# AUTHOR QUERY FORM



	Journal: Chaos	Please provide your responses and any corrections by annotating this
		PDF and uploading it to AIP's eProof website as detailed in the
	Article Number: CHA22-AR-DDCS2022-00825	Welcome email.
ng		

Dear Author,

Below are the queries associated with your article; please answer all of these queries before sending the proof back to AIP.

Article checklist: In order to ensure greater accuracy, please check the following and make all necessary corrections before returning your proof.

- 1. Is the title of your article accurate and spelled correctly?
- Please check affiliations including spelling, completeness, and correct linking to authors.
   Did you remember to include acknowledgment of funding, if required, and is it accurate?

Location in article	Query / Remark: click on the Q link to navigate to the appropriate spot in the proof. There, insert your comments as a PDF annotation.			
Q1	Please check that the author names are in the proper order and spelled correctly. Also, please ensure that each author's given and surnames have been correctly identified (given names are highlighted in red and surnames appear in blue).			
Q2	Please define SMOE at first occurrence.			
Q3	Please define CCN at first occurrence.			
Q4	Please include the dataset reference in the reference list and update the reference in the sentence beginning "The data that support"			
Q5	We were unable to locate a digital object identifier (doi) for Refs. Arrieta <i>et al.</i> (2020), Butterworth <i>et al.</i> (1930), Duan <i>et al.</i> (2009), L'Heureux <i>et al.</i> (2017), Srivastava <i>et al.</i> (2014), Yan <i>et al.</i> (2020), and Zhao and Di Lorenzo (2020). Please verify and correct author names and journal details (journal title, volume number, page number, and year) as needed and provide the doi. If a doi is not available, no other information is needed from you. For additional information on doi's, please select this link: http://www.doi.org/.			
Q6	Please provide publisher name for Refs. Montavon et al. (2019) and Selvaraju et al. (2017).			
Q7	The resolution of Figs 2,4,7,8,10,13 and 15 is low. If you are not satisfied with the way the figures appear in the proof, please provide new figure files of higher resolution.			
	Please confirm ORCIDs are accurate. If you wish to add an ORCID for any author that does not have one, you may do so now. For more information on ORCID, see https://orcid.org/.			
	G. Lancia–0000-0001-6185-7081			
	C. Spitoni			
	H. Dijkstra			

Please check and confirm the Funder(s) and Grant Reference Number(s) listed: Netherlands Science Foundation, OCENW.M20.277 Please add any additional funding sources not stated above:

Thank you for your assistance.

3

# Physics captured by data-based methods in El Niño prediction

Cite as: Chaos **32**, 000000 (2022); doi: 10.1063/5.0101668 Submitted: 2 June 2022 · Accepted: 19 September 2022 ·

- 4 Published Online: ■■ 2022
- 5 G. Lancia,<sup>1,a)</sup> I. J. Goede,<sup>2</sup> C. Spitoni,<sup>1,3</sup> and H. Dijkstra<sup>2,3</sup>

## AFFILIATIONS

- <sup>6</sup> <sup>1</sup>Department of Mathematics, Utrecht University, Budapestlaan 6, 3584 CD Utrecht, Netherlands
- <sup>2</sup>Institute for Marine and Atmospheric Research Utrecht, Department of Physics, Utrecht University, Princetonplein 5, 3584 CC
   Utrecht, Netherlands
- 9 <sup>3</sup>Center for Complex Systems Studies, Department of Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, Netherlands
- 10 Note: This article is part of the Focus Issue, Theory-informed and Data-driven Approaches to Advance Climate Sciences.
- 11 <sup>a)</sup>Author to whom correspondence should be addressed: g.lancia@uu.nl

#### ABSTRACT

12 On average once every four years, the Tropical Pacific warms considerably during events called El Niño, leading to weather disruptions

- 13 over many regions on Earth. Recent machine-learning approaches to El Niño prediction, in particular, Convolutional Neural Networks
- 14 (CNNs), have shown a surprisingly high skill at relatively long lead times. In an attempt to understand this high skill, we here use data 15 from distorted physics simulations with the intermediate-complexity Zebiak–Cane model to determine what aspects of El Niño physics
- are represented in a specific CNN-based classification method. We find that the CNN can adequately correct for distortions in the ocean
- adjustment processes, but that the machine-learning method has far more trouble  $\frac{1}{10}$  dealing with distortions in upwelling feedback
- 18 strength.
- 19 Published under an exclusive license by AIP Publishing. https://doi.org/10.1063/5.0101668

20 Tropical Pacific can periodically be subjected to an irregular vari-21 ation in sea surface temperature (SST), affecting the climate over 22 many regions on Earth. In the last decade, deep learning tech-23 niques, in specific Convolutional Neural Networks (CNNs), have 24 shown to be peculiarly accurate in El Niño predictions, even at 25 long lead times. In order to give a deeper understanding and an 26 interpretation of this high skill of CNN, we make use of data 27 from distorted physics simulations to determine what aspects 28 of El Niño physics can be captured and recognized in a specific 29 CNN-based classification method. We find that the CNN can cap-30 ture the wave adjustment and feedback process, but that the deep 31 learning method has far more trouble to dealing with distortions 32 in upwelling feedback strength.

#### 33 I. INTRODUCTION

Interannual climate variability is strongly dominated by the El
 Niño-Southern Oscillation (ENSO) in the Tropical Pacific. During
 an El Niño, the positive phase of ENSO, sea surface temperatures
 in the eastern Pacific increase by a few degrees with respect to

seasonally averaged values; the oscillation phase opposite to El Niño 38 is La Niña, with a colder eastern Pacific. A much used measure of 39 the state of ENSO is the NINO3.4 index, which is the area-averaged 40 Sea Surface Temperature (SST) anomaly [i.e., deviation with respect 41 to the mean seasonal cycle (SC)] over the region 170°W-120°W 42  $\times$  5°S–5°N. El Niño events typically peak in December, occur every 43 two to seven years, and their strength varies irregularly on decadal 44 time scales. The spatial pattern of ENSO variability is often deter-45 mined from principal component analysis (Preisendorfer, 1988), 46 detecting patterns of maximal variance. At least two different types 47 of El Niño events exist (Kug et al., 2009; and Zhang et al., 2019), with 48 the largest temperature anomalies either in the eastern Pacific (East-49 ern Pacific or EP El Niño's) or near the dateline (Central Pacific or 50 CP El Niño's). 51

As ENSO has distinct influences on the climate around the globe through well-known teleconnections (Diaz *et al.*, 2001), skillful predictions of up to a one year lead time are desired to be able to mitigate the effects (Balmaseda *et al.*, 1995). For ENSO predictions, often the Oceanic Niño Index (ONI) is used, which is defined as the three-month running mean of the NINO3.4 index. Both statistical models (those capturing behavior of past events) and 58



Q1

approve

dynamical models (i.e., those based on the underlying physical 59 60 conservation laws) are used for El Niño prediction (Latif, 1998; 61 Chen and Cane, 2008; Barnston et al., 2012; Saha et al., 2014; Timmermann et al., 2018; Tang et al., 2018; and Barnston et al., 62 2019). El Niño events are difficult to predict as they have an irregu-63 64 lar occurrence and each time have a slightly different development 65 (McPhaden et al., 2015; and Timmermann et al., 2018). Many ENSO 66 prediction evaluation studies (Barnston et al., 2012; and L'Heureux et al., 2017) have shown that dynamical models do better than statis-67 68 tical models, although there are exceptions (Newman and Sardesh-69 mukh, 2017). When initialized before the boreal spring, most models 70 perform much worse than when initialized in summer. The lat-71 ter notion has been indicated by the spring predictability barrier problem (McPhaden, 2003). 72

73 ENSO theory (Neelin et al., 1998) provides a framework to 74 understand the existence of such predictability barriers. The ENSO 75 phenomenon is thought to be an internal mode of the coupled 76 equatorial ocean-atmosphere system which can be self-sustained or 77 excited by small-scale processes, often considered as noise (Fedorov 78 et al., 2003). Bjerknes' feedbacks are central in the amplification 79 of SST anomalies, whereas equatorial ocean wave processes pro-80 vide a delayed negative feedback and are responsible for the time 81 scale of ENSO. The interactions of the internal mode and the exter-82 nal seasonal forcing can lead to chaotic behavior through nonlinear 83 resonances (Tziperman et al., 1994; and Jin et al., 1994). On the 84 other hand, the dynamical behavior can be strongly influenced by 85 noise, in particular, westerly-wind bursts (Lian et al., 2014). During 86 boreal spring and summer, the Pacific climate system is most sus-87 ceptible to perturbations leading to predictability barriers (Latif and 88 Barnett, 1994). The growth of perturbations from a certain initial 89 state has been investigated in detail from a much used intermediate-90 complexity model, the Zebiak-Cane (ZC) model (Zebiak and Cane, 91 1987). Applying the methodology of optimal modes (Mu et al., 2007; 92 Duan et al., 2009; and Yu et al., 2012), it was indeed shown that 93 spring is the most sensitive season for EP El Niños and likewise 94 summer for CP El Niños (Tian and Duan, 2015; and Hou et al., 95 2019

