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2 3 4	Estimation of surface and deep flows from sparse SSH observations of geostrophic ocean turbulence using Deep Learning
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8	Key Points:
9 10	• A Deep Learning framework is developed to estimate mesoscale ocean currents from temporally-sparse SSH observations
11 12	• The Deep Learning framework outperforms linear and dynamical SSH interpola- tion techniques.
13 14	• A skillful state estimation of unobserved deep flows from SSH observations is achieved via supervised Deep Learning
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### 16 Abstract

Satellite altimeters provide global observations of sea surface height (SSH) and present 17 a unique dataset for advancing our theoretical understanding of upper ocean dynamics 18 and monitoring its variability. Considering that mesoscale SSH patterns of 50–300 km in 19 size can evolve on timescales comparable to or shorter than satellite return periods, it is 20 challenging to accurately reconstruct the continuous SSH evolution as currently available 21 altimetry observations are still spatially and temporally sparse. Here we explore the pos-22 sibility of SSH interpolation via a Deep Learning framework using synthetic observations 23 24 from a quasigeostrophic model of mesoscale ocean turbulence. We demonstrate that Convolutional Neural Networks with Residual Learning are superior in SSH reconstruction to 25 linear and recently developed dynamical interpolation techniques. In addition, neural net-26 works can provide a skillful state estimate of unobserved deep ocean currents at mesoscales. 27 This conspicuous result suggests that SSH patterns of eddies do contain substantial infor-28 mation about the underlying deep ocean currents that is necessary for SSH prediction. Our 29 framework is highly idealized and several crucial improvements such as transfer learning, 30 diversification of training data, and modification of the loss function would be necessary 31 to implement before its ultimate use with real satellite observations. Nonetheless, by pro-32 viding a proof of concept based on synthetic data, our results point to Deep Learning as 33 a viable alternative to existing interpolation and, more generally, state estimation methods 34 for satellite observations of eddying currents. 35

### <sup>36</sup> Plain Language Summary

Satellite observations of sea surface height (SSH) are widely used to derive surface 37 ocean currents on a global scale. However, due to gaps in SSH observations, it remains 38 challenging to retrieve the dynamics of rapidly evolving upper-ocean currents. To overcome 39 this limitation, we propose a Deep Learning framework that is based on pattern recognition 40 extracted from SSH observations. Using synthetic data generated from a simplified model 41 of ocean turbulence, we demonstrate that Deep Learning can accurately estimate both 42 surface and sub-surface ocean currents, significantly outperforming the most commonly 43 used techniques. By providing a proof of concept, our study highlights the strong potential 44 of Deep Learning for estimating ocean currents from satellite observations. 45

# 46 **1** Introduction

Satellite-derived global observations of sea surface height (SSH) have shed light on many 47 dynamical processes including large-scale circulation, propagation of waves, and the evolu-48 tion of the mesoscale eddy field (Chelton et al., 2011; Fu et al., 2010). Since the satellite era, 49 an increasing amount of evidence points towards mesoscale eddies being a key component 50 of the global ocean circulation and the Earth's climate as a whole due to their influence 51 on mean currents, heat and salt transport, atmosphere-ocean interactions, and biological 52 productivity (Ferrari & Wunsch, 2009; Klein et al., 2019). Nonetheless, understanding and 53 monitoring the oceanic kinetic energy spectrum and the associated spectral energy fluxes 54 (Scott & Arbic, 2007; Aluie et al., 2018), understanding tracer dispersion (Abernathey & 55 Marshall, 2013) or inferring subsurface flows (Klein et al., 2009) remain challenging because 56 these quantities depend on higher-order SSH derivatives that are resolution-sensitive. 57

To increase the density of SSH observations, several altimeters have been put in orbit 58 but their 10-20 days repeat orbits and relatively coarse along-track resolutions allow to view 59 the ocean dynamics only down to relatively large mesoscale eddies of O(100) km wavelengths 60 (Wunsch, 2010; Chelton & Schlax, 2003). The upcoming Surface Water Ocean Topography 61 (SWOT) altimeter mission (Fu & Ubelmann, 2014) promises to observe ocean mesoscale 62 eddies and submesoscale fronts ( $\leq 50$  km) at unprecedented spatial resolutions, potentially 63 resolving 15-30km wavelengths. However, with its complete repeat cycle of 21 days, the 64 temporal resolution of the altimeter is insufficient to continuously capture the evolution of 65 submesoscale eddies, although the mesoscale eddy field can be partially resolved in both 66 space and time if data from several altimeters are used. The mismatch between the high 67 spatial resolution and the moderate temporal resolution presents a challenge for reconstruct-68 ing time-continuous maps of SSH. The SSH interpolation can be especially challenging in 69 regions with energetic baroclinic turbulence where the evolution of small-scale SSH anoma-70 lies can be fast compared to the satellite return periods, e.g. in such major currents as the 71 Antarctic Circumpolar Current, Kuroshio Extension, and Gulf Stream. 72

The existing gridded SSH products, e.g. AVISO (Ducet et al., 2000), are spatially 73 and temporally interpolated from the along-track altimetry measurements and hence their 74 accuracy and effective resolution are constrained by the density of observations and deficien-75 cies of the interpolation technique. The temporal SSH interpolation could be conceptually 76 viewed as reconstructing the phase-space trajectory given only partial observations of the 77 two endpoints separated in time. A major complication arises due to the chaotic nature 78 of ocean turbulence in which phase-space trajectories can be so well-mixed that there is a 79 large number of plausible trajectories passing within some close vicinity of any given end-80 points. Thus, the task of temporal interpolation, i.e. finding the true trajectory, becomes 81 increasingly more difficult with an increasing time separation between observations. Most 82 commonly used interpolation techniques, such as objective mapping or polynomial inter-83 polation, do not attempt to make use of any potential dynamical constraints present in 84 the data and perform well only for autocorrelated data while failing for sparse data. It is 85 thus crucial to develop frameworks to efficiently extract information about the oceanic eddy 86 dynamics from the spatially and temporally sparse SSH observations. Below we discuss 87 how the nature of baroclinic ocean turbulence can provide dynamical limitations for SSH 88 interpolation and why Deep Learning might be a viable alternative to other interpolation 89 techniques. 90

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# 1.1 SSH interpolation and the associated dynamical limitations

Spatiotemporal interpolation or gridding of SSH data is inherently linked to ocean physics as the success of a given technique ultimately should rely on the pertinence of its assumed model (either dynamical or statistical) that captures the essence of eddy propagation in space and time. To illustrate this point, imagine a coherent eddy moving in a turbulent field and several altimeter tracks passing through it at different times and directions. If

there is an accurate model of eddy propagation, it would allow pinpointing the observations 97 taken over this specific eddy and combining this information to better constrain the two-98 dimensional eddy shape. Thus, to extract the information from various altimetry tracks to qq the fullest extent, it is necessary to have an accurate model of eddy evolution. However, due 100 to the stratified nature of geostrophic ocean turbulence, the unobserved deep ocean flows 101 can affect the surface dynamics, and hence the SSH observations on their own may not be 102 self-sufficient to infer its evolution. Given the lack of subsurface information at eddy scales, 103 constructing a closed system of equations for SSH evolution is challenging. 104

105 Another complication for SSH interpolation arises due to the chaotic nature of baroclinic turbulence that implies an increasingly high sensitivity to initial conditions as time 106 progresses. Alternatively, with increasing time-separation between any two observations, the 107 relation between them becomes more convoluted because the phase-space trajectories are 108 well-mixed. Thus, at sufficiently large separation times, one could effectively treat observa-109 tions as independent samples, and hence interpolating between these observations would not 110 be plausible. While the chaos itself makes the connections between subsequent observations 111 highly nonlinear, combined with the fact that satellites only provide approximate and par-112 tial observations of the ocean, the temporal SSH interpolation becomes under-constrained, 113 i.e. it might not have unique solutions as not enough information is given. 114

