Towards an integrated observation and modeling system in the New York Bight using variational methods. Part II: Representer-based observing strategy evaluation

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Abstract

As part of an effort to build an integrated observation and modeling system for the New York Bight, this study explores observing strategy evaluation using a representer-based method. The representer of a single observation describes the covariance between the observed quantity and ocean state errors at all locations at any time within the assimilation window. It also describes the influence of the observation on control variable correction in a 4D variational data assimilation system. These properties hold for the combination of representers that is associated with a group of observations and functions of model variables that combines model variables (e.g., salt flux). The representer-based method is used here to identify which of a set of proposed tracks for an autonomous coastal glider is better for predicting horizontal salt flux within the Hudson Shelf Valley in a 2-day forecast period. The system is also used to compare different observation strategies. We show that a glider that traverses a regular transect influences a larger area than a continuously profiling mooring, but the mooring carries stronger influence at the observation location. The representer analysis shows how the information provided by observations extends toward the dynamically upstream and how increasing the duration of the analysis window captures more dynamical connections and expands the area of influence of the observations in data assimilation. Overall, the study demonstrates that the representer methodology can quantitatively contrast different observational strategies and determine spatial patterns and temporal extent of the influence of observations, both of which are helpful for evaluating the design of observation networks.

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1. Introduction

Ocean observation technologies developed in recent decades have significantly expanded the scope and density of data available for coastal oceanic research. While largely used to study the oceans directly, observations are also increasingly used to correct numerical models using methods of data assimilation developed to improve state estimation and ocean prediction. The capability to simultaneously deploy numerous instruments of differing types during intensive observing experiments, and the development of sustained integrated coastal ocean observing systems, have bolstered the demand for objective methods of evaluating observational strategies. Observing system design considerations are generally motivated by a need for targeted observation of a particular aspect of regional ocean circulation, or a desire to deploy instruments in an adaptive sampling mode to capture transient or moving features. Designing a targeted observation program in conjunction with a data assimilation (DA) system has the objective of selecting the most efficient observation types and locations to improve model analysis or forecast of a certain physical quantity of interest given known instrument capabilities and practical logistical constraints on their deployment and operation.

Targeted observation design is an active research topic in the numerical weather forecast community (Langland, 2005; Rabier et al., 2008), and there are different design approaches: singular vector-type techniques (Leutbecher, 2003; Palmer et al., 1998), adjoint sensitivity-type techniques (Bergot, 1999; Wu et al., 2007), observation sensitivity-type techniques (Baker and Daley, 2000; Langland and Baker, 2004), and ensemble transform-type techniques (Bishop and Toth, 1999; Bishop et al., 2001).

Singular vector techniques find and then constrain the most rapidly growing error structures associated with a norm over a finite time interval. The norm is chosen to describe a physical quantity of interest, e.g., forecast uncertainty or total energy. Adjoint sensitivity techniques identify the state variables and geographic locations to which a chosen physical quantity is most
sensitive. Both adjoint sensitivity and singular vector approaches identify where new information would diminish forecast error in a DA system, but neither take into consideration existing or planned observations. Where best to acquire new targeted observations to complement existing observations can be addressed in observation sensitivity and ensemble transform techniques. The Observation sensitivity approach determines the effect of each assimilated observation on the analysis and forecast of a chosen aspect using the adjoint of the DA and forecast system so that the added information of hypothetical observations can be obtained. Ensemble transform techniques use an ensemble of forecast simulations to retrieve the forecast error covariance and then seek the observation pattern which best minimizes forecast uncertainty.

In contrast to meteorology, there are relatively few published studies of targeted observations in oceanography. Most recent studies employing DA in oceanography emphasize state estimation, and to complement these targeted observation efforts have paid greatest attention to capturing certain ocean phenomena or variability in an analysis, rather than a forecast. Examples are works utilizing ensemble transform-type techniques (Ballabrera-Poy et al., 2007; Frolov et al., 2008; Hackert et al., 1998; Oke and Schiller, 2007; Sakov and Oke, 2008). Other approaches that have been taken in oceanography are simulated annealing ( Barth and Wunsch, 1990), adjoint sensitivity ( Shulman et al., 2005), array mode analysis ( Bennett, 1990; McIntosh, 1987).

Köhl and Stammer (2004) simplified the observation sensitivity technique by assuming that model state error is much smaller than observational error. Targeted observation is typically followed by DA, so Köhl and Stammer’s (2004) assumption of large observational error is somewhat contradictory and interpreting the result as observation sensitivity (as in Baker and Daley (2000)) is questionable. However, as we will show in the next section, the simplified technique is still consistent with computing the representer of the chosen feature of interest – it gives the error covariance between the chosen feature and ocean state at all locations and times. Then it is logical to observe the places where the correlation is the highest.

In the New York Bight (NYB), local forces (e.g. topography, river discharge and air–sea exchange) and remote forces (e.g. large scale shelf circulation) interact on a wide continental shelf to create a coastal zone with complicated dynamics and short time and space scales of variability ( Choi and Wilkin, 2007; Yankovsky, 2003). The region has been the subject of many studies, both modeling and observational ( Castelao et al., 2008a; Chant et al., 2008; Tilburg and Garvine, 2003; Wilkin et al., 2005; Wong, 1999; Yankovsky et al., 2000). The area has seen pioneering deployments of new observing instruments like autonomous underwater vehicles (gliders) ( Schofield et al., 2007), coastal High-Frequency (HF) Radar systems ( Kohut et al., 2006), cabled observatory moorings ( Glenn et al., 2000), and the comprehensive use of multiple satellites ( Schofield et al., 2004) together with ship-borne instruments during a series of intensive multidisciplinary observational programs ( Chant et al., 2008). The monitoring of water conditions in the NYB is operated on a quasi-continuous base, which makes the region ideal for experimenting with integrating observation and modeling capabilities.

