

# Unsupervised clustering identifies thermohaline staircases in the Canada Basin of the Arctic Ocean

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## METHODS PAPER

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## Abstract

Thermohaline staircases are a widespread stratification feature that impact the vertical transport of heat and nutrients and are consistently observed throughout the Canada Basin of the Arctic Ocean. Observations of staircases from the same time period and geographic region form clusters in temperature-salinity ( $T-S$ ) space. Here, for the first time, we use an automated clustering algorithm called the Hierarchical Density-Based Spatial Clustering of Applications with Noise (HDBSCAN), to objectively identify individual well-mixed staircase layers in data from Ice-Tethered Profilers (ITPs). Our method only requires prior knowledge of the typical layer thickness and expected salinity range of staircases. We compare our method to two previous studies that used less objective approaches to identify layers, and reproduce several results including the mean lateral density ratio  $R_L$  and that the difference in salinity between neighboring layers is a magnitude larger than the salinity variance within a layer. We find that we can accurately and automatically track individual layers in staircases across time and space between different profiles. In evaluating the algorithm's performance, we find evidence of different physical features, namely splitting or merging layers and remnant intrusions. Further, we find a robust dependence of  $R_L$  on pressure, whereas previous studies have reported constant  $R_L$ . Our results demonstrate that clustering algorithms are an effective and objective method of identifying staircases in ocean profile data.

## Impact Statement

Clustering algorithms are unsupervised machine learning methods that are used across many areas of data science. The use of such methods can automate the identification of certain features, thus allowing for analysis of datasets that are too large to analyze manually. Here, we show that a particular clustering algorithm called HDBSCAN can be used to automatically identify thermohaline staircases in hydrographic profiles from the Arctic Ocean. Compared to previous detection methods, HDBSCAN has the advantages of requiring minimal prior knowledge and of automatically connecting individual staircase "steps" across different hydrographic profiles. We expect that this method could be applied to many similar datasets, offering a straightforward way to identify and track layers in thermohaline staircases across the world's oceans.

## 1. Introduction

Thermohaline staircases, formed by differential diffusion rates of heat and salt, appear as a series of vertically well-mixed horizontal layers each separated by thin, strongly stratified interfaces. These structures have been observed throughout the world's oceans [43] as well as in saline lakes [27], while related double-diffusive staircases are thought to occur in gas giants such as Jupiter and Saturn [1, 32].

In particular, they are well known to occur in the Arctic Ocean [40, 16, 21]. Around 250 to 800 meters below the surface of the Arctic Ocean, there is a layer of water originating from the Atlantic, which is warmer and saltier than the topmost layer that is in contact with the sea ice above [40]. The core of the Atlantic Water (AW) is defined as the maximum subsurface temperature and is generally at a depth of 400 meters. Above this depth, in a region in which both temperature and salinity increase downwards, lie the Lower Halocline Waters (LHW) where the staircases are found [16].

Most of the world's oceans are *alpha* oceans which are stratified by temperature, with the warmest waters at the surface and colder waters at depth; this is in contrast to *beta* oceans such as the Arctic which are primarily stratified by salinity, and therefore the warm, salty AW is stable at depth [4]. Historically, the density stratification above the AW core has been strong enough to insulate surface waters from the warmth at depth [37]. However, the lower sections of Arctic staircases have been disappearing in recent years [21], indicating changes to this stratification. This change could have major consequences because if the heat in the AW were able to reach the surface, it is estimated that all Arctic sea ice would melt within five years [42]. Indeed, Arctic sea ice is steadily disappearing [6] and exposure to heat from below, in addition to the warming atmosphere above, would accelerate this decline [42]. Given their potential role in modulating the Arctic climate, it is important to be able to accurately identify thermohaline staircases in observations.

The first recorded observation of thermohaline staircases in the Arctic Ocean was made in 1969 at Ice Island T-3 [24]. This iceberg, located somewhat northeast of the Canada Basin (often defined as 72–84°N, 130–155°W, see e.g. Peralta-Ferriz and Woodgate [31]) was the site of dozens of hydrographic profiles that contain clearly visible staircases [25, 26, 23]. Subsequent observations have consistently indicated the presence of staircases in the Canada Basin, including from data collected during the Arctic Internal Wave Experiment (AIWEX) [28, 29, 30] and the Surface Heat Budget of the Arctic (SHEBA) experiment [36]. The frequency of such observations increased dramatically in 2004, when the introduction of autonomous Ice-Tethered Profilers made possible the continuous, year-round sampling of the Arctic Ocean water column [41].

Although many early studies identified staircases by visual inspection, the recent increase in available data has spurred researchers to turn to algorithmic approaches. Timmermans et al. [40] defined a point in a hydrographic profile to be within a well-mixed layer (henceforth for brevity simply “layer”) when the local vertical potential temperature gradient  $\partial\theta/\partial z$  is below  $0.005^\circ\text{C m}^{-1}$ , roughly an order of magnitude smaller than the overall gradient for a typical profile. They then manually sorted these points into different layers. Shibley et al. [37] extended this idea by including additional conditions. For each experiment, they manually determined different threshold values on both  $\partial\theta/\partial z$  and on the temperature difference between neighboring points. After identifying layers in this way, those authors only considered staircases that consisted of at least three layers. Van der Boog et al. [44] developed a staircase detection algorithm based on similar principles, but chose threshold values of vertical density gradients that were expected to be applicable to staircases in all of the world's oceans, not just the Arctic. Specifically, they set a vertical gradient threshold of  $\partial\sigma_1/\partial p \leq 0.0005 \text{ kg m}^{-3} \text{ dbar}^{-1}$  where  $\sigma_1$  is the density anomaly referenced to 1000. Then, from the subset of data that meets that condition, only mixed layers with a maximum variation of density anomaly of  $0.005 \text{ kg m}^{-3}$  or less, and whose neighboring interfaces had thicknesses of 30 dbar or less, were considered. Using a similar approach, Lu et al. [16] first defined the intersections between layers and interfaces as locations where the difference in the potential temperature gradient between two neighboring points is greater than  $0.003^\circ\text{C m}^{-1}$ , then disregarded the points within the interfaces. However, with the layer points that remained, those authors then followed the work of Padman and Dillon [29] and used valleys in histograms of salinity to guide their choice of boundaries between layers, some of which were manually adjusted.

All of these techniques first find a subset of the data points that are likely within layers based upon vertical gradient thresholds. This approach requires both sufficient knowledge of the staircases properties in order to select appropriate thresholds, as well as data with sufficient vertical resolution to accurately estimate the gradients. Furthermore, all these techniques, except for the van der Boog et al. [44] algorithm, require some amount of manual intervention to produce a final dataset of staircase

layers. These limitations motivate the search for a more objective, automated, and general approach to thermohaline layer detection.

Many studies, notably Timmermans et al. [40], have observed that a collection of profiles that includes well-mixed layers, such as density staircases, is associated with clustered patterns when plotted in temperature-salinity ( $T$ - $S$ ) space [35, 41, 46, 2]. These patterns occur where a staircase is present because all data points within a particular layer have approximately the same temperature and salinity values as other observations from the same layer, regardless of their vertical position within the layer. This fact suggests that staircases could be detected by directly identifying clusters in  $T$ - $S$  space.

Clustering algorithms are a type of unsupervised machine learning, and have been previously used in a variety of different oceanographic applications [38]. Examples include grouping observations from freely-drifting instruments in the Nordic Seas [14], studying surface wave variability in the North Atlantic [8], classifying the heat content of hydrographic profiles [18], resolving trapping in mesoscale eddies [17], defining spatial regions for Southern Ocean temperature profiles [12], detecting ENSO events [11], finding hot spots for mixing in the Southern Ocean [34], and identifying shifts in the North Atlantic circulation [7]. However, to our knowledge, they have never before been used to identify thermohaline staircases.

Here, we develop a method based on the Hierarchical Density-Based Spatial Clustering of Applications with Noise or HDBSCAN algorithm [3], to detect thermohaline staircases in Arctic hydrographic profiles. This method has several advantages: It identifies and automatically connects staircases across large hydrographic datasets, does not require fine vertical resolution, and requires only minimal prior knowledge of staircase properties, namely typical layer thicknesses and the expected salinity range. Most importantly, it exhibits excellent performance with no operator intervention once a handful of controlling parameters are set, and is thus suitable for application to very large datasets as well as being exactly reproducible. The purpose of this paper is to present this method, and so we will note possible implications of our results but will not explore them in great detail.

The structure of this paper is as follows. First, in Section 2, we introduce and explain our choice of the datasets used in our analysis. In Section 3, we introduce HDBSCAN and describe how we use it to identify staircases and how we choose the input parameters. Then, in Section 4, we apply this method to data from two different Ice-Tethered Profiler experiments, focusing on results that reproduce those from the studies of Timmermans et al. [40] and Lu et al. [16], hereafter denoted as T08 and L22, respectively. Finally, in Section 5, we use the comparison between our results and those of T08 and L22 to evaluate the performance of the clustering algorithm and give recommendations on when and how it can be best used to identify staircases.

## 2. Data

Ice-Tethered Profilers (ITPs) are automated, vertically profiling instruments that are connected via a wire cable to a surface buoy on an ice floe [41]. The wire extends from the surface, through the ice, down to depths of 500–800 m. The profiler travels up and down the wire roughly two to three times a day collecting high-resolution ( $\sim 25$  cm) measurements of salinity, temperature, and pressure with a salinity precision of  $\pm 0.005$  g / kg and a temperature precision of  $\pm 0.001$  ° C [40, 37, 2]. Each traverse, alternating up or down, is recorded as a separate profile.

In this paper, data from two different ITP experiments, ITP2 and ITP3, are analyzed; see Table 1 for a summary. Because the measuring instruments are located at the top of the profiler, we use only the up-going profiles in order to avoid the known distortion caused by the wake of the profiling unit in the down-going profiles [37]. Figure 1 shows the locations of all up-going profiles for each of the two ITP experiments. We choose to analyze ITP2 and ITP3 in particular in order to reproduce several results of T08 and L22, respectively.

