Article

An Information Spatial-Temporal Extension Algorithm for Shipborne Predictions Based on Deep Neural Networks with Remote Sensing Observations—Part I: Ocean Temperature

Kai Mao 1, Feng Gao 1,2,* , Shaoqing Zhang 1,3,4,5 and Chang Liu 1,6

1 College of Intelligent Systems Science and Engineering, Harbin Engineering University, Harbin 150001, China; maokai@hrbeu.edu.cn (K.M.); szhang@ouc.edu.cn (S.Z.); liuchang407@hrbeu.edu.cn (C.L.)
2 Qingdao Innovation and Development Center, Harbin Engineering University, Qingdao 266400, China
3 Key Laboratory of Physical Oceanography, MOE, Institute for Advanced Ocean Study, Frontiers Science Center for Deep Ocean Multiplespheres and Earth System (DOMES), Ocean University of China, Qingdao 266100, China
4 The College of Ocean and Atmosphere, Ocean University of China, Qingdao 266100, China
5 Ocean Dynamics and Climate Function Lab/Pilot National Laboratory for Marine Science and Technology (QINLM), Qingdao 266237, China
6 Qingdao Hatran Ocean Intelligence Technology Co., Ltd., Qingdao 266400, China

* Correspondence: gaofeng19@hrbeu.edu.cn

Abstract: For ships on voyage, using satellite remote sensing observations is an effective way to access ocean temperature. However, satellite remote sensing observations can only provide the surface information. Additionally, this information obtained from satellite remote sensing observations is delayed data. Although some previous studies have investigated the spatial inversion (spatial extension) or temporal prediction (temporal extension) of satellite remote sensing observations, these studies did not integrate ship survey observations and the temporal prediction is limited to sea surface temperature (SST). To address these issues, we propose an information spatial-temporal extension (ISTE) algorithm for remote sensing SST. Based on deep neural networks (DNNs), the ISTE algorithm can effectively fuse the satellite remote sensing SST data, ship survey observations data, and historical data to generate a four-dimensional (4D) temperature prediction field. Experimental results show that the ISTE algorithm performs superior prediction accuracy relative to linear regression analysis-based prediction. The prediction results of ISTE exhibit high coefficient of determination (0.9936) and low root mean squared errors (around 0.7 °C) compared with Argo observation data. Therefore, for shipborne predictions, the ISTE algorithm driven by satellite remote sensing SST can be as an effective approach to predict ocean temperature.

Keywords: shipborne predictions; information spatial-temporal extension; satellite remote sensing observations; deep neural networks; ship survey observations; ocean temperature

1. Introduction

The ocean environment has an important impact on human maritime operations. Having timely information about the current and future ocean environment is of great significance to ships that perform operations at sea. For ships on voyage, shipborne predictions that mean conducting variables predictions of ocean environment on board, are convenient approaches for obtaining marine information relative to receiving huge marine data from shore-based institutions.

In terms of ocean temperature, traditional methods of shipborne predictions are mainly based on statistical analysis of historical data, such as linear regression analysis-based prediction (LRAP). However, in general, traditional statistical methods cannot effectively capture the spatial characteristics of ocean data. Moreover, traditional statistical methods are not able to make effective use of observation data. This makes the prediction results
generated through traditional statistical methods less accurate. Under the condition of
shipborne predictions, using satellite remote sensing observations is an effective way to
obtain more accurate ocean temperature. However, satellite remote sensing observations
can only provide surface information and cannot directly provide subsurface information.
Moreover, in this context, the acquired satellite remote sensing observations are delayed
data points, and the real-time remote sensing information is hardly available. In order to
address these issues, it is necessary to conduct information spatial-temporal extension (ISTE)
of satellite remote sensing observations. As a result, four-dimensional (4D) prediction data
can be generated from two-dimensional (2D) observation data and shipborne predictions
driven by satellite remote sensing observations can be realized.

In fact, the information spatial extension (ISE) is equivalent to the spatial inversion
of remote sensing data while the information temporal extension (ITE) is equivalent to
the temporal prediction of remote sensing data. Previous studies have proposed various
algorithms about ISE or ITE, which mainly include empirical analysis methods and artificial
intelligence (AI) methods.

The algorithmic principle of Modular Ocean Data Assimilation System (MODAS) [1]
is a typical empirical analysis method for underwater inversion, which can effectively
portray the underwater temperature structure using satellite remote sensing observations.
With the rapid development of technology, AI represented by deep learning, has shown its
strength in many scientific fields, which include geoscience [2]. Subsequent researchers
have attempted to use AI methods to perform underwater inversion. Ali et al. [3] used
artificial neural networks (ANNs) to estimate the subsurface temperature structures from
surface variables. Lu et al. [4] combined a pre-clustering process and a neural network to
estimate the subsurface temperature anomaly using ocean surface variables at the global
scale. Han et al. [5] used a convolutional neural network (CNN) to estimate subsurface
temperature from satellite remote sensing observations. Sammartino et al. [6] proposed a
Multi-Layer-Perceptron (MLP) network to reconstruct the three-dimensional (3D) fields
of temperature.

It can be anticipated that the inversion accuracy will be improved using vertical
observations in the inversion process, similar to studies carried out by Wang et al. [7], which
combined Argo profiles with satellite observations to reconstruct weekly three-dimensional
temperature fields of the Pacific Ocean. In the situation of shipborne prediction, besides
satellite remote sensing observations, it is convenient to obtain the ship survey observations.
The ship survey observations data can provide subsurface vertical information. However,
these observations are only distributed along the ship route. Meanwhile, the observation
information of other locations is difficult to be obtained. In this context, using the limited
ship survey observations to supplement the remote sensing observations with a suitable
algorithm will further improve the prediction accuracy of the ocean environment.