Part I ( Zhang et al., 2010) of this study demonstrated the use of observations to correct a numerical model using 4Dimensional Variational (4DVAR) DA. In this paper, Part II, we explore two applications of a representer-based system to objectively assess and guide observation strategies. The first application considers long-term, repeated glider deployments for predicting horizontal salt flux within the Hudson Shelf Valley (HSV). Our motivation here is that horizontal tracer fluxes in the HSV potentially bring nutrient-rich deep water up to the euphotic zone and stimulate primary production on the inner shelf. The second application might be loosely thought of as a comparison of moored and mobile observation platforms, with added consideration of different dynamical regimes, with coverage and magnitude of the representer functions used to guide instrument choice and spacing.

A drawback of representer-based observing system evaluation is that it does not consider pre-existing observations that might make the “designed” mission redundant in a DA system. However, this is not a major concern because so few subsurface observations are routinely made in coastal regions. The methodology we describe is readily adapted to address how observations can be targeted at improving specific aspects of a forecast in a coastal ocean region. Our examples are somewhat idealized, but the methodology will be tested in earnest in future collaborative field work integrating models and observations in NYB.

This paper is organized as follows: Section 2 describes the theory of representer-based observing strategy evaluation; Section 3 describes the system setup; Section 4 applies the method to predicting salt flux within the HSV; Section 5 compares the influences of different observations; and Section 6 summarizes the work.

### 2. Representer-based observing strategy evaluation

Let us denote \( \Phi(t) \) to be the ocean state vector \( \begin{bmatrix} u & v & T & S \end{bmatrix}^T \) comprised of the velocity, temperature, salinity and sea surface height at all grid points at time \( t \). A representer is the error covariance between a single element of \( \Phi(t_0) \) at a particular grid point at time \( t_0 \), which we call a “point aspect of interest” in this paper, and all other elements of \( \Phi(t) \) (a 4-dimensional field) ( Bennett, 2002; Kurapov et al., 2009). We can transform the continuous space-based representer formulation in Bennett (2002) to a discrete space-based matrix formulation as

\[
\text{Representer} = \mathbf{M}^T \Lambda(\phi_0, x_0, t_0).
\]

where \( \mathbf{M} \) is the tangent linear model propagator and \( \mathbf{M}^T \) is the corresponding adjoint operator ( Moore et al., 2004), \( \mathbf{B} \) is the background error covariance matrix, \( \Lambda \) is an impulse vector with the same length as \( \Phi \), and

\[
\Lambda(\phi_0, x_0, t_0) = \begin{cases} 1 & \phi = \phi_0 \text{ and } x = x_0 \text{ and } t = t_0, \\
0 & \phi \neq \phi_0 \text{ or } x \neq x_0 \text{ or } t \neq t_0. 
\end{cases}
\]

\( \phi_0 \) is the variable of interest \( (\phi_0 \in [u \, v \, T \, S]^T) \), \( x_0 \) is the location of interest, and \( t_0 \) is the time of interest. Then \( \phi(\mathbf{x}_0, t_0) \) is the point aspect of interest.

This representer is based on the linearization around a nonlinear model trajectory. In variational DA, if the physical quantity of interest is the ocean state at a single observation location, the representer describes the influence of the observation in the model ( Bennett, 1990; Egbert and Erofeeva, 2002; Kurapov et al., 2009). In (1), \( \Lambda(\phi_0, x_0, t_0) \) can be considered as \( \partial L_0 / \partial \Phi(t_0) \), where \( L_0 \) is an objective function of a point aspect of interest, \( L_0 = \phi(\mathbf{x}_0, t_0) \). Hence, the representer gives the error covariance between \( L_0 \) and \( \Phi(t) \), and (1) becomes

\[
\text{rep} \left( \frac{\partial L_0}{\partial \Phi(t_0)} \right) = \mathbf{M}^T \frac{\partial L_0}{\partial \Phi(t_0)} = \text{cov}(L_0, \Phi(t)).
\]

(2)

Here we denote the linear representer operator as \( \text{rep} ( \cdot ) \). Notice that the units of (2) are \( \text{[L]} \cdot \text{[reset]} \). The middle term in (2) is similar to Eq. (13) in Köhl and Stammer (2004) except for the sampling operator and observation error covariance matrix that they applied after the representer.

Next, we extend the representer concept to more general circumstances. For \( a \) and \( b \) being any two independent point aspects of interest at time \( t_0 \), it can be shown (see Appendix) that
\[
\text{Crep} \left( \frac{\partial (a + b)}{\partial \Phi(t)} \right) = \text{cov}(a + b, \Phi(t)), \\
\text{Crep} \left( \frac{\partial (a - b)}{\partial \Phi(t)} \right) = \text{cov}(a - b, \Phi(t)), \\
\text{Crep} \left( \frac{\partial (ab)}{\partial \Phi(t)} \right) \approx \text{cov}(ab, \Phi(t)),
\]

and
\[
\text{Crep} \left( \frac{\partial (a/b)}{\partial \Phi(t)} \right) \approx \text{cov}(a/b, \Phi(t)).
\]

Here, Crep(.) denotes the combination of some representers. Note that in this paper we refer to the superposition of some representers as a combination of representers to draw a distinction between the representer of a single observation and the covariance information given by superposition of a group of representers.

