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A historical nutrient dataset (1895–2024) for the North Pacific: reconstructed from machine learning and hydrographic observations

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Key points:

- Rigorous data quality control procedures were applied to clean nutrient and hydrographic data collected from multiple sources in the North Pacific, following state-of-the-art practices.
- Three machine learning models demonstrated low errors across diverse validation strategies.
- We reconstructed a monumental database of ~473 million nutrient data points across 1.92 million stations (1895–2024), expanding the number of nutrient data points by a factor of 2,127–2,393 compared to original observations.

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Abstract

Nutrients play a critical role in oceanic primary productivity and the biological pump. However, compared to hydrographic parameters such as temperature and salinity, nutrient observations are limited due to their labor-intensive and costly measurements. Thus, nutrient observations are several orders of magnitude sparser than hydrographic observations. In this study, we first established a rigorous data quality control procedure to clean the hydrographic and nutrient (including NO_3^-, NO_2^-, DIP, and $Si(OH)_4$) observations collected from World Ocean Database (WOD) and CLIVAR and Carbon Hydrographic Data Office (CCHDO) in the North Pacific. Subsequently, the cleaned and high-quality CCHDO dataset was used to train three machine learning models—Random Forest, Light Gradient Boosting Machine (LightGBM), and Gaussian Process Regression—to establish relationships between nutrient concentrations and key variables, including space coordinates (longitude, latitude, and depth), time variables (year and month), and water mass properties (indexed by potential temperature and salinity). Validation shows that the reconstruction closely matches the observations, with RMSEs of <1.41, <0.071, <0.089 and <3.07 μmol kg^{-1} for NO_3^-, NO_2^-, DIP, and $Si(OH)_4$, respectively. The validated models were then applied to reconstruct nutrient concentrations from the hydrographic observations in WOD, most of which lacked direct nutrient measurements. This resulted in ~473 million reconstructed nutrient data points across 1.92 million stations for each nutrient, spanning from 1895 to 2024, representing a 2,127 to 2,393–fold increase compared to the original nutrient observations in the North Pacific (197,539 to 222,234). This new dataset will be valuable for studying nutrient variability under climate change and anthropogenic influences, and for providing transient boundary conditions in ocean biogeochemical models. The dataset generated in this study is openly available on Zenodo at https://zenodo.org/records/17451417.

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1 Introduction

Bio-essential elements such as nitrogen, phosphorus, and silicon constitute the fundamental material basis for marine ecosystems. Their concentrations govern primary and new production (e.g., Browning et al., 2023; Lipschultz et al., 2002; Moore et al., 2013) and subsequently regulate oceanic uptake of atmospheric CO_2 (Deutsch and Weber, 2012; Sigman and Hain, 2012). However, traditional nutrient data collection relies heavily on ship-based cruises and subsequent sample analysis, which are labor-intensive, inefficient, and costly (Du et al., 2021). Consequently, compared to the abundant hydrographic data collected from multiple platforms such as Conductivity-Temperature-Depth (CTD) and the Array for Real-time Geostrophic Oceanography (Argo) profilers, etc., nutrient observations are sparse in the ocean. These sparse nutrient observations limit our understanding of both small-scale and long-term nutrient variations and our comprehensive understanding of the mechanisms driving changes in oceanic production and ecosystem dynamics (Bidigare et al., 2009; Yasunaka et al., 2021; Karl et al., 2021).

To address this data sparsity, two main approaches have been commonly employed to augment the spatiotemporal coverage of the observed nutrient data. The first is objective analysis, which interpolates field measurements to generate broader spatial coverage, as implemented in products such as the World Ocean Atlas (WOA) (e.g., Reagan et al., 2023; Lee et al., 2023). The second is data fusion, which establishes statistical relationships between nutrients and environmental predictors such as temperature (e.g., Kamykowski, 1987; Kamykowski et al., 2002; Kamykowski, 2008), density (e.g., Dugdale et al., 1989; Switzer et al., 2003), oxygen, salinity, and chlorophyll *a* (Goes et al., 1999; Palacios et al., 2013; Sarangi et al., 2011). Statistical methods including cubic regression, multiple linear regression (Steinhoff et al., 2010; Arteaga et al., 2015; Madani et al., 2024; Zhong et al., 2024), and generalized additive models (Palacios et al., 2013) are frequently used in these efforts.

Recent studies have demonstrated the potential of machine learning for enhancing the spatial and temporal coverage of nutrient data. For instance, Możejko and Gniot

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(2008) used Artificial Neural Networks (ANNs) to model time series of total phosphorous concentrations in the Odra River. Self-organizing maps (SOMs) were used to estimate mixed layer nitrate and sea surface nutrients in the open ocean (Steinhoff et al., 2010; Yasunaka et al., 2014). Liu et al. (2022) applied Support Vector Regression, Random Forest Regression, and ANNs to reconstruct monthly surface nutrient concentrations in the Yellow and Bohai Seas from 2003 to 2019. Their results revealed pronounced seasonal and spatial variability in nutrient levels and underscored the influence of environmental drivers such as sea surface temperature and salinity. Similarly, Sundararaman and Shanmugam (2024) employed Gaussian Process Regression (GPR) models to estimate global ocean surface macronutrient concentrations using satellite-derived data, achieving high accuracy and demonstrating their suitability for large-scale marine ecosystem monitoring. Yang et al. (2024) employed a U-net and Earthformer to reconstruct the three-dimensional nitrate distribution by integrating surface data including wind speed, sea surface temperature, chlorophyll *a*, solar radiation, and precipitation in the Indian Ocean. These advancements highlight the expanding role of machine learning in marine biochemical data fusion and provide novel insights into nutrient dynamics and their ecological impacts.

