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Projected novelty in the climate envelope of the California Current at multiple spatial-temporal scales

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Abstract

A useful measure of general climate stress is where and when novel habitats emerge. Here we evaluate 'climate envelope novelty'–a spatial indicator of system-level habitat change–in the California Current System (CCS), by quantifying the emergence of novel ocean conditions in multivariate physical-biogeochemical space. We use downscaled climate projections from three earth system models out to 2100 under emission scenario RCP8.5, and detect novelty at multiple spatial-temporal scales using two methods (n-dimensional hypervolumes and extrapolation detection). Under high emissions, persistent novelty doesn't appear until around 2040 and then only in small patches of Southern California and the Pacific North West. However, novelty increases rapidly after this (especially in warmer seasons), so that by 2060 up to 50% of the CCS in an average year has shifted to a novel local climate, which increases to 100% by 2090. These results are for the average year, and the first years to experience these levels of novelty typically occur 20 years sooner. The ecosystem will increasingly experience novel combinations of warmer temperatures, lower dissolved oxygen (especially inshore), and a shallower mixed layer (especially offshore). The emergence of extensive local novelty year-round has implications for the required ubiquitous redistribution or adaptation of CCS ecology, and the emergence of extensive regional novelty in warmer months has implications for bioregional change and regionally emerging fisheries. One of our climate projections showed considerably less novelty, indicating that realistic uncertainties in climate change (especially the rate of warming) can mean the difference between a mostly novel or mostly analog future.

Introduction

Climate change is causing widespread ecosystem change, including changes to species distributions, species productivity, and food web dynamics [1–3]. It is estimated that by 2100 (and

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compared to a recent historical baseline) 10–40% of the terrestrial surface will be experiencing novel climates [4, 5], and almost all of the ocean surface will be experiencing novel or 'unusual' climate conditions [6, 7]. Given the assumption that the distribution, abundance, and success of species derives from the complementarity of the climate space and their fundamental niche [8], measuring the emergence and location of novel climates is a useful and comparatively simple method for evaluating the potential impacts of climate change on species and ecosystems [9–13].

Measuring climate novelty employs the conceptual model of a spatially-explicit 'climate envelope', where the observed climate of a location occupies a multivariate data space defined by numerous environmental variables [4, 5]. Change and novelty in the climate envelopes of two time periods (e.g. historical and future periods) can then be measured using multivariate tools, such as multivariate distance metrics or hypervolumes [14, 15]. Novel or 'no-analog' climates occur when climate conditions exceed the bounds statistically defined for the comparison (i.e. historical) climate. It is important that novelty is measured in multivariate space to quantify not just novel values of single climate variables, but novel combinations of variables [16–18].

The detection of multivariate novelty (or 'extrapolation') is increasingly used in model-based predictions, such as those in species distribution modelling [14, 19–22]. In these cases, the focus is typically on a specific species and its modelled niche, and comparing the observed (i.e. fitted) set of environmental conditions with a set intended for prediction. Detection of novelty in the prediction set indicates extrapolation of the observed environmental responses, which is useful for identifying data limitations and uncertainty of predictions [16, 20]. Projecting novelty of a climate envelope differs from these analyses, in that the region of the historical and future data remains fixed, and the entirety of the niche in that region is assumed measured, but otherwise the detection of novelty in the climate envelope–and detection of model-based extrapolation–are the same. Thus, projecting novelty of the climate envelope can indicate not only ecological impacts but also where and when climate-based projections of the region are likely to be less reliable due to extrapolation uncertainties [23].

Most studies of climate novelty have been in terrestrial systems, although the ocean is receiving increasing attention [7, 24, 25], and these studies typically [but not always; 26] use the comparatively coarse resolution of global climate models [4–6]. These coarse models may miss key changes arising from fine-scale processes, such as coastal upwelling in marine systems, and provide less insight on community-level impacts, such as those experienced by specific fisheries or ports [27, 28]. Our study uses three dynamically downscaled projections of the California Current System (CCS)–a dynamic and productive upwelling system–to determine future multivariate novelty in the physical-biogeochemical climate envelope at a finer 0.1˚ (10 km) horizontal resolution (compared to 0.5–1˚ for the global models). These projections come from a regional ocean circulation model coupled with a biogeochemical model that was forced by three earth system models (ESMs) under the RCP8.5 scenario [29].

We use a four-dimension climate envelope [8] incorporating broadly-relevant surface and sub-surface environmental information [30–33]: sea-surface temperature (SST); oxygen concentration at 100 m depth; iso-thermal layer depth (ILD) as a measure of mixed layer depth; and eddy kinetic energy (EKE); this set of variables is compared to a second set to estimate the effect of variable choice on estimated novelty. We compare two methods for calculating novelty: n-dimensional hypervolumes [34, 35] and extrapolation detection ['ExDet'; 14]; which differ in how novelty is quantified and how drivers are identified (Table 1; S1 Fig). The hypervolume method uses a geometric approach to calculate novelty while ExDet uses dimension reduction, and together cover the two fundamental approaches to the task. Novelty is quantified as the percentage of the CCS experiencing a novel climate at four spatial-temporal scales:

Table 1. Explanation of the four scales of novelty and how each was calculated. '*Hyper*' is hypervolume, '*ExDet*' is extrapolation detection.

Novelty scale	Regional	Regional monthly	Local	Local monthly
What this scale measures	Conditions entirely novel to the CCS region[1]	Conditions novel to the CCS region for that month of year[1]	Conditions entirely novel at a particular location[1]	Conditions novel at a particular location for that month of year[1]
Species most impacted by this scale of novelty	Any species adapted or acclimated to historical CCS conditions	Species with strong phenology[2]	Species with lower mobility[3]	Species with lower mobility and strong phenology[4]
The historical data set	Monthly values of the four covariates[5] from Jan 1980 to Dec 2009 for a given ESM projection[6] (360 months)	Same as 'regional', but only for a specific month from 1980 to 2009 (30 months)	Same as 'regional', plus:	Same as 'regional monthly', plus:
	ExDet: 7,696,080 observations of each covariate (21,378 unique locations)	*ExDet*: 641,340 observations	*ExDet*: 14 areas tested separately	*ExDet*: 14 areas tested separately
	Hyper[7]: 5% subset, 384,804 observations	*Hyper*: 32,495 observations	*Hyper*: latitude and longitude included as covariates	*Hyper*: latitude and longitude included as covariates
The future data set	Monthly values of the four covariates[5] at every location in the CCS for a specific month, from 2020–2100 for one of the three ESM projections[6] (21,378 observations of each variable); for hypervolume[7] at local scale also included latitude and longitude			
How novelty was quantified	*ExDet*: Compare Euclidean distance of future single variable values against historical values (novelty exists when ExDet values < 0; 'univariate extrapolation'), and compare Mahalanobis distance of all future variable values against historical set (novelty exists when ExDet > 1; 'combinatorial extrapolation'); Total novelty is the percentage of CCS pixels with univariate or combinatorial extrapolation[8]			
	Hyper: Compare all future variable values against an historical hypervolume, and test for inclusion (inside or outside; the 'inclusion test'); Total novelty is the percentage of CCS pixels outside the historical hypervolume			
How drivers of novelty were identified	*ExDet*: For a specific period and scale, mapping the 'most influential covariate' (MIC) output, calculated by ExDet			
	Hyper: For a specific period and scale, calculating a future hypervolume, and comparing overlap and centroid location of pair plots; and a 'drop one out' analysis			

[1] Compared to the historical period.