Existing methods for spatiotemporal SSH interpolation can be broadly split into two 115 distinct classes: methods that rely on a postulated dynamical model of SSH evolution and 116 purely data-driven methods. Both methods have their advantages and disadvantages. To 117 avoid prescribing a dynamical model, statistical models like objective interpolation (Davis, 118 1985; Le Traon et al., 1998; Ducet et al., 2000) rely on data only. Their premise is to in-119 corporate spatiotemporal correlations and measurement error into a statistical model and 120 provide the most likely estimate of the true continuous field under consideration. However, 121 this method does not rely on any dynamical model of the eddy propagation and hence can 122 lead to an unphysical behavior of the interpolated SSH field. Methods involving dynamical 123 ocean models are typically based on data assimilation, a procedure that minimizes the differ-124 ence between the observed and modeled fields by adjusting unknown variables like boundary 125 and initial conditions or external forcing (see e.g. reanalysis product by Carton & Giese, 126 2008). While resulting in SSH fields that are dynamically-constrained, this method suffers 127 from a drawback that it requires additional observations to constrain other essential model 128 variables like the subsurface flow and/or the density field. Also, data assimilation for com-129 plex ocean models at eddy-resolving scales is often under-determined and is computationally 130 demanding. 131

A recent study by Ubelmann et al. (2015) demonstrated that representing SSH prop-132 agation with a single equivalent barotropic mode in a quasigeostrophic model results in 133 significant improvements in the spatiotemporal interpolation of sparse SSH observations. In 134 particular, Ubelmann et al. (2015) considered a fundamental problem of reconstructing the 135 SSH distribution that occurred in between two observed SSH fields separated by about 20 136 days, a characteristic timescale required by a set of altimeters to reconstruct a spatial SSH 137 field. They found that integrating the earlier SSH observation forward in time (following 138 the assumed dynamics of an equivalent barotropic mode) and averaging it with the later 139 observed SSH anomalies that were integrated backward in time resulted in an improvement 140 compared to conventional linear interpolation methods. In follow-up work, Ubelmann et al. 141 (2016) generalized this temporal interpolation method to the spatiotemporal interpolation 142 of along-track SSH observations by essentially performing data-assimilation on the one-layer 143 QG model. The advantage of the dynamical interpolation method is that it relies on the 144 advection of potential vorticity – a non-linear process that is inherently present in ocean 145 dynamics and cannot be represented by linear or objective interpolation techniques. 146

A drawback of the dynamical interpolation is that it assumes that SSH evolves independently of deep ocean flows, considering the so-called equivalent barotropic mode dynamics (Berloff & Meacham, 1997). However, in many energetic regions of the ocean, e.g. in Gulf

Stream, Kuroshio or Antarctic Circumpolar Current, the currents are baroclinically unstable 150 and hence are necessarily composed of at least two dynamically interacting vertical modes, 151 the barotropic and baroclinic modes (see e.g. Chapter 6 in Vallis, 2017). To illustrate this 152 point, consider the conservation of quasigeostrophic potential vorticity  $q_1$  in the upper ocean 153 layer as a model of SSH evolution at mesoscales: 154

 $\frac{Dq_1}{Dt} = \underbrace{\frac{D}{Dt} [\nabla^2 \psi_1 - R_d^{-2} \psi_1) + \beta y]}_{\text{Depends on partially-observed } \psi_1} + \underbrace{R_d^{-2} \frac{D}{Dt} \psi_{b.t.}}_{\text{Depends on unobserved } \psi_2} \approx 0,$ (1)

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where 
$$\psi_{b.t.} = \frac{H_1\psi_1 + H_2\psi_2}{H_1 + H_2}$$
 and  $R_d^{-2} = \frac{f_0^2}{g'H_1} + \frac{f_0^2}{g'H_2}$ , (2)

 $\psi_1$  and  $\psi_2$  are the surface and deep ocean stream functions,  $\psi_{b.t.}$  is the barotropic streamfunction (depth-averaged transport),  $R_d$  is the Rossby baroclinic deformation radius,  $f_0$  and  $\beta$  are the Coriolis and beta-plane parameters, y is the meridional coordinate,  $H_1$  and  $H_2$ are the ocean layer depths, g' is the reduced gravity, and D/Dt is the material derivative accounting for advection by the surface flow (see Methods). Note that the surface streamfunction is directly proportional to SSH:  $\psi_1 = (q/f_0)SSH$ , where g is the acceleration due to gravity. On relatively short timescales, sources and dissipation of potential vorticity could be neglected and its approximate conservation provides a basic description of the eddy evolution. The terms in the equation 1 above have been grouped into those that only depend on the partially-observed  $\psi_1$  (or equivalently SSH) and terms that depend on the unobserved subsurface flow  $\psi_2$  (or on the barotropic flow  $\psi_{b.t.}$ ). By considering only the equivalent barotropic mode dynamics and taking  $\psi_1$  to be equal to the baroclinic mode, the dynamical interpolation method as described in Ubelmann et al. (2015, 2016) discards the term in the PV conservation equation that depends on the unobserved barotropic streamfunction, resulting in

$$\frac{D}{Dt} [\nabla^2 \psi_1 - R_d^{-2} \psi_1) + \beta y] = 0.$$
(3)

Since the discarded term is the only term that depends on the unknown streamfunction  $\psi_2$ . 157 it is possible to integrate the approximate PV-conservation equation forward and backward 158 in time given only  $\psi_1$  observations, as was done in Ubelmann et al. (2015). Even though 159 in many ocean regions both deep and surface geostrophic currents are dynamically active, 160 reconstructing SSH using the dynamical interpolation technique proved to be superior to lin-161 ear interpolation methods (Ubelmann et al. (2015)) because it relies, at least approximately, 162 on the fundamental PV-conservation constraint. Nonetheless, the dynamical interpolation 163 method can lead to significant errors (see Results), implying that the omitted term, while 164 being relatively small, can substantially impact SSH evolution on timescales comparable to 165 return periods of altimetry satellites. 166

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## 1.2 The rationale for Deep Learning approach.

A clear way of improving the dynamical interpolation algorithm would be to take into 168 account the contribution of the barotropic mode to SSH evolution. However, comprehen-169 sive measurements of deep ocean currents at eddy scales are missing, posing a significant 170 challenge of inferring them from only SSH observations. Without taking into consideration 171 the physical processes that have led to the generation of any given SSH snapshot, there is a 172 wide range of plausible ways in which  $\psi_1$  could be decomposed into baroclinic and barotropic 173 modes, each corresponding to the distinct configuration of PV anomalies in the deep and 174 surface layers. However, considering that PV anomalies are specifically due to baroclinic 175 instabilities obeying specific conservation laws (Eq. 1), the corresponding barotropic and 176 baroclinic modes are inherently entangled, providing at least partial constraints on how any 177 specific SSH pattern could be partitioned into modes. 178