However, many existing approaches rely solely on mathematical extrapolation or data fusion and often neglect the influence of physical seawater properties, such as water mass characteristics. Using the relationship between nutrient concentration and water masses (indexed by temperature and salinity), Du et al. (2021) successfully predicted the nutrient concentrations in the South China Sea. However, the water masses and their relationship with nutrients can also vary with space and time, which should also be taken into consideration. In addition, most research has predominantly focused on nutrient predictions at surface waters—driven by readily available remote-sensing measurements of sea surface temperature and chlorophyll *a*—while subsurface nutrient distributions remain poorly studied.

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The North Pacific Ocean is one of the largest marine biomes in the global ocean (Karl and Church, 2017), spanning a broad latitudinal range from tropical to subpolar regions. It includes a subtropical gyre characterized by extremely low surface nutrient concentrations due to Ekman convergence (e.g., Dave and Lozier, 2010; Browning et al., 2021; Dai et al., 2023), and subpolar gyres in the north with elevated nutrient concentrations driven by Ekman divergence. The North Pacific Ocean is influenced by multiple upwelling and current systems, including the equatorial and California upwelling systems, North Equatorial Current, Kuroshio Current, etc., which further change nutrient levels in these regions. In addition, the North Pacific Ocean exhibits abundant mesoscale eddies (Chelton et al., 2007), which play a critical role in redistributing nutrients and modulating biological activity (e.g., Benitez-Nelson et al., 2007; Ascani et al., 2013; Barone et al., 2022). The interaction of these multi-scale physical processes with biogeochemical processes results in highly dynamic nutrient variability in the upper ocean. Therefore, high-resolution and extensive nutrient datasets are essential to accurately resolve the nutrient dynamics. Although the WOA (Reagan et al., 2023) serves as a primary nutrient database and is widely used for boundary conditions in biogeochemical models, its applicability is constrained by relatively coarse spatial resolution (currently 1°) and climatological smoothing, which limit its ability to represent mesoscale and episodic features or to capture long-term variations.

In the North Pacific, Yasunaka et al. (2014) used the SOMs technique to generate monthly surface nutrient maps by integrating sea surface temperature, salinity, chlorophyll *a*, and mixed layer depth. These maps revealed seasonal and interannual variability in surface nutrient distributions in the northern North Pacific. To investigate long-term changes, Yasunaka et al. (2016) applied Optimal Interpolation to analyze the spatial and temporal evolution of surface nutrient concentrations. Lee et al. (2023) provided spatiotemporally gridded nitrate and phosphate data in northwest Pacific from 1980 to 2019 using the spatiotemporal kriging technique. Wang et al. (2023) used the

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deep neural network model to estimate nitrate concentrations in the upper northwestern Pacific Ocean using temperature and salinity as the primary input parameters.

In this study, we first collected nutrient data from public databases and applied rigorous quality control procedures. Using machine learning methods, we established relationships between nutrient concentrations and water mass properties, spatial coordinates, and temporal variables. We then evaluated the model performance through a comprehensive error analysis. Finally, the validated models were applied to reconstruct historical nutrient distributions across the North Pacific from 1895 to 2024.

2 Data and Methods

2.1 Observation data

Field observations were originally downloaded from the Climate and Ocean: Variability, Predictability, and Change (CLIVAR) and Carbon Hydrographic Data Office (CCHDO), which distributes vessel-based hydrographic data from programs such as the World Ocean Circulation Experiment (WOCE), Joint Global Ocean Flux Study (JGOFS), GO-SHIP, CLIVAR, and other repeat hydrography efforts (https://cchdo.ucsd.edu/). In total, 631 cruises were collected in the North Pacific, comprising 228,091, 197,617, 225,403, and 212,660 data points for $NO_3^- + NO_2^-$ (NO_x^-), NO_2^-, DIP, and $Si(OH)_4$, respectively (Table 1). The dataset spans from 1973 to 2022 and was downloaded on October 1 2024; any updates made after this date were not included in this study. The data cover a geographic range from 120.08°E to 95.17°W and from 2.05°S to 60.25°N. The study domain was slightly extended into the South Pacific to mitigate potential boundary effects during model development.

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Table 1. Information on nutrients and their associated hydrographic data collected from CLIVAR and Carbon Hydrographic Data Office (CCHDO) and the data information after quality control (QC).

