Abstract—Multi-satellite measurements of altimeter-derived Sea Surface Height (SSH) and Sea Surface Temperature (SST) provide a wealth of information about ocean circulation. In particular, mesoscale ocean dynamics can be characterized by strong spatio-temporal interactions between SSH and SST fields. Within an observation-driven framework, we investigate the extent to which mesoscale ocean dynamics may be decomposed into a superposition of dynamical modes, characterized by different relationships between SSH and SST fields. Formally, we develop a novel latent class regression model to identify dynamical modes from joint SSH and SST observation series. Applied to the highly dynamical Agulhas region, we demonstrate and discuss the geophysical relevance of the proposed mixture model to achieve a spatio-temporal segmentation of the upper ocean dynamics.

Index Terms—SST, SSH, Observation-driven model, Latent class regression, Mesoscale ocean surface dynamics

I. INTRODUCTION

In the last two decades, multi-satellite measurements of altimeter-derived Sea Surface Height (SSH) and multi-sensor measurements of Sea Surface Temperature (SST) have provided a wealth of information about ocean circulation and atmosphere-ocean interactions. As a depth-integrated quantity dependent upon the density structure of the water column, altimeter SSH estimations capture mesoscale structures, horizontal scales of 50 km to few hundred kilometers, and allow to retrieve surface currents using the geostrophy balance. This emerging and rich mesoscale circulation further stirs the large-scale SST fields. Accordingly, our picture of upper ocean dynamics has considerably evolved towards a complex system characterized by strong interactions, whose spatio-temporal variability extends over a wide range of scales. Furthermore, several studies (cf. [18], [19], [15], [17], [11]) rationalize and demonstrate that fields of SST can become an active tracer coupled to the dynamics leading to strong correlations with SSH fields.

Such a framework can possibly guide the investigation and implementation of improved statistical means to optimally combine existing multi-altimeter SSH measurements with other satellite medium to high resolution observations (e.g., microwave sea surface temperature and salinity, scatterometer winds), augmented by the growing available in situ data (e.g., [1], [8], [22]). Theoretically, the upper ocean turbulence for the horizontal scales between 50 km to few hundred kilometers is still consistent with the geostrophy turbulence theory. To some assumptions, as mentioned above, the upper ocean dynamics may be simply predicted from surface density horizontal variations possibly dominated by SST variations. For such a case, a linear transfer function shall be identified between SSH and SST fields to also possibly lead to the estimation of the subsurface flow (e.g., [14], [18]). This linear transfer function does not involve temporal differencing as in the maximum cross-correlation technique or alternate strategies (e.g., [4], [20], [7]).

This strongly advocates for observation-driven studies to explore and characterize the local relationships between SST, SSH and the derived surface currents from satellite-based routine observations. Yet, as illustrated in Fig. 1, a simple linear transfer function cannot be expected to solely govern the whole mesoscale dynamics in a particular ocean region. As revealed, an overall spatial correlation exists, but for instance, relationships between SST gradients and altimetry-derived surface currents differ. In the warmer SST frontal zone, SST gradients correspond to large surface currents (top of the image). In the colder frontal area, large SST gradients do not reflect in large surface currents (bottom of the image). Finally, over a clearly detected eddy (top-left of the image), associated SST gradients are weak.

Within an observation-driven framework, a plausible assumption is then to consider the local dynamics as a mixture model, consisting in the superposition of a finite set of linear transfer functions. In this paper, we propose to investigate such a model to (i) develop a probabilistic learning-based setting for the inference of such mixture models and the spatio-temporal segmentation of the identified dynamical modes between SST and SSH observations, and to (ii) evaluate the extent to which such mixture models are geophysically relevant to characterize the upper ocean dynamics over active ocean regions.

Hereafter we consider the Agulhas region, and the paper is organized as follows. Section II presents the proposed probabilistic learning-based model. In Section III, the application to satellite observations is evaluated. We further discuss and summarize the key results of our investigations in Section IV.