Although previous studies have carried out research on the fusion of satellite remote
sensing information and ocean observation vertical information, most of the vertical in-
formation comes from Argo grid data products, which means that these algorithms need
enough vertical information data. In the situation of shipborne predictions, the vertical
information data is limited along the ship route. For these special limited data, traditional
methods with statistical analysis are difficult to fuse the ship survey observations and
remote sensing observations [8]. Therefore, a new scheme for data fusion that can make
full use of limited ship survey observations is needed.

In order to obtain the future information of ocean environment, the ITE is required.
Temporal intelligent prediction can be seen as an ITE algorithm of remote sensing ob-
servations, which can use AI methods to predict the future data. Neetu et al. [9] proposed a
nonlinear data-adaptive approach known by the name of genetic algorithm for predicting
satellite-observed sea surface temperature (SST) in the Arabian Sea. Su et al. [10] proposed
a support vector machine approach that can estimate the subsurface temperature anomaly.
Zhang et al. [11] first adopts long short-term memory (LSTM) to predict SST. Xiao et al. [12]
proposed a machine learning method combining the LSTM deep recurrent neural network
model and the AdaBoost ensemble learning model (LSTM-AdaBoost) to predict the short and mid-term daily SST. Wei et al. [13] used ANNs to predict SST of the South China Sea. Sun et al. [14] proposed a time-series graph network (TSGN) for SST prediction that can jointly capture graph-based spatial correlation and temporal dynamics. All these previous studies have developed various algorithms and achieved great success, which greatly promoted the development of ITE algorithms for remote sensing observations. However, for the temporal intelligent prediction of ocean temperature, most previous studies only focused on SST prediction [9–19]. However, sea thermocline has a more important influence on the maritime operation, such as underwater navigation and hydroacoustic communication. A practical and effective prediction method should be applicable to the full range of water depths.

Deep learning, based on deep neural networks (DNNs), is a branch of machine learning. DNNs are ANNs structures with multiple layers, which can learn complex functions by combining nonlinear modules [20,21]. In geoscience, deep learning based on DNNs can better capture the spatial and temporal features of data that are difficult to extract by traditional methods with statistical analysis [2,22,23]. To address the issues above, this study proposes a DNN-based ISTE algorithm for remote sensing SST. The ISTE algorithm can effectively fuse the satellite remote sensing SST data, ship survey observations data and historical data of ocean temperature to generate 4D ocean temperature prediction data. The main contributions of this study are as follows: (1) compared with previous studies, this study effectively integrate the limited ship survey observations using DNNs, which can improve the underwater inversion accuracy of satellite remote sensing SST; (2) this study uses DNNs to achieve temperature predictions over the full water depth, including the mixed layer, thermocline and deep layer; (3) the ISTE algorithm proposed in this study could be a new effective approach for shipborne predictions.

The remainder of this article is organized as follows. Section 2 describes the ISTE principle and experimental details. Section 3 presents the experimental results and performance evaluation of the ISTE. A discussion is given in Section 4. Finally, Section 5 summarizes this study.

2. Materials and Methods

2.1. Data and Tools

Imagine that a ship was operating in the northeastern part of the South China Sea on 13 September 2016. The ship has downloaded global satellite remote sensing SST data for the day 10 September 2016. Three sets of vertical temperature observations measured by ship are available on 11 September 2016, 12 September 2016 and 13 September 2016, respectively. Additionally, historical data for global ocean temperature were stored on board. Based on the available information, we want to predict the 4D ocean temperatures from 13 September 2016 to 10 October 2016 within the region of 112–124°E and 13.5–23°N.

The remote sensing data of daily average SST for experiment come from the L4 satellite remote sensing grid data of Copernicus Marine Environment Monitoring Service (CMEMS) available online: https://resources.marine.copernicus.eu/product-detail/SST_GLO_SST_L4_REP_OBSERVATIONS_010_024/INFORMATION/ (accessed on 6 June 2021). These data were produced by running the Operational Sea Surface Temperature and Sea Ice Analysis system [24,25]. The remote sensing SST of experimental area is shown in Figure 1.

We use Argo data to simulate the ship survey observations, which come from the Chinese Argo Real-time Data Center. Available online: http://www.argo.org.cn/ (accessed on 10 October 2019). The type of Argo instrument used in the experiment is HM2000_TSI, which has small errors and high data quality. These Argo data can provide a temperature profile of 2000 m every 5 days. The Argo after 13 September 2016 will be used to evaluate the prediction effects. The Argo distribution is shown in Figure 2.
Remote Sens. 2022, 14, x 4 of 21

June 2021). These data were produced by running the Operational Sea Surface Temperature and Sea Ice Analysis system [24, 25]. The remote sensing SST of experimental area is shown in Figure 1.

Figure 1. Remote sensing SST for the experimental area of 10 September 2016.

We use Argo data to simulate the ship survey observations, which come from the Chinese Argo Real-time Data Center. Available online: http://www.argo.org.cn/ (accessed on 10 October 2019). The type of Argo instrument used in the experiment is HM2000_TS1, which has small errors and high data quality. These Argo data can provide a temperature profile of 2000 m every 5 days. The Argo after 13 September 2016 will be used to evaluate the prediction effects. The Argo distribution is shown in Figure 2.

Figure 2. The distribution of Argo buoys that are using for correction and evaluation. The yellow triangle represents the location of the acquired satellite remote sensing SST. The green pentagram represents the location where the ship survey data was acquired. The red dots represent the Argo data that were used to evaluate the prediction results. The moments of all observations are given in the figure.

