NOTES AND CORRESPONDENCE

Optimal Linear Fitting for Objective Determination of Ocean Mixed Layer Depth from Glider Profiles

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ABSTRACT

A new optimal linear fitting method has been developed to determine mixed layer depth from profile data. This methodology includes three steps: 1) fitting the profile data from the first point near the surface to a depth using a linear polynomial, 2) computing the error ratio of absolute bias of few data points below that depth versus the root-mean-square error of data points from the surface to that depth between observed and fitted data, and 3) finding the depth (i.e., the mixed layer depth) with maximum error ratio. Temperature profiles in the western North Atlantic Ocean over 14 November–5 December 2007, collected from two gliders (Seagliders) deployed by the Naval Oceanographic Office (NAVOCEANO), are used to demonstrate the capability of this method. The mean quality index (1.0 for perfect determination) for determining mixed layer depth is greater than 0.97, which is much higher than the critical value of 0.8 for well-defined mixed layer depth with that index.

1. Introduction

Upper oceans are characterized by the existence of a vertically quasi-uniform layer of temperature (T, isothermal layer) and density (ρ, mixed layer). Underneath each layer, there exists another layer with a strong vertical gradient, such as the thermocline (in temperature) and pycnocline (in density). The intense vertical turbulent mixing near the surface causes the vertically quasi-uniform layer. The mixed layer is a key component in studies of climate and the link between the atmosphere and deep ocean (Chu 1993). It directly affects the air–sea exchange of heat, momentum, and gases. The mixed layer (or isothemal layer) depth H_{mix} is an important parameter that largely affects the evolution of the sea surface temperature (SST) (Zhang and Zhang 2001).

Three criteria are available to determine H_{mix}: difference, gradient, and curvature. The difference criterion requires the deviation of T (or ρ) from its surface value to be smaller than a certain fixed value. The gradient criterion requires $\partial T/\partial z$ (or $\partial \rho/\partial z$) to be smaller than a certain fixed value. The curvature criterion requires $\partial^2 T/\partial z^2$ (or $\partial^2 \rho/\partial z^2$) to be maximum at the base of the mixed layer ($z = -H_{\mathrm{mix}}$). Obviously, the difference and gradient criteria are subjective. For example, in the difference criterion for determining H_{mix} for temperature, the fixed value varies from 0.5° (Wyrtki 1964) to 0.8°C (Kara et al. 2000). Defant (1961) was among the first to use the gradient method. He used a gradient of 0.015°C m^{-1} to determine H_{mix} for the temperature of the Atlantic Ocean, whereas Lukas and Lindstrom (1991) used 0.025°C m^{-1}. The curvature criterion is an objective method (Chu et al. 1997, 1999, 2000; Lorbacher et al. 2006), but it is relatively hard to use for noisy profile data because the curvature involves the calculation of the second derivative versus depth (Chu et al. 1999; Chu 2006). AU1

Thus, it is urgent to develop a simple objective method for determining mixed layer depth with the capability of handling noisy data. The objective of this paper is to present such a method based on the existence of a near-surface, quasi-homogeneous layer. We will show that the proposed method is easy to implement and that the method performs well against glider-based observations of the mixed layer.

2. Methodology

Assume a temperature profile that can be represented by $[T(z_i)]$. A linear polynomial is used to fit the profile

