An Objective Method for Probabilistic Forecasting of Multimodal Kuroshio States using Ensemble Simulation and Machine Learning

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ABSTRACT: This paper presents a method for detecting the ensemble means, spreads, and occurrence probabilities for each of the multiple Kuroshio states. This is accomplished by classifying the forecasts of the ensemble members with a Gaussian mixture distribution model, a machine learning method. Ensemble simulations with 80 members are conducted to reproduce possible occurrences of the multiple Kuroshio states, targeting the large meander event in 2017. To test its performance, first, the method is applied for the southernmost latitude, a conventional index that represents meander intensity. The results show that the Kuroshio initially taking the nearshore nonlarge meander state bifurcates into the large meander and offshore nonlarge meander states, which occur with similar probabilities. Both developments are accompanied by positive potential energy extraction rates, consistent with baroclinic instability. As a more objective approach, the method is then applied for the dominant modes derived from empirical orthogonal function (EOF) analysis of the sea surface height field in the entire Kuroshio region. Importantly, almost identical results can be achieved. In particular, the bimodality between the large meander and nonlarge meander is shown to appear on the axis of the first EOF mode. From a mathematical perspective, this mode can be interpreted as the singular vector which grows most rapidly following the time-evolution operator. Finally, the multimodality of the Kuroshio is reinterpreted as a phase transition phenomenon where the nearshore nonlarge meander constitutes the basic state.

KEYWORDS: Boundary currents; Classification; Kalman filters; Ensembles; Numerical weather prediction/forecasting; Data assimilation

1. Introduction

An interesting feature of the Kuroshio among the western boundary currents is the existence of multiple equilibria in its current path variability, as has been recognized in observations since the 1960s (Shoji 1963; Taft 1972; Kawabe 1985, 1995). The multiple equilibria are basically treated as bimodality, represented by large meander and nonlarge meander states (Fig. 1), whose dynamical interpretation has been provided by several theoretical studies (White and McCreary 1976; Masuda 1982; Yamagata and Umatani 1987; Yoon and Yasuda 1987). In particular, the large meander state, which causes a drastic change in the Kuroshio region, has attracted much attention. The large meander has been shown to be achieved for a range of inlet flow volumes of the Kuroshio (White and McCreary 1976; Masuda 1982; Yoon and Yasuda 1987; Tsujino et al. 2006; Usui et al. 2013), which could be controlled by the basin-scale wind field (Kurogi and Akitomo 2006; Akitomo 2008). In this context, it has recently been proposed that a possible mechanism causing the large meander could be baroclinic instability (Mitsudera and Grimshaw 1994; Qiu and Miao 2000; Endoh and Hibiya 2001; Endoh et al. 2011; Tanaka and Hibiya 2017; Tsujino et al. 2006; Fujii et al. 2008).

It is considered that the perturbation which marks the onset of this instability is a small meander generated southeast of Kyushu, the so-called “trigger meander” (e.g., Shoji 1972;

Solomon 1978). The trigger meander can be induced in a different way for each large meander event. For instance, the trigger meander could be caused by an anticyclonic eddy occurring southeast of Kyushu (Endoh and Hibiya 2001), a cyclonic eddy propagating from the southern recirculation of the Kuroshio (Usui et al. 2008), or frontal waves originating from a disturbance off Taiwan (Miyazawa et al. 2008; Usui et al. 2008). Further, several studies have suggested that the evolution of the large meander depends on the amplitude of the trigger meander (Kamachi et al. 2004; Komori et al. 2003; Miyazawa et al. 2005; Fujii et al. 2008). All of this therefore implies that the transition among the Kuroshio paths is highly sensitive to the initial condition representing the state before the transition, and hence the Kuroshio path variability could be conceived as a probabilistic phenomenon associated with uncertainty involved in the initial condition.

Accordingly, an ensemble forecast could be an effective means for providing a better forecast. Ensemble forecasts are widely utilized in short- and medium-range meteorological contexts (Mureau et al. 1993; Molteni et al. 1996; Buizza 2005), and they provide a statistical mean and variance for various simulations run from different initial conditions. In terms of the Kuroshio, Kamachi et al. (2004) show that predictions for the transition between the nonlarge meander and large meander paths can be improved by considering an ensemble mean of five members rather than only using a single simulation.

However, the ensemble mean does not always provide a realistic prediction, since the statistical average across all the members can hide distinctive features of the states produced by a subset of those members (e.g., Lalaurette 1999). This may

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FIG. 1. Topography of the Kuroshio region (by courtesy of Norihisa Usui). Black curves denote the typical current path (LM: large meander, oNLM: offshore nonlarge meander, nNLM: near-shore nonlarge meander); oNLM and nNLM are both often simply referred to as nonlarge meander. The gray rectangle demarcates the horizontal domain of our numerical simulation.

be problematic for predicting the Kuroshio path variability because each of the multiple equilibria occurs probabilistically. For example, Miyazawa et al. (2005) showed that simulations with 10 members run from similar initial conditions finally bifurcate into the large meander and nonlarge meander paths. The ensemble mean for that case could provide a midstate between them, which is merely an artifact. To resolve this problem, we need to define each statistical mean for each subset of members which share a similar state identified by a classification.

Such a classification of ensemble forecasts leads to prediction of the occurrence probability of multiple equilibrium states. This probabilistic forecast would have two advantages. One is that it is feasible to give probabilistic values to the possibilities of an event such as occurrence/nonoccurrence, which has been predicted in general operational forecasts. This can provide a probabilistic uncertainty gauge concerning the occurrence of phenomena associated with the Kuroshio path variation, such as heavy snowfall or atmospheric storm tracks under the large meander state (Nakamura et al. 2012). The other advantage is that this approach contributes to our collective understandings of the dynamics of multiequilibria in the Kuroshio path. While trimodality in the Kuroshio path is widely recognized in observations (Kawabe 1985, 1995), theoretical and numerical modeling studies to date have treated the transition between the large meander and nonlarge meander states (White and McCreary 1976; Masuda 1982; Yamagata and Umatani 1987; Endoh and Hibiya 2001), and that between the offshore and near-shore paths of the nonlarge meander state (Mitsudera et al. 2001; Ebuchi and Hanawa 2003; Waseda et al. 2003) separately. Examining how many states occur with what probabilities in the ensemble simulations may provide a key to resolve this puzzle.