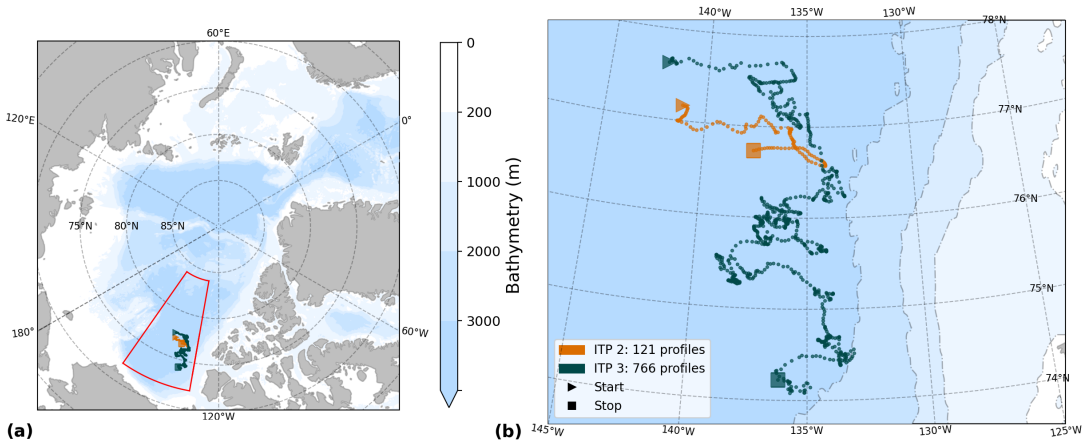
At this point we note some choices in the study relative to those of T08 and L22. Here we choose to work with pressure, a directly measured quantity, while both of those studies use depth, which is derived from pressure; as the conversion between pressure and depth is linear, this difference does not affect our



**Table 1.** Details of the Ice-Tethered Profilers (ITPs) used in this study.

| ITP | Start Date | Days in Operation | Starting Position       | Along-path Distance | Longest Span <sup>1</sup> | Total Profiles | Up-going Profiles |
|-----|------------|-------------------|-------------------------|---------------------|---------------------------|----------------|-------------------|
| 2   | 2004/8/19  | 40                | 77° 10.4'N, 141° 13.0'W | 390 km              | 191 km                    | 242            | 121               |
| 3   | 2005/8/23  | 382               | 77° 36.1'N, 142° 11.8'W | 2541 km             | 441 km                    | 1531           | 766               |

<sup>1</sup>The maximum distance between any two, not necessarily consecutive, profiles



**Figure 1.** A map showing the locations of all profiles used from ITPs 2 and 3, showing the whole Arctic in (a) and a zoomed-in view in (b). The red box designates the Canada Basin as defined by Peralta-Ferriz and Woodgate [31].

results or comparisons. Also note that although both of those earlier studies use potential temperature  $\theta$ , we choose instead to use conservative temperature  $\Theta$ , as recommended by TEOS-10 [19]. For the range of temperatures and salinities in the data we analyze, the difference  $|\theta - \Theta|$  is a systematic shift that is always less than  $0.05^\circ\text{C}$ . Because this shift is relatively constant, our results are not sensitive to this choice. Furthermore, TEOS-10 recommends using absolute salinity  $S_A$  over practical salinity  $S_P$ . Our results do not change significantly using one versus the other (see Supplementary Materials), so we choose to use  $S_P$  to make direct comparisons to the salinity ranges used by T08 and L22.

Staircases are only found in certain vertical ranges of the water column. However, as noted by L22, the salinity values of the layers are much more consistent across different profiles than their pressure or temperature characteristics, so we focus our analyses on a specific salinity range for each ITP. While choosing a range that is too small will potentially miss layers, running the algorithm on a liberally large range will not only take longer but may also return some clusters that do not correspond to meaningful thermohaline staircase layers. We therefore choose the salinity ranges which we know, from the earlier studies, contain the layers that we wish to identify, specifically  $34.05\text{--}34.75\text{ g/kg}$  for ITP2 following T08 and  $34.21\text{--}34.82\text{ g/kg}$  for ITP3 following L22.

As discussed in more detail below, the clustering algorithm does not distinguish between the different times and locations at which different profiles were taken. It follows that a dataset to be analyzed should not span larger temporal or spatial scales than the scales the staircases are known to be coherent across. T08, who analyzed much of the same data we do, found staircases that spanned the entire Canada Basin (approximately 800 km) and lasted at least 2 years. We define the longest span as the maximum distance between any two, not necessarily consecutive, profiles. We find the longest span ( $\leq 441\text{ km}$ ) and duration ( $\leq 382\text{ days}$ ) of the two ITPs we analyzed, see Table 1, are indeed smaller than the expected staircase coherence scales.

### 3. Methods

#### 3.1. The HDBSCAN clustering algorithm

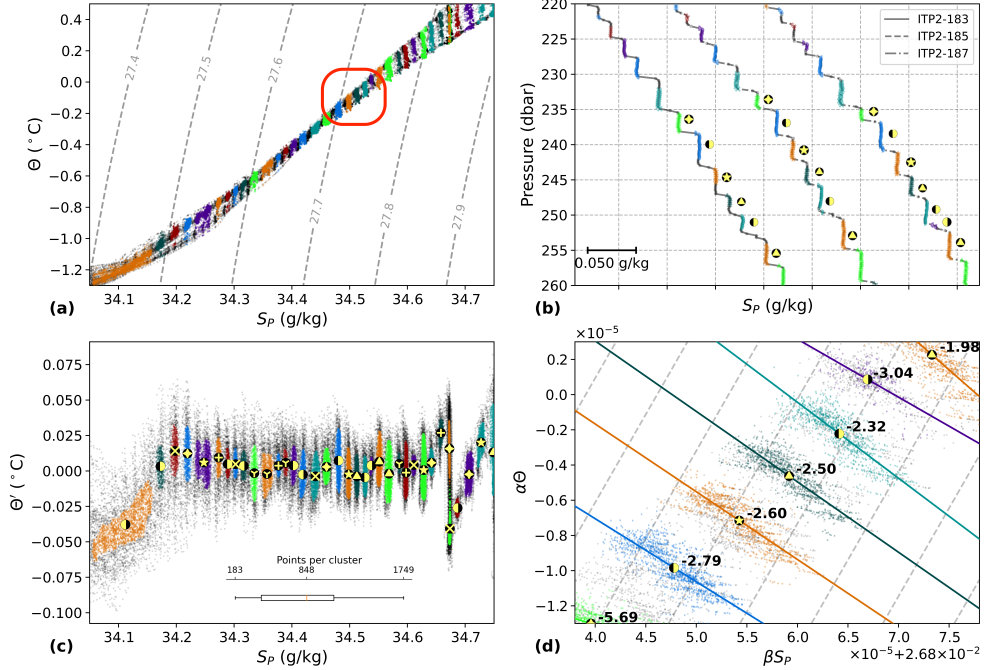
To identify  $T$ – $S$  clusters as evidence for staircases within the ITP data, we use the HDBSCAN algorithm to group spatial data into clusters based on the relative densities of data in different regions. Note that, within the context of clustering algorithms, we refer to “density” as the relative number of data points in a certain region of parameter space and not physical density  $\rho$  or density anomaly  $\sigma$ . HDBSCAN has one required input parameter  $m_{pts}$ , which is a threshold for the minimum number of points within a cluster. Algorithm-identified clusters in the ITP data are expected to correspond to staircase layers, with some exceptions as detailed in Section 3.3.

We choose HDBSCAN over other types of clustering algorithms for several reasons. Many previous oceanographic studies used partitioning algorithms such as  $k$ -means [14, 8, 11] or Gaussian mixture models [18, 12, 34, 7]; however, partitioning algorithms require one to specify the number of clusters *a priori*, which is not known for our application. The first reason for choosing HDBSCAN is that it does not have this requirement [9, 12]. Second, HDBSCAN allows points that lie outside a cluster to be categorized as “noise.” In our case, this is important because points in an interface between layers should not be assigned to any cluster. Third, unlike DBSCAN, which uses the same density threshold for all clusters throughout the domain [9, 3], HDBSCAN creates a hierarchy of clusterings with different thresholds and can therefore correctly identify clusters that vary significantly in both the number of points per cluster and the densities of points within the clusters [20]. Fourth, HDBSCAN can correctly identify arbitrarily shaped clusters, whereas partitioning algorithms like  $k$ -means generally find center-defined clusters, which, because points are assigned to clusters based on their distance from the cluster’s center point, are only equipped to find globular, or convex, clusters [10, 9]. This is important because the shapes of clusters associated with thermohaline staircases are not necessarily globular. Lastly, HDBSCAN only requires one input parameter ( $m_{pts}$ ) to be specified, implying limited subjectivity. All other possible input parameters were set to the default values provided by the Python package “hdbscan” following the recommendation of the authors of the algorithm [3, 22].

Having chosen a clustering algorithm, we now turn to specifying the two-dimensional space within which the clustering algorithm will operate. Figure 2(a) shows data from ITP2 in  $\Theta$ – $S_P$  space, where discrete groups of points, associated with individual layers and spanning multiple profiles, are apparent; these are colored according to their eventual partitioning into clusters. Note the occurrence of occasional gaps in  $\Theta$  values, seen in the salinity ranges 34.16 – 34.30 and 34.65 – 34.74 g/kg. These result from the uneven spatial coverage of the meandering drift path of the ITPs (see Figure 1) together with the tendency for the temperature to vary more horizontally within a particular layer than salinity [16]. In order to avoid HDBSCAN splitting such groups of points into multiple clusters for the same layer, for each temperature profile  $\Theta(z)$ , we define the local anomaly as

$$\Theta'(z) = \Theta(z) - \frac{1}{\ell} \int_{z-\ell/2}^{z+\ell/2} \Theta(z') dz' \quad (3.1)$$

where  $\ell$  is the width of a rectangular moving average window. Presenting the ITP2 data in  $\Theta'$ – $S_P$  space rather than  $\Theta$ – $S_P$  space, as in Figure 2(c), leads to groups that are more centered around zero along the temperature axis, without notable gaps. We choose to work in this space as it will allow HDBSCAN to group points more accurately. We also confirmed the difference between using  $\Theta$  or  $\theta$  and  $S_P$  or  $S_A$  did not significantly affect the results. Finally, we mention that HDBSCAN is sensitive to the aspect ratio of the axes; however, because the results were found to be satisfactory, we did not investigate this dependency.

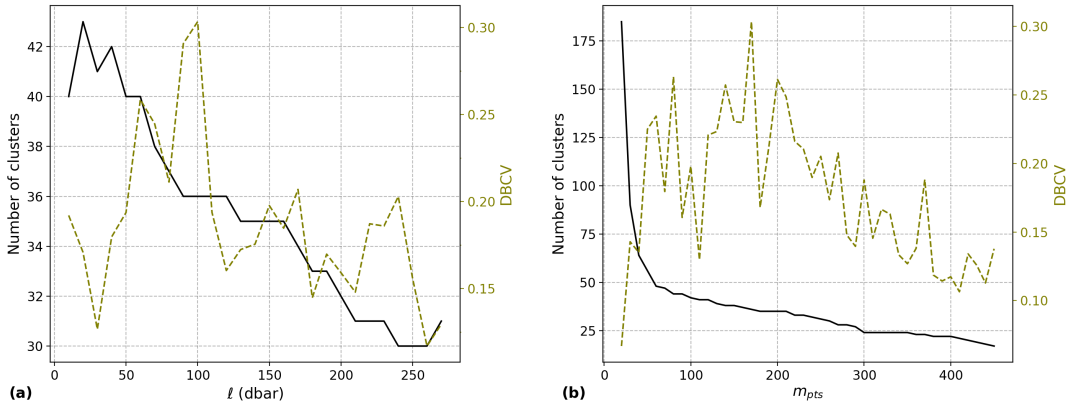


**Figure 2.** Results from the clustering algorithm with  $m_{pts} = 170$  and  $\ell = 100$  dbar run on 53042 data points in the salinity range 34.05–34.75 g/kg from all up-going ITP2 profiles. (a) The data in  $\Theta$ – $S_P$  space with dashed lines of constant potential density anomaly ( $\text{kg m}^{-3}$ ) referenced to the surface. The red box bounds the clusters marked in panels (b) and (d). (b) Profiles 183, 185, and 187 from ITP2 in a limited pressure range to show detail. Each profile is offset in  $S_P$  for clarity. (c) The spatial arrangement used as input for the algorithm where the gray points are noise and each color-marker combination indicates a cluster. The same color-marker combinations are used in each panel and the markers in panels (c) and (d) are at the cluster average for each axis. (d) A subset of the data in  $\alpha\Theta$ – $\beta S_P$  space with the linear regression line and inverse slope ( $R_L$ ) noted for each individual cluster and with dashed lines of slope  $\alpha\Theta/\beta S_P = 1$ .