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14. ABSTRACT

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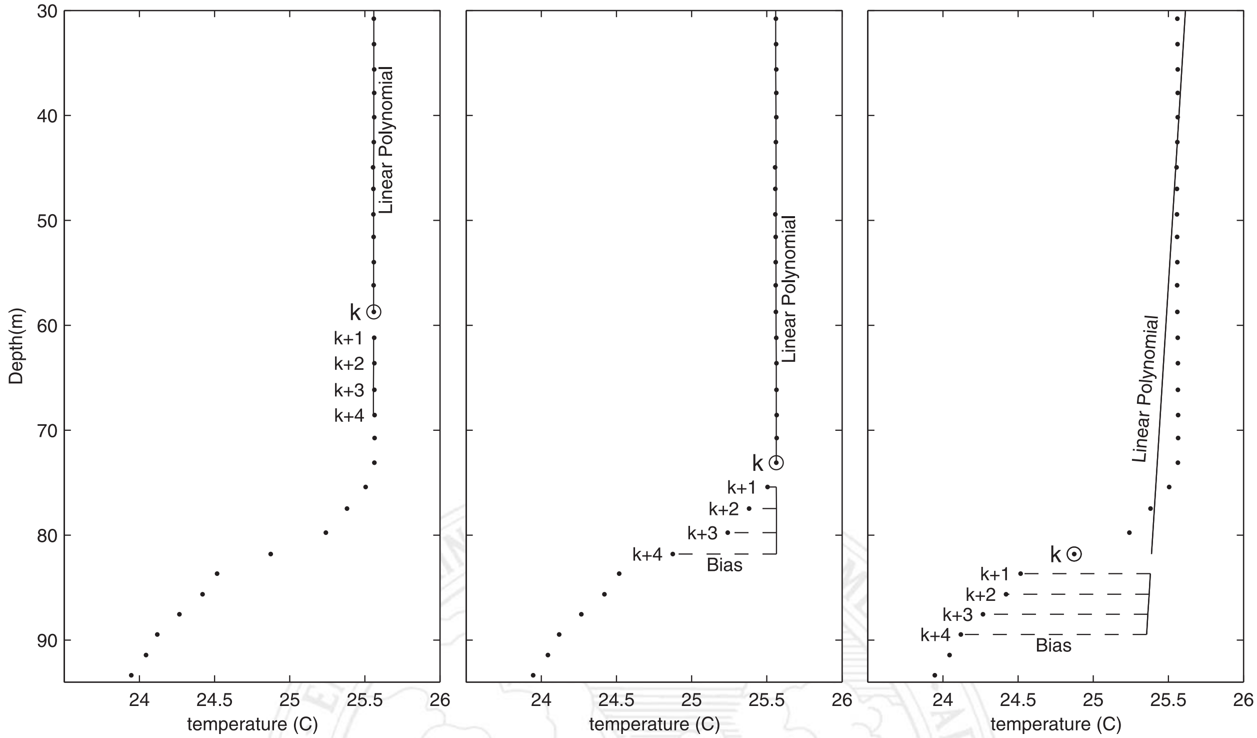

FIG. 1. Illustration of the optimal linear fitting (OLF) method: (a) z_k inside the mixed layer (small E_1 and E_2), (b) z_k at the mixed layer depth (small E_1 and large E_2), and (c) z_k below the mixed layer depth (large E_1 and E_2).

data from the first point near the surface (z_1) to a depth z_k (marked by a circle in Fig. 1). The original and fitted data are represented by ($T_1, T_2, \ldots, T_k$) and ($\hat{T}_1, \hat{T}_2, \ldots, \hat{T}_k$), respectively. The root-mean-square error E_1 is calculated by

$$E_1(k) = \sqrt{\frac{1}{k}\sum_{i=1}^{k}(T_i - \hat{T}_i)^2}. \tag{1}$$

The next step is to select n data points ($n \ll k$) from the depth z_k downward: $T_{k+1}, T_{k+2}, \ldots, T_{k+n}$. A small number n is used because below the mixed layer temperature has a large vertical gradient and because our purpose is to identify if z_k is at the mixed layer depth. The linear polynomial for data points ($z_1, z_2, \ldots, z_k$) is extrapolated into the depths ($z_{k+1}, z_{k+2}, \ldots, z_{k+n}$): $\hat{T}_{k+1}, \hat{T}_{k+2}, \ldots, \hat{T}_{k+n}$. The bias of the linear fitting for the n points is calculated by

$$\mathrm{Bias}(k) = \frac{1}{n}\sum_{j=1}^{n}(T_{k+j} - \hat{T}_{k+j}). \tag{2}$$

If the depth z_k is inside the mixed layer (Fig. 1a), the linear polynomial fitting is well representative for the data points ($z_1, z_2, \ldots, z_{k+n}$). The absolute value of the bias,

$$E_2(k) = |\mathrm{Bias}(k)|, \tag{3}$$

for the lowest n points is usually smaller than E_1 since differences between observed and fitted data for the lowest n points may cancel each other. If the depth z_k is located at the base of the mixed layer, $E_2(k)$ is large and $E_1(k)$ is small (Fig. 1b). If the depth z_k is located below at the base of the mixed layer (Fig. 1c), both $E_1(k)$ and $E_2(k)$ are large. Thus, the criterion for determining the mixed layer depth can be described as

$$\frac{E_2(z_k)}{E_1(z_k)} \rightarrow \max, \quad H_{\mathrm{mix}} = -z_k, \tag{4}$$

which is called the optimal linear fitting (OLF) method. The OLF method is based on the notion that there exists a near-surface, quasi-homogeneous layer in which the standard deviation of the property (temperature, salinity, or density) about its vertical mean is close to zero. Below the depth of H_{mix}, the property variance should increase rapidly about the vertical mean.