96 Deep learning methods (DLMs) are powerful statistical mod-97 els, which have now been used in a wide range of applications 98 such as speech recognition and image reconstruction (Goodfellow 99 et al., 2016). These methods include feed-forward Artificial Neural 100 Networks (ANNs), Recurrent Neural Networks (RNNs), Reservoir 101 Computers (RCs), and Convolutional Neural Networks (CNNs); 102 over quite some time now, DLMs have been applied to El Niño pre-103 diction (Dijkstra et al., 2019). The current work is motivated by the 104 high El Niño prediction skill of two types of DLMs. First, in Ham 105 et al. (2019), CNNs were trained on model data from the Climate 106 Model Intercomparison Project, phase 5 (CMIP5) using transfer 107 learning and subsequently trained on reanalysis data. The CNN-108 based scheme shows a better forecasting skill than most dynamical 109 models and this forecast skill remains high up to lead times of about 110 17 months. It is also able to successfully predict the type of El Niño 111 (CP or EP) patterns that develop. Second, in Petersik and Dijk-112 stra (2020), deep ensemble methods (Lakshminarayanan, 2017), in 113 particular, Gaussian Density Neural Networks (GDNNs) and Quan-114 tile Regression Neural Networks (QRNNs), were used in ENSO prediction. These methods also give a skillful model for the long-lead 115

time prediction of the ONI (and its uncertainty) using a relatively 116 small predictor set. 117

At the moment, there is an enormous effort to understand 118 119 the performance of DLMs generally referred to as explainable AI (Arrieta et al., 2020). The research described above shows that DLMs 120 are a very promising tool in ENSO prediction that can provide 121 useful skills of El Niño forecasts beyond the predictability barri-122 ers. The intriguing question is now what the DLMs capture of the 123 ENSO physics contained in the data. Addressing this question is 124 precisely the focus of this paper. We will approach this issue using 125 the Zebiak-Cane model, which is also routinely used for ENSO 126 prediction. The novel aspect of this work is that we use so-called 127 distorted physics experiments where different physical processes 128 (such as equatorial wave dynamics and ocean-atmosphere feed-129 backs) are perturbed. Using saliency analyses, determining which 130 input variables contribute most to the prediction skill, we then aim 131 to determine what part of the ENSO dynamics is represented by the 132 DLM. 133

#### II. MODELS AND METHODS

#### A. ENSO model

The Zebiak-Cane (ZC) model (Zebiak and Cane, 1987) rep-136 resents the coupled ocean-atmosphere system on an equatorial  $\beta$ -137 plane in the equatorial Pacific. In this model, a shallow-water ocean 138 component is coupled to a steady shallow-water (Gill, 1980) atmo-139 sphere component (Fig. 1). The atmosphere is driven by heat fluxes 140 from the ocean, depending linearly on the anomaly of the sea surface 141 temperature T with respect to a radiative equilibrium temperature 142  $T_0$ . We use the numerically implicit fully-coupled version of this 143 model, developed in van der Vaart et al. (2000) and slightly extended 144 in Feng and Dijkstra (2017). In this version, the zonal wind stress  $\tau^x$ 145 is written as 146

$$\tau^{x} = \tau^{x}_{ext} + \tau^{x}_{c},$$

$$\tau^{x}_{ext} = -\tau_{0} e^{-\frac{1}{2} \left(\frac{y}{L_{a}}\right)^{2}}.$$
(1)

Here, the external part  $\tau_{ext}^x$  represents a weak ( $\tau_0 \sim 0.01 \text{ Pa}$ ) easterly wind stress due to the Hadley circulation,  $L_a$  is the atmospheric Rossby deformation radius and y is the meridional coordinate. The zonal wind stress  $\tau_c^x$  is proportional to the zonal wind from the atmospheric model which, in turn, depends on sea surface temperature. 152

As shown in van der Vaart et al. (2000), the parameter mea-153 suring the strength of all ocean-atmosphere coupled feedbacks is 154 the coupling strength  $\mu$ . When  $\mu < \mu_c$ , where  $\mu_c$  indicates a crit-155 ical value, the Tropical Pacific climatology (a stationary state of the 156 model) is stable. However, if the coupling strength exceeds the crit-157 ical value  $\mu_c$ , a supercritical Hopf bifurcation occurs and sustained 158 oscillations occur with a period of approximately four years. A sea-159 sonal cycle is included in the model by varying  $\mu$  over time with a 160 specific amplitude  $\Delta \mu$  and with an annual period. 161

Apart from the coupled ocean-atmosphere processes, ENSO is162also affected by fast processes in the atmosphere, such as westerly-163wind bursts. These processes are considered as noise in the ZC164model. The representation of atmospheric noise in the model is similar to that in Feng and Dijkstra (2017), where the westerly-wind165

134

ARTICLE



**FIG. 1.** Schematic of the Zebiak–Cane model, where a shallow-water ocean model is coupled to a shallow-water atmosphere model through a mixed-layer ocean model with temperature T. The ocean-atmosphere coupling involves a heat flux  $Q_{re}$  and a wind-stress vector  $\tau$ .

bursts are represented by one Empirical Orthogonal Function pat-167 168 tern (with the associated principle component fitted to an AR(1) 169 process) in the zonal wind stress. The observation-based dataset in 170 Feng and Dijkstra (2017) contains weekly patterns of this windstress noise. In the ZC model, we randomly add one of such patterns 171 172 at each time step (of a week) to the zonal wind stress. The effect of 173 the noise on the model behavior depends on whether the model is 174 in the super- or sub-critical regime (i.e., whether  $\mu$  above or below 175  $\mu_c$ ). If  $\mu < \mu_c$ , the noise excites the ENSO mode, causing irregular 176 oscillations. In the supercritical regime, the cycle of approximately 177 four years is still present, but the noise causes an irregular amplitude 178 of ENSO variability.

While the ZC model is used for ENSO predictions, it also has
its limitations as it cannot capture either tropical basin interactions
(e.g., Atlantic and Indian Oceans) or tropical-extratropical interactions (it described only the dynamics of the Pacific). The model also
cannot represent adequately a Tropical Pacific seasonal cycle, and,
hence, such a seasonal cycle is prescribed in the model.

#### 185 B. Distorted physics simulations

186 The advantage of the ZC model is that the behavior of the 187 model can be connected to the physical processes in a very trans-188 parent way (Jin, 1997). In the distorted physics approach, we define 189 a "truth" by a reference simulation, using an external seasonal cycle, 190 prescribed noise in the wind-stress, and parameter settings such as 191 in Feng and Dijkstra (2017). Next, in subsequent distorted-physics 192 simulations, we change the representation of physical processes 193 in the model by varying parameters. We will focus on the main 194 processes setting the time scale and amplitude of ENSO.

An important memory component in the Tropical Pacific cli-195 mate system is the ocean adjustment to changes in the atmospheric 196 forcing. This is accomplished by equatorial wave dynamics and best 197 described by a basin mode response, where the basin mode consists 198 of a sum of one Kelvin and multiple Rossby waves. In the SST-mixed 199 ocean dynamics mode framework behind ENSO variability (Neelin 200 et al., 1998), the adjustment is crucial for the timing of El Niño 201 events. It plays also a crucial role in the recharge/discharge oscil-202 lator view of ENSO (Jin, 1997), where the equatorial heat content 203 is varied, usually measured by the warm water volume (WWV) in 204 observations. The temporal aspects of the adjustment can be con-205 trolled in the Zebiak–Cane model by putting a coefficient  $\delta$  before 206 the time derivatives of the ocean momentum equations (Neelin, 207 1991). In the extreme case where the time derivative is effectively 208 zero ( $\delta = 0$ ), the so-called "fast-wave" limit is reached. 209

Three of the most important positive Bjerknes' feedbacks are 210 the thermocline feedback, the zonal advection feedback, and the 211 upwelling (or Ekman) feedback (Dijkstra, 2005). The relative mag-212 nitude of these feedbacks determines which spatial SST perturbation 213 patterns are amplified. In addition, the feedbacks determine also 214 the mean state and seasonal cycle of the tropical Pacific climate 215 state (Dijkstra and Neelin, 1995). Specific feedback strengths can be 216 changed in the ZC model by varying the mean thermocline depth 217 (thermocline feedback), the mean zonal temperature gradient (zonal 218 advection feedback), or Ekman friction (upwelling feedback). We 219 will concentrate on the latter feedback, affecting the amplitude of 220 ENSO and which can be changed in the ZC model by adjusting the 221 222 parameter  $\delta_s$ .