Given Eqs. (3)–(6), it follows that
\[
\text{Crep} \left( \frac{\partial L}{\partial \Phi(t)} \right) = \text{cov}(L, \Phi(t))
\]
holds true for \( L \) defined as a combination of arithmetic operations (summation, subtraction, multiplication, and division) on ocean state variables at time \( t_0 \). For \( L \) constructed as a sum of contributions from several snapshots over certain time interval, \( L = L(\Phi(t)), t \in [t_1, t_2], \) the associated combination of representers can be simply obtained as a sum of individual representers because the system is linear. Eq. (7) is thus still valid.

Provided the feature of ocean dynamics of interest can be expressed as a function of model variables, e.g. salt transport across a certain cross-section, we can compute a combination of representers to give the error covariance between the feature of interest and ocean variables at all locations at any time in the integration window. The only restriction is that the linear assumption hold for the duration of the integration time window.

Suppose observations are to be gathered to determine some feature of regional ocean dynamics, with no other observations being available for this purpose. It is logical to deploy instruments at the place where the state variables have the highest error correlation with the ocean feature of interest. Assimilation of these observations into the model will lead to more precise description of the physical quantity of interest. Note that a representer extends over times that precede, span, and follow the interval when \( L \) is defined. Hence, representer-based observing system design can guide data acquisition for forecasting, nowcasting and re-analysis. However, representer computation depends on the chosen background error covariance, \( \mathbf{B} \), and the linearization around a particular nonlinear model trajectory. If \( \mathbf{B} \) or the base trajectory change due to changes in initial or boundary conditions, surface forcing, or underlying physics, a new set of representer functions should be computed, possibly leading to a different observation design.

The use of representers here differs from array mode analysis (Bennett, 2002). Our approach uses error covariance information given by representer functions to directly target relocatable observing system deployments without consideration of any pre-existing observing network.

3. System setup

3.1. Model configuration

The Regional Ocean Modeling System (ROMS, www.myroms.org), a free-surface, hydrostatic, primitive equation model, is used in this study. It consists of nonlinear forward, tangent linear and adjoint models and numerous drivers that utilize the component models for adjoint sensitivity, optimal perturbation, repre-

senter-based optimal observation, observation sensitivity, and 4DVAR DA applications (Broquet et al., 2009; Di Lorenzo et al., 2007; Moore et al., 2004, 2009; Powell and Moore, 2009; Powell et al., 2008, 2009; Zhang et al., 2009b).

The model domain (Fig. 1) extends from south of Delaware Bay northeastward to eastern Long Island. Two major rivers are included: the Hudson and Delaware. The model has 30 terrain-following vertical layers and 2 km horizontal resolution. The nonlinear forward control simulation with respect to which the tangent linear and adjoint models are linearized covers the year 2006 with initial conditions from Zhang et al. (2009a). It uses Chapman (1985) and Flather (1976) conditions for sea level elevation and the barotropic component of velocity on the model open boundaries, respectively. Steady along-shelf flow (Lentz, 2008) and tidal elevation and current extracted from a regional simulation (Mukai et al., 2002) were imposed on the open boundaries. Orlanski-type radiation conditions (Orlanski, 1976) were applied for 3D velocity and tracers. Vertical mixing was parameterized with the \( k-\varepsilon \) scheme of general length-scale method (Umlauf and Burchard, 2003) and quadratic bottom drag. Bulk formulae (Fairall et al., 2003) with meteorological conditions from the North American Regional Re-analysis (Mesinger et al., 2006) were applied to compute air–sea momentum and heat fluxes. River discharges were from USGS Water Data (http://waterdata.usgs.gov/nwis) scaled to include ungauged portions of the watershed.

3.2. Representer computation

Computation of the representer described by (1) involves integration of an adjoint model backward in time, application of a background error covariance, \( \mathbf{B} \), and forward integration of a tangent linear model. The adjoint forcing, \( \frac{\partial L}{\partial \Phi(t)} \), is applied to the time interval over which \( L \) is defined. The duration of the adjoint and tangent linear model integrations depends on the processes of interest, but is also constrained by the period for which the

Fig. 1. The model domain (black frame) and bathymetry of the New York Bight in grayscale. The short straight line across the Hudson Shelf Valley indicates the cross-section used to compute salt transport within the valley; the dash line is the so-called Endurance Line glider track regularly sampled by RU-COOL; the long straight black line is the hypothetical glider track; and the triangle indicates the location of the hypothetic mooring.
linearization holds. Zhang et al. (2009b) tested the linearity assumption in a model with the same domain but a higher horizontal resolution (1 km) and found that it is valid for 3 days. In the application presented below analyzing salt flux within the HSV, we integrated the adjoint model backward for 4 days to consider glider deployments 2 days prior to the defined \( L \).