Conventionally, classification of the Kuroshio paths has been conducted on the basis of indices originally defined by observational studies. For example, the southernmost latitude of the Kuroshio path defined from 136° to 140°E provides an index to discern the large meander state (Kawabe 1995; Yoshida et al. 2006). Further, the difference between the sea levels measured at tidal stations located in Kushimoto and Urugami is used as an index to discriminate between the large meander and nonlarge meander states (Moriyasu 1958; Kawabe 1980, 1989; Sekine and Fujita 1999). The sea level around Hachijo Island is further used as an index to distinguish nearshore and offshore paths in the nonlarge meander state (Kawabe 1985).

In terms of mathematical pattern recognition, the classification of states involves identifying clusters of state vectors for the respective states in a phase space (e.g., Bishop 2006). The dimensions of phase spaces are generally a function of the number of variables and grids. The use of an index means selecting one of the axes in the phase space. This axis, however, does not always appropriately function for all dynamical models, because it is chosen regardless of the characteristics of the trajectory of a dynamical model solution. An alternative approach for avoiding this problem could be to classify the states on the axes given by statistical dominant modes derived from the ensemble solutions.

In the present study, we develop a state-wise ensemble forecast method in combination with a dynamically consistent classification. We conduct ensemble simulations with 80 members, which is the maximum number technically possible on our current computer system. This ensemble size might not be sufficient, but it is still greater than what has been used in previous studies and hence we can simulate a larger number of possible states of the Kuroshio. To classify the ensemble members, we employ a mixture distribution model (MDM), which is a machine learning method capable of finding clusters of members and the respective means and variances in a phase space (e.g., Bishop 2006). In what follows, the MDM is first applied for the aforementioned southernmost latitude to test its performance and then subsequently applied for the phase space composed of statistical dominant modes derived by an empirical orthogonal function (EOF) analysis (e.g., Thomson and Emery 2014) targeting the sea surface height (SSH) field in the entire Kuroshio region instead of the conventional indices.

Since the EOF mode is just a statistical mode, we attempt to elucidate its physical meaning in terms of a dynamical system, compared with singular vector (SV) analysis. The latter approach can identify the solution with the maximum growth rate inherent to the time-evolution operator linearized at a certain time. Such analysis is often utilized to seek the initial state that has the largest impact on a target phenomenon (Mureau et al. 1993; Molteni et al. 1996; Buizza 2005). For example, Fujii et al. (2008) apply it to find the occurrence of the trigger meander prior to the development of the large meander. According to Enomoto et al. (2015), SV analysis can be defined in the ensemble space (hereafter, EnSV analysis), while maintaining theoretical consistency with the original. In this paper, we will see that our dominant EOF mode can be

regarded as the dominant SV mode developed from the initial state of the Kuroshio in our simulations, conducting the EnSV analysis.

The remainder of the paper is organized as follows. In [section 2a](#), the configuration of the ensemble forecasts is described. [Section 2b](#) provides an overview of MDM and the method for its application to our probabilistic forecast. [Section 2c](#) contains the EOF and EnSV analyses employed in this study. [Section 3](#) presents the results, demarcated into three parts. First, the mixture distribution model is applied for the southernmost latitude data ([section 3a](#)). Second, we apply our method for the SSH field for the entire Kuroshio region ([section 3b](#)). Third, we will see that our EOF mode can be interpreted as the SV mode ([section 3c](#)). Finally, conclusions are put forward in [section 4](#).

2. Methods

a. Ensemble forecast system

We have developed a regional ensemble forecast system for south Japan based on a parallelized version of the Princeton Ocean Model ([Jordi and Wang 2012](#)). This system is an improved version of the original developed by [Miyazawa et al. \(2012\)](#). The model covers the region of 28°–36°N and 128°–142°E with a resolution of 1/36° horizontally and 47 sigma levels vertically. The system covers a wider area and has a greater vertical resolution than the original. The model topography is derived from a 1/120° gridded product provided by the Japan Hydrographic Association, “JTOPO30.”

The model is driven by wind stress and heat fluxes, which are calculated from 6-hourly NCEP–NCAR reanalysis data ([Kalnay et al. 1996](#)) using bulk formulae ([Kagimoto et al. 2008](#)). The surface salinity flux is relaxed to surface salinity of monthly mean climatology (*World Ocean Atlas 2001*; [Conkright et al. 2002](#)), with a restoring scale of 10 m in space and 30 days in time. The lateral boundary conditions are given by outputs of a JAMSTEC operational ocean model (JCOPE2M; [Miyazawa et al. 2017](#)) with a horizontal resolution of 1/12°, which produces analysis data by assimilating satellite SSH anomaly, satellite sea surface temperature (SST), and in situ temperature and salinity (*T/S*) data based on a multiscale three-dimensional variational method ([Miyazawa et al. 2017](#)). No tide forcing is included in our model.

Eighty ensemble runs start from 1 January 2017. The initial conditions are given by temperature and salinity sampled from data of the JAMSTEC operational model in the period from 1 December 2016 to 28 February 2017 with a time interval of 2 days. For the first month, forecasts of the ensemble simulation converge near optimal values by assimilating the observational data using the local ensemble transformation Kalman filter (LETKF; [Hunt et al. 2007](#); [Miyoshi et al. 2010](#)).