### 3.2. Selecting values of input parameters

It remains to choose values for the method parameters. The HDBSCAN algorithm is deterministic; that is, given the same arrangement of input data and the same value of the  $m_{pts}$  parameter, it will find the same clusters every time. The exact arrangement of data in  $\Theta'$ – $S_P$  space that we feed into the algorithm depends on three factors: (1) the set of profiles that we include, (2) the salinity range that we decide to analyze, and (3) the window width  $\ell$  used to calculate the local anomaly of conservative temperature  $\Theta'$  in Equation (3.1). We discussed our method of selecting the profiles and salinity range previously in Section 2. Here, we explain how we select values for  $\ell$  and  $m_{pts}$ .

The results of a clustering algorithm can be judged on the basis of either external or internal validation. External validation methods involve comparing the clustering results to an external “ground truth,” while internal validation methods use the data themselves to provide a measure of quality for the clustering [22]. Although we compare our results with other studies, see Section 4, these do not constitute external validations since layer labeling for individual data points, necessary to make direct comparisons, is not available from those studies. We therefore tune our selection of  $\ell$  and  $m_{pts}$  using Density-Based Clustering Validation (DBCW) [22] as an internal validation. DBCW considers good clustering solutions to be those in which the lowest-density regions within the clusters are still denser than the highest-density regions of the surrounding noise points.



**Figure 3.** A parameter sweep showing the number of clusters found (solid lines) and DBCV (dashed lines) in ITP2 as a function of (a) 27 different values of  $\ell$  with  $m_{pts} = 170$  and (b) 44 different values of  $m_{pts}$  with  $\ell = 100$  dbar.

To evaluate algorithm performance, we performed a parameter sweep through different values of  $\ell$  and  $m_{pts}$ , and present the number of clusters found together with the DBCV scores in Figure 3. For the  $\ell$  dependence, see Figure 3(a), we find a downward trend in the number of clusters as  $\ell$  increases. DBCV scores tend to be larger in the middle of the  $\ell$  range, with the highest score occurring for  $\ell = 100$  dbar. We may also note that the choice of  $\ell$  shapes a large-scale feature of the  $\Theta'$ - $S_P$  plots. In Figure 2(c), a zig-zag pattern of increasing, rapidly decreasing, and then increasing again  $\Theta'$  is seen in the range of  $S_P \approx 34.63$ – $34.72$  g/kg. This pattern is due to the presence of the AW subsurface temperature maximum in  $\Theta$  profiles; it disappears when  $\ell$  is small while becoming more exaggerated for larger  $\ell$  (see Supplementary Materials). Staircases in the Canada Basin during this time period are known to have layers of around 5 m in height, or 5 dbar in pressure [40, 16]. The choice  $\ell = 100$  dbar, where the largest DBCV score occurs, thus corresponds to approximately twenty times the typical layer thickness. This value is found to be large enough that the staircases are completely smoothed out yet small enough that the features outside the analyzed pressure range do not significantly affect the moving average.

We now turn now to  $m_{pts}$ , which under the default settings of HDBSCAN sets the minimum number of points in a cluster [3]. If the value of  $m_{pts}$  is too small, the algorithm may erroneously split a cluster that represents one layer into multiple, smaller clusters, while a too-large value of  $m_{pts}$  would lead to the incorrect grouping of multiple discrete layers into a single cluster. Note that this upper bound on a reasonable  $m_{pts}$  depends greatly on the number of data points given to the algorithm: the more data points the algorithm is given, the higher the value of  $m_{pts}$  can reasonably be set. In the parameter sweep of Figure 3(b), we find the number of clusters decreases rapidly until  $m_{pts} \approx 60$ , then decreases at a much slower rate, while the highest DBCV scores occur for intermediate values of  $m_{pts}$ . As with  $\ell$ , we choose the value of  $m_{pts}$  having the highest DBCV score. For ITP2, this led to our selection of  $m_{pts} = 170$ .

Running HDBSCAN on ITP2 using the procedure outlined above with the choices  $\ell = 100$  and  $m_{pts} = 170$  leads to the clusters presented in Figure 2. Following the same parameter selection process for ITP3, we obtain the values  $\ell = 100$  dbar and  $m_{pts} = 580$  (see Supplementary Materials). Table 2 summarizes our input parameter choices and the resulting number of clusters and DBCV values for both ITP2 and ITP3.

### 3.3. Evaluating the clustering algorithm results

The DBCV score gives a measure of quality for the clusters in terms of their densities of points relative to the surrounding noise. However, DBCV does not take into account the properties of the clusters that we expect from the physical situation of staircases, such as their spans in  $\Theta$  and  $S_P$  or how far they are

**Table 2.** The values of parameters used to run the clustering algorithm over both datasets.

| ITP | Study to Reproduce     | Input Parameters   |                       |          |           | Results                         |        |
|-----|------------------------|--------------------|-----------------------|----------|-----------|---------------------------------|--------|
|     |                        | Number of Profiles | Salinity Range (g/kg) | $\ell$   | $m_{pts}$ | Number of Clusters <sup>1</sup> | DBCv   |
| 2   | Timmermans et al. [40] | 121                | 34.05–34.75           | 100 dbar | 170       | 36 (31)                         | 0.3034 |
| 3   | Lu et al. [16]         | 766                | 34.21–34.82           | 100 dbar | 580       | 43 (40)                         | 0.3862 |

<sup>1</sup>The first number is the total number of clusters found by the algorithm. The second is the number of clusters that were neither outliers in  $IR_S$  nor  $R_L$ .

from neighboring clusters. We therefore present two metrics to help predict whether each cluster will accurately represent what we expect from layers within staircases: the lateral density ratio  $R_L$  and the normalized inter-cluster range  $IR$ .

The relative strength of horizontal variations in salinity and temperature along the  $i$ th layer is described by the lateral density ratio

$$R_L^i = \frac{\beta \Delta S_P}{\alpha \Delta \Theta}, \quad (3.2)$$

where  $\beta = \rho^{-1} \partial \rho / \partial S_P$  is the haline contraction coefficient,  $\alpha = -\rho^{-1} \partial \rho / \partial \Theta$  is the thermal expansion coefficient, and  $\Delta S_P$  and  $\Delta \Theta$  are the variations in salinity and temperature, respectively, along a particular layer [33, 2]. We estimate  $R_L$  by finding the inverse slope of the best-fit line through each cluster in  $\alpha \Theta - \beta S_P$  space (see Figure 2(d)) [40, 5]. These lines are found using Orthogonal Distance Regression, which is more suitable than ordinary least squares in our case due to the presence of variability along both the  $\alpha \Theta$  and  $\beta S_P$  axes [45]; however, both methods yield similar results (not shown).

$R_L$  quantifies the relative importance of  $S_P$  and  $\Theta$  for the density of that layer [40, 2] and is known to be directly related to the ratio of the vertical fluxes of salinity and heat within a staircase [2]. The relative constancy of  $R_L$  values across time and space has been interpreted as reflecting the remarkable degree of lateral coherence of staircase layers [41]. Note that the lateral density ratio  $R_L$  is distinct from the density ratio,  $R_\rho$ , which is defined using the same equation (3.2) but with  $\Delta S_P$  and  $\Delta \Theta$  taken in the vertical direction [37]. For a cluster capturing a single complete layer, we expect the value of  $R_L$  to lie within a previously documented range [40]. Therefore, if a value of  $R_L$  lies significantly outside of this range, the cluster either reflects the erroneous grouping multiple layers into a single cluster, or else a physical merging or splitting of layers as discussed in Section 4.2.

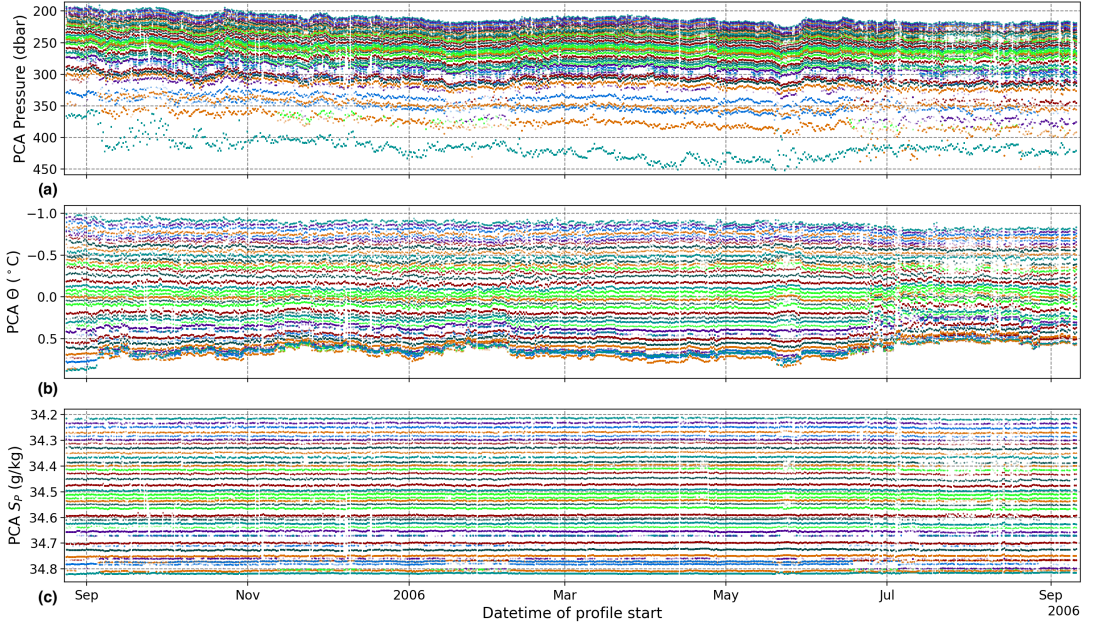
We also define a measure of the relative spread of a variable, such as temperature or salinity, within a cluster in comparison with the differences between adjacent clusters. Ordering the clusters sequentially in density, the normalized inter-cluster range for the  $i$ th cluster is given by

$$IR_v^i = \frac{v_{max}^i - v_{min}^i}{\min(|\bar{v}^i - \bar{v}^{i-1}|, |\bar{v}^i - \bar{v}^{i+1}|)}, \quad (3.3)$$

where  $i - 1$  and  $i + 1$  denote the adjacent clusters to either side,  $v$  is the variable of interest (i.e., pressure,  $\Theta$ , or  $S_P$ ),  $v_{max}^i$  and  $v_{min}^i$  are the maximum and minimum values of the variable  $v$  within cluster  $i$ , and  $\bar{v}^i$  denotes the mean value of  $v$  for cluster  $i$ . The numerator is the span between the maximum  $v_{max}^i$  and minimum  $v_{min}^i$  within cluster  $i$ . The denominator is the span between the mean of that cluster  $\bar{v}^i$  and the mean of either the cluster above or below, whichever is smaller. For clusters at either end of the variable space, we take the denominator to be the span between the mean of the  $i$ th cluster and that of its single neighbor.