Hence, we have already a good idea of how the behavior of 223 the model is distorted by varying the parameters  $\delta$  and  $\delta_s$ . Now, 224  $\delta$  is an artificial parameter enabling the variation of the equatorial 225 wave speeds and in the results below, we vary it from 0.5 to 1.5. The 226 upwelling feedback strength  $\delta_s$  is quite an uncertain parameter in 227 the ZC model and we vary it over the range  $\delta_s = 0.1$  to  $\delta_s = 0.6$ , 228 which is a plausble range, where an adequate mean state and vari-229 ability are obtained (van der Vaart et al., 2000). In the approach 230 below, we are interested in whether a CNN is able to capture ENSO 231 dynamics adequately when trained with data from distorted model 232 simulations. 233

#### C. CNN approach

Due to their versatility and peculiarity in solving binary and 235 multi-labels classification tasks by capturing and recognizing the 236 discerning patterns of the input data, CNNs (Convolutional Neural 237 Networks) can represent a powerful method for making forecast-238 ing of ENSO events with lead times of up to one and a half years 239 (Ham et al., 2019) or for solving a binary classification problem 240 in hybrid models with high complexity multi-resolution input data 241 (Yan et al., 2020). Unlike more sophisticated and popular ANNs 242 like CNN-LSTM and ConvLSTM, the predictions provided by the 243 244 CNN can be made explainable by means of saliency maps (Zhou et al., 2016; Selvaraju et al., 2017; Adebayo et al., 2018; Montavon 245 et al., 2019; and Mundhenk et al., 2019) that allow us to outline the 246 spatial locations of those signal patterns that mainly contribute to 247 making the CNN give the classes of output. Therefore, CNNs rep-248 resent the perfect choice for classifying the occurrence of ENSO 249



FIG. 2. Schematic illustrations of the CNN model; flow diagram (a) and the hidden layers (b).

events in ZC simulations and investigating in detail on which features contained in data can lead to highly accurate predictions. To
leverage the basic feature of the CNN of encoding the sequentiality
of the patterns contained in the input data, we feed the CNN with

simulated time series obtained via the Zebiak–Cane model. This synthetic dataset describes the temporal evolution in the NINO3.4 region of some physical observables of interest as the thermocline depth, the sea surface temperature, the wind speed, and the 257

wind-stress noise. The extraction of the instances from the ZC sim-258 259 ulations, therefore, consists in slicing the synthetic time series along 260 the time domain, i.e., the set of time series is chunked in a sequence 261 of overlapping time windows of 48 months and stride 1. As a result, 262 each single instance is a tensor of rank 2 whose dimensions are 263 the time-length (48 pixels, sampling frequency one month) and the 264 number of time-series features (the four physical observables of 265 interest). The labeling of the instances is performed by equipping each instance with the corresponding ONI-index value and so we 266 267 label one ENSO event whenever the ONI-index value is greater than 268 0.5 (El Niño event) or lower than -0.5 (La Niña event). The input 269 instances are then pre-processed via standardization (each feature 270 has now zero-mean and unit variance) and divided into training set 271 and test set; we validate the CNN model by means of the fivefold 272 cross validation. Therefore, we evaluate the AUC (Area Under the 273 Curve) of the receiver operating characteristic curve on each fold; 274 the mean value and the standard error mean will provide the degree 275 of accuracy of the CNN model and its error, respectively. The design 276 of our CNN is quite standard and it is composed by the sequence 277 of one convolutional layer (64 kernels, size 9) with a Rectified Lin-278 ear Unit (ReLu) activation function, followed by a maxpooling Layer 279 with pooling size 2 (Fig. 2). Dropout layers (Srivastava et al., 2014) 280 with a dropout rate of 0.50 are also employed to reduce overfitting, 281 but no stride is applied during the convolutions. After repeating two 282 times this block of hidden layers, the resulting feature map is flat-283 tened via a flattened layer; the final fully-connected layer with the 284 sigmoid activation function returns the output of the CNN. During 285 the training phase, the ADAM (Kingma and Ba, 2014) algorithm is 286 used as an optimizer for the binary-cross entropy loss function; the 287 batch size and learning rate are set equal to 128 and 0.005, respec-288 tively. The SMOE scale method (Mundhenk et al., 2019) is a robust 289 statistical measure of the activation values of CNNs arising at dif-290 ferent spatial locations (temporal locations in the domain of our instances). This statistics can be used to construct robust saliency 291 292 maps that appear to be much more efficient and computationally 293 faster than popular gradient methods. More specifically, this method 294 estimates the saliency of the input data at each temporal location; 295 the saliency values are returned as a score laying in the range [0, 1]. 296 Therefore, the closest is one score to the unit value, the more is the 297 saliency attributed to its temporal location. We, therefore, exploit 298 the capability of SMOE scale method to detect those patterns and 299 their spatial domains that mostly indicate the approaching or the 300 occurring of the ENSO events. Thus, we proceed with the analysis 301 of the profile of the saliency maps in order to evince possible analogies and differences between the patterns learnt during the training 302 303 phase and the patterns contained in the test dataset. In order to 304 complete the analysis provided by the SMOE scale method, we even 305 look at how the predictions can change when only a spectral sub-306 band of the input instances is propagated through the hidden layers. 307 With this approach, we aim to investigate how oscillations occurring 308 under a specific regime can really be a basic aspect of the prediction 309 provided by the CNN. Therefore, we can progressively apply a digi-310 tal Butterworth filter (Butterworth et al., 1930; and Hamming, 1998) 311 of order 3 as either a bandpass filter or low-pass filter to smooth 312 the input instance. The ensemble of bandpass filters is designed 313 to cover the whole spectral domain of any input instance and be 314 non-overlapping at the same time and, thus, we impose the cutoff

TABLE I. Frequency bands and cut-off frequencies for the bandpass and low-pass digital filters, respectively.

$ \begin{array}{c} [2,4) \\ [4,8) \\ \end{array} $	
[1,0]	
[8, 16] 8	
[16, 32) 16 [32, 48) 32	

frequencies of each filter to be in ratio 1:2. This means that, start-315 ing from the Nyquist frequency  $v_0$ , the first digital filter will have 316 its frequency band in  $\left[\frac{\nu_0}{2}, \nu_0\right]$ , the second one in  $\left[\frac{\nu_0}{4}, \frac{\nu_0}{2}\right]$ , and so on. 317 Again, when considering the low-pass digital filters, we will choose 318 the cut-off frequency according to a dyadic scale, i.e., the first filter 319 will have cut-off frequency  $v_0$ , the second one  $\frac{v_0}{2}$ , the third one  $\frac{v_0}{4}$ , 320 and so on. The full list of bandwidths (in periods) and cutoff fre-321 quencies is reported in Table I. Note that we will apply these digital 322 filtering techniques by repeating the same fivefold cross validation 323 with metrics AUC, as we do in the model validation; the CNN archi-324 tecture will not be altered during this step. Hence, by means of this 325 approach, we aim to reveal which time scale is dominant in those 326 patterns that characterize the ENSO events (e.g., a slow oscillating 327 trends against rapid oscillating deviations), i.e., we make an effort 328 to understand how the periodicity of the time-series features is an 329 essential characteristic of data that the CNN captures for solving 330 the classification task and how a distortion of it can give rise to a 331 decrease in the CNN capability of classifying the events El Niño and 332 La Niña. 333

RESULTS
---------

#### A. Distorted physics

III.

The model experiments broadly consist of two steps: first, the 336 ZC model is run for standard parameter values to produce reference 337 case data; and then it is run again but for a range of values around 338 the standard parameter value (shown in Table II) to get the distorted 339 data. This ultimately results in three different kinds of datasets: ref-340 erence case, distorted wave speed, and distorted upwelling feedback. 341 There are no simulations where more than one parameter is dis-342 torted at the same time. In the second step, the distorted datasets are 343 used as training data for the DLMs whose performance is then deter-344 mined by using the reference case as the test set. As a consistency 345 check, the DLMs are also trained on the reference case data and then 346 tested on reference case data. This should produce the highest per-347 formance because the DLMs are tested on data they have already 348 349 seen.

#### B. Equatorial wave dynamics: Saliency maps

Time series of the ONI for the different  $\delta$  values, as computed 351 from the ZC model are shown in Fig. 3. Changing the  $\delta$  value causes 352 the amplitude of the oscillation to become much smaller for  $\delta < 1$ , 353 so much even that by definition only ENSO neutral conditions 354 (-0.5 < ONI < 0.5) are present. Increasing  $\delta$  above the reference 355

334

335

**TABLE II.** Parameter settings of the ZC model used to generate the data used in the distorted physics experiments with the parameter step size shown within brackets. Parameter ranges are chosen to cover roughly a 50% increase and decrease compared to the reference value, step size is chosen to get around 10 points within this range. The parameters are from left to right: coupling strength  $\mu$ , wave speed parameter  $\delta$ , and upwelling feedback parameter  $\delta_s$ . The value of  $\mu = 2.7$  is subcritical in the ZC model.

