An Uncertainty-Aware Transformer Framework for Satellite-Driven Subsurface Thermohaline Reconstruction

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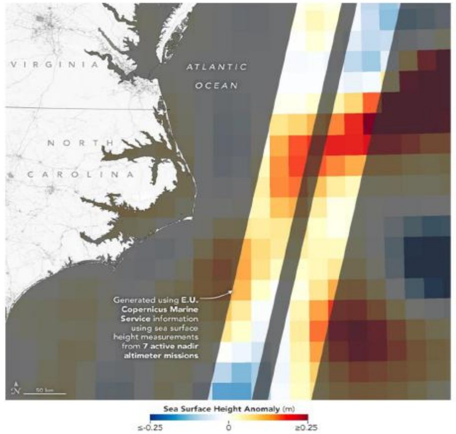
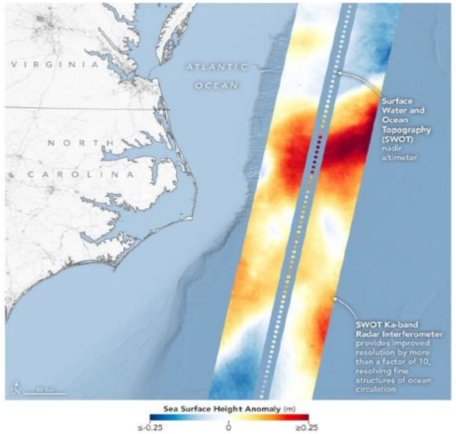
SSH is informative BUT spatially incomplete

- Subsurface observations are sparse and limited
- Sea Surface Height (SSH) reflects vertically integrated density
  → **key link (surface ↔ subsurface)**
- **But : Spatially incomplete (along tracks)**

Conventional altimetry



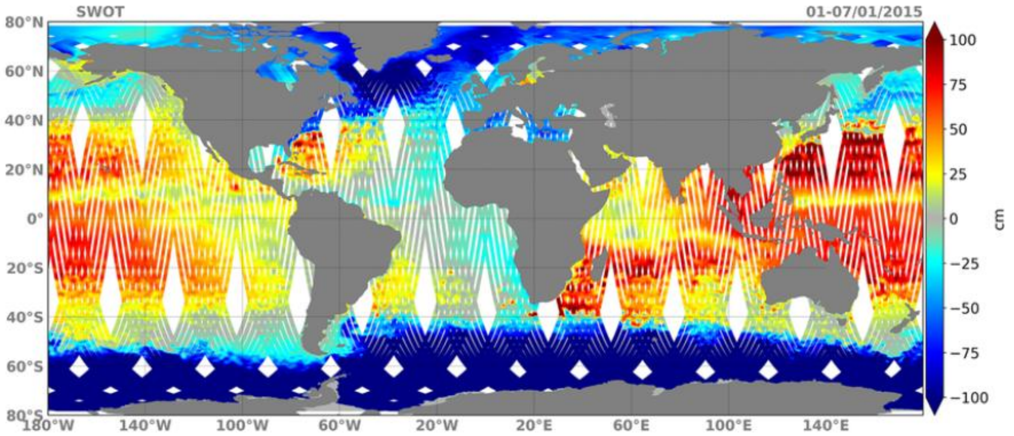
SWOT



Assessing the Impact of the Assimilation of SWOT Observations in a Global High-Resolution Analysis and Forecasting System – Part 2: Results (2021, Tchonang et al.,)

The Surface Water and Ocean Topography Mission: A Breakthrough in Radar Remote Sensing of the Ocean and Land Surface Water (2023, Fu)

Global SWOT SSH (cm) January 1–7, 2015.

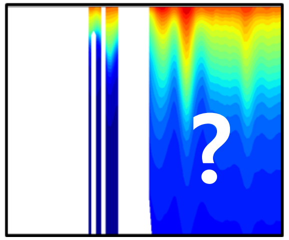


Challenges of Using SSH for Subsurface Constraints

Ill-posed mapping: SSH → T/S

SSH

Subsurface



SSH does not uniquely determine subsurface T/S

Require adjust T/S → May cause imbalance

Key Challenges
Non-uniqueness
Mapping limitation
Uncertainty quantification

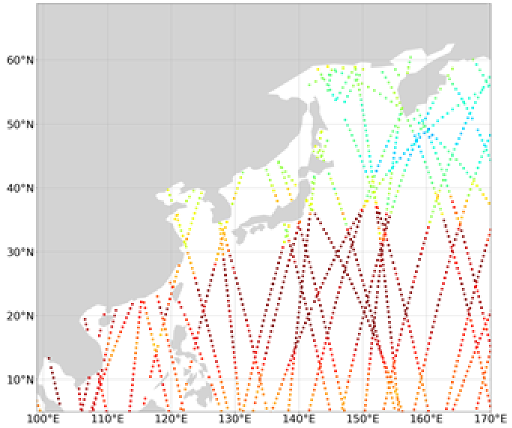
Existing Approaches & Limitations
Vertical displacement / multivariate / regression
→ Depend on fixed dynamics or statistics
→ Limited in complex ocean variability
→ **Limited in flexibility**
(e.g., coastal/tidal variability)

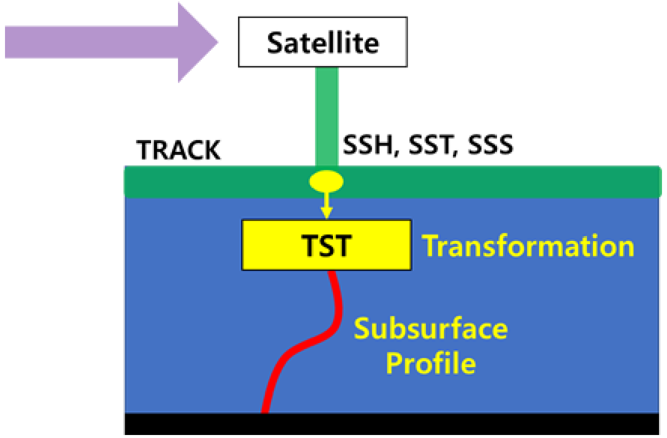
Toward Observation-Space Mapping for Subsurface Reconstruction

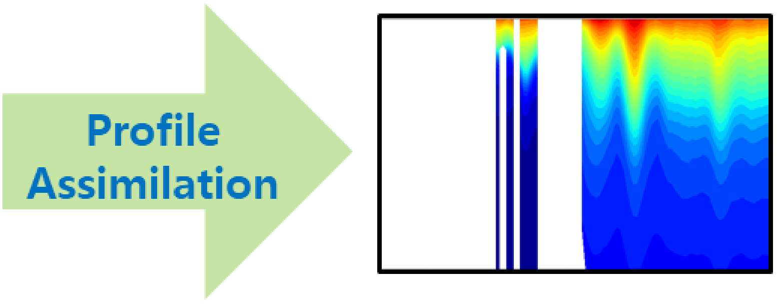
- **Existing ML** : Focus on field reconstruction

- **TST (Temperature and Salinity Transformer)**
  - Observation-space formulation
  - Suface → subsurface mapping
  - Nonlinear interactions

Key contribution
Observation-space mapping
Uncertainty-aware reconstruction
Scalable training

