

Machine Learning as an Antidote to Chaos: Decoding Ecological Complexity

Maike Sonnewald^{1,2,*}, Stephanie Dutkiewitz¹, Christopher Hill^{1,+}, and Gael Forget^{1,+}

²Harvard University, Department of Earth and Planetary Sciences, Cambridge, MA 02138, USA

¹Massachusetts Institute of Technology, Department of Earth, Atmospheric and Planetary Sciences, Cambridge, MA 02139, USA

*sonnewald@fas.harvard.edu

+these authors contributed equally to this work

ABSTRACT

The complex nature of ecology in the global ocean is leveraged to present the emergent biogeochemical provinces. A global framework based on unsupervised machine learning is presented that allows a robust and nested classification of biogeochemical provinces spanning global and regional scales. Similar ecology is identified in 20 year mean surface data from state of the art biogeochemical model DARWIN. Initially, a large number of global ecological niches are identified, using 51 species with a range of trait-based functional types and nutrient fluxes of N, P, Si and Fe coupled to physics from the ECCO State Estimate. Provinces are determined by nesting the niches according to their ecological similarity, and a minimum complexity is determined by comparison to the Longhurst provinces. The presented framework is applicable both globally and regionally as the degree of nesting can be adjusted according to the region of interest. A dynamic ocean ecology emerges, with gradual and sharp transitions between ecological provinces. Expected compositions are found in oligotrophic gyres or regions of upwelling and strong seasonality.

Introduction

Marine microbial ecosystems are a product of the physical, chemical and biological interactions. Patterns in Chl-a can be indicative of phytoplankton distribution, but current the question of the link to ecology remains unanswered. Biogeography and biodiversity have manifestations on the large scale (e.g., Barton et al., 2010; Dutkiewicz et al., 2009; 2011), mesoscale (e.g., Levy et al., 2014; 2015; Perruche et al., 2011), and submesoscale (Mahadevan, 2016). This is because ocean currents and mixing are key in setting aspects of this biogeography (Clayton et al., 2013; Levy et al., 2014; 2015). Indeed observations suggest highly complex pattern of community structure (deVargas, Lima-REF). Despite the importance of phytoplankton ecology in the climate and for fisheries, identifying key components setting ecosystem structure in the pelagic ocean is lacking. Here a framework is presented that leverages novel unsupervised machine learning techniques to provide the necessary tools to identify the underlying mechanisms that set the ecosystem structure at different location.

Defining provinces is one way to reduce the complexity of the physical, chemical and biological interactions that comprise ecosystems. Provinces are regions that are assumed to have some similarity in characteristics. For the terrestrial ecosystem, biomes are classified according to (usually easily identifiable) vegetation types, to explain patchiness and behaviors on different scales. A hierarchical approach to modeling is often used where landscapes are understood as “mosaics” of varying niches. In contrast to the terrestrial, the oceanic pelagic ecosystem responds directly and fluidly to pressure from oceanic and atmospheric dynamics, confounding mapping efforts. However, there have been several such attempts (Longhurst, Oliver and Irwin, SeaScapes REFS). Mapping the global provinces, it becomes possible to assess how sensitive they are to different sources of stress. Changes in currents can lead to changes in dispersal/niche boundaries. Other stressors include warming, changes in sea ice, reduced oxygen and pH.

Additionally, the hope is that similar mechanisms within a province are important for controlling the biogeochemical properties, such as Chl-a. EXPAND

Provinces have an advantage that if there are at least some in situ observations within the province, then there is an assumption that these will provide information about the rest of the province (EXPAND - BriNG IN HENSON WORK).

Previous studies that have classified provinces in the ocean have used bulk properties such as Chl-a or Primary pro-

duction along with physical characteristics (such as MLD and SST) and sometimes also optical properties (Oliver and Irwin). As such we will refer to these previously defined provinces as "biogeochemical provinces".**MORE - BRING IN LONGHURST/SEASCAPES**

There has not been an attempt to define the oceans in terms of ecological provinces based on plankton community structure. This is largely due to available data of ecological characteristics being sparse. However, new survey and greater ease of genomic data analysis will begin to improve our coverage of the ocean. Observations from efforts such as Tara Oceans feed into databases such as the Ocean Gene Atlas OGA, and subsequent work has made use of machine learning tools to help define communities (e.g. Lima-REF), but have not had sufficient coverage to define distinct provinces.

How emergent ecological niches are governed tells us what they key features are. A niche is defined as a set of physical and chemical surroundings. The term "niche" is used to refer to the spatially smallest such sets identified, and when niches are grouped together they are referred to as "provinces" of varying "complexity". This complexity is set by choosing how many niches to aggregate together into the provinces. The present work details the method to find an aggregate provinces of nested "complexity". To highlight what shapes the provinces, the discussion weights the effect of nutrient availability, ecological adaptability and pressure from physical oceanography such as currents. For the marine pelagic ecosystems, the biology is seen largely as passive regarding the physical niches, but can actively contribute to setting the availability of e.g nitrogen through fixation by diazotrophs. Similarly, allowing a range of cell sizes, with varying growth rates suggests that some niches can achieve high productivity despite a harsh environment by configuring the ecological interactions accordingly.

Following⁷, the purpose here is to leverage unsupervised learning as a tool to define distinct eco-provinces. Determining a useful classification, such a scheme needs to allow for both 1) global classification, and 2) a multiscale analysis that can be both spatially and temporally nested. The criteria of being global and multiscale are essential for a useful classification scheme. Such a scheme allows understanding controllers of community structure, monitoring changes and potentially help in conservation issues.