The inter-cluster range  $IR_v$  therefore quantifies the range of a given variable,  $v$ , within a cluster in comparison with the range to the nearest neighboring cluster. For a staircase, the salinity values within one layer are generally well separated from the salinity values of the neighboring layers [16]. Therefore,





**Figure 4.** The average (a) pressure, (b)  $\Theta$ , and (c)  $S_P$  for the points within each cluster for each profile (profile cluster average, PCA) across time. The clustering algorithm was run with  $m_{pts} = 580$  and  $\ell = 100$  dbar on 678575 data points in the salinity range 34.21–34.82 g/kg from all up-going ITP3 profiles.

we expect that the clusters with large  $IR_{S_P}$  could represent a part of a single layer that was erroneously divided into multiple clusters by the algorithm, or entirely different physical features, as discussed in Section 4.3.

We define outliers in both  $IR_{S_P}$  and  $R_L$  as points with a z-score (that is, the distance from the mean divided by the standard deviation) greater than two. While this approach is not guaranteed to find all erroneous clusters, outliers in  $IR_{S_P}$  and  $R_L$  give us an indication, based on simple and measurable physical characteristics, of particular clusters which may not represent a single, full layer and which therefore require closer inspection. Although such outliers could be manually adjusted to better capture single, complete layers, we take the approach of disregarding them when calculating statistics and trends.

## 4. Results

Now having presented the HDBSCAN clustering algorithm, our process of selecting  $\ell$  and  $m_{pts}$ , and metrics to identify erroneous clustering, we apply this method to data from ITP2 and ITP3.

### 4.1. Properties of detected layers

As a starting point, we examine the average value of pressure,  $\Theta$ , or  $S_P$  for each cluster found from profiles collected by ITP3. Inspired by L22, we plot those values over time in Figure 4. We find that the clustering algorithm is capable of tracking individual layers across hundreds of profiles collected over 382 days and 2541 km. A pattern emerges, where the pressures of individual layers appear to have more variability than temperature and salinity, consistent with T08. Moreover, we find that salinity varies less within a layer than between two neighboring layers, while the opposite is true for pressure and temperature (similar to L22; see their Figure 3). We find similar results for ITP2 (see Supplementary Materials).

**Table 3.** The median normalized inter-cluster ranges for the clusters for ITP2 and ITP3, calculated after removing outliers with  $z$ -score  $> 2$  in the respective variable.

|      | $\widehat{IR}_p$ | $\widehat{IR}_\Theta$ | $\widehat{IR}_{S_p}$ |
|------|------------------|-----------------------|----------------------|
| ITP2 | 8.394            | 4.087                 | 0.707                |
| ITP3 | 16.641           | 7.141                 | 0.927                |

More quantitatively, we find variations in salinity between clusters are approximately seven times larger than those within a cluster. That is, we compute the standard deviation of salinity within each cluster and find that the median is 2.2 mg/kg, while the median absolute difference between the average salinity of adjacent clusters is 15.4 mg/kg. This is in agreement with L22 who found inter-layer salinity variations to be an order or magnitude larger than those within a layer. Furthermore, the median normalized inter-cluster ranges (Equation 3.3) in Table 3 quantitatively confirm the qualitative patterns noted by T08 and L22 as  $\widehat{IR}_p, \widehat{IR}_\Theta > 1$  and  $\widehat{IR}_{S_p} < 1$  for both ITPs, where  $\widehat{\cdot}$  indicates the median.

#### 4.2. Outliers and splitting / merging layers

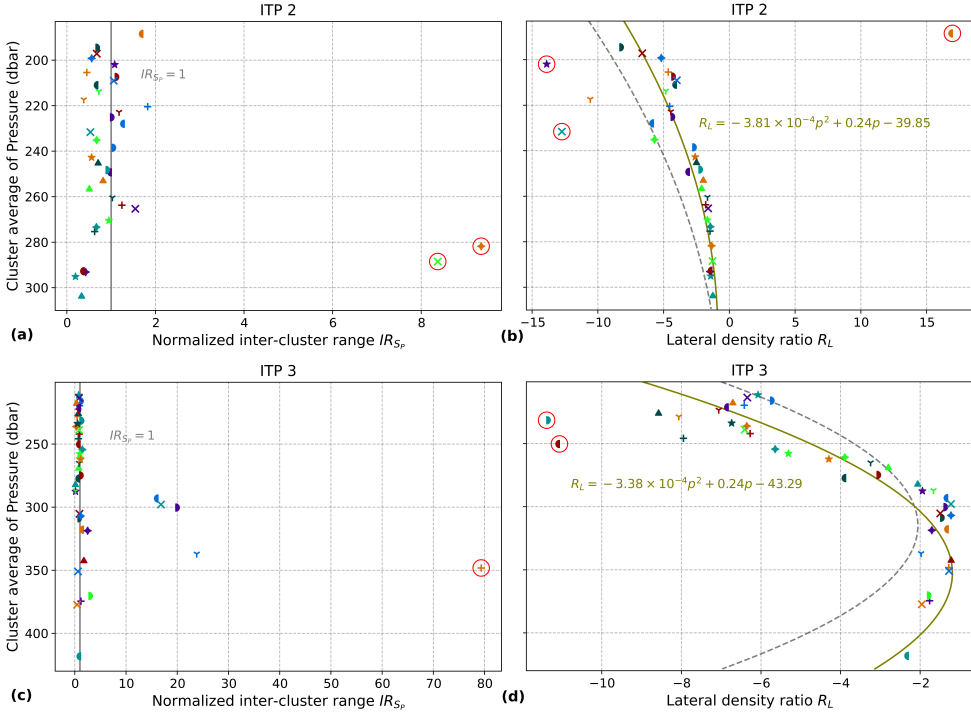
As discussed previously in Section 3.3, outliers have been identified in the inter-cluster salinity range  $IR_{S_p}$  as well as the lateral density ratio  $R_L$ . Figure 5 shows  $IR_{S_p}$  and  $R_L$  for both ITPs with outliers indicated by red circles. We find that these outliers can either be due to erroneous clustering or indicate the presence of different physical features such as the splitting or merging of thermohaline staircase layers, which is a well-known phenomenon [26, 29, 13].

We can learn more about these features from the illustrative sets of particular salinity profiles from ITP2 presented in Figure 6. Both sets of profiles span less than a week and we narrow the displayed pressure ranges so that the individual steps are visible. This figure shows that overall, the algorithm captures the layered structure very well, marking points within interfaces as noise. Nevertheless, it is imperfect. Near layer boundaries, the algorithm sometimes includes points from an interface within a cluster, and sometimes neglects to include points within a layer. Additionally, as seen in the first profile of Figure 6(b) around 236 dbar, the algorithm can also miss layers entirely, especially when the layer is particularly thin and only present in a small number of profiles. Occasional issues such as these are to be expected with any automated detection method.

Focusing on ITP2 as an example, we find two outliers in  $IR_{S_p}$  marked by an orange 4-pointed star and a green “x” in Figure 5(a). We can track the same clusters in Figure 2(c), indicated by orange or green dots with a 4-pointed star or a “x” at the center of the cluster. They both have an average  $S_p \approx 34.67$  g/kg but are separated in  $\Theta'$ . A series of individual salinity profiles associated with these outliers over approximately six days is shown in Figure 6(a). We find that these outliers correspond to a relatively thick single layer that was erroneously split across two clusters by the algorithm. We attribute this erroneous splitting to the zig-zag pattern in  $\Theta'-S_p$  space mentioned in Section 3.2 and note that it could be eliminated with a different selection of  $\ell$ . Although we can attribute these outliers in  $IR_{S_p}$  to an artifact of the method, there are other instances where such outliers indicate the presence of physical features, as we will discuss in Section 4.3.

Next, we examine outliers in  $R_L$ , defined in Equation 3.2, for ITP2, marked by red circles in Figure 5(b). These outliers correspond to clusters that appear to have multiple layers grouped together. For example, the outlier cluster marked by an orange half-circle in Figure 5(b) can be seen in Figure 2(c) spanning  $S_p = 34.054$ – $34.159$ , a much wider range than any other cluster. Similarly, in Figure 2(c), the outlier cluster marked by a purple star spans  $S_p = 34.233$ – $34.261$  and clearly encompasses what should be two distinct clusters. Some outliers in  $R_L$  are the result of erroneously clustering multiple layers together. On the other hand, the particular feature of the outlier cluster marked by a teal “x”, centered around 232 dbar with  $R_L = -12.7$  in Figure 5(b), indicates splitting or merging. As shown in Figure 6(b), it typically spans multiple stair steps, but the last few profiles it only spans a single, larger step.





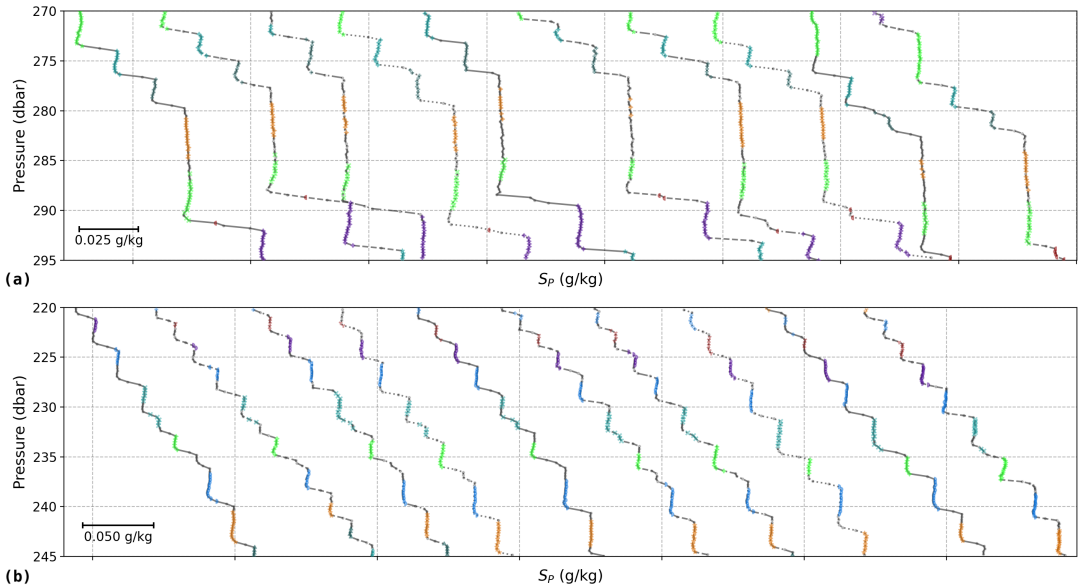
**Figure 5.** The value of each cluster’s normalized inter-cluster range for salinity  $IR_{S_p}$  in (a) and (c) and the lateral density ratio  $R_L$  in (b) and (d) as a function of the cluster’s average pressure. The colors and markers for ITP2 in (a) and (b) are the same as the clustering shown in Figure 2 and for ITP3 in (c) and (d), they are the same as shown in Figure 4. Markers circled in red indicate outliers with a z-score greater than 2. In (b), the solid curve is a 2nd-degree polynomial fit (equation given by the annotation) for the non-outlier points from ITP2 and the dashed curve is the same for ITP3. In (d), the solid curve is a 2nd-degree polynomial fit (equation given by the annotation) for the non-outlier points from ITP3 and the dashed curve is the same for ITP2.