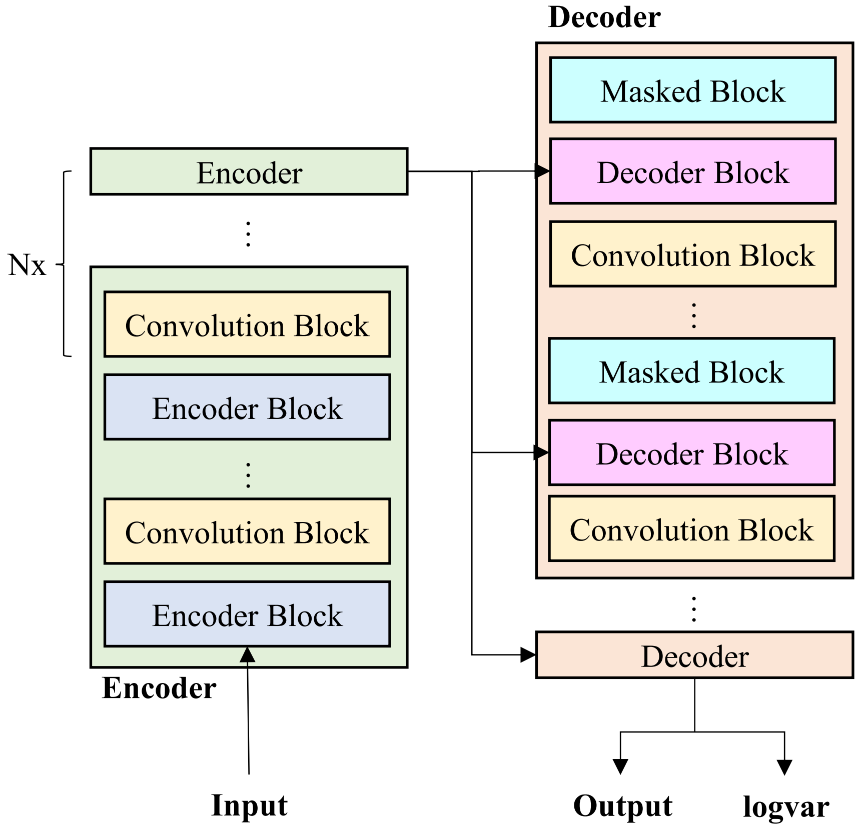






Subsurface Structure

Overview

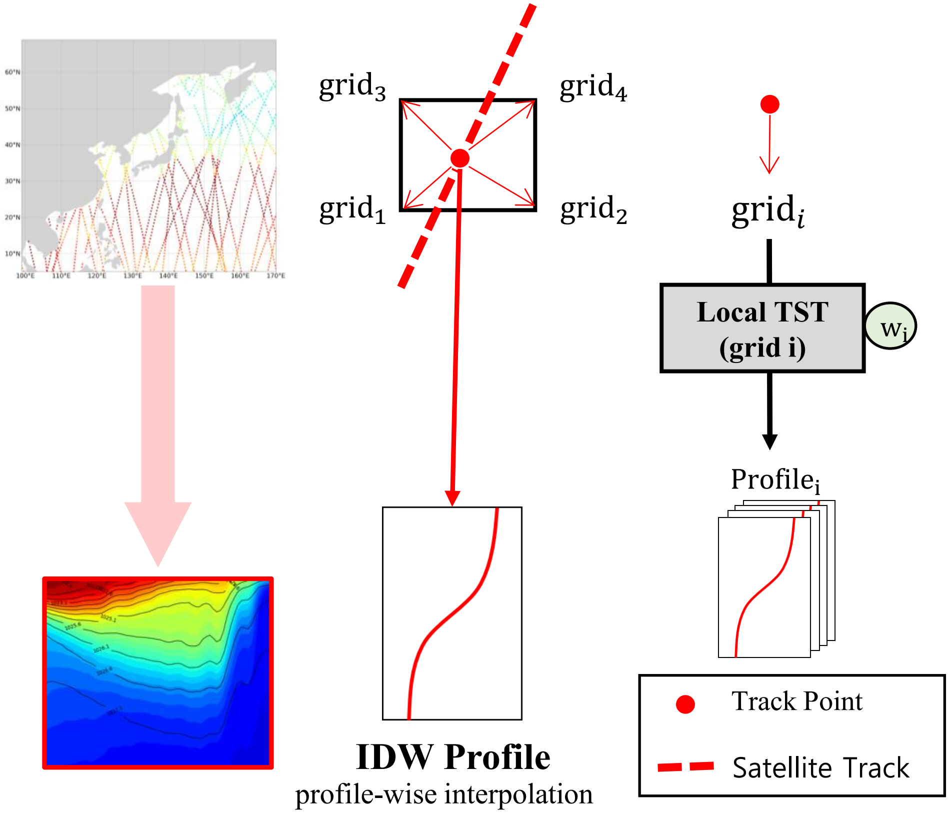


TST (Temperature and Salinity Transformer)
→ data-driven framework for DA

- **Input :** SSH, SST, SSS, Bathymetry, Time
- **Output :** Subsurface T/S profiles + Uncertainty

- **Architecture :**
  - Conv blocks for vertical structure
  - Hybrid attention across variables and depth

Grid-Wise Strategy for Track Reconstruction



- **Key idea**
  - Convert irregular → gridded mapping
- **Why grid-wise?**
  - Enables reliable uncertainty learning
  - Captures strong regional variability
- **Approach**
  - Train a local model for each grid
- **Application to satellite tracks**
  - Use 4 nearest grids
  - IDW (Inverse Distance Weighting) interpolation

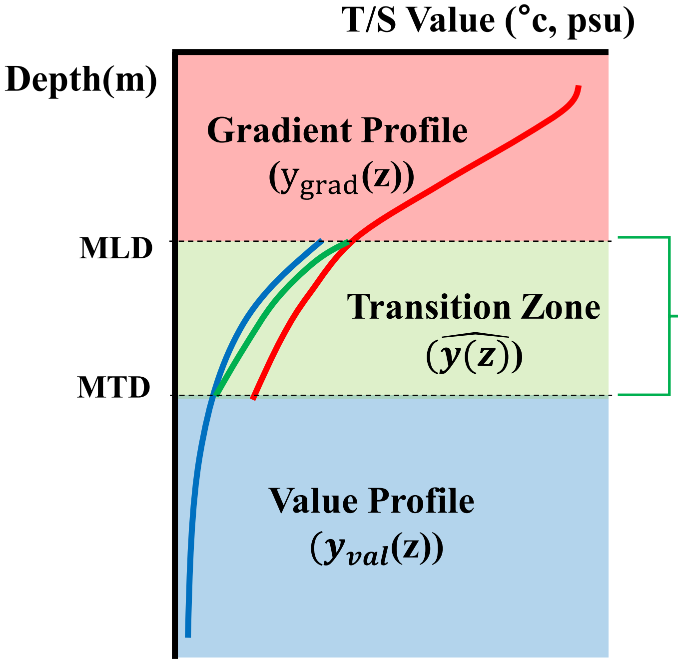
Convert irregular observations into a structured grid
(Train : ~200 min for ~8300 grids, Infer : ~2700 profiles/min)

Profile Generation

Surface: high variability → **gradient-dominated**

Deep: stable structure → **value-dominated**

Depth-dependent blending:
gradient (upper) + value (deep)

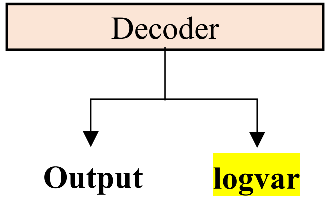


Value : T/S value at depth ($y_{val}(z)$)
Gradient : vertical change relative to surface ($y_{grad}(z)$)

σ : normalized depth $\sigma = \dfrac{z - z_{MLD}}{z_{MTD} - z_{MLD}}$

$$\boxed{\widehat{y(z)} = y_{grad}(z) \cdot S(\sigma) + y_{val}(z) \cdot (1 - S(\sigma))}$$

Uncertainty Calibration and Observation Error Estimate



log-variance(logvar)

Loss Function : $\mathcal{L}_{total} = \mathcal{L}_{Huber} + \mathcal{L}_{NLL} + \mathcal{L}_{cons}$

Heteroscedastic Negative Log-Likelihood (NLL)

$$\mathcal{L}_{NLL} = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{(y_i - \mu_i)^2}{2\sigma_i^2} + \frac{1}{2}\log\sigma_i^2\right]$$

$\boldsymbol{y_i}$: target

$\boldsymbol{\mu_i}$: predicted mean

$\boldsymbol{\sigma_i^2}$: predicted variance

1. Mis-scaled due to multi-component outputs

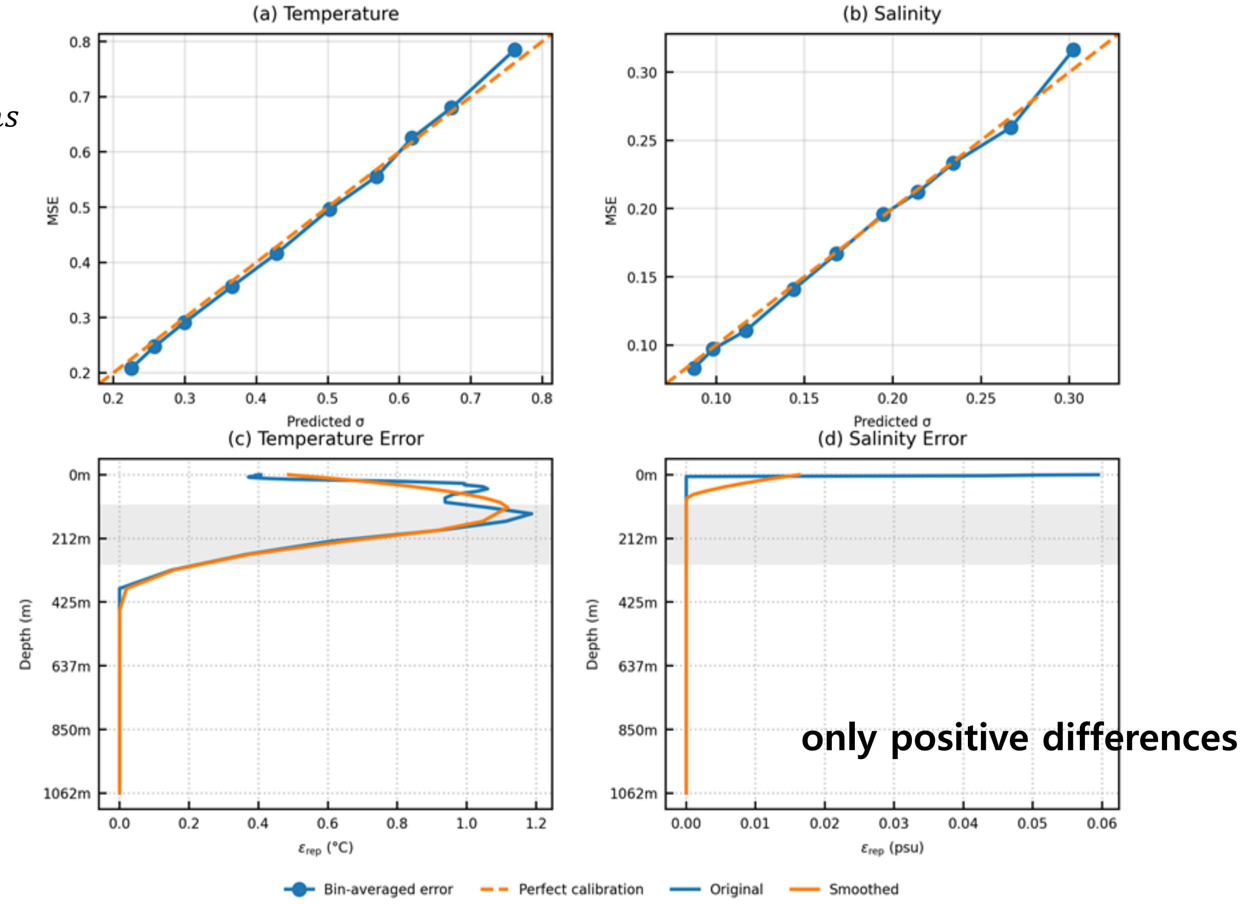
→ Variance Calibration (Linear regression)