The present work uses a 20 years of data from a global 3-dimensional physical/ecosystem model to explore a method to define eco-provinces. The train-based model covers 7 functional groupings of plankton over 16 size classes. A priori the model output are extremely complex and sorting out what the controlling mechanisms of the patterns and associated community structure is overwhelming. The present work demonstrates that the controls within eco-provinces can be understood by defining eco-provinces using machine learning techniques, including some of the likely controlling mechanism such as nutrient supply rates.

Model framework: DARWIN

The complexity at the heart of ecological niche construction makes it a problem well suited for machine learning applications. The approach here assumes the modeled ecology is correct, using the DARWIN model and treating the model data as truth. An Ecosystem-Optical model uses the physical model. The ecological niches are defined by the proportional presence of phytoplankton, zooplankton and nutrients (Nitrogen, Iron, Phosphate and Silica). The 51 plankton types (2 pico-prokaryotes, 2 pico-eukaryotes, 5 coccolithophores, 5 diazotrophs, 11 diatoms, 10 mixotrophic dinoflagellates, and 16 zooplankton) range from $0.6\mu\text{m}$ to $2500\mu\text{m}$ equivalent spherical diameter. Parameters influencing growth, grazing, and sinking are related to size (following Ward *et al.*, 2012) with specific differences between functional groups. The plankton distributions in this model compare well with both observations based on functional types as well as size distributions.

The physical component comes from the Estimating the Circulation and Climate of the Ocean (ECCOv4) global state estimate described by [Wunsch and Heimbach, 2013](#), [Forget *et al.*, 2015](#), see also [ECCO Consortium, 2017a](#), [ECCO Consortium, 2017b](#). The state estimate has a nominally 1° resolution, available at: [ecco.jpl.nasa.gov](#). A least-squares with Lagrange multipliers approach is used to obtain the state estimate. The result is a *free-running* version of the MIT General Circulation Model (MITgcm, [Adcroft *et al.*, 2004](#)), with adjusted initial and boundary conditions and internal model parameters. The ECCO state satisfies basic conservation laws for enthalpy, energy, salt, volume, and momentum while remaining largely within error estimates of a diverse set of global data [Wunsch and Heimbach, 2007](#), [Wunsch and Heimbach, 2013](#),[?]. Regions without data are filled in a dynamically consistent way using the dynamics, still relying on parameterizations but avoiding the use of untested statistical hypotheses e.g., [Reynolds *et al.*, 2013](#).

Dimensionality reduction: Finding the standout similar regions

By identifying the ecological niches in the 20 year average of the surface field, this work aims to provide a framework for looking at important relations between key features such as biomass of species. Like drawing a map of a complex mountainous region, careful thought needs to be given so the key features remain intact. The dimensionality of the data was initially reduced by including only the sum of biomass of each of the seven functional group and all source terms for the flux of the nutrients (Nitrogen, Iron, Phosphate and Silica). The summing into functional groups reduces the problem from a 55-dimensional space to all 11. The nutrient supply rates were included following earlier studies showing their key roles in setting community structure (e.g. Ward et al., 2012; 2013; Dutkiewicz et al 2012; 2014, in prep). The biomass and nutrient fluxes leave an 11 dimensional vector \mathbf{x} . If \mathbf{x} is a vector field on the model grid discretized sphere, where each element \mathbf{x}_i represents an 11-dimensional vector on the model's horizontal grid, each index i uniquely identifies a grid point on the sphere, with (lon,lat) = (ϕ_i, θ_i) . The components of the vector \mathbf{x}_i are the seven functional groups and 4 nutrient terms. The log of the biomass data is used, and if a cell has less than $12 * 10^{-4} mgChl/m^3$ it is discarded. The data is normalized and standardized such that all data exist on the same range [0 to 1]. This is done so the features (biomass and nutrient fluxes) do not get conditioned by features with wider range of possible values when computing distances that map the key relations between features. In ecological terms, this step is necessary because species that may have comparatively small biomass can be key ecological players facilitating relations that only emerge when the data is normalized and standardized.

The t-distributed Stochastic Neighbor Embedding (t-SNE) algorithm is used to make existing similar regions stand out more clearly by emphasizing their proximity in the high-dimensional parameter space in a lower dimensional representation. Previous work aiming to build deep neural networks for remote sensing applications employed t-SNE, demonstrating its skill in separating key features satelliteDNN. This is a necessary step to identify robust clusters in the biogeochemical data. Using a Gaussian kernel, t-SNE preserves the statistical properties of the data by mapping each high-dimensional object onto a 3D point in a way that ensures a high probability of similar objects being close and vice versa [van der Maaten & Hinton, 2008](#). Given a set of N high-dimensional objects $\mathbf{x}_1, \dots, \mathbf{x}_N$, the t-SNE does a reduction by minimizing the Kullback-Leibner distance [Kullback, 1987](#) between the likelihood of association between a low dimensional rendition and the high dimensional data. If \mathbf{x}_i is the i -th object in the N dim space and y_i is the i -th object in the low-dim space:

$$p_{j|i} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma_i^2)}{\sum_{k \neq i} \exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2/2\sigma_i^2)},$$

and the same for a reduced dimensional set:

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}.$$

This is done as:

$$KL(P||Q) = \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}$$

Figure 2a illustrates the effect of reducing the variables of phytoplantion, zooplankton and nutrients. While different in practice, the motivation for applying t-SNE is similar to a principal component analysis (PCA) decomposition, using a method to highlight attributes in the data and reduce the dimensionality. The t-SNE method was found to be much superior to PCA in delivering robust results. PCA did very little to make the applied clustering more able to identify robust and repeatable clusters. This is likely because the orthogonality assumption that underlies PCA is not appropriate for identifying key interactions between highly complicated and interacting features. [Lunga et al., 2014](#) demonstrates the effect of several dimensionality reduction techniques demonstrating how complex spectral features in remote sensing data can be highlighted employing SNE in the context of manifold learning.