[2] Species with strong phenology may not be able to move their dynamics in time to adapt to novel conditions (e.g. spring spawners, or migration of north pacific albacore into the CCS).

[3] Species with lower mobility may not be able to move in space to adapt to novel local conditions (e.g. kelp or groundfish).

[4] For example, juvenile salmon exiting fixed nursery grounds.

[5] SST, ILD, EKE, oxygen concentration.

[6] GFDL-ESM2M, HadGEM2-ES, IPSL-CM5A-MR.

[7] All variables were centred and scaled for hypervolume analyses, using their mean and standard deviation from the historical period.

[8] For both methods, a value of 100% novelty means that ocean conditions in every pixel of the CCS model are not represented in the historical conditions.

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1) regional; 2) regional-monthly; 3) local; and 4) local-monthly (Table 1). This approach evaluates the 'when and where' of ocean climate novelty in the CCS, and identifies and maps drivers of novelty. The expected value of this information is to identify areas of the CCS most likely to experience strong ecological stress and resulting impacts on ecosystem services, and provide broad context for evaluating the suitability of end-of-century model-based ecological projections.

Materials and methods

Analysis structure

We quantified multivariate novelty in the physical-biogeochemical climate envelope of the CCS in two ways: n-dimensional hypervolumes [34, 35] and extrapolation detection [14]. Both were used to define the historical conditions (1980–2009) of the CCS in multidimensional space, and calculate the extent of novelty in future conditions (each month within 2010–2100)

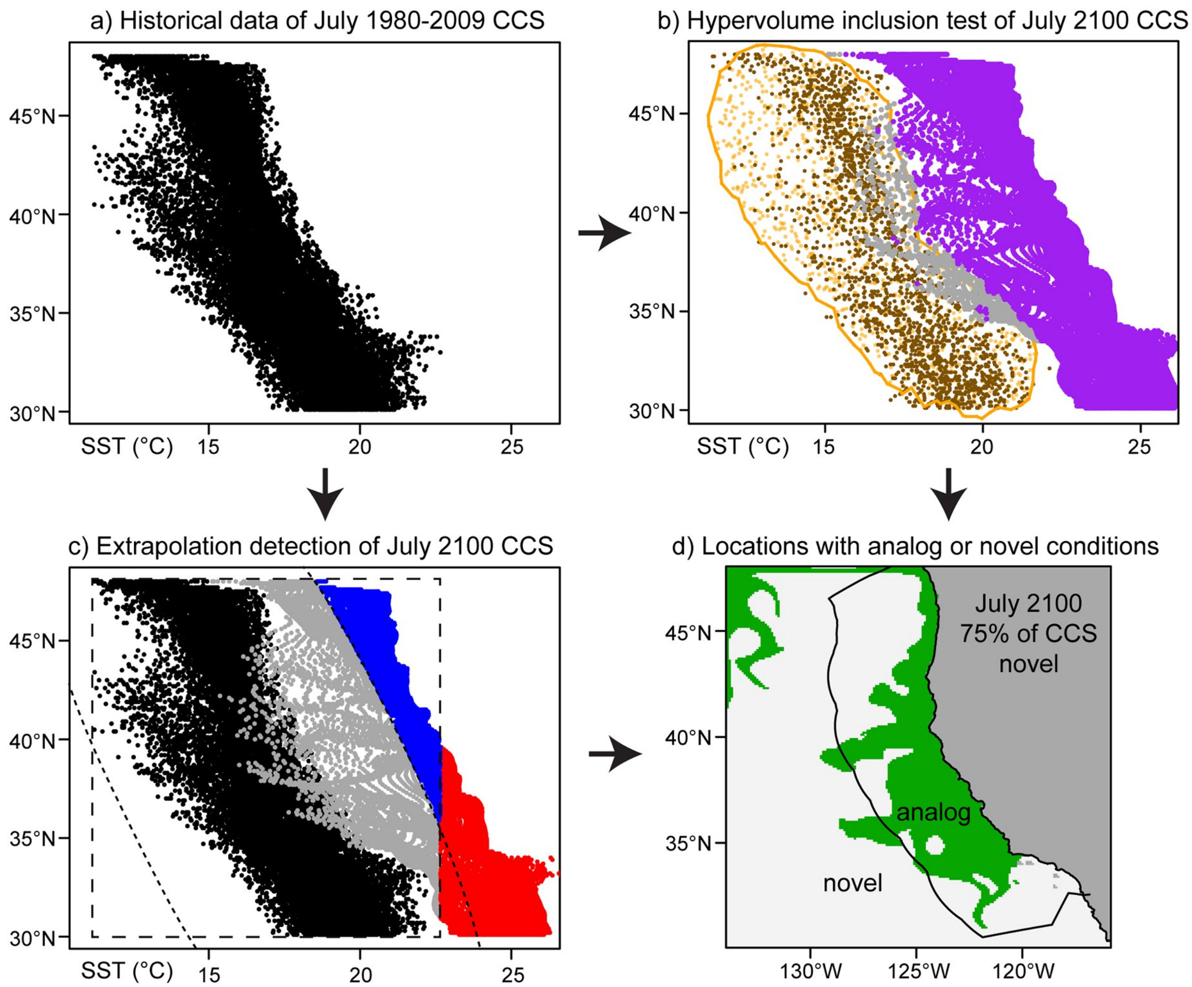

Fig 1. Schematic of how novel conditions were identified. This is a simplified example with two covariates (SST and Latitude), and calculating novelty in the CCS climate envelope in July 2100 compared to historical Julys using the IPSL projection. a) Historical conditions in the CCS are extracted from projections for the desired environment and spatial covariates, and for the temporal span of interest (annual or monthly; Table 1). b) The hypervolume method creates a hypervolume (orange line an alpha hull approximation) surrounding these historical values (in as many dimensions as covariates), and then tests whether future values of the covariates (at every location in the domain) lie within the historical hypervolume. Locations that lie within the historical hypervolume (grey dots) have future conditions analogous to historical, and those that lie outside the hypervolume (purple dots) have novel future conditions. Brown dots are a subset of historical observations and orange dots are random points (used for hypervolume creation) guaranteed to be in the hypervolume. c) The ExDet method detects univariate novelty by identifying locations with conditions that lie outside the range of historical values for single variables (dashed box; red dots), and calculates the Mahalanobis distance to detect combinatorial novelty (dashed oval; S4 Fig), i.e. locations 'outside' the maximum of this distance have novel combinations of variable values (blue dots). Locations are otherwise considered to have future conditions analogous to historical (grey dots). d) For each of these methods, novelty for any future month is calculated as the percentage of locations in the CCS domain experiencing novel conditions compared to historical. This map shows the result of the ExDet method, with 75% of the CCS in July 2100 experiencing novel conditions (grey area) and 25% analog conditions (green area). In this example (essentially a local-monthly scale, but lacking longitude), novelty represents SSTs warmer than experienced historically in July anywhere in the CCS, plus SSTs warmer than experienced at specific latitudes. The black line is the exclusive economic zone (EEZ). The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.