Since the QG model exhibits a highly non-linear and chaotic behavior, an analytical 179 approach to disentangle the modes has not been found but the evidence that data-driven 180

approach might be relevant has been presented in the literature. In particular, the surface 181 and subsurface flows from mooring observations are significantly correlated such that a 182 single Empirical Orthogonal Function (EOF) can explain a significant amount of variance 183 of the overall vertical velocity profile (Wunsch, 1997; de La Lama et al., 2016). Furthermore, 184 machine learning techniques such as self-organizing maps (Chapman & Charantonis, 2017), 185 as well as convolutional neural networks (Bolton & Zanna, 2019), have been successfully used 186 to estimate the subsurface flows from SSH data. However, the unknown term  $D\psi_{bt}/Dt =$ 187  $(\partial_t + \mathbf{u}_1 \cdot \nabla) \psi_{bt}$  in Eq. 1 can only provide a substantial contribution to the PV budget if  $\psi_{bt}$ 188 has a substantial component that is decorrelated from  $\psi_1$  because  $\mathbf{u}_1 \cdot \nabla \psi_1 \equiv 0$ , and  $\partial_t \psi_{bt} \ll$ 189  $\partial_t \psi_1$  for surface-amplified flows. Thus the key for a more accurate SSH interpolation lies 190 in estimating the component of  $\psi_2$  that is decorrelated from  $\psi_1$  – a problem that is tightly 191 linked to estimating eddy heat fluxes in baroclinically unstable flows. Using residual neural 192 networks, George et al. (2019) demonstrated that  $\psi_1$  indeed contains substantial information 193 about the decorrelated part of the subsurface streamfunction  $\psi_2$ , allowing to estimate about 194 60% of the variance in eddy heat fluxes only from SSH snapshots. Given that machine 195 learning methods can extract information from SSH patterns to estimate the component of 196  $\psi_{bt}$  that is uncorrelated with  $\psi_1$  for estimation of the eddy heat fluxes, it is plausible that 197 they could be used for SSH interpolation as well. 198

While ocean turbulence is chaotic and appears to be random and unpredictable, it does 199 not prohibit characteristics that are particularly beneficial for deep learning: the emergence 200 of underlying repeating patterns, self-similarities, and self-organization. We thus hypoth-201 esize that deep learning techniques could outperform conventional interpolation methods 202 including linear and dynamical interpolation. In this manuscript we use synthetic model 203 observations to present a proof of concept for using deep learning to shortcut the formal 204 process of data assimilation and reconstruct not only the interpolated SSH field but also the 205 corresponding unobserved deep ocean currents, thus providing a complete state estimate of 206 the baroclinic ocean turbulence. 207

The manuscript is organized in the following way. In Section 2, we present a range of 208 deep neural network architectures, outline a set of training experiments, and describe the 209 synthetic model of ocean turbulence that we used to evaluate the efficacy of Deep Learning 210 in SSH interpolation and state estimation of both surface and deep ocean streamfunctions. 211 In Section 3, we present examples of SSH estimates using deep neural networks and compare 212 213 their skills to linear and dynamical interpolation techniques. In Section 4, we discuss the broader implications of our results, outline the deficiencies and advantages of our Deep 214 Learning methodology, and propose possible improvements to generalize our method for its 215 ultimate use with real satellite observations. 216

### 217 2 Methods

We implement a range of deep neural network architectures to address a basic question 218 of interpolating SSH fields in baroclinic ocean turbulence. To exclude potential limitations 219 of real-world data, our study is entirely based upon synthetic data that we generate using 220 the quasigeostrophic (QG) model of baroclinic ocean turbulence. We find the QG model 221 to be optimal for our goals as it is pertinent to many energetic regions in the ocean while 222 being relatively simple such that a large volume of data can be generated for training and 223 testing; furthermore, the model allows us to directly benchmark deep learning against the 224 dynamical interpolation technique that also utilizes QG dynamics. Below we describe our 225 neural network architectures, the QG model used for the generation of training and testing 226 datasets, and the details of the dynamical interpolation that we implemented for direct skill 227 comparisons with deep learning and linear interpolation. 228



Figure 1. The ResNet architecture of a deep convolutional neural network with residual learning that was used for SSH interpolation and state estimation. The input consists of two SSH snapshots separated by 20 day. A set of convolutional layers are then applied to create an abstract representation of the input patterns in a bottleneck fashion: when image sizes decrease by a factor of two, the number of filters increases by a factor of two. Each convolutional layer is followed by the batch normalization and the application of the nonlinear function (Leaky Rectified Linear Unit). Residual learning blocks are saving the information from one layer and adding its identity to the output several layers ahead (blue arrows). The output from the final convolutional layer is subject to a global average pooling and flattening into a vector that is densely connected to the output of the appropriate dimension to represent either a single or multiple fields.

## 2.1 Deep Learning framework: Residual Convolutional Neural Networks

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Artificial neural networks are based on the idea of approximating the 'output' by taking 230 the 'input' variable and performing a large number of matrix additions and multiplications, 231 applying non-linearity functions, and either condensing or expanding the variable dimension 232 as it passes from layer to layer. The resulting network contains a large number of free 233 parameters that are later adjusted to optimize a given loss function, commonly taken as a 234 measure of difference between the prediction and the truth. Because we are trying to extract 235 information from the eddy patterns expressed in SSH fields, the choice of convolutional 236 237 neural networks (CNNs) is rationalized. In passing the information from layer to layer, CNNs define a set of filters (kernel matrices with prescribed dimensions) and convolve images 238 to produce increasingly more abstract levels of information that are passed on to the next 239 layer. Here we implement the ResNet architecture – a Convolutional Neural Network with 240 Residual Learning blocks (He et al., 2016). The Residual Learning is a process by which 241 the information is not only transferred sequentially from one layer to another but is also 242 transferred by skipping several layers via the so-called skip connections (blue arrows in Fig. 243 1). The presence of skip connections can result in better performances for a wide range of 244 computer vision problems (Targ et al., 2016). An example of the open-source implementation 245 of the ResNet architecture in Keras following He et al. (2016) was provided by Michael Dietz 246 here https://gist.github.com/mjdietzx/0cb95922aac14d446a6530f87b3a04ce, and we 247 have adjusted this code for our specific problem of SSH interpolation and state estimation. 248

A brief description of the ResNet architecture as shown schematically in Figure 1 fol-249 lows. The input consists of two SSH snapshots represented by a (32,32,2) matrix. The very 250 first convolutional layer takes the input and applies a set of 32 convolutional filters of size 251 (5,5) with a stride of (1,1), followed by the batch normalization, the nonlinearity function 252 taken to be the Leaky Rectified Linear Unit (Leaky ReLU), and the maximum 2D pooling 253 of size (2,2) with a stride of (2,2). Next, a series of residual learning blocks follow, each 254 consisting of two convolutional layers that take the input with M channels and apply N255 filters, each followed by batch normalization and Leaky ReLu, and at the very end of the 256 residual block, its initial input matrix is added to its output (see Figure 1). The architec-257 ture has a total of 16 residual blocks containing 52 convolutional layers. The first series 258 of residual blocks consist of 3 blocks that transform the input from M = 32 to M = 64259 channels while reducing the matrix rows and columns by a factor of two using the (2,2) max 260 pooling. Next, a set of 4 blocks transform the input to 128 channels, a set of 6 blocks to 261 256, and a set of 3 blocks to 512 channels, and the matrix dimension becomes (2,2,512). 262 Then, a global two-dimensional average pooling is applied to have a vector of length 512, 263 which is in some experiments subjected to a dropout rate of 20%. The resulting vector is 264 then densely connected to a vector of size 1024, which is finally reshaped to represent the 265 output SSH snapshot of size (32,32). For our state estimation experiments with 4 separate 266 fields appearing as the output matrix, the ResNet architecture remains the same except for 267 the final dense layer being of length 4096 and reshaped to the appropriate output size of 268 (32, 32, 4).269

We have explored more complex ResNets (going up to 161 convolutional layers) but 270 also simpler CNN architectures without residual learning as well as shallow feed-forward 271 networks (see Table 1). A brief description of the neural network architectures follows. FC: 272 feed-forward neural network with 2 hidden layers (254 and 512 neurons correspondingly), 273 batch normalization, and leaky ReLU as an activation function after each hidden layer. 274 FC\_Large: same as FC but with 512 and 1024 neurons in the hidden layers. VGG: 275 convolutional neural network with 32 (4x4) filters in the first layer, 64 (3x3) in the second, 276 128 (3x3) in the third, 256 (2x2) in the forth, with batch normalization and leaky ReLU 277 used after each layer and the two-dimensional global average pooling before connecting 278 to the dense layer. VGG\_Large: same as VGG but using a four times larger number 279 of filters in each convolutional layer. VGG\_Deep: same as VGG but repeating each 280 convolutional layer 3 times before proceeding to the next one. ResNet\_Small, ResNet, 281

and ResNet\_Large are residual neural networks with architectures as depicted in Figure 1
but with a total of 31,52, and 161 convolutional layers correspondingly; \_Dropout denotes
the use of 20% dropout rate in the last layer. We have implemented the architectures
in Tensorflow/Keras and provided the Python scripts along with the training data in the
Zenodo data repository (Manucharyan, 2020).

