

1 **State estimation of surface and deep flows from sparse**
2 **SSH observations of geostrophic ocean turbulence using**
3 **Deep Learning**

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7 **Key Points:**

- 8 • Deep Learning framework is developed for SSH interpolation in a baroclinically
9 unstable current.
- 10 • Residual Neural Networks outperform linear and dynamical SSH interpolation tech-
11 niques.
- 12 • Skillful estimation of unobserved deep flows from temporally-sparse SSH obser-
13 vations is plausible

14

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Abstract

Satellite altimeters provide global observations of sea surface height (SSH) and present a unique dataset for advancing our theoretical understanding of upper ocean dynamics and monitoring its variability. Considering that mesoscale and submesoscale SSH patterns can evolve on timescales comparable to or shorter than satellite return periods, currently available altimetry observations are still spatially and temporally sparse and hence it is challenging to accurately reconstruct continuous SSH evolution. Here we explore the possibility of SSH interpolation using Deep Learning — a machine learning approach that extracts information only from data. Using synthetic observations taken from an idealized quasi-geostrophic model of baroclinic ocean turbulence, we demonstrate that Convolutional Neural Networks with Residual Learning are superior in SSH reconstruction than the linear and recently developed dynamical interpolation techniques. Furthermore, the neural network can provide an accurate state estimate of unobserved deep ocean currents at mesoscales, suggesting that SSH patterns of eddies do contain substantial information about ocean interior that is necessary for SSH prediction. Our framework is highly idealized and several crucial improvements such as transfer learning and diversification of training data would be necessary to implement before its ultimate use with real satellite observations. Nonetheless, by providing a proof of concept, our results point to Deep Learning as a viable alternative to existing interpolation and more generally state estimation methods for satellite observations of baroclinic ocean turbulence.

Plain Language Summary

Satellite sea surface height (SSH) observations provide critical insights into the variability of ocean currents. However, these observations are spatially and temporally sparse, presenting a challenge for reconstructing time-continuous SSH maps particularly at resolutions containing relatively fast-evolving upper-ocean eddies. Further limitations are due to the fact that the evolution of SSH is not self-constrained as it is affected by unobserved deep ocean flows. In this study, we test a different approach to address poor temporal sampling of SSH: a machine learning framework that relies on pattern recognition in large-scale ocean turbulence. We demonstrate that deep artificial neural networks can generate a skillful state estimation of unobserved deep ocean currents and outperform conventional SSH reconstruction methods in an idealized model of ocean turbulence. In providing the proof of concept, our results strongly point at Deep Learning learning as a viable alternative to existing interpolation and state estimation methods for satellite oceanography.

1 Introduction

Satellite-derived global observations of sea surface height (SSH) has shed light on many dynamical processes including large-scale circulation, propagation of waves as well as on the evolution of the mesoscale eddy field (Chelton et al., 2011; Fu et al., 2010). Since the satellite era, an increasing amount of evidence points towards the mesoscale eddies being a key component of the global ocean circulation and significantly impact, among others, carbon sequestration, biological productivity, heat transport and thus the Earth’s climate as a whole (Ferrari & Wunsch, 2009). Nonetheless, understanding and monitoring oceanic energy spectrum and associated spectral energy fluxes (Scott & Arbic, 2007; Aluie et al., 2018), understanding tracer dispersion (Abernathy & Marshall, 2013) or inferring subsurface flows (Klein et al., 2009) still remains challenging because these quantities depend on higher-order SSH derivatives and hence require high resolution and accuracy. The regularly-gridded SSH data, e.g. AVISO (Ducet et al., 2000), is spatially and temporally interpolated from along-track altimetry measurement using objective mapping and hence its accuracy is constrained by the density of observations and by the deficiencies of the interpolation technique. To provide better coverage, several altimeters have been put in orbit but their 10-20 days repeat orbits and relatively coarse along-track resolutions allow to view the ocean dynamics only down to relatively large mesoscale eddies (Wunsch, 2010).

The upcoming Surface Water Ocean Topography (SWOT) altimeter mission (Fu & Ubelmann, 2014) promises to observe ocean mesoscale eddies and submesoscale fronts (50 km) at unprecedented spatial resolutions, potentially resolving 15-30km wavelengths. However, the temporal resolution of the altimeter (i.e., a complete repeat cycle of 21 days) is not sufficient to continuously capture the evolution of submesoscale eddies and fronts. The mismatch between the high spatial resolution and the moderate temporal resolution presents a challenge for reconstructing time-continuous maps of SSH. This task is especially challenging in eddy-rich regions where small-scale SSH anomalies can evolve relatively fast compare to satellite return periods, e.g. in the Antarctic Circumpolar Current, the Kuroshio Extension and the Gulf Stream, all of which are key players in the climate system. It is thus crucial to develop frameworks to efficiently extract information about oceanic eddy dynamics from the spatially and temporally sparse SSH observations.

1.1 SSH interpolation and 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 moving eddy 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 to pinpoint only those tracks that have passed over this specific eddy and combine this information to constrain the two-dimensional eddy shape. Thus, without a model of eddy evolution, or more generally SSH evolution, the information from various altimetry tracks could not be used in an optimal way. However, due to the stratified nature of geostrophic ocean turbulence, the unobserved subsurface flows can affect surface dynamics and hence the knowledge of the SSH field may not be self-sufficient to infer its evolution. Given the lack of subsurface information at eddy scales, constructing a reduced self-contained model of SSH evolution is challenging.

Existing methods for spatiotemporal SSH interpolation can be broadly split into two distinct classes: methods that rely on a postulated dynamical model of SSH evolution and purely data-driven methods, both having their advantages and disadvantages. To avoid prescribing a dynamical model, statistical models relying on data only, e.g. objective interpolation methods (Davis, 1985; Le Traon et al., 1998; Ducet et al., 2000). Their premise is to incorporate spatiotemporal correlations and measurement error into a statistical model that provides the most likely estimate of the true continuous state, given available observations.