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relative to this historical period (Fig 1; Table 1). For both methods, novelty was measured as the percentage area of the CCS experiencing novel climate. Our results are at a monthly and 0.1 horizontal resolution, which represents sustained and meaningful 'on the ground' change for ecological and human communities.

We quantified climate novelty at four spatial-temporal scales: 1) regional; 2) regional monthly; 3) local; and 4) local monthly (Table 1). At the 'regional' scale, a location is identified as experiencing novel climate conditions if those conditions were not observed anywhere in the CCS at any time during the historical period. At the 'regional monthly' scale, novelty represents conditions not historically observed anywhere in the CCS during a particular month of the year. At the 'local' scale, novelty represents conditions not historically observed at any time at a given location. And at the 'local monthly' scale, novelty represents conditions not historically observed at a given location during a particular month of the year. These four scales are useful to infer potential impacts on species within the CCS based on whether they can move in space (their mobility), move in time (their phenology), or both (Table 1); e.g. local novelty is likely to indicate the extent of stressors motivating species redistribution, and more-so for species with smaller ranges or lower mobility. The local-monthly scale encompasses all other scales of novelty, so can represent a metric of total novel area. Although regional novelty is relative to the extent of our domain, it has relevance to new environments and emerging fisheries for the U.S. West Coast. Having multiple scales also recognises that climate change can be expected to produce localized novelty at all latitudes, rather than just in the warmest margins of the domain [5].

Climate variables

A climate or niche envelope is defined by its axes (here, environment variables). Variable selection is a key decision that determines the volume and shape of the climate envelope–too many variables will tend to over-characterise each location, and lead to inflated, unmeaningful, or false novelty [5, 34]. Using fewer important variables for the desired climate niche seems to be the best approach [4]. We selected four climate variables from the projections to define the multi-dimensional space defining the CCS: sea-surface temperature (SST, ˚C); oxygen concentration at 100 m depth (mmol m^{-3}); iso-thermal layer depth (ILD, m) as a measure of mixed layer depth and defined by a 0.5˚C deviation from surface temperature; and eddy kinetic energy [EKE, $\log_e(m^2 s^{-2})$]. These are variables commonly used in species distribution models in the region, and with broad relevance for many pelagic and near-surface species [30–33]. Temperature in particular correlates with other important bioclimatic controls of ecological patterns and processes [4, 36, 37]. Other reasons to limit the covariate number to four were the considerable computational burden of the hypervolume calculation, and potential issues arising from correlated variables [35]. These reasons are less important for the extrapolation detection method, but for the sake of comparison among methods both used the same climate variables. We visually compared the trajectory of novelty calculated using this set of four climate variables with that calculated using a second set, which includes one biological variable (SST, bulk Brunt-Väisälä frequency, surface chlorophyll, and wind stress) to estimate the effect of variable choice on estimated novelty. This comparison set is detailed in S1 Fig. To quantify novelty at the local scales, geographic coordinates were also included for the hypervolume method (Table 1), as detailed below.

Climate projections of the CCS were obtained from a high-resolution (0.1˚) regional ocean circulation model coupled with a biogeochemical model (ROMS-NEMUCSC) that was forced by three earth system models (ESMs) under the RCP8.5 scenario [29]. The biogeochemical model is a Regional Ocean Modeling System (ROMS) configured for the CCS [38] coupled to the NEMUCSC model [39, 40]–an adapted version of the North Pacific Ecosystem Model for Understanding Regional Oceanography [NEMURO; 41]. The ESMs are Geophysical Fluid Dynamics Laboratory (GFDL) ESM2M, Hadley Center HadGEM2-ES, and Institut Pierre Simon Laplace (IPSL) CM5A-MR (abbreviated hereafter to GFDL, Hadley, and IPSL). These three models encompass the range of models in the Coupled Model Intercomparison Project (CMIP5) archive in terms of future physical and biogeochemical changes in the CCS. These models differ in the range of projected warming (GFDL projects a ~2˚C SST increase in the 21st century, compared to 3–4˚C for the other two models), and disagree on the sign of change in primary production; further characteristics and differences are detailed in Pozo Buil *et al.* [29]. Given that variability among climate models is greater than internal climate variability at decadal and century scales [42], the spread among these models is a robust estimate of climate uncertainty in the CCS. The historical period, against which future conditions were compared, was taken as the 1980–2009 period (30 years) of the climate projections. A 30-y period was selected to encompass representative climate conditions and variation, and approximately aligns with the end of model period forced by historical emission (2005). Our estimates of climate novelty are specific to the spatial domain of ROMS-NEMUCSC (30–48˚N and offshore to 134˚W), which encompass much (but not all) of the CCS. We used only RCP8.5 because this was the only emissions scenario available as downscaled projections. However, in the CCS most of the scenario uncertainty is contained within the model uncertainty, meaning that within the range of our three models under RCP8.5 lies much of the climate space contained within those models under RCP2.6 and 4.5, including for SST [see 29, 42]. Thus, our projections of climate novelty are likely representative of a broader range of potential futures than only the highest emissions scenario.

Hypervolumes

Our first approach to measure environmental novelty was the n-dimensional hypervolume, where 'n' is the number of independent axes used to define the potential multivariate space [34]. The hypervolume is an n-dimensional geographic shape that defines the subset of space defining a particular set of axis values. Hypervolumes are used in a variety of contexts to explore the niche, including using climate axes to quantify multivariate climate space and its change [15], although hypervolumes are underutilised for quantifying emerging novelty in the climate niche of a region using climate projections. We fit hypervolumes using the 'hypervolume' package v2.0.12 [35] in R v4.0.4 [43].

There are two main algorithms for delineating and evaluating the hypervolume function in the 'hypervolume' package: Gaussian kernel density estimation (KDE) and a support vector machine (SVM). The KDE method creates a continuous probabilistic output with a 'looser' fit to the boundary of the hypervolume, whereas the SVM method provides an 'in or out' output and is insensitive to outliers [35]. We chose the SVM method (and default algorithm values), because we deemed it more likely to detect similar but novel environmental conditions, and because it allowed an 'inclusion test' approach to measuring environmental change [34].

We quantified future novelty using the suitability projection set operation. This approach creates an historical period hypervolume, and calculates the suitability of locations based on future environmental conditions. Because the SVM algorithm creates a binary 'inside or outside' suitability, we measured future novelty as the percentage of CCS locations with environmental conditions outside the historical hypervolume, i.e. an inclusion test [34]. Hypervolumes were created using the 'hypervolume' function, and the suitability projection was done using the 'hypervolume_project' function [35]. The computational burden of hypervolumes was large, so we subsampled 5% of the historical data (consistent but randomly selected) to create the historical hypervolumes (Table 1). A comparison of using 5% and 20% of the data led to hypervolumes with very similar volumes and centroids, which indicates that the 5% hypervolumes are representative of the historical period (testing > 20% at our resolution was not computationally feasible). Aggregation of data is an alternative to subsampling, but we preferred to maintain our spatial and temporal resolution.

The environmental variables driving future change were evaluated through interpretation of the pairwise overlap of the historical (1980–2009) and future hypervolumes (2051–2060 and 2091–2100), and through a 'drop one out' analysis of hypervolume overlap. These analyses used the hypervolume overlap set operation, which measures Jaccard and Sorensen similarities (the relative volume of hypervolume intersection and union), plus the unique fractions of each hypervolume [35]. These metrics are comparable to the results of the inclusion test (i.e. novel percentage of CCS). Our 'drop one out' analysis estimates each variable's relative influence to novelty by measuring the overlap between historical and future hypervolumes when that variable is removed compared to the overlap measured in the full model (detailed in S2 Fig).