Applying t-SNE, the result is a 3D representation of the 11D feature vector. Fig. 2a illustrates this space, where the points are the 3D representation of every latitude and longitude point. If two points are close to each other in Fig. 2a, this is because their biomass and nutrient fluxes are similar, not due to geographical proximity. The colors on Fig. 2a are the clusters found using the Density-based spatial clustering of applications with noise (DBSCAN) proposed by [Ester et al., 1996](#). Looking for densely packed observations, the DBSCAN algorithm uses the distance in the 3D representation between points, setting a minimum distance for associated points (ϵ), and the number of similar points needed to be interesting. The DBSCAN method makes no assumptions about the shapes or numbers of clusters in the data:

1. A random datapoint y_i is selected.

2. The number of immediately neighbouring points within distance ε of y_i is measured.
3. The cluster boundary is determined repeating step 2 iteratively for all points identified as within distance ε . If the number of points is larger than the set minimum it is designated as a cluster.
4. A new point is chosen at random from the remaining unclassified data, and the method repeated.

The data that does not meet the minimum cluster member and distance ε distance metric are counted as "noise". DBSCAN is a fast and scalable algorithm, with a worst-case performance of $O(n)$. Setting the number of minimum points and the distance ε was done using the degree of connectedness (Fig. 1a) and how large a percentage of the global ocean is covered (Fig. 1b). A minimum number of points was set to an area of 100 gridpoints denoted by the black line in Fig. 1a and 1b. A distance ε was chosen to be at the "elbow"/kink where the connectedness increases suddenly. This is symmetric, and the point allowing maximal area coverage was preferred. When the minimum number of points to be designated as a cluster is chosen, the lower limit is set for what spatial scales the identified niches and provinces are relevant for. This step should be guided by the application at hand, which in the present case was set to 100 points.

Each cluster $j = 1, \dots, N$ is represented by the 11-dimensional characterizing vector of the cluster. The DBSCAN classification attributes each vector \mathbf{x}_i to a unique cluster if it is not "noise". The 115 clusters identified in Fig. 2a are presented in their geographical extent in Fig. 2b. Each colour corresponds to a geographically coherent combination of biogeochemical factors picked out by the unsupervised learning algorithm DBSCAN after processing by t-SNE. Striking features stand out in Fig. 2a in that globally coherent regions are identified.

To understand the ecological context of the niches, the intra-cluster ecology is assessed using the Bray-Curtis Dissimilarity metric (BC [Bray and Curtis, 1957](#)). BC is defined as:

$$BC_{n_i n_j} = 1 - \frac{C_{n_i n_j}}{S_{n_i} + S_{n_j}},$$

where BC is always measured comparing one species assemblage to another. $BC_{n_i n_j}$ refers to the dissimilarity of assemblage n_i compared to assemblage n_j , where the $C_{n_i n_j}$ is the minimum of biomass of a certain species present in both assemblages n_i and n_j while S_{n_i} refers to the sum over all the biomass present in both assemblages n_i and S_{n_j} represents the sum over all the biomass present in assemblage n_j . For each cluster identified in Fig. 2b, the coherence within each niche is illustrated in Fig. 4c. This is determined using the mean area averaged assemblage within one cluster, and determining the BC-dissimilarity of each gridpoint within the niche to the mean. The global mean intra-cluster BC-dissimilarity is 0.102 ± 0.0049 .

The context of much work to determine the global provinces of the ocean is referenced to the provinces presented by Longhurst in "Ecological Geography of the Sea". Longhurst defined 56 provinces that partitioned the pelagic ocean geographically². The provinces defined by Longhurst (1995; 1998; 2006) are not static in time, but assume that ocean physics have a dominant role in regulating the distribution of phytoplankton. The primary provinces Longhurst identified are: the Polar biome, the Westerlies biome, the Trade winds biome, and the Coastal biome. These are then subdivided into about ten further within each basin. The physical quantities used are the biological productivity (Chlorophyll), photic depth and mixed layer depth and sea temperatures at 0 and 50 meters. These values are set to five equal intervals. Longhurst remains the gold standard for work partitioning the pelagic ocean into provinces, however even though he calls these "Ecological" provinces, they are really "biogeochemical" in that there definitions involve bulk properties such as Chl-a, and not the more ecologically relevant community structure. For instance, Fig. 4b illustrates the intra-province BC-dissimilarity arrived at using the biomass data from this study. Using the Longhurst provinces, the global mean intra-province BC-dissimilarity is 0.227. This is significantly larger than for the clusters identified by the method presented here for defining eco-provinces, and moving forward the mean intra-province BC-dissimilarity from the Longhurst regions of 0.227 is used as a benchmark.

Decoding Complexity: Global Regions

The niches presented in Fig. 2a offer a considerable improvement on the Longhurst provinces, describing the ecologically shaped niches in a manner that unpicks the emergent boundaries given by the governing equations of the underlying physical and biogeochemical model. However, the utility of over hundred niches is limited as this number is overwhelming. One of the uses of provinces is to help us understand how global niches are set and governed, and to leverage the emergent properties presenting a framework that can be nested to the appropriate level of detail. The full complexity in Fig. 2a is only useful for more regional assessments. The necessary nested condition is achieved by sorting niches according to their ecological

dissimilarity, assessed using the BC-dissimilarity between clusters. This approach allows a nested architecture which reveals what degree of complexity is necessary.

