Statistical Inversion of Surface Ocean Kinematics from Sea Surface Temperature Observations

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(Manuscript received 29 March 2018, in final form 10 August 2018)

ABSTRACT

The sea surface temperature (SST) record provides a unique view of the surface ocean at high spatio-temporal resolution and holds useful information on the kinematics underlying the SST variability. To access this information, we develop a new local matrix inversion method that allows us to quantify the evolution of a given SST perturbation with a response function and to estimate velocity, diffusivity, and decay fields associated with it. The matrix inversion makes use of the stochastic climate model paradigm—we assume that SST variations are governed by a linear transport operator and a forcing that has a relatively short autocorrelation time scale compared to that of SST. We show that under these assumptions, the transport operator can be inverted from the covariance matrices of the underlying SST data. The accuracy of the results depends on the length of the time series, and in general the inverted properties depend on the spatial and time resolution of the SST data. Future studies could use the methodology to explore the interannual variability of SST anomalies; to estimate the scale dependency of ocean mixing; and to estimate anomaly propagation, both at the surface and in the interior. The methodology can be easily used with any gridded observations or model output with adequate time and spatial resolution, and it is not restricted to SST. The inversion code is written in Python and distributed as a MicroInverse package through GitHub and the Python Package Index.

1. Introduction

Sea surface temperature (SST) varies at different time and space scales, and these variations have been linked to the variability in several climate and environmental phenomena (Deser et al. 2010). In addition, the SST data provide valuable information on surface ocean kinematics as it is observed at high spatial and temporal resolution. It is therefore of interest to characterize SST variability and to use the SST data to characterize ocean kinematics. To this end we develop a local linear matrix inversion method (Jeffress and Haine 2014b,a) to quantify the evolution of the SST field with a response function and to derive the associated SST velocity, diffusivity, and decay fields.

In the past, several statistical methods have been used to assess SST variability and related predictability (Hasselmann 1976; Frankignoul 1985; Saravanan and McWilliams 1998; Buckley et al. 2014, 2015; Yamamoto and Palter 2016; Ærthun and Eldevik 2016; Ærthun et al. 2017; Roberts et al. 2017). In addition, sequential pairs of SST images have been used to infer surface velocities (Emery et al. 1986; Kelly 1989; Vigan et al. 2000a,b; Chen et al. 2008, and references therein). The former studies are usually motivated by climate-related questions, while the latter studies are often more operational in scope. Our methodology is statistical, and therefore similar to the former methods, although some aspects of it, such as usage of spatial covariances, have similarities with the latter approaches. In the following we introduce these approaches, before describing our methodology (see section 5 for more comparison between the different methods).
One of the most widely used statistical approaches to understand SST variability is the lagged correlation analysis, in which the anomaly propagation speed is derived from the time lag of maximum correlation between two locations (e.g., Sutton and Allen 1997; Arthun et al. 2017). These studies often report propagation speeds on the order of a few centimeters per second (cm s\(^{-1}\)), which are generally an order of magnitude slower than the mean current speeds in the ocean. Consequently, these studies find climate predictability over lead times of several years and attribute it to the slow SST (or upper-ocean heat content) anomaly propagation (Sutton and Allen 1997; Arthun et al. 2017). Despite its wide usage, the lagged correlation approach has several shortcomings. The lagged correlations tend to be weak unless the underlying data are low-pass filtered in time (Foukal and Lozier 2016). However, such filtering can be problematic, especially if applied over a time scale at which the forcing varies, because the separation between the forcing and the response becomes ambiguous. In fact, Foukal and Lozier (2016) demonstrated that the results of Sutton and Allen (1997) were likely an artifact of the filtering time scale that incorporated the effect of the changing North Atlantic Oscillation on the filtered SST anomaly field. Finally, a more fundamental problem with the lagged correlation approach is that by focusing on the peak correlation, one recovers only one travel time between two points, whereas an advective–diffusive system hosts a distribution of travel times. Such a travel-time distribution can be represented by a response function (Green’s function) that solves the SST anomaly equation for an impulse forcing (Jeffress and Haine 2014a). The ability to derive such a response function is one of the advantages of the matrix inversion presented here.

Another statistical approach is the linear matrix modeling, which is popular in statistical climate prediction (Penland and Magorian 1993; Penland and Sardeshmukh 1995; Penland and Matrosova 1998; Penland and Hartten 2014; Newman 2007; Alexander et al. 2008; Piterbarg and Ostrovskii 1997; Ostrovskii and Piterbarg 2000; Ostrovskii and Font 2003; Deser et al. 2003; Zanna 2012) and in analysis of model predictability (Tziperman and Ioannou 2002; Tziperman et al. 2008; Hawkins and Sutton 2009). Linear matrix modeling assumes that the time evolution of SST (or another parameter of interest) is governed by a linear transport operator and a white noise forcing. As we will show, the linear transport operator can be recovered from the covariance matrices of the SST anomaly vector at different time lags. Because the dimensions of the covariance matrices become very large as the spatial domain size increases, it is a common practice to build the inversion on empirical orthogonal functions (EOF) or some other reduced-size basis set. For example, Frankignoul et al. (1998) invert for the SST anomaly decay rate from autocorrelation by averaging SST over a large region in the North Atlantic. In that case, the transport operator is dominated by air–sea interaction, as the mean current and eddy activity are weak. A related approach moves one step further and focuses on the eigenvectors of the linear transport operator, also known as principal oscillation patterns (POP) (Hasselmann 1988; von Storch et al. 1995, and references therein).

Instead of using EOFs or POPs to reduce the degrees of freedom of a large dataset, it is possible to build the inversion upon covariances that are local in space. In this approach, one inverts a small covariance matrix for each grid cell and its immediate neighbors. For example, Piterbarg and Ostrovskii (1997), Ostrovskii and Piterbarg (2000), and Ostrovskii and Font (2003) perform such a local inversion and invert for velocity, diffusivity, decay rate, and mixed layer entrainment (which form their transport operator) in the North Pacific and in the North Atlantic. In this study we will also use a stencil that is local in space to solve for the transport operator but use a somewhat different approach than Piterbarg and Ostrovskii (1997), Ostrovskii and Piterbarg (2000), and Ostrovskii and Font (2003) in solving for it (see our section 5 for details).

In addition to the statistical approaches, different inversion methods are used to estimate ocean surface velocities from pairs of SST images (or even from single SST images given some additional constraints; e.g., Isern-Fontanet et al. 2017). These studies usually infer the ocean velocities by either using feature tracking (maximum cross correlation) or by solving the heat equation. The focus is also on short time scales (<1 day), and these studies neglect diffusion (or effectively include the effect of diffusion in the velocity estimates) and decay of the anomalies. Finally, it is worth noting that in the fluid dynamics community, there is a wide field of particle image velocimetry (for a recent review, see Westerweel et al. 2013) that focuses on estimating a flow field from a sequence of images through cross correlation.

Our approach is based on the linear matrix modeling framework (Jeffress and Haine 2014b,a). We assume that the SST variability behaves as a linear system with stochastic forcing (Hasselmann 1976), and it can be written as

\[
\frac{d}{dt} x(t) = B x(t) + f(t),
\]

where \( x(t) \) is an \( M \times 1 \) vector of global (\( M \) refers to spatial locations) SST anomalies from a climatology; \( B \) is a constant \( M \times M \) matrix operator containing all the
processes acting on the SST field; and \( f(t) \) is the \( M \times 1 \)

stochastic forcing vector, representing the sources and sinks of SST anomalies (see Table 1). Given a time series of SST anomalies, \( x(t) \), Eq. (1) provides a possibility for estimating \( \mathbf{B} \) via matrix inversion, as long as some information exists about \( f(t) \). As shown in detail in section 3c, we can exploit \( \mathbf{B} \) in two ways: it yields an estimate of the response function for an instantaneous step forcing with which one can derive, for example, travel-time distributions. And, with certain assumptions, it yields estimates of physical fields, such as SST velocity, diffusivity, and decay rate. We believe that using \( \mathbf{B} \) in these ways will be the most useful applications of the methods presented in this manuscript.