#	Architecture	Parameters	Data Samples	$\Delta T$ (days)	Skill
1	$\mathbf{FC}$	$1.2 \times 10^6$	$2 \times 10^5$	20	0.53
2	FC_Large	$6.3 imes10^6$	$2 \times 10^5$	20	0.54
3	VGG	$0.5 \times 10^6$	$2 \times 10^5$	20	0.63
4	VGG_Large	$4.6  imes 10^6$	$2 \times 10^5$	20	0.64
5	VGG_Deep	$1.4  imes 10^6$	$2 \times 10^5$	20	0.61
6	ResNet_Small	$0.9  imes 10^6$	$2 \times 10^5$	20	0.69
$\overline{7}$	ResNet_Large	$7 \times 10^6$	$2 \times 10^5$	20	0.72
8	$ResNet\_Large\_Dropout$	$7 \times 10^6$	$2 \times 10^5$	20	0.72
9	$ResNet_Dropout$	$4.7  imes 10^6$	$2 \times 10^5$	20	0.73
10	ResNet	$4.7  imes 10^6$	$2 \times 10^5$	20	0.75
11	ResNet	$4.7\times 10^6$	$2 \times 10^5$	40	0.44
12	ResNet	$4.7  imes 10^6$	$2 \times 10^5$	60	0.18
13	ResNet	$4.7 \times 10^6$	$1 \times 10^5$	20	0.71
14	$\operatorname{ResNet}$	$4.7  imes 10^6$	$4 \times 10^4$	20	0.65
15	$\operatorname{ResNet}$	$4.7  imes 10^6$	$2 \times 10^4$	20	0.58
16	$\operatorname{ResNet}$	$4.7  imes 10^6$	$8 \times 10^3$	20	0.55
17	$\operatorname{ResNet}$	$4.7  imes 10^6$	$4 \times 10^3$	20	0.44
18	ResNet	$4.7  imes 10^6$	$1 \times 10^3$	20	0.39
19	ResNet	$4.7\times 10^6$	$5  imes 10^2$	20	0.33

Table 1. List of neural network training experiments demonstrating the achieved prediction skill for temporal interpolation of SSH snapshots. Experiments 1-10 explore various architectures, 11-12 explore the skill deterioration with increasing time separation between the input images, and 13-19 explore skill dependence on the number of training examples. The architecture names correspond to function names in the provided NetworkArchitectures.py script that encodes their graphs using TensorFlow/Keras. The parameters column represents the number of trainable neural network parameters for corresponding architectures. The Data Samples column denotes the number of input-output examples that were used in neural network training. The  $\Delta T$  column denotes the time separation between the two input snapshots of SSH, and the skill column denotes the maximum achieved skill on validation data.

As a performance metric we define the model skill that is proportional to the loss function and normalized by the standard deviation of the SSH signal in the following way:

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$$Skill = 1 - \left(\frac{\overline{|SSH_{predicted} - SSH_{true}|^2}}{\overline{|SSH_{true}|^2}}\right)^{\frac{1}{2}}.$$
(4)

For reference, the maximum skill=1 is achieved when the predicted and true images are identical; the skill=0 corresponds to a prediction that makes the same error as assuming a spatially homogeneous SSH field, and negative skill implies an even worst fit. This definition of skill is more conservative than the correlation coefficient or the R-squared value; for example,  $\psi_2$  is correlated to  $\psi_1$  with an average correlation coefficient of 0.74 and the linear regression model has the R-squared of about 0.55 but the skill is only 0.33 if defined as in equation 4 above. It is thus important to compare the results from different publications using consistent metrics. Here we use the skill metric that is based on the RMS-error normalized by the standard deviation (Eq. 4) and, for consistency, we use the Mean Square Error (L2 norm) as the loss function for a neural network to minimize during training.

Coefficients of filter matrices, along with all other weights and biases involved in the neu-300 ral network architecture are then iteratively optimized using the Adam optimizer (Kingma 301 & Ba, 2014) to minimize the loss function that is the root-mean-square difference between 302 the predicted and true SSH images (or equivalently to maximize the skill). The parameter 303 optimization procedure requires evaluating neural network predictions for a large volume of 304 training data and hence the final optimized state of a particular neural network depends 305 only on the training data itself. To ensure that no overfitting have occurred, the neural net-306 work skill is evaluated for a group of three independent datasets: training, validation, and 307 testing. The training data are used only for the training purposes, the validation data are 308 used to evaluate the skill of the neural network and to identify a stoppage criterion for the 309 training, while the testing data are used at the very last step to define the skill of a trained 310 neural network. All three datasets are generated from different numerical simulations to 311 ensure that overfitting didn't occur. 312



2.2 Synthetic training data: quasigeostrophic model

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Figure 2. An example of the eddy field evolution over 20 days as generated by the QG model of a baroclinically unstable current. Top panels show surface streamfunction  $\psi_1$  (or SSH) and bottom panels show the corresponding deep ocean streamfunction,  $\psi_2$ , both being normalized by their respective standard deviations; the domain size is 1000x1000 km and rows correspond to streamfunction snapshots taken five days apart. Note that the eddy field dramatically changes over 20 days (SSH decorrelation time scale is about 10–20 days), implying that conventional linear or optimal interpolation methods would lead to significant errors if available observations are separated by more than the decorrelation timescale.

In the absence of high-quality and/or large volumes of data, neural networks are likely to overfit the training data and have poor skills when evaluated on the test data. To avoid these issues we choose to train neural networks on synthetic data generated using an idealized model of ocean turbulence – the two-layer quasigeostrophic (QG) model (Phillips, 1951; Vallis, 2017). The QG model is pertinent to baroclinically unstable flow and contains

the propagation dynamics of large-scale ocean eddies, including advection by the mean 319 flow, the beta drift, and the eddy interactions with the mean flow. Our choice of using the 320 two-layer model is rationalized because i) ocean currents are predominantly composed of 321 the barotropic and the first baroclinic mode (Wunsch, 1997; Smith & Vallis, 2001) and ii) 322 it is the minimal model demonstrating the difficulty of predicting SSH evolution without 323 direct observations of subsurface flows because both layers are necessarily dynamically active 324 during baroclinic instabilities, and iii) the dynamical interpolation method also relies on QG 325 dynamics, allowing to make a straight-forward performance comparison. 326

The quasigeostrophic model relies on the conservation of potential vorticity and simulates the mesoscale turbulence driven by baroclinic instabilities associated with the vertical shear of the mean flow, requiring a minimum of two vertically stacked shallow layers. The conservation laws for the top and bottom layer potential vorticities,  $q_{1,2}$ , are written in the following way:

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$$\frac{Dq_1}{Dt} = \frac{D}{Dt} [\nabla^2 \psi_1 - \frac{f_0^2}{g' H_1} (\psi_1 - \psi_2) + \beta y] = 0$$
(5)

$$\frac{Dq_2}{Dt} = \frac{D}{Dt} [\nabla^2 \psi_2 - \frac{f_0^2}{g' H_2} (\psi_2 - \psi_1) + \beta y] = -r_{Ek} \nabla^2 \psi_2, \tag{6}$$

where  $\psi_{1,2}$  is the top and bottom layer streamfunctions,  $f_0$  is the Coriolis parameter and 334  $\beta$  is its derivative in the meridional y-direction, g' is the reduced gravity,  $D/Dt = \partial/\partial t + \partial t$ 335  $\mathbf{u}\nabla$  is the material derivative using corresponding layer' geostrophic velocity u, and  $r_{Ek}$ 336 is the bottom drag coefficient. The relative importance of the discarded term in the PV-337 conservation budget in Eq. 1,  $D\psi_{bt}/Dt$ , could be estimated by comparing its magnitude to 338  $D\psi_1/Dt$ , where both material derivatives use the velocity in the top layer. The ratio of these 339 terms would scale roughly as the ratio of the characteristic amplitudes of the barotropic and 340 surface streamfunctions, which we find from numerical simulations to scale as the ratio of 341 layer depths in QG simulations of the baroclinic instabilities, i.e.  $[\bar{\psi}_{b.t.}^2/\bar{\psi}_1^2]^{\frac{1}{2}} \sim O(H_1/H_2)$ . 342 Since in most ocean regions the pycnocline is relatively shallow compared to the full depth 343 of the ocean, the flows are surface-amplified and the discarded term is relatively small but 344 non-negligible and can substantially impact the SSH evolution leading to significant errors 345 of the dynamical interpolation (see Results). 346

The QG model has been configured to represent baroclinically unstable currents such 347 as the Gulf Stream, Kuroshio, or Antarctic Circumpolar Current. Model parameters are 348 as follows: the Rossby deformation radius is 40 km, the ratio of mean layer depths is 0.2, 349 there is a steady uniform mean vertical shear of 0.2 m/s, beta plain parameter corresponds 350 to a latitude of 40 degrees, linear Ekman friction was prescribed in the bottom layer for 351 dissipation, and high-wavenumber motions are being filtered in Fourier space for all variables 352 (more details could be found in Flierl (1978); Arbic et al. (2012)). The model domain is 353 1000 km by 1000 km and periodic boundary conditions are used. We have explored various 354 resolutions and find that it is sufficient to use a relatively coarse grid of 32x32 to simulate 355 baroclinic instabilities and the chaotic evolution of relatively large mesoscale eddies. The 356 QG model is integrated forward in time managing an ensemble of noisy initial conditions 357 to produce a large volume of data: about 200,000 SSH snapshots separated by 10 days 358 (Figure 2). Over a timescale of 20 days, the correlation between SSH fields drops to about 359 0.4 and it is hard to identify any persisting eddies because their shapes and intensities have 360 dramatically changed due to interactions with other eddies (Figure 2). We ensure that the 361 data for training, validation, and testing come from distinct simulations to accurately access 362 the generalization skill of the neural network. 363

To evaluate the efficacy of neural networks, we consider the tasks of i) temporal interpolation where the input consists of two SSH snapshots separated by 20 days, ii) spatiotemporal interpolation with the same input as for the temporal interpolation but with SSH images having missing data, and iii) the state estimation of unobserved deep ocean flows from SSH snapshots. For the temporal separation of SSH images, we choose 20 days because it is of

the order of the return periods for existing altimeters and to be consistent with Ubelmann 369 et al. (2015), and we explore how the skill varies with increasing this timescale to 40 and 370 60 days (Table 1). For the spatiotemporal interpolation, we choose the area of missing data 371 to roughly correspond to that of the SWOT observations over its return period. For a 1000 372 km domain, SWOT would have about four crossings (each having a swath of 120 km) with 373 one inclination angle and another four with an opposite angle (see e.g. Figure 1 in Gaultier 374 et al. (2016)). While SWOT would have missing-data areas in the shape of a rhombus, here 375 for simplicity we have prescribed square shapes as there is no reason to assume this would 376 lose generality. 377

#### **2.3 Dynamical Interpolation**

We reproduce the dynamical interpolation methodology as outlined in Ubelmann et al. 379 (2015) and evaluate its skill distribution. The method consists of initializing the surface 380 streamfunction  $\psi_1 = (g/f_0)SSH$  and integrating a single-layer quasi-geostrophic equation, 381 i.e. Eq. 3. The domain size, boundary conditions, stratification parameters, and all other 382 parameters of the single-layer model are consistent with those of the two-layer model that 383 was used to generate the validation data. The model integration is performed for 10 days 384 forward in time starting from the SSH snapshot on day 0 and also backward in time starting 385 from the SSH snapshot on day 20. The backward in time integration is performed by 386 reversing the direction of the velocity field and changing the time variable to be negative. 387 The estimate of the SSH field on day 10 is then taken to be the arithmetic mean between 388 the SSH fields resulting from the forward and the backward integration. The skill of the 389 dynamical interpolation is evaluated on the testing data from the two-layer QG model and 390 used for comparison with linear and deep learning interpolation. 391

### 392 **3 Results**

407

We have explored various neural network architectures for the task of temporal SSH 393 interpolation, ranging from single hidden layer networks (FC) to convolutional networks 394 (VGG), to a more complex residual neural networks (ResNet) – all achieving skills com-395 parable to or higher than the linear and dynamical interpolation methods (Table 1). Sub-396 stantially decreasing neural network complexity leads to an only slight decrease in the skill 397 (e.g. compare experiment pairs [1, 2] or [6, 10] in Table 1), while substantially increasing the 398 complexity does not significantly improve the skill (e.g. compare experiment pairs [3,4] or 300 [7,10] in Table 1). The highest skill of 0.75 is achieved by the ResNet architecture (Fig. 1) with a total of 52 convolutional layers and about five million adjustable parameters, taking 401 about 1 hour to train on a Tesla T4 GPU on 200K data samples. We thus find the ResNet 402 architecture to be optimal for our tasks and we use it throughout the paper to present our 403 deep learning results, although we note that other superior architectures may exist. Below 404 we use ResNet to demonstrate the deep learning skill in spatiotemporal SSH interpolation 405 and state estimation. 406

### 3.1 Spatiotemporal SSH interpolation

Upon training separate ResNets to perform temporal and spatiotemporal interpolation 408 of SSH data, a significant performance skill is achieved with networks generating realistic 409 SSH images with small errors (see Figure 4). The average prediction skill for both simu-410 lations plateaus at about 0.75 and it isn't significantly smaller when evaluated on the test 411 dataset (Figure 3a). A few illustrative examples of eddy field evolution are shown in Fig-412 ure 4a, demonstrating the non-trivial SSH evolution that occurs in a chaotic QG model of 413 baroclinically unstable flow. In the top-raw example of Figure 4a, the strong positive SSH 414 anomaly in the center of the domain almost completely disappears after 20 days, yet the 415 neural network is still capable to reconstruct the SSH state at day 10. For such examples 416 when the eddy field changes dramatically with time, linear or objective interpolation tech-417



Figure 3. Performance comparison of the deep learning neural network (ResNet) with linear and dynamical interpolation techniques. (a) The evolution of the ResNet model validation and training skill during its training on temporal and spatiotemporal SSH interpolation (b) The dependence of the ResNet skill on the number of data samples used in training for the temporal SSH interpolation. (c) Comparison of skill distributions of the linear interpolation (LI), dynamical interpolation (DI), and the deep learning method evaluated on the testing dataset.



Figure 4. Examples of temporal (a) and spatiotemporal (b) interpolation of SSH data using the Deep Learning framework. Each row represents a randomly chosen interpolation example from the testing dataset. All panels share the same color bar and display streamfunction magnitudes normalized by the standard deviation of the entire dataset. The first and third column show panels with input SSH fields  $\psi_1(t)$  and  $\psi_1(t+20d)$ , second column shows the interpolated field  $\psi_1(t+10d)$ , and the fourth column shows the interpolation error. White regions in the case of spatiotemporal interpolation denote areas of obstructed input data.

niques perform poorly as they do not rely on any dynamical model of SSH evolution and 418 only make use of autocorrelation as a statistical model. Evaluated on a large number of 419 testing data (10K samples), the deep learning model outperforms the linear and dynamical 420 interpolation techniques, having not only a better average skill but also much more infre-421 quent occurrence of low-skill interpolations, i.e. much narrower skill-distribution tail in the 422 direction of small skills (Figure 3c). Noticeably, the linear interpolation skills can be so low 423 as to approach zero and even negative values, i.e. its prediction is no better than assuming 424 that SSH = 0 everywhere in the domain. The dynamical interpolation is much better than 425

the linear interpolation but still has a significant probability of poor interpolations in the skill range of about 0.4-0.6.