The background error covariance acknowledges correlations between the same variable (univariate) and different variables (multivariate) at different locations due to dynamical scales and processes. At the time of this study ROMS implements only a univariate \( B \). It is simulated by solving two diffusion equations (one for horizontal and the other for vertical) that impose decorrelation scales chosen here to be 20 km in the horizontal and 2 m in the vertical. Detailed descriptions of how the background error covariance is treated in ROMS are given by Powell et al. (2008) and Broquet et al. (2009). This neglect of multivariate correlations in \( B \) causes underestimation of the cross-variable information in the representer. However, we are mainly looking at the variables that \( L \) is defined from which makes the problem less severe. Consistent with the DA system in Part I, the representer approach here is based on the “strong constraint” assumption and neglects model error. Omitting model error presumably overestimates the covariance information in representer functions. The extent to which model error and multivariate background error covariances will change the result will be addressed in future work.

Before proceeding to analyze combinations of representers constructed for the NYB, we illustrate the interpretation of a simple representer computed for a single observation point. Fig. 2 (top row) shows surface salinity during 5 days in September 2006. The physical quantity of interest, \( \mathbf{x}_0 \), for the purposes of illustration was chosen to be salinity at position \( \mathbf{x}_0 = 73.7^\circ W, 40.3^\circ N \) (indicated by the triangle symbol in Fig. 2) at \( t_0 = 2006-09-18 00:00 \) UTC. To compute the representer for this simple \( L \) the adjoint model is forced by a delta function in salinity at the place of interest, i.e. \( \partial L / \partial \Phi(t_0) = \partial (\mathbf{S}, \mathbf{x}_0, t_0) \). Here, we integrate backward for 4 days then apply the univariate background error covariance with the length scales noted above. Fig. 2 (bottom row) shows the time evolution of surface salinity in the subsequent tangent linear model – the surface salinity representer for this \( L \).

The modeled salinity shows that the river plume has two branches. One branch curls southeastward having detached from the Long Island coast, while the other fresher branch flows southward along the New Jersey coast. The higher salinity water between them is a shoreward intrusion of mid-shelf water along the HSV. On 2006-09-18 00:00 UTC, the tip of the southwestern flowing branch reaches \( \mathbf{x}_0 \). Transport pathways strongly influence salinity patterns in the NYB (Zhang et al., 2009a) so we expect properties of water at the point of interest to be correlated with properties in the two plume branches. The surface salinity representer shows these patterns. At 2006-09-14 00:00 UTC, just after applying the background error covariance, the surface salinity representer has a circular pattern of high covariance in the New York Bight apex centered on a location clearly different from \( \mathbf{x}_0 \). The circular shape of the pattern stems from the smoothing effect of the background error covariance. The pattern subsequently transforms as the tangent linear model integration proceeds. By 2006-09-18 00:00 UTC, the time at which the aspect of interest is defined, the representer shows surface covariance develops a two-branch pattern with similarities to the plume. The highest covariance, not surprisingly, occurs near the point of interest itself, and decays proceeding upstream back along the plume trajectory. The error covariance with the other branch along the New Jersey coast is lower but still greater than in the intervening region influenced by higher salinity mid-shelf waters. The two branches are connected at the estuary entrance. In the vertical, high error covariance is concentrated in the surface 15 m (not shown), corresponding to the depth of the surface mixed layer.

The surface salinity representer identifies the area that, 4 days prior, supplies water to the point of interest, but has also identified that the same region is a source of water to the New Jersey coastal current at this time. Couched in terms of DA, the representer indicates that observations made at the point of interest would impact the assimilation increments in both branches of the flow emanating from New York Harbor. This simple representer gives error

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**Fig. 2.** Surface salinity (top) and surface salinity representer (bottom) at different times in 2006. The triangles in the last column indicate the point of interest at which \( L \) is defined; and gray dash lines are 20, 40 and 60 m isobaths.
covariance patterns readily interpreted in terms of the local circulation. Next, we turn our attention to formulating representatives that will aid the evaluation of observing strategies.

4. Targeted observations

4.1. Background

Flow variability within the HSV is correlated with local wind and sea level elevation (Mayer et al., 1982; Nelson et al., 1978) and the mean flow in the valley is shoreward (Zhang et al., 2009a). Because of seasonal variation in the wind, stratification, and possibly the remotely forced along-shelf circulation, the shoreward ocean water intrusion in the HSV intensifies in winter (Harris et al., 2003; Nelson et al., 1978). Fig. 3 shows seasonal averages of the salinity and current at 20 m from the nonlinear forward simulation of 2006. At the cross-section indicated by the short black line the current at 20 m is shoreward along the valley in spring and winter with the strongest intrusion in winter. In summer and fall, the circulation at the cross-section is roughly parallel to the isobaths crossing the valley. Fig. 4 shows time series of the vertically integrated subsurface (below 10 m) salt flux across the cross-section over 2006. Shoreward salt flux dominates the winter and spring seasons (October–April) which is consistent with observations by Nelson et al. (1978). Subsurface mid-shelf waters have higher nutrient concentrations and shoreward flow in the HSV followed by mixing or upwelling to the surface has likely consequences for local biogeochemical processes.

4.2. Representer-based glider track design

Recognizing the influence of the HSV on local biogeochemistry and sedimentation, we have formulated an example of representor-based observing system design aimed at evaluating tracks for glider missions intended to observe HSV transport processes. The question we ask is: where are the most suitable places to routinely deploy two gliders in order to better predict, 2 days in the future, the along-valley salt flux across a selected cross-section? The cross-section we choose is indicated by the short lines plotted in Fig. 3. We define the objective function, $L$, as the vertically integrated subsurface salt flux 2 days after the glider deployment, and apply the representer system to obtain the error covariance and the error correlation between $L$ and variables everywhere at the deployment time. Observations made where and when the error correlation is the highest should have the greatest impact on the model-based analysis. We assume there are no other observations in the environs of the cross-section.