The LETKF method in the present system is a successor to the original version ([Miyazawa et al. 2012](#)). In short, LETKF updates the ensemble mean and deviations from the mean of the forecasts of the ensemble members with the following equations:

$$\bar{\mathbf{x}}^a = \bar{\mathbf{x}}^f + \mathbf{X}^f \mathbf{w}^a, \quad (1)$$

$$\mathbf{x}^{a(i)} = \bar{\mathbf{x}}^a + \mathbf{X}^f \mathbf{W}^{a(i)}, \quad (2)$$

where $\mathbf{x}^f$ and $\mathbf{x}^a$ are n -dimensional vectors that represent a forecast and an analysis for each ensemble member, respectively, where n is the number of model grids times the number of variables. The term $\mathbf{X}^f$ is an $n \times m$ matrix that contains m columns of deviations from the ensemble mean, where m is the ensemble size. The weight $\mathbf{w}^a$ is an m -dimensional vector optimized by the observation data and ensemble forecasts, and $\mathbf{W}^{a(i)}$ is an $m \times m$ matrix calculated from the ensemble forecasts.

The observational data to be assimilated by LETKF are satellite SSH anomaly (*Jason-2*, *Jason-3*, *CryoSat-2*, *SARAL/Altika*), SST (*Himawari-8*, *WindSat*, *Global Change Observation Mission–Water 1*, and *Global Precipitation Measurement*), and *T/S* data (*Global Temperature–Salinity Profile Program*). In LETKF, observational data located outside a specified radius of each model grid point are not assimilated. Following [Miyoshi et al. \(2007, 2010\)](#), the distance is defined horizontally $\tilde{d}_h$ and vertically $\tilde{d}_v$, and set to be $\tilde{d}_h \equiv \delta_h 2\sqrt{10/3}$ and $\tilde{d}_v \equiv \delta_v 2\sqrt{10/3}$, respectively, where δ_h and δ_v are chosen to be 36 km and 2000 m, respectively ([Miyazawa et al. 2012](#)). Observation errors of the data are enhanced by multiplying by a factor, $\exp\{0.5[(d_h/\tilde{d}_h)^2 + (d_v/\tilde{d}_v)^2]\}$, where d_h and d_v are respectively horizontal and vertical distances from the target model grid. LETKF is applied every 2 days with a time window of ± 5 days for sea surface height and ± 1 day for temperature and salinity. Note that this time interval is sufficiently shorter than the typical transition time scale of the multimodal states of the Kuroshio path variation.

Following assimilation, we conduct ensemble forecast runs from 1 February to 14 June 2017, during which the large meander has not occurred in the real ocean. Note that all the members experience unique atmospheric forcing and boundary conditions. This means that we examine the probabilistic behavior of the Kuroshio associated with only intrinsic variabilities in the ocean. In terms of an operational forecast, this experimental setting may be a substantive constraint, given that a change in the wind field can cause the transition of the Kuroshio state (e.g., [Kurogi and Akitomo 2006](#)). However, understanding the probabilistic variability intrinsic to the ocean may provide useful information for forecasts with stochastic forcings in the future.

b. Clustering method

The MDM technique can be used to decompose a general probability distribution into multiple distributions. Although any type of distribution could be a possible candidate for each distribution, here we consider the Gaussian distribution. An advantage of this choice is that we can estimate a set containing the mean and variance of each cluster, which provides the spatial pattern characterizing the cluster and its uncertainty. This estimation can be regarded as an extension of the conventional ensemble mean and spread to a multimodal system. The use of the Gaussian distribution has another advantage. Recall that stochastic approaches in ocean modeling are generally premised on the Gaussian distribution as many data assimilation techniques including the LETKF method adopt this. Such a stochastic approach is justified for linear systems

FIG. 2. Example of 2-class Gaussian MDM. The original distribution is expressed by the sum of the two Gaussian distributions whose means are μ_1 and μ_2 , and variances are σ_1 and σ_2 .

with random noise, but may not work in fully nonlinear contexts. In such cases, multiple Gaussian distributions may be needed to approximate the distribution governing the forecast in terms of curve fitting. In other words, the need for multiple Gaussian distributions to represent an original distribution implies the system being fully nonlinear.

The MDM method with a Gaussian distribution is called the Gaussian MDM. Because this method has been applied widely in the literature, we only provide key procedural information; interested readers may refer to Bishop (2006) for theoretical details. The Gaussian MDM represents an arbitrary probability distribution as a linear combination with Gaussian functions having different parameters. Let $\mathcal{N}(\mathbf{x}|\mu, \Sigma)$ be a multivariate Gaussian distribution with a set comprising mean μ and covariance matrix Σ for a D -dimensional variable $\mathbf{x}$. With this notation, the Gaussian MDM with K -class decomposition can be expressed as

$$p(\mathbf{x}|\{\pi_k\}, \{\mu_k\}, \{\Sigma_k\}) = \sum_{k=1}^K \pi_k \mathcal{N}_k(\mathbf{x}|\mu_k, \Sigma_k), \quad (3)$$

where π_k is the mixing coefficient. The bracket $\{A_k\}$ for an arbitrary variable, A_k , means a set of the variable, i.e., $\{A_k\} = (A_1, A_2, \dots, A_K)$. An example of a 2-class Gaussian MDM applied to a bimodal distribution for a one-dimensional variable is shown in Fig. 2. The task here is to seek optimal parameters, μ_k , Σ_k , and π_k in (3), that best reproduce the original distribution.

