 satellite observation space is being non-linearly dimensionally reduced to 384 vector space. ViT is a sequence of self-attention (Vaswani et al., 2023), and feed-forward layers paralleled with skip connections. The mechanism of ViT (Dosovitskiy et al., 2021) takes non-overlapping contiguous image patches of resolution NxN pixels, where N=16 for this work, along with their positional encoding as an input. Without the positional encoding, the output feature vector from ViT is invariant to the arrangement of these NxN patches. But with positional encoding, it learns the relative position of the objects in the image. This becomes helpful if we want the model to learn the relationship between the patches. Thus it learns how a particular arrangement of cloud distribution usually occurs, and it learns the constrained settings behind the appearance of a given cloud distribution. Therefore, the ViT architecture can identify long-range spatial dependencies (Khan et al., 2022) by learning relevant information in the image. The activation function used in the ViT is Gaussian error linear units (Hendrycks & Gimpel, 2023) (GELU), as the GELU function behaves smoother when values are closer to zero and thus is more effective at learning complex patterns in the data.

Further, $h_j$ is non-linearly projected to $z_k$ with $k = 1,...,K$ using a three-layer multilayer perceptron activated by GELU followed by $l_2$ normalization and a linear layer. Here $z = \{z_1, z_2, z_3, ..., z_K\}$ is the final output dimension of the pipeline. The feature space dimensions are decided based on input dimensions, the complexity of information context, and neural network complexity. Caron et al. (2021) suggest that if the training dataset size is much less than 1.3 million ImageNet datasets (Russakovsky et al., 2015), then the final dimensions of $z_k$ be reduced compared to the default dimensions of 65536. We iterated on
a smaller $K$ dimension of 128 and a higher $K$ dimension of 8192; in this case, we visually found the latter working better to understand the similarity between cloud fields. Our intuition is giving the final output feature more dimensions gives the model more freedom to observe small semantic details of cloud distributions. Also, since the loss function used here (explained in section 1.3) is non-contrastive, higher dimensional features are still computationally inexpensive. Our aim here is not to find the optimal feature vector size but a functional size that can optimize the network and smoothly converge the training. Therefore, the optimal dimension size of the dimensionally reduced atmospheric fields in self-supervised learning is not the focus of this work. Figure S2.1 (Schematic diagram of N1) shows two different branches in the network: student and teacher. The point to note here is that they have the same general architecture and pipeline, but the parameters (weights and biases) learned during training are different.

### 1.3. Upper branch of the network

The upper branch of the network, represented in Figure S2.1 (Schematic diagram of N1), by the student transformer $g_s$ and further projected by multi-layer perceptron (MLP) (Rumelhart et al., 1986), ingests one random augmented global crop of the parent satellite image and outputs feature vector $z_s$. $z_s$ is normalized and converted to a probability distribution. This means that the original feature vector $z_s$ (which has 8192 dimensions); some values could be negative or greater than one, but after applying soft-max (Bridle, 1989), it normalizes to (0,1), and all the 8192 dimensions will add to one. Additionally, the larger input components will correspond to larger probabilities. This probability distribution of the feature vector $z_s$ is an input to the cross entropy loss function described
later. The soft-max probability for an input \( x_i \) of the student network can be described as

\[
P_s^{(i)} = \frac{\exp(\frac{1}{\zeta_s} Z_s^{(i)})}{\sum_{m=0}^{k} \exp(\frac{1}{\zeta_s} Z_s^{(m)})}.
\]  

(1)

where \( \zeta_s \) is the temperature parameter for the student network and is set to 0.1. The \( \zeta \) parameter controls the sharpening of the probability distribution. A higher value of \( \zeta \) implies smoothed probability.

1.4. Lower branch of the network

The lower branch of the network represented in Figure S2.1 (Schematic diagram of N1) by the teacher transformer applies function \( g_t \) to the other remaining global crop of the parent satellite image, and the MLP projects outputs feature vector \( z_t \). Unlike \( p_s \), before normalizing \( p_t \) individually with soft-max, vector \( z_t \) is centered around the mean properties of all images in a batch. A batch refers to the number of samples propagating through the neural network before updating the model parameters. Centering is done to prevent any feature from dominating, as the mean will be somewhere in the middle of the batch sample properties. While applying the temperature \( \zeta_t \) parameter for the teacher, it is kept lower to 0.05 to sharpen the probability of \( z_t \) artificially. Therefore, the feature vector \( z_t \) of the teacher branch went through centering and sharpened soft-max before being input to the loss function.

1.5. Cross entropy loss of the network

When the feature vectors of the two branches capture similar information from the global crops of the satellite parent image, the loss becomes lower and vice-versa. That’s
how the network branches are encouraged to focus on the common image characteristics, progressively making the feature vectors similar.

\[
\min_{\theta_s} \sum_{x \in \{x_1, x_2\}} p_t(x) \log(p_s(x))
\] (2)

This is achieved through the cross-entropy loss function applied on the centered and sharpened probability distribution of the teacher branch \(p_t\) and smoothened distribution of the student branch \(p_s\). As shown in equation 2, the loss function minimizes \(\theta_s\), i.e., the student network’s parameters (weights and biases). Teacher network parameters or \(p_t\) guide the student network during the training phase, as discussed in subsection 1.6.