99 However, this method does not rely on any dynamical model of the eddy propagation and
 100 hence can lead to unphysical behavior of the interpolated SSH field. Methods involving dy-
 101 namical ocean models are typically based on data assimilation, a procedure that minimizes
 102 the difference between observed and modeled fields by adjusting unknown variables like
 103 boundary and initial conditions or external forcing (see e.g. reanalysis product by Carton &
 104 Giese, 2008). While resulting in SSH fields that are dynamically-constrained, the drawback
 105 of this method is that it requires additional observations to constrain other essential model
 106 variables like the subsurface flow and density field. Also, data assimilation for complex
 107 ocean models at eddy-resolving scales is often under-determined and is computationally
 108 demanding.

109 Recent work by Ubelmann et al. (2015) demonstrated that representing SSH propa-
 110 gation with a single equivalent barotropic mode in a quasigeostrophic model results in
 111 significant improvements in spatiotemporal interpolation of sparse SSH observations. In
 112 particular, Ubelmann et al. (2015) considered a fundamental problem of reconstructing
 113 SSH distribution that occurred in between two observed SSH fields separated by about 20
 114 days, a characteristic timescale required by a set of altimeters to reconstruct a spatial SSH
 115 field. They found that integrating the earlier SSH observation forward in time (follow-
 116 ing assumed dynamical of an equivalent barotropic mode) and averaging it with the later
 117 observed SSH anomalies that were integrated backward in time, resulted in improvement
 118 compared to conventional linear interpolation methods. In a follow-up work, Ubelmann et
 119 al. (2016) generalized this temporal interpolation method to spatiotemporal interpolation of
 120 along-track SSH observations by essentially performing data-assimilation on the one-layer
 121 QG model. The advantage of the dynamical interpolation method is that it relies on the
 122 advection of potential vorticity – a process that is inherently non-linear and thus cannot be
 123 accurately represented by linear or objective interpolation techniques that do not take into
 124 account the dynamical constraints imposed on ocean flows.

125 A drawback of the dynamical interpolation is that it assumes that the surface stream-
 126 function evolves independently of subsurface streamfunction, considering the so-called equiv-
 127 alent barotropic mode dynamics (Berloff & Meacham, 1997). However, in many energetic
 128 regions of the ocean, e.g. in Gulf Stream, Kuroshio or Antarctic Circumpolar Current, the
 129 currents are baroclinically unstable and hence are by necessity composed of at least two
 130 dynamically interacting vertical modes, barotropic and baroclinic modes (see e.g. Chapter
 131 6 in Vallis, 2017). To illustrate this point, consider the conservation of quasigeostrophic
 132 potential vorticity q_1 in the upper ocean layer as a model of SSH evolution at mesoscales:

$$133 \quad \frac{Dq_1}{Dt} = \underbrace{\frac{D}{Dt}[\underbrace{r^2}_{1} + \underbrace{R_d^2}_{1}]}_{\text{Depends on partially-observed } \psi_1} + \underbrace{R_d^2 \frac{D}{Dt} \psi_{b:t.}}_{\text{Depends on unobserved } \psi_2} = 0; \quad (1)$$

$$134 \quad \text{where } \psi_{b:t.} = \frac{H_1 \psi_1 + H_2 \psi_2}{H_1 + H_2} \text{ and } R_d^2 = \frac{f_0^2}{g^\theta H_1} + \frac{f_0^2}{g^\theta H_2}; \quad (2)$$

135 ψ_1 is the surface streamfunction directly proportional to SSH, ψ_2 is the subsurface stream-
 136 function, $\psi_{b:t.}$ denoting the barotropic streamfunction (depth-averaged transport), R_d is the
 137 Rossby baroclinic deformation radius, f and β are the Coriolis and beta-plane parameters,
 138 H_1 and H_2 are the ocean layer depths, g^θ is the reduced gravity, and $D=Dt$ is the material
 139 derivative accounting for advection by the surface flow (see Methods). On relatively short
 140 timescales, sources and dissipation of potential vorticity could be neglected and its approxi-
 141 mate conservation provides a basic description of eddy evolution. The terms in the equation
 142 1 above have been grouped into those that only depend on the partially-observed ψ_1 (or
 143 equivalently SSH) and terms that depend on the unobserved subsurface flow ψ_2 (or on the
 144 barotropic flow $\psi_{b:t.}$). It is now clear that by considering only the equivalent barotropic
 145 mode dynamics and taking ψ_1 to be equal to the baroclinic mode, the dynamical interpo-
 146 lation method as described in Ubelmann et al. (2015, 2016) discards the term in the PV
 147 conservation equation that depends on the unobserved barotropic streamfunction. Since

148 the discarded term was the only one that depended on the unknown streamfunction, ψ_2 , it
 149 is possible to integrate the approximate PV-conservation equation forward and backward
 150 in time given only ψ_1 observations, as was done in Ubelmann et al. (2015). Even though
 151 in many ocean regions both deep and upper-ocean currents are dynamically active, recon-
 152 structing SSH using the dynamical interpolation technique performed well, being superior
 153 to linear interpolation methods because it relied, at least approximately, on the fundamen-
 154 tal PV-conservation constraint. Nonetheless, the dynamical interpolation method can lead
 155 to significant errors (see Results), implying that the omitted term, while being relatively
 156 small, can substantially impact SSH evolution on timescales comparable to return periods
 157 of altimetry satellites.

158 1.2 Rationale for Deep Learning approach.