Effect	$\mu$	δ	$\delta_s$
Distorted wave speed	2.7	0.5-1.5 (0.1)	0.3
Distorted wave speed	2.7	0.5-1.5 (0.1)	0.3
Distorted upwelling feedback	2.7	1.0	0.1-0.6 (0.05)
Distorted upwelling feedback	2.7	1.0	0.1-0.6 (0.05)
Reference	2.7	1.0	0.3

356 value of 1.0 initially leads to an increase in the oscillation amplitude and it then decreases again for higher values of  $\delta$ . This is 357 358 expected because the ENSO period depends on the speed of Rossby 359 and Kelvin waves crossing the Pacific basin. In the study of the classification performance of the CNN, we take a prediction lead time 360 361 of 9 months. The propagation of the  $\delta$ -distorted data through the 362 CNN can lead to substantial changes when testing the accuracy of 363 the model on the reference data. By construction, the AUC score 364 [Fig. 4(a)] attains excellent results at  $\delta = 1.0$  (AUC 0.94) as the CNN is trained on the reference data. The AUC scores tend to remain 365 366 relatively high (peak of AUC 0.91 at  $\delta = 0.8$ ) as the  $\delta$  parameter is 367 slightly decreased from its reference value. Instead, as  $\delta$  is reduced up to value 0.5, we can observe a severe degradation of the accu-368 369 racy with respect to the reference case; from  $\delta = 0.7$ , the evaluation 370 of the AUC metrics decreases monotonically (AUC 0.66 at  $\delta = 0.5$ ). 371 At values  $\delta > 1.0$ , we observe a total reduction of the AUC values. 372 Specifically, models trained for  $\delta = 1.1$ , and  $\delta = 1.2$  show low AUCs 373 as 0.58 and 0.56 but the lowest value (AUC value 0.51) is reached 374 at  $\delta = 1.5$ . The evaluation of the loss function (when the reference 375 data are propagated through the CNN models) confirms the sce-376 nario expressed above [see Fig. 4(b)]. Indeed, the global minimum 377 value is achieved at  $\delta = 1.0$  and a relative minimum is also present at  $\delta = 0.8$ . When  $\delta$  is decreased or augmented toward the bound values 378  $\delta = 0.5$  and  $\delta = 1.5$ , respectively, we can observe the loss function 379 tends to reach higher values. In particular, an increase or decrease in 380 the AUC along the  $\delta$  domain is followed by a decrease or an increase 381 in the loss function. 382

The application of the combined SMOE Scale on the mean 383 instances (namely, the instances obtained by averaging all samples of 384 the test data of the reference case) can help identify which patterns in 385 the data are captured by the CNN to generate (accurate or degraded) 386 ONI predictions. The reason for analyzing the mean instance is that 387 it represents the main patterns in the feature time series; the inter-388 pretation of the saliency maps of all instances would turn out to be 389 really impractical. The mean instances of both the events El Niño 390 and La Niña are represented in Figs. 5(a) and 6(a), respectively. 391 Therefore, after propagating the mean instance through the trained 392 CNN model, we get the activated feature maps and compute the 393 saliency map by means of the SMOE scale method. Next, we indi-394 vidualize the regions (months) of the saliency maps achieving the 395 highest values; at the same regions of the mean instance, we can 396 397 identify those time-series patterns that are mainly captured by the CNN model. 398

Taking into account the event El Niño, the saliency map of 399  $\delta = 1$  reference case [green line in Fig. 5(a)] shows two peaks with 400 an intensity of 0.6 and 0.9 around months 18 and 36, respectively 401 (note that the instances are 48 months long and that the lead time is 402 9 months). These two regions turn out to be the most salient along 403 the whole domain of the mean instance. At month 18, we find a 404 peak in the thermocline depth [Fig. 5(a), green line] and a trough in 405 both sea surface temperature [Fig. 5(a), orange line] and wind speed 406 [Fig. 5(a), indigo line]. Conversely, in the neighborhood of month 407 36, we find the thermocline is descending toward a trough, while 408 both sea surface temperature and wind speed are reaching a peak 409 value. Both these two combinations of patterns represent the main 410 characteristic that mostly defines the event El Niño according to the 411 recognition activity of the CNN model. 412

Likewise, we can find some similar results for the event class La Niña. The spatial locations, where the saliency map [Fig. 6(b), green line] achieves values close to unity corresponding to one interval domain (months 0–7) of the mean instance [see Fig. 6(a)] where the thermocline depth attains a peak while both 417



FIG. 3. Several time series of ONI calculated from ZC model simulations using  $\delta$  parameter values of 0.5, 1.0, and 1.5, respectively.

Chaos **32**, 000000 (2022); doi: 10.1063/5.0101668 Published under an exclusive license by AIP Publishing



**FIG. 4.** The AUC score (a) and the loss function (b) as a function of the equatorial wave speed  $\delta$ . Each point represents the mean AUC over five different folds; error bars are evaluated via the standard error mean.

418 the sea surface temperature and the wind speed descend toward a 419 trough.

When considering other distorted cases, such as  $\delta = 0.5$  and 420 421  $\delta = 0.8$  (where waves are propagating faster than the reference case), 422 the combination of peaks in the thermocline and troughs in the 423 sea surface temperature (and vice versa) still represents those rele-424 vant time-series patterns that the CNN model captures during the 425 learning phase. If we focus our attention on the event El Niño, the saliency map of case  $\delta = 0.8$  [see Fig. 5(b), orange line] shows at 426 months 30-38 a broad region with intensity larger than 0.8, whereas 427 428 the saliency map of case  $\delta = 0.5$  [Fig. 5(b), blue line] shows intensities close to unity in the region 0-10 months. In the first case, we 429 430 find that the high saliency region corresponds to a peak in the ther-431 mocline and a trough in both the sea surface temperature and the 432 wind speed, while in the latter case, we find the thermocline depth



**FIG. 5.** The mean instance considering all the El Niño event instances in the test data (reference case) (a). Saliency maps of CNN models (b) and (c) trained with the wave distorted data (variation of  $\delta$ ) considering the cases (b)  $\delta = 0.5, 0.8, 1.0, 1.2, 1.5$  and (c)  $\delta = 0.7, 0.8, 0.9, 1.0$ .

shows a soft minimum value as opposed to the high-valued peak in the sea surface temperature and wind speed. 434

Similar results are also obtained for the event La Niña. The 435 saliency map of case  $\delta = 0.5$  [see Fig. 6(b), blue line] shows at 436 months 35-40 a saliency region with intensity higher than 0.85. In 437 Fig. 6(a), we see that this high saliency region corresponds to a peak 438 in the thermocline depth and a trough in both the sea surface tem-439 perature and the wind stress. The saliency map of case  $\delta = 0.8$  [see 440 Fig. 6(b), orange line] reveals a broad high-valued peak (maximum 441 intensity 0.81) around month 18 and a flat salient region (intensity 442 close to 0.9) at months 40-48. By looking at those temporal regions 443



**FIG. 6.** The mean instance considering all the event La Niña instances in the test data (reference case) (a). Saliency maps of CNN models (b) and (c) trained with the wave distorted data (variation of  $\delta$ ) considering the cases (b)  $\delta = 0.5, 0.8, 1.0, 1.2, 1.5$  and (c)  $\delta = 0.7, 0.8, 0.9, 1.0$ .

in Fig. 6(a), we find a peak in both the sea surface temperature and
the wind stress together with a deep trough in the thermocline depth
around month 18, whereas the domain months 40–48 show a soft
trough in the thermocline and a prominent peak in both sea surface
temperature and wind speed.

449 A deeper insight into the region  $\delta = 0.7-1.0$  (where the AUC 450 takes the highest values) reveals that all CNN models tend to capture 451 a specific type of time-series patterns when they have to deal with 452 the recognition of the event El Niño. For all cases considered in this 453 interval, the saliency maps indicate as interesting the region months 454 32–38 [see Fig. 5(c)], where the values attained are larger than 0.8. 455 Thus, we find that the results previously discussed for both cases  $\delta = 0.8$  and  $\delta = 1.0$  (where we discussed the behavior of the mean 456 instance around month 36) are still valid even when we consider 457 both cases  $\delta = 0.7$  and  $\delta = 0.9$ . Interestingly, the case  $\delta = 0.9$  shows 458 a recognition activity that is similar to that of the model trained 459 under the reference case because the saliency maps appear to be par-460 tially overlapped [see both the pink and the green line of Fig. 5(c) at 461 months 32–38]. Moreover, the saliency map of case  $\delta = 0.9$  points 462 out some other aforementioned details of interest, e.g., those corre-463 sponding to the peak with intensity 0.6 at month 18, as shown by the 464 pink line in Fig. 5(c). 465

For La Niña event, instead, the saliency map of case  $\delta = 0.7$ 466 [Fig. 6(c), cyan line] presents some analogies with case  $\delta = 0.8$ 467 [Fig. 6(c), orange line], individualizing one highly salient region at 468 months 40–48 with an intensity around. Similarly to case  $\delta = 1.0$ 469 [Fig. 6(c), green line], the saliency map of case  $\delta = 0.9$  [Fig. 6(c), 470 pink line] individualizes a salient region in proximity of the left edge 471 of the instance domain (months 0-5) with an intensity around to 472 0.95. It is interesting to note that both saliency maps of cases  $\delta = 0.9$ 473 and  $\delta = 1.0$  are overlapped at the middle region (months 15–35); 474 both two CNN models show a similar approach to capturing some 475 low relevant features to identify the event La Niña. 476