This illustrates that we can use outliers in  $R_L$  to identify clusters that are not single, complete layers and to find instances of potential splitting or merging.

### 4.3. Remnant intrusions revealed by temperature

Direct comparisons with other layer detection methods can also be used to identify interesting physical features. To demonstrate this, here we directly compare average layer characteristics computed by HDBSCAN to those reported by L22, both using data from ITP3. L22 used 758 profiles from ITP3 while we used all 766 available up-going profiles. Based on the gaps in Figure 3 of L22, we believe that the eight missing up-going profiles are from July 2006. Figure 7 shows the average  $\Theta$  and  $S_P$  for each cluster found in our study and by L22 based on the values in their Table A1 after converting  $\theta$  to  $\Theta$ . We initially find 43 clusters and, after eliminating outliers in  $IR_{S_p}$  and  $R_L$  as described in Section 3.3, we find 40 clusters. While L22 identified only 34 thermohaline layers, we find close agreement between those and the clusters we found for  $S_P \lesssim 34.74$  g/kg. Below where this salinity occurs in the water column, we find five more clusters than L22.

The differences between these two results appears to be related to the presence of *remnant intrusions*, anomalous layers that are thought to represent an intermediate stage in staircase formation. Such features are known to appear near the bottom of staircases around the AW core and have been analyzed in detail



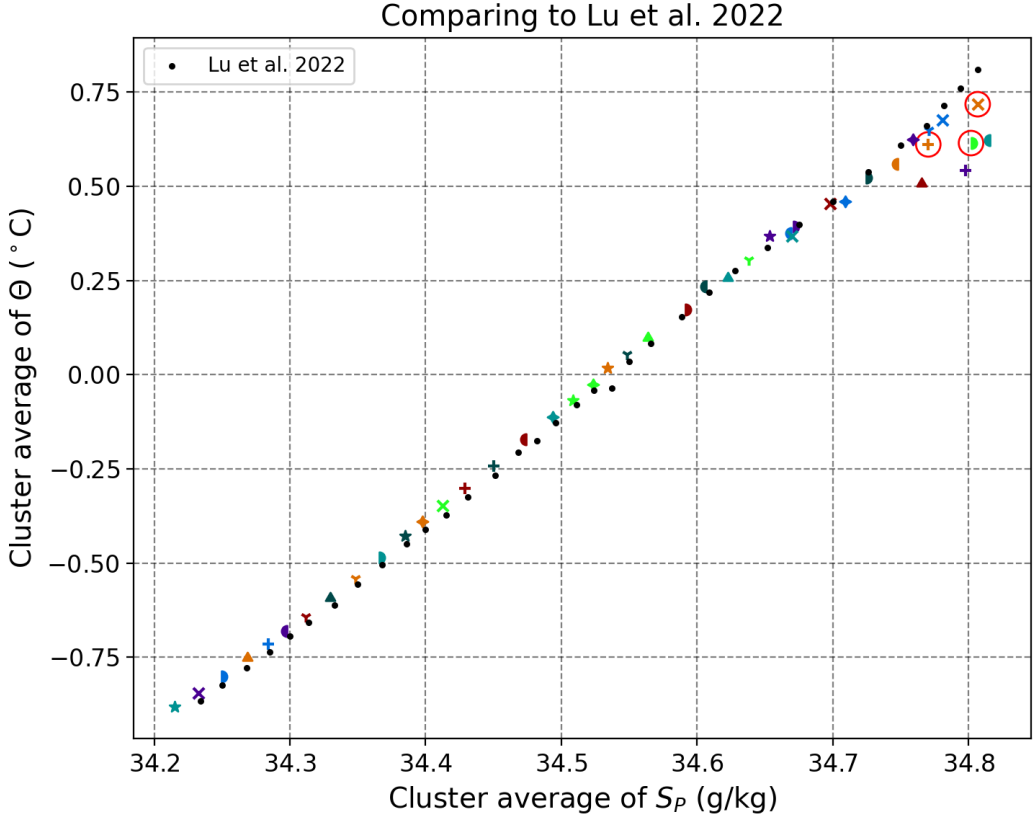
**Figure 6.** Individual  $S_P$  profiles from ITP2, chosen to show examples of outlier clusters in  $IR_{S_P}$  and  $R_L$ . (a) Profiles 67, 69, 73, 75, 81, 83, 91, 93, 97, and 99, collected between August 31 - September 5, 2004. (b) Profiles 87, 89, 95, 97, 99, 101, 103, 105, 109, and 111, collected between September 3-7, 2004. The colors and markers are the same as the clustering shown in Figure 2. The gray dots are noise points and the black lines show the profiles. Each profile is offset in  $S_P$  for clarity.

by Bebieva and Timmermans [2]. They are characterized by homogeneous salinity, which leads the method of L22 to treat them as single layers. However, they have a temperature structure that is inverted (warmer above colder) compared to the typical gradient within a thermohaline staircase. The warm and cold sections are distinct enough for the clustering algorithm to split the structure into multiple clusters, each of which is homogeneous in salinity and relatively homogeneous in temperature. Figure 8 shows an example of a remnant intrusion where the method of L22 gives results that differ from ours; the layer spanning approximately 320–340 dbar is constant in  $S_P$ , but decreases in  $\Theta$  with depth and is divided into two clusters using our method.

Such remnant intrusions exist between the active intrusions of the AW core and the staircase layers of the LHW. Staircases may be formed from intrusions but such features have distinctly different patterns of heat and salt flux than double-diffusively driven staircases [2]. The disagreement between our results and those of L22 highlights the difficulty of detecting remnant intrusions. While neither method is designed to automatically distinguish between these and staircase layers, the method presented here offers the opportunity to identify them when evaluating outlier clusters. Moreover, although Table 3 supports the suggestion by L22 that salinity is the most appropriate variable by which to identify staircase layers, the case of the remnant intrusions illustrates why it remains important to consider temperature as well.

#### 4.4. Dependence of $R_L$ on pressure

Lastly, we revisit Figure 5(b,d) where the distribution of points suggest a dependence of  $R_L$  on pressure. This is in contrast to previous studies which have found a constant  $R_L$  for the depth range we analyze [40, 41, 2]. For ITP2 in panel (b), after removing the five outliers indicated across panels (a) and (b), we use a second-degree polynomial fit to find  $R_L = -3.81 \times 10^{-4} p^2 + 0.24p - 39.85$ , where  $p$  is pressure, with a coefficient of determination  $R^2 = 0.67$ . For ITP3 in panel (d), we remove the three outliers in panels (c) and (d) then find quite the similar dependence of  $R_L = -3.38 \times 10^{-4} p^2 + 0.24p - 43.29$  with a

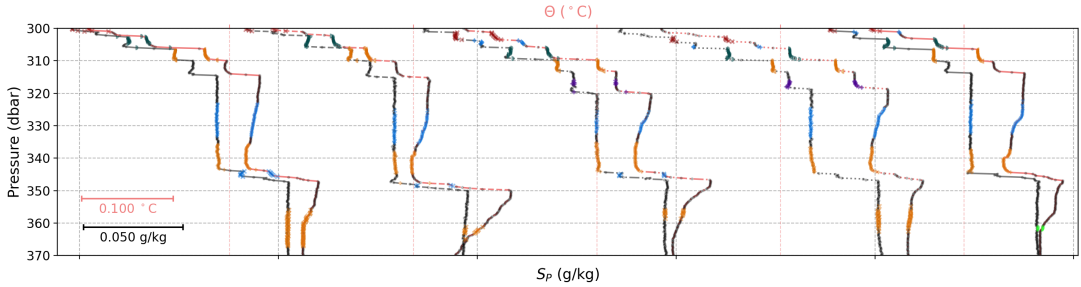


**Figure 7.** The average  $\Theta$  and  $S_p$  for the 34 layers found by Lu et al. [16] in black dots and for the 43 layers found in our study using data from ITP3 and the same colors and markers as in Figure 4. Clusters circled in red are outliers in either  $IR_{S_p}$  or  $R_L$ .

coefficient of determination  $R^2 = 0.84$ . Comparing these two curves in Figure 5(b,d), we find most of the difference can be explained by a downward shift of roughly 20 dbar in the upper water column to 50 dbar in the lower water column from ITP2 to ITP3. Note that a second-degree polynomial was chosen here as a simple parametric model to capture the apparent non-linear dependence of that  $R_L$  on pressure.

By contrast, T08 concluded there was no vertical dependence of  $R_L$ . They analyzed data from ITP1 through ITP6, which sampled the Canada Basin during the period from 2004 to 2007, and found a constant value of  $R_L = -3.7 \pm 0.9$ . Their Figure 6(a) shows five values of  $R_L$  for ITP2 that range from -3.5 to -3.0. While Bebieva and Timmermans [2] found that  $R_L$  changes below the depth of the temperature maximum, those authors also found in their Figure 3(b) that  $R_L$  is constant in the depth range we consider in this study. Although we find that  $R_L$  depends on pressure, our results agree with those of T08 on the magnitude of  $R_L$ , as we find the mean value for all non-outlier clusters of ITP2 to be  $-3.55$  with a standard deviation of 2.24, and so we compare more of our results to those of T08.

We reproduce several of the figures from T08 in Figure 2. The combinations of color and markers for the clusters are the same in Figures 2, 5, and 6. In Figure 2(a), we plot data from ITP2 in  $\Theta$ - $S_p$  space, reproducing Figure 5(a) from T08. Those authors noted that points from each particular layer clustered along lines in  $\Theta$ - $S_p$  space that cross isopycnals and when we mark the clusters found by the algorithm, those layers become visually distinct. Figure 2(b) shows profile 185 in the same depth range as Figure 4 from T08, plus the up-going profiles taken by ITP2 immediately before and after. This illustrates that



**Figure 8.** Individual profiles 313, 315, 317, 319, and 321 from ITP3, collected between November 10-12, 2005, and were chosen to show an example of a temperature inversion. The colors and markers of the individual points are the same as the clustering shown in Figures 4 and 7. The gray dots are outliers. The black lines on the left of each pair are the  $S_P$  profiles while the red lines on the right are for  $\Theta$ . Each profile is offset in both  $S_P$  and  $\Theta$  for clarity.

the clustering algorithm is indeed marking points within those particular layers as in the same cluster and points within interfaces as noise. It also shows that the clustering algorithm tracks the same layers across neighboring profiles even though the pressure at which those layers are found varies. Figure 2(c) shows the ITP2 data on the axes used by the clustering algorithm. In Figure 2(d), we plot the clusters bounded by the box in Figure 2(a) in  $\alpha\Theta - \beta S_P$  space, reproducing Figure 6(a) from T08. The dashed lines of slope 1 correspond to isopycnals as  $\Delta\rho = -\alpha\Delta\Theta + \beta S_P$ . Overall, the panels in Figure 2 are close visual matches for those particular figures in T08.