We structure this paper as follows: first we derive an inversion method for solving the transport operator \( \mathbf{B} \) in section 2, we discuss decomposing \( \mathbf{B} \) and the numerical implementation of the inversion in section 3, and we evaluate the inversion method in section 4 (and in appendix B). We compare the chosen methodology to other approaches in section 5 and conclude in section 6.

2. Theory

Using different time lags, several methods exist for estimating \( \mathbf{B} \) from Eq. (1). We focus on one that is similar to the widely used linear inverse model, it reads

\[
\mathbf{B} = \frac{1}{\tau} \log([x(t + \tau)x^T(t)]/[x(t)x^T(t)])^{-1}. \tag{2}
\]

Here, the multiplication of \( x \) and its transpose results in covariance matrices, \([ ]^{-1}\) denotes a matrix inverse, and \( \log \) denotes a matrix natural logarithm (see section 3b for numerical implementation). There are four time scales: \( \Delta t \) is the data sample rate, \( \tau \) is a time lag (an integer multiple of \( \Delta t \)), \( \tau_f \) is the forcing decorrelation time scale, and \( \tau_c \) is the decorrelation time of the SST anomalies themselves. Here \( \tau \) lies between \( \tau_f \) and \( \tau_c \). Note that throughout the derivation, we assume an infinitely long time series of \( x \), but we discuss the error associated with finite-length observational time series in section 4b(1).

Equation (1) is an inhomogeneous first-order linear differential equation and can be solved using the variation of constants method. At time lags 0 and \( \tau \), the solutions are

\[
x(t) = \int_{-\infty}^{0} e^{-\mathbf{B}t'} f(t + t') dt' \tag{3}
\]

and

\[
x(t + \tau) = e^{\mathbf{B}\tau} x(t) + \int_{-\tau}^{0} e^{-\mathbf{B}t'} f(t + \tau + t') dt', \tag{4}
\]

where \( t' \) is the integration variable. Here we see that the eigenvalues of \( \mathbf{B} \) need to have negative real parts in order for the anomalies and memory of prior forcing to decay. Multiplying Eq. (4) by \( x^T(t) \) gives

\[
x(t + \tau)x^T(t) = e^{\mathbf{B}\tau} x(t)x^T(t) + \int_{-\tau}^{0} e^{-\mathbf{B}t'} f(t + \tau + t')x^T(t) dt'. \tag{5}
\]

Substituting Eq. (3) for \( x^T(t) \) in the right-hand side integral gives

\[
x(t + \tau)x^T(t) = e^{\mathbf{B}\tau} x(t)x^T(t) + \int_{-\tau}^{0} \int_{-\infty}^{0} e^{-\mathbf{B}t'} f(t + \tau + t')f^T(t + t') e^{-\mathbf{B}t''} dt'' dt'. \tag{6}
\]

For forcing, \( f(t) \), with an autocorrelation time scale \( \tau_f < \tau \), the forcing covariance term disappears because \( \tau + \tau' \to 0 \), while \( \tau'' \to 0 \); therefore, the two forcing terms are separated by time at least \( \tau (\tau < \tau' - \tau') \) and thus not correlated. Equation (6) simplifies to

\[
x(t + \tau)x^T(t) = e^{\mathbf{B}\tau} x(t)x^T(t). \tag{7}
\]
Solving for $\mathbf{B}$ gives Eq. (2). If the forcing autocorrelation is not smaller than $\tau$, then the double integral term in Eq. (6) becomes the error term.

The derivation of Eq. (2) is only one possibility to solve for $\mathbf{B}$ from Eq. (1). Generally, one can solve for $\mathbf{B}$ by combining solutions to Eq. (1) at relevant time lags so that the forcing term disappears because its autocovariance vanishes after a sufficient lag. A comparison of other methods to estimate $\mathbf{B}$ from Eq. (1) is left for future work.

3. Implementation

Here we move from the theoretical realm of the previous section to a practical realm. In particular, we always have a finite-length time series and are left with an estimate $\mathbf{B}$ of the true transport operator $\mathbf{B}$. In this study we use the daily record of global SST at 0.25° horizontal resolution between 1982 and 2016 [NOAA OISST; Reynolds et al. 2007; $M = O(10^5)$ wet points]. In particular, we base the main analysis on the Advanced Very High Resolution Radiometer (AVHRR)-only version of the OISST data, which blend the AVHRR satellite measurements with ship and buoy observations, and interpolate to fill the gaps. In appendix C we also perform the analysis using the OISST dataset that also includes the data from the Advanced Microwave Scanning Radiometer for EOS (AMSR-E) instrument. Indeed, the procedure for finding $\mathbf{B}$ is not data specific and could be applied to any gridded tracer data with adequate time and spatial resolution, and for which Eq. (1) is a reasonable assumption.

Further, we assume that we can use a local five-point stencil ($K = 5$; Fig. 1) to estimate $\mathbf{B}$, even though Eq. (2) is strictly valid only when $\mathbf{x}(t)$ is global and $[\mathbf{x}(t) \mathbf{x}^T(t)]$ describes a global covariance matrix. This assumption is effectively used in forward numerical modeling as well, and it is motivated by the fact that the SST evolution is governed by partial differential equations, which are local in nature—that is, $\mathbf{B}$ is sparse and has only $O(K)$ nonzero elements per row. The advantage is twofold. Given the finite, noisy observations, a local method might be more accurate because the global $M \times M$ covariance matrix could be dominated by random covariances in the far field (which disappear in the case of infinite time series). Computationally, the local method is also more feasible, as we can solve for the elements of $\mathbf{B}$ by iterating Eq. (2) for $M$ times using covariance matrices of size $K \times K$ instead of directly solving for $\mathbf{B}$ using the $M \times M$ covariance matrix.

a. Preprocessing of the input data

In this study we are interested in characterizing the mechanisms behind the oceanic part of SST variability.

![Fig. 1. Illustration of the five-point stencil, and the notation used in Eqs. (10) and (11).](image)
relationship at around spatial scales of 1000 km in the North Pacific (see their Fig. 2). We perform the high-pass filtering by removing an area average of 8° longitude × 4° latitude surrounding each location. Different choices of filter size have very little impact on the results [see section 4b(4)]. This spatial high-pass filtering leaves an SST record where the forcing term \( f(t) \) is mainly due to oceanic instabilities (see section 3c and appendix A). Even after spatial filtering, the problem of choosing an appropriate \( \tau \) remains: we describe our procedure for optimizing \( \tau \) in section 3d.

b. Technical implementation

The inversion is implemented in parallel Python code, which inverts the OISST record in roughly an hour on a standard UNIX cluster using \( O(10) \) cores, of which most of the time is spent in data input/output (I/O).

In terms of the matrix operations (matrix division and matrix logarithm), we rely on their Python implementations in the numpy.linalg package. The package provides the logm function for the matrix logarithm, which is similar to, for example, logm in MATLAB. However, Python does not provide an upper-level method for matrix division, so we employ a dot product between the numerator and the pseudoinverted denominator (pseudoinverse with numpy.linalg.pinv). This procedure is similar to, but less error prone than, the denominator (pseudoinverse with numpy.linalg.pinv).