For the cases  $\delta = 1.2$  and  $\delta = 1.5$  (where waves are propagating 477 slower), the saliency maps [Fig. 5(b), red and purple line] reveal that 478 the region around month 18 is no longer salient as in the reference 479 case for El Niño event. For case  $\delta = 1.2$ , we find a salient region at 480 months 36-48, where the saliency map takes values larger than 0.8. 481 This corresponds to the presence of one broad peak in both the sea 482 surface temperature and the wind speed with a less important contri-483 bution (than in the reference case) in the thermocline depth located 484 at months 32–48. For case  $\delta = 1.5$ , we can observe that the saliency 485 map is similar and almost completely overlapped with that of case 486  $\delta = 0.5$ ; in this case, the analysis of the most salient time-series pat-487 terns will lead to some results that have already been discussed for 488 the case  $\delta = 0.5$ . 489

When considering the event La Niña, the saliency map of case 490  $\delta = 1.2$  [see Fig. 6(b), red line] attains values with an intensity close 491 492 to unity at months 0-10. This temporal domain is characterized by 493 the opposite feature, i.e., a broad peak in the thermocline depth and a trough in the sea surface temperature, located at months 0-10. 494 The same feature can be also found for the case  $\delta = 1.5$ . Indeed, the 495 saliency map [see Fig. 6(b), purple line] shows high saliency regions 496 at either months 0-10 (intensity values close to unity) and month 36 497 (a peak with a maximum of 0.81). In particular, at month 36, the sea 498 surface temperature and the wind speed reach a deeper trough with 499 respect to that of region months 0-10. 500

# C. Equatorial wave dynamics: Filtering of the instances via Butterworth digital filter

The application of a bandpass filter on all the instances 503 included in the test dataset (reference case data) reveals that the 504 propagation of one specific frequency band through the CNN mod-505 els can retrieve most of the AUC scores obtained with the non-506 filtered data, as shown in Fig. 7. In specific, the model trained under 507 the reference case turns out to be very sensitive to the frequency 508 band corresponding to periods 8-16 months, where the AUC is 509 equal to 0.80 [Fig. 7(a), green line]. On the contrary, the complete 510

501





degradation of AUC scores is attained when propagating lower and 511 higher frequency bands, e.g., both intervals 16-32 months and 2-4 512 513 months, where the AUC value is equal to 0.61 and 0.58, respectively. Similar results can be found for other cases taken under consider-514 515 ation, as the case  $\delta = 0.5$  and  $\delta = 0.8$  [Fig. 7(a), blue and orange 516 lines]. For both these cases, the band 8-16 months turns out to be 517 the most predictive one with a net degradation of AUC score as soon 518 as slower frequency bands are considered.

519 In particular, case  $\delta = 0.8$  still shows some analogies with the 520 reference case; the frequency band 8–16 months is still the most pre-521 dictive with an AUC score of 0.80, and net degradation occurs at 522 either lower or higher frequency bands. Such a result offers further 523 details in interpreting the saliency maps, i.e., the CNN models tend





**FIG. 8.** Evaluation of AUC when the ROAR method (a) or the replacing at random strategy is applied (b); on the x axis, the ratio of pixels is replaced and on the y axis the AUC value.

to capture oscillating trends with specific carrier frequencies within 524 the low-medium band of frequencies. It is important to highlight 525 that the presence of details on a shorter frequency scale (i.e., period 526 16-32 months) is still fundamental and needed to allow the CNN 527 to make an accurate classification of the ENSO events. The smooth-528 ing of the sample instances with a low-pass filter [Fig. 7(b)] reveals 529 the instances tend to substantially lose many of their discriminating 530 patterns at cutoff frequencies as 8 or 16 months. For example, in the 531 cases  $\delta = 0.8$  and  $\delta = 1.0$  [Fig. 7(b), orange and green lines], we can 532 observe a decrease in the predictive power with degradation of 0.1 533 AUC at 8 months and 0.3 AUC at 16 months. Hence, medium-low 534 frequency patterns (4-8 months) as those contained in the thermo-535 cline depth or in the wind-noise time series can play an important 536 role in the detection of the events. 537



FIG. 9. Several time series of ONI calculated from ZC model simulations using  $\delta_s$  parameter values of 0.1, 0.3, and 0.6 using  $\mu = 2.7$ .

#### 538 D. Equatorial wave dynamics: ROAR

539 To ensure the correct implementation of the combined SMOE 540 Scale and guarantee the validity of the results obtained, we used (and 541 adapted to this analysis) the metrics ROAR (Remove and Retain) introduced in Mundhenk et al. (2019). The replacement in the vali-542 543 dation sets of an increasing amount of salient spatial locations with 544 zero-valued pixels rapidly deteriorates the predictive characteristics 545 of the data; as shown in Fig. 8. It is important to remember that the CNN models do not make use of any bias term neither in the convo-546 547 lutional layers nor in the dense layers. Accordingly, the CNN model 548 considers the zero-valued patterns as absolutely non-informative, 549 i.e., the propagation of such a pattern through the CNN is designed 550 to prevent the activation of any stimulus along the hidden layers. In Fig. 8(a), we can observe that the removal of the top 50% salient 551 552 pixels via ROAR (actually 24) guarantees a considerable decrease in 553 the AUC; under the reference case model, the AUC scores present a loss equal to 0.20. Contrary to this, when randomly replacing the 554 555 50% pixels with zero-valued pixels, we can still observe a slighter 556 decrease in the AUC curve under the reference, i.e., a loss equal to 557 0.03 [see Fig. 8(b)]. Likewise, similar results can be found when even 558 considering all the other distorted physics cases.

## 559 E. Upwelling feedback: Saliency maps

560 We next consider the distortion of the model data due to a wrong representation of the upwelling feedback, represented by the 561 562 parameter  $\delta_s$  in the ZC model. Figure 9 shows that the ONI's ampli-563 tude increases (decreases) for larger (smaller) values of  $\delta_s$ . This behavior is expected because the upwelling feedback is a positive 564 565 one, enhancing the existing sea surface temperature anomaly further and consequently increasing the amplitude of the ONI. The 566 567 AUC score vs  $\delta_s$  curve [Fig. 10(a)] reveals that a particular tuning 568 of the parameter  $\delta_s$  strongly affects the accuracy of the CNN models 569 when trained with distorted data. By construction, the AUC score 570 attains the highest score at the reference value  $\delta_s = 0.3$  (AUC 0.94). 571 For  $\delta_s < 0.3$  the profile of the curve suggests a net degradation in the 572 AUC scores with the lowest score attained at  $\delta_s = 0.15$  (AUC 0.5), 573 whereas at  $\delta_s > 0.3$  the AUC scores remain stable, but still attain val-574 ues lower than 0.7. The profile of the AUC has a plateau at values of 0.6 as  $\delta_s$  goes toward the boundary value  $\delta_s = 0.6$ . The evaluation of 575

the loss function [Fig. 10(b)] as a function of the parameter  $\delta_s$  con-576 firms the results obtained above. At  $\delta_s = 0.3$ , the global minimum 577 is achieved, and the net degradation occurring at lower and higher 578  $\delta_s = 0.3$  are still present; the loss function increases monotonically 579 in both cases. Similarly to the analysis provided for the distortion 580 of the  $\delta$  parameter, we next consider the mean instances (of the 581 test data of the reference case) and their saliency maps [Figs. 11(a) 582 and 12(a)]. 583

For the event El Niño, we can observe that different regions 584 of saliency can be associated to different variations of  $\delta_s$ , i.e., for 585  $\delta_s < 0.3$  the saliency maps [Fig. 11(b), blue and orange lines] 586 indicate the left part of the instance as the most predictive, 587 while for  $\delta_s > 0.3$  the right part [Fig. 11(b), red and purple 588 lines]. In particular, the saliency map of cases  $\delta_s = 0.10$  and 589  $\delta_s = 0.25$  [Fig. 11(b), blue and orange lines] turns out to be 590 very salient at 0-8 months, with intensity above 0.8. In that 591 region, the mean instance presents a peak occurring in both the 592 sea surface temperature and the wind speed time-series features. 593 On the contrary, for cases  $\delta_s = 0.45$  and  $\delta_s = 0.60$ , the saliency 594 maps [Fig. 11(b), red and purple lines] achieve intensities larger 595 than 0.8 around 32-48 months and capture one single broad 596 oscillating peak in both the sea surface temperature and the wind 597 speed time-series features. 598

For the event La Niña, we refer to Fig. 12. In particular, the 599 saliency maps of cases  $\delta_s = 0.10$  and  $\delta_s = 0.25$  [Fig. 12(b), blue and 600 orange lines] present intensities larger than 0.8 at 42–48 months. 601 It is interesting to observe that the saliency map of case  $\delta_s = 0.25$  602 presents a plateau around 32–48 months; in opposition to the event El Niño, the CNN here captures a deep trough in the sea surface 604 temperature time-series feature. 605

### F. Upwelling feedback: Filtering of the instances via 606 Butterworth digital filter 607

The application of bandpass and low-pass filters on the sample instances brings to light a result similar to the analysis done for the parameter  $\delta$ , as shown in Fig. 13. When applying a bandpass filter with bandwidth 8–16 months, the case  $\delta_s = 0.25$  [Fig. 13(a), orange line] can partially retrieve the original prediction with AUC 0.70, whereas for other cases such as  $\delta_s = 0.6$  [Fig. 13(a), purple line] the 613



**FIG. 10.** The AUC score (a) and the loss function (b) as a function of the upwelling feedback parameter  $\delta_s$ . Each point represents the mean AUC over five different folds; error bars are evaluated via the standard error mean.

original prediction can be retrieved only by oscillations lying within the frequency band corresponding to 32–48 months. The smoothing of the instances via low-pass filter [Fig. 13(b)] shows that the removal of high-frequency patterns oversimplifies the data; and so, the classification task cannot be solved by the information contained in the low-frequency data only.