Parameter estimation is conducted following the expectation–maximization (EM) algorithm (Dempster et al. 1977; McLachlan and Krishnan 2007). This algorithm is executed in the following E- and M-steps after giving initial μ_k , Σ_k , and π_k for the K classes. For the E-step, we calculate the so-called “responsibility” of each class (posterior probability of given $\mathbf{x}$), defined as

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}_k(\mathbf{x}_n|\mu_k, \Sigma_k)}{\sum_{k=1}^K \pi_k \mathcal{N}_k(\mathbf{x}_n|\mu_k, \Sigma_k)}, \quad (4)$$

which is positive definite. The responsibility for $\mathbf{x}_n$ (n is the number of samples) tends to be small with distance from the

mean. For the M-step, the parameters, μ_k , Σ_k , and π_k , are updated by calculating

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^N \gamma_{nk} \mathbf{x}_n, \quad (5)$$

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^N \gamma_{nk} (\mathbf{x}_n - \mu_k)(\mathbf{x}_n - \mu_k)^T, \quad (6)$$

$$\pi_k = \frac{N_k}{N}, \quad (7)$$

where $N_k = \sum_{n=1}^N \gamma_{nk}$ and N is the size of samples. The mixing coefficient defined in (7) indicates the fraction of the number of samples belonging to k -class among the total number of samples and hence can be regarded as the occurrence probability of k -class. The responsibility γ_{nk} plays the role of a weight in (5) and (6). The E- and M-steps are repeated until the likelihood function defined as

$$\ln p(\mathbf{X}|\text{params}) = \sum_{n=1}^N \ln \left\{ \sum_{k=1}^K \pi_k \mathcal{N}_k(\mathbf{x}_n|\mu_k, \Sigma_k) \right\} \quad (8)$$

reaches a maximum, where params is a shorthand for the parameters shown on the left-hand side of (3).

The MDM itself cannot determine the total number of classes, since K is a given parameter. This yields a problem whereby the MDM with a large K is misjudged as a better model since the likelihood function becomes large with increasing K . To avoid an erroneous outcome, here, we determine the optimal K that maximizes the Akaike information criterion (AIC) and Bayesian information criterion (BIC) defined as

$$\text{AIC: } \ln p(\mathbf{X}|\text{params}) - M, \quad (9)$$

$$\text{BIC: } \ln p(\mathbf{X}|\text{params}) - \frac{M}{2} \ln N, \quad (10)$$

respectively, where

$$M \equiv K + DK + \frac{D}{2}(D+1)K \quad (11)$$

(e.g., Bishop 2006). These information criteria penalize the MDM having a large K . Although these criteria generally tend to select a small K , this property may not be particularly crucial in clustering the Kuroshio path, because it has three states at most.

In the machine learning domain, the MDM is recognized as a kind of latent variable model. Self-organizing maps (SOMs) and k -means clustering, which are often used in ocean research (Straus et al. 2007; Leloup et al. 2007; Yoshida et al. 2014), also belong to this group. We provide brief details in what follows; see Bishop (2006) for a more in-depth treatment. If we focus only on results, all the methods estimate a mean value using a formula which is identical to (5). In the k -means method, the weights (responsibility) are given as 0 or 1, while in the SOM, they are given as Gaussian functions on the latent space.

The responsibility in the Gaussian MDM [Eq. (4)] indicates the likelihood (between 0 and 1) of a sample n belonging to a

class k . A higher value means that a sample n is more likely to be within a class k . The continuous nature of such responsibility values means that the Gaussian MDM is capable of measuring ambiguity in similarity among samples. In contrast, k -means clustering does not allow for any ambiguity, since it defines responsibility as taking a value of only 0 or 1. Taking an example of a 2-class decomposition, all the states including an indiscernible state are classified into either of the classes in k -means clustering. Indeed, k -means clustering applied for the classification of the Kuroshio state in Yoshida et al. (2014) formally discriminates the states that are located in very close proximity to each other in a phase space.

c. EOFs and singular vectors

We will conduct the EOF analysis in section 3b and the obtained EOF mode is reinterpreted by the singular vector in section 3c. This reinterpretation exploits the mathematical identity between the EOF analysis and SV analysis, which is essentially the same as that already argued in previous studies (e.g., Kelly 1988), except for using the ensemble members. The reader familiar with this identity may skip the details of the mathematical argument, and just note the method of our EOF analysis and the aim of the SV analysis here.

In section 3b, we classify the Kuroshio states using the SSH data for the entire Kuroshio region in terms of pattern recognition. This classification seeks to demarcate the SSH data in the phase space whose dimension is the number of horizontal grids (506×290). However, expecting that the typical Kuroshio paths have large SSH variances, we extract statistical modes by applying the EOF analysis for the SSH field. As a first step, we coarsened the grid resolution to have 10 times larger spacing between grid points in both the zonal and meridional directions to remove finescale fluctuations. The resultant coarsened grids have a horizontal resolution of $0.27^\circ \times 0.27^\circ$, which is sufficient to represent the large-scale Kuroshio path variations. Defining a data matrix $\mathbf{Z}$ with size $n \times m$, where n is the number of horizontal grids and m is the ensemble size ($m = 80$), we perform the EOF analysis for the covariance matrix $\mathbf{ZZ}^T$. Solving the eigenvalue problem for this covariance matrix yields a set of m eigenvalues and corresponding eigenvectors that provide horizontal mode structures (EOF modes).

The equivalence between the EOF analysis and SV analysis can be shown as follows. We begin by briefly reviewing the SV analysis. Let $\mathbf{y}$ and $\mathbf{z}$ be n -dimensional vectors of disturbance defined at an initial time (initial disturbance) and a subsequent time (final disturbance), respectively. The linear temporal evolution from $\mathbf{y}$ to $\mathbf{z}$ may be expressed as

$$\mathbf{z} = \mathbf{M}\mathbf{y}, \quad (12)$$

where $\mathbf{M}$ is an $n \times n$ matrix representing the time-evolution operator of the dynamical system linearized at the initial time. To identify the initial disturbance that enlarges the norm, we pose a cost function with the constraint of $\mathbf{y}^T\mathbf{y} = 1$ such that

$$J(\mathbf{p}) \equiv \mathbf{z}^T\mathbf{z} + \lambda(1 - \mathbf{y}^T\mathbf{y}), \quad (13)$$

where λ is a Lagrange multiplier. With the aid of (12), maximizing this cost function with respect to $\mathbf{y}$ leads to

$$\mathbf{M}^T\mathbf{M}\mathbf{y} = \lambda\mathbf{y}, \quad (14)$$

which is an eigenvalue problem with λ as the eigenvalue and $\mathbf{y}$ as the eigenvectors. The corresponding $\mathbf{z}$ can be obtained using the relation (12). The solutions $\mathbf{y}$ and $\mathbf{z}$ are referred to as the right and left singular vectors, respectively. The task in the SV analysis is to identify these singular vectors.