	Original data information		Data information after QC	
	Data	Stations	Data	Stations
Temperature	328502	15274	327688	15125
Salinity	311871	15274	328275	15269
NO_x^-	228091	9588	214943	9120
NO_2^-	197617	8233	197539	8228
DIP	225403	9623	222234	9474
$Si(OH)_4$	212660	8220	210447	8121

Hydrographic data for nutrient reconstruction were obtained from the World Ocean Database (WOD; Mishonov et al., 2024), which compiles observations from various platforms, including Autonomous Pinniped Bathythermograph (APB), Conductivity-Temperature-Depth profiler (CTD), Drifting Buoy (DRB), Glider (GLD), Mechanical Bathythermograph (MBT), Moored Buoy (MRB), Ocean Station Data (OSD), Profiling Float (PFL), and Undulating Oceanographic Recorder (UOR). Since nutrient reconstruction models rely on relationships with water masses, only samples containing both temperature and salinity measurements were used; therefore, most APB observations, which record only temperature, were excluded. Among these platforms, CTD, OSD, and PFL provided the majority of usable data. Additionally, several marginal seas—including the South China Sea, the Yellow Sea, the Sea of Japan, and the Sea of Okhotsk—were excluded from this study because they are semi-enclosed and strongly influenced by terrestrial inputs. The spatial domain was consistent with that used for the CCHDO dataset, while the temporal coverage extended from 1875 to 2024. In total, 577,215,683 data points from 2,284,448 stations across 40,113 original cruises were collected (Table 2).

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Table 2. Information on hydrographic data collected from World Ocean Database, and the data information after quality control (QC).

Platform	Original data information			Data information after QC		
	Data	Stations	Cruises	Data	Stations	Cruises
APB	692302	46454	189	543714	37209	154
CTD	157914052	315177	8785	135584007	297036	8415
GLD	119302218	288840	384	69834989	285778	380
OSD	8885341	592225	21169	6942902	505780	17671
PFL	284781001	700798	9511	255423345	680531	9099
UOR	3373799	26699	7	3304158	25813	6
MRB	1459032	293734	65	1019565	88487	19
DRB	807938	20521	3	0	0	0
Total	577215683	2284448	40113	472652680	1920634	35744

2.2 Data quality control

Given that the data were collected from multiple platforms using various methods over a long-time span and broad spatial range, quality control (QC) was essential (Du et al., 2021; Wang et al., 2025). Following the QC procedures developed by the World Ocean Database (WOD) (Garcia et al., 2024), we applied comprehensive QC protocols (Fig. 2) to both CCHDO and WOD datasets, including hydrographic and nutrient variables.

Four levels of QC were applied to identify and remove potentially erroneous or low-quality records from the CCHDO and WOD datasets. The first level targeted individual measurements, including several checks. (1) A range check was conducted by defining depth-dependent acceptable value ranges for each parameter; data falling outside these ranges were flagged as invalid. This check was applied to temperature, salinity, NO_x^-, NO_2^-, DIP, and $Si(OH)_4$. Note that the NO_x^- denotes the sum concentration of NO_2^- and

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NO_3^-. At stations lacking direct NO_x^- measurements, NO_x^- concentrations were derived by summing discrete NO_2^- and NO_3^- observations. (2) An empirical relationship check was performed to verify consistency among paired variables based on predefined acceptable domains, including temperature–salinity, temperature–NO_x^-, temperature–NO_2^-, temperature–DIP, temperature–$Si(OH)_4$, salinity–NO_x^-, salinity–NO_2^-, salinity–DIP, salinity–$Si(OH)_4$, NO_x^-–DIP, and NO_x^-–$Si(OH)_4$. (3) A six-standard-deviation check was conducted by calculating the mean and standard deviation at each depth level; values falling beyond six standard deviations were flagged as outliers. (4) A gradient check assessed the vertical gradients of each parameter at each depth level across stations; data showing abnormal gradients exceeding five standard deviations from the mean were flagged as questionable. (5) A depth/potential density (σ_θ) inversion check was applied to detect unrealistic reversals in parameters such as temperature and nutrients, which typically exhibit monotonic relationships with depth or σ_θ in stratified waters; measurements violating preset thresholds for depth–temperature, depth–NO_x^-, depth–DIP, depth–$Si(OH)_4$, σ_θ–temperature, σ_θ–NO_x^-, σ_θ–DIP, and σ_θ–$Si(OH)_4$ were flagged. (6) A spike check was implemented to identify abrupt deviations (spikes) between a measurement and its adjacent vertical neighbors; if the difference exceeded a defined threshold, the data point was flagged as suspect. This check was applied to temperature, NO_x^-, DIP, and $Si(OH)_4$. (7) Only measurements with an original quality flag of 'good' from CCHDO and WOD were retained, while those marked as questionable or erroneous were flagged as outliers.