1.6. Optimization for convergence

The loss function minimization happens progressively layer by layer, derivating the loss function with respect to \(\theta_s\) parameters and adjusting parameter values in each layer by backpropagation. At the end of the minimization, we obtain a configuration of parameters for the student network that will be ready for the next iteration with a new batch of images. Stochastic gradient descent (Bottou, 2012) (SGD) is only applied to the student network parameters \(\theta_s\), and the teacher parameters \(\theta_t\) are built through past iterations of the student network (Caron et al., 2021). As shown in equation 3, \(\theta_t\) is the exponential moving average (EMA) of \(\theta_s\) with \(\lambda\) following a cosine scheduled from 0.996 to 1 during training.

\[
\theta_t = \lambda \theta_t + (1 - \lambda) \theta_s
\] (3)

During optimization, a collapse can occur regardless of the input provided to the model; the output becomes constant or is predominantly influenced by a single dimension. In other words, the model’s predictions across different dimensions or features become uni-
form, leading to zero ideal loss value. Therefore, centering and sharpening introduced in subsection 1.3 and 1.4 and EMA (subsection 1.6) are the easiest acceptable ways to prevent collapsing in the described teacher-student framework.

1.7. Training and libraries

To set up this architecture, we use the software package DINO from Facebook Artificial Intelligence Research (FAIR) (Caron et al., 2021) based on PyTorch. The open-source VISSL computer vision library (Goyal et al., 2021) adapted the DINO neural network to our requirements. Based on sensitivity tests on training loss, visualization of dimensionally reduced feature space, and ablation study of the original network on longer training showing improving performance, we train the model up to 800 epochs. Training the neural network for 800 epochs on 4 V100 GPUs took 16.5 hours or 66 core hours.
S2 Network architectures

Figure S2.2 (N2 outputs).  a) Sparse 2D feature space obtained from N2 by applying the tSNE algorithm on $z_x$ features of 51,000 satellite images. The perplexity and epsilon derived from auto-configuration for t-SNE runs is 30 and 1150. b) Same as b but using direct clustering on the satellite images using N2. Here, the labels are overlaid on the continuous feature space from N1 for comparison with Figure 2.b in the main article.

2. Discrete network (N2)

We briefly describe the functional mechanism of the discrete neural network (N2) and its learning scheme. Refer to section 3 from (Chatterjee et al., 2023) for a detailed network description. The data loading nature of N2 remains the same as of N1 (subsection 1.1 of text S2). The general architecture has a pipeline similar to the continuous approach setup, with the image processing backbone here being a convolutional residual network with 50 layers of depth (ResNet-50, (He et al., 2015)), followed by a projection head of MLP with ReLU activations (Fukushima, 1975) and a linear layer. Therefore, similar to Figure S2.1 (Schematic diagram of N1), there are two branches. For the upper branch, the features obtained at the end of the pipeline (like $Z_s$ in
the continuous approach) are clustered using spherical k-means (where k=7), and features are allocated a pseudo-label (L) according to their closest centroid. Further, the features obtained from the lower branch are compared with the calculated upper branch centroids using cosine distance ($D_L$). Finally, L from the upper branch and $D_L$ from the lower branch are inputs of the cross-entropy loss function as discussed in subsection 1.5 of text S2 and is progressively minimized during training. We call the labels as pseudo-labels during the training stage as they can change to minimize the loss function better. Finally, at the end of the training, we collect the labels for each satellite image and further evaluate their separation using auxiliary datasets.
S3 Identify the optimal class

Figure S3 (Metric scores). Results of three different metric scores of distortion, silhouette, and Calinski-Harabasz, shown along with varying cluster numbers along the abscissa. The vertical-dashed line is drawn at cluster 7, which shows the chosen inflection point for the optimal cluster.

Text S3: Determination of optimal cluster number

We apply the following metrics to two-dimensionally reduced representations (using tSNE) on $h_j$ from N1 to identify the best optimal cluster:

1. **Distortion metric**: The distortion metric considers the cluster’s tightness by computing the sum of squared distances (SSD) from each point to its assigned center, which tends to decrease toward 0 as we increase the number of clusters (K). This shows an exponential shape leveling off such that the shape of the curve results in an elbow, but
the optimal cluster or the point of inflection represents the point where adding additional clusters stops adding useful information. Also, adding clusters beyond the inflection point also makes the clusters harder to separate; thus, we start to observe diminishing returns by increasing $k$. The elbow blue line curve in figure S3 (Metric scores) shows $k = 7$ as the sweet spot of optimal clustering.