The historical data for global daily average ocean temperature come from the HYCOM reanalysis data products which were generated by HYCOM model and Navy Coupled Ocean Data Assimilation system. Available online: https://www.hycom.org/ (accessed on 9 September 2020). The HYCOM reanalysis data has assimilated available satellite altimeter data, satellite remote sensing data of SST, and other data from XBT, Argo buoys and mooring buoys. In the reanalysis data, there are dynamical constraints between neighboring grid points. The purpose of ANN training is to mine the hidden patterns in the training sample dataset.

The ANN tool used in this study is Pytorch, which has been widely used in many scientific fields. Available online: https://pytorch.org/ (accessed on 10 October 2020). The training sample is chosen from the reanalysis data from the years of 2006–2015. The grid size is 150 × 120 horizontally. The horizontal resolution is 9 km. We use a stretched terrain-following coordinate in the vertical direction and the grid has 20 layers vertically. In order to evaluate the improving effects of ISTE, we have also carried out a prediction experiment using LRAP. 2.2. Information Spatial-Temporal Extension Algorithm

The ISTE process can be seen as a regression problem, whereas FC (Fully Connected) DNNs are very effective in data fitting and pattern capturing. Through data training, FC-DNNs can approximate the nonlinear mapping relationship between the samples and labels. Since FC-DNNs have superior advantages, we choose FC-DNNs as the network architectures for ISTE.
The historical data for global daily average ocean temperature come from the HYCOM reanalysis data products which were generated by HYCOM model and Navy Coupled Ocean Data Assimilation system. Available online: https://www.hycom.org/ (accessed on 9 September 2020). The HYCOM reanalysis data has assimilated available satellite altimeter data, satellite remote sensing data of SST, and other data from XBT, Argo buoys and mooring buoys. In the reanalysis data, there are dynamical constraints between neighboring grid points. The purpose of ANN training is to mine the hidden patterns in the training sample dataset.

The ANN tool used in this study is Pytorch, which has been widely used in many scientific fields. Available online: https://pytorch.org/ (accessed on 10 October 2020). The training sample is chosen from the reanalysis data from the years of 2006–2015. The grid size is 150 × 120 horizontally. The horizontal resolution is 9 km. We use a stretched terrain-following coordinate in the vertical direction and the grid has 20 layers vertically. In order to evaluate the improving effects of ISTE, we have also carried out a prediction experiment using LRAP.

2.2. Information Spatial-Temporal Extension Algorithm

The ISTE process can be seen as a regression problem, whereas FC (Fully Connected)-DNNs are very effective in data fitting and pattern capturing. Through data training, FC-DNNs can approximate the nonlinear mapping relationship between the samples and labels. Since FC-DNNs have superior advantages, we choose FC-DNNs as the network architectures for ISTE.

A FC-DNN consists of an input layer, multiple hidden layers, and an output layer. Its architecture is shown in Figure 3.

Figure 3. The schematic diagram of the FC-DNN architecture.

The ISTE algorithm is composed of ISE process, intelligent correcting (IC) process and ITE process. The general scheme uses the satellite remote sensing SST data to generate an initial estimation field by ISE. Then, the limited observations with vertical temperature information were used to correct the initial estimation field to obtain an initial correction field. Finally, use the initial correction field for ITE. In this way, 4D ocean temperature prediction data can be obtained. The overall flows of ISTE are shown in Figure 4.
A FC-DNN consists of an input layer, multiple hidden layers, and an output layer. Its architecture is shown in Figure 3.

Figure 3. The schematic diagram of the FC-DNN architecture.

The ISTE algorithm is composed of ISE process, intelligent correcting (IC) process and ITE process. The general scheme uses the satellite remote sensing SST data to generate an initial estimation field by ISE. Then, the limited observations with vertical temperature information were used to correct the initial estimation field to obtain an initial correction field. Finally, use the initial correction field for ITE. In this way, 4D ocean temperature prediction data can be obtained. The overall flows of ISTE are shown in Figure 4.

Figure 4. The schematic diagram of the ISTE operational process.

The procedures of ISTE are described below.

1. Train the Reconstruction DNN using historical ocean temperature data.
2. Put the satellite remote sensing SST into the trained Reconstruction DNN to generate the initial estimation field.
3. Train the Correction DNN using the initial estimation field and historical ocean temperature data.
4. Put the ship survey observations into the trained Correction DNN to generate the initial correction field.
5. Train the Extrapolation DNN using historical ocean temperature data.
6. Put the initial correction field into the trained Extrapolation DNN to generate the final prediction field.

As mentioned above, the ISTE process requires the construction of Reconstruction DNN, Correction DNN and Extrapolation DNN. All the three DNNs adopt fully connected forms, and they are described in the following subsections.

2.2.1. Reconstruction DNN

Since there are correlations between the SST and the subsurface temperature, we can then use the Reconstruction DNN to fit these correlations. Thus, when the SST have been known, the subsurface temperature can be predicted through the Reconstruction DNN.

To speed up training and prevent overfitting, we use temperature anomalies as training samples and training labels. Temperature anomaly is the anomaly relative to the multi-year temperature average. This is the reason why previous studies prefer to use temperature anomalies [9,12,16,18].

For the Reconstruction DNN, we set the number of hidden layers to 16 and the number of neurons for each layer to 48. The learning rate is 0.001 and the epoch is 1000. The activation function is ReLU, the optimizer is Adam, and the loss function is MSELoss. The input layer is SST anomaly with 18,000 neurons, and the output layer is the subsurface temperature anomaly at a certain depth with 18,000 neurons.