Calibration using independent validation dataset

2. Mismatch due to sampling and scale differences

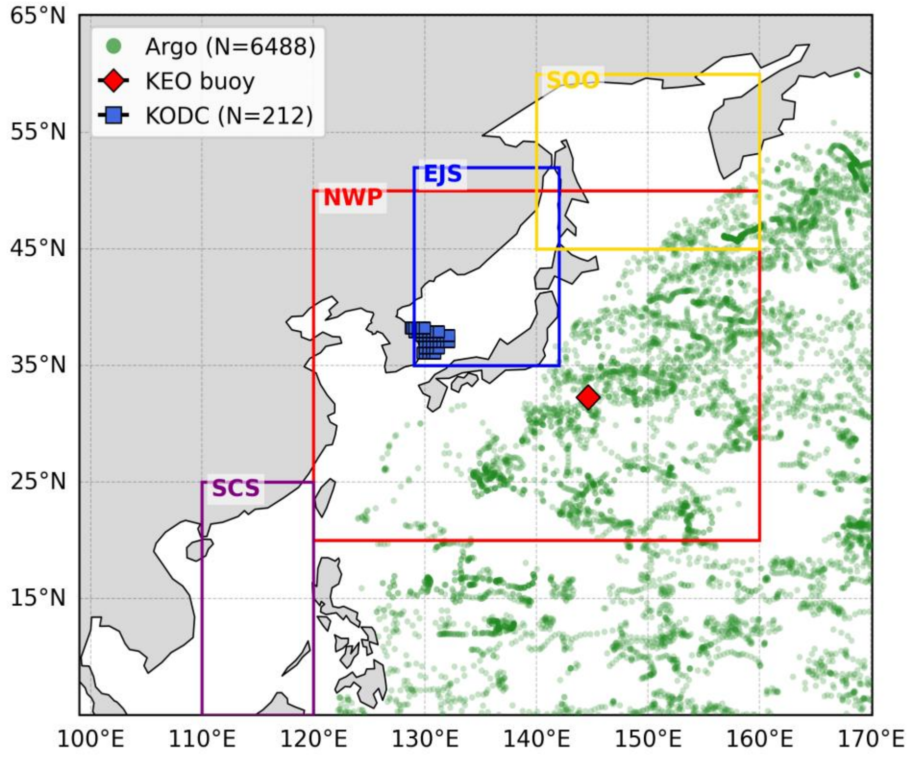
→ Representativeness Error ($\boldsymbol{\varepsilon_{rep}}$)

$$R^2 = \sigma^2 + \varepsilon_{rep}^2 \quad \textbf{OR} \quad R^2 = \beta\sigma^2$$



Logvar (4 outputs) → Calibration → Representativeness Error → **Proxy for Observation Error**

Data and Experiments



* KODC and KEO are local observations

Data Split:

Training : 2010 – 2019
Val : 2020
Test : 2021-2022

Experiments:

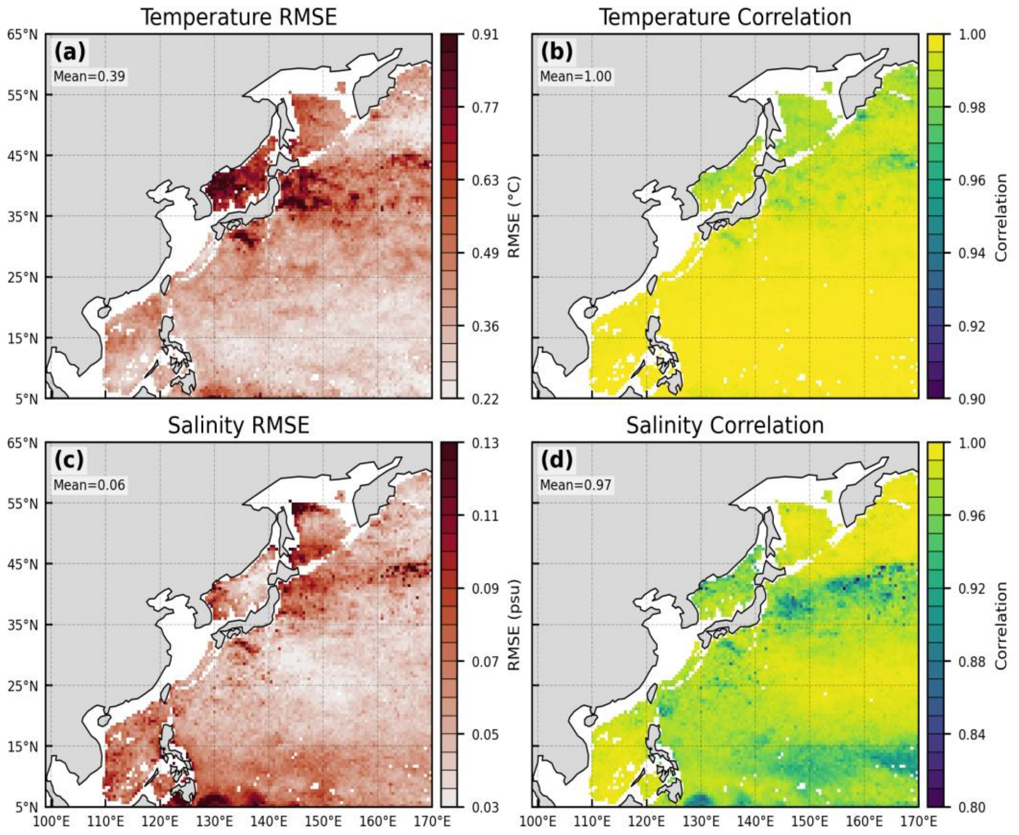
EXP1 (Model-based)
GLORYS surface → GLORYS subsurface

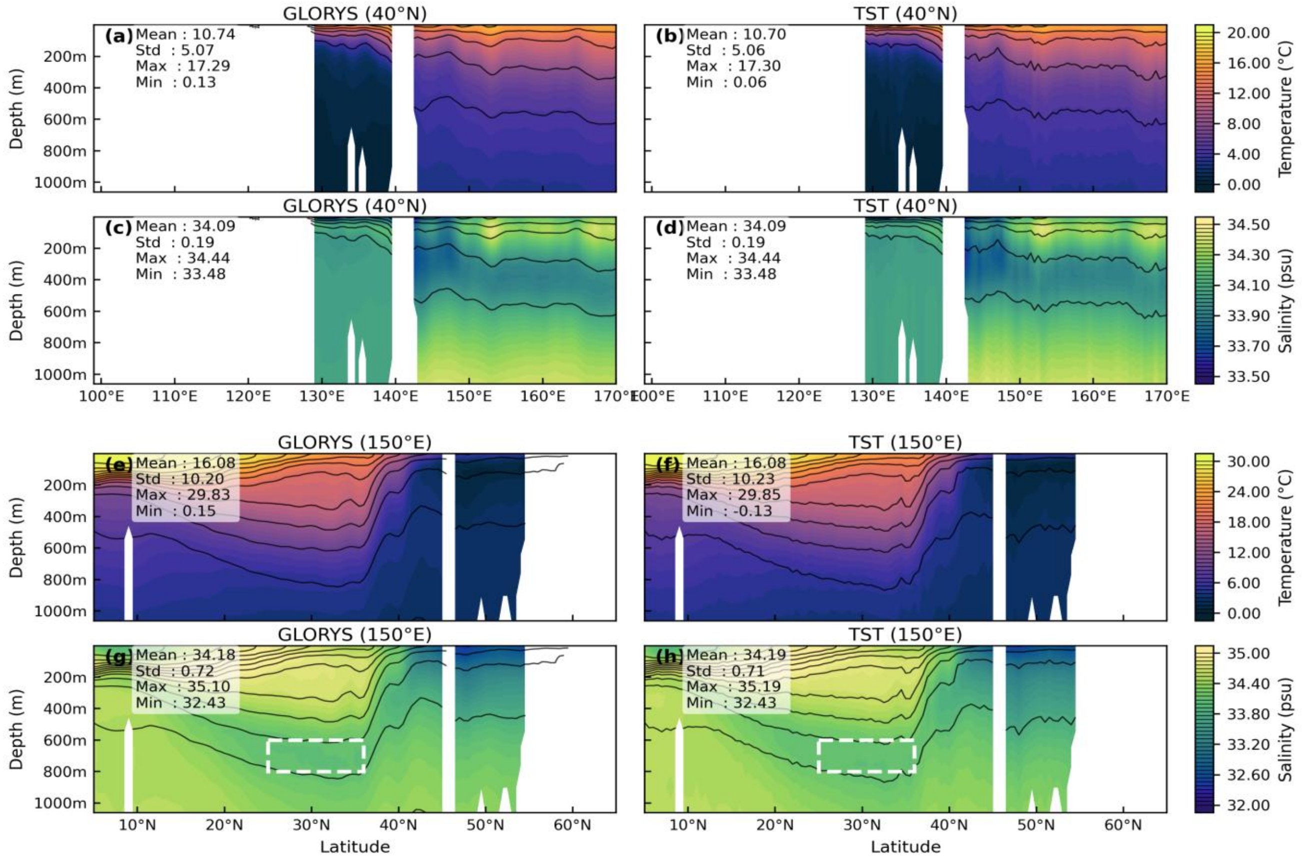
EXP2 (Observation-based)
Satellite surface → In-situ subsurface