3. Glider data

Two Seagliders (Eriksen et al. 2001) were deployed in the western North Atlantic Ocean (Fig. 2a) by the Naval Oceanographic Office (NAVOCEANO) (Mahoney et al.

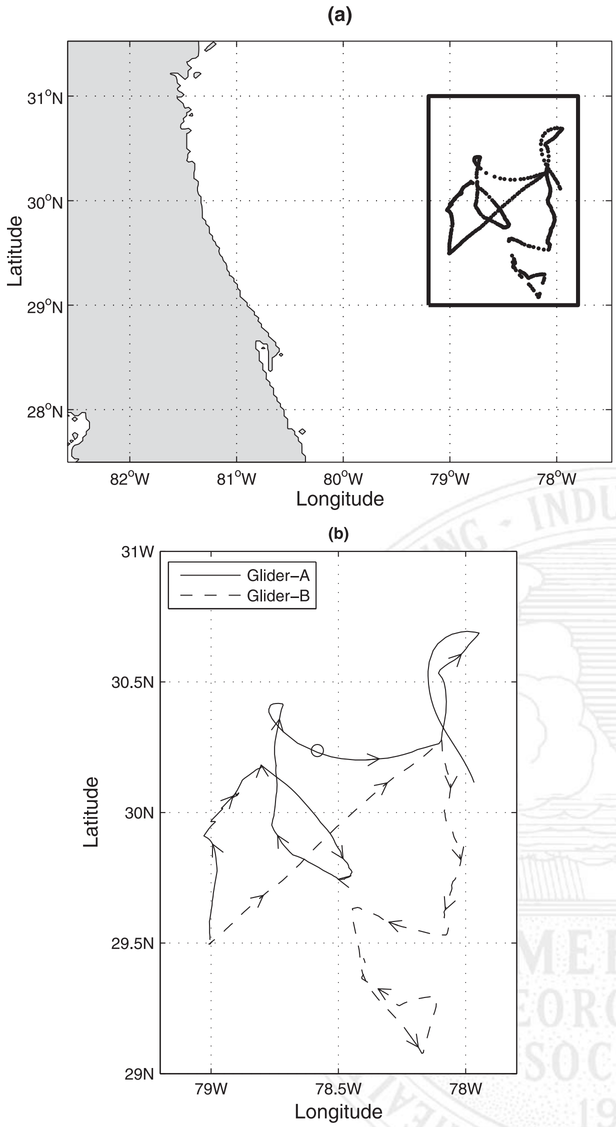

FIG. 2. (a) Location of the glider data and (b) drifting paths of two gliders with the marked station for demonstration in section 4.

2009) from two nearby locations on 14 November 2007: one at 29.5°N, 79.0°W (glider A) and the other at 29.6°N, 79.0°W (glider B). Glider A (solid curve) moved toward the northeast to 30.25°N, 78.1°W, turned anticyclonically toward the south, and finally turned cyclonically at 29.6°N, 78.4°W. Glider B (dashed curve) moved toward the north to 30.0°N, 79.0°W, turned northeast and then anticyclonically, and finally turned cyclonically (Fig. 2b). Our purpose is the objective determination of the mixed layer depth, not the description of the flow pattern and eddy structure.

The temperature profile data observed by the two deployed gliders underwent quality control (QC) procedures

