

1 **Oceanic harbingers of Pacific Decadal Oscillation**
2 **predictability in CESM2 detected by neural networks**

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5 **Key Points:**

- 6 • Artificial neural networks (ANNs) predict Pacific Decadal Oscillation (PDO) per-
7 sistence and transitions in CESM2.
- 8 • Explainable AI unveils regions used by ANNs for predicting the PDO on inter-
9 annual timescales.
- 10 • Predictable PDO transitions can be preceded by a heat build up in off-equatorial
11 western Pacific.

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12 **Abstract**

13 Predicting Pacific Decadal Oscillation (PDO) transitions and understanding the asso-
14 ciated mechanisms has proven a critical but challenging task in climate science. As a form
15 of decadal variability, the PDO is associated with both large-scale climate shifts and re-
16 gional climate predictability. We show that artificial neural networks (ANNs) predict PDO
17 persistence and transitions with lead times of 12 months onward. Using layer-wise rel-
18 evance propagation to investigate the ANN predictions, we demonstrate that the ANNs
19 utilize oceanic patterns that have been previously linked to predictable PDO behavior.
20 For PDO transitions, ANNs recognize a build-up of ocean heat content in the off-equatorial
21 western Pacific 12-27 months before a transition occurs. The results support the con-
22 tinued use of ANNs in climate studies where explainability tools can assist in mechanis-
23 tic understanding of the climate system.

24 **Plain Language Summary**

25 The Earth’s oceans are capable of storing large amounts of heat with spatial pat-
26 terns of ocean heat lasting for decades at a time. One such pattern is called the Pacific
27 Decadal Oscillation (PDO). As these patterns indicate how heat is distributed over the
28 globe, they are associated with increased predictability of extreme weather events as well
29 as being an important factor for marine ecosystems. Predicting when the PDO will shift
30 from one pattern to the other has proven a tricky proposition in climate science as mech-
31 anisms from the atmosphere and the ocean both play a role. Here we show that artifi-
32 cial intelligence can predict PDO transitions over 12 months in advance. We also inves-
33 tigate the predictions and show that they are related to known physical mechanisms —
34 our models are making the right predictions for the right reasons. We leverage past knowl-
35 edge, and the new discoveries from artificial intelligence to speculate how ocean patterns
36 can lead to PDO predictability.

37 **1 Introduction**

38 The Pacific Decadal Oscillation (PDO; Mantua et al., 1997; Zhang et al., 1997) is
39 recognised as one of the most important sources of predictability on decadal timescales
40 (Cassou et al., 2018). As such it has been linked to increased predictability of surface
41 variables, including precipitation and temperature, as well as being an important fac-
42 tor in marine ecosystems and resource management. The PDO is not itself considered

43 a single mode of variability, but a manifestation of several different forcings operating
44 on different timescales: the integration of stochastic atmospheric forcing associated with
45 the Aleutian low; tropical-subtropical atmospheric teleconnections associated with the
46 El Nino Southern Oscillation (ENSO) phenomenon; the re-emergence of winter-to-winter
47 sea surface temperature (SST) anomalies; and ocean gyre dynamics (Newman et al., 2016,
48 and the references therein). In its positive phase, the PDO manifests as a pattern of neg-
49 ative SST anomalies in the central and western North Pacific Ocean, surrounded by pos-
50 itive anomalies around the eastern edge, extending southward to around 20°N (Figure 1a).

51 While the combination of mechanisms that contribute to the PDO are considered
52 to be largely understood, challenges still exist in the realm of PDO predictability (Cassou
53 et al., 2018). This is especially true in predicting PDO transitions, i.e. when the PDO
54 shifts from one phase to the other. Stochastic models (Deser et al., 2003; Newman et al.,
55 2003; Schneider & Cornuelle, 2005), linear inverse models (LIMs; Newman, 2007; Alexan-
56 der et al., 2008; Dias et al., 2019), atmosphere-only models (Farneti et al., 2014) and fully
57 coupled climate models (Meehl & Hu, 2006; Meehl et al., 2014) have been used to recre-
58 ate the relevant processes that contribute to PDO variability and by comparing to ob-
59 servations, attempt to estimate how these processes can lead to predictability. This has
60 lead to a single robust theory for PDO transitions: studying periods of mega-droughts,
61 Meehl and Hu (2006) posited that tropical SST anomalies drive surface wind-stress anoma-
62 lies in the off-equatorial Pacific ($\sim 25^\circ$) via atmospheric teleconnections, forcing oceanic
63 Rossby waves that propagate westward on decadal timescales. This results in a build-
64 up of ocean heat content in the off-equatorial western Pacific. If an ENSO event sub-
65 sequently switches the sign of the tropical Pacific SST anomaly, this off-equatorial heat
66 is redistributed via Kelvin waves throughout the equatorial region, leading to a transi-
67 tion in the PDO. Meehl et al. (2016) investigate this mechanism in the context of the
68 Interdecadal Pacific Oscillation (IPO; similar to the PDO but the spatial domain spans
69 the full meridional extent of the Pacific), finding that initialized hindcasts with the Com-
70 munity Climate System Model, Version 4, (CCSM4; Gent et al., 2011) show skill in sim-
71 ulating past IPO transitions with this mechanism appearing to coincide with those par-
72 ticular transitions. Since the PDO is considered the North Pacific manifestation of the
73 IPO, the mechanism outlined above is directly relevant to understanding and predict-
74 ing PDO transitions (Farneti et al., 2014; Lu et al., 2021).