159 A clear way of improving the dynamical interpolation algorithm would be to include
 160 the contribution of the barotropic mode to SSH evolution. However, comprehensive mea-
 161 surements of deep ocean currents at eddy scales are missing, posing a significant challenge of
 162 inferring them from only SSH observations. Without taking into consideration the physical
 163 processes that have lead to the generation of any given SSH snapshot, there is a wide range
 164 of plausible ways in which ψ_1 could be decomposed into baroclinic and barotropic modes,
 165 each corresponding to the distinct configuration of PV anomalies in the two layers. How-
 166 ever, considering that PV anomalies are specifically due to baroclinic instabilities and they
 167 obey specific conservation laws (Eq. 1), the barotropic and baroclinic modes are inherently
 168 entangled and this must provide at least partial constraints on how any specific SSH pattern
 169 could be partitioned. Since the QG model exhibits highly non-linear and chaotic behavior,
 170 an analytical approach to disentangle the modes has not been found but the evidence that
 171 data-driven approach might be relevant has been presented in the literature. In particu-
 172 lar, mooring observations demonstrate that surface and subsurface flows are significantly
 173 correlated such that a single empirical orthogonal function (EOF) can explain a signifi-
 174 cant amount of variance of the overall vertical velocity profile Wunsch (1997); de La Lama
 175 et al. (2016). Furthermore, machine learning techniques such as self-organizing Chapman
 176 & Charantonis (2017), as well as convolutional neural networks (Bolton & Zanna, 2019),
 177 have been used to estimate subsurface flows from SSH data. However, the unknown term
 178 $D\psi_{bt} = D_t(\psi_{bt} + \mathbf{u}_1 \cdot \nabla \psi_{bt})$ in Eq. 1 can only provide a substantial contribution to the PV
 179 budget if ψ_{bt} has a substantial component that is decorrelated from ψ_1 because $\mathbf{u}_1 \cdot \nabla \psi_1 = 0$,
 180 and $D_t \psi_{bt} \ll D_t \psi_1$ for surface-amplified flows. Thus the key for a more accurate SSH in-
 181 terpolation lies in estimating the component of ψ_2 that is decorrelated from ψ_1 – a problem
 182 that is tightly linked to estimating eddy heat fluxes in baroclinically unstable flows. Us-
 183 ing residual neural networks, George et al. (2019, under review) have demonstrated that
 184 ψ_1 indeed contains substantial information about the decorrelated part of the subsurface
 185 streamfunction ψ_2 , allowing to estimate about 60% of the variance in eddy heat fluxes only
 186 from SSH snapshots. Given that machine learning methods can extract information from
 187 SSH patterns to estimate the component of ψ_{bt} that is uncorrelated with ψ_1 when esti-
 188 mating the eddy heat fluxes, here we hypothesize that machine learning techniques could
 189 outperform the dynamical interpolation methods.

190 2 Methods

191 Here we present a machine learning framework that mimics the task of dynamical inter-
 192 polation, i.e. reconstructs the SSH snapshot that occurred between two given SSH snapshots
 193 separated by 20 days (Ubelmann et al., 2015). We use machine learning as a tool to shortcut
 194 the formal process of data assimilation and to establish if there are substantial possible con-
 195 nections between the dynamical evolution of eddies and spatiotemporal interpolation. We
 196 are interested in providing a proof-of-concept machine learning framework and understand-
 197 ing its dynamical limitations, i.e. those that are not subject to insufficiency or poor quality
 198 of data. We develop and test our method in an idealized framework of predicting SSH snap-

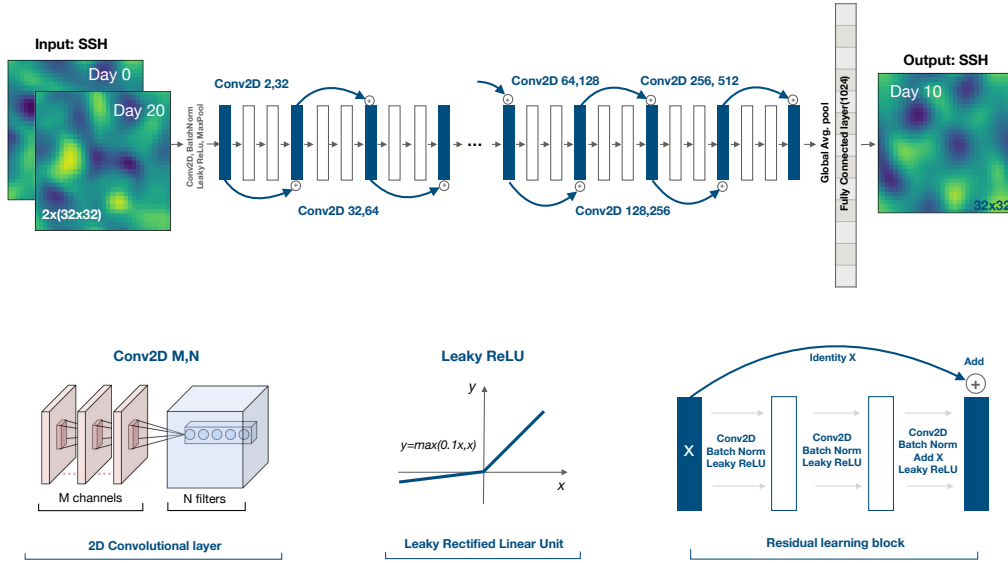


Figure 1. Architecture of the Deep Learning neural network with residual learning (slightly modified from the well-known ResNet50 architecture He et al. (2016)). The input consists of two SSH snapshots separated by 20 days (in case of SSH input with missing data, those values are set to zero). A set of convolutional layers are then applied to create abstract representation of the input patterns in a bottleneck fashion: when image sizes decrease by a factor of two, the number of filters increase 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. The output from the convolutional layer is subject to global average pooling and flattening into a vector that is finally densely connected to the output.

199 shots that were generated by a quasigeostrophic (QG) model of baroclinically unstable flow.
 200 We find the QG model to be optimal for our goals as is pertinent to many energetic regions
 201 in the ocean while being relatively simple that a large volume of data can be generated for
 202 training and testing; furthermore, the model allows us to directly benchmark machine learn-
 203 ing against the dynamical interpolation technique that also utilizes QG dynamics. Below
 204 we describe our neural network architecture for spatiotemporal SSH interpolation and the
 205 QG model used for the generation of training and testing datasets.