The SST anomaly data in this study come from historical reanalysis data and the purpose is to mine the physical patterns in the reanalysis data. As the ocean has different properties at different depths, we use a layer-training scheme. For example, the training sample is the SST anomaly, and the training label is the temperature anomaly in the 10th depth layer. After the Reconstruction DNN is trained, the 10th depth layer temperature anomaly of 10 September 2016 can be generated by inputting the SST anomaly of 10 September 2016 to the Reconstruction DNN.
2.2.2. Correction DNN

The initial estimation field can be obtained through the Reconstruction DNN. Since the initial estimation field is only produced by learning the historical pattern, it inevitably has some errors. However, we can reduce the errors by fusing the vertical temperature information into the initial estimation field. The vertical temperature information can be provided by ship survey observations.

In fact, it is not possible to obtain observations for all grid points. This requires us to correct the initial estimation field using the limited observations. It has proved to be feasible and effective to perform IC process for the initial field using the limited observations [26]. The IC algorithm can perform horizontal extension of the limited observation information. In this way, the purpose of using the limited observations to correct the initial field can be realized.

The Correction DNN has 2 hidden layers, the number of neurons for each layer is 48. The learning rate is set to 0.01 and the epoch is set to 500. The activation function is ReLU, the optimizer is Adam, and the loss function is MSELoss. The input layer is the observation point increment with 3 neurons, which is the difference between the temperature at observation location in the reanalysis data and the temperature at observation location in the initial estimation field. The output layer is the entire field increment with 18,000 neurons, which is the difference between the temperature of reanalysis data and the temperature of initial estimation field. More details about the IC algorithm can be found in the study carried out by Mao et al. [26].

Through training, we can obtain a Correction DNN that can fit nonlinear mapping function $\eta$ between the entire field increment and the observation point increment:

$$
E = \eta(X_o),
$$

where $E$ is the entire field increment, $X_o$ is the observation point increment.

Then, the initial correction field $A_1$ can be calculated by

$$
A_1 = M_1 - E,
$$

where $M_1$ is the initial estimation field.

2.2.3. Extrapolation DNN

With reference to the operation of the numerical model, the temperatures at the moments to be predicted are related to the initial field. We can use the Extrapolation DNN to fit the relationship between the initial field and the temperature field at different moments. In this way, once we have obtained the initial field, we can use the trained Extrapolation DNN to make temporal prediction.

Assume $A_p$ is the target temperature field to be predicted, the time gap is $\Delta t$. We believe that $A_p$ is related to $A_1$, that is:

$$
A_p = P_{\Delta t}(A_1),
$$

where $P_{\Delta t}$ represents the mapping function within $\Delta t$ time.

$P_{\Delta t}$ cannot be calculated directly, but can be fitted by trained Extrapolation DNN. For example, if the temperature of 10 September 2016 is the initial field, suppose we want to predict the temperature of 13 September 2016. We can take the temperature of 10 September in the past years as the samples and the temperature of 13 September in the past years as the labels. The mapping function $P_{\Delta t}$ between 10 September and 13 September can be fitted through data training.

The Extrapolation DNN has 2 hidden layers and the number of neurons for each layer is 64. The learning rate is set to 0.002 and the epoch is set to 500. The activation function is ReLU, the optimizer is Adam, and the loss function is MSELoss. The input layer is the temperature of initial correction field. The number of neurons in the input layer is
18,000. The output layer is the temperature field at the time to be predicted. The number of neurons in the output layer is 18,000. It should be noted that due to the large fluctuations in thermocline, overfitting tends to occur with the same parameter settings. Therefore, the training process in thermocline needs to add the dropout setting. Here, we set the dropout value to 0.1. Once the Extrapolation DNN has been trained using historical data, the temperature at any time can be predicted.

3. Results

Figure 5 shows the results of the inversion and correction. With the help of DNNs, which is a powerful tool, it is possible to achieve obvious correcting effect with a small amount of vertical information data.

![Temperature of 20th layer](image1)

![Temperature of 20th layer](image2)

![Temperature of 15th layer](image3)

![Temperature of 15th layer](image4)

![Temperature of 10th layer](image5)

![Temperature of 10th layer](image6)

Figure 5. Cont.
Figure 5. The results of the inversion and correction. Subfigures (a,c,e,g) show 4 layers of the initial estimation field. Subfigures (b,d,f,h) show 4 layers of the initial correction field. Using the maximum water depth as a reference, 20th layer is the surface layer of the ocean, 15th layer represents approximately 100 m water depth, 10th layer represents approximately 500 m water depth and 5th layer represents approximately 1000 m water depth.

Then, we used a series of Argo observations at different times to evaluate the prediction results through statistics. The evaluation criteria used for following analysis are reported in Table 1:

Table 1. The criteria for evaluation. m is the prediction results, a is the Argo data, $a_{mean}$ is the mean value of Argo data, n is the number of observation points.

| Evaluation Criteria                        | Formulas                                      |
|--------------------------------------------|-----------------------------------------------|
| Absolute Error (AE)                        | $AE = |m - a|$                                   |
| Mean Absolute error (MAE)                  | $MAE = \frac{\sum_{i=1}^{n}|a_i - a_{\text{mean}}|}{n}$ |
| Mean Absolute Percentage Error (MAPE)      | $MAPE = \frac{\sum_{i=1}^{n}|a_i - a_{\text{mean}}|/a_{\text{mean}}}{n} \times 100$ |
| Root Mean Square Error (RMSE)              | $RMSE = \sqrt{\frac{\sum_{i=1}^{n}(a_i - m)^2}{n}}$ |
| Coefficient of Determination ($R^2$)       | $R^2 = 1 - \frac{\sum_{i=1}^{n}(a_i - m)^2}{\sum_{i=1}^{n}(a_i - a_{\text{mean}})^2}$ |

3.1. Mixed Layer

Figure 6 is the prediction errors for mixed layer. We use 0 m, 10 m, 20 m, and 30 m depths to present the prediction errors for mixed layer. The results show that the ISTE method shows a clear superiority over the LRAP method. Compared with the LRAP method, the largest improvement of prediction accuracy in ISTE is at 10 m depth with 52% reduction in error. Additionally, the smallest improvement of prediction accuracy in ISTE is at 30 m depth with 16% reduction in error.