75 While stochastic climate models and LIMs model the climate system as linear, it
76 has been suggested that predictive skill, especially of oceanic variability, could be gained
77 using methods that better capture non-linearities in the system (Newman, 2007). Ar-
78 tificial neural networks (ANNs), a form of unsupervised machine learning, offer such a
79 non-linear framework and have proven skillful at predicting processes in the climate sys-
80 tem such as identifying the forced response to climate change, ENSO evolution and Madden-
81 Julian Oscillation teleconnections (Barnes et al., 2020; Ham et al., 2019; Toms et al., 2020;
82 Mayer & Barnes, 2021). Specifically in the case of oceanic predictability, Ham et al. (2019)
83 used a convolutional neural network to predict ENSO evolution, showing significantly
84 higher forecast skill than previous dynamical forecasts, while also identifying spatial SST
85 patterns corresponding to increased predictability. Similarly, Nadiga (2021) demonstrated
86 how reservoir computing (a form of recurrent neural networks) increases predictability
87 of oceanic variability in the North Atlantic Ocean on the interannual timescale, espe-
88 cially during period of infrequent or missing data. Together, these studies suggest that
89 neural networks are effective for investigating and predicting climate processes related
90 to oceanic variability. These, along with explainable AI (XAI, methods designed to aid
91 the interpretation of the decision-making process of a neural network) can identify sig-
92 nals associated with a neural network’s prediction.

93 In this study we show that ANNs are effective tools for predicting persistence and
94 transitions in the PDO. In our analysis we examine predictions with lead-times from 12
95 months onward. Recall the PDO is considered a combination of forcings that propagate
96 on different timescales, from stochastic atmospheric forcing on the timescale of days to
97 weeks, to oceanic Rossby wave propagation on multi-year scales (Newman et al., 2016).
98 We examine predictability on the shorter than “decadal” timescales to avoid averaging
99 out the forcings on shorter timescales that may contribute to predictive skill. We choose
100 to still use the PDO terminology, however, as we are investigating predictability of the
101 PDO spatial pattern across various timescales.

102 Furthermore, we investigate mechanisms identified by the ANNs that lead to pre-
103 dictability, both long-term persistence and predicting transitions. Most notably, we lever-
104 age explainable AI methods to attribute patterns of ocean heat content anomalies to in-
105 creased PDO predictability. We emphasize that not only are we concerned with optimiz-
106 ing an ANN to solve a prediction problem, but we also explore the decision making pro-
107 cess of the ANN to uncover potential sources of predictability (Toms et al., 2020).

2 Data and Methods

2.1 Data

We use monthly mean sea surface temperature (SST) and ocean heat content (OHC) from the Community Earth System Model Version 2 (CESM2; Danabasoglu et al., 2020) pre-industrial control run for the Coupled Model Intercomparison Project, Phase 6 (CMIP6; Eyring et al., 2016). The presence of realistic ENSO and PDO variability in CESM2 was demonstrated by Capotondi et al. (2020). We use the full 2000 year run, with the large amount of data available (24000 months) desirable for training the ANNs. OHC is calculated as the vertical heat content integral from the surface to 100 m depth (Fasullo & Nerem, 2016). Both OHC and SST are interpolated to a $4^\circ \times 4^\circ$ grid and we deseasonalize both the SST and OHC fields by subtracting their respective monthly mean annual cycles at each grid point. Furthermore for OHC (the input for the ANNs), we standardize each grid point by dividing it by its monthly standard deviation and apply a 6-month running mean.

The PDO is calculated from the deseasonalized SSTs, defined as the leading empirical orthogonal function (EOF) of the North Pacific (110E-260E, 20N-60N) monthly SSTs. This EOF, projected onto the global deseasonalized SST field, is presented in Figure 1a. In contrast to previous studies where the PDO index is defined using low pass filters with between 5–11 year cut-offs, here the PDO index is defined as the 6-month running mean of the principal component time series. This is because PDO transitions are considered to be influenced by interannual variability associated with e.g. ENSO (Meehl et al., 2016, 2021) and we want our ANNs to be able to account for these processes. The distribution of phase durations in CESM2 is shown in Figure 1b, demonstrating that there are a large number of phases of shorter duration, with decreasing samples as phase duration increases. The PDO representation in CESM2 is considerably improved over previous versions of the model, with periods of long term persistence similar to the observational record. However, the PDO within CESM2 contains extended periods of rapid fluctuation (Capotondi et al., 2020). We choose to retain and investigate these periods because the observational record is relatively short, and furthermore it has been posited the PDO will become weaker and of shorter phase under climate change (Li et al., 2019), hence high frequency PDO variability may become more relevant in future climate scenarios.