206 2.1 Deep Learning framework: Residual Convolutional Neural Networks

207 Artificial neural networks are based on the idea of approximating the ‘output’ by taking
 208 the ‘input’ variable and performing a large number of matrix additions and multiplications,
 209 applying non-linearity functions, and either condensing or expanding the variable dimen-
 210 sion as it passes from layer to layer. The resulting network contains a large number of free
 211 parameters that are later adjusted to optimize a given loss function, commonly taken as
 212 a measure of difference between the prediction and the truth. Because we are trying to
 213 extract information from eddy patterns expressed in SSH fields, the choice of convolutional
 214 neural networks (CNNs) is rationalized. In passing information from layer to layer, CNNs
 215 define a set of filters (kernel matrices with prescribed dimensions) and convolve images

216 to produce more abstract levels of information that is passed on to the next layer. Here
 217 we implement the ResNet50 architecture – a Convolutional Neural Network with Residual
 218 Learning blocks (He et al., 2016). The Residual Learning is a process by which the infor-
 219 mation is not only transferred sequentially from one layer to another but is also transferred
 220 via skip connections that add the identify of the current layer to the layer that is a few
 221 ahead (see Fig. 1); the presence of skip connections can result in better performance for a
 222 wide range of computer vision problems (Targ et al., 2016). We note that we have explored
 223 several simpler architectures like shallow neural networks with only dense connections, and
 224 simpler VGG-type architectures without residual learning but have achieved significantly
 225 poorer performance; we thus present the network architecture that have lead to a signifi-
 226 cant skill, although there is always a possibility that superior neural network architectures
 227 may exist. The graph of the architecture used in this study, outlining all hyperparam-
 228 eters together with the Python code of its implementation in Tensorflow/Keras as well
 229 as the training datasets can be found here [https://drive.google.com/drive/folders/](https://drive.google.com/drive/folders/1tZrplLw2m19CB1YcQABj6pn0a7_-H63n?usp=sharing)
 230 [1tZrplLw2m19CB1YcQABj6pn0a7_-H63n?usp=sharing](https://drive.google.com/drive/folders/1tZrplLw2m19CB1YcQABj6pn0a7_-H63n?usp=sharing).

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

$$233 \quad Skill = 1 - \frac{\sqrt{\overline{SSH_{predicted} - SSH_{true}}^2}}{\sqrt{\overline{SSH_{true}}^2}}; \quad (3)$$

234 For reference, the maximum skill=1 is achieved when the predicted and true images are
 235 exactly the same; the skill=0 corresponds to a prediction that makes the same error as
 236 assuming a spatially homogeneous SSH field, and negative skill implies an even worst fit.
 237 This definition of skill is more conservative than the correlation coefficient or R-squared
 238 value; for example, ρ_2 is correlated to ρ_1 with an average correlation coefficient of 0.74 and
 239 the linear regression model has R-squared of about 0.55 but the skill of only 0.33 if defined
 240 as in equation 3 above. It is thus important to compare results from different publications
 241 using consistent metrics. Here we stick with the skill metric that is based on the RMS-error
 242 normalized by the standard deviation as it is a natural choice for a neural network loss
 243 function to minimize during training.

244 Coefficients of filter matrices, along with all other weights and biases involved in the neu-
 245 ral network architecture are then iteratively optimized using the Adam optimizer (Kingma
 246 & Ba, 2014) to minimize the loss function that is the root-mean-square difference between
 247 the predicted and true SSH images (or equivalently to maximize the skill). The parameter
 248 optimization procedure requires evaluating neural network predictions for a large volume of
 249 training data and hence the final optimized state of a particular neural network depends only
 250 on the training data itself. To test if a general dependence was found the neural network
 251 skill is estimated for a group of three independent datasets: training, validation, and testing
 252 sets. Training data is used only for training purposes, validation data is used to evaluate
 253 the skill of the neural network and to identify a stoppage criterion for the training, while
 254 the test data is used at the very last step to define the skill of a trained neural network. All
 255 three datasets were generated from different numerical simulations to ensure that overfitting
 256 didn't occur and that a general law was found.

257 **2.2 Synthetic training data: quasigeostrophic model**

258 Deep neural networks typically require a large volume of training data to identify a
 259 general law. In the absence of high-quality or sufficiently large volume of data neural
 260 networks are likely to overfit the training data and have poor skill when evaluated on the test
 261 data. To avoid these issues we choose to train neural network on synthetic data generated
 262 using an idealized model of ocean turbulence – the two layer quasigeostrophic (QG) model
 263 (Phillips, 1951; Vallis, 2017). The QG model is pertinent to baroclinically unstable flow
 264 and contains the propagation dynamics of large-scale ocean eddies, including advection by
 265 mean flow, beta drift, and eddy interactions with mean flow. Our choice of using the

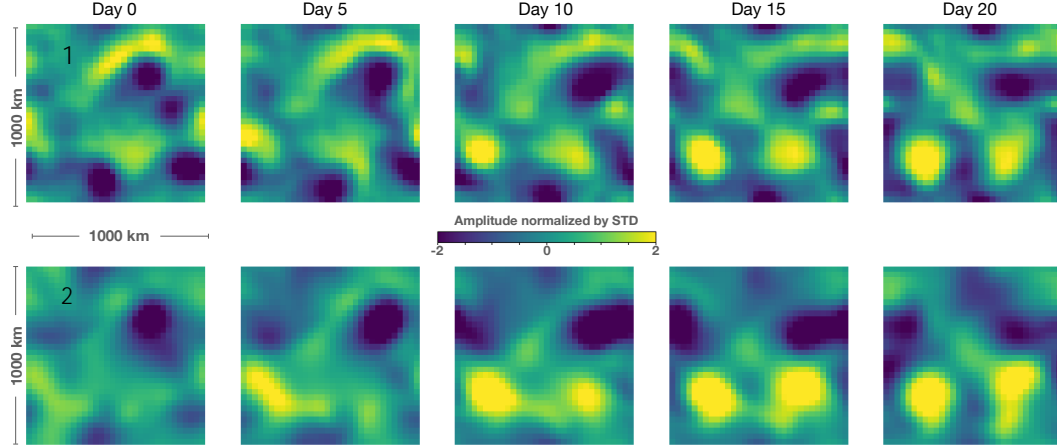


Figure 2. An example of the eddy field evolution over the course of 20 days as generated by the QG model of a baroclinically unstable current. Top panels show surface streamfunction ψ_1 (or SSH) and bottom panels show the corresponding deep ocean streamfunction ψ_2 , both being normalized by their respective standard deviations; domain size is 1000x1000 km and rows correspond to streamfunction snapshots taken 5 days apart. Note that the eddy field dramatically changes over the course of 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.