After examining the differences between the two in detail (see Supplementary Materials), it remains unclear why the values of  $R_L$  we found for clusters in ITP2 data differ from T08. However, we believe that the quantitative agreement in magnitude for the values of  $R_L$  and the qualitative match between the clustering results and the features in Figure 2 show that the clustering method reproduces those results from T08. Overall, these findings suggest that the clustering algorithm is accurately revealing a dependence of  $R_L$  on pressure in the data we analyzed from ITP2 and ITP3. Since  $R_L$  is directly related to the ratio of the vertical fluxes of salinity and heat within a staircase [2], this could indicate a pressure dependence of that ratio of vertical fluxes.

## 5. Discussion

In this paper, we have presented an automated method based on the HDBSCAN clustering algorithm to identify well-mixed layers in thermohaline staircases in Arctic Ocean hydrographic data. Comparison with results from previous studies was favorable, and suggests this method is able to produce trustworthy results when applied to large datasets. This study contributes to a growing set of examples of clustering algorithms being used in oceanography [e.g., 14, 8, 18, 17, 12, 11, 34, 7, 38]. The continued and extended use of clustering algorithms in oceanography and related fields is an important development, since discovering and detecting features in all manner of datasets becomes more challenging as they grow ever larger.

Special attention was given herein to the identification of outliers using parameters output by the method itself. We found that clusters which are outliers in the lateral density ratio  $R_L$  often indicate multiple layers that are erroneously clustered together, but can also highlight potential instances of layer splitting or merging. By introducing the normalized inter-cluster range  $IR_V$ , we quantitatively showed that the pressure and temperature values vary more within a layer than the difference between the values of neighboring layers, while the opposite is true for salinity. Because we know that the practical salinity  $S_P$  values in a particular layer are well separated from those of neighboring layers, we identified clusters with notably large values of  $IR_{S_P}$ , as likely to be either only part of a layer that was erroneously split by the algorithm or a remnant intrusion. An apparently new result from this study is the pressure

dependence of the lateral density ratio  $R_L$ , seen in both ITP2 and ITP3. The reasons for this dependence are unclear and are worthy of further study.

The method we presented here has certain advantages over other staircase detection techniques. For example, all of the other methods referred to herein [40, 37, 44, 16] require setting one or multiple thresholds on gradients in temperature, salinity, or density which are used to identify sections of profiles where layers may be present. However, choosing reasonable values for these thresholds requires prior knowledge of the staircase properties, which may not be available before identifying staircases in that particular region and time period. In addition, while the other techniques require resolution high enough to resolve small-scale vertical gradients, the method presented here—which does not distinguish between individual profiles—only requires that a sufficient number of data points be available in order to detect clusters. Therefore, this technique could potentially find staircases in datasets that have too low a resolution to resolve the steps in any particular profile. Compared to other staircase detection methods which involve manual intervention, the one we presented here is objective, repeatable, and can easily accommodate larger datasets. Finally, the method automatically connects layers across profiles, a task that is a completely manual process in all other staircase detection techniques cited above except for L22. Consequently it could be readily used to examine the large-scale, lateral properties of layers in thermohaline staircases.

The clustering algorithm has several limitations. Because this method relies on having a large number of related data points, it is not applicable to identifying stair steps in independent individual profiles. It cannot be used to examine sets of profiles spanning temporal or spatial scales larger than those on which stairs are known to be coherent. Moreover, as the clustering algorithm does not consider profiles individually, it may miss layers which are only present in a small number of profiles, as may occur especially for layers that split or merge. Finally, although our method captures the overall structure of the staircase layers well, it sometimes miscategorizes points, especially near the boundaries between layers and interfaces.

The method presented here could be used in conjunction with other staircase detection methods. For example, if a different detection method were used to identify which data points in a collection of profiles are in layers, the clustering algorithm could be run on just the layer points to automatically connect the layers across profiles. Additionally, the clustering algorithm could be used on a large collection of datasets to identify which subsets contain staircases; then a more specifically tuned staircase detection method could be used on just that subset, reducing the amount of manual, time-consuming analysis.

Because the method can be scaled to larger datasets, a natural extension would be to apply it to more ITP profiles. Furthermore, although we have focused on identifying upper-ocean Arctic thermohaline staircases, it could also be useful in other oceanic regimes. Staircases with steps on the order of 50 m thick have been observed in the Arctic between depths of 2000–3000 m [39], much deeper than ITPs measure, while the Argo network of autonomous profiling floats has captured staircases in regions all over the world [43]. This method could also be adjusted to identify other structures that appear in  $\Theta$ – $S$  space such as different types of layers or water masses, or even structures that can appear in different spaces such as  $\Theta$ – $O_2$  [34]. On the technical side, another topic of future study would be to adapt this method to automatically distinguish between well-mixed layers and intrusions. Finally, there may be methods other than the DBCV validation process used herein that may be better able to guide the choice of parameters, potentially improving the detection fidelity.

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**Competing Interests.** The authors declare none.

**Data Availability Statement.** Replication code can be found on Zenodo: <https://zenodo.org/record/8173386>. The Ice-Tethered Profiler data were collected and made available by the Ice-Tethered Profiler Program (Toole et al. [41], Krishfield et al. [15]) based at the Woods Hole Oceanographic Institution (<https://www2.whoi.edu/site/itp/>).

**Ethical Standards.** The research meets all ethical guidelines, including adherence to the legal requirements of the study country.

**Author Contributions.** Conceptualization: M.G.S., N.G., E.R., J.M.L.; Data Curation: M.G.S.; Formal Analysis: M.G.S.; Funding Acquisition: N.G.; Investigation: M.G.S.; Methodology: M.G.S.; Software: M.G.S.; Supervision: N.G., E.R., J.M.L.; Validation: M.G.S., N.G., E.R., J.M.L.; Visualization: M.G.S.; Writing – Original Draft: M.G.S.; Writing – Review & Editing: M.G.S., N.G., E.R., J.M.L.; All authors approved the final submitted draft.

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## METHODS PAPER

# Supplementary Materials for: Unsupervised clustering identifies thermohaline staircases in the Canada Basin of the Arctic Ocean

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**Keywords:** Arctic Ocean, clustering algorithm, machine learning, thermohaline staircases, ice-tethered profilers

## S. Supplementary materials

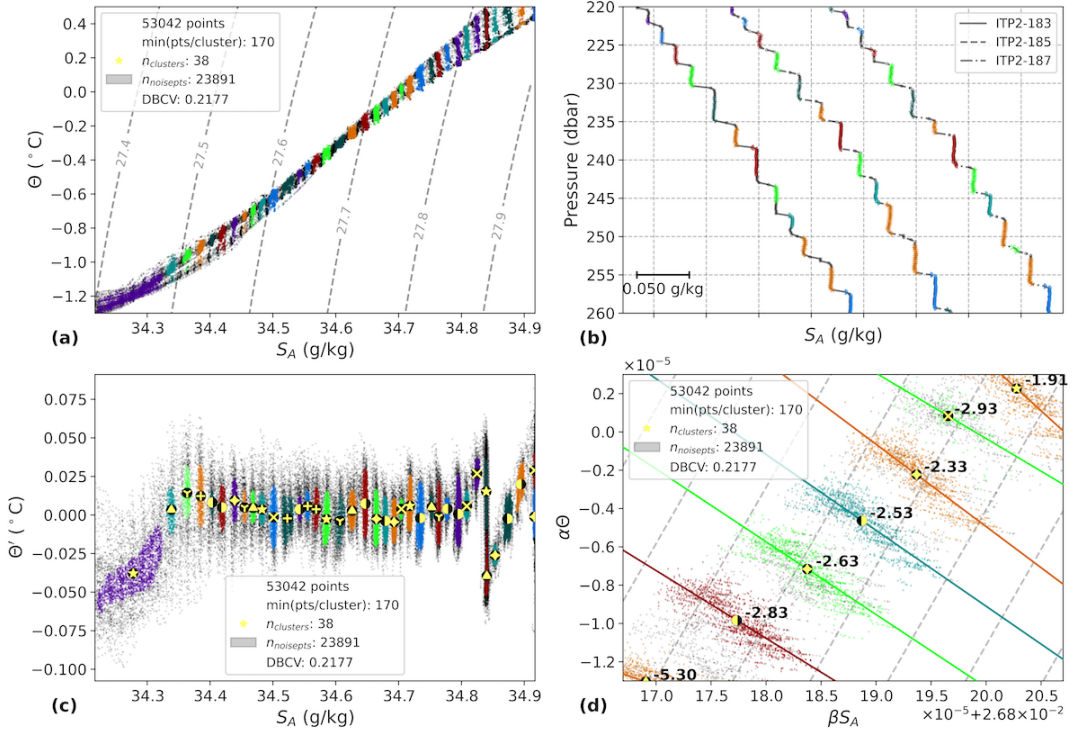
### S.1. Practical salinity $S_P$ vs. absolute salinity $S_A$

TEOS-10 recommends storing values of practical salinity  $S_P$  in databases in order to maintain continuity with older records and also because  $S_P$  is practically a measured quantity [4]. In contrast, absolute salinity  $S_A$  is a calculated variable defined as "the mass fraction of dissolved non-H<sub>2</sub>O material in a seawater sample at its temperature and pressure," and is recommended for use in publications [2]. For this study, we ultimately chose to work with  $S_P$  because the two studies to which we make direct comparisons, T08 and L22, used  $S_P$ . Specifically, when we define the ranges of  $S_P$  to filter to before running the clustering algorithm, we were able to directly take the values of  $S_P$  from T08 and L22 without having to first convert to  $S_A$ .

To investigate the difference between using  $S_P$  vs.  $S_A$  on our results, we recreated Figure 2, but replacing  $S_P$  with  $S_A$  on all the axes, as shown in Figure S.1. We still filtered the ITP2 data to be in the practical salinity range  $S_P$  34.05–34.75 g/kg to make sure we used the same data points. However, then we plotted those data points in  $\Theta'$ – $S_A$  space in panel (c) to run the clustering algorithm using the same  $m_{pts} = 170$ . This resulted in 38 clusters (as opposed to 36) with a DBCV score of 0.2177 (as opposed to 0.3034). In panel (d), the values of  $R_L$  displayed made minor changes of (from left to right): +0.39, -0.04, -0.03, -0.03, -0.01, +0.14, and +0.07.

We also reproduced Figure 5(a,b) in Figure S.2 using the clustering shown in Figure S.1. The two outliers in  $IR_{S_A}$  in Figure S.2(a) do not correspond to outliers in Figure 5(a) because these have very high  $IR_{S_A}$ , over 20, which skews the mean as used when calculating the z-score. The dark green star and the red triangle in Figure S.2(a) correspond to the two outliers in Figure 5(a) where they are marked by an orange 4-pointed star and a green "×". These pairs of points have very similar values of  $IR_{S_A}$  and  $IR_{S_P}$ , respectively.