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c. Output

The aim of the inversion is to estimate the transport operator \( \mathbf{B} \), which provides two valuable insights into the underlying data. They are

1) ESTIMATE OF THE RESPONSE FUNCTION \( \mathbf{G} \)

The transport operator \( \mathbf{B} \) provides the means to estimate the response function (Green’s function) \( \mathbf{G}(t) \). This \( M \times M \) response function is the solution to Eq. (1) for an impulsive forcing at each location,

\[
\frac{d}{dt} \mathbf{G}(t) - \mathbf{B} \mathbf{G}(t) = \delta(t),
\]

where \( \mathbf{I} \) is an \( M \times M \) identity matrix and \( \delta \) is the Dirac delta function. The solution to Eq. (8) is

\[
\mathbf{G}(t) = e^{\mathbf{B}t},
\]

and \( \mathbf{G}(t) \) describes the global evolution of an impulse forcing at time \( t = 0 \). In future work we plan to use \( \mathbf{G}(t) \) to estimate the distribution of travel times of surface temperature and salinity anomalies, and the related predictability.

2) DISCRETIZATION OF \( \mathbf{B} \)

The transport operator \( \mathbf{B} \) describes the spatial discretization of the different terms in the partial differential equation governing the evolution of SST anomalies, and we can estimate these terms by decomposing \( \mathbf{B} \). We assume that the SST anomalies are created by stochastic atmospheric and oceanic forcing, after which their evolution is governed by horizontal advection, diffusion, and local decay (which represents surface interaction with the atmosphere and the ocean thermocline). Such a system can be described with an advection–diffusion–relaxation equation, which we derive in appendix A.

We relate the elements of \( \mathbf{B} \) to spatially discretized advection, diffusion, and decay terms in Eq. (A6), using a five-point stencil [four cells surrounding the central cell \((i, j)\) at right angles; Fig. 1]. The central column, vector \( \mathbf{B}_h \), of the \( 5 \times 5 \) matrix \( \mathbf{B} \), contains the elements of interest, that is, those that involve cross covariances between the central cell \( h \) and the four surrounding cells. We denote the cell location in the vector \( \mathbf{B} \) with a superscript and the cell location in the spatial grid by a subscript. Using central differences for the spatial discretization, we arrive at

\[
\begin{align*}
\hat{B}^h_{i,j+1} &= \frac{\kappa^x}{\Delta x^2} - \frac{1}{2\Delta y} \left( u - \frac{\partial \kappa^x}{\partial y} \right), \\
\hat{B}^{i+1,j} &= \frac{\kappa^y}{\Delta y^2} - \frac{1}{2\Delta x} \left( u - \frac{\partial \kappa^y}{\partial x} \right), \\
\hat{B}^h_{i,j} &= \frac{2\kappa^x}{\Delta x^2} - \frac{2\kappa^y}{\Delta y^2} - r, \\
\hat{B}^{i-1,j} &= \frac{\kappa^x}{\Delta x^2} + \frac{1}{2\Delta x} \left( u - \frac{\partial \kappa^x}{\partial x} \right), \\
\hat{B}^{h}_{i,j-1} &= \frac{\kappa^y}{\Delta y^2} + \frac{1}{2\Delta y} \left( v - \frac{\partial \kappa^y}{\partial y} \right).
\end{align*}
\]

Here the local stencil and the parameters \((u, v), (\kappa^x, \kappa^y)\), and \( r \) are centered at location \((i, j)\) containing the values of the time mean velocity vector, the time mean diffusivity tensor (with off-diagonal elements set to 0), and the time mean decay rate, respectively. The values \( \Delta x \) and \( \Delta y \) are the grid sizes of the underlying data in the zonal and meridional directions, respectively. Note that both a north–south- and east–west-oriented stencil or a 45° rotated stencil provide very similar results. Further, one could use a larger discretization stencil; for example, a nine-point stencil can be used to solve for the full diffusivity tensor (Jeffress and Haine 2014b). However, implementation of such a nine-point stencil returned noisy estimates of the velocities and diffusivities with the OISST data. We hypothesize that these noisy estimates
are due to random covariances in the corner cells, which are relatively far away from the central cell (see Fig. 1). Indeed, the results improve when the data points in the stencil are interpolated to an equal distance from the central cell. However, such an interpolation adds another layer of complexity and should be ideally done with raw data (not processed data such as OISST), which is why we restrict ourselves to the five-point stencil in this manuscript.

Estimates of velocity, diffusivity, and decay rate at each location \((i,j)\) are found from Eq. (10) given an estimate of \(B\) in the five-point stencil:

\[
\hat{u}^* = u^* + \epsilon_B^u = \Delta x (B_{i-1,j} - B_{i+1,j}),
\]

\[
\hat{v}^* = v^* + \epsilon_B^v = \Delta y (B_{i,j-1} - B_{i,j+1}),
\]

\[
\hat{k}^* = \hat{k}^* = \epsilon_B^k = \Delta x^2 \left( \frac{B_{i-1,j} + B_{i+1,j}}{2} \right),
\]

\[
\hat{\rho} = \rho + \epsilon_B^\rho = -\frac{2}{\Delta x^2} \frac{\hat{B}_{i,j}^x}{\Delta y^2} - \frac{2}{\Delta y^2} \frac{\hat{B}_{i,j}^y}{\Delta x^2} + \sum_{ij} \hat{B}.
\]  

(11)

Here, the \(\epsilon\) terms represent the error arising from estimating \(B\) from a finite time series (of length \(N\)) on a local stencil. We estimate the effective velocity \(\hat{u}^* = u - (\partial \hat{k}^*/\partial x)\), \(\hat{v}^* = v - (\partial \hat{k}^*/\partial y)\) instead of \(u, v\) because the \(\hat{k}^*/\hat{x}, \hat{k}^*/\hat{y}\) are indistinguishable from the velocity components. For notational convenience, we henceforth remove the asterisks and refer to the effective velocity simply as velocity. Iterating Eq. (11) for all \(M\) locations yields a complete estimate of the velocity, diffusivity, and decay rate fields. We do not apply the method at boundary locations or impose any boundary conditions. The result is an open boundary that allows SST anomalies to flow freely out of the domain at the edges.

The aforementioned discretization implies that both diffusivity and velocity are estimated at a horizontal scale of \((2\Delta x, 2\Delta y)\). Thus, when the inversion method is used with model data (see appendix B), one expects to recover the gridscale \((\Delta x, \Delta y)\) diffusivity only if there are no velocity–temperature fluctuations at the \((2\Delta x, 2\Delta y)\) scale.

d. Optimizing \(\tau\)

As mentioned in section 1, a sensible choice for \(\tau\) is between the forcing decorrelation time scale \(\tau_1\) and the decorrelation time scale of the SST anomalies \(\tau_s\). In other words, one wants to assure that \(\tau\) is large enough so that the covariances in Eq. (2) are not caused by the forcing, that is, \(\tau_1 < \tau\), and do not vanish; that is, \(\tau < \tau_s\). In addition to these upper and lower limits, the discretization on the local five-point stencil imposes additional requirements. In particular, \(\tau\) must be less than the time it takes for the flow to propagate information beyond the local five-point stencil. Therefore, we require that \(uv/\Delta x < 1, uv/\Delta y < 1, \kappa^x/\Delta x^2 < 1, \) and \(\kappa^y/\Delta y^2 < 1\), which leads to an upper limit for \(\tau\); that is, \(\tau_{\text{max}} = \min(\Delta x/\kappa, \Delta y/\kappa, \Delta x^2/\kappa^x, \Delta y^2/\kappa^y)\). Note that the same constraints were used by Piterbarg and Ostrovskii (1997). In practice we first evaluate the \(\tau_{\text{max}}\) given the inverted velocity field (using maximum velocities over all \(\tau\)) and then impose the \((\kappa^x, \kappa^y)\) restrictions; the results are reported at the specific \(\tau_{\text{max}}\) at each location (Fig. 2).