While the deep learning technique is superior to other methods, it is important to note 428 that it still does not provide a perfect reconstruction and has a limit in skill bounded by 429 about 0.85 (Fig. 3c). The dynamical evolution of the ocean flow considered in our study 430 is inherently chaotic, i.e. the phase-space trajectories become well-mixed to the extent 431 that the sensitivity to initial conditions increases exponentially with time. Thus, if SSH 432 snapshots of a turbulent eddy field are separated by sufficiently large time (greater than 433 the characteristic Lyapunov exponent timescale), there should be no physical or statistical relationship between these snapshots and hence no interpolation technique could achieve a 435 skill significantly above zero. Indeed, given the same neural network architecture and the 436 same volume of training data, the interpolation skill deteriorates dramatically from 0.75 to 437 0.44 and 0.18 as the time separation between the input SSH snapshots increases from 20 to 438 40 and 60 days correspondingly (Table 1). 439

The sensitivity to the number of data samples used in training demonstrates that for 440 the ResNet architecture, about 20-30K data samples are needed to achieve a skill compa-441 rable to the dynamical interpolation skill, and using a larger number of training samples 442 leads to a significant skill improvement (Figure 3b). However, the skill continues to increase 443 slowly with the number of samples (Figure 3b), with the best power-law fit for the case of 444 20-day SSH separation being skill ~  $N^{0.09}$ , where N is the number of training samples. 445 Extrapolating the power-law would imply that achieving the perfect skill = 1 would re-446 quire  $O(10^7)$  training samples – a number beyond what the author's computing capabilities, 447 though not impossible to reach on modern supercomputers. Nonetheless, estimating the 448 necessary number of samples is only a hypothetical consideration as it is not clear if the 449 power-law would remain the same with the increasing volume of data. In addition, it is not 450 possible to exclude the existence of superior neural network architectures that could lead to 451 faster convergence. 452

#### 453

#### 3.2 State estimation of the unobserved deep ocean flows at mesoscales

Here we assess the efficacy of the Deep Learning framework in addressing the state 454 estimation problem, i.e. estimating all dynamical variables in the ocean turbulence model, 455 which in our case of a two-layer QG model implies estimating both the surface stream 456 function  $\psi_1$  (or equivalently SSH) and the deep ocean streamfunction  $\psi_2$ . Conventionally, 457 for state estimation, one needs to postulate the dynamical model and only then implement 458 the techniques e.g. variational data assimilation or the ensemble Kalman filter techniques 459 to estimate the unknown variables and parameters in the model at all times and everywhere 460 within the model domain. However, we demonstrate here that the deep learning framework 461 can provide an alternative to conventional data assimilation methods. The neural network 462 is capable of skillful reconstruction of  $\psi_2$  based on two SSH snapshots separated by 20 463 days, with an average skill of 0.7 for day 0 and a skill of 0.8 for day 20 (Figure 5). While 464 the neural network provides skillful predictions for all state variables with skills ranging 465 from 0.65 to 0.85, the best prediction skill is achieved for the deep flow at day 20 while 466 the worst prediction is for deep flow at day 0 (compare orange and red curves in Fig5c). This temporal asymmetry is expected in chaotic and dissipative quasigeostrophic dynamics, 468 making it more difficult to estimate the past state by observing the future as opposed to 469 estimating the future by observing the past. Thus, the two SSH snapshots must indeed be 470 ordered in time as the PV-evolution equations allow time reversal only for sufficiently small 471 time intervals at which the dissipation effects can be neglected. 472

It is important to note that only the component of  $\psi_2$  that is uncorrelated with  $\psi_1$  can affect the SSH evolution because the tendency due to the advection of the surface streamfunction by the surface flow is identically zero (see Eq. 5). However,  $\psi_2$  is highly correlated with  $\psi_1$ , with an average correlation coefficient is about 0.84, which is why reconstructing



Figure 5. Examples of state estimation using Deep Learning neural network (a) and its statistical skill distribution for surface and subsurface variables at different times (b). As in the case of SSH interpolation, the neural network receives as input two SSH snapshots separated by 20 days,  $\psi_1(t)$  and  $\psi_1(t + 20d)$  (top row, first and third columns), but reconstructs not only the surface streamfunction at the intermediate time,  $\psi_1(t + 10d)$  (top row, second column), but also the subsurface flow at all three times: t, t + 10d, and t + 20d. Note that  $\psi_1$  and  $\psi_2$  are linearly correlated with a correlation coefficient of 0.8, which is why the bottom rows in panel (a) show  $\tilde{\psi}_2$ , the component of the reconstructed deep flow that is not linearly correlated with the surface flow. The errors for reconstructing the day 10 surface and deep streamfunctions are shown in the last column. The probability density function of the neural network skill distribution is plotted in panel (b) for all predicted variables.

its full amplitude is a relatively trivial exercise. To evaluate the network ability to predict 477 the decorrelated component, we define it as  $\psi_2 = \psi_2 - A\psi_1$ , where the constant A is the 478 average linear regression coefficient between  $\psi_1$  and  $\psi_2$ . Indeed, using two SSH snapshots as 479 the input, the neural network does provide a skillful estimate of  $\psi_2$  with a relatively small 480 error (Fig5a). However, further exploring the limits of neural networks, we identify that 481 they are capable of reconstructing an instantaneous relation between the SSH field and deep 482 ocean streamfunction. We train the ResNet model using a single SSH snapshot as the input 483 and the decorrelated component  $\psi_2$  of the corresponding deep ocean streamfunction as the 484 output to achieve a prediction skill of 0.56, while a skill of 0.7 is achieved if using  $\psi_2$  as the 485 output. 486

### $_{487}$ 4 Discussion

Our study explored the efficacy of deep learning in reconstructing the unobserved state 488 variables of the chaotic ocean turbulence. The motivation for addressing the specific problem 489 of SSH interpolation came from the present-day use of relatively rudimentary techniques of 490 reconstructing continuous fields from sparse satellite data. Using synthetic data from an 491 idealized model of baroclinic ocean turbulence, we presented the proof of concept for using 492 deep neural networks as an efficient technique to extract non-trivial information from sparse 493 SSH observations. Specifically, we demonstrated that residual convolutional neural networks 494 can reconstruct SSH snapshots at the intermediate time between the 20 days separated 495 observations with an average skill of 0.75, significantly outperforming the commonly used 496 linear interpolation (skill=0.35) and dynamical interpolation (skill=0.6) techniques. We 497 also demonstrated that the deep learning technique is flexible enough to address a more 498 general problem of state estimation that includes reconstruction of the unobserved deep 499 ocean streamfunction using only SSH snapshots. Nonetheless, there is an inherent lack of 500 information in SSH-only observations that prevents any interpolation or state estimation 501 methodology from achieving a perfect skill. After all, if SSH snapshots are separated by 502 a sufficiently long time, there should not be any relation between them due to the chaotic 503 nature of baroclinic ocean turbulence. Indeed, the ResNet could only achieve a maximum 504 skill of about 0.85 for interpolation between SSH snapshots separated by 20 days, and the 505 skill dramatically decreased to about 0.2 for the snapshots separated by 60 days. The lack 506 of the perfect interpolation skill suggests the existence of a dynamical barrier associated 507 with the inherent lack of information in SSH data, although it is not possible to deduce 508 this with certainty due to potential deficiencies of the neural network architecture and the 509 limited volume of training data. 510