The distinction between intra- and inter-province BC-dissimilarity is used to mean that the intra-province BC-dissimilarity refers to the mean dissimilarity within a province itself. The inter-province BC-dissimilarity refers to how similar one province is to each other province. Fig. ?? illustrates the symmetric BC matrix where 0 (black: perfect correspondence) and 1 (white: completely dissimilar). Each line in this plot demonstrates patterns in the data. Fig. 3b demonstrates the geographical implications of the BC results from Fig. 3a for individual niches. For a niche in the low nutrient oligotrophic region, Fig. 3b demonstrates that large areas are reasonably similar symmetrically around the equator and in the Indian Ocean, but the higher latitudes are markedly different along with upwelling areas.

The emergent niches are globally coherent across the globe as Fig. 3b demonstrates. Some configurations are very "common", and using methods from genetics such as "connectivity" we can sort the > 100 niches according to which niche they are most similar to one another. Using a set number of "provinces" P , the P most dominant ones are used to organize the remainder of the niches into the province most similar to them. This organization according to the BC-dissimilarity allows the nested approach to global ecology. The complexity of the regions can be anything up to the full complexity from Fig. 2a.

What level of complexity is appropriate for the global ocean? The Longhurst provinces are leveraged as our benchmark in Fig. 4a (green line). Moving from a complexity of 1, the niches are aggregated, and the intra-province BC dissimilarity is assessed. The entire operation represented schematically in Fig. 1c is repeated ten times, as a slight difference could arise from using t-SNE. The computational cost associated limits the number, with the mean (black line) and 2σ (blue area) in Fig. 4a representing the presented method. A complexity of 12 is demonstrated to keep the intra-province BC-dissimilarity both below the Longhurst benchmark and shows a small 2σ . For a complexity of 12, the mean intra-seasonal BC-dissimilarity is 0.198 ± 0.013 , as seen in Fig. 4d.

Emergent minimal complexity: Chaos decoded

Taking the minimum complexity of 12 as determined in Fig. 4a, the global provinces that emerge can be assessed. With knowledge of the geographical locations of the 12 provinces, we revisit the overwhelming complexity in the 55D original data. The present complexity can now be leveraged to gain insight into the the ecology.

Fig. 5c shows the geographical projection of the identified 12 provinces, named from A to L. The identified provinces are all unique. There is some symmetry around the equator in the Atlantic and Pacific ocean, and similar, but augmented regions exist in the Indian ocean. Coherence with global physical regimes as presented in Sonnewald *et al.*, 2019, features that stand out include Western Boundary Currents (WBCs), the Antarctic Circumpolar Current (ACC), known upwelling regions on the Eastern side of the ocean basins and the subtropical gyres. Taking the geographical extents of the provinces A to L, the ecological assemblages for each province are shown in the bar plot in Fig. 5a. The nutrient fluxes are similarly shown in Fig. 5b, and have been scaled by N in the Redfield ration.

Provinces are seen have very similar phytoplankton biomass, but very different communities (e.g. D, H and K). These three regions are very different, with H being present mainly in the equatorial Indian ocean and having a larger population of diazotrophs. Province D is found in several basins, but is prominent in the Pacific surrounding the very highly productive region around the Equatorial upwelling. The shape of this province in the Pacific is reminiscent of planetary wavetrains. Province D has very few diazotrophs but more coccolithophores. Province K is found only in the high Arctic ocean, and is dominated by diatoms. The nutrient levels in each province are somewhat similar, with K having more Si, and H and D having very little. There is less N compared to P in province H. If only Chl were used to define provinces D, H and K they could not be distinguished. It is notable that the zooplankton biomass in the three regions are very different, with K having very little, but D and H having relatively similar levels. The phytoplankton biomass is similar, but is not sufficient to predict the zooplankton, in this manner using just Chl to define provinces would not capture this.

It is apparent that some provinces that have very different biomass are actually very similar in terms of their ecological community structure. This is seen in provinces D and E. These are close to each other, notably in the Pacific, where E is closer to the highly productive province J. There is again not a clear connection between phytoplankton biomass and zooplankton abundance. In this manner, monitoring Chlorophyll is not a sufficient predictor of zooplankton biomass and does not translate

to knowledge of higher trophic levels.

Diatoms only exist where there is silica supply; generally the higher the silica the higher the diatom biomass. However, the proportion of diatom biomass relative to other phytoplankton is dictated by how much more N, P, Fe are supplied, relative to the diatoms demands. This is because diatoms are the fastest growers, but are limited by silicon. If this limitation were not present diatoms would dominate in all but the lowest nutrient supply regions. Diatoms are seen in the provinces A, J K, and L together with silicon supply. As expected, diatoms are found in the polar regions. Province L spans the southern Southern Ocean and province K is a region in the Arctic Ocean. The very productive region J has diatoms, and provinde A is often an extension of J outside of the Equatorial regions.

The diazotrophs are able to coexist with other phytoplankton where there is excess of Fe, P relative the the demands of the non-diazotrophs. It is notable that there is higher diazotroph biomass where the amount Fe,P supply are relatively larger. In this manner, the diazotroph biomass in province H is larger than in J, although the overall biomass in J is larger. It is worth noting that provinces J and H are very different, with H located in the equatorial Indian Ocean.

The patterns demonstrated in the lowest level of complexity would be very difficult to determine is the biomass data were not separated into provinces. The simultaneous comparison of a plethora of maps, compared to Fig. 5c, 5a and 5b is daunting. What the provinces also highlight effectively, is that chlorophyll is not a good proxy for productivity, and leads to questions about how accurate the use of chlorophyll is as a proxy for biomass.

Conclusion

Using unsupervised learning, the niches in the 20 year mean surface ocean are determined using the DARWIN model. Major things to highlight in this section I will put down after feedback on the above.