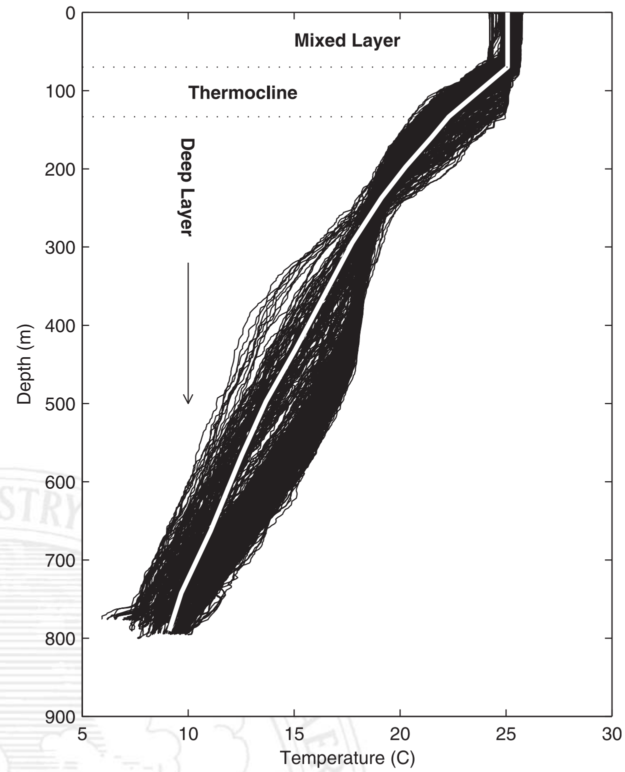

FIG. 3. Temperature profiles (total of 467) collected from the two gliders.

prior to analysis by the OFL method. These QC procedures consisted of a min–max check (e.g., disregarding any temperature data less than −2°C or greater than 35°C), an error anomaly check (e.g., rejecting temperature data deviating more than 7°C from climatology), a glider-tracking algorithm (screening out data with obvious glider position errors), a max-number limit (limiting a maximum number of observations within a specified and rarely exceeded space–time window), and a buddy check (tossing out contradicting data). The climatological dataset used for the quality control is the Navy's Generalized Digital Environmental Model (GDEM) climatological temperature and salinity dataset. After the QC, there were 467 profiles available for OLF analysis for determining the mixed layer. The vertical resolution of the profile is around 1 m. All the profiles are deeper than 700 m and clearly show the existence of layered structure: mixed layer, thermocline, and deep layer (Fig. 3). F3

4. Verification

Lorbacher et al. (2006) proposed a quality index ($\mathrm{QI}_{\mathrm{mix}}$) AU2 for determining H_{mix},

$$\mathrm{QI}_{\mathrm{mix}} = 1 - \frac{\mathrm{rmsd}(T_k - \hat{T}_k)|_{(H_1, H_{\mathrm{mix}})}}{\mathrm{rmsd}(T_k - \hat{T}_k)|_{(H_1, 1.5\times H_{\mathrm{mix}})}}, \qquad (5)$$