EnSV analysis (Enomoto et al. 2015) reformulates SV analysis using the ensemble members. Considering the ensemble size of m , we have m initial and final disturbances such that

$$\mathbf{Y} \equiv (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_m), \quad (15)$$

$$\mathbf{Z} \equiv (\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_m). \quad (16)$$

Using these disturbances, we express $\mathbf{y}$ as a linear combination of $\mathbf{Y}$:

$$\mathbf{y} = \mathbf{Y}\mathbf{p}, \quad (17)$$

where $\mathbf{p}$ is an m -dimensional vector. Further, from (12), we have

$$\mathbf{z} = \mathbf{Z}\mathbf{p}. \quad (18)$$

Then, the cost function (13) can be expressed as a function of $\mathbf{p}$ and maximizing it with respect to $\mathbf{p}$ leads to the following generalized eigenvalue problem:

$$\mathbf{Z}^T\mathbf{Z}\mathbf{p} = \lambda\mathbf{Y}^T\mathbf{Y}\mathbf{p} \quad (19)$$

For the case where $n = m$ and $\mathbf{Y}$ is linearly independent, $\mathbf{y}$ and $\mathbf{z}$ defined in (17) and (18), respectively, are consistent with the left and right singular vectors in the original SV analysis, respectively. Note that if $\mathbf{Y}$ is orthonormal, Eq. (19) simply becomes

$$\mathbf{Z}^T\mathbf{Z}\mathbf{p} = \lambda\mathbf{p}. \quad (20)$$

Enomoto et al. (2015) examine the reliability of EnSV analysis in an ensemble simulation with initial conditions that are orthonormal.

Our EOF analysis is the dual problem for the EnSV analysis for the case where $\mathbf{Y}$ is the orthonormal. This can be confirmed if we express (20) in the dual formalism:

$$\mathbf{p} = \frac{1}{\sqrt{\lambda}}\mathbf{Z}^T\mathbf{z} \quad \text{and} \quad \mathbf{ZZ}^T\mathbf{z} = \lambda\mathbf{z}, \quad (21)$$

and

$$\mathbf{z} = \frac{1}{\sqrt{\lambda}}\mathbf{Z}\mathbf{p} \quad \text{and} \quad \mathbf{Z}^T\mathbf{Z}\mathbf{p} = \lambda\mathbf{p}. \quad (22)$$

The formula on the left of (22) is the same as (18), where it is normalized by $\sqrt{\lambda}$ to give the dual formalism in a symmetric expression. We find that our EOF analysis concerns the eigenvalue problem shown on the right of (21). Given the theoretical consistency between the EnSV and original SV analyses, the EOF modes can be regarded as the left singular vectors. However, $\mathbf{Y}$ is practically not orthonormal and thus

FIG. 3. SSH fields for member (a),(c) 3 and (b),(d) 76 at (top) initial and (bottom) near end date of forecast run (black contours). Units are meters. Thick black contours denote 0 m. Color shading denotes the ensemble mean of SSH for all the members.

the singular vectors based on a certain initial state can be somehow different from the EOF modes. In section 3c, we examine how these modes are similar to each other.

3. Application

a. Conventional Kuroshio large meander index

All the members initially take the nonlarge meander path but about 2 months later some members take the large meander path (Fig. 3). This can be clearly confirmed in a time series diagram of the southernmost latitude of the current axis within the longitudinal range of 136°–140°E, where the current axis is defined as the contour of SSH of 0 m (Fig. 4). This value is chosen subjectively so as to visualize a well-developed meander path, but we will adopt a more objective approach in the next subsection. At the beginning of the forecast, the southernmost latitudes for all the members are located near the coast, but they diverge with the passage of time and finally bifurcate as is evident in the histogram at the end date (Fig. 5). After the bifurcation, a conventional single ensemble mean merely shows a state like the offshore nonlarge meander, ignoring the possibility of the occurrence of the large meander (shades in Figs. 3c,d).

Applying Gaussian 2-class MDM for the southernmost latitude data at the end date, we find that the mean and spread are 30.2°N and 0.7°, respectively, for one of the classes and 32.4°N

and 0.5°, respectively, for the other (Fig. 5). Both AIC and BIC select 2 classes as optimal. Although these means and spreads are obtained from clustering in one-dimensional data, the corresponding spatial fields can be estimated by exploiting the responsibility γ_{nk} , which contains information on the clusters. That is, writing $\tilde{\mathbf{x}}$ for the horizontal SSH field, the corresponding means and spreads, which are denoted by $\tilde{\boldsymbol{\mu}}_k$ and $\tilde{\boldsymbol{\Sigma}}_k$, respectively, are formulated as

$$\tilde{\boldsymbol{\mu}}_k \equiv \frac{1}{N} \sum_{n=1}^N \gamma_{nk} \tilde{\mathbf{x}}_n, \quad (23)$$

$$\tilde{\boldsymbol{\Sigma}}_k \equiv \frac{1}{N} \sum_{n=1}^N \gamma_{nk} (\tilde{\mathbf{x}}_n - \tilde{\boldsymbol{\mu}}_k)(\tilde{\mathbf{x}}_n - \tilde{\boldsymbol{\mu}}_k)^T. \quad (24)$$

Note that these formulas are formally the same as those in (5) and (6), although there are differences with respect to the variables with tilde. The means for these two classes calculated in (23) clearly indicate the large meander and nonlarge meander states (Fig. 6). Given that most of the SSH contours for the nonlarge meander state pass through south of Hachijo Island (Fig. 6b), the initial nearshore nonlarge meander state is most likely to evolve into either the large meander or offshore nonlarge meander state, at least, in this ensemble experiment.