While the resulting \(\tau_{\text{max}}\) generally respects the constraints from the autocorrelation time scale, \(\tau_1 < \tau < \tau_{\text{max}}\), in several regions, the upper limit is not respected \((\tau < \tau_s)\). At daily time resolution, such regions are found in the tropics and in the eastern rims of the subtropical gyres where \(\tau_s\) approaches \(\Delta t\) (minimum possible \(\tau\)) (Fig. 3a). Elsewhere, the autocorrelation time scale is well above the local \(\tau\) (Fig. 2). However, at lower time resolutions, \(\tau_s\) approaches \(\Delta t\) also in the midlatitudes (Figs. 3b–d), suggesting that the inversion might be less feasible when the time resolution grows large.

In this context note that the usefulness of the inversion for inferring oceanic properties is limited by the processes affecting the SST variability. Specifically, the transport operator \(B\) has to dominate the SST variability at time scale \(\tau\), otherwise estimating \(B\) via the inversion is not possible. In regions like the eastern rims of the subtropical gyres at daily time resolution, most of the SST variability is dominated by the atmosphere at all time and spatial scales, making it practically impossible to tease out an oceanic signal even with the spatial filtering (Fig. 3).

4. Results

First we provide estimates of the inverted velocity, diffusivity, and decay fields, after which we evaluate the sensitivity of the inversion to \(\tau, \Delta t\), and the spatial resolution of the SST data. For an idealized test case we refer to appendix B.

a. General description

1) VELOCITY

We expect the inverted velocity field at 0.25° resolution to capture the velocity at which mesoscale eddies (in the extratropics) and linear Rossby waves (in the tropics) propagate. Both features move at the Rossby wave speed Doppler shifted by the depth-averaged background flow (Klocker and Marshall 2014).
Indeed, both the inverted velocity field and the eddy velocity field [derived from the sea surface height–based eddy atlas of Chelton et al. (2011); similar to Fig. 1a in Klocker and Marshall (2014)] show a comparable structure dominated by ubiquitous westward propagation (Figs. 4a,b). Outside the tropics (i.e., poleward of 20°S–20°N), the root-mean-square error (RMSE) between the two velocity fields is 3 cm s$^{-1}$ for both velocity components. In the tropics the inversion velocities are notably smaller than the eddy velocities (Figs. 4a,b) with an RMSE of 9 and 5 cm s$^{-1}$ for zonal and meridional velocities, respectively. A more detailed analysis, and an inversion of sea level anomaly data (not shown), reveals that in the extratropics the SST-based velocities closely follow the velocity estimates from the eddy atlas and sea level anomaly–based inversion (i.e., record the Rossby wave speed) but that this relationship breaks in the tropics. There, the SST-based velocities are close to the underlying current velocities, and we suggest that the 0.25° resolution is enough in the tropics to see the deformation of the SST field by the strong zonal jets (and their shear).

As expected for the surface flow, the sea surface height–based geostrophic estimates (OSCAR; ESR 2009; Bonjean and Lagerloef 2002), and drifter data (Laurindo et al. 2017), render much higher velocities and different circulation features than the inversion- or eddy-atlas-based velocity estimates (Figs. 4b–d). Globally, a comparison to inverted velocities yields RMSE of $(u = 6 \text{ cm s}^{-1}, v = 4 \text{ cm s}^{-1})$ for OSCAR velocities and $(u = 11 \text{ cm s}^{-1}, v = 8 \text{ cm s}^{-1})$ for drifter velocities.

In appendix B we show that the velocities are unreliable when the decay term becomes large compared to the advection (specifically if $r \Delta x / u > 1$, $r \Delta y / v > 1$). This condition is respected in most of the global ocean, except in the subpolar regions in both hemispheres and in

![Figure 2](http://journals.ametsoc.org/doi/pdf/10.1175/JTECH-D-18-0057.1)

**FIG. 2.** Optimized $\tau$ after applying velocity- and diffusivity-based restrictions as discussed in section 3d. Areas that are under sea ice cover (more than 15% ice concentration) more than 50% of the time are masked with light gray.

![Figure 3](http://journals.ametsoc.org/doi/pdf/10.1175/JTECH-D-18-0057.1)

**FIG. 3.** SST autocorrelation $e$-folding time scale with changing time resolution $\Delta t$. Autocorrelation is calculated from the spatially high-passed daily OISST anomaly data (spatial filter is 4° in latitude, 8° in longitude), and we show the time (days) at which autocorrelation drops below $e^{-1}$. 

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FIG. 4. Comparison of different velocity estimates. (a) Inverted velocity field, (b) velocity field estimated from the daily atlas of sea surface height–based eddy tracks (covering 1993–2016; Chelton et al. 2011), (c) satellite altimetry–based OSCAR velocity climatology (mean over 1993–2016; ESR 2009; Bonjean and Lagerloef 2002), and (d) drifter velocity climatology (based on data from surface drifters between 1979 and 2015; Laurindo et al. 2017). Color illustrates speed, and the streak lines are plotted with the Python matplotlib streamplot function. Gray shading in (a) indicates areas where the inversion becomes unreliable as the SST autocorrelation drops below 1 day, and gray shading in (b) indicates regions where the velocity estimate is based on fewer than 10 eddies.
the tropical western Pacific Ocean and in the northern Indian Ocean: in these regions the velocity estimates are noisy and unreliable, which is evident also by visual inspection of the streamlines there (Fig. 4a). Note that despite the spatial filtering, an atmospheric imprint on the velocities remains a possibility, especially if the intrinsic oceanic variability is weak.

2) DIFFUSIVITY

Diffusivity peaks in the most energetic regions of the ocean in boundary currents and in the tropics (Fig. 5b) as one would expect based on the eddy kinetic energy distribution (e.g., Klocker and Abernathey 2014). We note that the inversion produces negative diffusivities in regions where the SST variability is reduced to white noise after the data is high-pass filtered, that is, $\tau_x < \tau$ (this issue is reduced when AMSR-E data are included; see appendix C). Ocean diffusivities are mainly $O(100) \text{ m}^2 \text{ s}^{-1}$, while peak values are a few thousand square meters per second ($\text{m}^2 \text{ s}^{-1}$). The ratio between the two diffusivity components is somewhat noisy, but in general it is close to unity, suggesting isotropic diffusion, and the anisotropic regions tend to coincide with strong ocean currents (see the contours in Fig. 5b). A closer look at these regions (not shown) suggest that the anisotropy is mainly due to suppression of the across-stream diffusivity component (Ferrari and Nikurashin 2010; Naveira Garabato et al. 2011; Klocker and Abernathey 2014; Abernathey and Marshall 2013; Cole et al. 2015; Rypina et al. 2012).

FIG. 5. (a) Inverted speed, (b) mean diffusivity, and (c) decay time scale. Gray shading indicates areas where the inversion becomes unreliable as the SST autocorrelation drops below 1 day. In (b) the cyan contour indicates regions where $\kappa_x > 2 \kappa_y$ and the purple contour indicates regions where $\kappa_y > 2 \kappa_x$. 