620 As confirmed by the filtering of the instances, the frequency bands 4-8 months and 8-16 months represent the main frequency 621 622 bands in the reference case ( $\delta_s = 0.3$ ). Capturing one of these two 623 can retrieve a considerable amount of skill. The case  $\delta_s = 0.25$ focuses a large amount of relevant patterns mainly in the frequency 624 625 band 8-16 months. The filtering with a low-pass digital filters also 626 reveals that a cut-off frequency of 16 months can reduce the AUC in 627 both cases, but a cut-off frequency of 8 months leads to a degrada-628 tion for the reference case only. In the latter scenario, we register 629 a loss of 0.1 AUC, i.e., a degradation on the same order of magnitude as when testing the reference case data and the data of 630



**FIG. 11.** The mean instance (a) of all the El Niño event instances in the test data (reference case). Saliency maps of CNN models (b) trained with the upwelling distorted data (variation of  $\delta_s$ ). In specific, cases  $\delta_s = 0.10, 0.25, 0.30, 0.45, 0.60$  are considered.

case  $\delta_s = 0.25$ . Hence, this example shows how a manipulation in the intrinsic characteristic of the instances can lead to a reduction and oversimplification of the instances, i.e., the distortion of the periodicity of data provokes a reduction or missing of some patterns that are fundamental in the classification of the reference case data.

#### G. Comparison of CNN and GDNN

To provide a comparison, we also applied the distorted physics 637 approach in the Gaussian Density Neural Network (GDNN) as used 638 in Petersik and Dijkstra (2020). The Gaussian density terminology 639 refers to the network's purpose of predicting a Gaussian distribution 640 by producing both a mean and standard deviation as output. The 641 variable to be predicted (or target variable) is also the ONI at a (lead) 642 time in the future. The features used in the GDNN are described by 643 Petersik and Dijkstra (2020): ONI, network graph connectivity met-644 ric  $c_2$ , adjusted Hamming distance  $\mathcal{H}^*$  (measure of change in the 645 network graph) and a seasonal cycle (SC) in the form of a cosine. 646 The warm water volume (WWV, volume of water above the 20 °C 647 thermocline) is not available in the output of ZC model, and, there-648 fore, the thermocline depth itself was used here. All feature datasets 649 are normalized before training. 650

Training the GDNN consists of a number of ensemble members that are trained in parallel. Each of the members is trained for 100 iterations over 500 epochs with a batch size of 100. The training starts with a random selection of hyperparameters within 654



**FIG. 12.** The mean instance (a) of all the La Niña event instances in the test data (reference case). Saliency maps of CNN models (b) trained with the upwelling distorted data (variation of  $\delta_s$ ). In specific, cases  $\delta_s = 0.10, 0.25, 0.30, 0.45, 0.60$  are considered.

bounds defined by the user and is then optimized using the ADAM
algorithm (Kingma and Ba, 2014) with a user specified learning rate,
dropout, and Gaussian noise. The resulting ensemble members each
predict a mean and standard deviation of the target variable and
these predictions are then averaged over the ensemble for the final
prediction. Again, the lead time is 9 months in the result below.

661 We use two different measures for the performance of the GDNN: the RMSE and the Pearson correlation; also, the loss func-662 tion is shown (see Fig. 14). Different simulations give different 663 664 networks and give different performance values. The GDNN's, when 665 trained on distorted physics data, still perform consistently when varying  $\delta$  or  $\delta_s$ . However, a change in the ONI's amplitude in the 666 667 training data (such as for higher than reference  $\delta_s$ ) is poorly corrected for, leading to a large overestimation of the predicted variable 668 669 [e.g., see  $\delta_s = 0.40$  in Fig. 14(a)]. The model only tolerates a difference in amplitude between test and training dataset ONI if only a 670 671 small distortion of the variable is used (e.g.,  $\delta_s = 0.35$ ). The ability 672 to compensate for the period but not the amplitude is explained by the relatively simple architecture of the GDNN. Whereas the former 673 674 only requires a scalar addition to the input, the latter would require 675 some linear combination of (co)sines to be learned by the neural 676 network.

The attempt of comparing the capability of both CNN and GDNN in detecting El Niño events is made complicated by the intrinsic design of both models. Although both models are trained



**FIG. 13.** The AUC score for different values of  $\delta_s$  for the event El Niño as a function of (a) the bandpass frequency range and (b) the cut-off frequency, obtained by filtering the data by (a) bandpass Butterworth digital filter and (b) a low-pass Butterworth digital filter.

to solve the same problem, we have to take into account that the 680 CNN model is a binary classifier, while the GDNN is designed to 681 solve regression problems. In addition, the fact that both models 682 optimize the same loss function does not ensure a relation or a simi-683 larity about what the two models learn during the training phase can 684 be found. The two models could focus on capturing totally different 685 features of data, because the outputs of the two models represent two 686 different probabilities, i.e., the CNN estimates the probability of the 687 event itself, whereas the GDNN estimates the probability distribu-688 tion of the ONI index. However, the ENSO events are based on the 689 behavior of the ONI index and we can exploit this fact to make the 690 outputs of the GDNN more close to those of the CNN. After train-691 ing the GDNN, we can use the estimation on the Gaussian density 692



**FIG. 14.** Performance of the GDNN when trained on distorted ZC model data using several values of (a)  $\delta_s$  and (b)  $\delta$ .

to estimate the probability of El Niño events, i.e., the probability that
the absolute value of ONI index is greater than 0.5 °C. Thereafter,
we can use the AUC metric to compare the performance of the two
models.

As we can see in Fig. 15, the GDNN model appears to be less 697 698 accurate than the CNN model. The reference case data show a lower 699 AUC [compare to Fig. 3(a)] and we can observe a general reduction 700 of 0.1 AUC with respect to the results obtained with the CNN model. When feeding the GDNN model with ZC data with a different tun-701 702 ing of parameters  $\delta$ , we can observe that GDNN tends to be more 703 degraded at  $\delta < 1$ , then the CNN model [compare to Fig. 8(a)]; in 704 fact, the AUC can lose up to 0.21 with respect to the reference case. 705 Note that the same tuning of parameter  $\delta$  would reveal a plateau in 706 the AUC score whose values are much closer to that one attained 707 in the reference case. When considering the distortion of parame-708 ter  $\delta_s$  we can still appreciate a degradation at values lower than 0.3. 709 However, the decrease in the AUC scores appears milder ( $\sim 0.1$ ) 710 with respect to that shown for the CNN model. On the contrary, 711 as  $\delta_s > 0.3$ , there is a significant reduction in the AUC scores; with respect to the reference case, the AUC scores can now be reduced up 712 713 to 0.2.

### 714 IV. SUMMARY AND DISCUSSION

This work was strongly motivated to understand the high skill in ENSO prediction obtained with the CNN approach in



**FIG. 15.** AUC metric for the GDNN when considered as a classifier for both the wave distorted case (a) and the upwelling distorted case (b). On the *x* axis, the values of ZC parameters ( $\delta$ ,  $\delta$ <sub>s</sub>) and on the *y* axis the AUC score.

Ham et al. (2019), in particular, at long lead times. Although heat 717 maps were presented in Ham et al. (2019), their analysis does not 718 connect immediately to the detailed processes of ENSO dynamics, 719 720 which is also difficult because of the wide range of data they used. In this paper, we introduced distorted physics simulations with the 721 well-known Zebiak-Cane (ZC) model (Zebiak and Cane, 1987) to 722 determine how a CNN can perform on real data when trained on 723 data from "wrong" model simulations. 724

The behavior of the ZC model can be elegantly described by a 725 delay-differential equation (Suarez and Schopf, 1988; and Jin, 1997) 726

$$\frac{dT(t)}{dt} = aT(t) - bT(t-d) - cT^{3}(t)$$
(2)

for the eastern Pacific temperature T as a function of time t. Here, the constant a indicates the strength of the positive feedbacks, bthat of the delayed negative feedback (with a delay d due to equatorial wave dynamics), and c measures the strength of the nonlinear equilibration. 731

Chaos **32**, 000000 (2022); doi: 10.1063/5.0101668 Published under an exclusive license by AIP Publishing

Q3

By distorting the  $\delta$  parameter in the ZC model, we modify the 732 733 delay d in (2) and, hence, mostly the adjustment processes in the equatorial Pacific. When the equatorial wave speeds are distorted, there is an asymmetry in the skill of the CNN. For faster waves  $\delta < 1$ , 736 the performance remains good, whereas for  $\delta > 1$  (slower waves), it 737 deteriorates. For example, in case  $\delta = 1.2$ , the El Niño event appears 738 to be mainly constituted by slower oscillations, even though the 739 behavior of the large-scale thermocline depth and sea surface tem-740 perature is similar to the reference case. However, the loss of details 741 on shorter time scales leads the model to still reasonably solve the 742 classification task.

