Supplementary Materials for

A Sea Surface Data-based Machine Learning Model for Rapid 3D Mapping of Underwater Sound Speed.

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Supplementary Text

This supplementary section provides additional details about the Deep Neural Network (DNN) and K-nearest neighbor (KNN) model training and a comprehensive analysis of the models used in our study to predict underwater sound speed.

The DNN model's architecture, illustrated in Fig. 1, features an input layer (dense_24_input) accepting an 8-dimensional vector, followed by fully connected layers with decreasing nodes: dense_24 (320 nodes), dense_25 (160 nodes), dense_26 (80 nodes), dense_27 (40 nodes), and dense_28 (20 nodes). Each dense layer is accompanied by a batch normalization layer, enhancing training efficiency. The final layer (dense_29) consists of a single node outputting continuous values for the predicted underwater sound speed. This design enables the DNN to capture both simple and complex features critical for modeling marine relationships.

The learning curve for the DNN model, shown in Fig. 2A, demonstrates improved prediction accuracy over training epochs. Both training and cross-validation MAE metrics decrease sharply initially, indicating effective learning. The close alignment of training and validation errors suggests that the model is well-suited to the task, with minimal overfitting. After the initial rapid decrease, metrics plateau as the model converges on the loss function's minimum. The stabilization of cross-validation MAE indicates the application of early stopping, which halts training before overfitting occurs, conserving computational resources and enhancing generalization to new data.

The learning curve for the KNN model, illustrated in Fig. 2B, shows a significant decrease in both training and cross-validation RMSE as dataset size increases, indicating improved accuracy. The initial steep decline suggests substantial learning gains from early data additions. As more examples are introduced, convergence of training and cross-validation RMSE implies good generalization, with similar performance on seen and unseen data. The eventual plateau of the cross-validation RMSE suggests that additional data may not significantly improve model performance beyond a certain point, providing insight into optimal training dataset size and balancing performance with computational resources.

It includes additional performance metrics, detailed comparisons, and explanations of each model's effectiveness. We present an extended evaluation using Root Mean Squared Error (RMSE), R-squared (R^2) scores, and Pearson correlation coefficients (r) to offer a thorough understanding

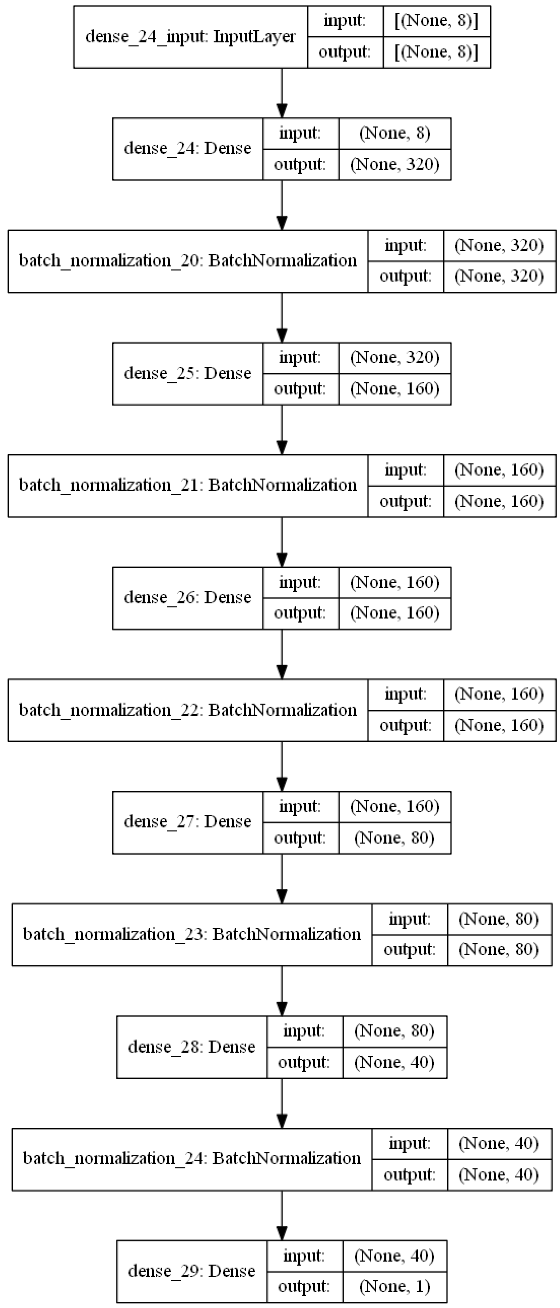
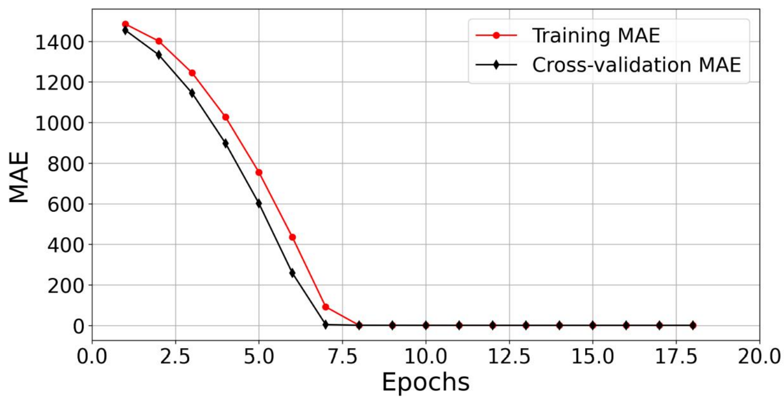