The work flow of the system is depicted in Fig. 5. Firstly, a forward nonlinear simulation (control run) is carried out and we assume the simulated result is the truth. Secondly, $L_c$, the “true” subsurface salt flux through the cross-section averaged over 1 day (the 4th day after nominal time zero) and the corresponding adjoint forcing, $\partial L_c/\partial \Phi(t)$, are computed from the control run. Thirdly, a representer computation is conducted with 4-day adjoint model integration and 1-day tangent linear model integration. This gives the error covariance field at day = 1, two days prior to the interval over which $L$ is defined. Steps 2 and 3 were then repeated with the nominal day $t$ advanced by two days at a time over the entire period of 2006 until a total of 180 combinations of representatives were computed. This ensemble of combinations of representatives was grouped into two sets for winter–spring (October–April) and summer–fall (May–September). The error correlation associated with each salinity representer was normalized by the product of the standard deviations of $L$ and detided model variables. Each individual correlation map suggests the most suitable observation locations for the corresponding time, and would be valuable for adaptive sampling and individual glider mission control. Here we form an average of all the correlation maps to measure the overall relevance of a glider track with $L$ were the track be occupied on repeated missions throughout the season. To avoid the cancelation of positive and negative correlations, we computed the root-mean-square (RMS) average of all the correlation fields in each season set, which we call the relevance function to aid the distinction. Salinity relevance functions at 20 m depth in both seasons are presented in Fig. 6.

The average correlation map for summer–fall (Fig. 6a) has highest relevance north of the cross-section and the relevance contours

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**Fig. 3.** Seasonal averages of salinity (in color) and current (arrows) at 20 m depth. Gray lines are 20, 40, 60 m isobaths and the thick black lines indicate the cross-section of the Hudson Shelf Valley used to compute the salt flux. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

**Fig. 4.** Time series of the modeled subsurface (below 10 m) along-valley salt flux within the Hudson Shelf Valley during 2006. The thin gray line is the daily-averaged time series and the thick black line is 24-day low-pass filtered. Positive is shoreward.
are nearly circular. In winter–spring, the highest relevance occurs east of the cross-section and is elongated roughly along shelf. These positions are consistent with the circulation in Fig. 3. In summer and fall, subsurface current is southward to southwestward, so upstream to the cross-section is somewhat to the north. In winter and spring, circulation at the cross-section is shoreward along the HSV and upstream to the cross-section is to the east or southeast. Moreover, the relevance in winter–spring season is higher because the current within the HSV is much stronger and consistently onshore at that time.

Guided by the information in the relevance patterns we chose optimal glider tracks for 2 gliders for each biseasonal period and present these in Fig. 6 (triangles) along with a traditional design approach that would simply operate gliders on both sides of the cross-section (circles). We emphasize that the optimal track is not obtained from a robust optimization algorithm but chosen intuitively according to the relevance pattern. We call it “optimal” here to distinguish it from the traditional track. True optimization would require an algorithm that took into consideration constraints on glider operation.

4.3. Twin experiments

We evaluate whether the proposed optimal sampling strategy is indeed advantageous with a set of DA twin experiments, the workflow for which is depicted in Fig. 5. For each member in the ensemble we took temperature and salinity vertical profiles from the control run along two tracks: traditional, and optimal according to the season. Both sets of “observations” were taken 2 days from the nominal time zero (Fig. 5), and had the same quantity of data to make the comparison fair. We then conducted a perturbed nonlinear forward simulation by starting from the end of day = 1 with initial conditions obtained from the model state 5 days prior (day − 4 in Fig. 5). Forcing was unchanged from the control run. The subsurface salt flux at the cross-section at day = 4, $L_b$, therefore differs from the truth, $L_t$. The two sets of observations were assimilated using Incremental Strong-constraint 4DVAR (IS4DVAR) DA described in Part I (Zhang et al., 2010). The DA window is 1 day and the “glider-measured” temperature and salinity profiles were the only data assimilated. The adjusted initial conditions given by the two DA analyses were used to initialize two forecast simulations. For the 180 members of the ensemble we therefore have the true salt flux at the section at day = 4, $L_o$, the prior conditions to the DA from the perturbed simulation, $L_p$, and two forecast realizations (one each for the optimal and traditional sampled data sets), which we denote $L_a$.

The added skill of the DA system for the two data sets (Fig. 7) uses a metric defined as

$$S = 1 - \frac{|L_a - L_t|}{|L_b - L_t|}.$$  \hspace{1cm} (8)

$S = 0$ would not indicate that the forecast is of no value, only that DA did not improve it. When $S > 0$, DA has improved the forecast $L$ compared to the prior value. For both seasons, the system assimilating optimally sampled observations gives a statistically better 2-day prediction of the salt flux. In summer–fall the improvement in $L$ for the optimal track is comparable to that obtained with the traditional tracks, but for winter–spring the improvement in the prediction using optimal tracks is much greater. This reflects differences in relevance functions. In summer–fall when the inner shelf is stratified and circulation is highly responsive to variable winds the relevance function is weak. Moreover, the areas of high relevance are close in the optimal and traditional sampling locations (Fig. 6) so the information is not appreciably different. This suggests that the proposed semi-routine deployment approach is not suitable for summer–fall and a strategy more adaptive to daily conditions might be preferable, whereas the winter–spring optimal sampling strategy is clearly superior.