743 By distorting the parameter  $\delta_s$ , we basically modify the feedback 744 parameter a in (2) and, hence, the amplitude of the El Niño events. 745 However, also the stability properties of the background climate 746 state are changed as seen through the shift in the Hopf bifurcation 747 with  $\delta_s$  (van der Vaart *et al.*, 2000). For increasing  $\delta_s$  and constant  $\mu$  (as is done here), the background destabilizes as can also be seen 748 749 in Fig. 9. The case  $\delta_s = 0.1$  (reference case  $\delta_s = 0.3$ ) offers a clear 750 example about how the manipulation in the upwelling feedback can 751 degrade the AUC, i.e., the distortion of the patterns in the data leads 752 to a misplacement and misalignment and reduce the capability of 753 the network in capturing the right patterns at the right (temporal) 754 location. For other cases (e.g.,  $\delta_s = 0.25$ ,  $\delta_s = 0.45$ , and  $\delta_s = 0.6$ ), the 755 skill of the CNN predictions is reduced less, because the right com-756 bination of peaks and valleys in the time series are present. Indeed, 757 the absence of oscillating terms located at the frequency band 4-8 758 months does not allow the CNN to capture all the relevant patterns 759 but only a part of them.

The results indicate that the accuracy of the classification of 760 761 the El Niño and La Niño events for lead times of 9 months using a CNN approach is strongly related to the capability of the CNN 762 763 to capture the wave adjustment and feedback processes. The exact 764 combination of specific patterns like peaks and valleys occurring at 765 specific regions of the time domain of all features is essential to gen-766 erate skill in the CNN predictions. The distorted physics approach 767 can be very useful to look at how a CCN based prediction scheme 768 can represent additional processes. For example, it is well known 769 that connections between the Indian-Pacific (Izumo et al., 2010) and 770 Atlantic-Pacific (Ham et al., 2013) and extratropical-tropical con-771 nections (Zhao and Di Lorenzo, 2020) are important for the skill 772 of ENSO predictions. The latter interactions have been described as 773 ocean-atmosphere meridional modes and can influence ENSO and 774 tropical variability on decadal time scales from both hemispheres 775 independently (Amaya, 2019). Also, the effect of climate change on ENSO prediction skills, and how a CNN would capture this, 776 777 is an interesting future line of work. However, one cannot use the 778 Zebiak-Cane model for such studies and needs to do such distorted 779 physics simulations with more sophisticated global climate models.

#### 780 ACKNOWLEDGMENTS

781 The work by H.D. was sponsored by the Netherlands Science 782 Foundation (NWO) through Project No. OCENW.M20.277.

#### AUTHOR DECLARATIONS 783

#### **Conflict of Interest** 784

785 The authors have no conflicts to disclose.

#### Author Contributions

All authors contributed to the design of this study. Results were 787 mainly obtained by G.L. and I.G. The paper was jointly written with 788 contributions from all authors. 789

G. Lancia: Data curation (supporting); Formal analysis (support-790 791 ing); Methodology (lead); Visualization (equal); Writing - original draft (equal); Writing - review & editing (equal). I. J. Goede: Data 792 curation (lead); Formal analysis (equal); Investigation (equal); Visu-793 alization (equal); Writing - original draft (equal); Writing - review 794 & editing (equal). C. Spitoni: Formal analysis (equal); Supervision 795 (equal); Writing - original draft (equal); Writing - review & editing 796 (equal). H. Dijkstra: Formal analysis (lead); Methodology (equal); 797 Supervision (lead); Writing – original draft (equal); Writing – review 798 & editing (equal). 799

DATA	AVA	ILABII	.ITY

The data that support the findings of this study are openly available in github at https://github.com/glancia93/Physics-captured-bydata-based-methods-in-El-Nino-prediction\_PyCODE, Ref.

#### REFERENCES

- Adebayo, J., Gilmer, J., Muelly, M., Goodfellow, I., Hardt, M., and Kim, B., "Sanity checks for saliency maps," arXiv:1810.03292 (2018).
- Amaya, D. J., "The Pacific meridional mode and ENSO: A review," Curr. Clim. Change Rep. 5, 296-307 (2019).
- Arrieta, A. B., Díaz-Rodríguez, N., Del Ser, J., Bennetot, A., Tabik, S., Barbado, A., Garcia, S., Gil-Lopez, S., Molina, D., Benjamins, R., Chatila, R., and Herrera, F., "Explainable artificial intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI," Inf. Fusion 58, 82-115 (2020).
- Balmaseda, M. A., Davey, M. K., and Anderson, D. L. T., "Decadal and seasonal dependence of ENSO prediction skill," J. Clim. 8, 2705-2715 (1995).
- Barnston, A. G., Tippett, M. K., L'Heureux, M. L., Li, S., and DeWitt, D. G., "Skill of real-time seasonal ENSO model predictions during 2002-11: Is our capability increasing?," Bull. Am. Meteorol. Soc. 93, 631-651 (2012).
- Barnston, A. G., Tippett, M. K., Ranganathan, M., and L'Heureux, M. L., "Deterministic skill of ENSO predictions from the North American multimodel ensemble," Clim. Dyn. 53, 7215-7234 (2019).
- Butterworth, S., "On the theory of filter amplifiers," Wireless Eng. 7, 536-541 (1930).
- Chen, D. and Cane, M. A., "El Niño prediction and predictability," J. Comput. Phys. 227, 3625-3640 (2008).
- Diaz, H. F., Hoerling, M. P., and Eischeid, J. K., "ENSO variability, teleconnections and climate change," Int. J. Climatol. 21, 1845-1862 (2001).
- Dijkstra, H. A., Atmospheric and Oceanographic Sciences Library (Springer, 2005), Vol. 28, p. 480.
- Dijkstra, H. A. and Neelin, J., "Coupled ocean-atmosphere models and the tropical climatology. II: Why the cold tongue is in the east," J. Clim. 8, 1343-1359 (1995)
- Dijkstra, H. A., Petersik, P., Hernández-García, E., and López, C., "The application 834 of machine learning techniques to improve El Niño prediction skill," Front. 835 836 Phys. 7, 153 (2019).
- Duan, W., Liu, X., Zhu, K., and Mu, M., "Exploring the initial errors that cause a significant 'spring predictability barrier" for El Niño events," J. Geophys. Res. 114, C04022 (2009)
- Fedorov, A., Harper, S., Philander, S., Winter, B., and Wittenberg, A., "How 840 predictable is El Niño?," Bull. Am. Meteorol. Soc. 84, 911-919 (2003). 841

Chaos 32, 000000 (2022); doi: 10.1063/5.0101668 Published under an exclusive license by AIP Publishing 32.00000-14