Figure 7 shows the results of the Gaussian MDM application at each time. Information criteria indicate that a branch to the

FIG. 4. Time series diagram of the southernmost latitude of the Kuroshio current axis defined as the 0-m contour in SSH for each ensemble run. Color gradient from blue to red is based on the values at the end date.

large meander and nonlarge meander occurs about 3 months (28 April 2017) after the start of the forecast. These two states are found to be robust, as their spreads rarely overlap in the duration after the branch (Fig. 7a). This experiment shows that the nonlarge meander tends to occur with a larger probability near the end of the forecast (Fig. 7b). This higher occurrence probability for the nonlarge meander state is consistent with the fact that the real Kuroshio path took the nonlarge meander state at that time (Usui 2019).

How does the initial Kuroshio state develop into the final large meander and offshore nonlarge meander states? To examine the temporal evolution toward each final state, we group the ensemble members using the responsibility γ_{nk} at the end date. That is, the members assigned by $\gamma_{nk} > 0.9$ are defined to be in k group, where k is 1 or 2 due to the 2-class decomposition. The group showing the large meander state is referred to as the LM group. We further divide the group showing the nonlarge meander state into the nearshore nonlarge meander and offshore nonlarge meander groups, which are referred to as the nNLM group and oNLM group, respectively. In this discrimination, we follow the conventional definition that the nearshore nonlarge meander occurs north of Hachijo Island, while the offshore nonlarge meander is to the south. There are 35 LM groups, 28 oNLM groups, and 12 nNLM groups. Note that the remaining five members are dropped out by the criterion $\gamma_{nk} > 0.9$.

Further, to examine whether the transitions to the bimodal states can be induced by baroclinic instability, we calculate the so-called potential energy (PE) extraction rate, which indicates the transfer of potential energy from the background state to the eddy field. Denoting variables with overbar and prime for the background and eddy fields, respectively, the PE extraction rate can be expressed as

$$-\frac{g}{\bar{\rho}_z} \mathbf{u}' \cdot \nabla \bar{\rho}, \quad (25)$$

where g is the gravitational force, ρ is the density of seawater, and $\mathbf{u}$ is the horizontal velocity vector (e.g., Vallis 2006). Also, $\bar{\rho}_z$ is the vertical derivative of $\bar{\rho}$ and ∇ is the horizontal gradient operator. This formula shows that energy is transferred into the eddy (background) field for positive PE extraction rate values. In general usage, the PE extraction rate is defined by the temporal average of (25) and the variables denoting the background and eddy fields are regarded as time mean and deviation from it (e.g., Masina et al. 1999; Wells et al. 2000; Miyazawa et al. 2004). However, since this definition does not provide an appropriate result for a developing field, Tsujino et al. (2006) proposed a different approach, in which a variable at a certain time represents the background field, while the deviation from it at the subsequent time represents the eddy field. Therefore, we calculate the PE extraction rate

FIG. 5. Normalized histogram of the southernmost latitudes at the end date. Solid and dashed curves denote the probability distributions estimated by 2-class Gaussian MDM.

FIG. 6. Mean (contour) and standard deviation (gray shade) for the different classes identified by Gaussian MDM applied for the southernmost latitude data. The black dot denotes the location of Hachijo Island.

following this latter approach and take the ensemble average for each group. Further, prior to the calculation of the PE extraction rate, all the variables are horizontally smoothed using a Gaussian filter with a 0.5° scale to reduce the influence of small-scale phenomena such as warm water intrusions.

The LM group evolves following a pattern frequently captured by previous studies (e.g., Tsujino et al. 2006). First, a trigger meander occurs southeast of Kyushu just after starting the forecast run. The development of this trigger meander seems to be supported by a large positive PE extraction rate in its southern side (shade in Fig. 8a), suggesting the induction of cold inshore water by anticyclonic circulation into the southern flank of the trigger meander. This trigger meander moves to the downstream, anchored off Kii Peninsula (Fig. 8b). At this stage, the trigger meander begins to develop to the large meander, accompanied by a positive PE extraction rate in its western side (Fig. 8c). This feature is consistent with the baroclinic instability shown in previous studies (Tsujino et al. 2006; Fujii et al. 2008). At the final stage, growth of the large meander ceases, while the positive PE extraction rate still governs in the western side of the large meander (Fig. 8d).

Figure 9 shows the temporal evolution for the oNLM group. This group shows the trigger meander accompanied by a large positive PE extraction rate in its southern side (Fig. 9a). The trigger meander, however, is located just east of Kyushu, which is somewhat north compared to the LM group. The positive PE extraction rate associated with the trigger meander moves to the downstream, while the signal of the trigger meander migration itself is obscured in the SSH field (Fig. 9b). At the developing stage of the offshore nonlarge meander, the positive PE extraction rate is widely extended along the Kuroshio path east of Kii Peninsula (Fig. 9c), similar to what has been reported previously (Fujii et al. 2008). This horizontal structure in the PE extraction rate persists to the stage of the offshore nonlarge meander (Fig. 9d). With this group, the occurrence of a negative anomalous SSH field is notable just behind Kii Peninsula and it merges into a large negative core at the trough of the meander (Figs. 9b–d). This subsequent process is consistent with the coalescence of high potential vorticity water

generated by the sharp coastal topography of Kii Peninsula with the existing cyclonic circulation associated with the meander (Waseda et al. 2003).

According to extant literature, the offshore nonlarge meander is a transient phenomenon that repeats the near-shore and offshore paths on a time scale of several months (Mitsudera et al. 2001; Ebuchi and Hanawa 2003; Waseda et al. 2003). Since the period of our forecast run is about 5 months, it is possible that our nonlarge meander states are also transient phenomena. The nNLM group, however,

FIG. 7. Time series of (a) mean and spread (standard deviation) and (b) mixing coefficient for the probability distribution decomposed by Gaussian MDM. The optimal number of classes is diagnosed by information criteria.