266 two-layer model is rationalized because i) ocean currents are predominantly composed of
 267 the barotropic and the first baroclinic mode (Wunsch, 1997; Smith & Vallis, 2001) and ii)
 268 it is the minimal model demonstrating the difficulty of predicting SSH evolution without
 269 direct observations of subsurface flows because both layers necessarily are dynamically active
 270 during baroclinic instabilities, and iii) the dynamical interpolation method also relies on QG
 271 dynamics which allows to make a fair performance comparison.

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

$$277 \quad \frac{Dq_1}{Dt} = \frac{D}{Dt} [r^{-2} \psi_1 + \frac{f_0^2}{g^0 H_1} (\psi_1 - \psi_2) + \gamma] = 0 \quad (4)$$

$$278 \quad \frac{Dq_2}{Dt} = \frac{D}{Dt} [r^{-2} \psi_2 + \frac{f_0^2}{g^0 H_2} (\psi_2 - \psi_1) + \gamma] = r_{EK} r^{-2} \psi_2; \quad (5)$$

279 where $\psi_{1,2}$ is the top and bottom layer streamfunctions, f_0 is the Coriolis parameter and
 280 ψ is its derivative in the meridional y -direction, g^0 is the reduced gravity, $D=D_t = \partial_t +$
 281 $\mathbf{u} \cdot \nabla$ is the material derivative using corresponding layer' geostrophic velocity \mathbf{u} , and r_{EK}
 282 is the bottom drag coefficient. The relative importance of the discarded term in the PV-
 283 conservation budget in Eq. 1, $D_{bt} = D_t$, could be estimated by comparing its magnitude
 284 to $D_{\psi_1} = D_t$, where both material derivatives use velocity in the top layer. The ratio of
 285 these terms would scale roughly as the ratio of characteristic amplitudes of the barotropic
 286 and surface streamfunctions, which we find from numerical simulations to scale as the ratio
 287 of layer depths in QG simulations of baroclinic instabilities, i.e. $[\frac{-2}{b;t} = \frac{-2}{1}]^{\frac{1}{2}} \sim O(H_1 = H_2)$.
 288 Since in most ocean regions the pycnocline is relatively shallow compared to the full depth
 289 of the ocean, the flows are surface-amplified and the discarded term is relatively small but

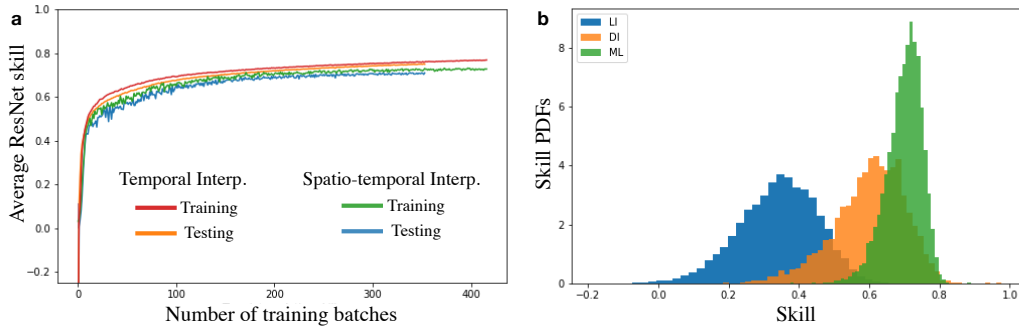


Figure 3. a) The evolution of the ResNet50 model skill during its training; 10 training mini-batches correspond to one epoch, while the actual number of batches is 128 and the total number of samples used in training is about 80,000; testing was conducted on 10,000 samples. b) comparison of skill distributions of the linear interpolation (LI), dynamical interpolation (DI), and the machine learning method evaluated on the test data set. Note that the lack of skills close to 1 hint at the existence of a dynamical barrier for SSH interpolation likely due to the chaotic nature of QG equations; i.e. the information content about the predicted SSH image is decreasing with the increased amount of time separation between the input image as the phase space trajectories are being mixed to the point where the dependence of initial conditions is being lost.

290 non-negligible and can substantially impact the SSH evolution leading to significant errors
 291 of the dynamical interpolation (see Results).

292 The QG model has been configured to represent baroclinically unstable mid-latitude
 293 currents such as the Gulf Stream or Kuroshio. Model parameters are as follows: the Rossby
 294 deformation radius is 40 km, the ratio of mean layer depths is 0.2, there is a steady uni-
 295 form mean vertical shear of 0.2 m/s, beta plain parameter corresponds to a latitude of
 296 40 degrees, linear Ekman friction was prescribed in the bottom layer for dissipation, and
 297 high-wavenumber motions are being filtered in Fourier space for all variables (more details
 298 could be found in Flierl (1978); Arbic et al. (2012)). The QG model is integrated forward in
 299 time using an ensemble of noisy initial conditions to produce a large volume of data: about
 300 100,000 SSH snapshots separated by 10 days (Figure 2). Over a timescale of 20 days, SSH
 301 fields become substantially decorrelated such that it is hard to identify any persisting eddies
 302 because their shapes and intensities have been dramatically changed due to interactions
 303 with other eddies (Figure 2). We ensure that the data for training/validation/testing comes
 304 from distinct simulations to accurately access the generalization skill of the neural network.