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The largest diffusivities occur in the tropical eastern Pacific and tropical Atlantic. Note that Klocker and Abernathey (2014) argued that these regions are dominated by linear Rossby waves and therefore an eddy-diffusivity closure (see appendix A) is not valid. However, we suggest that while linear waves themselves do not mix diffusively, mixing caused by wave breaking can be represented by a diffusive closure. Therefore, we relate the tropical maximum in diffusivity to mixing by breaking Rossby waves.

In appendix B we show that because of the central differencing scheme, the inversion overestimates diffusivities at large Peclet numbers, particularly when $u \Delta x / \kappa^i > 1$ and $u \Delta y / \kappa^i > 1$. Since the meridional velocities $v$ are small, the latter limit is practically never met, but in the tropics $u$ is large and $u \Delta x / \kappa^i$ peaks around 3. We can correct for the related error in $\kappa^x$ by deriving a relation (exponential) between the Peclet number and the error; to this end we use the results from appendix B (Fig. B1a). The correction (not shown) is zero for most of the ocean and therefore does not affect the main geographical features in Fig. 5b. However, 10% of the $\kappa^x$ errors are over 50%. These largest errors are found in the tropics, and there the correction decreases the peak magnitude of $\kappa^x$ to around 3000 m$^2$ s$^{-1}$, which is similar to values of $\kappa^y$ in the same region.

3) Decay time scale

Patterns of the local decay time scale reflect the patterns of the SST autocorrelation (cf. Figs. 3, 5c) and one can indeed derive a close relation between the two (not shown). The decay time scale peaks at both frontal regions, suggesting that frontal perturbations are long lived, and in eddy-rich locations it is similar to eddy lifetime (cf. Fig. 5c to Fig. 5 in Chelton et al. 2011). In regions with strong atmospheric coupling (e.g., tropical Indian Ocean and tropical western Pacific), the decay time is short even when the velocities are small, as the atmosphere effectively controls the upper-ocean temperature anomalies.

In appendix B we show that the decay time scale is overestimated ($\tau$ is underestimated) when $\kappa^i/(r \Delta x^2)$, $u/(r \Delta x)$ and $\kappa^y/(r \Delta y^2)$, $v/(r \Delta y)$ exceed 100. However, these restrictions are respected in the inverted data, except in a small region in the Agulhas retroflection, suggesting that the peak decay time scales there might be overestimated (Fig. 5c).

b. Sensitivity

1) Sensitivity to the length of the time series

The B-based estimates of velocity, diffusivity, and decay rate all include a convergence error [see Eq. (11)]. The convergence error is expected to decrease as the number of (independent) samples increases [Jeffress and Haine (2014b) report $1/\sqrt{N}$ dependency, where $N$ is the total number of samples].

Figure 6 shows the inverted velocity, diffusivity, and decay fields based on a $2^5$-yearlong SST anomaly time series (1985–2016; Figs. 6a–c), and the error when these fields are the means of shorter segments ($2^1$–$2^4$ yr) over the same time period (Figs. 6d–o).

The error is smallest in regions with the strongest oceanic variability, and it decreases throughout the ocean as the length of the time series increases. In particular, the area-averaged root-mean-square error (Fig. 7) decreases roughly as the inverse of the square root of the length of the time series (similar to Jeffress and Haine 2014b). For example, moving from a 2-yr-long time series to a 8-yr-long time series would halve the error.

Apart from the error caused by the length of the time series, the shorter segments of the time series reveal interannual- to decadal-scale variability that is larger than the error compared to the long time series (not shown). Assessing this variability is left for a future study.

2) Effect of $\tau$

In section 3d we created an objective set of parameters to optimize $\tau$. Here we show that the optimization is indeed well justified and demonstrate the need for the spatial high-pass filtering of the SST data.

Diffusivity estimates in Figs. 8a and 8b show that at long $\tau$, the original (green) and the high-pass-filtered (orange) data approach a background global average around 500 m$^2$ s$^{-1}$. However, the two sets of data approach the background value from different directions. Diffusivity decreases toward the background value when the inversion is based on the original data, while it increases toward the background value when diffusivity is inverted from the high-pass-filtered data. This difference follows from the imprint of atmospheric variability in the original data; the oceanic variability starts to dominate only when one moves beyond the atmospheric autocorrelation time scale.

The decay time scale increases with $\tau$ because anomalies that have a lifetime shorter than $\tau$ are not accounted for by the inversion (Fig. 8c). High-pass filtering reduces the mean decay time scale, because it removes some of the large and persistent SST anomalies, such as those related to El Niño–Southern Oscillation in the tropical Pacific.

Velocity distributions are largely independent of $\tau$, except zonal velocities, which show a peak around $\tau = 8$ days (Figs. 8d–f). This reflects the global mean time that it takes for an anomaly to propagate from a...
central cell to the surrounding cells in the five-point stencil. In addition, high-pass filtering increases westward velocities, because it removes any eastward-propagating atmospheric anomalies present in the original data, leaving behind mostly westward-propagating eddies [see also section 4b(4)].

3) EFFECT OF TIME RESOLUTION

Here we assess the sensitivity of the inversion to the time resolution and low-pass filtering (in time) of the input data (Fig. 9). This assessment is relevant because many of the observed surface parameters are archived at resolutions $\Delta t > 1$ day, and a number of studies use low-pass-filtered (in time) data. Here we do not optimize $\tau$. We take $\tau = \Delta t$ when the time resolution changes, because $\tau_s$ (and therefore the upper limit for $\tau$) approaches $\Delta t$ at lower time resolutions (see Fig. 3). For data that are low-pass filtered in time, we take $\tau = \frac{1}{2}$ of the filter length, to avoid aliasing: low-pass filtering propagates information forward and backward in time and essentially part of an anomaly at a given time step is felt half a filter-length later (and before).

Both diffusivity and velocity estimates decrease with increasing $\Delta t$. We suggest that this is because any deformation (caused by mixing or advection) of the SST field that takes place on time scales shorter than $\Delta t$ is averaged out and is therefore not manifested in the inverted results. Low-pass filtering leads to an increase in diffusivity and speed with the filter length, up until the point when the signal leaves the local stencil (around 10 days). The increase in decay time scale is similar in both cases and because the anomalies cannot be shorter lived than $\Delta t$ or half of the filter length.

Altogether these results suggest that with the caveats discussed above, one can base the inversion on data with a lower time resolution, and, for example, carry out the inversion based on satellite-derived sea surface salinity data or Argo float–based products (both are usually available on a 5–7-day time resolution).

4) EFFECT OF SPATIAL SCALES

Here we assess the effect of the spatial resolution of the anomalies by applying both high-pass and low-pass spatial filters to the original SST data, which have a
This assessment is motivated by the varying spatial resolution between different tracer datasets. Physically, one might expect the spatial scales of the anomalies to matter for the anomaly propagation; for example, one would expect larger-scale SST anomalies to decay slower because of their larger heat content and ability to influence the atmosphere above. Alternatively, large-scale anomalies would be expected to be relatively slow because of a lack of coherent flow at large spatial scales.

Overall, the inversion appears insensitive to the size of the high-pass filter (green; Fig. 10), which supports our assumption of the scale separation between atmospheric and oceanic influence on SST anomalies. At the global scale, one achieves similar results with any filter that is below the atmospheric scales but still above the local stencil size. In the rest of this study, we used a 4° × 8° filter (latitude × longitude) because it preserves the equatorial waves that are $O(100)$ km in scale but still removes the atmospheric signals that are generally an order of magnitude larger.