The local scale measures whether ocean conditions are novel to a specific location, and was quantified by including geographic coordinates (latitude and longitude) as additional axes to the climate envelope (Table 1); thus, local novelty was identified as (for example) novel combinations of SST and latitude (see Fig 1). This is a suitable strategy for quantifying local novelty, as the values of the geographic coordinates do not change through time, so only contribute to novelty as new combinations with climate variables.

Extrapolation detection

Our second approach to measure environmental novelty was extrapolation detection [14], calculated using the 'dsmextra' R package v.1.1.5 [44]. Extrapolation detection ('ExDet') is most often used in a species distribution modelling context to identify when covariate values used for prediction extrapolate beyond the observed values used for model fitting [14, 21, 23]. In our analyses, the extent of extrapolation was used to measure the extent of environmental change of a fixed geographic domain. A similar method has been used to evaluate the distribution of climatic novelty across terrestrial North America [5].

ExDet measures novelty with both univariate and combinatorial extrapolation (Fig 1), with univariate being extrapolation along each axis (measured using Euclidean distance), and combinatorial being new combinations of covariates within the extent of the axes of the historical period (measured using the Mahalanobis distance). This method is less computationally expensive than hypervolumes, so we were able to use all data to define the historical climate envelope (Table 1).

The environmental variables driving future change were evaluated by the 'most influential covariate' metric, which identifies the covariate that changes the Mahalanobis distance the most when removed [14]. We used a different method to measure the local scale for the ExDet method. We evaluated adding geographic coordinates as additional axes (as for hypervolumes), but it was clear that the Mahalanobis distance underestimated local novelty, particularly novel SSTs at specific latitudes (Fig 1, and detailed in S3 and S4 Figs). Instead, we divided the CCS into 14 areas based on latitude and distance from shore (S5 Fig), and quantified ExDet for each area separately (Table 1). Total novelty was then the sum of the novel area within each of the 14 areas. This number of areas was selected to balance sufficiently distinguishing the inshore-offshore and north-south gradients in ocean conditions and having sufficient data (within an area) to properly represent the historical climate.

Results

Increasing novelty

Trajectories of the novel CCS area are shown in Fig 2a for one ESM projection, for the month of August, for the two analysis methods (hypervolume and ExDet), and at all four scales. At

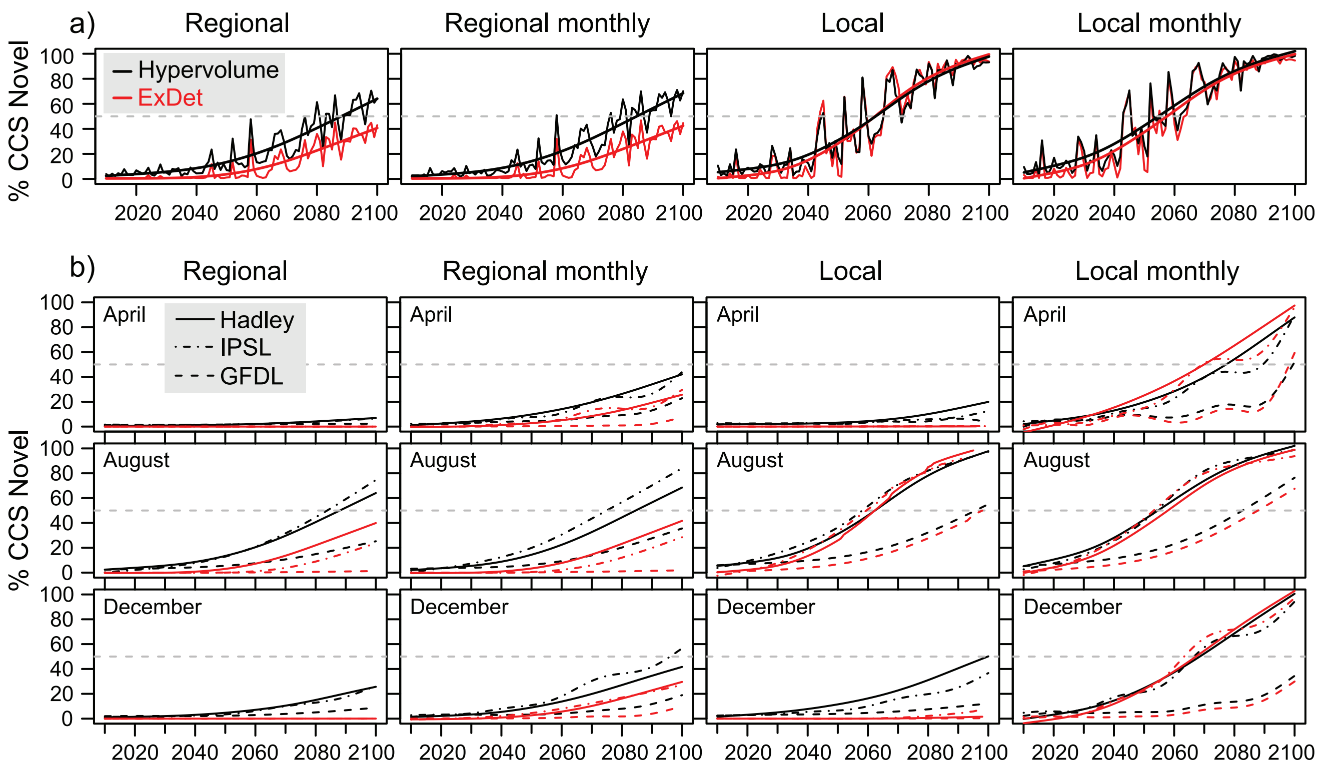

Fig 2. Projected percentage of the CCS experiencing novel conditions. Novelty is shown at the four scales (regional, regional-monthly, local, local-monthly), from 2010 to 2100 (compared to the 1980–2009 period). In a) we show novelty in August under Hadley, and both the yearly percentages (jagged lines) and a GAM smoothed trend, as estimated by hypervolumes (black line) and ExDet (red line). Coupled climate models are not intended to be used to forecast what happens in specific years, so while the frequency and magnitude of spikes in novelty will likely reflect reality, the exact years in which they happen will not. In b) we show just the smoothed trends for all three projections (line type) for three representative months. As a visual aid, the dashed grey line indicates 50% novelty.

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the regional scale, the area of our CCS domain experiencing climate novelty increases steadily to 40–65% by 2100. In other words, by the end of the century (under Hadley, a model that exhibits relatively strong projected warming [29]) 40–65% of the domain in August is experiencing an ocean climate not experienced anywhere or anytime in the domain during 1980–2009. The regional-monthly scale shows similar novelty, because August is one of the warmest months of the year. Novelty at the local scale is higher, with 90–100% of our CCS domain experiencing novel conditions (i.e. when accounting for additional novel combinations of space and climate), compared to any month (local scale) or only to August conditions (local-monthly scale). Fig 2a also shows the strong interannual variation in novelty (even among consecutive years); take, for example, the hypervolume estimate of the local scale in Fig 2a–although the smoothed trend for novelty reaches 50% by 2065, the first year to experience 50% novelty is 2045. The smoothed trend illustrates the novel area in the average year, and it's clear that years of exceptional novelty fluctuate around this trend.