305 3 Results

306 3.1 Spatiotemporal SSH interpolation

307 Two separate neural networks were trained to perform two types of interpolation tasks
 308 to identify SSH field: i) temporal interpolation where the input consists of two SSH snap-
 309 shots separated by 20 days, and ii) spatiotemporal interpolation with the same input as
 310 for the temporal interpolation but with SSH images having missing data. For the temporal
 311 separation of SSH images we chose 20 days because it is of the order of the return periods
 312 for existing altimeters and to be consistent with Ubelmann et al. (2015). For the spatiotem-
 313 poral interpolation, we choose the area of missing data to roughly correspond to that of
 314 the SWOT observations over its return period. For a 1000 km domain, SWOT would have

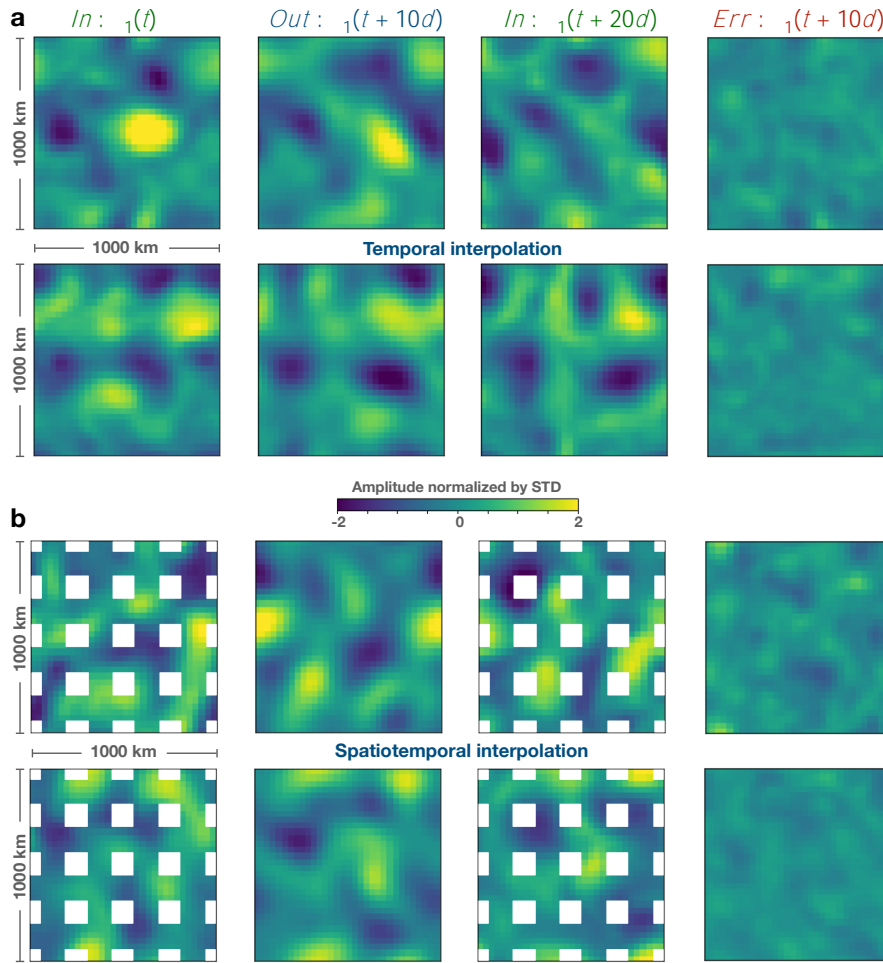


Figure 4. Examples of temporal (a) and spatiotemporal (b) interpolation of SSH data using the Deep Learning framework. Each row represents a randomly chosen interpolation example from the testing dataset (for a statistical distribution of prediction skill see Figure 3). The input SSH fields, $\eta_1(t)$ and $\eta_1(t+20d)$ are separated by 20 days and plotted in the first and the third columns correspondingly, while the predicted SSH field at day 10 ($\eta_1(t+10d)$) is plotted in the second column; the prediction error is plotted in the fourth column. White regions in the case of spatiotemporal interpolation denote areas of missing data. Domain size for both input and prediction is 1000km by 1000km. SSH data for training and testing was generated using baroclinically unstable QG model of ocean turbulence with configuration pertinent to midlatitude ocean jets (see Methods).

315 about four crossings (each having a swath of 120 km) with one inclination angle and another
 316 four with an opposite angle (see e.g. Figure 1 in Gaultier et al. (2016)). While SWOT would
 317 have missing-data areas in the shape of a rhombus, here for simplicity we have prescribed
 318 square shapes as there is no reason to assume this would lose any generality.

319 The neural networks were trained using about 100K data samples, both achieving a sig-
 320 nificant performance skill and producing realistic SSH images with small errors (see Figure
 321 4). The average prediction skill for both simulations plateaued at about 0.7 and it wasn't
 322 significantly smaller when evaluated on the test dataset (Figure 3 a), implying that a gen-
 323 eralized dependence has been found. A few illustrative examples of eddy field evolution are
 324 shown in Figure 4a, demonstrating the non-trivial SSH evolution that occurs in a chaotic

325 QG model of baroclinically unstable flow. In the top-row example of Figure 4a, the strong
 326 positive SSH anomaly in the center of the domain almost completely disappeared after 20
 327 days, yet the neural network was still capable to reconstruct the SSH state at day 10. For
 328 such examples when the eddy field changes dramatically with time, linear or objective in-
 329 terpolation techniques perform poorly as they do not rely on any dynamical model of SSH
 330 evolution and only make use of autocorrelation as a statistical model. Evaluated on a large
 331 number of testing data (10K samples), the machine learning model outperformed the linear
 332 and dynamical interpolation techniques, having not only a better average skill but also much
 333 more infrequent occurrence of low-skill interpolations, i.e. much narrower skill-distribution
 334 tail in the direction of small skills (Figure 3b). Noticeably, the linear interpolation skill can
 335 be so low that it has values reaching zero, i.e. its prediction is no better than assuming that
 336 $SSH = 0$ everywhere in the domain. The dynamical interpolation is much better than that
 337 but still has a significant probability of poor interpolations in the skill range of about 0.4-0.6.
 338 While the machine learning technique is superior to other methods, it is important to note
 339 that it still does not provide a perfect reconstruction and has a limit in skill abounded by
 340 about 0.8. Since we are utilizing only surface observations while SSH evolution depends also
 341 on the unknown subsurface flow, it is, of course, expected that the interpolation skill would
 342 not be perfect: it is inherently a partial information problem. In addition to having partial
 343 observations, the chaotic nature of the flow also must be contributing to the skill limitation:
 344 if the SSH images are separated by a sufficiently large amount of time (greater than the
 345 characteristic Lyapunov exponent timescale), there should be no physical or statistical rela-
 346 tionship between them and no interpolation technique could have a skill significantly above
 347 zero. Yet, the 20-day separation timescale, which is of the order of the return periods for
 348 existing altimeters, still allows one to extract sufficient information even for highly energetic
 349 baroclinically unstable flows.