Figure 1: **Architecture of Deep Neural Networks (DNN) model.**

(A)



(B)

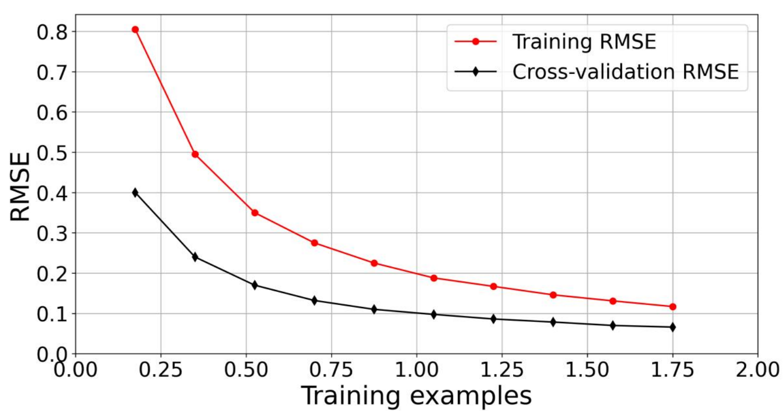


Figure 2: **Learning curves for**, (**A**) DNN model training (average). (**B**) K-NN model training.

Table 1: Comparative Performance Metrics of DNN and KNN Models

Region	DNN Model		KNN Model	
	RMSE	R^2	**RMSE**	R^2
Top Layer (0-50 m)	3.3549	0.9749	0.4404	0.9996
Upper Layer (0-400 m)	3.2585	0.9682	0.2568	0.9998
Deep Layer (beyond 400 m)	1.1297	0.9949	0.0367	1.0000
All Depths	1.4621	0.9918	0.0855	1.0000

of the models' strengths and limitations. The Pearson correlation coefficient measures the linear relationship between predicted and actual values, with coefficients near +1 or -1 indicating strong positive or negative correlations, respectively, while values close to 0 suggest minimal linear correlation. Our evaluation aims to identify the more effective model and determine the depths at which each model excels in predicting sound speed. We conducted depth-specific assessments across various strata: the top layer (0-50 m), the upper layer (0-400 m), and the deep layer (beyond 400 m), as well as a comprehensive evaluation encompassing all depth ranges.

Table 1 provides a detailed comparison of the KNN and DNN models' predictive performance across various ocean depths. To visualize model performance, we generated scatter plots illustrating the relationship between predicted sound speeds and those determined using CTD data. Figure **??** presents these scatter plots side-by-side for both models across different ocean layers, offering insights into their performance across varying depths.

The scatter plots in Fig.3 and the statistical metrics in Table1 highlight the strengths and weaknesses of each model. The KNN model demonstrates higher prediction accuracy, particularly in the upper layer (0-400 m), as evidenced by tight clustering around the line of best fit in Fig.3F, with an impressive R^2 of 0.9998. This indicates that the KNN model effectively handles the noisy and high-dimensional nature of ocean data. In contrast, while competitive, the DNN model shows greater dispersion, particularly in shallower layers, reflecting its sensitivity to data complexity. This is visible in the scatter plots for the top layer (0-50 m) Fig.3A and the upper layer (0-400 m) Fig. 3B, which exhibit more spread-out points, corresponding to higher RMSE and lower R^2 scores.