II. METHODS

A. Approach

As mentioned above, the SST may not be always considered as a passive scalar tracer decoupled to the upper ocean dynamics. Considering SSH to define the large scale flow streamfunction, couplings between SSH and SST are expected. In the Fourier domain, couplings can be expressed as (cf. [12])

\[ \mathcal{F}_H(\text{SSH}) = -\gamma |k|^\alpha \mathcal{F}_T(\text{SST}) \]

(1)

where \( k \) is the horizontal wavenumber vector, \( \mathcal{F}_H \) and \( \mathcal{F}_T \) are filters of SSH and SST respectively. As expressed, the filtered SSH is a smoothed version of the filtered SST. The
\[ \hat{U}, \hat{V} = \sum_{k=1}^{K} \mathcal{F}_k(SST) \] (2)

where \( \mathcal{F}_k \) now characterizes the \( k^{th} \) mode of local coupling between the SST and the streamfunction. We still assume that each dynamical mode \( \mathcal{F}_k \) is parameterized by a linear filter. Using a matrix formulation, Eq. (2) is rewritten as a patch-based linear regression such as

\[ Y_i = \sum_{k=1}^{K} X_i H_k \] (3)

where \( Y_i \) encoded as a 3-dimensional vector given by the SSH value and the surface current \((U, V)\) at spatio-temporal location \( i \). As chosen, \( h \) is set according to the Rossby radius of the study region, which states the mean size of the mesoscale ocean structures like eddies. For the Great Agulhas current region, we set it up to 200 km, i.e. \( h = 4 \) for the spatial resolution of the data in this study.

Given a joint series of SST and SSH satellite observations, our goal becomes first to identify the underlying set of dynamical modes subject to the proposed patch-based setting in Eq. (3), and second, to extract spatial segmentations of these dynamical modes. As described below, we rely on a probabilistic formulation using a latent class model.

B. Latent class regression model

Our objective is to identify \( K \) different dynamical modes (hidden variable \( Z \)) from a joint set of SST patches (\( p \)-dimensional vector \( X \)) and SSH with zonal and meridional surface currents (3-dimensional vector \( Y \)). In this paper, we
assume that the conditional likelihood of $Y$ given $X$ and the dynamical mode $Z = k$ is given by
\[
p(Y|X, Z = k) \propto N_k(Y; X\beta_k, \Sigma_k)
\] (4)
where $N_k$ represents a multivariate Gaussian probability density function with mean $X\beta_k$ and covariance $\Sigma_k$. Hence, the conditional likelihood of $Y|X$ resorts to a mixture of Normal distributions such as
\[
p(Y|X, \theta) = \sum_{k=1}^{K} \lambda_k N_k(Y; X\beta_k, \Sigma_k)
\] (5)
where $\lambda_k$ is the prior probability of mode $k$. To simplify the notations, we store the overall parameters of model (5) in $\theta = (\lambda_1, \ldots, \lambda_K, \beta_1, \ldots, \beta_K, \Sigma_1, \ldots, \Sigma_K)$. In the literature, this model is referred to as a “latent class regression” or “clusterwise regression” (cf. [10]). By construction, it imposes that $0 \leq \lambda_k \leq 1$, $\sum_{k=1}^{K} \lambda_k = 1$ and $\Sigma_k$ is positive defined. The maximum likelihood estimation procedure for model parameters $\theta$ is given below.