350 3.2 State estimation of unobserved deep ocean flows at mesoscales

351 Here we assess the efficacy of the Deep Learning framework in addressing the state
 352 estimation problem, i.e. estimating all dynamical variables in the ocean turbulence model,
 353 which in our case of a two layer QG model implies estimating both surface and subsurface
 354 layer streamfunctions. Conventionally, for state estimation one needs to postulate the dy-
 355 namical model and only then implement techniques e.g. data assimilation or the ensemble
 356 Kalman filter techniques in order to estimate unknown variables and parameters in the
 357 model at all times and everywhere within the model domain. However, we demonstrate
 358 here that the machine learning framework is capable to estimate both ψ_1 and ψ_2 with a
 359 high average skill of about 0.7 (Figure 5). It is important to note that while ψ_2 is highly
 360 correlated with ψ_1 (average correlation coefficient is about 0.8) it is the decorrelated part,
 361 $\tilde{\psi}_2 = \psi_2 - A \psi_1$, that is dynamically important for the SSH evolution. The neural network
 362 is capable of skillful reconstruction of $\tilde{\psi}_2$ based on two SSH snapshots separated by 20 days,
 363 with an average skill of 0.7 for day 0 and a skill of 0.8 for day 20 (Figure 5). It is thus
 364 clear that mesoscale eddy patterns imprinted in SSH do provide substantial information on
 365 deep ocean currents or equivalently information on the partitioning between the baroclinic
 366 and barotropic modes even for baroclinically unstable flows. Nonetheless, since both lay-
 367 ers are dynamically active and no subsurface information is given by satellite observations,
 368 there is an inherent lack of information that is contained in sparse SSH observations and
 369 this prevents any interpolation or state estimation methodology from achieving a perfect
 370 skill. After all, if SSH snapshots are separated by a sufficiently long time, there should
 371 not be any relation between them due to the chaotic nature of ocean mesoscale turbulence.
 372 Nonetheless, we have demonstrated here that the 20 day separation even for a strong baro-
 373 clinically unstable current with a dynamically active subsurface flow does contain sufficient
 374 information for skillful interpolation and state estimation.

375 In providing a skillful state estimate from snapshots only, the deep neural network can
 376 essentially encode the underlying model equations and then utilize the information from
 377 subsequent SSH snapshot to even better constrain subsurface flows (see bottom panel in

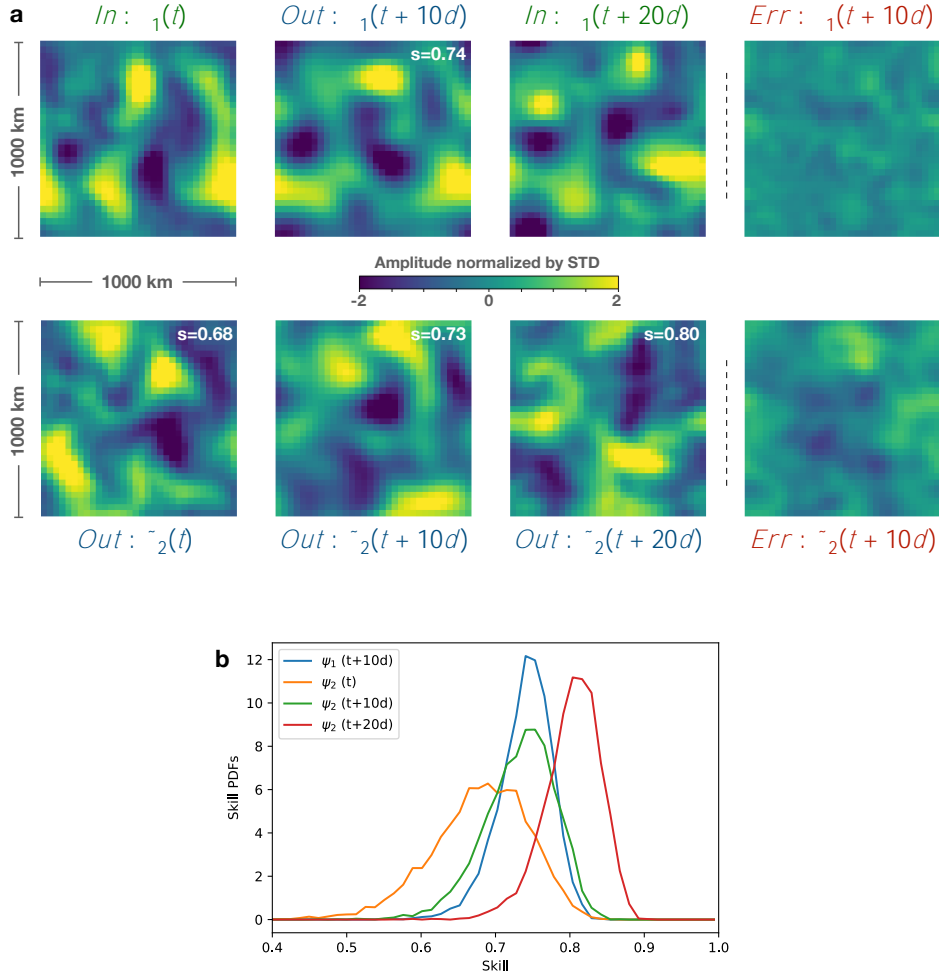


Figure 5. Examples of state estimation using Deep Learning neural network (a) and its statistical skill distribution for surface and subsurface variables at different times (b). As in the case of SSH interpolation, the neural network receives as input two SSH snapshots separated by 20 days, $\psi_1(t)$ 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, $\psi_2(t; t+10d; t+20d)$. Note that ψ_1 and ψ_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 subsurface streamfunctions are shown in last columns. The probability density function of the neural network skill distribution is plotted in panel (b) for all predicted variables. Note, while the neural network provides skillful predictions for all variables (skill ranges from 0.65 to 0.85), the best prediction skill is achieved for subsurface flow at day 20 and the worst prediction is for subsurface flow at day 0.