2. **Silhouette metric:** Apart from taking cluster closeness into account, this metric also considers distances between points of one cluster and the nearest other cluster center. This means that in order to have a good silhouette score, clusters generally need to be tighter and farther apart from each other. If the Silhouette coefficient for each point is close to 0, it means that the point is between two clusters; if it is close to -1, then that point is in the wrong cluster, and if it is close to +1, it is in the correct cluster. The average silhouette coefficient calculated for all 51,000 samples shows two local maxima at values of 0.37 ($k=3$) and 0.36 ($k=7$), as shown in Figure S3 (Metric scores). Note that the values are not close to one, meaning the cluster doesn’t lie very far from each other, further suggesting the continuous nature of cloud organizations.

3. **Calinski-Harabasz metric:** In comparison, the Calinski-Harabasz metric assesses the separation and compactness of the clusters. It denotes the ratio of the sum of inter-cluster dispersion and the sum of intra-cluster dispersion for all clusters. A good clustering result has a high Calinski-Harabasz Index value. The maximum lies at cluster 7, having a score of 43000.

In summary, the two metrics directs towards $k=7$, and the difference between the two maxima ($k=3$ and 7) in silhouette is insignificant. Therefore, we take the common agree-
ment of $k=7$ as the optimal cluster number and train N2 (section 2) from scratch using 7 clusters.
S4 Visualizing the internal layers of the trained network

Text S4 Here, we investigate whether N1 learns reasonable visual features of satellite images. This will help us to understand our network’s decision-making and may boost our confidence in the neural network’s final representations $Z_k$. From a human perspective, cloud system distributions may appear to be relatively chaotic and noisy, and while trying to decide their visual characteristics, we may pay attention to some or all of the following: the organizational semantics of convective organization, the semantics of the clear sky regions, deep convective cell distributions, open and closed cells, and shallow convection distributions. Similarly, to build trust in the network’s performance, it is crucial to see what the trained N1 architecture has learned to pay attention to when deciding the features $h_j$ of cloud system distributions.
Figure S4 (Visualization of different layers). Four cloud systems with different organizations are selected as examples. Their respective self-attention maps from the final head of the teacher ViT trained with 8 x 8 patches are shown in layers 1 - 6. The color bar indicates the range of the Gaussian error linear units (GELU) activation function for the activation maps. Higher values indicate more important features. All experiments are run with a default of six self-attention heads.
Given a satellite image, the activation space in a neural network allows us to visualize whether a neuron should be activated, indicating what part of the image is important for the network. The self-attention layers in ViT try to decompose the input samples and learn relatively independent features. Thus, this experiment aims to see whether the activation space reveals the abstract patterns that we, as humans, can make sense of while deciding the feature's importance. In this setup, we use a single satellite image sample and pass it through the trained model, freezing the weights. The granularity (N x N), or the number of pixels in a single patch, is controlled by the patch size, which is 8 x 8 pixels in this experiment.

Figure S4 (Visualization of different layers) shows that layer one activates at the dominant convective cells and deactivates at thin spread-out convection while layer 2 activates the thin spread convection. Layer three seems to try to learn and activate the clear sky features. In contrast to layer one, layer four activates the rest of the prominent convections. Like layer two, layer five tries to look at the rest of the thin-spread convection. Layer six is uncertain and is not obvious to our eyes, and it may somehow try to deactivate for all the clear sky regions in the majority of cases and look for boundary semantics in the satellite image. Examining other example cases shows the same consistency, and therefore, it can be concluded that although the cloud system distributions are different, each attention map has learned to pay attention to relatively different, consistent, sensible semantics of the cloud systems distribution and further indicates that we can trust the embedding space of the network.
S5 Environmental characteristics of human labels and neighbors

Figure S5. Comparison of 52 human labels (hl) environmental conditions with their nearest 30 neighbors (nn) using ERA-5. The top to bottom rows shows weighted-average and standard deviation profiles of cloud water content (clwc, kg kg$^{-1}$), cloud cover (cc), and relative humidity (rh, %) with the exception of cc variability shown in the interquartile range.

Text S5 Figure 3.c in section 4.2 of the main manuscript showed the occurrences of 30 nearest neighbors of human-labeled satellite images (mentioned as human crops below).
with machine-identified seven classes. Here, we aim to assess their existing environmental conditions. This complementary experiment can further help to trust human crops’ relative positions in the feature space. If the human crops and the neighbors have a similar homogenous distribution of their physical properties, this implies that the human crops are in the consistent region of the feature space. Here, we take the ERA-5 vertical profile of cloud water content, cloud cover, and relative humidity (Fig. S5) to compare the weighted averaged vertical profiles between human labels and their 30 nearest neighbors. When calculating these properties for human-labeled scenes, we weigh them with the level of agreement. In this way, the contribution of well-agreed organizations will contribute more than less agreed cloud organizations. We observe that there is hardly any difference in the vertical profiles except for the relative humidity of sugar and cloud cover for flowers. This may be due to quantitatively using 30 times more data.

References


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