Fig. 7 also shows that assimilating the optimal observations does not necessarily give a better prediction of salt flux on other days; e.g. the first and the fourth day predictions of salt flux of the two systems are indistinguishable for both seasons. This is not surprising because the objective function, $L$, was defined as day 2 of the forecast salt flux, and the system as we have configured it accordingly places less weight on other days. This highlights that the representer-based system is very dependent on the objective function, which should be carefully defined to meet the purpose of the application.
5. Comparison of observation influences

Observation influence is a measure that operational oceanographers and policy makers discuss with regard to integrating observing systems (Kaiser and Pulsipher, 2004), designing new observation networks (Oke and Schiller, 2007), or evaluating existing observations (Frolov et al., 2008). In this section we explore the use of the representer system to compare observation influences.

The representer associated with a single observation describes the potential model state increment that the observation can generate in a 4DVAR assimilation system. As implied by the indirect representer method (Bennett, 2002), this property extends to the representer associated with a linear combination of observations. Here, we restate the property to aid explanation in the following applications.

An outcome of DA is correction of the model state error at the observation locations and times. We can quantify this by a gain function, \( G \), which for a single observation is \( G_0 = \phi_0(x_0, t_0) - \phi(x_0, t_0) \). \( \phi_0(x_0, t_0) \) is observed quantity in the model and \( \phi(x_0, t_0) \) is the truth. The gain function of a group of observations can be the superposition of the gain functions of each individual observation and therefore a function of model state errors. In 4DVAR, assimilation corrects the ocean state not only at the observation locations but also at other locations and times through the dynamical and statistical connections that are embedded in the system, as the representer function depicts. The extent and magnitude of the influence on model state increments than can be generated by assimilating the observations is what we intend to quantify.

The initial condition, \( \Lambda(\phi_0, x_0, t_0) \), to the adjoint model in computing the representer of a single observation can be considered as the derivative of the corresponding gain function with respect to model state everywhere at the observation time, \( \partial G_0/\partial \Phi(t_0) \). The resulting representer gives the error covariance of \( G_0 \) and model states everywhere at all locations, and therefore outlines the influences of the observation in a 4DVAR system (Bennett, 2002). For a group of observations, we can obtain their influences in a 4DVAR system by combining the representers associated with each observation. The mathematical basis for this is essentially the same as in Section 2.

We present three examples to demonstrate this representer-based observation influence. We consider (i) the area and strength of influence of two different observing strategies, (ii) how the same observation strategy has differing influence for different dynamical regimes, and (iii) how the influence alters with different DA windows. Note that these examples are not aimed at the design of a particular realistic observation network, but rather are presented to qualitatively compare the influences of some typical elementary components of an observational system.

5.1. Comparison of glider and mooring observations

Giders and moorings are two instrument platforms commonly deployed in the NYB to measure vertical profiles of temperature and salinity. We compare their influences in this section. Fig. 1 shows a track typical of the so-called ‘Endurance Line’ cross-shelf glider section surveyed approximately 10 times per year by the RU-COOL (Castelao et al., 2008a). We consider a hypothetical glider transect slightly north of the nominal real track and assume a one-way mission takes 3 days, which is roughly the time it takes a real glider to traverse the shelf. To this we compare a hypothetical mooring that continuously observes temperature and salinity throughout the water column located at the 20-m isobath of the glider track.

Our analysis uses 60 days of simulated ocean conditions in April and May, 2006, from the forward control simulation introduced in Section 3. Full water column vertical temperature and salinity profiles were sampled from the control run at every model time step (180 s); at a single fixed location in the case of the mooring, and at locations traversing the shelf over 3 days in the case of the glider. The 2-month period was then separated to twenty 3-day windows and a representer computation was conducted in each window. Assuming model state error everywhere is proportional to ocean state anomaly and with the constant scale between model state error and ocean state anomaly neglected, we define the gain function as an overall measure of the model state error at the observation locations and times,

\[
G = \frac{1}{N} \sum_{i=1}^{N} \left[ \frac{(T_i - \bar{T})^2}{O_{ti}} + \frac{(S_i - \bar{S})^2}{O_{si}} \right],
\]

where \( N \) is the total number of samples, \( T_i \) and \( S_i \) are observed temperature and salinity, respectively, the overbar denotes temporal mean at each observation location, and \( O_{ti} \) and \( O_{si} \) are error covariance of each temperature and salinity observation, respectively. This definition of gain function is similar to the observational cost function of 4DVAR DA (Part I). With this definition, the influence of each observation in the group is essentially scaled by the model state error at the observation location and time. The resulting total influences ought to be explained as model-error-scaled influences of the group observations.

The representer computation is as in Section 4. For each combination of representers, the adjoint model is integrated backward for 3 days with adjoint forcing, \( \partial G(t) \), throughout the integration period, the background error covariance is applied at the nominal \( t = 0 \) for the interval, and the tangent linear model is integrated forward for 6 days to show the observation influences in both analysis (the first 3 days) and forecast (the last 3 days) periods. The RMS of the ensemble of 20 error covariance fields was...
then computed for different relative times in the 6-day window. Fig. 8 shows the RMS average temperature error covariance at the surface through time.