C. Model learning

To learn the model parameters $\theta$ of Eq. (5), we resort to a classical maximum likelihood criterion and use an iterative EM procedure (cf. [9]). It relies on the maximization of the log-likelihood given by
\[
\mathcal{L}(\theta) = \sum_{i=1}^{n} \log \left( p(Y_i|X_i, \theta) \right)
\] (6)
where $n$ is the number of observations. From a given initialization, the EM procedure iterates an E-step (Expectation-step) and M-step (Maximization step). At a given iteration, using the Bayes theorem, the E-step resorts to the computation of the posterior likelihoods of the latent variable $Z_i$ for each observation $i$ given current parameter estimate $\hat{\theta}$:
\[
\hat{\pi}_{ik} = \frac{\hat{\lambda}_k N_k \left( Y_i; X_i\hat{\beta}_k, \hat{\Sigma}_k \right)}{\sum_{j=1}^{K} \hat{\lambda}_j N_j \left( Y_i; X_i\hat{\beta}_j, \hat{\Sigma}_j \right)} , \forall k.
\] (7)
The M-step then comes to the maximization of the expectation of the log-likelihood conditionally to the current parameter estimate $\theta$. This leads to update the prior probabilities as
\[
\hat{\lambda}_k = \frac{\sum_{i=1}^{n} \hat{\pi}_{ik}}{n} , \forall k.
\] (8)
The updated regression parameters $\hat{\beta}_k$, $\forall k$ are derived by fitting $K$ separated linear regressions using a weighted least square criterion on the $n$ observations where the weights are given by the posterior likelihoods given in Eq. (7) as in [21]. Then, we maximize $\mathcal{L}$ with respect to $\Sigma_k$ and obtain
\[
\hat{\Sigma}_k = \frac{\sum_{i=1}^{n} \hat{\pi}_{ik} \left( Y_i - X_i\hat{\beta}_k \right)^\top \left( Y_i - X_i\hat{\beta}_k \right)}{\sum_{i=1}^{n} \hat{\pi}_{ik}} , \forall k.
\] (9)
The algorithm iterates the E-step and M-step until a negligible increase of the log-likelihood $\mathcal{L}$ which is strictly growing. A critical aspect of the latent class regression is the choice of $K$, the number of clusters. Different statistical criteria state the selection of parameter $K$ as a trade-off between the likelihood and the complexity of the model (cf. [16]). However, the optimization of these criteria makes no effort to distinguish the error explained by the regression fit and the error explained by the cluster process. In practice, there is an actual potential for overfitting with latent class regression (cf. [5]). Moreover, for a given number of clusters $K$, the problem of consistent estimation of the parameters in the latent class regression turned out to be difficult (cf. [13]). Therefore, we suggest different evaluations of the EM algorithm. The idea is to use random values $\hat{\pi}_{ik}$ as initialization values of the EM procedure and select parameter estimates corresponding to the greatest likelihood (see [3] for more details).

The EM procedure is applied to a training dataset formed by a set of joint SST patches $\{X_i\}_{i \in \{1,...,n\}}$ and SSH with surface current data $\{Y_i\}_{i \in \{1,...,n\}}$, which refer to randomly selected space-time positions in the considered time series of sea surface observations. Overall we typically consider a sample with $n = 10^5$ observations to balance between the representativeness of the training set and the computational complexity of the EM estimation.

D. Segmentation maps and SSH/current predictions

We exploit the inferred model with parameter $\hat{\theta}$ to perform a spatio-temporal segmentation of the underlying dynamical modes. More precisely, for any spatial location $s$ and time $t$, we evaluate the posterior likelihood that the dynamical mode is of type $k$ such as
\[
\hat{\pi}_{sk}(t) = P \left( Z_s(t) = k|X_s(t), Y_s(t), \hat{\theta} \right)
\] (10)
which is equivalent to Eq. (7). Then, the pixel at location $s$ and time $t$ will be assigned to the most likely dynamical mode. One can also estimate for each time $t$, the relative spatial occurrence of each dynamical mode using (8) such as
\[
\hat{\lambda}_k(t) = \frac{\sum_{i=1}^{n(t)} \hat{\pi}_{sk}(t)}{n(t)}
\] (11)
where $n(t)$ represents the number of pixels for a given map at time $t$. Finally, the estimation of the SSH and surface current at the spatial location $s$ and time $t$ is given by the fuzzy regression
\[
\hat{Y}_s(t) = \sum_{k=1}^{K} \hat{\pi}_{sk}(t) X_s(t)\hat{\beta}_k.
\] (12)

III. RESULTS

A. Remote sensing data

As SSH and surface geostrophic current data, we use the daily delayed time Maps of Absolute Dynamic Topography (MADT) produced by Collecte Localisation Satellites (CLS) available online at http://www.aviso.oceanobs.com/. This information combines the signal of several altimeters onto a 1/3 degree Mercator projection grid. We use the 2004 data since four altimeters were available (Jason-1, Envisat or ERS-2, Topex/Poseidon and GFO). As SST data, we use optimally interpolated microwave SSTs provided by Remote Sensing System (RSS) available online at http://www.ssmi.com/.
combines the signal of three microwave radiometers (TMI, AMSR-E and WindSAT) which are robust to the presence of clouds. The spatial resolution is $1/4 \times 1/4$ degrees and the temporal resolution is the same as the MADT data, i.e. daily. We bilinearly interpolate the MADT data onto the SST grid. We focus on the Agulhas region between longitudes $5^\circ E$ to $65^\circ E$ and latitudes $30^\circ S$ to $48^\circ S$.