In Figure S.2(b), we see that there are two outliers in  $R_L$  circled, both of which correspond to outliers found when using  $S_P$ . The purple star in Figure S.2(b) corresponds to the orange left half circle in Figure 5(b), while the dark green "Y" in Figure S.2(b) corresponds to the teal "×" in Figure 5(b). A notable difference is that the purple star outlier in Figure 5(b) (which spans  $S_P = 34.233$ – $34.261$  in Figure 2(c) encompassing what should be two distinct clusters) is no longer present in Figure S.2(b). Comparing Figures 2(c) and S.1(c), we see that it is now replaced by two clusters, the dark green left half circle and the red right half circle, neither of which are outliers in  $R_L$ .



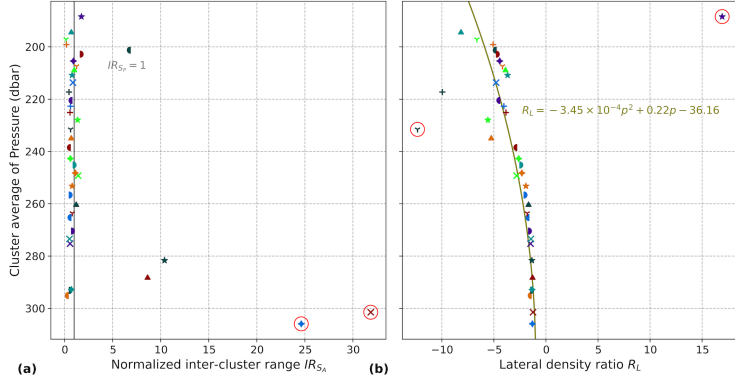
**Figure S.1.** Results from the clustering algorithm with  $m_{pts} = 170$  and  $\ell = 100$  dbar run on 53042 data points in the  $S_P$  range 34.05–34.75 g/kg from all up-going ITP2 profiles. This is the same as Figure 2, but the clustering algorithm was run on absolute salinity  $S_A$  instead of practical salinity  $S_P$ . (a) The data in  $\Theta - S_A$  space with dashed lines of constant potential density anomaly ( $\text{kg m}^{-3}$ ) referenced to the surface. (b) Profiles 183, 185, and 187 from ITP2 in a limited pressure range to show detail. Each profile is offset in  $S_A$  for clarity. (c) The spatial arrangement used as input for the algorithm where the gray points are noise and each color-marker combination indicates a cluster. The same color-marker combinations are used in each panel and the markers in panels (c) and (d) are at the cluster average for each axis. (d) A subset of the data in  $\alpha\Theta - \beta S_A$  space with the linear regression line and inverse slope ( $R_L$ ) noted for each individual cluster and with dashed lines of slope  $\alpha\Theta/\beta S_A = 1$ .

We also see that the 2nd-degree polynomial fit in Figure S.2(b) is similar to that in Figure 5(b). We conclude that the difference between using  $S_A$  vs.  $S_P$  does not significantly affect our results.

## S.2. Varying the value of $\ell$

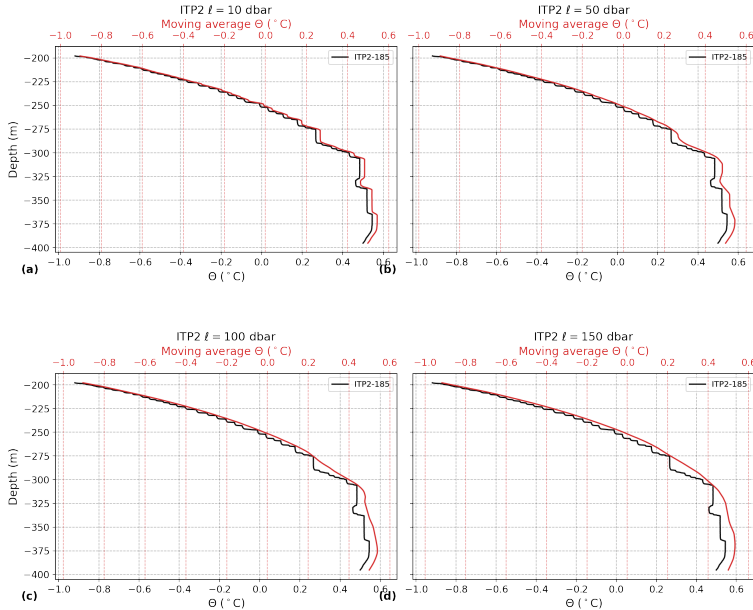
We define the local anomaly of a temperature profile  $\Theta'$  as the original profile minus a version of that profile smoothed with a moving average. Subtracting a smoothed profile from the original profile in this way gives temperature differences that are centered around zero and leads to more continuous clusters (compare Figures 2(a) and 2(c)), allowing HDBSCAN to group these points more accurately.

When calculating  $\Theta'$  with Equation 3.1, we use a moving average with window size  $\ell$ , so the resulting profile has dead regions  $\ell/2$  in size with no data at the top and bottom. Therefore,  $\ell$  cannot be larger than twice the distance available in the profile, either above or below the pressure range to be analyzed, whichever is smaller. As  $\ell$  increases, the moving average profile gets flatter, meaning  $\Theta'$  becomes closer to the original profile, just shifted in temperature space. Choosing a very small  $\ell$  will give a moving average temperature profile that will closely match the original temperature profile, meaning that the  $\Theta'$



**Figure S.2.** The value of each cluster’s normalized inter-cluster range for salinity  $IR_{S_A}$  in (a) and the lateral density ratio  $R_L$  in (b) as a function of the cluster’s average pressure for ITP2. This is the same as Figure 5(a,b), but the clustering algorithm was run on absolute salinity  $S_A$  instead of practical salinity  $S_P$ . The colors and markers are the same as the clustering shown in Figure S.1. Markers circled in red indicate outliers with a  $z$ -score greater than 2.

profile will be very close to zero. This eliminates any effect temperature might have on the clustering results.

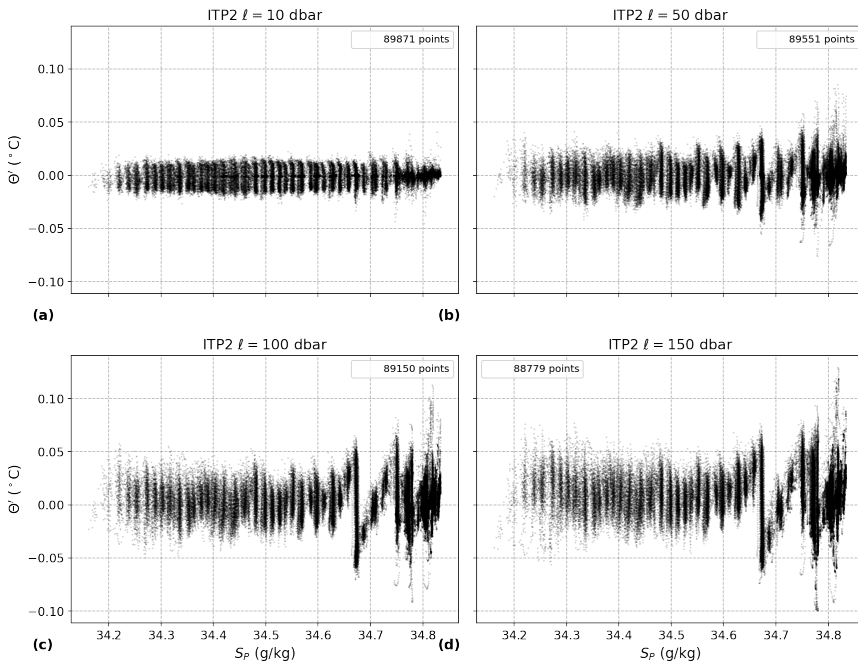


**Figure S.3.** The original profile 185 from ITP2 and the smoothed version of that profile for 4 different values of  $\ell$ : (a) 10 dbar, (b) 50 dbar, (c) 100 dbar, and (d) 150 dbar. The  $\Theta$  axes on each panel are offset slightly to show both lines.

In Figure S.3, we show 4 pairs of profiles, restricted to the 200-400 dbar pressure range to show detail. All profiles are number 185 from ITP2, the example profile featured in Figure 2(b). Each panel shows both the original profile and the moving average profile with the values of  $\ell$ : 10, 50, 100, and

150 dbar. The original and moving average profiles are slightly offset for clarity. When  $\ell = 10$  dbar, the moving average profile still clearly contains some of the larger stair steps. When  $\ell = 150$  dbar, almost all of the features in the original profile are gone.

We noted a feature in 2(c) where the cluster average  $\Theta'$  increases starting at  $S_P \approx 34.63$  g/kg until it jumps sharply to negative  $\Theta'$  values around  $S_P \approx 34.67$  g/kg, then increases again until  $S_P \approx 34.72$  g/kg. This zig-zag pattern is due to the choice of  $\ell$  and the presence of the AW subsurface temperature maximum in  $\Theta$  profiles. In Figure S.4, we show the ITP2 data used in the study in  $\Theta'$ - $S_P$  space for the same 4 values of  $\ell$  as in Figure S.3. This clearly illustrates that the zig-zag pattern is not present for low  $\ell$  and becomes more pronounced as  $\ell$  increases. We find the most reasonable clusterings occur when  $\ell$  is chosen to be small enough that the features outside the pressure range we analyze do not significantly affect the moving average, yet large enough that the stair steps are completely smoothed out.



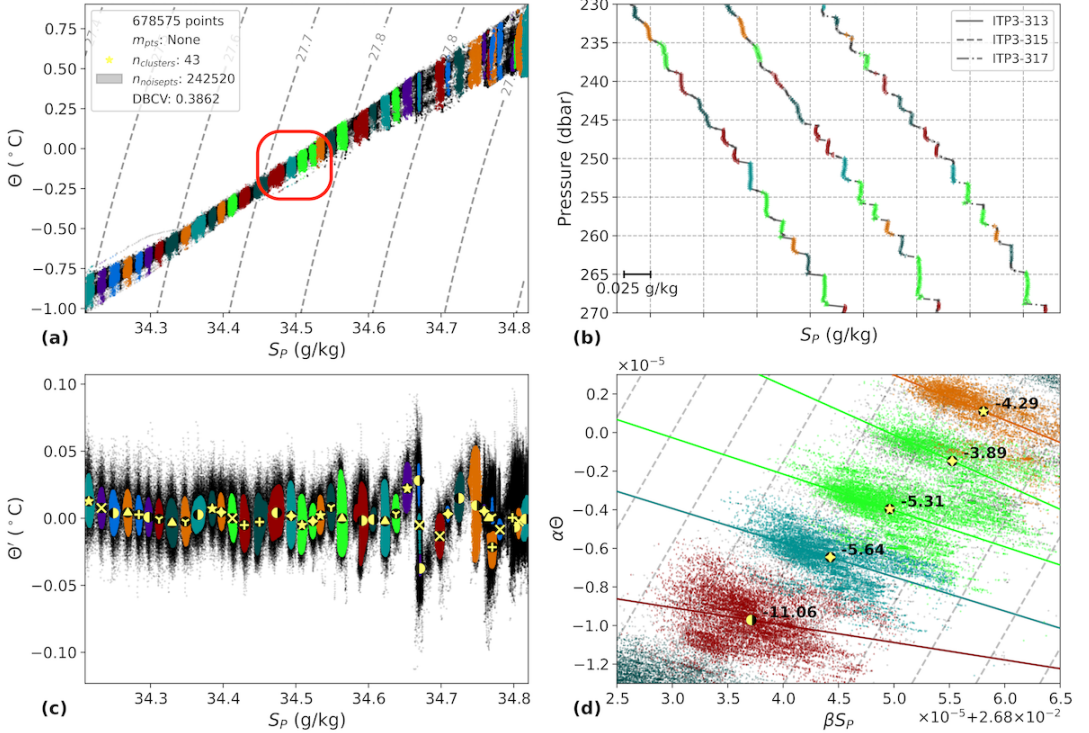
**Figure S.4.** Data from ITP2 between 200–400 dbar plotted in  $\Theta'$ - $S_P$  space for 4 different values of  $\ell$ : (a) 10 dbar, (b) 50 dbar, (c) 100 dbar, and (d) 150 dbar.