Realistic experiment with irregular observations

Experiment 1 : Model-based (GLORYS)

INPUT : GLORYS (SSH, SST, SSS) + Bathymetry
TARGET : GLORYS T/S



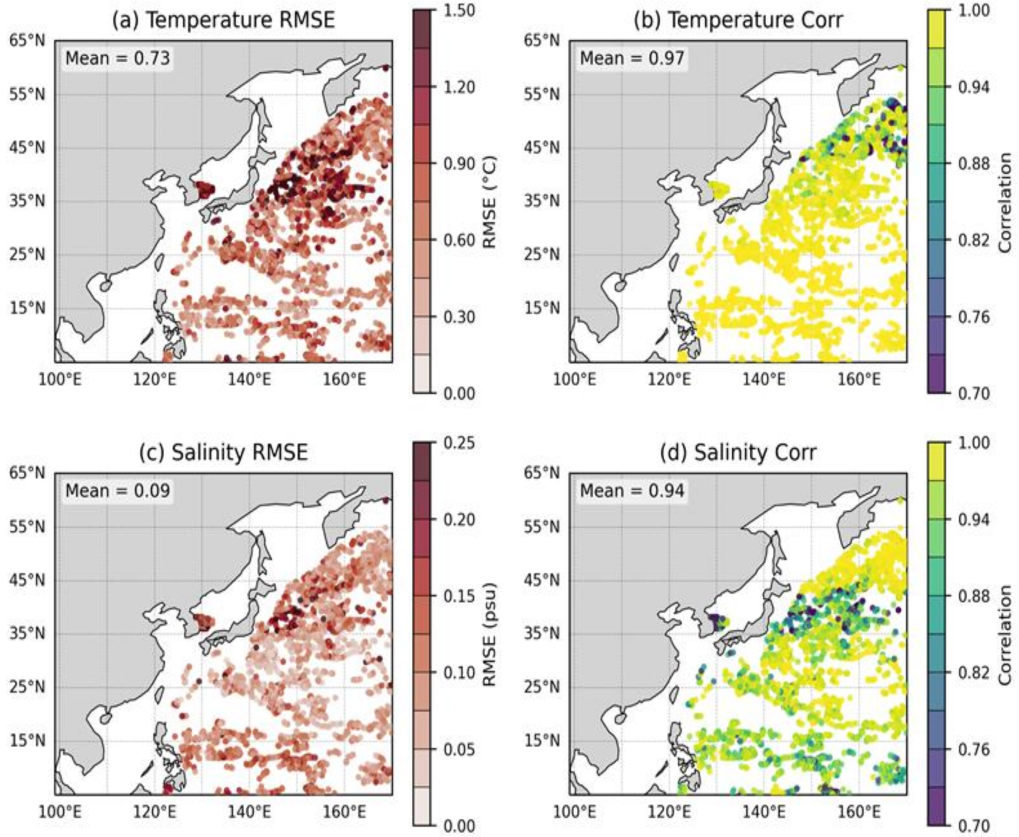


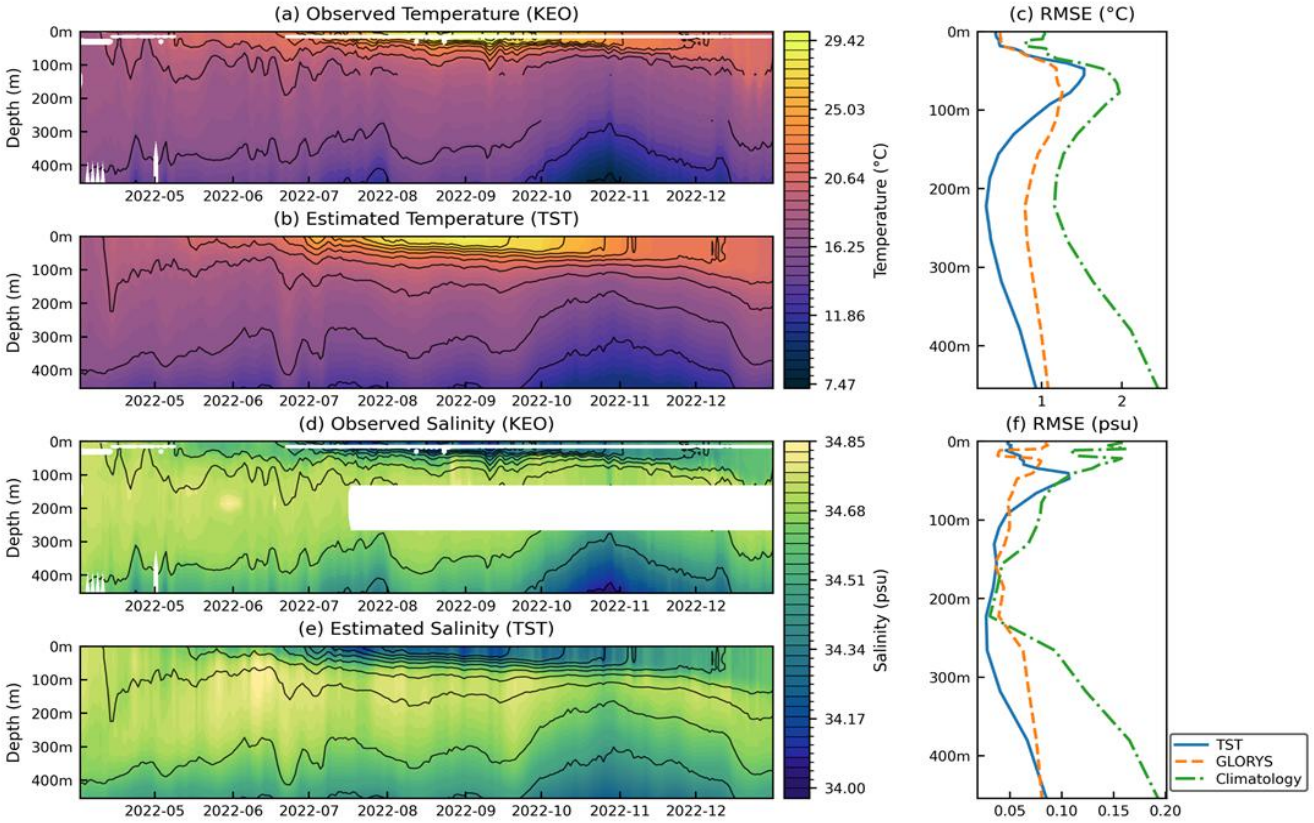
Accurate subsurface T/S reconstruction under GLORYS conditions

(RMSE, Corr, Densitiy consistency, NPIW Core)

Experiment 2 : Observation-based

INPUT : Satellite (SSH, SST, SSS) + Bathymetry
TARGET : In-situ T/S (Argo, KODC, KEO)