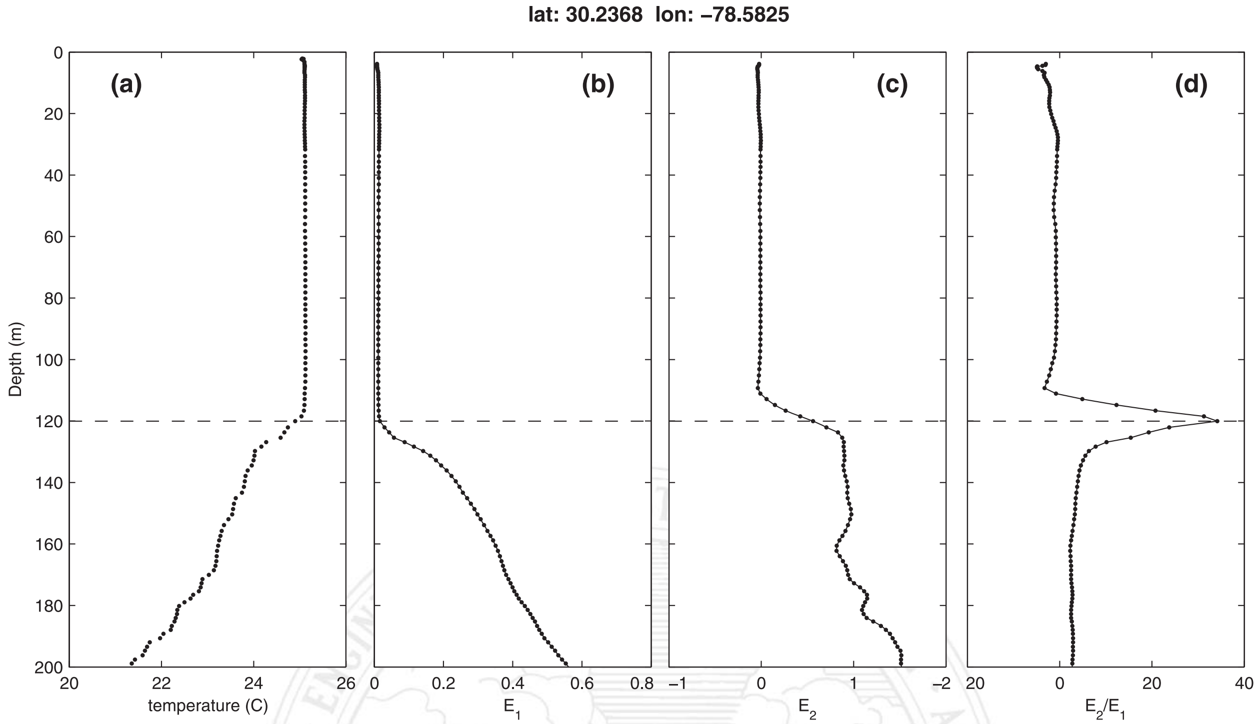

FIG. 4. Determination of H_{mix} using the OLF method: (a) temperature profile at the station (marked in Fig. 2b) by glider A, (b) calculated $E_1(k)$ by Eq. (1), (c) calculated $E_2(k)$ by Eqs. (2) and (3), and (d) ratio $E_2(k)/E_1(k)$. It is noted that the depth of the maximum ratio corresponds to the mixed layer depth.

which is one negative root-mean-square difference (rmsd) between the observed and fitted temperature in the depth range from the surface to H_{mix}, to the rmsd between the observed and fitted temperature in the depth range from the surface to $1.5 \times H_{mix}$. Its value of 1.0 represents "high-quality" computation of H_{mix} and progressively lower values imply that either larger volumes of stratified water present above the level of H_{mix}. Note that H_{mix} is well defined if $QI_{mix} > 0.8$, H_{mix} can be determined with uncertainty for QI_{mix} in the range of 0.5–0.8, and H_{mix} cannot be identified for $QI_{mix} < 0.5$. For the curvature criterion, QI_{mix} was above 0.7 for 70% of the profile data, including conductivity–temperature–depth (CTD) and expendable bathythermograph (XBT) data obtained during the World Ocean Circulation Experiment (Lorbacher et al. 2006).

The OLF method [i.e., (1)–(4)] was used to calculate H_{mix} from 467 quality-controlled profiles observed by the two Seagliders. With high vertical resolution (1 m), we chose $n = 4$. The value of H_{mix} was calculated for each profile. One station from glider A, located at 30.2368°N, 78.5825°W (marked in Fig. 2), is taken as the example for illustration. The observational temperature profile is shown in Fig. 4a. From the surface downward to any depth z_k, a linear fitting for the data of $(T_1, T_2, \ldots, T_k)$ provides the calculated data $(\hat{T}_1, \hat{T}_2, \ldots, \hat{T}_k, \ldots, \hat{T}_{k+4})$. The errors $E_1(k)$ (Fig. 4b) and $E_2(k)$ (Fig. 4c) are easily calculated using Eqs. (2) and (3). The location of the mixed layer depth in the profile corresponds to the maximum value of $E_2(k)/E_1(k)$ (Fig. 4d).

The calculated mixed layer depths from all 467 temperature profiles were plotted versus time in Fig. 5a (glider A) and Fig. 5b (glider B). Glider A (B) was drifting in the northwest (southeast) part of the region 29°–31°N, 78°–79°W. In this $1° \times 2°$ area, the fluctuations in the mixed layer depth are smaller before 25 November 2007 compared to the fluctuations in the mixed layer depth observed after this date. The mixed layer depth oscillates between 50 and 90 m before 25 November 2007, and between 58 and 136 m for glider A (Fig. 5a) and between 25 and 110 m for glider B after 25 November 2007. The surface wind and buoyancy forcing may be responsible for the spatial temporal variability of the mixed layer depth; however, determining the cause of this variability is beyond the scope of this paper. Figure 6a shows the histogram of mixed layer depths for all 467 temperature profiles. The distribution is quite symmetric. The mode is around 70 m, with the maximum mixed layer depth around 136 m and minimum mixed layer depth near 25 m. The quality index (QI_{mix}) is computed for each profile using Eq. (5). The histogram of 467 values of QI_{mix} (Fig. 6b) shows strong negatively skewed