For ISTE, the mean prediction error at 10 m depth is the smallest with the MAE of 0.4554 °C, whereas the mean prediction error at 30 m depth is the largest with the MAE of 1.0784 °C. This is probably because the fluctuations are smallest at 10 m, making it easier for the DNN to capture the pattern hidden in historical data. For 30 m depth, it is closer to the thermocline, which is more volatile and less regular. This results in DNNs not being able to capture data patterns well.

It is also understandable that the error for the sea surface is not the smallest. The sea surface is more influenced by the atmosphere and has more disturbances than the 10 m depth. Therefore, the prediction error at the sea surface is not the smallest.
Figure 6. (a–d) The prediction errors at different depths for the mixed layer with Argo buoys as reference.

We also notice that the prediction error is relatively stable in the first 15 days near the sea surface, with an error of around 0.5 °C, whereas there is a significant increase in prediction error after 15 days. As the ISTE algorithm itself does not have the problem of error accumulation over time, this abrupt increase may be due to changes in the background field outside the predicted region. Compared with numerical models, ISTE lacks the information on external changes given by the boundary field. This may lead to a sharp increase in prediction error when there is a dramatic change in the ocean–atmospheric environment outside the region.

3.2. Thermocline

Figure 7 shows the prediction error for the thermocline. The mean prediction error of ISTE is generally below 1 °C, but there are several extreme errors that greater than 2 °C. This demonstrates that the predictions for the thermocline are more unstable compared with the mixed layer.
formation on external changes given by the boundary field. This may lead to a sharp increase in prediction error when there is a dramatic change in the ocean–atmospheric environment outside the region.

3.2. Thermocline

Figure 7 shows the prediction error for the thermocline. The mean prediction error of ISTE is generally below 1 °C, but there are several extreme errors that greater than 2 °C. This demonstrates that the predictions for the thermocline are more unstable compared with the mixed layer.

Figure 7. (a–d) The prediction errors at different depths for the thermocline with Argo buoys as reference.

The prediction error was greatest at 100 m depth, with an MAE of 0.9843 °C. The prediction error was least at 200 m depth, with an MAE of 0.5902 °C. However, the improvement of ISTE is the smallest at 200 m depth relative to LRAP, where the mean prediction error is reduced by only 20%.

Comparing the predictions of ISTE and LRAP, it can be found that the improvement brought by ISTE is not as visually obvious as the mixed layer and the reduction in mean prediction error is relatively small. This is mainly due to two reasons. The first reason is that the underwater inversion accuracy for SST from satellite remote sensing inevitably decreases when the depth reaches below 50 m, which leads to increasing errors in subsequent prediction. The second reason is that due to the large fluctuations of the thermocline itself. Neither regression nor DNN methods can fully fit the variation pattern. However, even so, the DNN method outperform regression method in terms of mining temperature variation patterns and reducing prediction errors.

3.3. Deep Layer

Figure 8 shows the prediction errors at the deep layer. The mean prediction error of ISTE remains largely within 0.4 °C. The results show that ISTE still plays a relatively stable
role at the deep layer. At the depths of 300, 400, 500, and 1000 m, the prediction errors are smaller than those of LRAP. The results demonstrate that ISTE outperforms LRAP in general. We can also see that as depth increases, ISTE brings very limited improvement at deep layer. This is due to a number of reasons. The temperature fluctuation at deep layer is smaller and therefore the prediction errors are smaller in magnitude. In addition, the reanalysis data used for training does not guarantee high accuracy at deep layer. All these reasons lead to a poorer performance of ISTE at deep layer than in the mixed layer and thermocline.

![Prediction error at 300 m depth](image)
![Prediction error at 400 m depth](image)
![Prediction error at 500 m depth](image)
![Prediction error at 1000 m depth](image)

**Figure 8.** (a–d) The prediction errors at different depths for the deep layer with Argo buoys as reference.

Although the prediction performance of ISTE at the deeper layers has been reduced, this does not largely affect the value of ISTE applications. It is mainly the mixed layer and thermocline that have a significant impact on human activities at sea, such as sonar detection, offshore fishing, and so on. The improved prediction performance of ISTE for the mixed layer and thermocline will help humans to have a better understanding of the underwater information.
3.4. Vertical Profiles

In order to detect the prediction effect in vertical structure, we compare the prediction results with the Argo observation data. In fact, the Argo observations we use are from four Argo buoys, which produce observations every five days. Therefore, we divided the observations into 5 groups to test the prediction effect, as shown in Figures 9–13. Here, we only present the prediction results for water depths less than 1000 m. The Argo profiles are plotted from all Argo data, the LRAP and ISTE profiles are plotted based on interpolation of the grid data.

![Image](a)

![Image](b)

![Image](c)

![Image](d)

**Figure 9.** Comparison of prediction results from different prediction methods with Argo profiles for vertical temperature within 15 September–18 September (a) 15 September; (b) 16 September; (c) 17 September; (d) 18 September.

The time of group 1 is within 15 September–18 September. In this early stage, ISTE generally match the vertical structure of Argo temperature profiles. In terms of comparing the prediction errors at different depths, the deep layer errors are much smaller than the mixed layer and thermocline. Figure 9a,c,d show that the ISTE temperature profiles are closer to the Argo temperature profiles compared with LRAP.