**B. Characterization of ocean surface dynamics**

As explained in Section II-C, we first extract the SST patches $\{X_i\}_{i \in \{1, \ldots, n\}}$ and the associated SSH with surface current data $\{Y_i\}_{i \in \{1, \ldots, n\}}$ for a random sample of $n = 10^5$ space-time locations over all the possible ones ($\sim 5 \times 10^6$). Then, we fit the latent class regression model and learn model parameters $\theta$ according to the EM procedure. We consider $K = 4$ hidden dynamical modes, i.e. four different linear transfer functions between SST, SSH and surface current. This parameterization is regarded as a trade-off between the interpretation of model parameters and the goodness of the fit. This leads to dynamical modes which are spatio-temporally well-segmented. Given the estimated model parameters $\hat{\theta}$, we determine from Eq. (10) the posterior likelihood $\hat{p}_{ik}(t)$ of each spatio-temporal location $(s, t)$ to be assigned to any dynamical model $k$. From these posterior likelihoods, we determine the segmentation map of each dynamical mode as illustrated in Fig. 3. The animations of the time series of these daily maps in the Agulhas current over 2004 are available here: http://perso.telecom-bretagne.eu/ronanfablet/data/.

A first qualitative analysis of these maps highlights clear spatio-temporal clusters that can be interpreted from a geophysical perspective in terms of different dynamical modes. Also reported are the current, height and temperature statistics for each mode (cf. Fig. 4). The first dynamical mode (red) characterizes very strong current magnitude and warm waters. It is primarily associated with the main Agulhas current that flows down the East coast of Africa through the Agulhas ridge. This mode also involves mesoscale eddies, the so-called warm core Agulhas rings. An example is visible near the location $37^\circ S$, $32^\circ E$ in Fig. 3(a). It corresponds to the eddy identified in the upper left corner of Fig. 1(b) with strong surface currents, low temperature gradients and middle-range SSH values around 0.5 m (cf. Fig. 4(a)) which are discriminative features of this first cluster. The second cluster (green) mainly relates to the eastward Agulhas return current that hits a part of the South Atlantic current. It creates a subtropical front varying from $39^\circ S$ to $44^\circ S$ with strong eastward currents, middle-range SST gradients and large SSH values (about 1 m) as observed in the upper part of Fig. 1(b). The third (cyan) and fourth (blue) modes correspond to weaker surface currents. The third mode is characterized by mid-temperatures and westward currents whereas the fourth one involves colder temperatures and eastward currents. Let us stress that the third cluster involves large SST gradients but weak surface currents such as identified in the lower-part of Fig. 1(b).

Furthermore, the time-dependent segmentation maps of each dynamical mode outlines that we can track the dynamical structures associated with each dynamical mode. We can also analyze the temporal evolution of the relative proportions of the associated locations within the study region, given by parameter $\lambda_k(t)$ in Eq. (11). As obtained, the dynamical modes clearly depict off-phase seasonal variations in 2004 (cf. Fig. 5). Modes 1 (red) and 2 (green) are apparently associated with the intensification of Agulhas current during the Austral summer and of the Agulhas return current during the Austral winter.

We further investigate the geophysical consistency of the identified dynamical modes from the analysis of the surface
currents predicted by the fitted latent class regression model. In Fig. 6, we report a comparison to the true MADT surface currents. Overall, a good agreement is obtained between MADT surface currents and the predictions of the proposed model. The global correlation coefficient is 0.76, and can locally be very large as illustrated in the right column of Fig. 6 (corresponding to the zone depicted in Fig. 1). As found in Fig. 3 this zone involves the four dynamical modes. The mixture model then enables us to retrieve both the large warm eddy (upper left) associated with weak SST gradients, the relatively large surface currents along the large warmer SST gradients (upper part), as well as the rather weak currents along the large but colder SST front (lower part of the zone). By contrast, a single linear transfer function would result in underestimating the surface currents within the warm eddy (upper left) and overestimating the currents of the colder frontal zone (results not shown here).