The variation in novelty between calendar month, scale, and ESM projection is summarised in Fig 2b. Generally, only the months with warmer SSTs (especially Aug-Oct) showed moderate regional novelty by 2100 (20–60% of the CCS), with cooler months and especially Spring (April-June) showing little regional novelty. Novelty at the regional-monthly and local-monthly scales was considerable for all months, indicating that future conditions in CCS will be increasingly novel for any given time of year. The highest novelty occurred at the local-monthly scale, with 40–100% of the CCS in every month of the year experiencing conditions by 2100 that are novel for that month at a given location. These timelines are for the smoothed 'average' trends in novelty, and the first years to reach a given value occur considerably earlier, e.g. the first years to exhibit 50% local-monthly novelty occur 5–40 years before the 'average' year (typically 20 years). Novelty was generally lower under the GFDL projection, which exhibits a lower magnitude of warming than the other two models [29], and the ExDet method estimated lower novelty than the hypervolume method at the regional scales. The comparison model using a different set of climate variables (but keeping SST) showed similar trends, although novelty was higher in some months, with regional novelty reaching 100% for the warmest months (S1 Fig).

Location of novelty

Maps showing novel areas are demonstrated in Fig 3, using the IPSL projection for three example months at all scales. These maps combine the regional-monthly and local scales

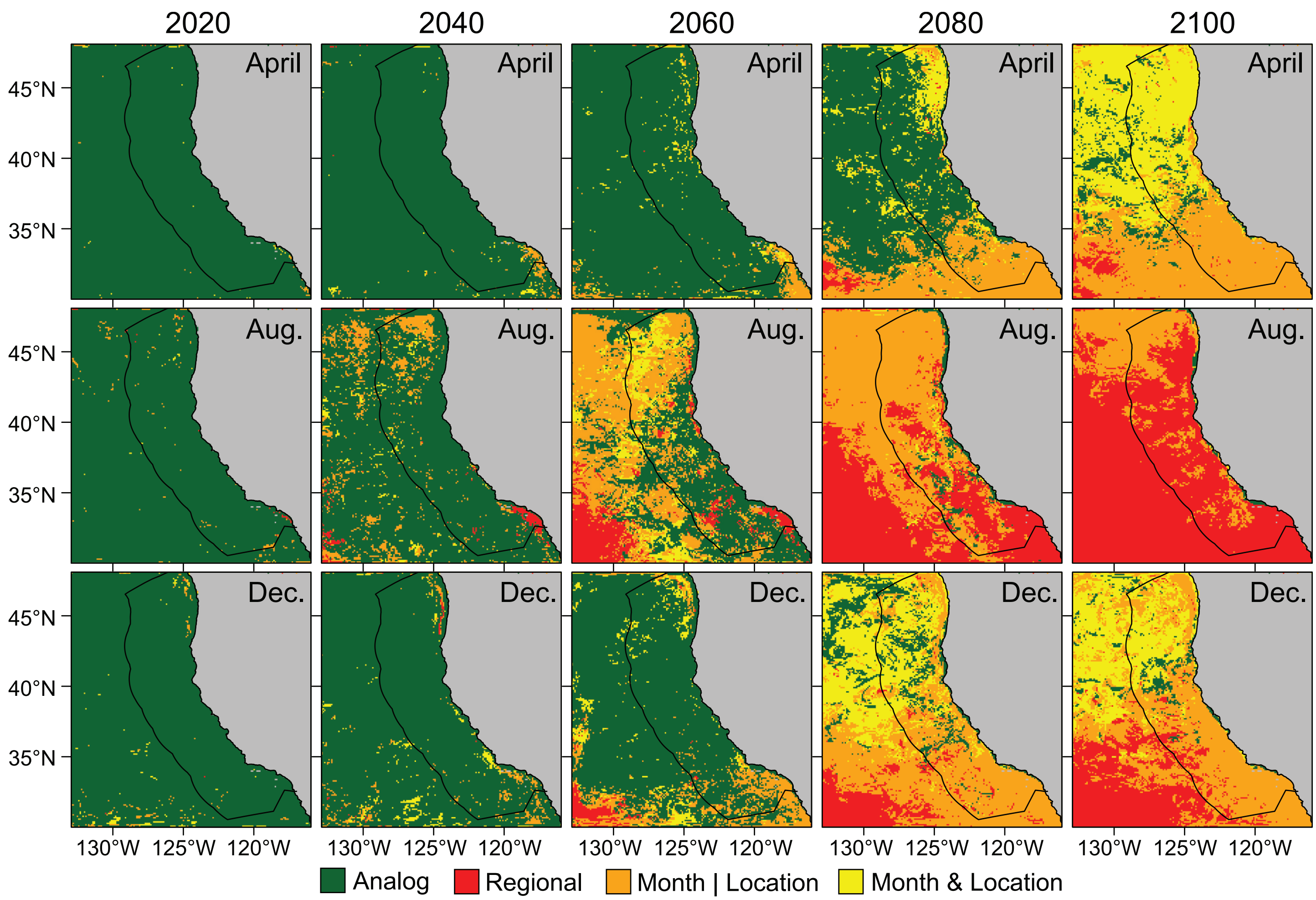

Fig 3. Maps of locations with novel or analog climates. Maps are shown for three example months at the end of five decades, under IPSL. Colors represent an analog climate (green), or climate novel to the region (red), novel to a given location or month of the year (orange), or novel at a given location and month of the year (yellow). The maps show each pixel's majority classification over a 5-year period ending in the specified year (e.g. 2016–2020). These maps use the hypervolume method, and the ExDet method is shown S6 Fig. The black line is the exclusive economic zone (EEZ). The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.

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because some locations were novel at both scales, and rather than choose a category to take precedence we combined them; but the local scale was typically the more abundant scale. Novelty appears simultaneously in Southern California and the Pacific Northwest, highlighting that, although the climate in the northern CCS will have been experienced previously elsewhere in the CCS, the climate will be new for that location and time of year. Regional climate novelty is more common in the southern area (the warmest part of the domain). The central coastal area retains analog conditions the longest, but virtually the entire region is novel by 2090–2100 in every month. The ExDet method estimates a similar extent, but with reduced regional novelty (S6 Fig).

Drivers of novelty

Drivers of novelty for the hypervolume are inferred from pair plots of historical and future hypervolumes. Fig 4 shows hypervolumes for the month of July, under the IPSL projection, and at the local-monthly scale. Most of the difference between hypervolume extents is on the SST axis, indicating that SST is the key driver of future climate novelty (and explains why regional novelty occurs predominantly in the warmer south). The relationship between SST and latitude/longitude shows that novel SSTs at a given location are also the main driver of increasing local novelty. The other three climate variables contribute to future climate novelty but less than SST. The future CCS experiences lower oxygen concentration and shallower ILD in general (note the shift between centroids in Fig 4), including novel low oxygen-shallow ILD space. We also see novel shallow ILD-high EKE climate space. The strongest ILD effect (but not contributing to novelty) is the loss of deep ILD values, especially offshore. Drivers of novelty are also inferred using a 'drop one out' comparison of fractional overlap between historical and future hypervolumes. This shows that SST contributes 40–95% of the estimated novelty in the climate niche (S2 Fig). This percentage increases over time and is higher with a higher rate of warming (i.e. a lowest influence under GFDL and highest under Hadley). Other variables individually contribute 0–25% to hypervolume novelty.