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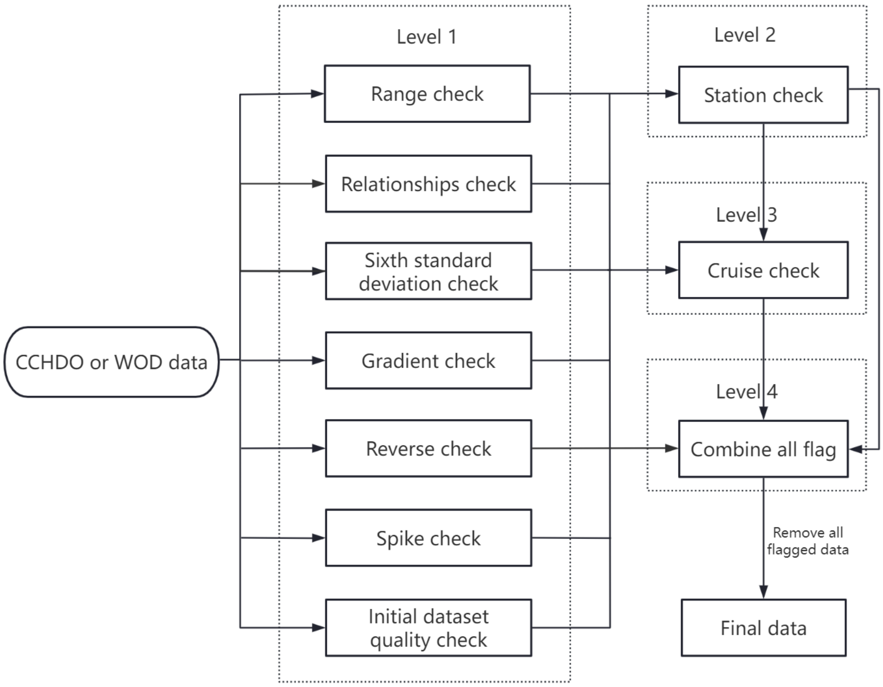

Figure 1. Data quality control procedures for temperature, salinity and nutrients collected from the CLIVAR and Carbon Hydrographic Data Office (CCHDO) and the World Ocean Database (WOD) datasets.

Building on the individual-level QC, we implemented additional QC at the station and cruise levels. At the station level, if a station profile contained more than 20% flagged data points, all data from that station were flagged as questionable. At the cruise level, if over 30% of a cruise's data were flagged, all data from that cruise were flagged. The final step integrated flags from all three levels (individual, station, and cruise), and any data flagged at any level were excluded. This hierarchical QC protocol effectively eliminates low-quality data. Although this approach may discard some high-quality measurements, the large volume of available data necessitates strict QC to ensure reliability.

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After quality control, the CCHDO dataset retained 214,943 (9,120), 197,539 (8,228), 222,234 (9,457) and 210,447 (8,123) data points (stations), accounting for 94.2% (95.1%), 100.0% (99.9%), 98.6% (98.5%) and 99.0% (98.8%) of the original data points (stations) for NO_x^-, NO_2^-, DIP, and $Si(OH)_4$, respectively (Table 1). The retained stations cover nearly the entire North Pacific Ocean (Fig. 2a). The retained data spanned from 1972 to 2023. Most observations were collected after 1980, with a substantial increase after 1990 (Fig. 2b). Seasonally, the number of stations in June, July, and August was approximately three times greater than that in March and December (Fig. 2c).

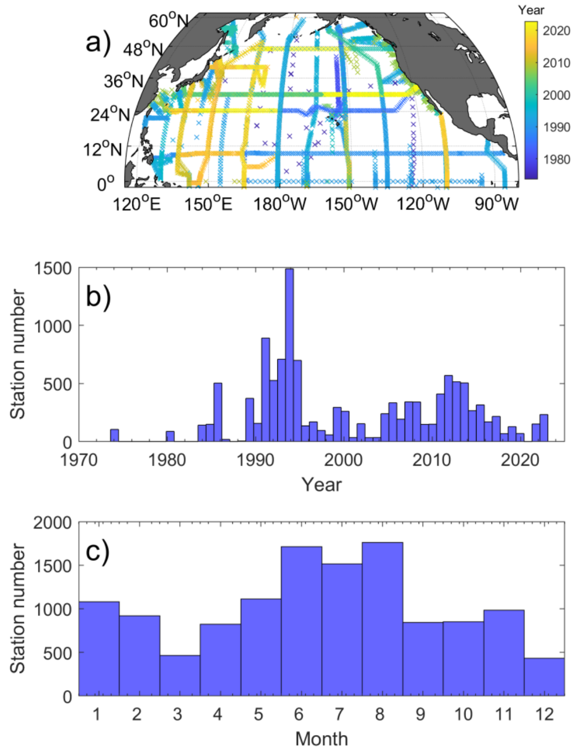

Figure 2. Spatial and temporal distributions of NO_x^- (nitrate plus nitrite) after quality control in the North Pacific. a) Distribution of NO_x^- data locations, with points color-coded by year; b) station counts per year; c) station counts per month.

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Following quality control, the final WOD dataset comprised 472,652,680 temperature and salinity data points from 1,920,634 stations across 35,744 cruises, spanning 1895 to 2024. These represent 81.9% of the original observations, 84.1% of the original stations, and 89.1% of the original cruises, respectively (Table 2). Spatially, station counts per 1°×1° grid cell range from 1 to 31,851, with a mean of 249 stations per cell (Fig. 3a). High sampling densities are found off eastern Japan and western North America, resulting from high frequency observations from CTD and OSD platforms, whereas elevated counts in the southwestern North Pacific primarily result from MRB observations. Temporally, fewer than 300 stations per year were collected before 1930. The annual number of stations exceeds 10,000 after 1964 and peaked at approximately 100,000 in 2021 (Fig. 3b). Seasonally, station numbers are highest from May to August (Fig. 3c). Overall, the collected WOD dataset provides 2127–2393 times more observations and 202 times more station records than the CCHDO dataset.