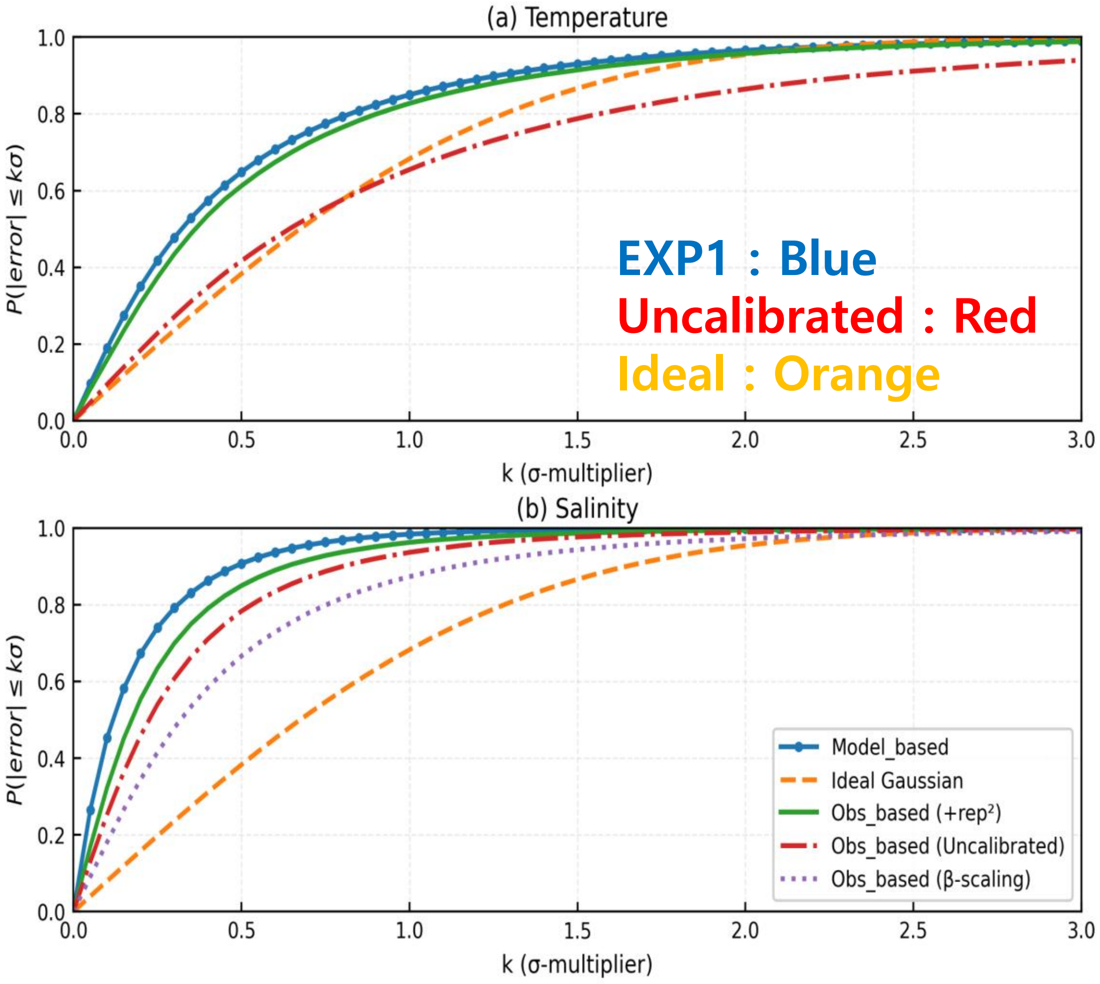


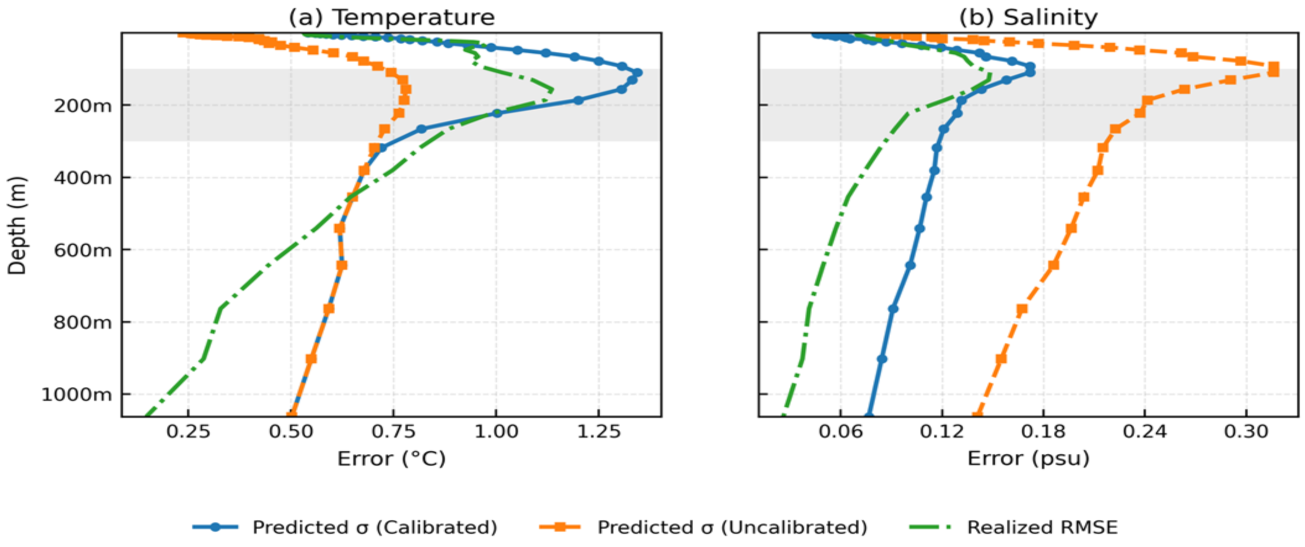


Consistent subsurface T/S reconstruction under real observation conditions
(Independent in-situ validation in observation space)

Experiment 2 : Observation-based

INPUT : Satellite (SSH, SST, SSS) + Bathymetry
TARGET : In-situ T/S (Argo, KODC, KEO)



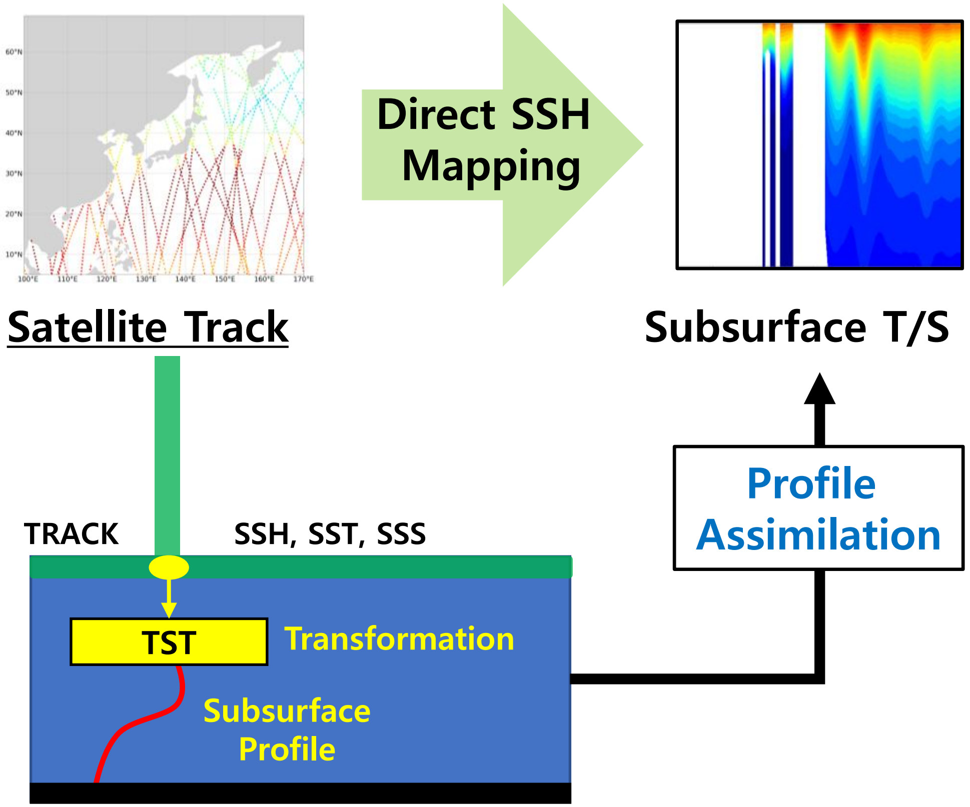


TST provides a proxy for observation error

- Reflects data quality
- Calibrated to realistic reference (EXP1)
- Consistent with observed errors across depth

Discussion and Conclusion

TST : observation-space mapping from satellite surface to subsurface T/S



Key Contributions
- Physically consistent mapping
- Observation-space (point-wise)
- Uncertainty-aware (for DA)

Limitations
- Reanalysis-trained (bias risk)
- Limited high-frequency variability

Future Work
- Global extension
- DA integration (MOM6)

Thank you!