378 Figure 5). It important to note the asymmetry in reconstructing subsurface velocities: at
 379 earlier times the skill is substantially worse (compare the orange and red curves in bottom
 380 panel of Figure 5). This asymmetry is expected in a chaotic and dissipative quasigeostrophic
 381 dynamics that makes it more difficult to estimate past state by observing the future as
 382 opposed to estimating future by observing the past. Thus, the two SSH snapshots must
 383 indeed be ordered in time as the PV-evolution equations only allow time reversal only for
 384 sufficiently small time intervals at which the dissipation effects can be neglected.

385 4 Discussion

386 Here we presented the proof of concept for using Deep Learning as an efficient tool to
 387 extract non-trivial information from sparse SSH observations, specifically demonstrating its
 388 utility in the spatiotemporal interpolation of SSH data and more generally in the state esti-
 389 mation that includes deep ocean currents apart from SSH. The Residual CNN outperformed
 390 the commonly used dynamical interpolation method. While it is challenging to precisely
 391 interpret the algorithm that was ultimately learned by the neural network, its success seems
 392 to be associated with its ability to predict subsurface flows only from individual snapshots of
 393 mesoscale eddy patterns. This separates machine learning from other methods that are in-
 394 capable of dis-entangling the highly-nonlinear relation between surface and subsurface flows
 395 and hence gives machine learning the edge in constructing a more accurate model of SSH
 396 evolution, resulting in higher quality interpolation.

397 Here we only considered the case of mesoscale turbulence and for the case of subme-
 398 soscale turbulence, the question remains open as to how SWOT’s 2D high-resolution swath
 399 measurements could be used to enhance the resolution of SSH data. While we expect the
 400 machine learning framework to perform well in reconstructing large and small mesoscale ed-
 401 dies, its limitations still need to be understood when considering mesoscale and submesoscale
 402 turbulence as a continuum. The main difficulty arises because the persistence timescale for
 403 submesoscale eddies is substantially shorter than for mesoscale eddies and no technique can
 404 bypass the inherent loss of the dependence on initial conditions for a chaotic system.

405 We have used a model of baroclinic turbulence as a synthetic training data because it
 406 presents a hard test for temporal SSH interpolation due to its chaotic nature and an a priori
 407 unknown impact of the dynamically active bottom layer on SSH evolution. We recognize
 408 that ocean regions where SSH variability is dominated by waves or other processes unrelated
 409 to baroclinic instabilities, a neural network that was trained to represent baroclinically
 410 unstable currents could perform poorly. Thus, it is necessary to develop more general
 411 training datasets that are more representative of the SSH dynamics for any given region of
 412 interest. Those could be ranging from more realistic mesoscale-resolving general circulation
 413 models to simplified stochastic QG-based models Samelson et al. (2019). Note, however,
 414 that it is essential for the synthetic model not to be overly simplistic to the point that
 415 it misrepresents the nature of SSH variability. The drawback of Deep Learning is that it
 416 generally requires a large number of data for training. Nonetheless, there are continuously
 417 improving methods aimed at addressing this practical issue, e.g. transfer learning (Pan &
 418 Yang, 2009) or one-shot learning (Fei-Fei et al., 2006).

419 A way towards ultimately developing the gridded SSH product using machine learning
 420 could be through training networks on a wide range of idealized and realistic models and
 421 then fine-tuning a much smaller number of neural network parameters using existing satellite
 422 data. However, since the true two-dimensional SSH state is not known at any particular time,
 423 the fine-tuning of a neural network cannot be achieved by defining a simple loss function as
 424 was done for synthetic data. Thus, the neural network ultimately would need to use a loss
 425 function that is based purely on observations, without invoking a dynamical model to provide
 426 a true state. This issue could be addressed for example using reinforcement learning, where
 427 two-dimensional SSH fields generated by the neural network would be rewarded or penalized
 428 based on the accuracy of their projection on the observed altimetry tracks that were left

429 out from the input set of tracks. Developing deep learning SSH interpolation techniques
 430 that would stir away from solely relying on dynamical models to provide training data
 431 is a necessary next step towards practical implementation with real satellite observations.
 432 Nonetheless, our work presents an important proof of concept, demonstrating that SSH
 433 observations do contain dynamically-relevant information about subsurface flows and hence
 434 with deep learning it is possible to build a skillful self-contained model of SSH evolution
 435 and as a consequence improve existing SSH estimates.

436 Finally we note another potentially important application of deep learning for state esti-
 437 mation at eddy-resolving scales. Since mesoscale-resolving data assimilation requires large
 438 computations, providing an accurate initial guess could substantially reduce the number of
 439 iterations necessary for optimization. It might be possible to accelerate data assimilation
 440 methods by providing the machine learning estimate as a first guess that is already close to
 441 reality. We thus see the synergy between machine learning and conventional state estima-
 442 tion methods as a potential framework for constructing improved state estimates, combining
 443 the best of the two paradigms: fast data-driven state estimation with machine learning and
 444 fine-tuning to ensure its strict consistency with a given dynamical model achieved by data
 445 assimilation.

446 Acknowledgments

447 G.E.M. thanks Charles Trimble for providing support at the California Institute of Technol-
 448 ogy. L.S. and P.K. acknowledge support from NASA. Discussions with Clement Ubelmann,
 449 Laure Zanna, and participants of the 2019 SWOT Science Team Meeting are highly appre-
 450 ciated. The code to numerically simulate baroclinic QG turbulence was originally written
 451 by Glenn Flierl. The neural network architecture and training scripts coded in Tensor-
 452 flow/Keras along with the synthetic model datasets that were used in this study can be down-
 453 loaded here: https://drive.google.com/drive/folders/1tZrplLw2m19CB1YcQABj6pn0a7_-H63n?usp=sharing
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