While it is challenging to interpret the SSH interpolation algorithm that was ultimately 511 learned by the deep neural network, its superiority over other methods could be associated 512 with its ability to estimate the unobserved deep currents because they directly affect the 513 SSH evolution (Eq. 5). Taking only a surface streamfunction snapshot as the input, we 514 demonstrated that the ResNet can estimate the underlying deep ocean streamfunction with 515 an average skill of 0.7, which is high enough for a skillful estimate of the component of the 516 deep streamfunction that is not linearly correlated with the surface streamfunction. Apart 517 from deep learning, no other methods have been reported in the literature that can skillfully 518 estimate the uncorrelated component of the deep ocean currents at mesoscales. The success 519 of those neural network architectures that rely specifically on 2D convolutions for pattern 520 extraction implies that it may be the eddy shapes that contain the information necessary 521 to infer deep ocean currents. 522

A possible physical interpretation in terms of the eddy shapes could be drawn from considering the ocean dynamics in terms of the barotropic and baroclinic modes that are nonlinearly coupled and continuously exchange energy (Larichev & Held, 1995). The surface streamfunction (or SSH) is simply the weighted sum of the barotropic and baroclinic modes while the lower layer streamfunction is their difference. The key question here is: are instantaneous observations of only surface streamfunction sufficient enough to reconstruct

the corresponding barotropic and baroclinic modes? This presents an under-constrained 529 problem as there are two unknown modes while there is only one equation connecting their 530 sum to the SSH field and there are no analytical laws that could be inferred from the QG 531 dynamics to provide any additional constraints on the instantaneous relationship between 532 the modes. Nonetheless, the distinct dynamical evolution of each mode can lead to dif-533 ferences in their characteristic spatial patterns that could be discerned by deep learning 534 algorithms. The baroclinic mode experiences a direct energy cascade and its spatial struc-535 tures should appear more elliptical or elongated because it is stirred by the barotropic flow, 536 especially at scales of the order of or smaller than the Rossby deformation radius. On the 537 contrary, the barotropic mode experiences an inverse kinetic energy cascade manifested in 538 eddy merging and a tendency towards axisymmetrization (Melander et al., 1987). While 539 the two modes continuously interact by exchanging energy, the barotropic mode ends up 540 strongly dominating the baroclinic mode at large scales and their amplitudes become com-541 parable at scales of the order of the Rossby deformation radius (see Figure 4a in Larichev & 542 Held, 1995). This implies that the barotropic mode should dominate large-scale relatively 543 axisymmetric eddy patterns, the baroclinic mode dominates smaller-scale relatively more el-544 liptical patterns, while both modes are present at the deformation scale. Thus, our tentative 545 rationalization of the deep learning success is that by using convolutional filters, the neural 546 networks are effectively extracting SSH patterns at different length scales and classifying 547 them into barotropic and baroclinic modes. After estimating the mode amplitudes based on 548 individual SSH snapshots and learning from many synthetic examples of SSH evolution in 549 time, the neural networks are then capable to effectively integrate the QG equations forward 550 or backward in time for a skillful temporal interpolation between the two SSH snapshots. 551 While the complexity of deep learning algorithms makes it impossible to interpret them, 552 our hypothetical two-step process of the mode decomposition followed by the forward and 553 backward integration provides a plausible dynamical rationalization for the superiority of 554 deep learning over methods that ignore the influence of deep ocean flows on SSH evolution. 555

We chose to use the quasigeostrophic simulations of baroclinic turbulence as the syn-556 thetic training dataset because it presents a hard test for the temporal SSH interpolation due 557 to its chaotic nature and an a priori unknown impact of the dynamically active bottom layer 558 on SSH evolution. However, for the case of submesoscale turbulence (length scales smaller 559 than about 100 km), the question remains open as to how SWOT's 2D high-resolution 560 swath measurements could be used to enhance the resolution of SSH data. While we ex-561 pect the deep learning framework to perform well in reconstructing both large and small 562 mesoscale eddies, its limitations still need to be understood when considering mesoscale 563 and submesoscale turbulence as a continuum. It is thus necessary to develop more general 564 training datasets that are representative of the SSH dynamics for any given region or pro-565 cess of interest. Including satellite observations from Synthetic Aperture Radars or of sea 566 surface temperatures in addition to the SSH observations could provide additional information for improved reconstruction of SSH. The training datasets could be assembled ranging 568 from more realistic submesoscale-resolving general circulation models to simplified stochas-569 tic models in various parameter regimes (Samelson et al., 2019). While diversifying the 570 training datasets should increase the versatility of neural network interpolation methods, 571 the crucial constraint of their performance would likely come from the chaotic evolution of 572 submesoscale eddies that occurs on substantially shorter timescales compared to mesoscale 573 eddies. 574

While we have demonstrated the efficacy of supervised deep learning using synthetic 575 data, its practical utility in interpolating real-world SSH observations remains to be tested. 576 The drawback of deep learning is that it requires a large volume of training data, although 577 there are continuously improving methods aimed at addressing this practical issue, e.g. 578 transfer learning (Pan & Yang, 2009), data augmentation (Perez & Wang, 2017), one-shot 579 learning (Fei-Fei et al., 2006). A way towards ultimately developing the gridded SSH product 580 using deep learning could be through training networks on a wide range of idealized and 581 realistic models and then fine-tuning a much smaller number of neural network parameters 582

using existing satellite data. However, since the true two-dimensional SSH state is not known 583 at any particular time, the fine-tuning of a neural network cannot be achieved by defining a 584 simple loss function as was done with synthetic data. Thus, the neural network ultimately 585 would need to use a loss function that is based purely on observations, without invoking a dynamical model to provide a true state. This issue could be addressed for example using 587 reinforcement learning, where two-dimensional SSH fields generated by the neural network 588 would be rewarded or penalized based on the accuracy of their projection on the observed 589 altimetry tracks that were left out from the input set of tracks. Developing deep learning 590 SSH interpolation techniques that would steer away from solely relying on dynamical models 591 to provide training data is a necessary next step towards practical implementation with real 592 satellite observations. Nonetheless, our work presents an important proof of concept that 593 SSH observations do contain dynamically-relevant information about subsurface flows, and 594 hence with deep learning it should be possible to build a skillful model of SSH evolution 595 and as a consequence improve the existing SSH estimates. 596

Finally, we note another potentially important application of deep learning for state 597 estimation at eddy-resolving scales. Since mesoscale-resolving data assimilation methods 598 require large computations, providing an accurate initial guess would substantially reduce 599 the number of iterations necessary for optimization. Thus, it might be possible to acceler-600 ate data assimilation methods by providing a deep learning estimate as a first guess that 601 is already close to reality. Note that data assimilation and neural networks are similar 602 approaches in that they both use iterative procedures to find the optimal set of unknown 603 parameters to minimize the error between the predicted and true fields. The critical dif-604 ference is that data assimilation methods are based on a concrete physical model or its 605 linearization, and hence the predicted fields conform to the desired physical constraints but 606 the reconstruction skill relies on the accuracy of the model. Contrarily, the deep learning 607 approach does not rely on a physical model as it is optimizing a complex non-linear mapping 608 function that is general enough to map the input to the output. Hence, the deep learning 609 predictions do not have to obey any dynamical constraints unless those have been explicitly 610 incorporated in the loss function. Thus, we see the synergy between deep learning and 611 conventional state estimation methods as a potential framework for constructing improved 612 state estimates, combining the best of the two paradigms: fast data-driven state estimation 613 via deep learning and fine-tuning by conventional data assimilation methods to ensure the 614 strict consistency with an assumed dynamical model. 615

# 616 Data Availability

<sup>617</sup> The neural network architectures coded in Tensorflow/Keras and the training datasets are <sup>618</sup> published in the following Zenodo repository: https://doi.org/10.5281/zenodo.3757524

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### 626 References

- Abernathey, R. P., & Marshall, J. (2013). Global surface eddy diffusivities derived from satellite altimetry. *Journal of Geophysical Research: Oceans*, 118(2), 901–916.
- Aluie, H., Hecht, M., & Vallis, G. K. (2018). Mapping the energy cascade in the north
   atlantic ocean: The coarse-graining approach. *Journal of Physical Oceanography*, 48(2),
   225–244.
- Arbic, B. K., Scott, R. B., Flierl, G. R., Morten, A. J., Richman, J. G., & Shriver, J. F.