Despite these challenges, the DNN model performs well at greater depths, maintaining strong monotonic relationships in deeper layers (beyond 400 m), as shown in Fig. 3C and Fig. 3G. The KNN model achieves a perfect R^2 at these depths, indicating excellent linear accuracy and effective

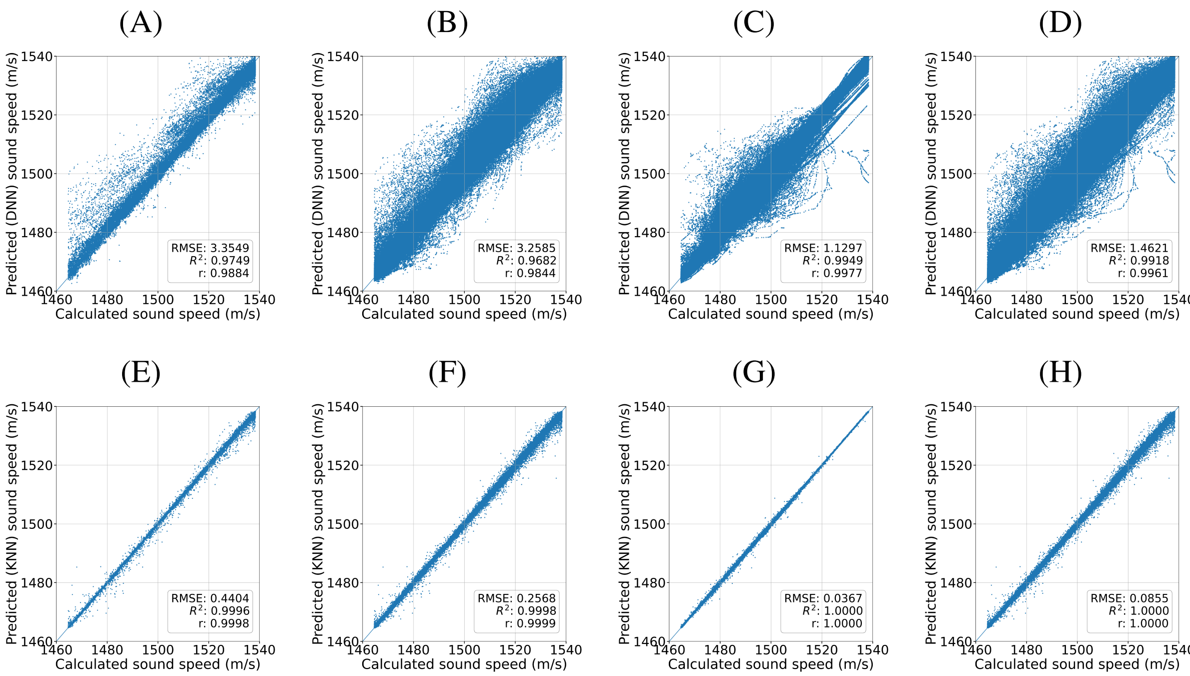


Figure 3: **Comparative Scatter Plots of Predicted Sound Speed Values:** (**A**-**D**) DNN Model and (**E**-**H**) KNN Model. (**A**,**E**) Top layer (0-50 m), comparing predictions for shallower waters; (**B**,**F**) Upper layer (0-400 m), showing results for the top to mid-depth regions; (**C**,**G**) Deep layer (beyond 400 m), depicting outcomes for deeper zones; (**D**,**H**) All depths combined.

maintenance of data rank order.

The DNN model, though slightly more scattered, still shows robust predictive performance with a high R^2 of 0.9949, as seen in Fig. 3C. Across all depths, the KNN model maintains high prediction consistency with perfect R^2 in Fig. 3H, reflecting its ability to accurately predict sound speed while preserving the natural order of the data. The DNN model, despite a wider spread in Fig. 3D and an RMSE of 1.4621, still demonstrates a strong linear relationship with actual values (R^2 of 0.9918).

These scatter plots confirm the statistical metrics from the table and highlight the importance of Spearman's ρ values in understanding the models' ability to capture non-linear and rank-ordered relationships. The KNN model consistently shows high accuracy and strong monotonic relationships across depths, while the DNN model's better performance in deeper waters suggests a need for depth-specific adjustments in shallower layers.