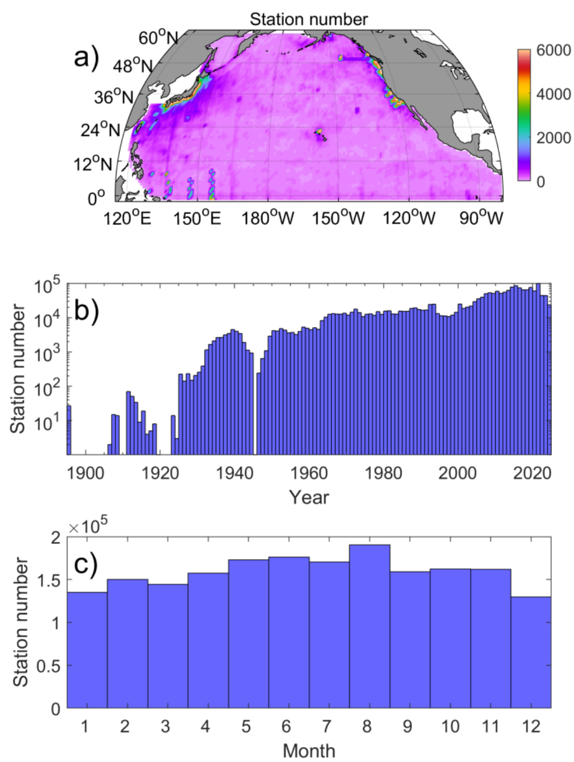

Figure 3. Spatial and temporal distribution of the World Ocean Database (WOD) data after quality control. a) Station counts per 1°×1° grid cell; b) station counts per year; c) station counts per month.

2.3 Machine learning and nutrient reconstruction

After rigorous data quality control, CCHDO data were used to train machine learning models. Three algorithms including Random Forest (RF), Light Gradient Boosting Machine (LightGBM), and Gaussian Process Regression (GPR) were applied to establish the relationship between environmental parameters and nutrient concentrations. These methods are widely used in marine science (Hu et al., 2021; Huang et al., 2022; Yu et al., 2022; Chen et al., 2023; Sundararaman and Shanmugam, 2024). The use of diverse models helps decrease algorithm selection bias. RF is an ensemble technique based on bagging, which builds multiple independent decision trees and aggregates their outputs by voting or averaging (Liaw and Wiener, 2002). Its strengths include high predictive accuracy and reduced overfitting owing to the large number of trees. RF has been applied to predict global primary production (Huang et al., 2021), chlorophyll concentrations (Madani et al., 2024), nutrients (Chen et al., 2023; Chen et al., 2024), dissolved iron (Huang et al., 2022), surface ocean $p\mathrm{CO_2}$ (Chen et al., 2019), and N_2 fixation rates (Yu et al., 2024).

LightGBM is an ensemble learning algorithm based on Gradient Boosting Decision Trees (GBDT). Compared to standard GBDT, LightGBM employs a leaf-wise tree growth strategy and a histogram-based binning technique to improve predictive accuracy and computational efficiency (Ke et al., 2017). It has been successfully applied to predict water levels (Gan et al., 2021), salinity (Dong et al., 2022; Wang et al., 2022), and chlorophyll *a* concentration (Su et al., 2021). GPR is a non-parametric Bayesian approach that infers relationships by defining a prior distribution over functions via kernel-based covariance matrices, rather than estimating fixed coefficients. This flexibility allows GPR to capture complex, nonlinear input–output relationships and to quantify prediction uncertainty. GPR has been used in

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oceanography to estimate global dissolved oxygen and nutrient concentrations (Sundararaman and Shanmugam, 2024).

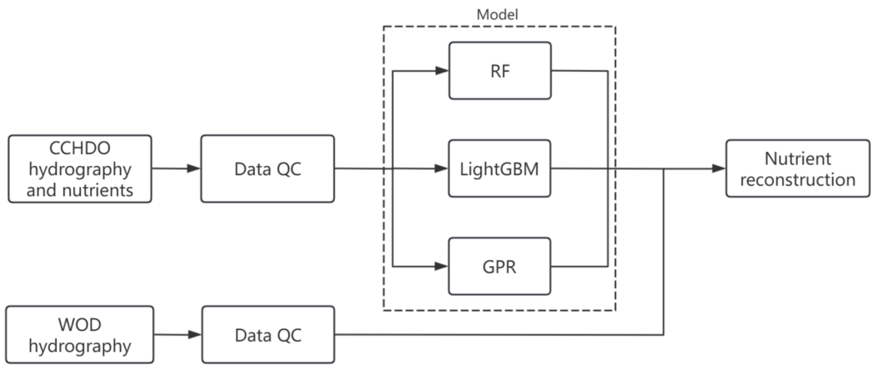

Figure 4. Flowchart of the machine learning framework and its application to WOD hydrographic data for nutrient reconstruction.