In the analysis period (the first two columns in Fig. 8) the glider observations have influence over a wider area than the mooring, but the strength of influence of the mooring at the observation location is about twice that of the glider. This result is consistent with most oceanographers’ intuition on the likely relative value of the two instruments, but is quantified by the representer analysis. During the forecast period (the last two columns in Fig. 8), the influence of the glider observations decays, while that of the mooring stays strong. At day 6, 3 days into the forecast, the influence of the mooring at the observation location is more than three times stronger than that of the glider, and the area of influence of the mooring expands quickly along the shelf over the forecast period, whereas that of glider observation expands little. Thus, it appears that at day 6 the mooring has greater overall surface influence than the glider.

In Fig. 9, we plot the influence of data from the two instruments along the vertical cross-section along the glider track. As inferred from Fig. 8, the glider influence extends across the shelf while the mooring has greater magnitude but less spatially extensive influence centered at the observation location. An interesting feature in Fig. 9 is that both cross-sections at day 0 show rather greater influence in the surface and bottom boundary layer than in the middle of the water column. This suggests that dynamical connections in the boundary layers, caused by the wind-driven coastal upwelling and downwelling, extend the scope of influence of observations – a consequence of the ocean physics embodied in the adjoint and tangent linear models.

5.2. Influence of glider observations in different wind regimes

Wind-driven coastal upwelling and downwelling are common phenomena in the inner shelf of the NYB (Castelao et al., 2008b; Wong, 1999; Yankovsky and Garvine, 1998), and effective observational strategies for these distinct dynamical regimes are of interest to operational oceanographers. In this section, we take the hypothetical glider track of Section 5.1 as an example and demonstrate how its influence differs in upwelling and downwelling regimes.

The 20 combinations of glider representers from Section 5.1 were separated into two groups according to the average wind direction in the 3-day observation windows (southerly wind drives upwelling on the New Jersey coast; northerly wind drives downwelling). The RMS of the temperature error covariance fields of each group, at the sea surface, is presented in Fig. 10. The influence in the analysis window (days 0–3) during upwelling is about twice as strong as that in the downwelling regime. Coastal upwelling pulls deep cold water to the surface and downwelling pushes offshore surface water onshore, so surface temperature anomalies are stronger during upwelling and model surface temperature error in the upwelling regime is larger. Because the combination of representers computed here is the model-error-scaled influence, the influence of the glider observations on correcting model state errors is therefore larger in the upwelling regime.

At day 0, the influence of the observations extends further southward along the coast during upwelling and further northward during downwelling because the model captures the dynamical upstream of the observed quantities. The upstream information embodied in the observations and revealed by the representer analysis concurs with the identification of dynamical upstream regions by adjoint sensitivity (Zhang et al., 2009b) and this information would subsequently influence the 4DVAR assimilation. As time proceeds into the forecast window (the last two columns in Fig. 10), the area of influence propagates in the respective downstream direction for the two regimes.

5.3. Comparison of different data assimilation windows

An advantage of 4DVAR DA is its ability to propagate information, e.g. observation innovation, over time, both backward and for-
ward. Ideally, we would like the information to be propagated as long as possible in order to fully exploit the dynamical connections captured by the adjoint and tangent linear models. But the duration that the information can propagate, namely the DA window, is somewhat constrained by the linearization in 4DVAR systems. For the same observations, different lengths of the DA window will result in different observation influence. To show this, we present a simple example using the representer-based estimate of observation influence.

We formed four groups of combinations of representers for observations along the hypothetical glider track. Each group has 20 combinations of representers. The adjoint models in the 4 groups were initialized at the same times and integrated backward in time for 0, 1, 2 and 3 days, and the tangent linear models were
integrated forward for 3, 4, 5 and 6 days, respectively, bringing them all to day = 6. To make the comparison fair, we assumed all glider observations were made at the instant of the initial times of the adjoint models; this ensured all representer windows received equivalent amounts of data.

The RMS of the error covariance fields in each group give the average surface temperature influences in Fig. 11. Day = 3 is the observation time in each representer computation, and day = 6 is the ending time of the tangent linear integration. Comparing the plots in each row shows that the longer the window the larger the area of influence. At day 3, the average influence in the 0-day window group is confined around the glider track and results entirely from the background covariance immediately extending the observational information to neighboring points. As the window becomes longer, the influence spreads out, especially along the coast, reflecting the added information introduced by the adjoint and tangent linear models in regions that are dynamically upstream to the data locations. The average influence in the 3-day window group covers almost the entire New Jersey coast. Note that the small covariance value (0.01) at the edges of the area of influence results from the ensemble averaging process. The covariance of any ensemble member is larger, but with area of influence that is smaller in extent and skewed toward the upstream region for the flow at that particular time.

The combination of representers of the 0-day window is analogous to observation influences in sequential DA, e.g., 3DVAR and Kalman filter-type DA methods. In those methods information about the dynamical upstream is not exploited; there is no backward in time propagation of observation innovation. In 4DVAR, the adjoint model propagates the observation innovation backward according to the linearized dynamics and identifies where corrections should be made to the dynamically upstream initial conditions, boundary conditions, or surface forcing. The Kalman smoother shares some of these properties.