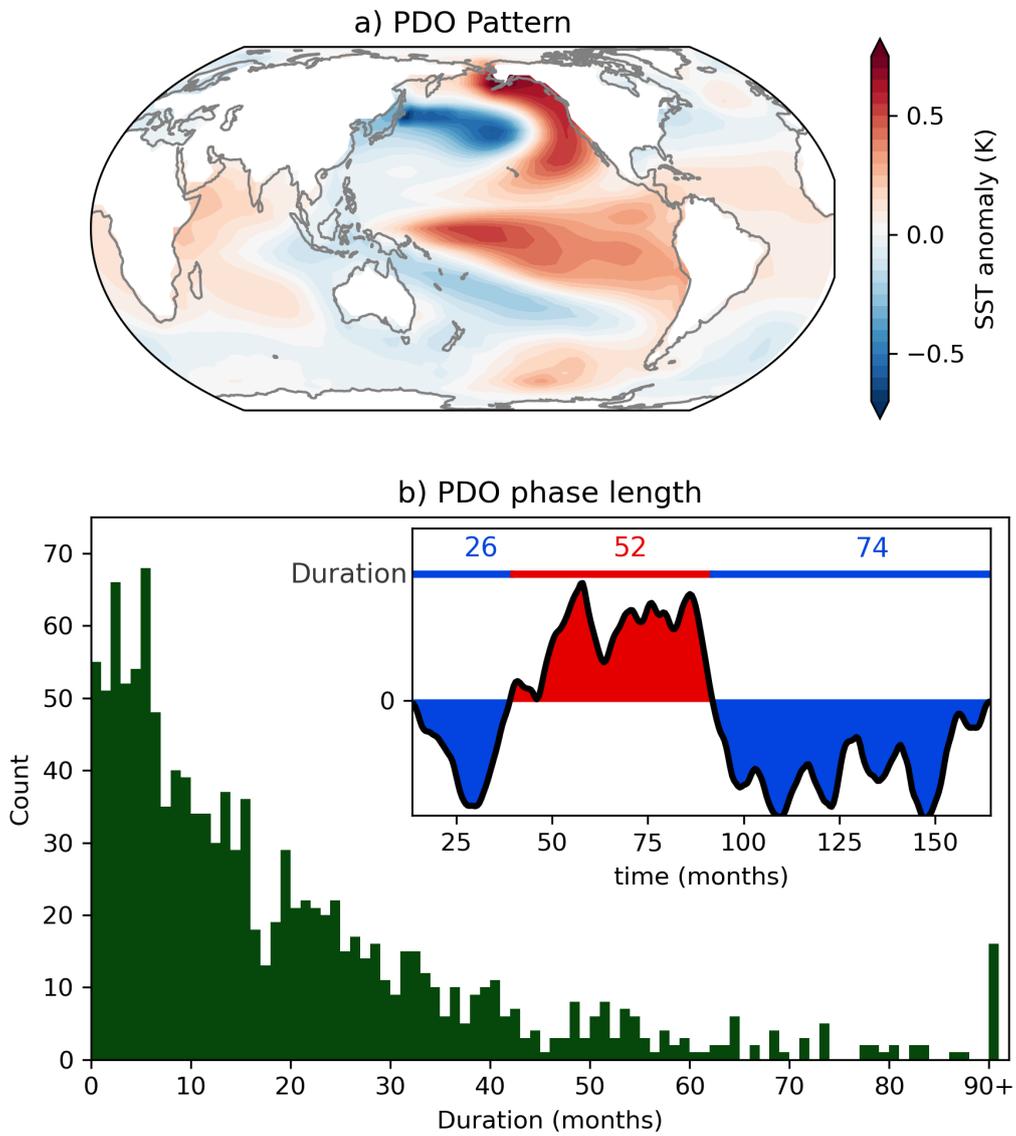


Figure 1. a) North Pacific PC 1 projected onto global de-seasoned SST. b) Histogram showing distribution of PDO phase lengths in CESM pre-industrial control run. Inset: slice of PDO index showing PDO phase length as number of months between phase changes.

2.2 Artificial Neural Network

We use a single layer artificial neural network (ANN) to predict whether a PDO phase transition will occur within 30 months, i.e. for some input, the output is a classification (yes or no) of whether a PDO transition will occur within the following 30 months. An overview of neural networks is provided in the supplement as well as our rationale for using a 30 month lead time in this study. The input layer to the ANN is three maps of deseasoned and standardized $4^\circ \times 4^\circ$ OHC anomalies, four months apart i.e. if the ANN is predicting PDO transition occurrence within some month $\tau = 0$, the three input maps are $\tau = -38$, $\tau = -34$, and $\tau = -30$ months. The input fields are flattened and concatenated resulting in an input vector of 12150 pixels. The input vector is fed into a densely connected hidden layer with 8 nodes which utilize the Rectified Linear Unit (ReLU) activation function. Finally, this is fed into an output layer of two nodes with softmax activation, representing the prediction. We interpret the ANN's prediction as the node with the higher value, and this value is termed the "ANN's confidence". For example, if the output is 0.63 on the persistence node, and 0.37 on the transition node, this represents a prediction of persistence with 0.63 confidence. For training, we use the categorical cross entropy loss function. We have found that setting the problem up as a binary classification task – will it or will it not transition in the next 30 months – yields insights into the mechanisms for PDO transition predictability. With that said, we have explored other architectures as well, including setting the problem up as a regression task whereby the network must predict the number of months until the next transition. In this instance, the network struggles to differentiate weak PDO states that may flip sign in the coming months from those weak PDO states that are on their way to persist for years. Since the main goal of this work is to identify mechanisms that offer PDO transition predictability, we present results from the binary classification architecture here although the regression architecture warrants further exploration.

We split the data into training and validation, using the first 90% (1800 years, 21600 samples) for training and final 10% (200 years, 2400 samples) for validation. Since there are more samples where transitions occur than persistence (see Figure 1b, there are more short duration phases than long), we manually balance the classes in both the training and validation sets. To generate the training data we use all of the persistence samples in the training set, and randomly grab an equal number of transition samples from the training set. We do the same from the validation set. This results in 9386 training sam-

173 ples (4693 of each class) and 1110 validation samples (555 of each class) for each neu-
174 ral network. We train 60 networks total with identical architecture and vary only the
175 random seed which controls how the weights in each network are initialized. Here we present
176 results as averages from the best 3 networks. Full model specifications, descriptions and
177 analysis of all 60 networks is included in Table S1 and the supplement text. After train-
178 ing, we use the ANN to make predictions of both training and validation data. As we
179 are able to rank an ANN's output by confidence, when presenting results as composites
180 we choose to discard the 50% least confident predictions. Since the network is less con-
181 fident about these predictions, removing them from our analysis suggests our results will
182 focus on those with the strongest signals.