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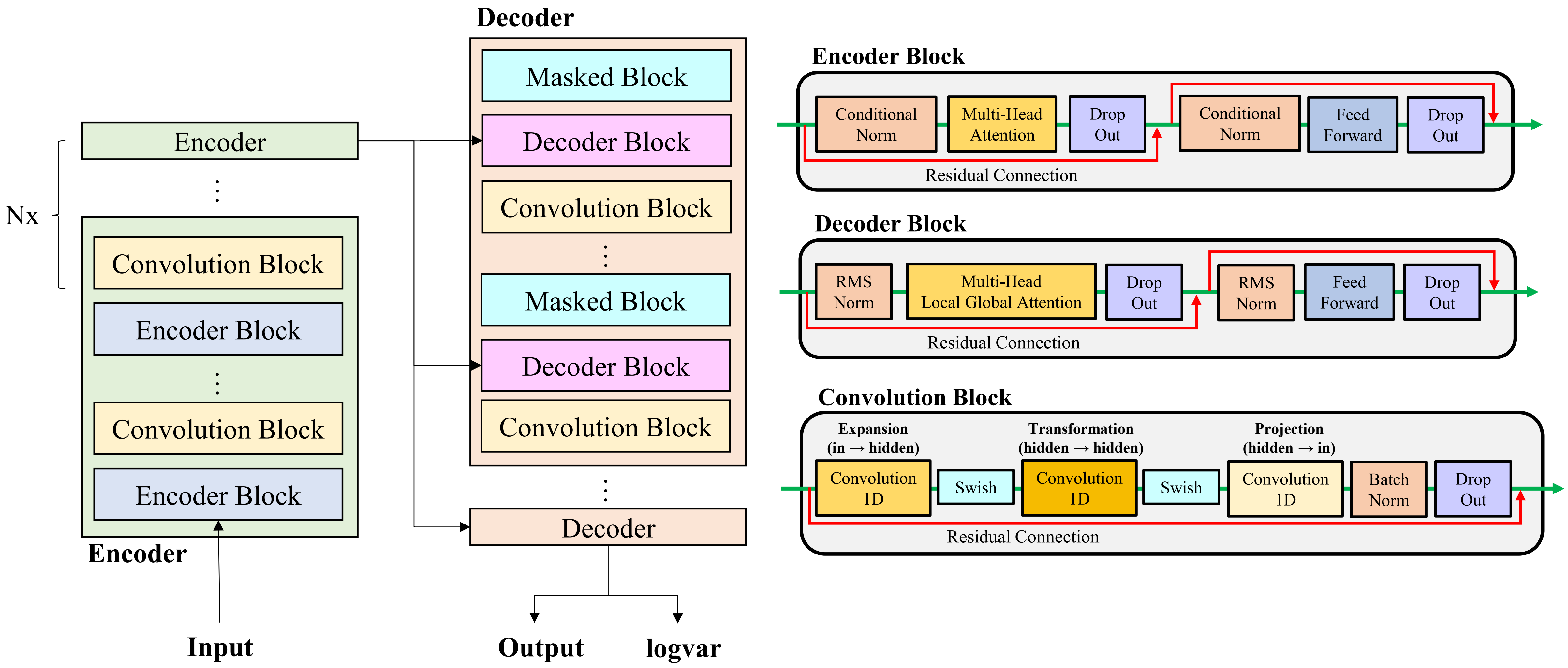
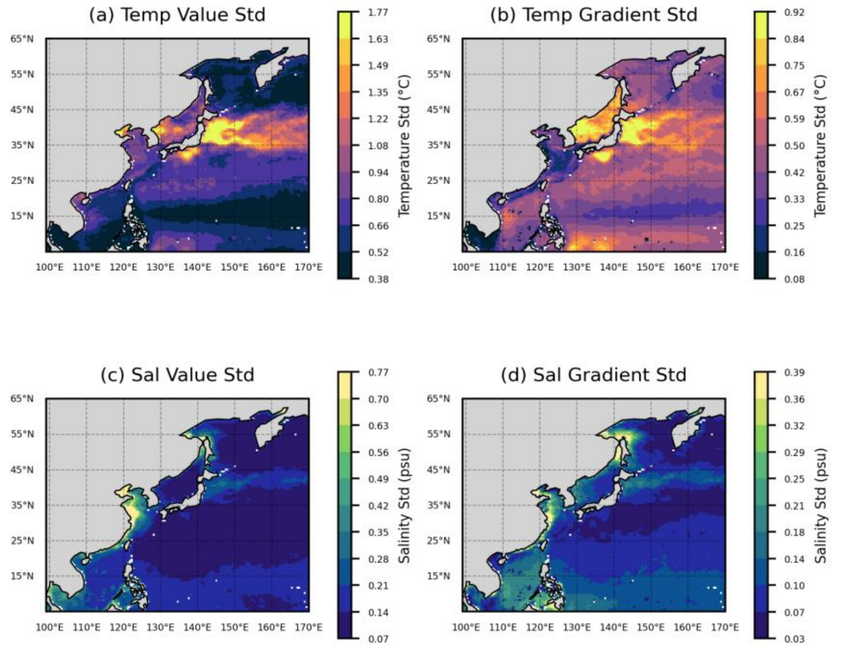
Method

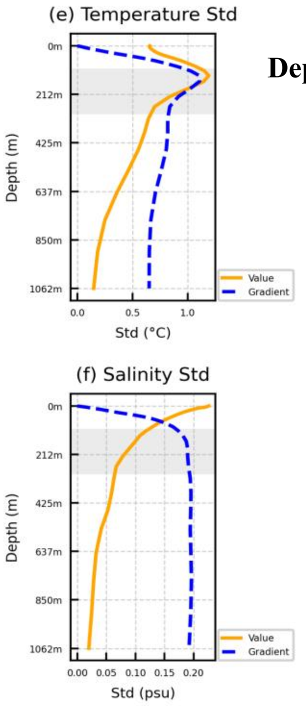
Architecture

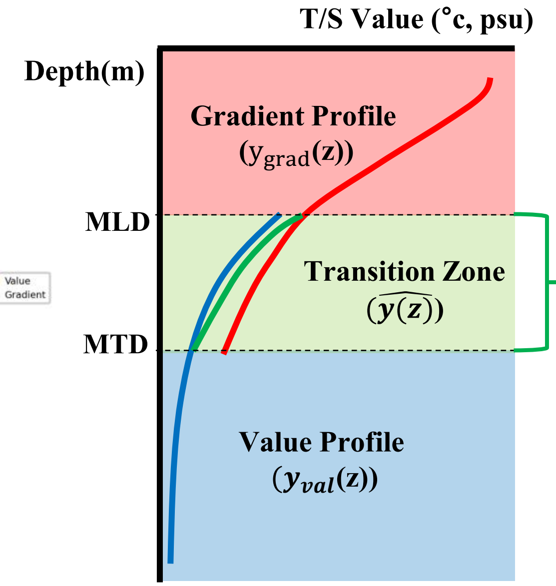


Method

Profile Generation







$$\sigma = \frac{z - z_{MLD}}{z_{MTD} - z_{MLD}}$$

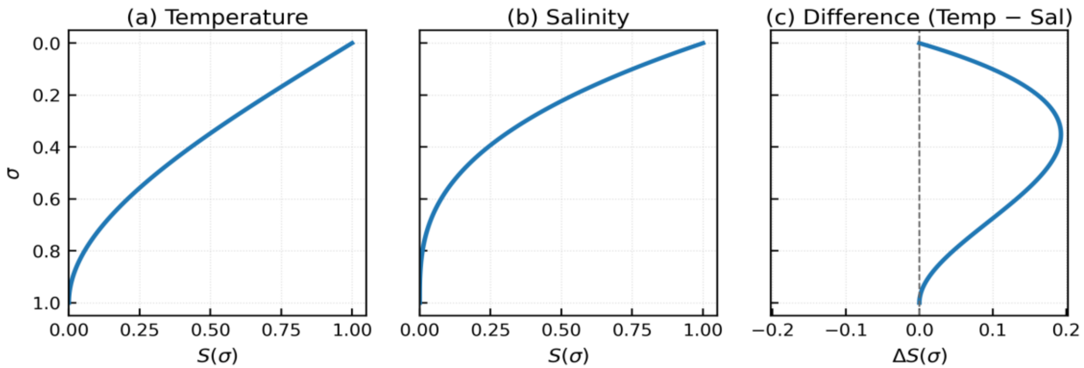
$$\widehat{y(z)} = y_{grad}(z) \cdot S(\sigma) + y_{val}(z) \cdot \left(1 - S(\sigma)\right)$$

$S(\sigma)$: **Similarity Function**

$$S_{base}(\sigma) = \begin{cases} 1, & \sigma \le 0 \\ (1 + a\sigma)(1 - \sigma)^b, & 0 < \sigma < 1 \\ 0, & \sigma \ge 1 \end{cases}$$

$$S(\sigma) = \mathcal{E} + (1 - 2\mathcal{E}) S_{base}(\sigma)$$

$$y(z) = \begin{cases} y_{grad}(z) \ldots (0 < z < MLD) \\ \widehat{y(z)} \ldots (MLD < z < MTD) \\ y_{val}(z) \ldots (MTD < z) \end{cases}$$