The time of group 2 is within 20 September–23 September. In this stage, the SST prediction by ISTE is significantly better than that of LRAP, just like Figure 9. This proves that we have used the observations effectively.
Figure 10. Comparison of prediction results from different prediction methods with Argo profiles for vertical temperature within 20 September–23 September. (a) 20 September; (b) 21 September; (c) 22 September; (d) 23 September.

Figure 11. Cont.
Figure 11. Comparison of prediction results from different prediction methods with Argo profiles for vertical temperature within 25 September–28 September. (a) 25 September; (b) 26 September; (c) 27 September; (d) 28 September.

Figure 12. Comparison of prediction results from different prediction methods with Argo profiles for vertical temperature within 30 September–3 October. (a) 30 September; (b) 1 October; (c) 2 October; (d) 3 October.
Figure 13. Comparison of prediction results from different prediction methods with Argo profiles for vertical temperature within 5 October–8 October. (a) 5 October; (b) 6 October; (c) 7 October; (d) 8 October.

Figure 10b shows that both ISTE and LRAP present large errors at the thermocline. The maximum error is even more than 2 °C. This may be due to the emergence of temperature changes in this region that are significantly different from its climatic state.

The time of group 3 is within 25 September–28 September. Figure 11b still shows obvious prediction errors at the thermocline. Meanwhile, the prediction errors of SST are smaller. This also proves that the thermocline temperature is much more difficult to predict than SST. It exhibits more instability.

The time of group 4 is within 30 September–3 October. We notice a significant increase in the prediction error of the ISTE for the SST. This is because the sea surface is more sensitive to the atmospheric environment as time progresses. The accumulated influence of external factors thus leads to a weakening of the correlation between the initial field and the temperature field to be predicted, which in turn increases the prediction error.

The time of group 5 is within 5 October–8 October. We can see that the prediction effect of ISTE generally keep its stability. Additionally, the overall prediction errors of ISTE are smaller than those of LRAP.

Figures 9–13 show that ISTE predicts the structure of the vertical temperature profile in the experimental area well. This demonstrates that ISTE can predict the temperature over the full water depth.
3.5. Statistical Analysis

The above results are the result of training using a 10-year sample of data. In addition to this, sensitivity tests were conducted using 5 and 8 years of sample data, respectively. All the statistical analysis results are shown in Table 2.

Table 2. Statistical analysis results.

| Method       | MAE   | MAPE | RMSE  | $R^2$  |
|--------------|-------|------|-------|--------|
| LRAP         | 0.6316| 4.5% | 0.9252| 0.9894 |
| ISTE_5years  | 0.4974| 3.9% | 0.7495| 0.9931 |
| ISTE_8years  | 0.4845| 3.8% | 0.7549| 0.9930 |
| ISTE_10years | 0.4949| 3.9% | 0.7199| 0.9936 |

The results show that the ISTE method has a much smaller prediction error. In terms of training results for the 10-year sample, the MAE of ISTE is 0.4949 °C. Compared with LRAP, the MAE of ISTE is reduced by 0.14 °C, whereas the MAPE of ISTE is reduced by 0.6%. ISTE exhibited a lower RMSE of 0.7199 °C, with a 0.21 °C reduction relative to LRAP. ISTE also exhibited a higher $R^2$ of 0.9936, with an improvement of 0.0042 relative to LRAP.

From the results we can also see that the sample length did not have a significant effect on the prediction results, which indicates that the prediction results are not sensitive to the sample length. However, in terms of the characteristics of DNNs, we should use as many sample data as possible to ensure the stability of the data training.

The above experimental results fully demonstrate the effectiveness of the ISTE algorithm, which is significantly better than the traditional LRAP algorithm for the prediction accuracy of ocean temperature.

4. Discussion

Ocean dataset is different from the dataset in other fields such as image and finance. Ocean dataset has its own inherent physical patterns. In terms of ocean temperature, the hidden patterns in temperature data are theoretical vertical modes [27,28] or empirical modes [29] in oceanography. The variation of thermocline or currents are all correlated with the ocean vertical structure changes. It is the correlation between different depth layers that justifies the use of sea surface information to predict the subsurface information [30,31]. Thus, AI methods are used to learn these hidden patterns in historical sample data through DNNs and to provide rapid prediction for humans.

In the process of ISE, traditional empirical analysis methods cannot make full use of all SST grid points simultaneously to produce the target inversion field. Besides this, traditional empirical analysis methods can only analyze linear relationships between the SST and subsurface temperature [8], whereas the AI method are different from the traditional empirical analysis method and have excellent performance that traditional empirical analysis methods do not have.

The driving factor of AI method is the entire SST field, which is a nonlinear correlation with the subsurface temperature field. DNNs can better reflect the spatial correlation characteristics between each grid point of temperature field and capture more structural characteristics of temperature field. Thus, DNN-based ISE can produce a better reconstruction result of temperature field.

In the IC process, the fusion of ship survey observations is superior to traditional linear interpolation. The IC algorithm can largely compensate for missing effective information using the patterns that are mined from historical data. Therefore, the IC process can make full use of the limited ship survey observations to correct the initial estimation field, and thus produce an initial correction field.

For ITE, the DNN-based algorithm can approximate the dynamical equations to some extent. It can fit the pattern of historical data and achieve an approximate prediction. This algorithm establishes a one-to-one mapping relationship between the moment to be
predicted and the initial field. The advantage of this algorithm is that there is no error accumulation over time. The stability of the prediction error can be guaranteed.