183 To investigate the decisions made by the ANNs, we use the neural network attri-
184 bution technique called layer-wise relevance propagation (LRP; Bach et al., 2015). LRP
185 propagates the prediction from an ANN back through the network and provides in our
186 case, a map of relevance values corresponding to the input grid, with positive values in-
187 dicated points that were relevant to the specific prediction, and negative values indi-
188 cating points that detracted from the prediction. The higher the value, the more “rel-
189 evant” the grid point. The utility of LRP in climate predictability studies has been dis-
190 cussed by Toms et al. (2020); Mamalakis et al. (2021) and used in studies by e.g. Mayer
191 and Barnes (2021); Toms et al. (2021); Sonnewald and Lguensat (2021). Here, we present
192 composites of LRP maps for predictions when the network is correct and confident. Each
193 relevance map is first normalized by the prediction confidence (i.e. LRP map is divided
194 by the winning confidence) before compositing, then the composite map is scaled by its
195 maximum absolute value so that the composite map has a maximum absolute relevance
196 value of 1.

197 **3 Results**

198 **3.1 Detecting Persistence**

199 The average total accuracy of the best three ANNs is 65%, with average conditional
200 accuracy for predicting persistence of 55% (given no transition occurs, the ANN correctly
201 predicts no transition). While this accuracy is above that expected by random chance,
202 the low conditional accuracy across all persistence samples is likely due to the set up of
203 this problem. Consider a sample that transitions 31 months after input; this sample would

204 be designated persistence. However, a sample that transitions 29 months after input would
 205 be classified as a transition, despite the similarity of the input samples. Because of this,
 206 the samples that persist just beyond 30 months have very low accuracy while those with
 207 much longer phase duration (potentially more indicative of long-term PDO persistence)
 208 are more rare but have higher prediction accuracy (62% for durations > 40 months).
 209 This is demonstrated in Figure 2. In panel a we show the average distribution of phase
 210 duration (green line) with the blue line demonstrating the number of samples correctly
 211 identified by the ANN in the validation data. The increase of samples at month 30 is due
 212 to our method of balancing the number of samples per class for our neural network in-
 213 puts. Recall that the number of samples in the transition class (area under green curve
 214 for durations 0-30 of months) is equal to the number of samples in the persistence class
 215 (area under green curve for durations of 30+ months), and to achieve this we sub-sampled
 216 the transition samples while maintaining all persistence samples. The sub-sampling main-
 217 tains the shape of the distribution of phase duration in the transition class but reduces
 218 its size, resulting in a jump in the number of samples at phase duration > 30 months.
 219 Panel b shows the accuracy as a function of phase duration (i.e. blue divided by green).
 220 For example, when a transition occurs 10 months after input, (i.e. duration of 10 months
 221 on the horizontal axis), the ANNs are correct and predict a transition around 75% of the
 222 time. Similarly, when a transition occurs 60 months after input (i.e. the correct predic-
 223 tion is that no transition occurs within 30 months), the ANNs are correct around 90%
 224 of the time. To compare the results to random chance, the dashed line indicates accu-
 225 racy of 0.5, with shading indicating the 5th-95th percentile range for each phase dura-
 226 tion bin. For samples around the cut off of 30 months, there is a dramatic drop in ac-
 227 curacy. However, as duration increases so does prediction accuracy with high accuracy
 228 for samples between 45 and 65 months. Note for samples of duration above 70 months
 229 accuracy is again very low. We propose that this is because these samples will occur early
 230 in a PDO phase (i.e. very soon after a transition) and hence having a weak PDO pat-
 231 tern for the ANNs to discern. It is hence difficult for the ANN to differentiate between
 232 these samples and those where the sign flips very soon after input. We hence propose
 233 that the ANNs have learned patterns relating to persistence especially for samples where
 234 the phase is of longer duration. We also consider the accuracy of the predictions with
 235 the top 50% confidence values, shown in the dashed red line in Fig. 2. This shows that
 236 predictions with higher confidence are more likely to also be accurate, especially for the

237 regime we consider here (transitions that occur in 12-27 months). As higher confidence
 238 corresponds to higher accuracy, this implies that our networks have learned when pat-
 239 terns are more likely to lead to predictability.

240 Figure 3 shows the composite maps for correct predictions for cases when the PDO
 241 persists in its positive phase. The LRP heatmap of relevance values calculated for month
 242 $\tau = -30$ (the last input month) are shown in Figure 3a, while Figures 3b and 3c dis-
 243 play the standardized OHC anomaly at the input month ($\tau = -30$) and the final month
 244 ($\tau = 0$). OHC anomalies at both the input time and the prediction show a positive PDO
 245 pattern in the North Pacific, with the horse-shoe shaped positive anomalies surround-
 246 ing negative anomalies, verifying that indeed the ANNs have predicted a persisting pat-
 247 tern. Furthermore, the large magnitude anomalies in the North Pacific at input (Fig. 3b)
 248 are suggestive of PDO persistence as they correspond to a high magnitude PDO index
 249 which takes time to decay. It is thus encouraging that the largest relevance values in the
 250 LRP heatmap in Fig. 3a align with the positive horse-shoe shape in 3b. This suggests
 251 that the ANNs recognize large positive OHC anomalies in the North Pacific ocean as be-
 252 ing an indicator that the PDO will persist on the interannual timescale, and this is con-
 253 sistent with our physical understanding.