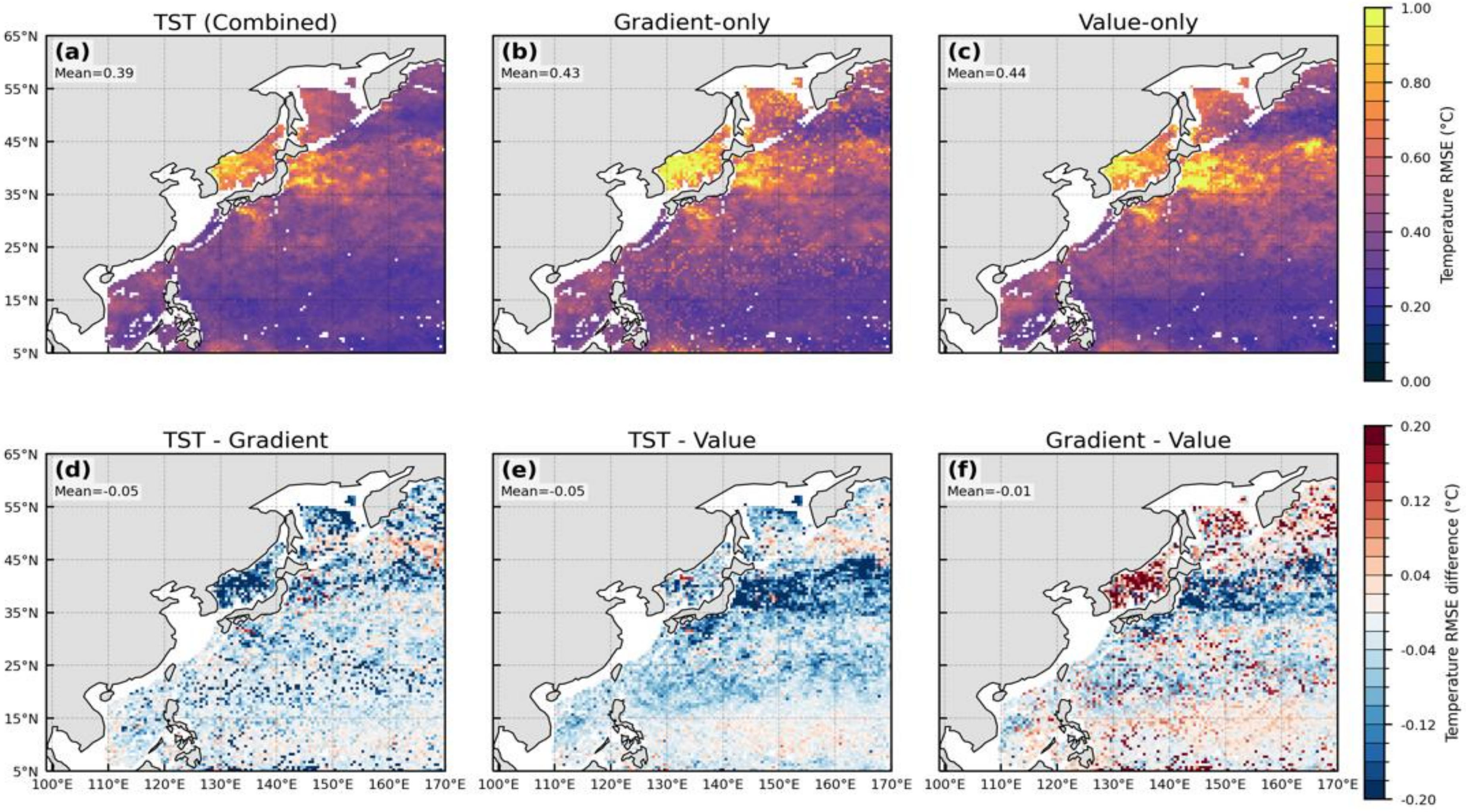


Value : predicts absolute temperature and salinity at depth ($y_{val}(z)$)
Gradient : vertical changes relative to the surface ($y_{grad}(z)$)

- Value and gradient representations describe different aspects of variability
- Gradient emphasizes surface-intensified structure
- Value provides a stable representation in deeper layers

Method

Profile Generation



Experiment 1 : Model-based Validation under GLORYS Conditions

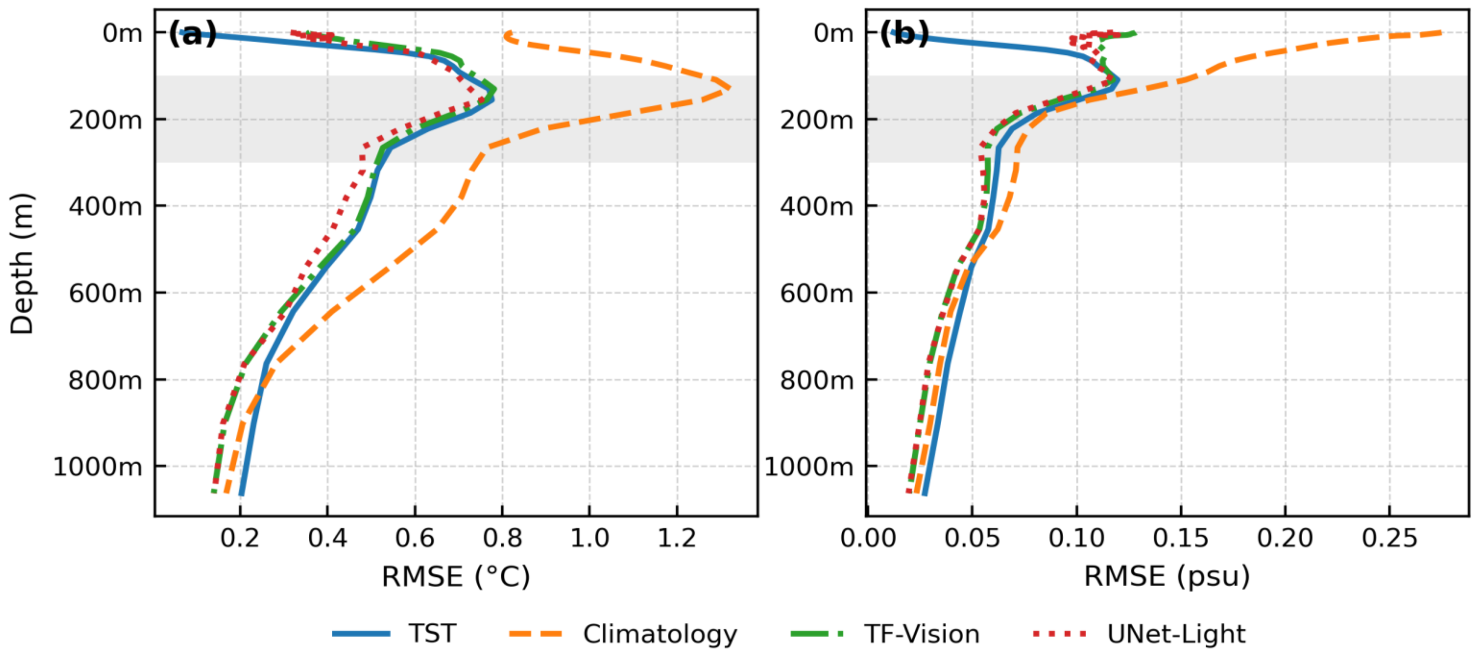


Fig. 9. Depth-dependent RMSE profiles of (a) temperature and (b) salinity (0–1000 m) for TST (blue), TF-Vision (green), UNet-Light (red), and the climatology baseline (orange). The climatology baseline is derived from the 10-year (2010–2019) monthly mean GLORYS reanalysis fields and represents a reanalysis-based low-frequency reference state rather than a static constant profile. The vertical grid is non-uniform, with 24 of the 36 model levels located above 130 m, resulting in enhanced resolution within the upper ocean and thermohaline.

Experiment 1 : Model-based Validation under GLORYS Conditions

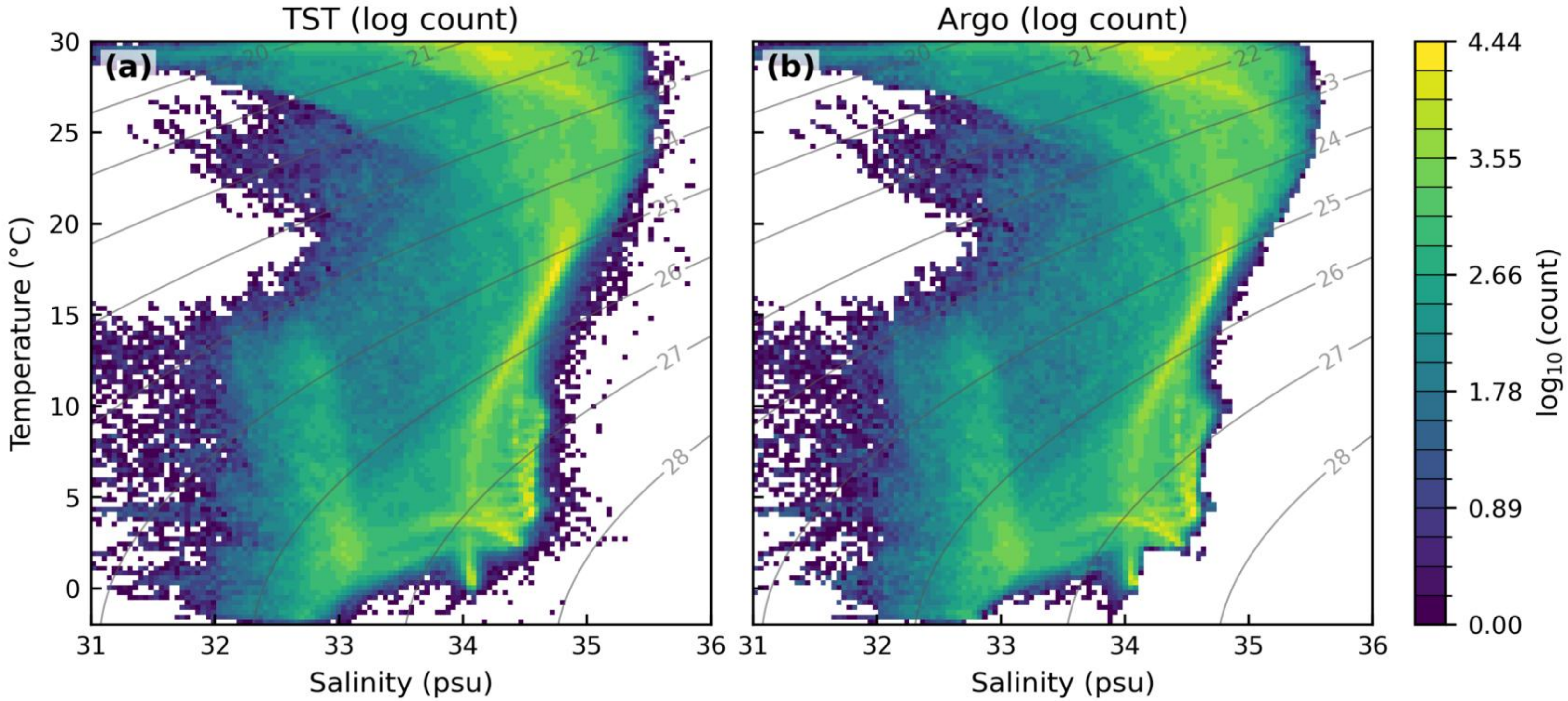


Fig. 10. Temperature–salinity (T–S) distributions from TST predictions (left) and the GLORYS reference fields (right) for 2021–2022. Colors indicate the logarithmic density of samples in T–S space, and black contours denote potential density anomaly (σθ), computed using TEOS-10. The diagrams illustrate the overall thermohaline structure of the northwestern Pacific, including the characteristic salinity minimum associated with North Pacific Intermediate Water (NPIW).