In this study, we used spatial coordinates (longitude, latitude, depth), temporal variables (month and year), and water mass properties (represented by potential temperature and salinity) as environmental predictors of nutrient concentrations. The time predictors used month and year with decimals to capture seasonal, interannual, and long-term variability. The North Pacific contains distinct water masses, including North Pacific Subtropical Water, North Pacific Intermediate Water, Antarctic Intermediate Water, Western South Pacific Central Water, North Pacific Deep Water, and Pacific Deep Water, as well as Circumpolar Deep Water (e.g., Talley et al., 2011; Fuhr et al., 2021). These water masses mix to form different water types associated with distinct nutrient concentrations (Fig. 5). Water types have been found to be an important parameter to reconstruct nutrient concentrations in the South China Sea (Du et al., 2021). Thus, potential temperature and salinity serve as proxies for water mass identification.

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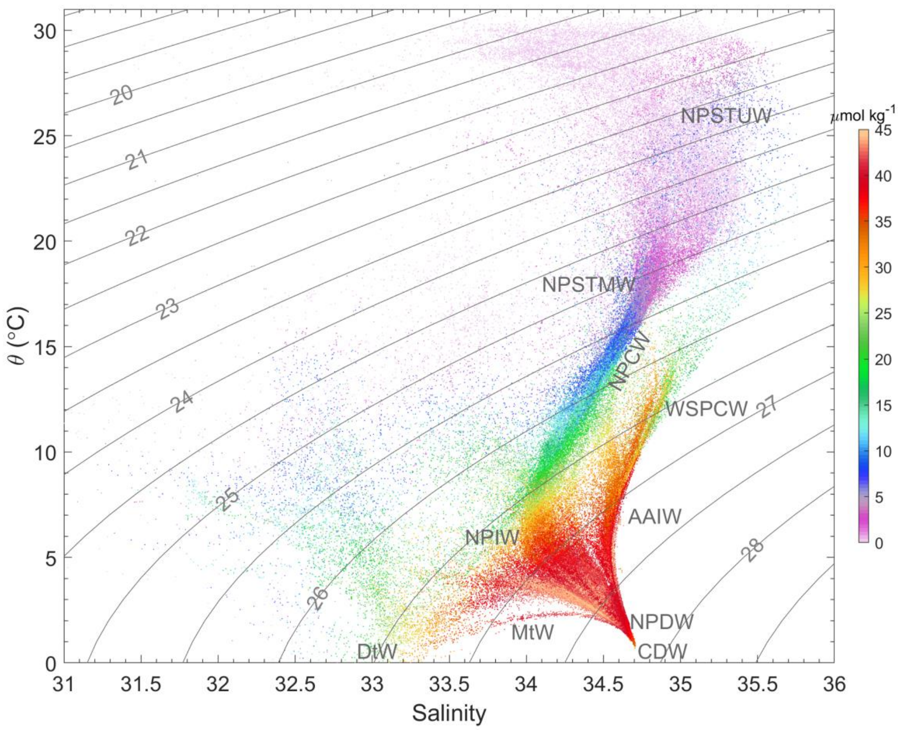

Figure 5. The water masses (indicated by salinity and potential temperature (θ)) and NO_x^- ($NO_3^- + NO_2^-$; color shading) relationships in the North Pacific. The temperature and salinity data were collected from the CCHDO dataset. The gray contour lines and number denote the potential density anomaly. The typical water masses are shown as follows: North Pacific Central Water (NPCW), North Pacific Subtropical Underwater (NPSTUW), North Pacific Subtropical Mode Water (NPSTMW), North Pacific Intermediate Water (NPIW), Dichothermal Water (DtW), Mesothermal Water (MtW), Antarctic Intermediate Water (AAIW), Western South Pacific Central Water (WSPCW), Pacific Deep Water (PDW), and Circumpolar Deep Water (CDW). The water masses and their acronyms are follow the classifications in Talley et al. (2011) and Fuhr et al. (2021).

3 Results

3.1 Error estimation

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Leave-one-out cross-validation was used to quantify model reconstruction errors. The CCHDO dataset was divided into training and testing subsets for model development and performance evaluation, respectively. To assess how data partitioning affects error metrics, we implemented four validation methods based on different data-selection strategies (Fig. 6a). The first three methods involved partitioning the CCHDO dataset into training (80%) and testing (20%) subsets. These methods employed three data selection strategies: (1) sample-random, by withholding 20% of individual samples; (2) station-random, by withholding 20% of stations; and (3) cruise-random, by withholding 20% of cruises. Predictions for the held-out subsets, generated using their respective spatial, temporal, and water mass property data, were compared against the actual withheld nutrient measurements to calculate error metrics. These partitioning strategies were designed to evaluate potential errors under the sparse and non-uniform spatiotemporal distribution of observations: Error 1 represented an optimistic estimate (validation data are likely colocated with training data in space and time), Error 3 represented a conservative, generalized scenario (validation data are independent of training data), Error 2 provided an intermediate estimate (validation data may share spatial/temporal context with training data within the same cruise). The choice of error metric (Error 1, 2, or 3) should be guided by the degree of extrapolation in the intended application relative to the training data's spatiotemporal distribution.