254 3.2 Detecting Transitions

255 We now consider the ANNs's ability to predict PDO transitions within CESM2.
 256 The average conditional accuracy for predicting a transition (i.e. given a transition oc-
 257 curs, the ANN predicts a transition) is 74%. The conditional accuracy of transitions 12-
 258 27 months after input (given a transition occurs 12-27 months after input, the ANN pre-
 259 dicted the transition) is 69%. This is apparent in Figure 2b, with high accuracy for tran-
 260 sitions that occur very soon after input (duration of 0-12 months on the horizontal axis)
 261 with reduced accuracy for transitions that occur in the 12-27 month window (duration
 262 of 12-27 months on the horizontal axis). These later transitions are hence more difficult
 263 for the ANNs to learn because they must learn to detect precursors of transitions more
 264 than 12 months before it occurs. Up to 27 months, accuracy values fall on or above the
 265 95th percentile of random chance. This suggests that when correct, the ANNs have learned
 266 patterns that lead to PDO transitions and furthermore, that they can recognize them
 267 more than 12 months in advance.

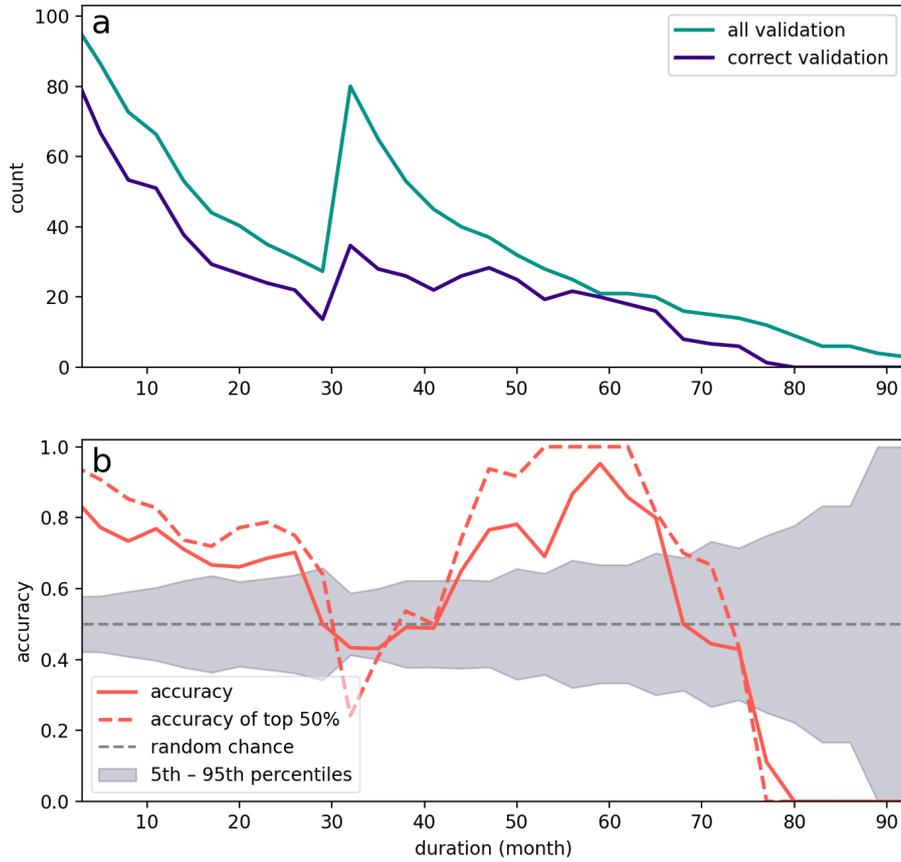


Figure 2. a: Average distribution of phase duration in the validation data for the three ANNs, green shows all the validation data and blue is number correctly predicted by the ANN with data binned into 3 month averages. b: Red line is accuracy of each phase duration bin (blue divided by green from above), red dashed line is accuracy of each phase duration when we only consider samples with highest 50% confidence. Grey dashed line indicates accuracy of 0.5, or random chance, with shading indicated 5th–95th percentile range for random chance.