Result

Experiment 2 : Observation-based Validation (Real-World)

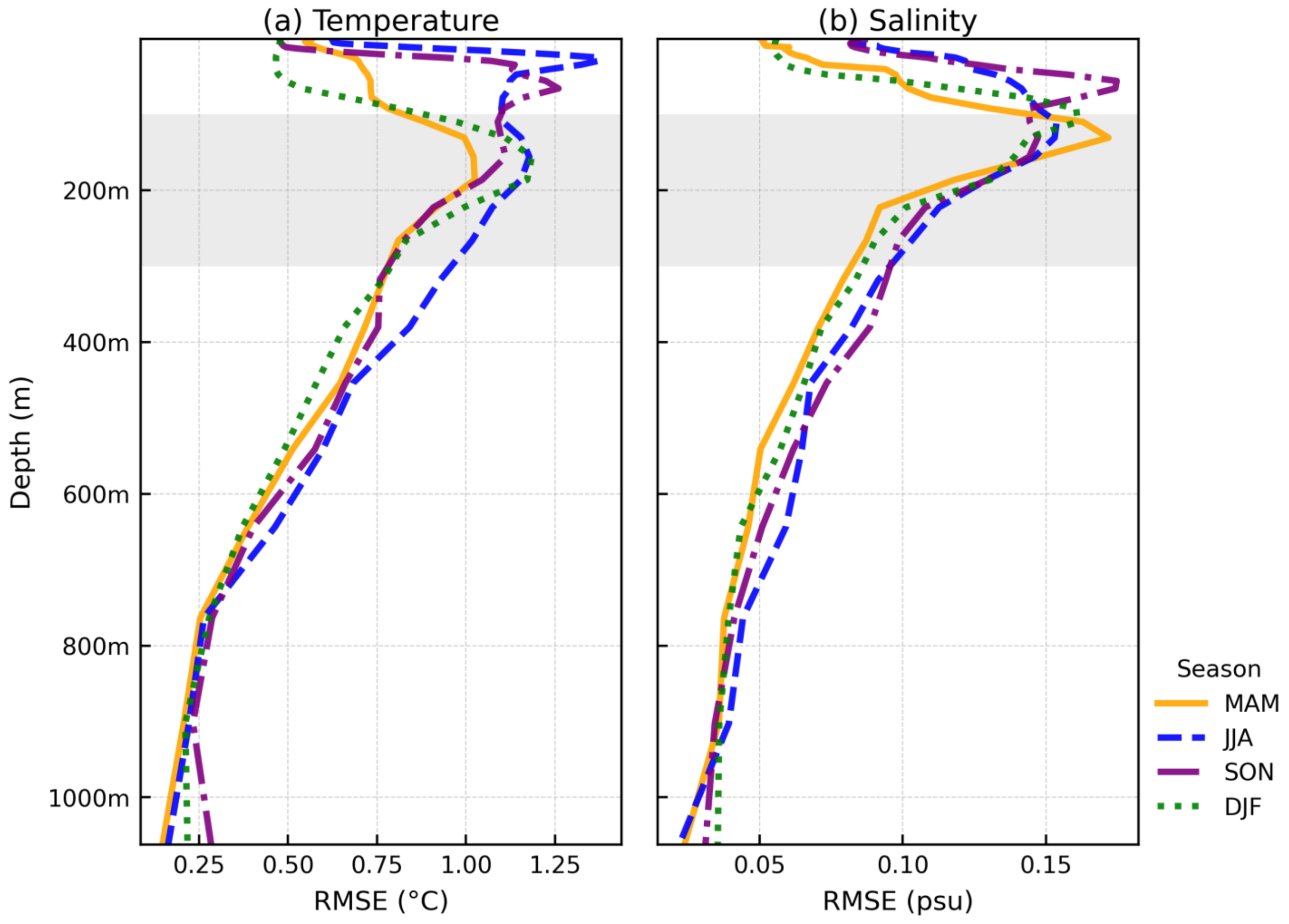


Fig. 13. Depth-dependent RMSE profiles for (a) temperature and (b) salinity across seasons (MAM, JJA, SON, and DJF). Temperature errors are largest within the upper thermohaline (100–300 m), particularly during summer (JJA) when vertical stratification is strongest. In contrast, salinity exhibits comparatively weak seasonal variation throughout the water column, indicating a stable representation of subsurface water-mass structure across seasons.

Result

Experiment 2 : Observation-based Validation (Real-World)

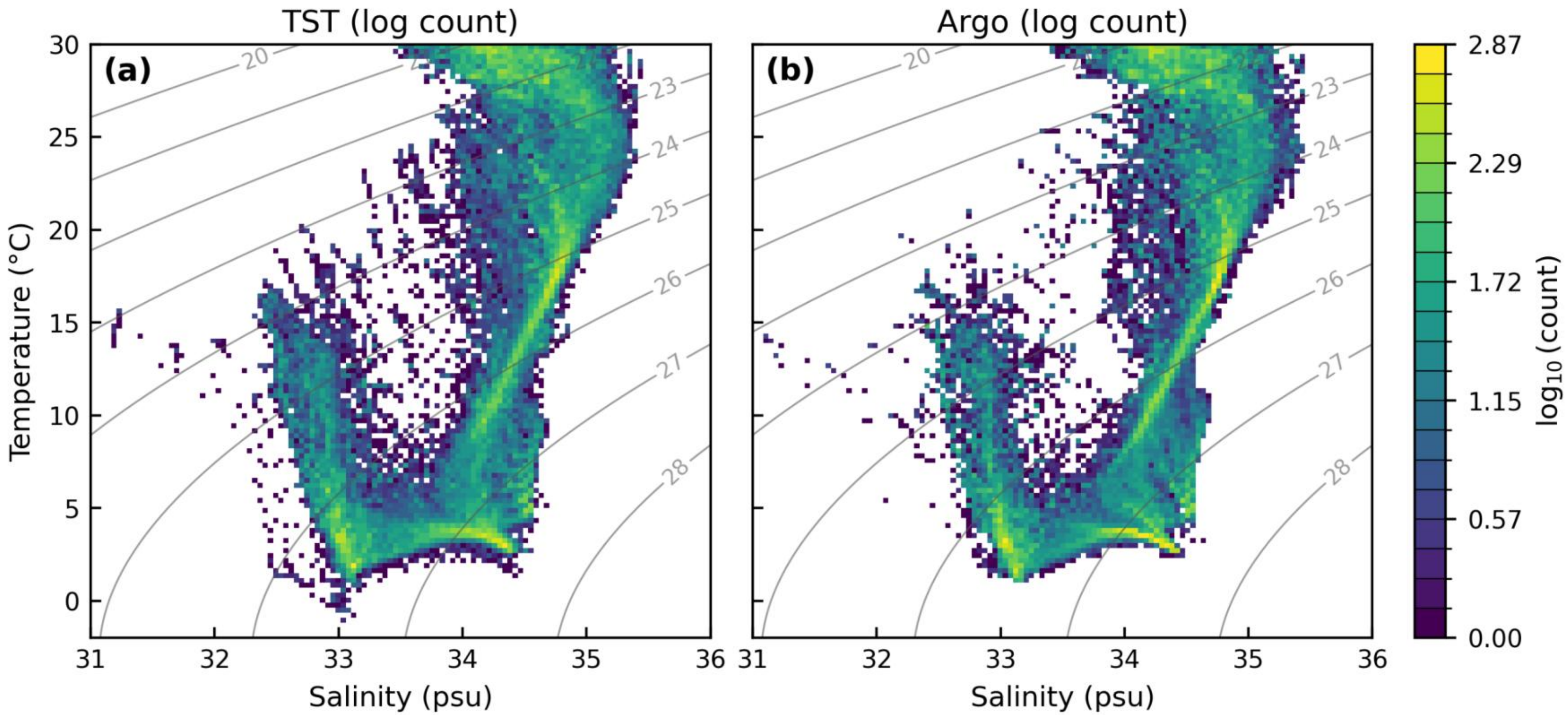


Fig. 14. Temperature–salinity (T–S) distributions from TST reconstructions (left) and Argo observations (right), shown as log-scale sample densities. Density contours indicate water-mass structure. TST reproduces the primary thermohaline distribution of the basin, including both cold, fresh subpolar waters and warm, saline subtropical waters, demonstrating physically consistent large-scale water-mass relationships.