I suggest emphasizing the following conclusions:

1. The method is successful in creating a global and nested classification that works globally, basin-by-basin, and on regional scales. The smallest scale can be adjusted on the base of the used model.
2. Ecological provinces are identified that conform to firmly established biological regions with well studied ecological dynamics. These are nominally given the names "seasonal/upwelling" and "light limited Polar" for the HNLC regions, the most productive province by biomass is the "semi-seasonal/upwelling", and the less productive regions are the "oligotrophic" and "oligotrophic adjacent" provinces. The are unique
3. Some paragraphs highlighting the use of provinces: (a) reducing the complexity of studying the system; (b) provinding broad regions that can be studied as a whole for (for instance what are the controls on the community structure); (c) providing a context for the sparse sampling: what region can observations be extrapolated too (i.e can also help identify where new timeseries stations should be located); (d) provide a framework for monitoring change
4. The regions that fail to be identified as within a niche by the developed method are seen to be highly seasonal, or associated with very few datapoints, likely failing the "minimum" criterion of DBSCAN.

Future work:

1. provinces boundaries will move – use same methods on a time varying field
2. link eco-provinces to provinces that can be more easily detected, for for instance space. how do combinations of Chl, PAR, MLD etc link to the eco-povinces here defined by community structure

The complicated interactions that dictate the spatial and temporal spaces of niches and provinces will be the topic of further work, with a focus on the climatological and regional ocean.

Acknowledgements

This work was supported by grant .

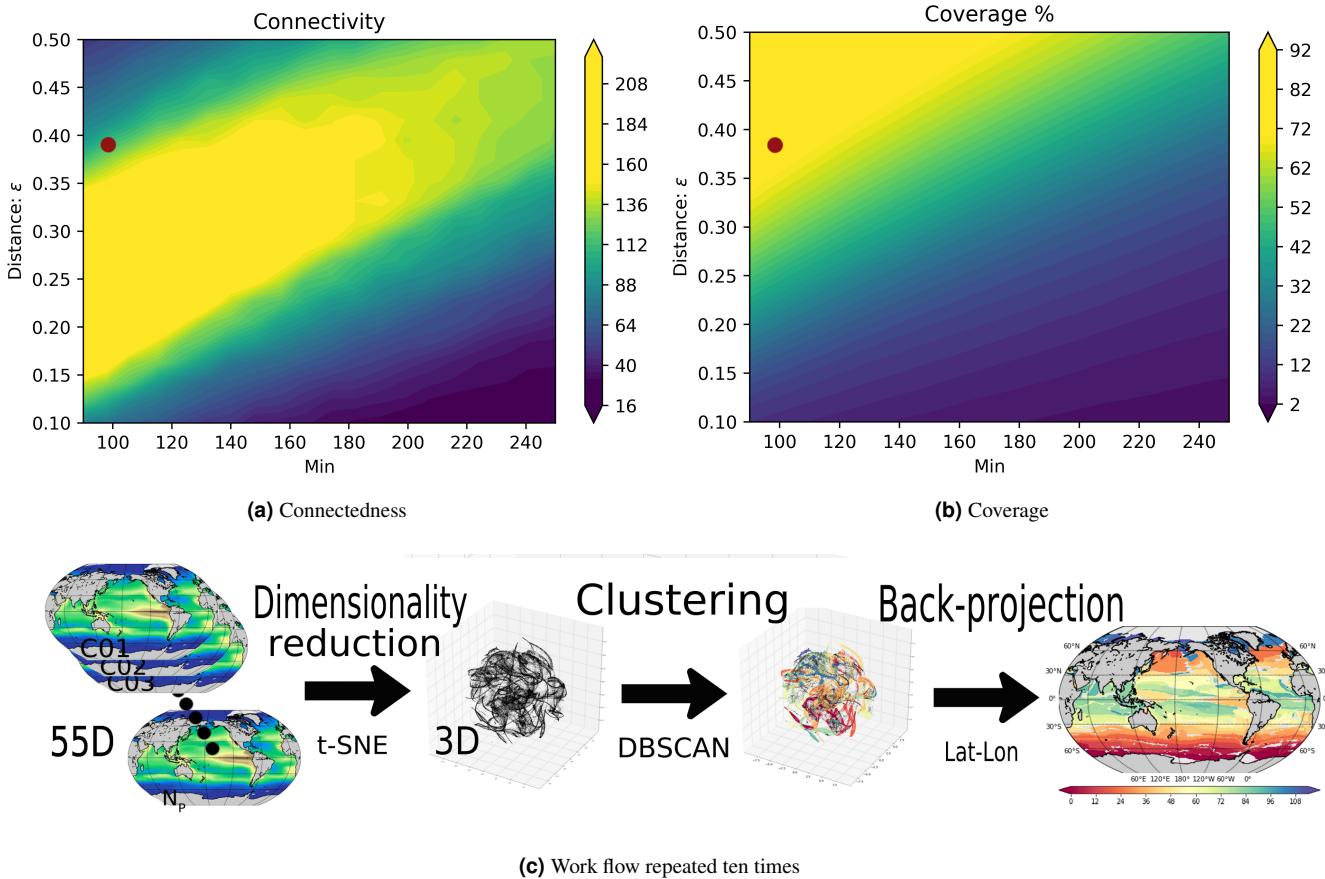


Figure 1. Setting the parameters for t-SNE the resultant number of found clusters is used as a measure of the connectedness (Fig. 1a) and the percentage of the data assigned to a cluster (Fig. 1b). The red dot illustrates the optimal combination of coverage and connectedness. The minimum number was set on the basis of minimum number relevant for ecology. Lower panel is Fig. 1c is a sketch of the work-flow; The raw 55D model data has sum of biomass of functional groups taken. Negligible values and persistent ice cover areas are discarded. Data is normalized and standardized. The 11D data is given to the t-SNE algorithm to highlight statistically similar feature combinations. DBSCAN selects the clusters carefully setting parameter values. The data is finally projected back onto a lat-long projection. Note this is repeated 10 times as a slight stochastic element is possible through the application of t-SNE.