- (2012). Nonlinear cascades of surface oceanic geostrophic kinetic energy in the frequency
   domain. Journal of Physical Oceanography, 42(9), 1577–1600.
- Berloff, P. S., & Meacham, S. P. (1997). The dynamics of an equivalent-barotropic model of the wind-driven circulation. *Journal of marine research*, 55(3), 407–451.
- Bolton, T., & Zanna, L. (2019). Applications of deep learning to ocean data inference and subgrid parameterization. *Journal of Advances in Modeling Earth Systems*, 11(1), 376–399.
- Carton, J. A., & Giese, B. S. (2008). A reanalysis of ocean climate using simple ocean data assimilation (soda). *Monthly Weather Review*, 136(8), 2999–3017.
- Chapman, C., & Charantonis, A. A. (2017). Reconstruction of subsurface velocities from
   satellite observations using iterative self-organizing maps. *IEEE Geoscience and Remote Sensing Letters*, 14(5), 617–620.
- Chelton, D. B., & Schlax, M. G. (2003). The accuracies of smoothed sea surface height
   fields constructed from tandem satellite altimeter datasets. Journal of Atmospheric and
   Oceanic Technology, 20(9), 1276–1302.
- Chelton, D. B., Schlax, M. G., & Samelson, R. M. (2011). Global observations of nonlinear
   mesoscale eddies. *Progress in Oceanography*, 91(2), 167–216.
- <sup>650</sup> Davis, R. E. (1985). Objective mapping by least squares fitting. *Journal of Geophysical* <sup>651</sup> *Research: Oceans*, 90(C3), 4773–4777.
- de La Lama, M. S., LaCasce, J. H., & Fuhr, H. K. (2016, 09). The vertical structure of ocean eddies. *Dynamics and Statistics of the Climate System*, 1(1). Retrieved from https://doi.org/10.1093/climsys/dzw001 (dzw001) doi: 10.1093/climsys/dzw001
- Ducet, N., Le Traon, P.-Y., & Reverdin, G. (2000). Global high-resolution mapping of
   ocean circulation from topex/poseidon and ers-1 and-2. Journal of Geophysical Research:
   Oceans, 105(C8), 19477–19498.
- Fei-Fei, L., Fergus, R., & Perona, P. (2006). One-shot learning of object categories. *IEEE* transactions on pattern analysis and machine intelligence, 28(4), 594–611.
- Ferrari, R., & Wunsch, C. (2009). Ocean circulation kinetic energy: Reservoirs, sources,
   and sinks. Annual Review of Fluid Mechanics, 41, 253–282.
- Flierl, G. R. (1978). Models of vertical structure and the calibration of two-layer models. *Dynamics of Atmospheres and Oceans*, 2(4), 341–381.
- Fu, L.-L., Chelton, D. B., Le Traon, P.-Y., & Morrow, R. (2010). Eddy dynamics from satellite altimetry. *Oceanography*, 23(4), 14–25.
- Fu, L.-L., & Ubelmann, C. (2014). On the transition from profile altimeter to swath
   altimeter for observing global ocean surface topography. Journal of Atmospheric and
   Oceanic Technology, 31(2), 560–568.
- Gaultier, L., Ubelmann, C., & Fu, L.-L. (2016). The challenge of using future swot data
   for oceanic field reconstruction. Journal of Atmospheric and Oceanic Technology, 33(1),
   119–126.
- George, T., Manucharyan, G., & Thompson, A. (2019, Nov). Deep learning to infer eddy heat
   *fluxes from sea surface height patterns of mesoscale turbulence*. EarthArXiv. Retrieved
   from eartharxiv.org/erhy2 doi: 10.31223/osf.io/erhy2
- He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition.
  In Proceedings of the ieee conference on computer vision and pattern recognition (pp. 770–778).
- Kingma, D. P., & Ba, J. (2014). Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980.
- Klein, P., Isern-Fontanet, J., Lapeyre, G., Roullet, G., Danioux, E., Chapron, B., ... Sasaki,
   H. (2009). Diagnosis of vertical velocities in the upper ocean from high resolution sea
   surface height. *Geophysical Research Letters*, 36(12).
- Klein, P., Lapeyre, G., Siegelman, L., Qiu, B., Fu, L.-L., Torres, H., ... Le Gentil, S. (2019).
   Ocean-scale interactions from space. *Earth and Space Science*, 6(5), 795–817.
- Larichev, V. D., & Held, I. M. (1995). Eddy amplitudes and fluxes in a homogeneous model of fully developed baroclinic instability. *Journal of physical oceanography*, 25(10),

687 2285-2297.

- Le Traon, P., Nadal, F., & Ducet, N. (1998). An improved mapping method of multisatellite altimeter data. *Journal of atmospheric and oceanic technology*, 15(2), 522–534.
- Manucharyan, G. (2020, April). State estimation of surface and deep flows from sparse SSH
   observations of geostrophic ocean turbulence using Deep Learning. Zenodo. Retrieved
   from https://doi.org/10.5281/zenodo.3757524 doi: 10.5281/zenodo.3757524
- Melander, M., McWilliams, J., & Zabusky, N. (1987). Axisymmetrization and vorticity gradient intensification of an isolated two-dimensional vortex through filamentation. Jour nal of Fluid Mechanics, 178, 137–159.
- Pan, S. J., & Yang, Q. (2009). A survey on transfer learning. *IEEE Transactions on knowledge and data engineering*, 22(10), 1345–1359.
- Perez, L., & Wang, J. (2017). The effectiveness of data augmentation in image classification using deep learning. *arXiv preprint arXiv:1712.04621*.
- Phillips, N. A. (1951). A simple three-dimensional model for the study of large-scale
   extratropical flow patterns. *Journal of Meteorology*, 8(6), 381–394.
- Samelson, R., Chelton, D., & Schlax, M. (2019). The ocean mesoscale regime of the
   reduced-gravity quasi-geostrophic model. *Journal of Physical Oceanography*(2019).
- Scott, R. B., & Arbic, B. K. (2007). Spectral energy fluxes in geostrophic turbulence: Implications for ocean energetics. *Journal of physical oceanography*, 37(3), 673–688.
- Smith, K. S., & Vallis, G. K. (2001). The scales and equilibration of midocean eddies:
   Freely evolving flow. *Journal of Physical Oceanography*, 31(2), 554–571.
- Targ, S., Almeida, D., & Lyman, K. (2016). Resnet in resnet: Generalizing residual architectures. arXiv preprint arXiv:1603.08029.
- Ubelmann, C., Cornuelle, B., & Fu, L.-L. (2016). Dynamic mapping of along-track ocean al timetry: method and performance from observing system simulation experiments. *Journal* of Atmospheric and Oceanic Technology, 33(8), 1691–1699.
- Ubelmann, C., Klein, P., & Fu, L.-L. (2015). Dynamic interpolation of sea surface height
   and potential applications for future high-resolution altimetry mapping. Journal of At mospheric and Oceanic Technology, 32(1), 177–184.
- <sup>716</sup> Vallis, G. K. (2017). Atmospheric and oceanic fluid dynamics. Cambridge University Press.
- Wunsch, C. (1997). The vertical partition of oceanic horizontal kinetic energy. Journal of Physical Oceanography, 27(8), 1770–1794.
- <sup>719</sup> Wunsch, C. (2010). Toward a midlatitude ocean frequency-wavenumber spectral density <sup>720</sup> and trend determination. *Journal of Physical Oceanography*, 40(10), 2264–2281.