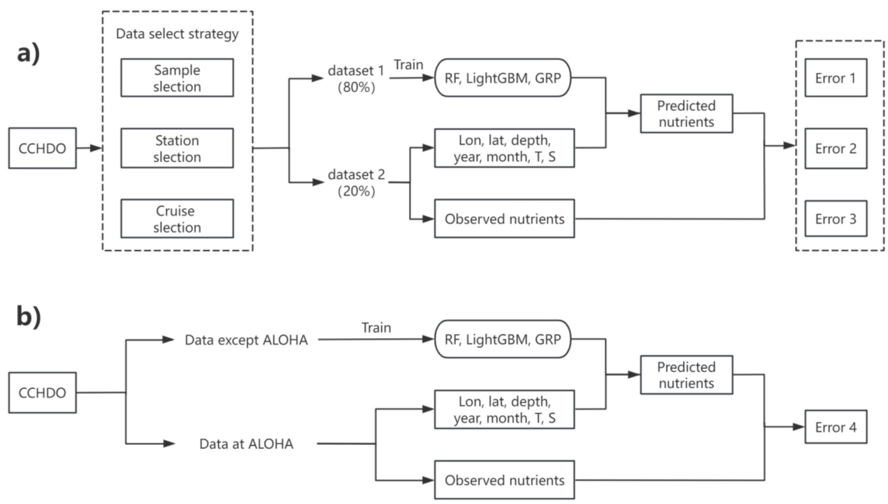

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Figure 6. Schematic of the error estimation procedure. a) Error estimation based on three types of data selection strategy; b) assessing temporal error evolution by excluding the data at Station ALOHA.

The validation results for reconstructed NO_x^- versus observations under the first three data-selection strategies are shown in Fig. 7. RF and GPR exhibited nearly identical performance, with regression slopes of 0.992–0.998, R^2 >0.992, and Root Mean Squared Errors (RMSE) between 0.734 and 1.313 μmol kg^{-1} (Fig. 7a, c, d, f, g, i). LightGBM showed slightly lower accuracy (slope: 0.991–0.995; R^2: 0.991–0.996; RMSE: 0.780–1.419 μmol kg^{-1}) (Fig. 7b, e, h). Across different data-selection strategies, sample-random (Error 1) yielded the lowest errors (RMSE: 0.734–0.983 μmol kg^{-1}) (Fig. 7a–c), station-random (Error 2) was intermediate (RMSE: 0.908–1.313 μmol kg^{-1}) (Fig. 7d–f), and cruise-random (Error 3) produced the highest errors (RMSE: 1.243–1.424 μmol kg^{-1}) (Fig. 7; Table 3). This gradient in error estimates underscores the necessity of employing different data-selection strategies for a comprehensive error assessment. The high slopes and R^2 values (>0.99) achieved across all algorithms and data-selection strategies confirmed the robustness of the nutrient reconstructions.

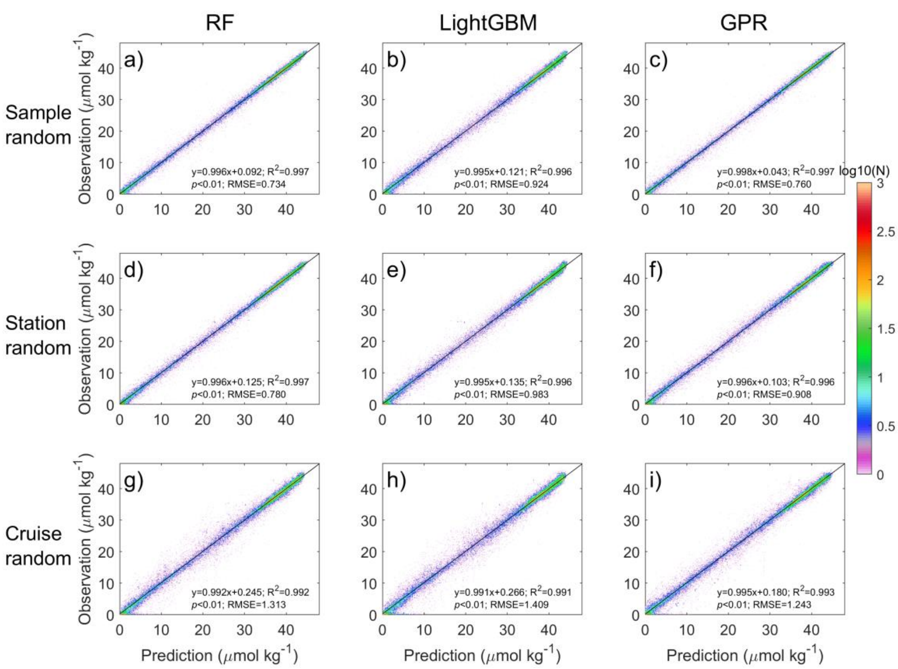

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Figure 7. Validating the reconstructed NO_x^- concentrations using leave-one-out cross-validation with different data selection strategies and machine learning methods. Plots shown in row 1 correspond to the sample random strategy (a-c), row 2 correspond to the station random strategy (d-e), and row 3 correspond to the cruise random strategy (g-i). Plots shown in column 1 correspond to the Random Forest (RF; a, d, and g), column 2 correspond to the LightGBM (b, e, and h), and column 3 correspond to the Gaussian Process Regression (GPR; c, f, and i). The black lines and text show the fitted linear regressions, regression equations, coefficient of determination (R^2), p values, and Root Mean Squared Errors (RMSE). The color represents the data density (N, number of observations). Note that the logarithmic scale of N is applied.