In contrast, low-pass filtering reveals strong filter size dependence of the inversion (orange; Fig. 10). We interpret this dependence as a shift from a mixed ocean–atmosphere signal when no filter is used (0.25° scale) to one dominated by the atmosphere at larger filter sizes. The low-pass-filtered diffusivities (orange; Figs. 10a,b) approach an asymptotic value $O(10^5)$ m$^2$ s$^{-1}$ that is relatively close to effective diffusivities reported in the upper troposphere and lower stratosphere [$O(10^6)$–$O(10^8)$ m$^2$ s$^{-1}$; Haynes and Shuckburgh 2000a,b]. The decay time scale increases with the low-pass filter size (orange; Fig. 10c), because of the increase in the spatial autocorrelation length scale, which translates to a larger autocorrelation time scale. The speed of the anomalies increases with the size of the low-pass filter (orange; Fig. 10f) primarily because of increasing eastward velocities in the midlatitudes, and increasing westward velocities in the tropics (note the increasing spread of

![Fig. 7. Area-weighted RMSE in ice-free regions where $\min(k_x, k_y) > 0$ calculated from Fig. 6. Here we have ignored regions in which the decay time scale is outside 0.1%–99.9% range of its values, because very few points skewed the statistics otherwise. The dashed gray line ($1/\sqrt{N}$, where $N$ is the length of the segment) is shown for guidance.](http://journals.ametsoc.org/doi/pdf/10.1175/JTECH-D-18-0057.1)

![Fig. 8. Effect of the forcing decorrelation time scale $r$ given the original data and spatially high-pass-filtered data. We illustrate the area-weighted global distribution with the median shown by the solid line, and the area between 25% and 75% quartiles shown by the shading.](http://journals.ametsoc.org/doi/pdf/10.1175/JTECH-D-18-0057.1)
the zonal velocity in Fig. 10d). Increasing eastward propagation in the midlatitudes is unlikely to have an oceanic origin, because Rossby waves propagate westward. However, the midlatitude atmosphere has eastward-moving anomalies (weather systems), albeit they move with speeds much faster than the inversion suggests. Therefore, we argue that the eastward-moving anomalies in the atmosphere, together with a lagged response from the ocean mixed layer, produce midlatitude SST anomalies that seem to propagate eastward at speeds faster than the underlying ocean current speeds [see Nilsson (2000, 2001), who suggests that the SST anomaly speed depends on the speed of the atmospheric temperature/heat flux anomaly and the ratio between the heat capacities of the atmosphere and the ocean]. The largest low-latitude increase in the westward anomaly propagation coincides with the trade wind–related surface wind stress maxima in the tropical North Atlantic and in the tropical Pacific (Risien and Chelton 2008). Similar to the midlatitudes, we suggest that the lagged ocean mixed layer response to wind stress anomalies produces relatively fast, westward-propagating SST anomalies.

Fig. 9. Effect of averaging and low-pass filtering in time. We illustrate the area-weighted global distribution with the median shown by the solid line, and the area between 25% and 75% quartiles shown by the shading.

Fig. 10. Effect of spatial high- and low-pass filtering, where axis is the filter size in latitude and the filter size in longitude is twice that. As in Fig. 9, we illustrate the area-weighted global distribution with the median shown by the solid line, and the area between 25% and 75% quartiles shown by the shading. Note the logarithmic y scale for diffusivity.
5. Discussion

As mentioned in section 1, a widely used approach to linear matrix modeling is to estimate the linear matrix operator from a reduced number of EOFs instead of the full SST field. Another related method is to analyze the leading eigenvectors, POPs, of the transport operator $B$ (which again is often inverted from the EOF components). While these methods are useful for prediction, they are not guaranteed to represent the underlying physical processes in the ocean. For example, EOF patterns of the global sea surface temperatures do not describe a purely oceanic variability but often variability linked to some coupled ocean–atmosphere modes. In this study we aim to gain physical insight into the oceanic processes that relate to the SST variability. Therefore, we argue that here the relevant linear matrix operator is the one rooted in the local covariances rather than one estimated from EOFs of the global SST field.

Previously, Piterbarg and Ostrovskii (1997), Ostrovskii and Piterbarg (2000), and Ostrovskii and Font (2003) applied a linear matrix modeling approach very similar to ours to the SST field. It appears that the main differences between their approach and ours are in the implementation of the methodology. For example, they used a nine-point stencil, and instead of our logarithmic relation between the SST covariance matrices [Eq. (2)], their derivation ends with a set of nine discretized equations that depend linearly on the covariance matrices (Piterbarg and Ostrovskii 1997). Their results are qualitatively similar to ours in the North Pacific and in the North Atlantic (which are the domains they cover). However, quantitatively, the results differ, which is partly explained by their coarser and shorter SST dataset, and partly because they do not spatially high-pass filter the data.

The ability to invert for the diffusivity globally is intriguing, and it would be interesting to relate our results to other approaches in estimating ocean mesoscale diffusivity. While we leave a detailed comparison for further studies, we want to point out some correspondence with prior works that use higher moments of tracer time series to infer oceanic mixing. For example, Hughes et al. (2010) and David et al. (2017) use skewness and kurtosis of potential vorticity to identify jets and mixing barriers, and based on idealized simulations Hughes et al. (2010) further suggest a linear relation between diffusivity and kurtosis of potential vorticity (in the sense that higher kurtosis equals higher diffusivity). We suggest that future studies should attempt to link these higher moments of temporal variability to properties of spatial variability. For example, it is clear that the local spatial covariance drops in the presence of mixing barriers, but it would be fruitful to understand how spatial covariance relates to the local time variability in general.

In this study the velocity estimates are primarily linked to the mesoscale eddy propagation, because the OISST product does not resolve submesoscale features. However, note that any velocity estimation that is based on deformation of the tracer field is fundamentally limited. A deforming tracer field holds information only about the velocity component perpendicular to the tracer contours, which causes the deformation, while no information exists about the velocity component that is parallel to the tracer contours. This is of particular importance in temperature-based estimates, because temperature is an active tracer affecting the density field, which is why the velocity field itself tends to align with the temperature field (because of geostrophy).

Rhines and Young (1983) estimated that a time scale for the tracer alignment with the velocity field is $(LU/\kappa)^{1/3}(LU)$, where $L$, $U$, and $\kappa$ are spatial, velocity, and diffusivity scales, respectively. Reasonable choices for the scales lead to alignment in a few days in the region of strong currents ($L = 10^4$ m, $U = 1$ m s$^{-1}$, $\kappa = 10^5$ m$^2$ s$^{-1}$) and a few months in more quiescent regions ($L = 10^5$ m, $U = 0.05$ m s$^{-1}$, $\kappa = 10^5$ m$^2$ s$^{-1}$). This suggest that SST-based estimation of the full ocean velocity field is difficult in the boundary current regions, where the SST field quickly aligns with the velocity field, but perhaps it is feasible in regions of slow currents, where the least alignment is expected (for more see, e.g., Turiel et al. 2009, their Fig. 9).

On the other hand, our estimates are a function of the spatial and temporal resolution of the SST dataset. For example, given hourly time resolution and submesoscale \cite{OISST} spatial resolution, one could detect structures that are directly advected by the mean current. In such a case, MicroInverse would return the underlying current velocities. In our analysis the tropical regions seem to be at the border of this limit, as the retrieved velocities are closer to the current velocities than the local wave speeds. We believe that at finer temporal and spatial scales, our statistical estimate would converge to estimates from feature tracking. The advantage of MicroInverse over the feature tracking (especially maximum covariance) methods is the lack of region-specific tuning needed for the method to work (Heuzé et al. 2017), and the ability to estimate also diffusivity and decay rate. The advantage of feature tracking is the ability to work on image pairs rather than time series.