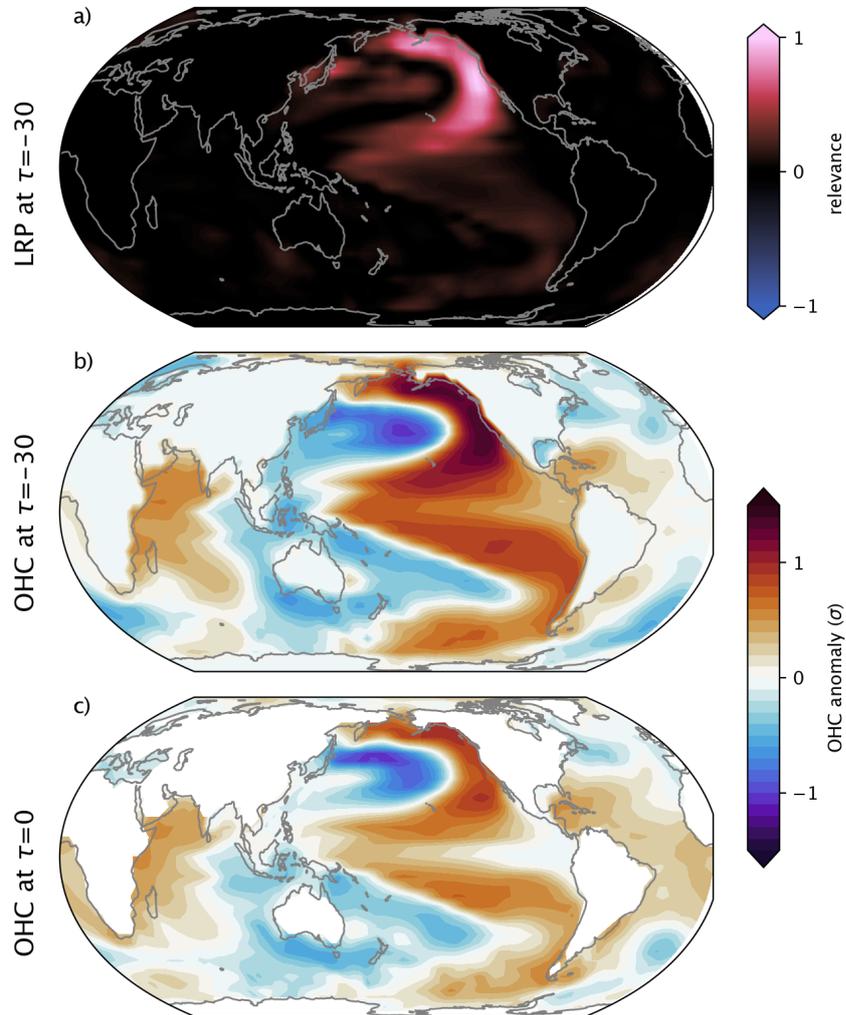


Figure 3. Composite maps when ANN correctly and confidently predicts persistence. a) Composite mean of LRP maps at final input month ($\tau=-30$). Red areas correspond to positive relevance and blue to negative relevance. b) Composite mean of OHC input maps at $\tau=-30$. Color scale is OHC anomaly in units of standard deviation σ at each grid-point. c) Composite mean of OHC at predicted month, color scale as in b).

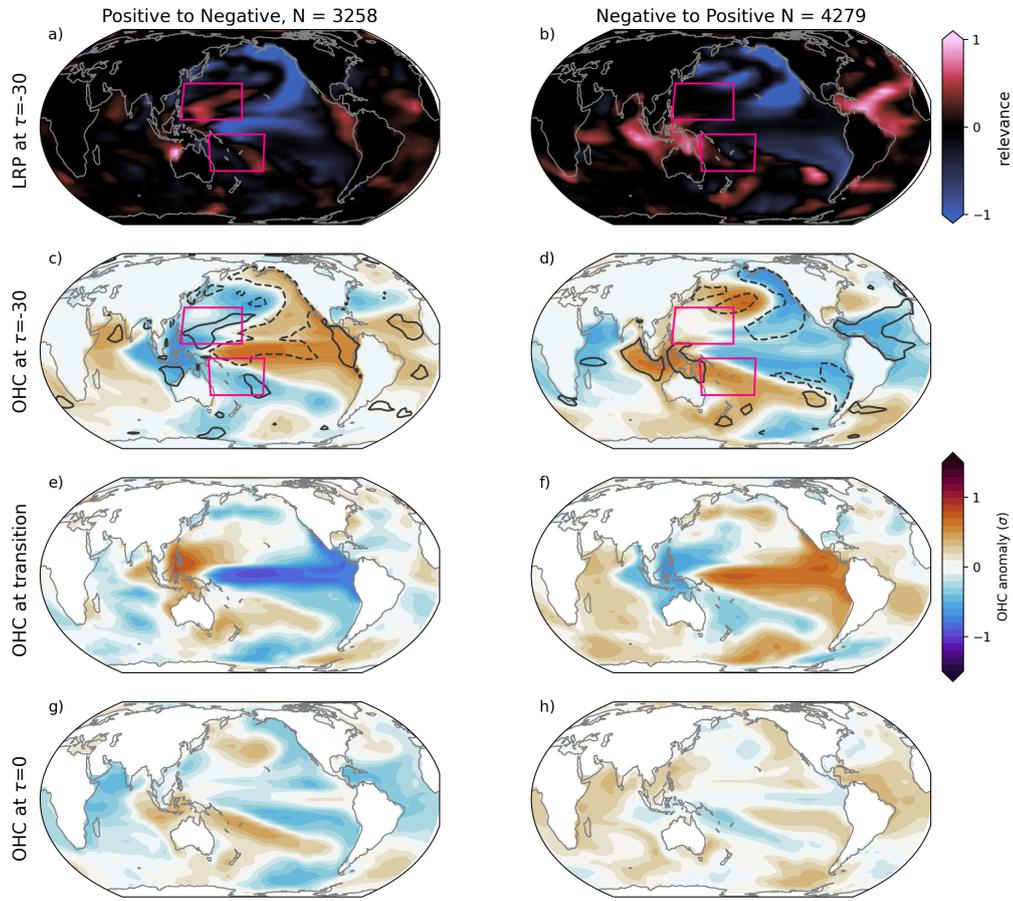


Figure 4. Composite maps of correct and confident predictions of PDO transition when transition occurs 12-27 months after input. Left column is positive to negative transitions, and right column is negative to positive transitions. Number of samples in each column is included in the title. Panels a) and b) are composite LRP 30 months before predictions. Red regions correspond to highest relevance and blue to lowest. Pink boxes highlight regions where OHC build-up is considered to precede PDO transitions (125E-180E, 5N-30N, and 150E-200E, 5S-30S). Panels c) and d) are the composite OHC maps 30 months before prediction, with color scale OHC anomaly in units of standard deviation. Dashed contours in c) and d) correspond to regions with highest 5% relevance in a) and b) respectively with dotted contour the lowest 5%. Panels e) and f) show composite OHC when transition occurs and panels g) and h) show OHC at the predicted month.