Drivers of novelty for ExDet are inferred using the most influential covariate (MIC) metric (Fig 5) which is typically mapped [44]. MIC only identifies the most influential covariate so likely underestimates contributions of other variables (especially when one variable is more often novel, e.g. SST in Hadley). As observed for hypervolumes, SST is the dominant driver of novelty and contributes to novelty in all areas (but least at inshore Southern California for GFDL and IPSL). Oxygen concentration influences inshore novelty, and ILD influences offshore novelty. A mid-century exploration of MIC shows a similar pattern (S7 Fig). ExDet estimates novelty as both univariate and combinatorial novelty, and at all scales (and more so at the regional scales) novelty is predominantly univariate.

Discussion

Under a high emissions scenario, two of our three downscaled projections indicate it takes around 50 years for 50% of the CCS domain to experience novel conditions in the average year (for a given location and time of year) and 90 years for ~100%. However, the first years to experience these levels of novelty typically occur around 20 years sooner. Under high emissions, consistent novelty doesn't appear until around 2040 and only in small patches of Southern California and the Pacific North West, but novelty increases rapidly after this especially in warmer seasons. These trajectories are based on mean monthly climate conditions and are thus sustained periods of novelty with the potential for considerable stress on ecological and human communities. The warmest months show the fastest emergence of novelty, and in these months the ocean environment is not only new locally but often new to the CCS domain.

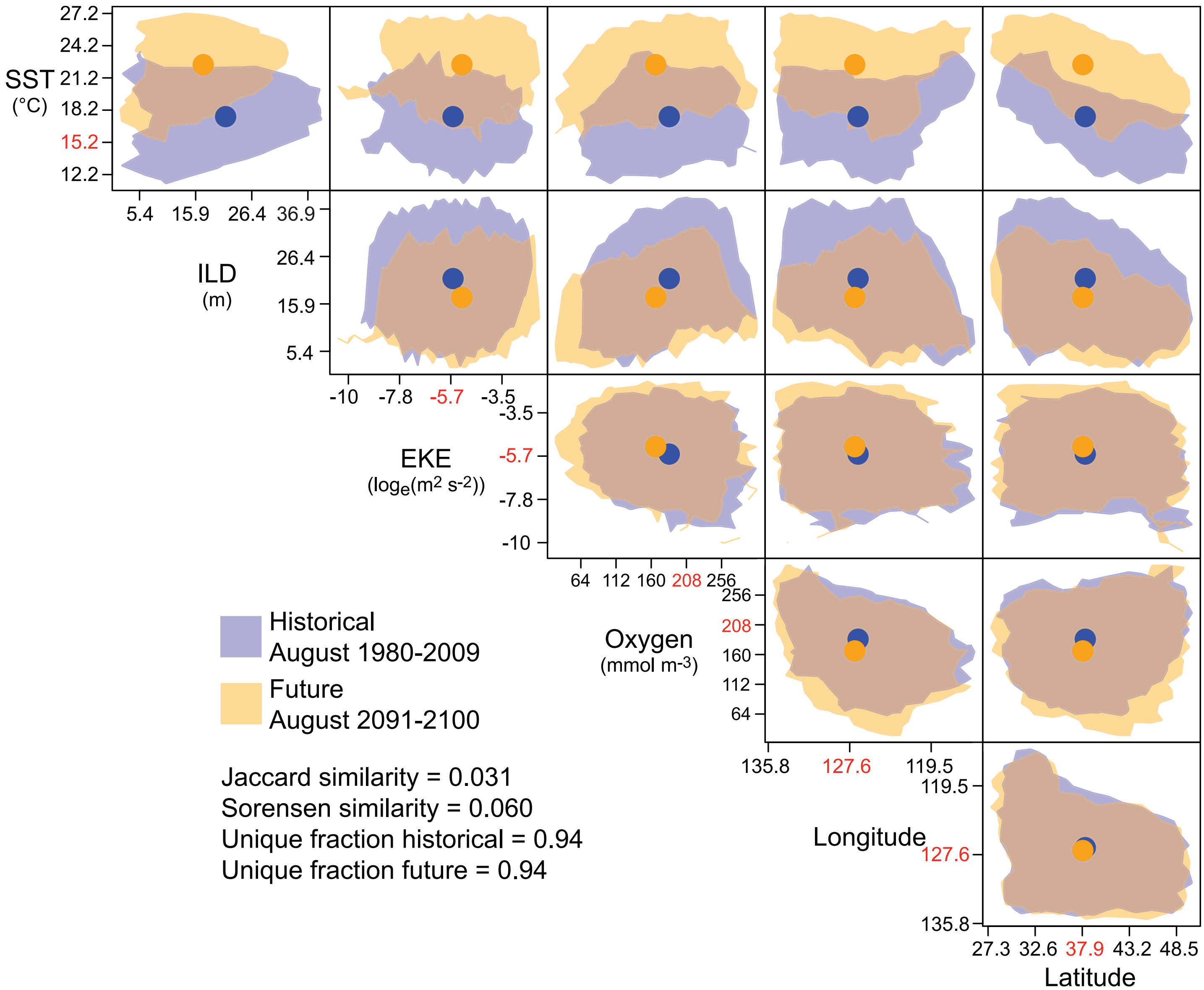

Fig 4. Historical and future end-of-century hypervolumes visualized as pair plots. These hypervolumes respectively represent 30 years and 10 years of August climate conditions combined. This is for the IPSL projection and at the local-monthly scale; results are similar across months. Filled circles are hypervolume centroids. Overlap metrics of the two hypervolumes are given, i.e. 94% of each six-dimensional hypervolume is unique to that period, with very low similarity measures. Mean historical values for each variable are indicated in red font.

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The GFDL projection shows meaningfully less novelty, because GFDL exhibits the slowest rate of warming in the CCS [29]. In fact, the difference in warming between GFDL and the other two projections sometimes meant the difference between a mostly analog or mostly novel ocean climate. This result highlights the potential for non-linear or threshold impacts in biological and human systems due to a changing climate [45–47], and climate novelty may be a key indicator of the novel communities [8, 45] or physical climate thresholds [46] that can lead to these strong changes.