Author contributions statement

M. Sonnewald developed the method and ran the analysis, she wrote the main body of the text.

Must include all authors, identified by initials, for example: A.A. conceived the experiment(s), A.A. and B.A. conducted the experiment(s), C.A. and D.A. analysed the results. All authors reviewed the manuscript.

Additional information

To include, in this order: **Accession codes** (where applicable); **Competing interests** (mandatory statement).

The corresponding author is responsible for submitting a **competing interests statement** on behalf of all authors of the paper. This statement must be included in the submitted article file.

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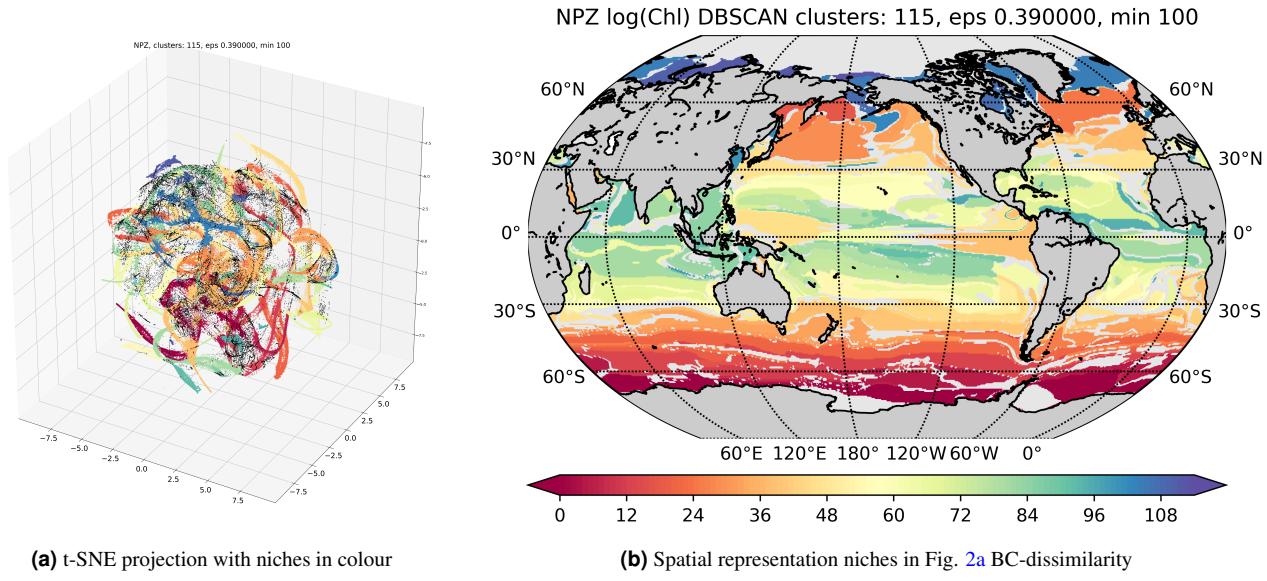


Figure 2. The left Fig. 2a showing nutrient, phytoplankton and zooplankton data as rendered by the t-SNE algorithm, and colored by niche using DBSCAN. Each point represents one point in the high dimensional space, with the vast majority of points captured as is demonstrated in the appendix. Axes refer to the "t-SNE" dimensions 1, 2 and 3. The right Fig. 2b shows the geographical projection of the niches discovered by DBSCAN onto the origin lat-lon grid. Colours should be considered arbitrary but correspond to Fig. 2a.