268 Figure 4 shows the composite result for correct prediction of PDO transitions when
 269 the transition occurs 12-27 months after input. We choose this window because it means
 270 the ANNs must recognize patterns that signal transitions at least 12 months in advance
 271 while there no loss in accuracy due to the 30 month cutoff. Positive to negative tran-
 272 sitions are displayed in the left column and negative to positive transitions are displayed
 273 in the right column. Figures 4a and 4b are the LRP maps for the final input map (month
 274 $\tau = -30$) with Figure 4c and 4d the corresponding OHC. We highlight the strongest
 275 relevance regions from the LRP maps by superimposing LRP contours (Fig. 4a and 4b)
 276 onto the OHC (Fig. 4c and 4d), with solid lines contours outlining highest 5% relevance
 277 values. Similarly, dashed contours encircle regions with the lowest 5% relevance values.
 278 Furthermore, we include pink squares in Fig. 4a-d to emphasize the regions where a build-
 279 up of OHC has been suggested in the literature to precede a PDO transition (Meehl et
 280 al., 2016). Lastly, to track the OHC evolution throughout the transition process, pan-
 281 els 4e and 4f show the OHC when the transition occurs, and 4g and 4h the OHC at month
 282 $\tau = 0$. Note in Figure S3-S4 we show the LRP maps and associated OHC for each in-
 283 put grid ($\tau = -38$, $\tau = -34$ and $\tau = -30$) but we do not include them here as they
 284 are very similar but with lower relevance values.

285 Large negative anomalies in the northern and southern off-equatorial western Pa-
 286 cific precede the positive to negative PDO transitions (Fig. 4c), while large positive anoma-
 287 lies precede negative to positive transitions in the southern off-equatorial western Pa-
 288 cific (Fig. 4d). Together, these suggest the presence of a build up of OHC in either the
 289 northern or southern off-equatorial Pacific at least 12-27 months before a PDO transi-
 290 tion occurs. In conjunction with the anomalies in Fig. 4c, the ANNs have recognized the
 291 northern region of heat content build up, with high relevance in the LRP composite in
 292 Fig. 4a. Conversely for negative to positive transitions, the ANNs mostly focus on the
 293 large positive anomalies over the maritime continent as well as the negative anomalies
 294 in the Atlantic, as shown by the high relevance values in Fig. 4b. The large relevance
 295 values in the Atlantic could signify the ANN detecting Atlantic teleconnections driving
 296 PDO transitions, which we discussion further in section 4. We also speculate that the
 297 lack of high relevance in the specific regions previously posited to contain anomalies lead-
 298 ing to transitions (Meehl et al., 2016, pink boxes in Fig. 4b) could be due to a westward
 299 shift of these anomalies in CESM2 leading to the high relevance values in the maritime
 300 continent. Conversely, the larger number of samples in Fig. 4b compared to positive to

301 negative transitions ($N = 4279$ for negative to positive compared to $N = 3258$ for positive
302 to negative), results in weaker relevance signals. In supplement figure S6 we show
303 by k-means clustering the LRP maps that there are indeed several distinct patterns within
304 the LRP composite likely corresponding to different transition regimes detected by the
305 ANNs, and cluster three of Fig. S6 (middle column) shows high relevance correspond-
306 ing to the off-equatorial western Pacific for negative to positive transitions. So there ap-
307 pear to be different OHC patterns leading to PDO predictability. Furthermore the re-
308 gions of high relevance in the composite in Fig. 4b suggest that the ANNs are using the
309 OHC anomalies in these regions for its correct predictions, hence, we suggest future in-
310 vestigation into how these OHC anomaly patterns may preempt PDO transitions. Fur-
311 thermore, the ANNs appear to be better at predicting negative to positive transitions
312 than positive to negative transitions as there are more correct samples in the latter cat-
313 egory (note there approximately the same number of transitions in each category). It
314 is unclear whether this is due to PDO representation in CESM2, or whether there are
315 fundamental differences in the transition process.

316 At the month the PDO transition occurs, note the large equatorial anomalies via
317 La Nina and El Nino (Fig. 4e and 4f respectively). Furthermore, the anomalies in the
318 western off-equatorial Pacific have switched sign in each panel at the transition as well.
319 These factors are consistent with the mechanism posited by e.g. Meehl et al. (2016), that
320 an ENSO event following the OHC build-up causes the OHC to be redistributed by equa-
321 torial Kelvin waves. This redistribution of heat, and the associated atmospheric telecon-
322 nections, effect a PDO transition. Lastly, after the transition occurs (Fig. 4g and 4h),
323 OHC anomalies have largely shifted into the opposite PDO phase pattern as we would
324 expect.