In this study we have used OISST data that are preprocessed (interpolated and filtered) to yield a complete dataset on a regular latitude–longitude grid. In principle MicroInverse could be used with less-processed data.
products, for example, pure satellite images. Control on the filtering and interpolation routines is desirable, and one could use existing methods to estimate covariance matrices with missing data (Dempster et al. 1977; Schneider 2001), instead of calculating them directly with interpolated data [as in Eq. (2)]. An added benefit of satellite images over processed data products is the higher spatiotemporal resolution.

6. Conclusions

We developed a local linear matrix inversion method to assess ocean kinematics. Given a gridded time series of tracer data, one can use this inversion method to estimate a mean transport operator that governs the evolution of tracer anomalies. One can then use the transport operator to derive a global response function (Green’s function) and to estimate physical fields such as velocity, diffusivity, and decay time scale.

In this paper we applied the inversion to the 35-yearlong daily SST record (OISST, 1982–2016; Reynolds et al. 2007) at 0.25° horizontal resolution. We show that the inversion is in general feasible at 0.25° resolution as long as the time resolution is below the SST decorrelation time scale. The decorrelation time scale of the SST field is O(10) days, which suggests that it could be feasible to invert other data products that have approximately weekly time resolution (such as Argo data). The inversion is also relatively robust to the length of the time series (error decreases as an inverse square root of the length of the time series), enabling assessments of subdecadal variability.

However, care should be taken with the combination of spatial and time resolution of the input data. The inversion of high-spatial-resolution data but low-time-resolution data should be avoided, as one would expect anomalies to leave a local stencil within a time step, which would cause underestimation of diffusivity and velocity. In such a case it would make more sense to regrid the data to a coarser spatial resolution if a higher time resolution is not available. The opposite scenario—high time resolution but low spatial resolution—is not as problematic, although the assumption of separating atmospheric and oceanic SST imprints by spatial scales becomes invalid as the spatial resolution decreases.

Finally, the inversion method provides several avenues for future work. Propagation of temperature anomalies, and their lifetimes, has been a long-standing research question with direct implications for predictability. The global response function can be used to assess the lifetime of anomalies, and to find regions where there might be potential predictability linked to temperature anomalies alone (similar to, e.g., Wang and Chang (2004), but using a local stencil rather than EOFs to derive the transport operator). Another research question is the estimation of subgrid-scale diffusivity; here the ability to estimate horizontal diffusivity from different observational, as well as model products, can provide a new understanding of the scale dependency of diffusivity. One could also investigate changes in the velocity and diffusivity at depth, with, for example, Argo-based products, or perform the inversion on isopycnal surfaces to estimate diffusivities along isopycnals.

Acknowledgments. We thank Peter Cornillon and an anonymous reviewer for their useful suggestions, which helped to improve the paper. We also thank M. Almansi, A. Gnanadesikan, R. Gelderloos, M.-A. Pradal, and A. Saberi for the fruitful discussions and feedback. A.N. and T.H. were supported by a grant from the NSF Directorate for Geosciences (1536554). NOAA Optimum Interpolation SST data (NOAA OISST) are provided by NOAA/OAR/ESRL PSD, Boulder, Colorado, from its web site (at https://www.esrl.noaa.gov/psd/). The Meso-scale Eddy Trajectory Atlas products were produced by SSALTO/DUACS and distributed by AVISO+ (http://www.aviso.altimetry.fr/) with support from CNES, in collaboration with Oregon State University with support from NASA. The data and further details are available online (at https://www.aviso.altimetry.fr/en/data/products/value-added-products/global-mesoscale-eddy-trajectory-product.html). The OSCAR data were obtained from JPL Physical Oceanography DAAC (https://podaac.jpl.nasa.gov/dataset/OSCAR_L4_OC_third-deg) and developed by ESR. The drifter-based climatology of surface currents can be found online (http://www.aoml.noaa.gov/phod/dac/dac_meanvel.php). The inversion code with examples is distributed under the name MicroInverse (https://github.com/AleksiNummelin/MicroInverse), and the code to generate the data and figures in this paper is distributed through Github (https://github.com/AleksiNummelin/MicroInverse_paper). Please contact the lead author for help with MicroInverse implementation.

APPENDIX A

Derivation of Perturbation Advection–Diffusion Equation

Here we derive Eq. (A5) assuming that an advection–diffusion–relaxation equation with a decay term describes the evolution of the SST field. Throughout the derivation we denote the time series of SST anomaly matrix (continuous in space) with $\mathbf{x}(t)$, which relates to the time series of SST anomaly vector $\mathbf{x}(t)$ used...
elsewhere in the text via \( \mathbf{x}(t) = \mathbf{y}(t) \); that is, element \( h \) in vector \( \mathbf{x}(t) \) points to element \( (i, j) \) in \( \mathbf{y}(t) \). We begin the derivation by writing down the advection–diffusion–relaxation equation in its Reynolds decomposed form with an overbar denoting the time mean and with a prime denoting a fluctuation from the time mean; for brevity we drop the explicit time dependency notation.

\[
\frac{\partial}{\partial t} (\mathbf{X} + \chi') + \nabla \cdot [(\mathbf{U} + \mathbf{U}') (\mathbf{X} + \chi')] - D \nabla^2 (\mathbf{X} + \chi') - \bar{r}(\mathbf{X} + \chi') = \mathbf{f} + \mathbf{f}'.
\]  

(A1)

where \( \mathbf{U} \) is a velocity vector, \( D \) is a constant uniform molecular diffusivity, \( r \) is the inverse decay time scale, and \( \mathbf{f} \) is the forcing. Here we have included the fluctuation in the decay time scale \( r' \) in the forcing fluctuation \( \mathbf{f}' \) term. We note that \( \nabla \cdot \mathbf{U} = 0 \) and average over time,

\[
\frac{\partial \mathbf{X}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{X} + \nabla \cdot (\mathbf{U} \mathbf{X}) - D \nabla^2 \mathbf{X} - \bar{r} \mathbf{X} = \mathbf{f}.
\]  

(A2)

By taking the difference, Eq. (A1) – Eq. (A2), we are left with the equation describing the anomaly evolution,

\[
\frac{\partial \mathbf{X}'}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{X}' - \nabla \cdot (\mathbf{U} \mathbf{X}') - D \nabla^2 \mathbf{X}' - \bar{r} \mathbf{X}' = \mathbf{f}'.
\]  

(A3)

We then parameterize the velocity–tracer fluctuation covariance terms in Eq. (A3) with eddy diffusivity closure \( \mathbf{U} \mathbf{X}' = -\bar{r} \nabla \mathbf{X} \) (where \( \bar{r} \) is the time mean eddy diffusivity). By Reynolds decomposing \( \mathbf{X} \) we can write

\[
\mathbf{U} \mathbf{X}' - \overline{\mathbf{U} \mathbf{X}} = -\bar{r} \nabla (\mathbf{X} + \chi') + \bar{r} \nabla \mathbf{X} = -\bar{r} \nabla \mathbf{X}'.
\]  

(A4)

Substituting Eq. (A4) into Eq. (A3), taking \( \mathbf{\kappa} = \bar{r} \mathbf{I} \), and leaving only the linear terms on the left hand side, we get

\[
\frac{\partial}{\partial t} \mathbf{X}' + \mathbf{U} \cdot \nabla \mathbf{X}' - \nabla \cdot (\mathbf{U} \mathbf{X}') - \bar{r} \mathbf{X}' = \mathbf{f}' - \nabla \cdot (\mathbf{U} \mathbf{X}).
\]  

(A5)

As we see from Eq. (A5), the right-hand side includes not only the fluctuations in the atmospheric forcing \( \mathbf{f} \) but also the term, \( \nabla \cdot (\mathbf{U} \mathbf{X}) \), as a result of velocity fluctuations acting on the time mean tracer field. This term describes the emergence of SST anomalies by anomalous advection of a mean SST gradient ( \( \mathbf{U} \cdot \nabla \mathbf{T} \)), and by divergence and convergence in the anomalous velocity field ( \( \nabla \cdot (\mathbf{U} \mathbf{X}) \)). Note that allowing for time variability in the diffusivity field (or explicitly treating the time variability in the decay field) simply adds additional terms to the right-hand side of Eq. (A5).