Through experiments, it can be found that the sea thermocline temperature (STT) is more difficult to be predicted compared with SST. The reason is that the ocean is different from a general data set. The real ocean is a 3D fluid affected by gravity, which forms a layered structure due to the difference in density, as shown in Figures 9–13. When the ocean is affected by external forces, it will cause sharp fluctuations in the thermocline. The SST change is relatively stable compared with STT and the SST changing regulations is easier to be captured by DNNs, which can lead to better prediction effects. Therefore, since the thermocline has stronger volatility and uncertainty, the STT changing regulations with time is more difficult to be captured compared with SST.

Taken together, the ISTE algorithm can makes full use of satellite remote sensing observations and limited ship survey observation data. Then, achieve the spatial and temporal extension of available information. In fact, this process achieves 4D temperature prediction. Therefore, the ISTE algorithm can be as an effective shipborne prediction method. The prediction performance of ISTE is significantly better than the traditional LRAP methods.

In this article, only an experimental study of the ISTE algorithm for temperature prediction has been carried out. In practice, we can obtain more types of observational data, including sea surface height (SSH) and sea surface salinity (SSS). Based on these facts, we will consider these factors in the next step.

1. Develop ISE algorithms that can fuse all satellite remote sensing data, including SST, SSH and SSS.
2. Develop IC algorithms with temperature and salt constraints.
3. Develop multi-factor coupled ITE prediction algorithms.
4. Consider exploring more advanced DNN structures that combine multiple neural networks.

We expect that these works will further improve the prediction accuracy for ocean environment. The more advanced technology will enable the ISTE algorithm to be used in a wider application context, including weather prediction and climate prediction.

5. Conclusions

Satellite remote sensing data can provide data with high temporal and spatial resolution, but they are limited to the surface and cannot provide underwater information. For shipborne prediction, it is convenient to obtain ship survey observations to access accurate vertical information. The ISTE algorithm can be used to fully integrate the satellite remote sensing data and ship survey observation data to achieve a 4D ocean environment prediction.

This paper demonstrates the effectiveness of the ISTE algorithm through prediction experiments on ocean temperatures. The experimental results show that the $\text{MAE}$ of ISTE is around $0.5 \, ^\circ\text{C}$, the $\text{MAPE}$ is around $4\%$, the $\text{RMSE}$ is around $0.7 \, ^\circ\text{C}$ and the $R^2$ is 0.9936, Relative to the observations. Compared with the traditional LRAP method, the prediction accuracy of ISTE has been significantly improved.

The ISTE algorithm is a convenient, practical, and effective method for shipborne prediction. We anticipate that the DNN-based ISTE algorithm will help humans to obtain timely information about the ocean environment and further benefit relevant marine operations, including but not limited to sonar detection and offshore fishing.

**Author Contributions:** Conceptualization, K.M., S.Z. and C.L.; methodology, K.M.; formal analysis, K.M., F.G., S.Z. and C.L.; funding acquisition, F.G. and C.L.; investigation, K.M., F.G., S.Z. and C.L.; resources, F.G., S.Z. and C.L.; software, K.M.; supervision, F.G., S.Z. and C.L.; validation, F.G., S.Z. and C.L.; visualization, K.M.; writing—original draft preparation, K.M.; writing—review and editing, K.M., F.G., S.Z. and C.L. All authors have read and agreed to the published version of the manuscript.
Funding: This research is supported by the National Natural Science Foundation of China (Grant No. 41830964) and the Shandong Province’s “Taishan” Scientist Project (ts201712017) and Qingdao “Creative and Initiative” frontier Scientist Program (19-3-2-7-zhc).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Acknowledgments: The authors would like to thank the China Argo Real-time Data Center, HYCOM, and CMEMS for providing the free data.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Fox, D.N.; Teague, W.J.; Barron, C.N.; Carnes, M.R.; Lee, C.M. The Modular Ocean Data Assimilation System (MODAS). J. Atmos. Ocean Technol. 2002, 19, 240–252. [CrossRef]

2. Reichstein, M.; Camps-Valls, G.; Stevens, B.; Jung, M.; Denzler, J.; Carvalhais, N. Deep learning and process understanding for data-driven Earth system science. Nature 2019, 566, 195–204. [CrossRef] [PubMed]

3. Ali, M.M.; Swain, D.; Weller, R.A. Estimation of ocean subsurface thermal structure from surface parameters: A neural network approach. Geophys. Res. Lett. 2004, 31, L20308. [CrossRef]

4. Lu, W.; Su, H.; Yang, X.; Yan, X.H. Subsurface temperature estimation from remote sensing data using a clustering-neural network method. Remote Sens. Environ. 2019, 422, 213–222. [CrossRef]

5. Han, M.X.; Feng, Y.; Zhao, X.L.; Sun, C.J.; Hong, F.; Liu, C. A Convolutional Neural Network Using Surface Data to Predict Subsurface Temperatures in the Pacific Ocean. IEEE Access 2019, 7, 172816–172829. [CrossRef]

6. Sammartino, M.; Nardelli, B.B.; Marullo, S.; Santoleri, R. An Artificial Neural Network to Infer the Mediterranean 3D Chlorophyll-a and Temperature Fields from Remote Sensing Observations. Remote Sens. 2020, 12, 4123. [CrossRef]

7. Wang, H.Z.; Wang, G.H.; Chen, D.K.; Zhang, R. Reconstruction of Three-Dimensional Pacific Temperature with Argo and Satellite Observations. Atmos. Ocean 2012, 50, 116–128. [CrossRef]

8. Zhou, C.; Ding, X.; Zhang, J.; Yang, J.; Ma, Q. An objective algorithm for reconstructing the three-dimensional ocean temperature field based on Argo profiles and SST data. Ocean Dyn. 2017, 67, 1523–1533. [CrossRef]