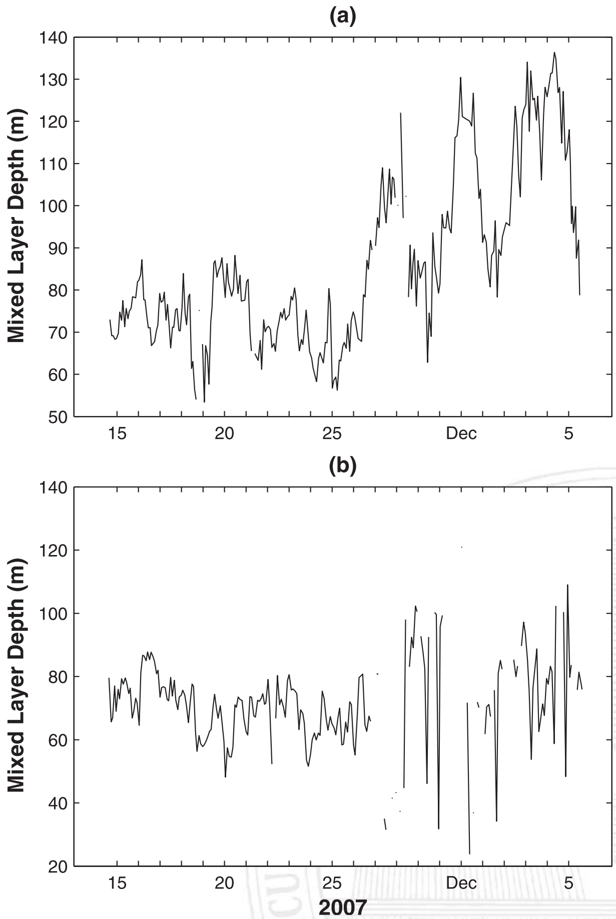

FIG. 5. Mixed layer depth along the track of (a) glider A and (b) glider B.

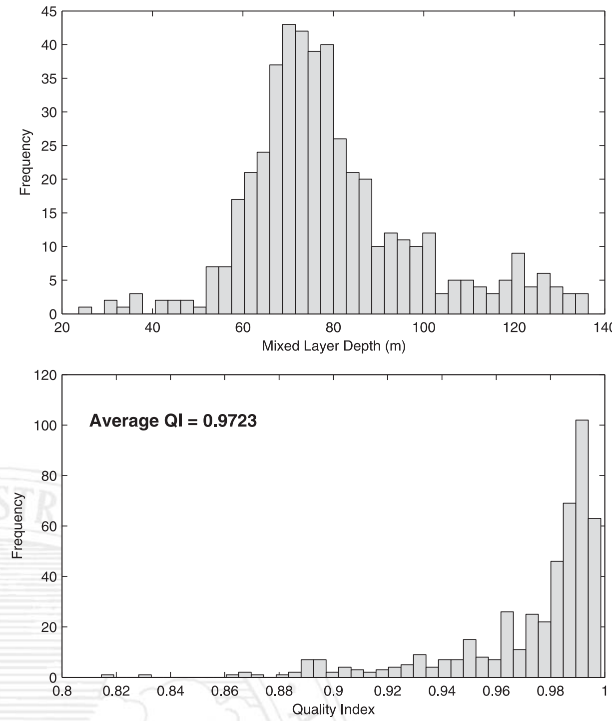

FIG. 6. Histograms of (a) H_{mix} and (b) quality index QI_{mix}.

distribution with most values larger than 0.98 and an averaged value of 0.9723. The minimum value of QI_{mix} is 0.82 for only one profile. High QI_{mix} values show the capability of OLF to determine mixed layer depth from profile data.

5. Conclusions

In this study, we established a new simple method to identify mixed layer depth from profile data. First, a linear polynomial is used to fit the profile data from the first point near the surface to a depth. Then, the error ratio of absolute bias of data points below that depth versus the root-mean-square error of data points from the surface to that depth between observed and fitted data is computed. Next, the mixed layer depth that corresponds to the maximum ratio of the bias to the root-mean-square error is found. Three advantages of this approach are as follows: (a) determination of mixed layer depth (H_{mix}) depends on downward profile data from the surface and not on any particular surface variables such as the sea surface temperature; (b) the procedure is totally objective without any initial guess (no iteration); and (c) no differentiations (first or second) are calculated for the profile data. With these features, the OLF method is capable of determining H_{mix} objectively and with high accuracy. This method has been verified using glider data. Feasibility studies should be conducted for other types of data such as conductivity–temperature–depth (CTD), expendable bathythermograph (XBT), and Argo profiles.

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