Finally, by combining the right-hand side under the \( \mathbf{f}' \) term and dropping the mean and the fluctuation notation, we arrive at

\[
\frac{\partial}{\partial t} \mathbf{X} + \mathbf{U} \cdot \nabla \mathbf{X} - \nabla \cdot (\mathbf{U} \mathbf{X}) - \bar{r} \mathbf{X} = \mathbf{f},
\]  

(A6)

which forms the basis for our discussion in section 3c.

APPENDIX B

Idealized Sensitivity Analysis

Here we provide two simple illustrations of the inversion method by inverting results from a numerically solved advection–diffusion–relaxation equation. We use the FiPy (Guyer et al. 2009) Python package to integrate the forward equation [Eq. (A6)] into a 50 \times 50 gridcell domain. In the first test case, we carry out multiple simulations, varying the constant velocity, diffusivity, and decay fields. In the second case, we use a similar approach but advect the temperature field with the observed OSCAR velocity field. Detailed results are presented below for both cases.

a. Constant velocity field

In the first test case, we use constant velocity, diffusivity, and decay fields, and start from an initial condition of 25 Gaussian SST anomalies within the domain. We apply no forcing and as the velocity field is constant in time, the right-hand side of Eq. (A6) vanishes. Each anomaly initially has a peak value of 1 K. We integrate forward with a time step of 900 s for a total of 6000 s, saving the output at every time step. The long integration time compared to the decay time guarantees that by the end of the simulations, less than 1% of the initial anomaly is present at any given location. We note that because the velocity field is constant and there is no eddy diffusivity \( \mathbf{\kappa} \) arising from the velocity–temperature fluctuation covariance, the diffusivity entirely arises from the subgrid-scale diffusivity \( D \).

After generating this idealized dataset, we invert it choosing \( \tau = 1 \). The results in Fig. B1 show that for the observed parameter space, the inversion returns the expected parameters in general. There are a few exceptions. First, diffusivity is sensitive to large Peclet numbers (\( y \) axis; \( u \Delta x / \alpha \)), because we discretize the diffusive flux operator with a central differencing scheme in the inversion. Second, velocity estimates become erroneous when the decay term becomes large (\( r \Delta x / u > 1 \)) compared to the advection. In such a case, the decay dominates the covariance matrix, because the signal decays before it has the chance to move around with the advection. Third, decay time estimates become
erroneous if advection and diffusion dissipate the signal faster than the decay has time to affect it (upper-right corner of Fig. B1c).

b. OSCAR velocity field

In the second test case, we also keep the diffusivity and decay fields constant but use the OSCAR velocity field (ESR 2009). We focus on a 50 × 50 gridcell subdomain (similar to the more idealized case) in the Southern Pacific (30°–46°S, 157°–173°W) away from the boundary currents. We modify the original OSCAR data by first making the velocity fields divergence free [following Marshall et al. 2006; Abernathey and Marshall (2013), with no flux boundary conditions]. We then randomly sample the velocities in time to form a new dataset with 1-day time resolution (which is then linearly interpolated to the time step scale). The resampling of the velocity field was done because of the constraints discussed in section 3d: The original OSCAR velocities are 5-day averages with decorrelation time scale $\tau_f$ of several weeks, and since we require $\tau > \tau_f$, we cannot satisfy $u\tau/\Delta x > 1$, $u\tau/\Delta y > 1$. In other words, anomalies leave the local stencil in less than the forcing decorrelation time scale.

We relax the SST field toward an atmospheric temperature field that is constant in time, but has a meridional gradient of 10 K. Because there are no time fluctuations in this relaxation term, the atmospheric part of the forcing term in Eq. (A6) is zero. However, since the OSCAR velocities vary in time, the $V \cdot U\nabla$ term is the forcing that creates the SST anomalies. We use daily outputs and create a 10-year-long time series.

After generating the data for the second test case, we carry out the inversion and optimize $\tau$ following the procedure laid out in section 3d. Figure B2 shows the results for subgrid-scale diffusivity $D$ ranging from 250 to 1500 m$^2$ s$^{-1}$.

Accuracy and precision of the diffusivity estimates (Figs. B2a–d) increases as a logarithmic function of $D$. Inversion overestimates small diffusivities, because the Peclet number is close to 1 (see previous test case) but also because small $D$ allows for large velocity–temperature fluctuation covariance that contributes to the eddy diffusivity (note that inversion of the OISST field, Fig. 5b, suggest that that the eddy diffusivity is around 500 m$^2$ s$^{-1}$ in this region). As the subgrid-scale diffusivity increases, the temperature field becomes relatively smooth and the velocity–temperature fluctuation covariance small, and the inverted diffusivity is mostly due to the subgrid-scale diffusivity alone. As expected from the previous test case, estimates of the decay time scale are relatively accurate and precise compared to the diffusivity and velocity fields, and appear robust to changes in the subgrid-scale diffusivity (Figs. B2e–h). Finally, velocity estimates are rather accurate, but not very precise (Figs. B2i–l). This is because the velocity field itself is highly variable (as we randomly sampled the field) and consequently there is also large variability in the alignment of the temperature and velocity fields both in time and space (see section 5). Note that the velocity estimation also grows less accurate as the subgrid-scale diffusivity begins to dominate the deformation of the SST field over the influence of the highly variable velocity field.
In all cases the precision is in large part controlled by the length of the time series (not shown; similar to what was found with the OISST data), but also by $\tau$. Choosing a larger $\tau$ improves especially the accuracy of diffusivity estimates, as the solution asymptotes to a true value [similar to section 4b(2)], but at the same time precision decreases because the covariance matrix becomes noisier with increasing lag.

**APPENDIX C**

**Comparison between NOAA OISST AVHRR Only and OISST AVHRR + AMSR-E Products**

Here we compare the two NOAA OISST products available, using the period 2003–11 when there are additional data from the AMSR-E instrument. AVHRR is an infrared instrument, but there are data gaps in cloudy
regions where it cannot see the surface. AMSR-E is a microwave instrument that can penetrate the clouds, but the data are available for only 2003–11 (full years). Including the AMSR-E data is expected to yield better results, as the data coverage is more complete. Both datasets went through the same pre- and postprocessing independently; that is, the data were spatially high-pass filtered and the climatologies were removed, and afterward $\tau$ was optimized as described in section 3d.

The comparison appears in Fig. C1, which demonstrates that while the underlying patterns are practically the same, the inclusion of AMSR-E data leads to larger velocities and diffusivities, and to a longer decay time scale. Note the differences in the boundary currents where the inclusion of AMSR-E data yields stronger velocities and in the interior where they yield fewer negative diffusivities. The inclusion of AMSR-E data also diminishes regions with decay time scales below the time resolution of the input data (1 day), shrinking the regions with unreliable results. In general, the anomalies also have longer lifetimes, which is likely due to fewer gaps in the data.

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