### S.3. Clusters from ITP3

In Figure S.5, we create a figure similar to that of Figure 2, but for ITP3. In Figure S.6, we create a figure similar to that of Figure 3(a), but for ITP3. Note that the run with  $m_{pts} = 710$  had a DBCV score of 0.3885, which is slightly higher than the run at  $m_{pts} = 580$  with a DBCV score of 0.3862. However, because the differences in DBCV were not great, we decided to use  $m_{pts} = 580$  to reduce computation time as the clustering algorithm takes longer to run with higher values of  $m_{pts}$ .

### S.4. Clusters across time for ITP2

In Figure S.7, we create a figure similar to that of Figure 4, but for ITP2.

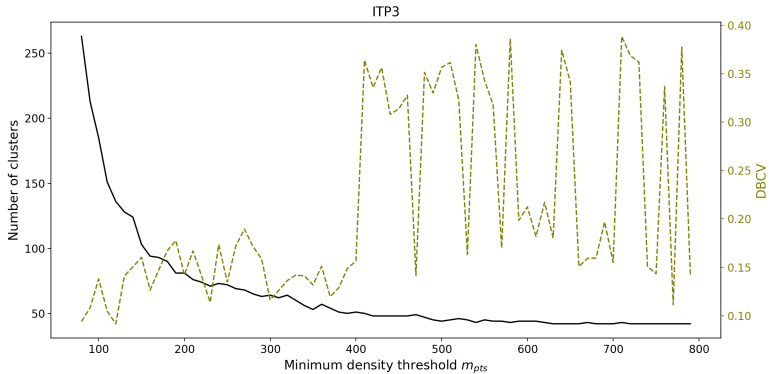


**Figure S.5.** Results from the clustering algorithm with  $m_{pts} = 580$  and  $\ell = 100$  dbar run on 678575 data points in the  $S_P$  range 34.21–34.82 g/kg from all up-going ITP3 profiles. (a) The data in  $\Theta$ – $S_P$  space with dashed lines of constant potential density anomaly ( $\text{kg m}^{-3}$ ) referenced to the surface. (b) Profiles 313, 315, and 317 from ITP3 in a limited pressure range to show detail. Each profile is offset in  $S_P$  for clarity. (c) The spatial arrangement used as input for the algorithm where the gray points are noise and each color-marker combination indicates a cluster. The same color-marker combinations are used in each panel and the markers in panels (c) and (d) are at the cluster average for each axis. (d) A subset of the data in  $\alpha\Theta$ – $\beta S_P$  space with the linear regression line and inverse slope ( $R_L$ ) noted for each individual cluster and with dashed lines of slope  $\alpha\Theta/\beta S_A = 1$ .

### S.5. Differences from T08

Figure 6 from Timmermans et al. [6] shows clusters in  $\alpha\Theta$ – $\beta S_P$  space with panel (a) showing five values of  $R_L$  for ITP2, which range from -3.5 to -3.0, and panel (b) showing 12 values of  $R_L$  for ITP5, which range from -3.9 to -2.4. It is unclear whether their reported  $R_L = -3.7 \pm 0.9$  applies to data from ITP2, ITP5, both, or all six ITPs they included in their study. It is not explicitly stated whether that value applies to just the clusters shown in that figure or it includes the dozens of clusters they identified earlier in their study. T08 never explicitly state that they did not find a trend in  $R_L$  with respect to depth. However, given that T08 reported one overall value of  $R_L$  and that Bebieva and Timmermans [1] (which extended the work of T08) show a constant value of  $R_L$  in the depth range we consider, we assume T08 also found a constant value of  $R_L$ .

There are several factors that could explain why our results for  $R_L$  differ from those of T08. The fact that they used potential temperature  $\theta$  while we worked with conservative temperature  $\Theta$  is not relevant, since when we repeat our calculations using  $\theta$  instead of  $\Theta$ , the values of  $R_L$  we find are negligibly different. It is unclear whether T08 calculated the values of  $\alpha$  and  $\beta$  for each point or for each layer. We calculated  $\alpha$  and  $\beta$  for each point in each profile individually using functions from the Gibbs Seawater (GSW) Oceanographic Toolbox, the Python implementation of TEOS-10 [4], while T08 used



**Figure S.6.** A parameter sweep showing the number of clusters found (solid lines) and DBCV (dashed lines) in ITP3 as a function of 72 different values of  $m_{pts}$  with  $\ell = 100$  dbar.

the McDougall [3] algorithm coded by Morgan [5] as GSW was not yet released. This difference in the calculation of  $\alpha$  and  $\beta$  may conceivably explain why the clusters we show in Figure 2(d) are tilted several degrees compared to those shown in Figure 6(a) from T08, and why the values of  $R_L$  found here are all less negative than corresponding values in Figure 6(a) of T08. The difference in calculating  $\alpha$  and  $\beta$  may also account for the shift in the ranges of  $\beta S_P$  between the two figures. Both plots show a span in  $\beta S_P$  of  $4.0 \times 10^{-5}$ , but our plot ranges from  $2.6838 \times 10^{-2}$  to  $2.6878 \times 10^{-2}$ , while theirs ranges from  $2.7002 \times 10^{-2}$  to  $2.7042 \times 10^{-2}$ . Because the clustering algorithm only considers  $\Theta'$  and  $S_P$ , any difference in calculating  $\alpha$  and  $\beta$  would not affect the clusters we found, only the values of  $R_L$ .

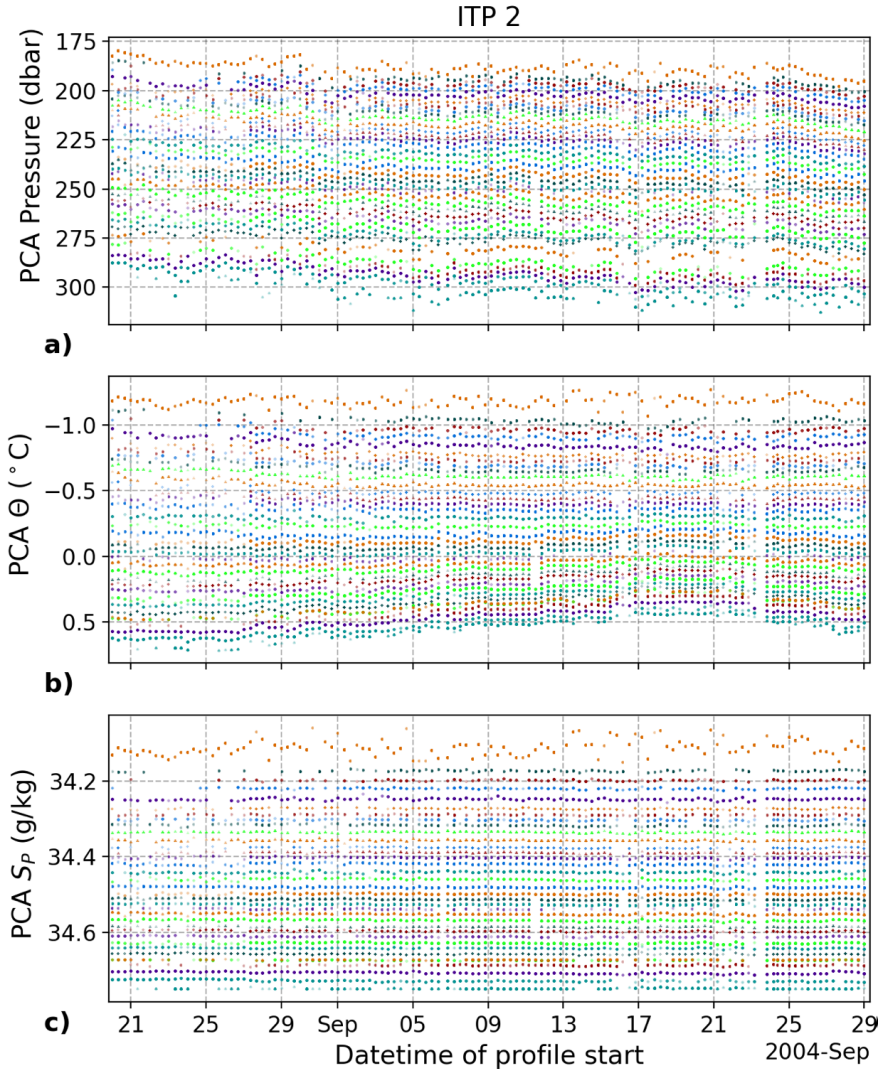
### S.6. Differences from L22

L22 used 758 profiles from ITP3 while we used all 766 available up-going profiles. The reasons 8 profiles were not used was not stated, nor could we determine exactly which profiles they are. Based on the gaps in Figure 3 of L22, we believe that the 8 missing up-going profiles are from July 2006. We do not, however, believe that this difference of 8 profiles accounts in any significant way for the differences between our results and those of L22.

Instead, we believe the reason our results differ from those of L22 has to do with the difference in the methods used to identify layers. Because the method used by L22 to delineate different layers only considered salinity, they would not separate layers with temperature inversions. Remnant intrusions are homogeneous in salinity but, compared to stair steps, are inverted in temperature and have different patterns of heat and salt flux. They tend to be present near the bottom of the staircase, which is indeed where we find the largest differences between our results and those of L22. A remnant intrusion's pattern of a section of warmer water above a section of colder water is distinct enough for the clustering algorithm to find two clusters. However, if only salinity is considered, as L22 did, it would appear to be one regular staircase layer. Whether a remnant intrusion represents one or multiple layers is subjective, and we do not claim that one method is superior to the other. Here, in fact, it is the disagreement between these two methods is arguably the most interesting point, because it indicates that a specific physical process is operating.

While we agree with L22 that salinity is the best measured quantity by which to identify the layers of a staircase, it is still important to consider temperature. Another topic of future study would be to adapt this method to automatically distinguish between well-mixed layers and intrusions.





**Figure S.7.** The average (a) pressure, (b)  $\Theta$ , and (c)  $S_P$  for the points within each cluster for each profile (profile cluster average, PCA) across time. The clustering algorithm was run with  $m_{pts} = 170$  and  $\ell = 100$  dbar on 53042 data points in the salinity range 34.05–34.75 g/kg from all up-going ITP2 profiles.

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