FIG. 8. Temporal evolution of ensemble mean SSH (contour) and vertically integrated PE extraction rate (shade) for LM group. Units of SSH and PE extraction rate are meters and $10^{-7} \text{ m}^2 \text{ s}^{-3}$, respectively. Note that the density in the calculation of the PE extraction rate is divided by a reference density. The black dot denotes the location of Hachijo Island.

shows a robust straight path along the Japanese coast for the vast majority of the period, while fluctuating occasionally (not shown). This suggests that the offshore and nearshore nonlarge meander states are distinctive modes in the Kuroshio although the analysis period might be too short to authoritatively confirm this.

b. Case of SSH field

Here, we conduct a classification of the Kuroshio states using the EOF analysis for the SSH data in the entire Kuroshio region. Table 1 shows the eigenvalues derived from the EOF analysis for the data. Eigenvalues are rapidly reduced within the first three dominant modes, indicating that the characteristics of the Kuroshio path based on SSH can be sufficiently expressed in a few dimensions. In particular, modes higher than the fourth mode contribute little, i.e., less than 10%. For this reason, we classify the SSH field in the space composed of the three dominant EOF modes.

Figure 10 shows a scatterplot of the solutions of all ensemble members in the phase space constructed by the three dominant EOF modes. Those plots are obtained by the projections of the SSH field to each mode. Applying MDM with 2-class decomposition derives two means with variances (shown as red and blue dots and lines in Fig. 10). The choice of 2 classes is justified

based on results from both the AIC and BIC. The corresponding horizontal fields for the two means calculated using (23) contain the large meander and nonlarge meander states similar to those in Fig. 6 (not shown).

These two clusters tend to be confined along the first-mode axis (Figs. 10b–d). This can be confirmed more clearly by the histogram of the solutions on each eigenmode, which shows that only the first mode has clear bimodality in the solutions (Fig. 11a). Furthermore, this bimodality well separates the aforementioned LM and NLM groups, whereas these groups are not clearly distinguishable on other mode axes (dot and cross symbols in Figs. 11a–c). This means that the horizontal distribution of the first mode represents the difference between these two states. In fact, the first mode has a strong amplitude in the large meander region (Fig. 11d) and its negative (positive) sign indicates the lower (higher) pressure anomaly associated with the large meander (nonlarge meander). At the same time, the first mode also has an extremum at the outlet of the Kuroshio, whose positive sign represents an outflow stuck to the Japanese coast typical in the large meander (Fig. 11d).

Then, is it possible to distinguish the nearshore and offshore paths of the nonlarge meander? According to previous studies, these nonlarge meander are defined as states

FIG. 9. As in Fig. 8, but for oNLM group.

with outlet paths located north and south of Hachijo Island, respectively (e.g., Kawabe 1995). Therefore, considering that the current velocity is proportional to the SSH gradient, the mode that can distinguish the two states should have an extremum near Hachijo Island. Such a feature is found in both the first and third modes (Figs. 11d,f), but the first mode should be excluded since it merely reflects the difference in the outlet flows between the large meander and nonlarge meander states.

Therefore, we consider further classification of the nonlarge meander on the third-mode axis. As a first step, this requires removing the members with the large meander state because they are also projected on this axis. As per section 3a, the responsibility γ_{nk} yielded in the three-dimensional classification in the EOF space can be leveraged to accomplish this. That is, we only retain those members showing the nonlarge meander state that satisfies $\gamma_{nk} > 0.9$, where k group indicates the nonlarge meander state. The histogram for those members on the third-mode axis has a minimum point at about 1.0 (Fig. 11c). If we divide the members into two groups by this value, the ensemble mean of the group that has a larger (smaller) value on the third-mode axis shows the nearshore (offshore) nonlarge meander state (Fig. 12). The members belonging to each group are the same as the aforementioned nNLM and oNLM groups. Note that the second mode may indicate fluctuations of the meander position along an east–west direction.

c. Comparison with singular vectors

To examine the extent to which our first EOF mode is consistent with the first SV mode, we apply EnSV analysis to our simulation results. We assume that the temporal evolution of the Kuroshio state is governed by a linear process in the duration from the time of the occurrence of the trigger meander (25 February 2017) to the end date (14 June 2017). This assumption may be strong, but could be reasonable if we consider that the development of the Kuroshio state from the nearshore nonlarge meander state is caused by baroclinic instability. The EnSV mode is obtained by solving (19) because $\mathbf{Y}$ defined here is not orthonormal. Since this calculation involves an inverse matrix of $\mathbf{Y}^T\mathbf{Y}$, computational error becomes large if $\mathbf{Y}$ includes linearly dependent members. To mitigate this problem, we thus only use 41 members that have cross correlations less than 0.9. Note that $\mathbf{Z}$ is also composed of the same members.

TABLE 1. Eigenvalues for EOF modes at the end date.

Mode No.	Eigenvalue (contribution)
1	9.0 (39%)
2	4.6 (20%)
3	2.3 (10%)
4	1.3 (5%)
5	1.0 (4%)

FIG. 10. Scatterplot of ensemble solutions at the end date in phase space consisting of three dominant EOF modes derived from SSH: (a) three-dimensional plot, and (b)–(d) projection to two-dimensional spaces composed of different modes. Red and blue dots with lines denote the means and standard deviations identified by Gaussian MDM. Some lines indicating standard deviation are obscured due to the view angle or tiny length.

The first EnSV mode for the final disturbance is shown in Fig. 13b. As expected from the theoretical argument on the duality, this mode has a similar horizontal structure to the first EOF mode. Because of nonidentical elements in $\mathbf{Y}^T\mathbf{Y}$ and removal of some members, the correlation of the first EnSV mode with the first EOF mode remains at 0.78, but is still higher than those with other dominant EOF modes (Table 2). Interestingly, the total field calculated as ensemble mean minus (plus) the first EnSV mode represents the large meander state (nonlarge meander state) (Figs. 13d,f). The corresponding EnSV mode for the initial disturbance tends to have a larger amplitude in the upstream region of the Kuroshio (Fig. 13a) and the total field in the initial state corresponding to the large meander state (nonlarge meander state) has a signal of the trigger meander located southeast (east) of Kyushu although it is somewhat obscured (Figs. 13c,e), compared with the result from the classification (Figs. 8a and 9a).