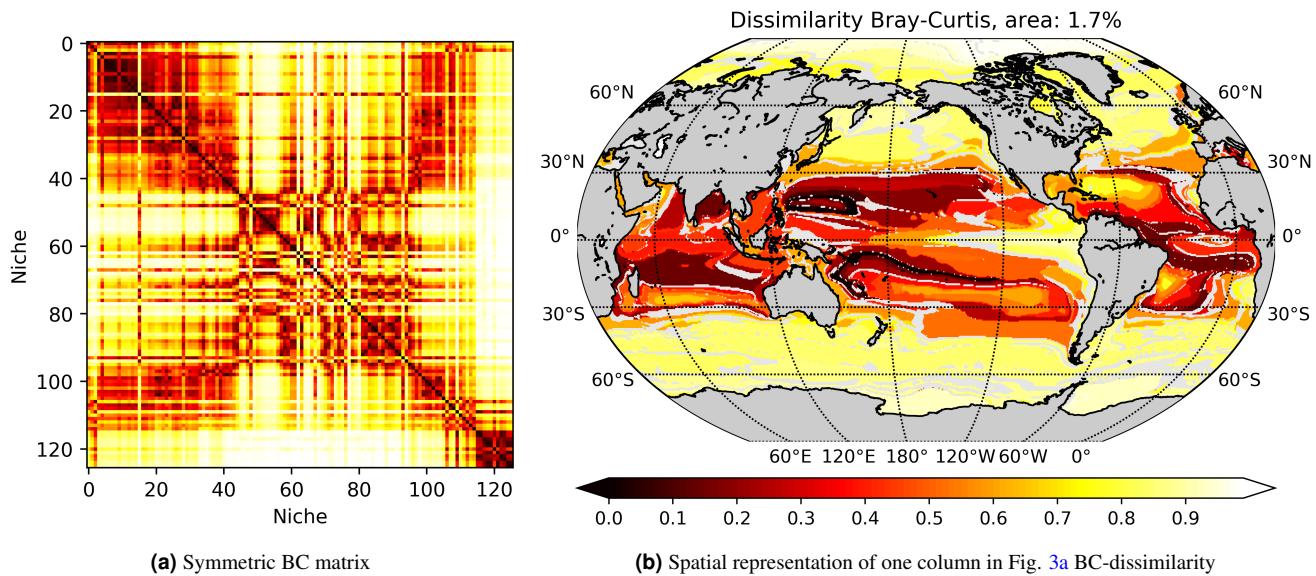


Figure 3. The left Fig. 3a Bray-Curtis Dissimilarity metric evaluated for **every niche compared to every other** for the global surface 20 year mean. Note the expected symmetry of the values. The spatial projection of one column (or row) is illustrated in the right Fig. 3b. The global distribution of Bray-Curtis Dissimilarity metric evaluated for one niche compared to every other for the global surface 20 year mean. Note the example shows an oligotrophic gyre example where other basins have similar regions and there is some symmetry across the equator. Black (Bray-Curtis = 0) denotes an identical region, while white (Bray-Curtis = 1) denotes no similarity.

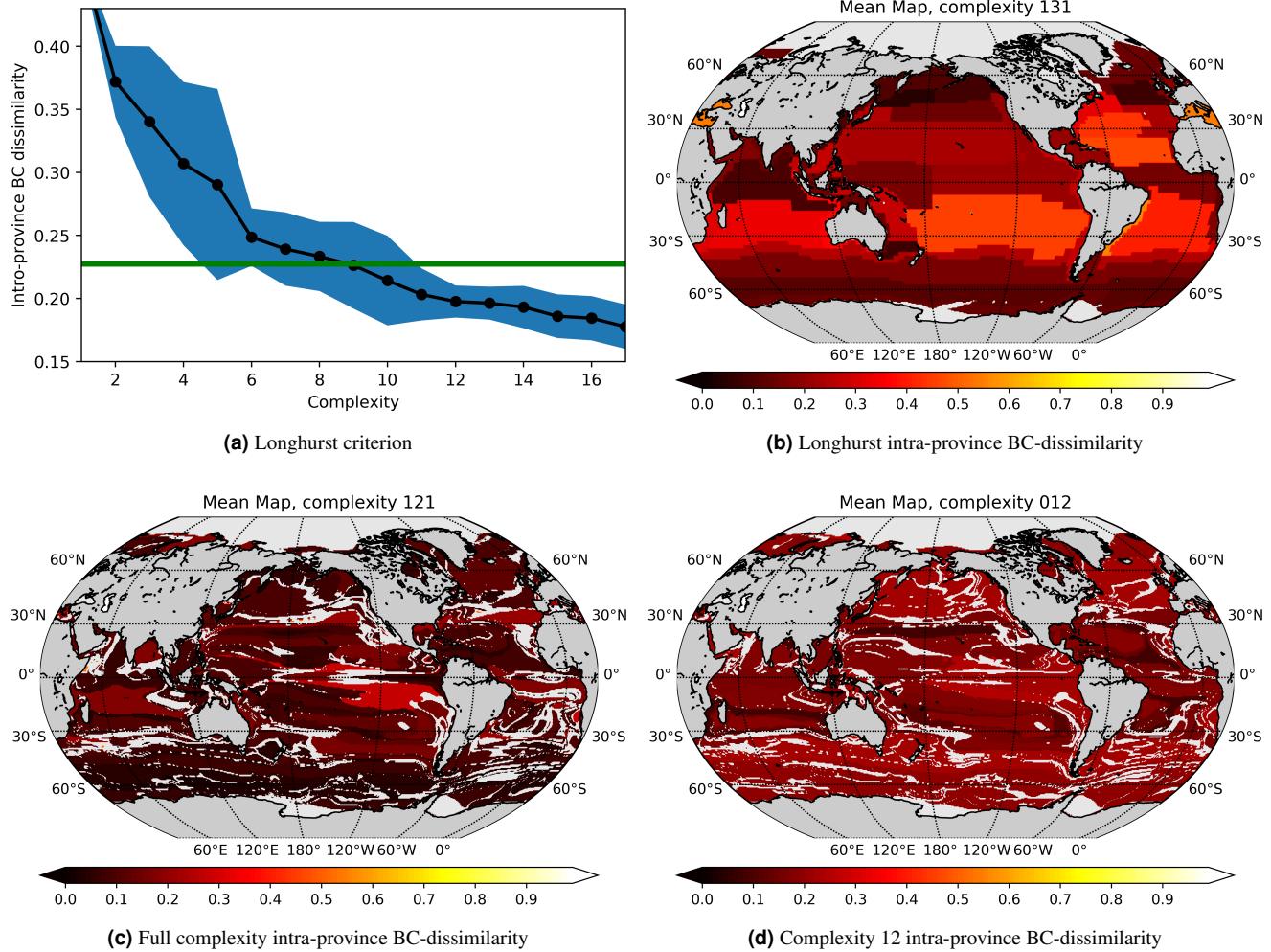
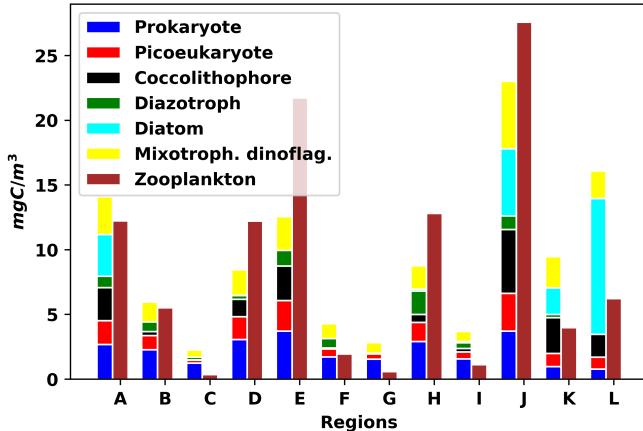
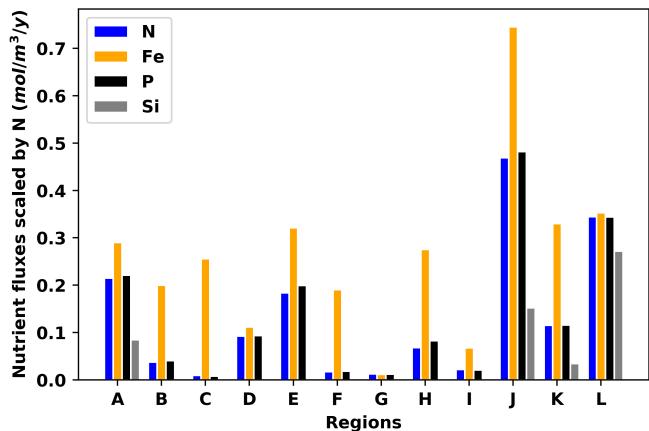