325 The evolution of OHC throughout the PDO transition and corresponding LRP heatmaps
326 suggest that not only are PDO transitions preceded by OHC build-up in the off-equatorial
327 western Pacific 12-27 months before the transition, but for positive to negative transi-
328 tions, our ANNs detect this heat build up as relevant to its predictions. Furthermore,
329 we suggest that this is also the case for negative to positive transitions but it is likely
330 that regimes where this is detected by the ANNs are averaged out in the composite (Fig
331 S6). Conversely, there are other signals detected in the relevance maps (Figs 4a and 4b),
332 and in addition the OHC anomalies are not consistently strong in the off-equatorial re-
333 gions (Fig. 4d) which suggests that there are likely mechanisms other than that proposed

334 by Meehl et al. (2016) that contribute to PDO transitions. The ability of the ANNs to
335 apparently detect a known precursor to PDO transitions supports their use in climate
336 variability problems to identify and possibly discover regions leading to predictability.

337 **4 Discussion and Conclusion**

338 We show that PDO transitions are preceded by large amplitude OHC anomalies
339 in either the northern or southern off-equatorial western Pacific 12-27 months before the
340 transition occurs. Furthermore, using LRP we show that these anomalies are detected
341 by the ANNs and were relevant to their correct predictions of positive to negative tran-
342 sitions. This finding is similar to the work of Meehl et al. (2016) however in their anal-
343 ysis they suggest that OHC must build up in the off-equatorial western Pacific over a
344 period of 10-15 years before a transition occurs. The transition predictions analyzed here
345 only have inputs 12-27 months before the transition occurs, yet the ANNs do make cor-
346 rect predictions above random chance, implying that perhaps the timescale of the OHC
347 build-up is less important than the fact that the anomaly is present. This is similar to
348 the finding of Lu et al. (2021) whose network analysis did not necessarily require OHC
349 to build-up over a long period of time as long as it reached a certain threshold. More-
350 over, as we have applied 6 month smoothing, it is perhaps surprising that mechanisms
351 contributing to PDO transition predictability were able to be detected by the ANNs. This
352 suggests that the decadal scale of OHC build-up, and the interannual scale of ENSO in-
353 teract cooperatively and hence filtering out shorter duration signals may hinder the de-
354 tection of mechanisms relating to PDO transitions. This was also suggested by Lu et al.
355 (2021), who found their method less likely to detect their “early warning signal” when
356 an 11-year low pass filter is applied. Note that if we only focus on transition predictions
357 for long PDO phases, i.e. the PDO must persist for a minimum 2.5 years before and fol-
358 lowing a transition, our results are essentially unchanged (see Figure S7). We use 2.5 years
359 here as a balance between sample size and long duration phases.

360 The maps in Figures 3 and 4 are presented as composite means of correct predic-
361 tions. As we have suggested, the signals detected by LRP and presented in these figures
362 may not necessarily be cooperating on every prediction. We check for this by using clus-
363 ter analysis on the LRP composites in Figure 4. Figures S5-S6 show how k-means clus-
364 tering highlights different signals in the LRP maps. Notably, the off-equatorial western
365 Pacific is highlighted in at least one cluster for both positive-to-negative transitions and

366 negative-to-positive transitions. Interestingly, there are regimes when the Atlantic Ocean
367 seems to be a highly relevant region for predictability. Since Atlantic teleconnections are
368 hypothesized to influence both PDO variability and ENSO events, and an ENSO event
369 is considered to be required to trigger a PDO transition (Kucharski et al., 2016; Chikamoto
370 et al., 2020; Johnson et al., 2020; Meehl et al., 2020) it is not unrealistic that Atlantic
371 OHC signals could assist in predicting PDO transitions. In particular, teleconnections
372 from the Atlantic are considered a key influence for triggering El Nino events (Ham et
373 al., 2013) whereas La Nina events are thought to be largely triggered by a preceding El
374 Nino event. In Figure 4b, the neural networks concentrate relevance in the Atlantic basin
375 preceding the El Nino event (and PDO transition) in Figure 4f. Given this, it appears
376 that the neural network recognizes the precursors of the El Nino event required for the
377 transition during negative to positive transitions. This highlights the ANNs’s ability to
378 detect distinct mechanisms contributing to predictability.

379 We show how ANNs and interpretability techniques can aid in the discovery and
380 investigation of mechanisms behind climate predictability. In the future, we suggest in-
381 vestigating regions highlighted here as potentially connected to PDO transitions, such
382 as the Atlantic Ocean. This is especially important in examining the possibility of dif-
383 ferent pathways that can lead to PDO transitions and hence we support the continued
384 use of methods such as ANNs and k-means clustering in objectively identifying poten-
385 tial regimes. In a broader sense, we encourage the future use of ANNs and XAI in cli-
386 mate predictability studies. We have shown that they are not just a tool for maximiz-
387 ing prediction accuracy, but also as a way of investigating potential mechanisms that lead
388 to predictability, and to advance our understanding of our chaotic climate system.

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392 The authors declare that they have no conflicts of interest.

393 Analysis was carried out in Python 3.7 and 3.9, ANNs were developed using Ten-
394 sorFlow (Abadi et al., 2016), while LRP visualizations were created with iNNvestigate
395 (Alber et al., 2019). Colormaps were used from CMasher (van der Velden, 2020). Re-
396 gridding was achieved using Climate Data Operators (CDO; Schulzweida, 2019).

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402 Data Availability: CESM2 pre-industrial control output for CMIP6 (doi:10.22033/ESGF/CMIP6.7627
 403) is freely available from Earth System Grid <https://esgf-node.llnl.gov/projects/cmip6/>
 404 .

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