The application of EnSV analysis here is the same as that of SV analysis in Fujii et al. (2008), except that we used the ensemble members. Those authors examine the temporal evolution of the Kuroshio in a single simulation in two cases, in which the first SV mode for the initial disturbance is added to and subtracted from the background initial state, respectively; their results suggest that those different conditions yield the different development of the Kuroshio state, as we have seen above. This suggests that the first SV mode is well represented by the first EnSV mode obtained from a limited number of the members and hence the first EOF mode can be interpreted as the first SV mode.

4. Summary and conclusions

This paper proposed a method to identify the ensemble mean, spread, and occurrence probability of each distinct and possible Kuroshio path. This was accomplished by classifying the ensemble

FIG. 11. Normalized histogram of SSH projected onto (a)–(c) three dominant EOF modes and (d)–(f) horizontal distributions of these modes at the end date. Values for each projection are normalized by the square root of the corresponding eigenvalue. Dots and crosses denote the values for the members belonging to the LM group and other groups (oNLM and nNLM groups), respectively, obtained from the 2-class decomposition in the MDM method applied to the large meander index (see section 3a). The histogram without gray shade in (c) denotes the projection to the third mode after removing the solutions containing the large meander state (see text in section 3b). The horizontal distribution of each mode is normalized so that the norm is unity. Contours in the (d)–(f) denote ensemble means for all the members in meters. The black dots in (d)–(f) denote the location of Hachijo Island.

members with Gaussian MDM. The number of possible Kuroshio paths (clusters) is selected according to the AIC and BIC. This method was successful in detecting the bimodality between the large meander and nonlarge meander states in the ensemble forecast targeting the large meander event in 2017, by classifying the ensemble members in the southernmost latitude, a conventional index to represent meander intensity. We also showed that a nearly identical result can be achieved when we apply the

classification in the phase space composed of the dominant EOF modes for the SSH field over the Kuroshio region.

The classification in the EOF space may provide an alternative method, free from any conventional indices, to identify possible Kuroshio path states. The first EOF mode is found to work as an index that classifies the large meander and nonlarge meander states, while the third EOF mode can be used to further distinguish between the nearshore and offshore paths

FIG. 12. Ensemble mean SSH for (a) nNLM group and (b) oNLM group. Units are meters. The black dot denotes the location of Hachijo Island.

FIG. 13. Horizontal distribution of SSH disturbance derived from ensemble singular vector analysis and corresponding total fields at (left) initial date (25 Feb 2017) and (right) final date (14 Jun 2017). (a),(b) The SSH disturbances (color) and ensemble means (contours). Contour intervals for the ensemble mean are 0.1 m. The total fields defined by the sums of the ensemble mean (c),(d) minus and (e),(f) plus the disturbances.

in the nonlarge meander state. Those EOF modes can be interpreted as the SV modes that represent linearly growing solutions for the time-evolution operator in the dynamical system (section 3c). In this sense, these EOF modes are not merely statistical, but can be regarded as having a physical meaning.

The fact that significant clusters representing the large meander and nonlarge meander states appear on the axis of the first EOF mode may help understanding the transition process among the multiple equilibria in the Kuroshio path. In a general theory for a phase transition, the multiple equilibria can be explained as possible realizations of a dominant mode which grows due to some instability (e.g., Haken 1977). Recall that our ensemble forecast showed the bifurcation into the large meander and offshore nonlarge meander states from the nearshore nonlarge meander state accompanied by the occurrence of the PE extraction rate consistent with baroclinic instability (section 3a). Given that, additionally, the two Kuroshio states after the bifurcation are in a direction close to that of the first SV mode, the trimodality in the Kuroshio paths may be explained by a phase transition mechanism with a basic state of the nearshore nonlarge meander state, triggered by baroclinic instability such as the pitchfork branch in a general dynamical system (e.g., Drazin 2002). Although this warrants

further theoretical attention, if this is tenable, the difference in persistence between the large meander and offshore nonlarge meander states (Kawabe 1995; Mitsudera et al. 2001; Waseda et al. 2003) is characterized by the difference in the nonlinear properties for the respective states.

Since we only conducted the ensemble forecast for the large meander event in 2017, caution needs to be observed in generalizing the results. Different transitions may occur in the ensemble forecast for a different large meander event. In particular, the occurrence probability of a state may change since it depends on the initial conditions, which could be different in a different period. However, if the multimodality in the Kuroshio is an intrinsic phenomenon, a similar bifurcation to what was found here will occur, although the occurrence probability of each state may be different from that in the present study. Otherwise, the multiple Kuroshio states are just forced phenomena, which is inconsistent with the fact that

TABLE 2. Correlation between the most dominant mode of EnSV and EOF modes at the end date.

EOF1	EOF2	EOF3
0.78	−0.36	0.36

numerical models for the Kuroshio under uniform external forcing can reproduce multimodality responsive to nonlinear parameters (Yoon and Yasuda 1987; Akitomo 2008).

The classification method with the Gaussian MDM and the EOF analysis could be applied in other contexts because it is independent of numerical model selection. Probabilistic forecasting of the El Niño–Southern Oscillation or Indian Ocean dipole, which researchers have attempted to simulate with huge ensemble sizes in recent years (Doi et al. 2019; Tompkins et al. 2017), may be possible candidates. In addition, our method could contribute to the development of probabilistic ocean dynamics theory, through comparison with a stochastic ocean model to predict probability distribution functions consistent with the ensemble simulations (Bessires et al. 2017).

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