Figure 4. How complex should the bioge geochemistry be? The top left Fig. 4a shows the intra-province BC-dissimilarity of the Longhurst provinces (green line). The black line illustrates the intra-province BC-dissimilarity of increasing complexity. The 2σ is from 10 repeats of the province recognition process. For Fig. 4b, 4d and 4c the intra-province BC-dissimilarity is assessed as the mean BC dissimilarity of the individual gridpoint communities compared to the mean niche with no reduction in complexity. For Fig. 4b, the global mean intra-province BC-dissimilarity is 0.227. This is the benchmark for the ecologically motivated sorting presented in this work (green line in Fig. 4a). For the full complexity in the niches discovered by DBSCAN, Fig. 4c illustrates that an intra-province BC-dissimilarity of 0.099 is reached, while sorting into a complexity of 12 as suggested by Fig. 4a gives an intra-province BC-dissimilarity of 0.200 is reached as demonstrated in Fig. 4d.

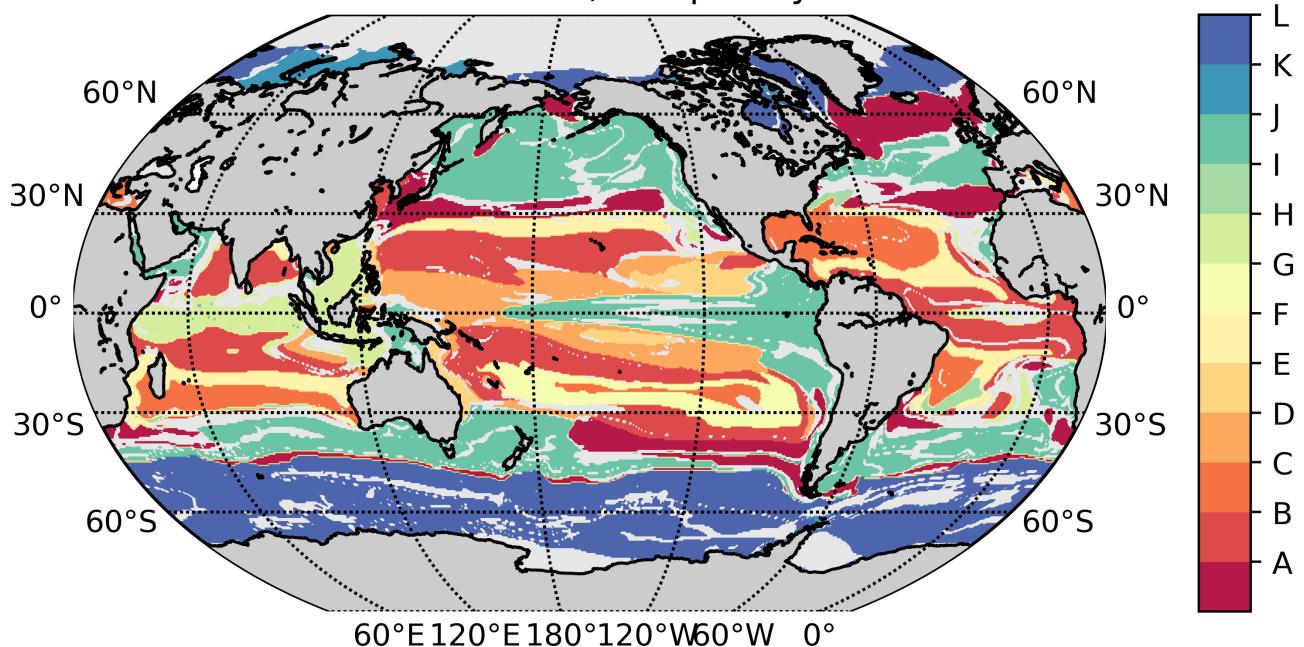


(a) Ecological ensemble



(b) Nutrient fluxes

Sorted Clusters, complexity 12



(c) Global provinces

Figure 5. Sorting the niches into the 12 most dominant provinces named from A to L. Top left Fig. 5a showing ecological ensemble in the 12 provinces. Top right Fig. 5b the nutrient fluxes. Bottom panel Fig. 5c. Note the distinction between Polar, subtropical gyres and dominantly seasonal/upwelling regions in the bottom panel.

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