9. Neetu; Sharma, R.; Basu, S.; Sarkar, A.; Pal, P.K. Data-Adaptive Prediction of Sea-Surface Temperature in the Arabian Sea. IEEE Geosci. Remote Sens. Lett. 2011, 8, 9–13. [CrossRef]

10. Su, H.; Wu, X.; Yan, X.H.; Kidwell, A. Estimation of subsurface temperature anomaly in the Indian Ocean during recent global surface warming hiatus from satellite measurements: A support vector machine approach. Remote Sens. Environ. 2015, 160, 63–71. [CrossRef]

11. Zhang, Q.; Wang, H.; Dong, J.; Zhong, G.; Sun, X. Prediction of sea surface temperature using long short-term memory. IEEE Geosci. Remote Sens. Lett. 2017, 14, 1745–1749. [CrossRef]

12. Xiao, C.; Chen, N.; Hu, C.; Wang, K.; Chen, Z. Short and mid-term sea surface temperature prediction using time-series satellite data and LSTM-AdaBoost combination approach. Remote Sens. Environ. 2019, 233, 111358. [CrossRef]

13. Wei, L.; Guan, L.; Qu, L.Q. Prediction of Sea Surface Temperature in the South China Sea by Artificial Neural Networks. IEEE Geosci. Remote Sens. 2020, 17, 558–562. [CrossRef]

14. Sun, Y.J.; Yao, X.; Bi, X.; Huang, X.C.; Zhao, X.G.; Qiao, B.Y. Time-Series Graph Network for Sea Surface Temperature Prediction. Big Data Res. 2021, 25, 100237. [CrossRef]

15. Patil, K.; Deo, M.C.; Ravichandran, M. Prediction of sea surface temperature by combining numerical and neural techniques. J. Atmos. Ocean. Technol. 2016, 33, 1715–1726. [CrossRef]

16. Patil, K.; Deo, M.C. Prediction of daily sea surface temperature using efficient neural networks. Ocean Dyn. 2017, 67, 357–368. [CrossRef]

17. Yang, Y.; Dong, J.; Sun, X.; Lima, E.; Mu, Q.; Wang, X. A CFCC–LSTM model for sea surface temperature prediction. IEEE Geosci. Remote Sens. Lett. 2017, 15, 207–211. [CrossRef]

18. Aparna, S.G.; D’Souza, S.; Arjun, N.B. Prediction of daily sea surface temperature using artificial neural networks. Remote Sens. 2018, 39, 4214–4231. [CrossRef]

19. Zhang, K.; Geng, X.; Yan, X.H. Prediction of 3-d ocean temperature by multilayer convolutional LSTM. IEEE Geosci. Remote Sens. Lett. 2020, 17, 1303–1307. [CrossRef]

20. LeCun, Y.; Bengio, Y.; Hinton, G. Deep learning. Nature 2015, 521, 436–444. [CrossRef]

21. Ma, L.; Liu, Y.; Zhang, X.L.; Ye, Y.X.; Yin, G.F.; Johnson, B.A. Deep learning in remote sensing applications: A meta-analysis and review. ISPRS J. Photogramm. 2019, 152, 166–177. [CrossRef]

22. Schmidhuber, J. Deep learning in neural networks: An overview. Neural Netw. 2015, 61, 85–117. [CrossRef] [PubMed]

23. Dong, S.; Wang, P.; Abbas, K. A survey on deep learning and its applications. Comput. Sci. Rev. 2021, 40, 100379. [CrossRef]
24. Merchant, C.J.; Embury, O.; Bulgin, C.E.; Block, T.; Corlett, G.K.; Fiedler, E.; Good, S.A.; Mittaz, J.; Rayner, N.A.; Berry, D.; et al. Satellite-based time-series of sea-surface temperature since 1981 for climate applications. Sci. Data 2019, 6, 223. [CrossRef]

25. Good, S.; Fiedler, E.; Mao, C.; Martin, M.J.; Maycock, A.; Reid, R.; Roberts-Jones, J.; Searle, T.; Waters, J.; While, J.; et al. The Current Configuration of the OSTIA System for Operational Production of Foundation Sea Surface Temperature and Ice Concentration Analyses. Remote Sens. 2020, 12, 720. [CrossRef]

26. Mao, K.; Gao, F.; Zhang, S.; Liu, C. An Initial Field Intelligent Correcting Algorithm for Numerical Forecasting Based on Artificial Neural Networks under the Conditions of Limited Observations: Part I—Focusing on Ocean Temperature. J. Mar. Sci. Eng. 2022, 10, 311. [CrossRef]

27. Dewitte, B.; Reverdin, G.; Maes, C. Vertical structure of an OGCM simulation of the equatorial Pacific Ocean in 1985–94. J. Phys. Oceanogr. 1999, 29, 1542–1570. [CrossRef]

28. Stewart, K.D.; Hogg, A.M.; Griffies, S.M.; Heerdegen, A.P.; Ward, M.L.; Spence, P.; England, M.H. Vertical resolution of baroclinic modes in global ocean models. Ocean Model. 2017, 113, 50–65. [CrossRef]

29. Wunsch, C. Multi-year ocean thermal variability. Tellus A 2020, 72, 1–15. [CrossRef]

30. Pauthenet, E.; Roquet, F.; Madec, G.; Sallée, J.B.; Nerini, D. The thermohaline modes of the global ocean. J. Phys. Oceanogr. 2019, 49, 2535–2552. [CrossRef]

31. He, Z.; Wang, X.; Wu, X.; Chen, Z.; Chen, J. Projecting Three-Dimensional Ocean Thermohaline Structure in the North Indian Ocean from the Satellite Sea Surface Data Based on a Variational Method. J. Geophys. Res. Oceans 2021, 126, e2020JC016759. [CrossRef]