The geographic scale of regional climate novelty in the CCS are similar to those for terrestrial environments [5, 8], and the 100% local-monthly novelty estimates for two of our three

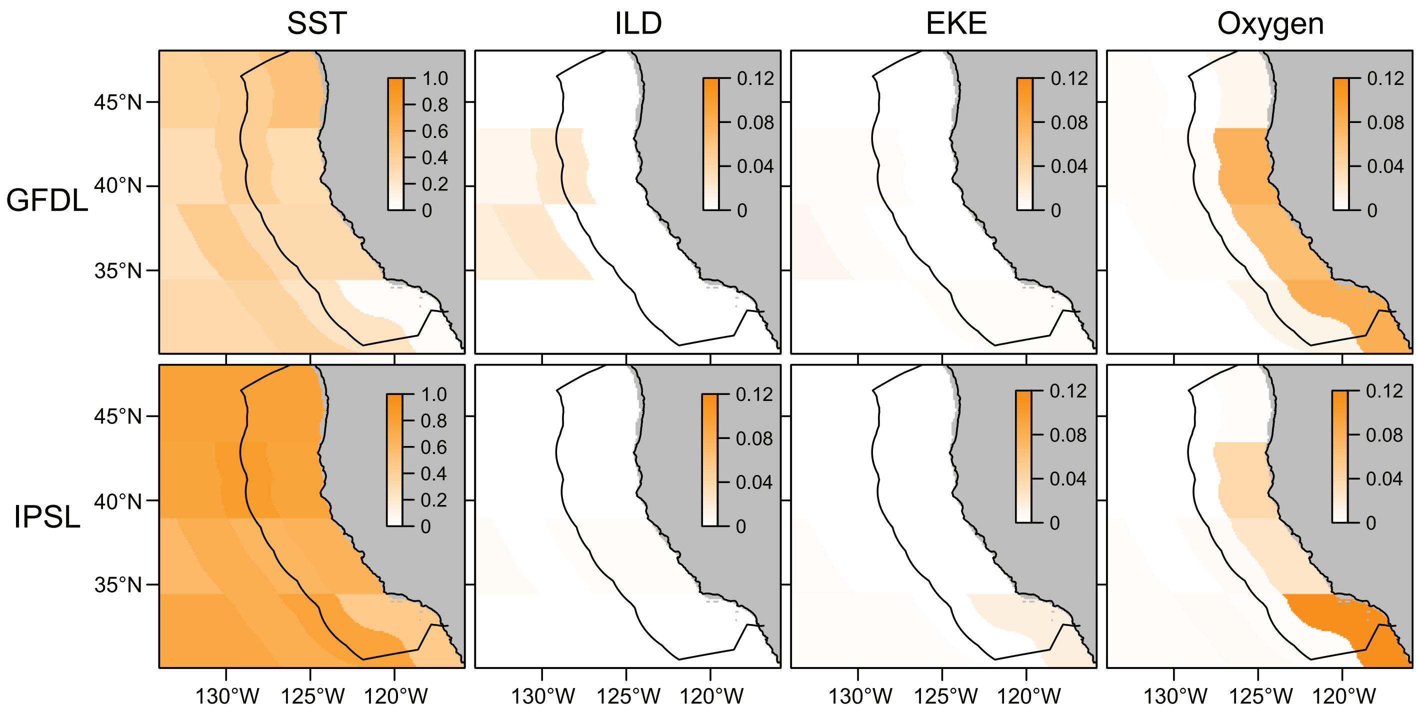

Fig 5. Maps of MIC (most influential covariate) values estimated by the ExDet method for the GFDL and IPSL projections. These are based on 2091–2100 July values at the local-monthly scale. Values are the proportion of months (n = 10) that each cell identified each variable as the MIC. This was calculated as the mean of the pixel-level proportions inside each of the 14 grid cells. Note the different color scale for SST (0–1) and the other covariates (0–0.12). Hadley is not shown because it was almost exclusively SST. A mid-century version showing a similar pattern is presented in S7 Fig. The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.

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projections support 'time of emergence' analyses indicating that the majority of the late 21st century ocean could experience unusual physical and biogeochemical conditions [6, 48]. Our four scales of novelty allow us to evaluate the likely impacts of this novelty further: the extreme novelty at the local-monthly scale indicates that in 50–100 years under a high emission future ecological communities will need to shift or adapt ubiquitously throughout the CCS (shift to maintain a similar climate, or adapt to maintain their same location and phenology); the novelty patterns at the local scale indicate that (ignoring phenological processes) most of the stress to shift or adapt will occur in the warmer months; the novelty patterns at the regional scale indicate that about half of the locally novel area is also entirely new to the domain, indicating the potential for new ecological communities to shift into the CCS (predominantly in the south); and the novelty patterns at the regional-monthly scale indicates the considerable change likely to occur to the seasonality of processes (such as spawning and migration) in the CCS, given that a considerable area of the CCS year-round will be entirely novel for that month. These proposed changes are supported by the extensive information showing large range shifts for species on the US West Coast [30], the arrival of new species moving poleward, but especially in warmer temperate waters [49], and observed warming-related phenological changes in the CCS [50].

It can be challenging to identify all multivariate instances of novelty, but our results indicate that the future CCS will experience novel values and combinations of increased SST, reduced oxygen concentration, shallower mixed layer, and increased eddy kinetic energy (Fig 4), in agreement with global physical and biogeochemical trends [29, 51–53]. For the CCS, nearshore oxygen declines are projected to have the most impact (i.e. take on novel values) in the GFDL and IPSL models, although Hadley does not show the same oxygen declines [29] or related novelty. Thus, near-shore species such as Pacific sardine and northern anchovy will be especially exposed to environments with novel metabolic capacity [33]. The projected loss of deeper ILD values (particularly offshore) is consistent with surface intensified warming and increased stratification both regionally and globally [52].

A global niche-based projection of biogeochemical provinces (defined by their historical environmental conditions) indicated that the coastal and offshore CCS 'provinces' would spatially shift but increase in area under RCP8.5 [24]. That study highlights that: 1) our CCS domain is part of a larger marine system, and that regional novelty in our system likely represent conditions historically experienced outside our domain; and 2) globally novel habitats typically arise in equatorial regions. However, given the scale of the movement and dispersal processes driving ecosystem function and structure, it is novelty at the ecosystem (or provincial) scale that is most relevant to understanding impact and change to ecological and human communities [9]. So, even if the CCS province remains an identifiable province, the ecosystem or province within the marine domain off the U.S. West Coast could undergo large future change, based on our projections of ocean climate novelty.

Our analysis of novelty is intended to create a multivariate indicator of environmental stress in the CCS due to climate change. The indicator indicates where and when this stress occurs, and, by looking at multiple scales, how this novelty may impact the CCS ecology. Much like the emergence of environmental conditions from historical variation [6, 54], novelty indicates where and when ecosystems and communities will have severe exposure to climate change. For example, novelty indicators could be part of climate response strategies to inform where to allocate resources for monitoring of regionally emerging fisheries or for assessing future infrastructure and regulatory change needs. Our selected climate variables do not represent change or stress for all species or ecological processes in the CCS, and additional variables (e.g. bottom temperature, pH, or nutrients) could be included or substituted to evaluate other components of the ecosystem. Given the importance of SST in driving novelty (Fig 4, S2 Fig), change in SST can be a key univariate indicator, but the potential for novel habitats in SST/oxygen/surface mixing space indicates the value of multivariate indicators. The multivariate approach also elucidates model uncertainty as models may all agree on change in univariate space (e.g., for SST) but not in multivariate space (e.g., for SST-oxygen; Fig 4). Novelty in a climate envelope could also be used as an index of current or 'nowcast' climate stress, by comparing current or forecast environmental conditions to a set of historical observations and at sub-monthly time scales.