6. Summary

This paper is the second part of a project developing integrated observation and modeling capabilities in coastal ocean prediction for the NYB. Part I demonstrated how 4DVAR data assimilation using ROMS improves ocean state estimates in a realistic pseudo-real-time setup. This Part is dedicated to the complementary objective of using an integrated observation-modeling system to improve observing system design.

A representer function describes the error covariance between a local feature of interest and variables at all locations at any time. In 4DVAR data assimilation, the representer expresses the influence of a single assimilated observation and can be used in the process of cost function minimization in observation space (Bennett, 2002). To extend the application of the representer beyond an isolated observation, we have shown that the combination of representers associated with a function that combines model variables, such as salt flux, has properties similar to an isolated observation. It describes the error covariance between the physical quantity of interest described by the function and model variables at all locations at any time within the assimilation window. Assuming there are no complementary observations and model performance is roughly uniform, then where the correlation is highest is logically a more optimal place to acquire observations in order for the model to describe the feature of interest more precisely. Similarly, the combination of representers associated with a group of observations outlines the influence of the observations as a whole in a 4DVAR data assimilation system. To consider how a combination of representers might guide the choice of observational strategies, we sought an “optimal” glider track for better model prediction of salt flux across a cross-section of the Hudson Shelf Valley 2 days after the glider deployment. An ensemble of combinations of representers were computed and grouped into two biseasonal periods (sum-

![Fig. 11. Contours of representer-based influence of a glider section (black straight lines) at day 3 (top row) and day 6 (bottom row) in systems with different durations of the data assimilation window. The contour lines are 0.01, 0.1, 0.5 °C. The observations were taken at day 3.](image-url)
mer–fall, and winter–spring) that share similar characteristics in the mean circulation. Optimal glider tracks were then picked heuristically for both seasons according to the correlation maps. Data assimilation twin experiments verified that glider observations taken along the proposed ‘optimal’ paths led to greater skill in term of predicting the salt flux 2 days after the observations were obtained.

A representer-based system was presented that measures the influence of a group of observations in a 4DVAR data assimilation system, and this was used to compare the data influence for different observing strategies. We compared the influences of equivalent amounts of data acquired by a repeat glider cross-shelf section versus a fixed mooring. The glider section has a wider area of influence while the mooring has stronger influence in the environs of the observation location. We compared the influence of the same routine glider section in different dynamical regimes: wind-driven coastal upwelling and down-welling. The area of influence of the glider data is shifted toward the dynamical upstream: southward along the coast in upwelling and northward along the coast in down-welling. We evaluated the influence of duration of data assimilation window lengths, obtaining a result that agrees with intuition that a longer assimilation window introduces more dynamical connections and extends the influence of observations to a larger area.

This work demonstrates the capability of representer-based systems to aid in developing more optimal observation strategies and quantifying the extent of influence of a set of observations. The method can be used to help design the positioning of a single instrument or an observation network. We emphasize that the notion of what observing strategy is optimal depends on the physical quantity of interest, but the system we have described is flexible in its ability to consider quite arbitrary arithmetic functions of the ocean state, including fluxes and transports, and regional spatial means or time averages.

The work in this paper approaches the design problem from one perspective; namely, identifying observing system characteristics that enhance forecast skill when the data are subsequently adopted in a 4DVAR assimilation system. True optimization of observing system design must take into consideration other constraints that are instrumental and logistical.

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Appendix. Derivation of Eqs. (3)–(6)

Suppose $a$ and $b$ are two independent variables at particular locations of interest, $x_1$ and $x_2$, respectively, at time $t_0$, that is, $a = \phi_1(x_1, t_0)$ and $b = \phi_2(x_2, t_0)$, and $N$ is the number of all possible ocean states. We have two assumptions: (i) the ocean state given by the control nonlinear simulation is a valid estimate of the ensemble mean of a set of ocean states, that is, $a_0 = a$, and $b_0 = b$, where subscript $0$ stands for the value given by the control simulation and overbar the ensemble mean and (ii) the deviation of all possible ocean states from the mean is small and the product of two or more state deviations (e.g. $ab'$) is negligible.

Derivation of Eq. (3):

$$\text{Crep} \left( \frac{\partial(a + b)}{\partial(\Phi(t_0))} \right) = \text{rep} \left( \frac{\partial a}{\partial(\Phi(t_0))} + \frac{\partial b}{\partial(\Phi(t_0))} \right)$$

$$= \text{cov}(a, \Phi(t)) + \text{cov}(b, \Phi(t))$$

Derivation of Eq. (4) is very similar to that of Eq. (3) and therefore neglected here.

Derivation of Eq. (5):

$$\text{Crep} \left( \frac{\partial(ab)}{\partial(\Phi(t_0))} \right) = b_0 \text{rep} \left( \frac{\partial a}{\partial(\Phi(t_0))} \right) + a \text{rep} \left( \frac{\partial b}{\partial(\Phi(t_0))} \right)$$

Applying aforementioned assumptions, we have

Derivation of Eq. (6):

$$\text{Crep} \left( \frac{\partial(a/b)}{\partial(\Phi(t_0))} \right) = \frac{1}{b_0} \text{rep} \left( \frac{\partial a}{\partial(\Phi(t_0))} - \frac{a_0}{b_0} \text{rep} \left( \frac{\partial b}{\partial(\Phi(t_0))} \right) \right)$$

Applying aforementioned assumptions, we have

References
