Geoscientific Model Development

Supporting Information for

A Novel Method for Sea Surface Temperature Prediction using a Featural Granularity-Based and Data-Knowledge-Driven ConvLSTM Model

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Text S1: LSTM Model

This sequential architecture processes flattened SST grids ($64 \times n \times m \rightarrow 64 \times N, N = n \times m$). Dual LSTM layers (512→256 units) capture temporal dependencies, with Dropout (0.3) mitigating overfitting. A fully connected layer outputs $48 \times N$ predictions, reconstructed into 48 $n \times m$ SST fields. The model minimizes a mean square error (MSE) loss via Adam optimization.

Text S2: Bidirectional LSTM (BiLSTM)

Utilizing bidirectional processing, this model ingests 64-month SST sequences ($64 \times N$). Two BiLSTM layers (128→64 units) with batch normalization (BN) extract forward/backward temporal dynamics. Predictions are generated through a dense layer ($48 \times N$ output) and spatially reconstructed. Training employs adam optimization with the loss function of root-mean-squared error(RMSE).

Text S3: Spatiotemporal CNN Model

Operating directly on SST data ($64 \times n \times m \times 1$), this architecture combines 3D convolutions (32 filters, 5×5×5 kernels) with ConvLSTM2D (64 units) to jointly model spatiotemporal patterns. Transposed convolutions upsample outputs to 48 data. RMSprop optimization prioritizes frontal zone accuracy through MSE loss.

Text S4: Deep Neural Network (DLNN)

Flattened SST sequences ($64 \times N$) undergo PCA dimensionality reduction (retaining 95% variance)(k). Three dense layers (2048→1024 units) with LeakyReLU activations and Dropout (0.4) learn nonlinear mappings. Outputs are reshaped into 48 SST data, with Huber loss enhancing robustness to outliers.

Text S5: ConvGRU Model

Core structure follows the described 5-layer configuration: Five stacked ConvGRU2D layers (50 filters, 7×7 kernels each) with recurrent Dropout (0.5) and batch normalization. Final Conv2D layers (50→1 channels) refine spatial features. A recursive prediction mechanism iteratively generates 48 data by sliding the input window. The Adam scheme was adopted as the optimizer.

Text S6: (GMNN, Liang et al., 2023)

Proposed by Liang et al. (2023), the Graph Memory Neural Network (GMNN) is a spatiotemporal prediction model tailored for SST forecasting, emphasizing the integration of spatial, temporal, and attribute features of oceanographic data. Its workflow involves three key stages: first, historical SST data are converted into time-ordered graph sequences (each graph includes spatial adjacency, temporal indices, and SST attribute values) as input; second, a dual-module encoder is used—with iterative GNN layers as the graph encoder to extract spatial correlations through node-edge message passing, and an LSTM as the temporal encoder to capture temporal dynamics across graph sequences; finally, a decoder with fully connected layers and a multi-output strategy maps the fused spatiotemporal features to future SST predictions. This design enables GMNN to effectively model the complex spatiotemporal dependencies in SST fields.

Table S1 Parameter Specifications

Model	Input Dim	Output Dim	Core Architecture	Optimizer	Loss Function
LSTM	(64, N)	(48,N)	LSTM(512)→Dropout(0.3)→LSTM(256)→Dense (48N)	Adam (lr=0.001)	MSE
BiLSTM	(64,N)	(48,N)	BiLSTM(128)→BN→BiLSTM(64)→BN→Dense (48N)	Adam (lr=0.001)	RMSE
CNN	(64,n,m,1)	(48,n,m,1)	Conv3D(32,5^3)→MaxPool3D(2)→ConvLSTM2D (64)→Conv3DTranspose(1,3^3)	RMSprop (lr=$2e^{-4}$)	MSE
DLNN	(64,k)	(48,N)	Dense(2048)→LeakyReLU→Dropout(0.4)→Dense(1024)→Dense(48N)	RMSprop (lr=10^{-4})	Huber (δ=0.5)
ConvGRU	(64,n,m,1)	(48,n,m,1)	5×ConvGRU2D(50,7×7)→BN→Dropout(0.5)→Conv2D(50,7×7)→Conv2D(1,7×7)	Adam (lr=0.001)	0.6×SSIM+ 0.4×MSE
GMNN	(56,n,m)	(48,n,m)	3 × GNN(128)→LSTM(64, dropout=0.2) → Dense(128)→Dense(64)→Dense(48 N)	Adam (lr=0.001)	MSE

Rerference

Liang, S., Zhao, A., Qin, M., Hu, L., Wu, S., Du, Z., and Liu, R.: A Graph Memory Neural Network for Sea Surface Temperature Prediction, 10.3390/rs15143539, 2023.