We also characterize each dynamical mode from global correlation statistics with respect to the true MADT data and a SQG-like hypothesis (cf. Table I). In the study area, recent spectral power law analysis of SSH fields (cf. [23]) explore the consistency with the SQG theory, to be mainly revealed near the edge of the large Agulhas current system. Following our analysis, about 90% of the variability of the MADT surface currents is captured by the linear transfer function for the second and fourth dynamical modes. As derived, these dynamical modes share some agreement with the SQG hypothesis (global correlation coefficients of 0.63 and 0.68, respectively). Note that the fourth dynamical mode also indicates a strong correlation between SST and SSH fields. Mostly excluded from the core Agulhas system, this result somehow confirms the previously reported spectral analysis (cf. [23]). By contrast, the SQG hypothesis poorly fits the first and third modes, with global correlation coefficients of 0.33 and 0.27, respectively.

**IV. CONCLUSION AND PERSPECTIVES**

In this paper, we propose an observation-driven framework to identify and discriminate ocean surface dynamical modes. We rely on a latent class regression model, where the hidden dynamical modes are characterized by a local linear transfer function between SST, SSH and surface current. This probabilistic setting resorts to locally model the distribution of the SSH and sea surface currents conditionally to the SST as a Gaussian mixture of linear transfer functions. The statistical parameters of the model are estimated using a maximum likelihood approach.

We applied the proposed methodology to the 2004 daily $1/4 \times 1/4$ degrees satellite image series of microwave SSTs and SSHs. The reported results retrieved a relevant spatio-temporal decomposition of ocean surface dynamics in the

**TABLE I**

<table>
<thead>
<tr>
<th>Correlation</th>
<th>Cluster 1</th>
<th>Cluster 2</th>
<th>Cluster 3</th>
<th>Cluster 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(U,V)$ and $(U,V)_{\text{SQG}}$</td>
<td>0.92</td>
<td>0.88</td>
<td>0.63</td>
<td>0.88</td>
</tr>
<tr>
<td>$(U,V)$ and $(U,V)_{\text{Latent}}$</td>
<td>0.33</td>
<td>0.63</td>
<td>0.27</td>
<td>0.68</td>
</tr>
<tr>
<td>SST and SSH</td>
<td>0.58</td>
<td>0.82</td>
<td>0.90</td>
<td>0.94</td>
</tr>
</tbody>
</table>
Aguilhas region according to four dynamical modes: (i) the main Aguilhas current and warm core rings characterized by strong currents and hot temperatures where the SST is weakly correlated with SSH, (ii) the return Aguilhas current with lower temperatures and currents but where the SST is dynamically coupled, (iii) local fronts regions where strong SST gradients do not seem to affect the current velocities, and (iv) a weaker dynamical mode where SST is strongly correlated to SSH.

As a key methodological contribution, the proposed mixture model quantitatively helps to extend previous theoretical studies which showed that linear transfer functions could characterize the mesoscale ocean surface couplings between SST and SSH. Such a fully observation-driven approach is coupled with a simple yet flexible parametric probabilistic model, to decompose and define the mixture of linear transfer functions. As analyzed, some modes can recover some SQG-like dynamical properties.

As an extension of this work, we plan to further evaluate the latent class regression model on other strongly active ocean regions such as the Gulf Stream system. The objective will then be to characterize more precisely each component of the different current systems and extract shared dynamical modes. Future work will also investigate more detailed physical interpretation of the proposed latent class regression model to refine the proposed analysis with available in situ subsurface information. As foreseen, such an improved model shall then possibly address both (i) the higher resolution prediction of mesoscale ocean surface currents from SST spatio-temporal fields (and improve the non geostrophic components estimation as in [20], [7]), and (ii) the extraction of new local and global descriptors of ocean surface dynamics from satellite sea surface observations (cf. [2]).

V. ACKNOWLEDGMENTS

We would like to thank the Archiving, Validation and Interpretation of Satellite Oceanographic (AVISO) and the RSS projects for respectively providing the altimeter-derived SSH and surface current, and the microwave SST data.

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Fig. 6. Surface currents from the Maps of Absolute Dynamic Topography (MADT) (a) and from the proposed latent class regression model (c) for the 1\textsuperscript{st} of January 1, 2004 in the Agulhas current with their zoom (b,d) for the zone depicted in Fig. 1.