Hypervolumes and ExDet gave similar results for novelty at the local-monthly scale, but at other scales they were meaningfully different (Fig 2b). One likely reason for this is ExDet underestimating combinatorial extrapolation. A two-variable assessment showed that using the maximum of the Mahalanobis distance from the observations [44] can be conservative for identifying novel combinations, and especially so when the relationship between variables is not elliptical, i.e. variables are not normally distributed (S3 and S4 Figs). It is also possible that the support vector machine algorithm we used for the hypervolumes is prone to overestimating novelty, given its close fit to observations and sensitivity to parameter correlation. While both tools are useful (and could act as upper (hypervolumes) and lower (ExDet) estimates of novelty), the potential for underestimation by ExDet appears high, so we feel that hypervolumes show greatest potential for measuring local-scale novelty due to their ability to identify concavities and holes in environmental space. The advantage of ExDet and dimension reduction using the Mahalanobis distance is the ability define a higher-dimension climate envelope without issues of collinearity or computation time. Preliminary testing shows that the area of applicability approach [22] and hypervolumes can give similar estimates of novelty. Hypervolumes are, however, computationally intense, and subsetting or aggregation of large climate datasets is required.

Extrapolation detection has developed predominantly for model-based assessment, e.g. novelty of prediction data relative to observations in species distribution models [14], and hypervolumes can be used the same way. Thus, there is great value in exploring species- and model-specific projections of novelty using these tools. Such analyses would better identify important environmental variables for a species (e.g. bottom temperature for benthic species), and identify novelty in terms of both novel data due to environmental change, and novel data due to imperfect observation of the species' niche. It is likely that imperfect observation is the driver of novelty in the short-term, but, as the projection horizon increases, environmental change becomes the more important driver of novelty in model prediction. Although the accuracy of projections of environment-driven models (such as species distribution models) will depend entirely on the structure and data of the specific model, our results indicate that: 1) emerging multivariate novelty will lead to environments not previously observed for a species; and 2) there will be an increasing mismatch between historically important locations and times-of-year and the experienced climate envelope. Both of these will create novel challenges for species, and challenge our predictive models (especially correlative ones) which are not 'trained' for novel climates [19, 23]. The potential for the rapid emergence of regional and local novelty in the CCS during this century highlights the value of incorporating multivariate climate novelty in long-term ecological projections [55], and in the adaptive management processes [26] used to develop robust and resilient management strategies for the marine environment [56].

Supporting information

S1 Fig. Projected novelty using alternate variables. Shows the percentage of the CCS experiencing a novel climate, based on a different combination of ocean climate variables: SST (˚C), bulk Brunt-Väisälä frequency (s^{-1}; averaged over the top 200 m), surface chlorophyll ($\sqrt[4]{mg\ m^{-3}}$), and wind stress ($N\ m^{-2}$). This is for comparison with Fig 2, which is based on SST, ILD, EKE, and oxygen concentration. The general trends are similar, but the hypervolume estimates of novelty in warmer months at the regional scales are increased for this set of variables, due mainly to increased novelty in bulk frequency (and perhaps inflated due to considerable correlation between this variable and SST).
(JPG)

S2 Fig. The 'drop one out' assessment of variable contribution. Shows the relative influence of climate variables on novelty at the local monthly scale (for July; results are similar across months), as measured using the hypervolume method. The line plots show the percentage area novel for each ESM projection at this scale (as in Fig 2; black = hypervolume, red = ExDet), and the bar plots show relative contribution of each climate variable to this novelty. This contribution is measured as the change in overlap ('fraction unique') of the hypervolumes for the historical period (1980–2009) and future decades (2021–2030, and onwards to 2091–2100; x-axis indicates start date only), as each covariate is dropped singly from the future hypervolumes (a 'drop one out' analysis). Relative novelty was measured as $1 - Cov/Full$, where *Cov* is the unique fraction of the future hypervolume when dropping a specific covariate, and *Full* is the unique fraction without removing any covariates. For each hypervolume comparison values summed close to 1, but were rescaled to sum exactly to 1 for ease of interpretation. The large relative influence of SST indicates that this is the most spatially expansive source of novel

climate in the CCS, and increasingly so to the end of the century. This is an imperfect estimate of influence, because removing one variable will also remove any novel combinations with other variables.
(JPG)

S3 Fig. An evaluation of the 'local' assessment of novelty for the ExDet method. a) Plotted ExDet values (colors) at the regional-monthly scale for July 2100 under IPSL. Most of the values were within 0–1, meaning that they are considered analog to the historical period (cells with univariate extrapolation [ExDet < 0] are colored light grey). b) When latitude and longitude are added as additional covariates (as done for hypervolumes), we see the ExDet values increase offshore and in the north, indicating that ocean climate is more different locally than regionally, but ExDet is still < 1 and thus considered analog. c) By plotting the range of SST values against latitude for the historical (black) and future period (red), we see clear evidence of novelty (new values of SST at specific latitudes). It is clear that the previous analysis (b) detected the univariate extrapolation of SST (black dashed line) but did not identify as novel the new combinations of space and SST (combinatorial extrapolation; see S4 Fig). d) However, if we split the region into 14 grid cells (S5 Fig), and calculate ExDet for each cell separately (i.e. the regional-monthly scale in each cell), the local novelty is now identified, with much of the region now considered to be experiencing locally novel conditions. This agrees closely with the hypervolume result, and we deem (d) the more effective method of calculating local novelty for ExDet. Note that the extrapolation identified in d) does not perfectly match the novel SST-latitude areas, because c) lacks information on the longitudinal novelty of SST. The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.
(JPG)

S4 Fig. Visualizing the Mahalanobis distance for detecting ExDet combinatorial novelty. In our two-variable example (Fig 1, S3 Fig), there is a relationship between SST and latitude (subset of the 1980–2009 period, black dots). A prediction set of a regular grid covering this space was used to properly identify what ExDet treats as univariate extrapolation (red dots), combinatorial extrapolation (blue dots), and as analog values (grey dots). Analog conditions are those with a Mahalanobis distance less than the maximum distance in the observations, which can clearly be a conservative measure of novelty (i.e. much of the grey area should be considered novel).
(JPG)

S5 Fig. The 14 areas used to partition the ROMS domain for the ExDet analysis at the local scales. The blue dashed line is the EEZ. The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.
(JPG)

S6 Fig. ExDet maps of novelty. Shows locations with novel (red, orange, yellow) or analog climates (green), for three example months at the end of five decades, under IPSL. This is for the ExDet method. Colors represent a climate novel to the region (red), novel to a given location or month of the year (orange), or novel at a given location and month of the year (yellow). The maps show each pixel's majority classification over a 5-year period ending in the specified year (e.g. 2016–2020). The appearance of lines in some of the novelty patterns are due to the grid used for the spatial analysis (S5 Fig). The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from

https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.
(JPG)

S7 Fig. MIC maps for 2051–2060. Shows the MIC (most influential covariate) values estimated by the ExDet method, based on 2051–2060 July values at the local-monthly scale, for the three ESM projections. Values are the proportion of months (n = 10) that each cell identified each variable as the MIC. At the coarse local scale, this was calculated as the mean of the pixel-level proportions inside each grid cell. Note the different color scale for SST (0–1) and the other covariates (0–0.12). Compare this with Fig 5 in the main article. The coastline data are sourced from https://naturalearthdata.com/downloads/110m-physical-vectors/110m-coastline, and the EEZ from https://nauticalcharts.noaa.gov/data/us-maritime-limits-and-boundaries.html.
(JPG)

S1 Table. Dataset IDs.
(DOCX)

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