804

800

801

802

803<sub>Q4</sub>

786

805 806

807 808 809

> 810 811 812

813<sub>Q5</sub> 814

817

818

819

820

821

822

823

824

825

826

827

828

829

830

831

832

833

837

838 839

907

908

909

910

911

912

913

914

915

916

917

918

919

920

921

922

923

924

925 926

927

928 929

930

931

932

933

934

935

936

937

938

939

940

941

942

943

944

945

946

947

948

949

950

951

952

953

954

955

956

957

959

960

- 842 Feng, Q. Y. and Dijkstra, H. A., "Climate network stability measures of El Niño 843 variability." Chaos 27, 035801 (2017).
- 844 Gill, A., "Some simple solutions for heat-induced tropical circulation," Q. J. R. 845 Meteor. Soc. 106, 447-462 (1980).
- 846 Goodfellow, I., Bengio, Y., and Courville, A., Deep Learning (MIT Press, 2016).
- 847 Ham, Y.-G., Kim, J.-H., and Luo, J.-J., "Deep learning for multi-year ENSO 848 forecasts," Nature 573, 568-572 (2019).
- Ham, Y.-G., Kug, J.-S., Park, J.-Y., and Jin, F.-F., "Sea surface temperature in the 849 850 north tropical Atlantic as a trigger for El Niño/southern oscillation events," 851 Nat. Geosci. 6, 112-116 (2013).
- 852 Hamming, R. W., Digital Filters (Courier Corporation, 1998), pp. 561-569.
- 853 Hou, M., Duan, W., and Zhi, X., "Season-dependent predictability barrier for two 854 types of El Niño revealed by an approach to data analysis for predictability," 855 Clim. Dyn. 53, 5561-5581 (2019).
- 856 Izumo, T., Vialard, J., Lengaigne, M., de Boyer Montegut, C., Behera, S. K., Luo, 857 J.-J., Cravatte, S., Masson, S., and Yamagata, T., "Influence of the state of the 858 Indian Ocean Dipole on the following year's El Niño," Nat. Geosci. 3, 168-172 859 (2010).
- 860 Jin, F.-F., "An equatorial recharge paradigm for ENSO. I: Conceptual model," J. 861 Atmos. Sci. 54, 811-829 (1997).
- 862 Jin, F.-F., "An equatorial recharge paradigm for ENSO. II: A stripped-down 863 coupled model," J. Atmos. Sci. 54, 830-8847 (1997).
- 864 Jin, F.-F., Neelin, J., and Ghil, M., "El Niño on the devil's staircase: Annual 865 subharmonic steps to chaos," Science 264, 70-72 (1994).
- 866 Kingma, D. P. and Ba, J., "Adam: A method for stochastic optimization," 867 arXiv:1412.6980[cs] (2014).
- 868 Kug, J.-S., Jin, F.-F., and An, S.-I., "Two types of El Niño events: Cold tongue El 869 Niño and warm pool El Niño," J. Clim. 22, 1499-1515 (2009).
- 870 Lakshminarayanan, B., Pritzel, A., and Blundell, C., "Simple and scalable pre-871 dictive uncertainty estimation using deep ensembles," in Advances in Neural 872 Information Processing Systems, edited by I. Guyon, U. V. Luxburg, S. Bengio, 873 H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (Curran Associates, 874 Inc., 2017), Vol. 30, pp. 6402-6413.
- 875 Latif, M., "Dynamics of interdecadal variability in coupled ocean-atmosphere 876 models," J. Clim. 11, 602-624 (1998).
- 877 Latif, M. and Barnett, T. P., "Causes of decadal climate variability over the North 878 Pacific and North America," Science 266, 634-637 (1994).
- 879 L'Heureux, M. L., Takahashi, K., Watkins, A. B., Barnston, A. G., Becker, E. 880 J., Di Liberto, T. E., Gamble, F., Gottschalck, J., Halpert, M. S., Huang, 881 B., Mosquera-Vásquez, K., and Wittenberg, A. T., "Observing and pre-882 dicting the 2015/16 El Niño," Bull. Am. Meteorol. Soc. 98, 1363-1382 883 (2017).
- 884 Lian, T., Chen, D., Tang, Y., and Wu, Q., "Effects of westerly wind bursts 885 on El Niño: A new perspective," Geophys. Res. Lett. 41, 3522-3527, https://doi.org/10.1002/2014GL059989 (2014). 886
- 887 McPhaden, M. J., "Tropical Pacific Ocean heat content variations and ENSO persistence barriers," Geophys. Res. Lett. 30, 2705-2709, https://doi.org/10.1029/ 888 889 2003GL016872 (2003).
- 890 McPhaden, M. J., Timmermann, A., Widlansky, M. J., Balmaseda, M. A., and Stockdale, T. N., "The curious case of the El Niño that never happened: A per-891 892 spective from 40 years of progress in climate research and forecasting," Bull. 893 Am. Meteorol. Soc. 96, 1647-1665 (2015).
- 894 Montavon, G., Binder, A., Lapuschkin, S., Samek, W., and Müller, K.-895 R., "Layer-wise relevance propagation: An overview," in Explainable 896 AI: Interpreting, Explaining and Visualizing Deep Learning (E, 2019), 897 pp. 193-209.
- 898 Mu, M., Sun, L., and Dijkstra, H. A., "The sensitivity and stability of the ocean's 899 thermohaline circulation to finite amplitude perturbations," arXiv:0702083v1 900 [arXiv:physics] (2007), pp. 1-40.
- 901 Mundhenk, T. N., Chen, B. Y., and Friedland, G., "Efficient saliency maps for 902 explainable AI," arXiv:1911.11293 (2019).

- Neelin, J., "The slow sea surface temperature mode and the fast-wave limit: Ana-903 904 lytic theory for tropical interannual oscillations and experiments in a hybrid coupled model," J. Atmos. Sci. 48, 584-606 (1991). 905 906
- Neelin, J., Battisti, D. S., Hirst, A. C., Jin, F.-F., Wakata, Y., Yamagata, T., and Zebiak, S. E., "ENSO theory," J. Geophys. Res. 103, 14261-14290, https://doi.org/10.1029/97JC03424 (1998).
- Newman, M. and Sardeshmukh, P. D., "Are we near the predictability limit of tropical Indo-Pacific sea surface temperatures?," Geophys. Res. Lett. 44, 8520-8529, https://doi.org/10.1002/2017GL074088 (2017).
- Petersik, P. J. and Dijkstra, H. A., "Probabilistic forecasting of El Niño using neural network models," Geophys. Res. Lett. 47, 1-8, https://doi.org/10.1029/2019 GL086423 (2020).
- Preisendorfer, R. W., Principal Component Analysis in Meteorology and Oceanography (Elsevier, Amsterdam, 1988).
- Saha, S., Moorthi, S., Wu, X., Wang, J., Nadiga, S., Tripp, P., Behringer, D., Hou, Y.-T., Chuang, H.-Y., Iredell, M., Ek, M., Meng, J., Yang, R., Mendez, M. P., Van Den Dool, H., Zhang, Q., Wang, W., Chen, M., and Becker, E., "The NCEP climate forecast system version 2," J. Clim. 27, 2185-2208 (2014).
- Selvaraju, R. R., Cogswell, M., Das, A., Vedantam, R., Parikh, D., and Batra, D., "Grad-cam: Visual explanations from deep networks via gradient-based localization," in Proceedings of the IEEE International Conference on Computer Vision ( 2017), pp. 618-626.
- Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R., "Dropout: A simple way to prevent neural networks from overfitting," J. Mach. Learn. Res. 15, 1929-1958 (2014).
- Suarez, M. and Schopf, P., "A delayed action oscillator for ENSO," J. Atmos. Sci. 45, 3283-3287 (1988).
- Tang, Y., Zhang, R.-H., Liu, T., Duan, W., Yang, D., Zheng, F., Ren, H., Lian, T., Gao, C., Chen, D., and Mu, M., "Progress in ENSO prediction and predictability study," Natl. Sci. Rev. 5, 826-839 (2018).

Tian, B. and Duan, W., "Comparison of the initial errors most likely to cause a spring predictability barrier for two types of El Niño events," Clim. Dyn. 47, 779-792 (2015).

- Timmermann, A., An, S.-I., Kug, J.-S., Jin, F.-F., Cai, W., Capotondi, A., Cobb, K., Lengaigne, M., McPhaden, M. J., Stuecker, M. F., Stein, K., Wittenberg, A. T., Yun, K.-S., Bayr, T., Chen, H.-C., Chikamoto, Y., Dewitte, B., Dommenget, D., Grothe, P., Guilyardi, E., Ham, Y.-G., Hayashi, M., Ineson, S., Kang, D., Kim, S., Kim, W., Lee, J.-Y., Li, T., Luo, J.-J., McGregor, S., Planton, Y., Power, S., Rashid, H., Ren, H.-L., Santoso, A., Takahashi, K., Todd, A., Wang, G., Wang, G., Xie, R., Yang, W.-H., Yeh, S.-W., Yoon, J., Zeller, E., and Zhang, X., "El Niño-Southern oscillation complexity," Nature 559, 535-545 (2018).
- Tziperman, E., Stone, L., Cane, M. A., and Jarosh, H., "El Niño chaos: Overlapping of resonances between the seasonal cycle and the Pacific ocean-atmosphere oscillator," Science 264, 72-74 (1994).
- van der Vaart, P. C. F., Dijkstra, H. A., and Jin, F. F., "The Pacific cold tongue and the ENSO mode: A unified theory within the Zebiak-Cane model," J. Atmos. Sci. 57, 967-988 (2000).
- Yan, J., Mu, L., Wang, L., Ranjan, R., and Zomaya, A. Y., "Temporal convolutional networks for the advance prediction of ENSO," Sci. Rep. 10, 1-15 (2020).
- Yu, Y., Mu, M., and Duan, W., "Does model parameter error cause a significant spring predictability barrier for El Niño events in the Zebiak-Cane model?," J. Clim. 25, 1263-1277 (2012).
- Zebiak, S. and Cane, M., "A model El Niño-southern oscillation," Mon. Weather Rev. 115, 2262-2278 (1987).
- Zhang, Z., Ren, B., and Zheng, J., "A unified complex index to characterize two types of ENSO simultaneously," Sci. Rep. 9, 8373 (2019). 958
- Zhao, Y. and Di Lorenzo, E., "The impacts of extra-tropical ENSO precursors on tropical Pacific decadal-scale variability," Sci. Rep. 10, 1-12 (2020).
- 961 Zhou, B., Khosla, A., Lapedriza, A., Oliva, A., and Torralba, A., "Learning deep 962 features for discriminative localization," in Proceedings of the IEEE Conference 963 on Computer Vision and Pattern Recognition (IEEE, 2016), pp. 2921-2929.

Chaos 32, 000000 (2022); doi: 10.1063/5.0101668 Published under an exclusive license by AIP Publishing