Reconstruction errors for NO_2^-, DIP, and $Si(OH)_4$ are summarized in Figs. S1–S3 and Table 3. Across methods, RMSE values were below 0.079 μmol kg^{-1} for NO_2^-, 0.089 μmol kg^{-1} for DIP, and 3.07 μmol kg^{-1} for $Si(OH)_4$. DIP and $Si(OH)_4$ exhibited similar error trends: RMSE increased from sample-random to station-random to cruise-random selection. In contrast, NO_2^- reconstruction exhibited lower accuracy than NO_x^-, DIP, and $Si(OH)_4$, with regression slopes of 0.48–0.68 and R^2 values of 0.32–0.72. RF and LightGBM outperform GPR for NO_2^-. The poorer NO_2^- performance likely reflects its generally low concentrations (mostly <0.5 μmol kg^{-1}) and high biological variability.

Table 3 The Root Mean Squared Errors of nutrient reconstruction from different error evaluation strategies (unit: μmol kg^{-1}).

Data selection strategy	NO_x^-			NO_2^-			DIP			$Si(OH)_4$		
	RF	LightGBM	GPR	RF	LightGBM	GPR	RF	LightGBM	GPR	RF	LightGBM	GPR
Sample random	0.724	0.924	0.760	0.049	0.054	0.079	0.056	0.070	0.055	1.90	2.30	1.53
Station random	0.780	0.983	0.908	0.065	0.068	0.072	0.058	0.071	0.065	2.07	2.45	2.20
Cruise random	1.313	1.409	1.243	0.054	0.057	0.071	0.080	0.089	0.084	2.79	3.07	2.94
ALOHA validation	0.701	0.842	0.674	—	—	—	0.066	0.079	0.064	2.13	2.48	2.32

A fourth validation step assessed the model's temporal performance at Station ALOHA. To test this, we withheld all observations from ALOHA (which, since 1988,

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represent 8.52%, 8.45%, and 8.11% of the total $Si(OH)_4$, NO_x^-, and DIP records, respectively) from model training. We then reconstructed nutrient concentrations using space, time, and water-type predictors at Station ALOHA. NO_2^- was excluded due to insufficient observations. For NO_x^-, the regression slopes between reconstruction and observations were 0.99, 0.98, and 0.99, with RMSEs of 0.701, 0.842, and 0.674 µmol kg^{-1} for RF, LightGBM, and GPR, respectively; R^2 values exceeded 0.997 for all models (Fig. 8a). RF and GPR slightly outperformed LightGBM. All models accurately reproduced the NO_x^- profiles (Fig. 8b). The reconstruction errors for DIP were 0.066, 0.079, and 0.064 µmol kg^{-1} for RF, LightGBM, and GPR, respectively. The corresponding errors for $Si(OH)_4$ were 2.13, 2.48, and 2.32 µmol kg^{-1} (Table 3, Figs. S4–S6).

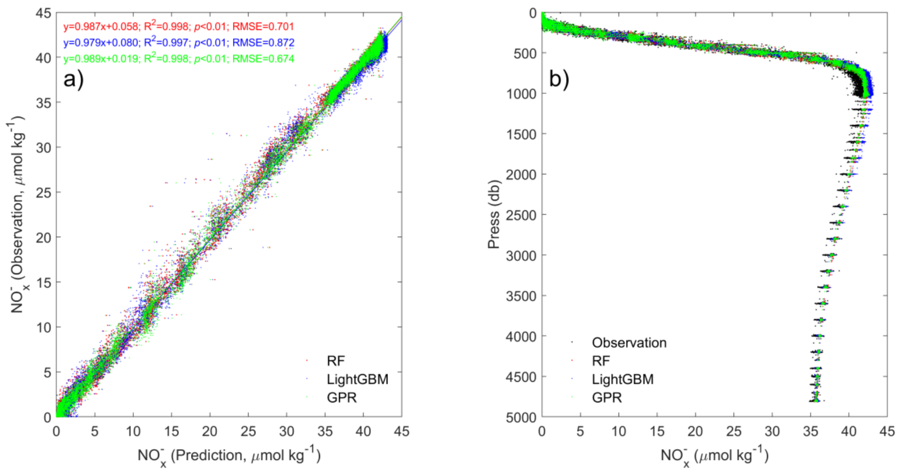

Figure 8. Validating the reconstructed nutrient concentrations at Station ALOHA. a) Reconstructed NO_3^- + NO_2^- (NO_x^-) vs. observations: Random Forest (RF; red dots), LightGBM (blue dots), and Gaussian Process Regression (GPR; green dots). b) Profiles of observed (black dots) and reconstructed NO_x^- from RF (red dots), LightGBM (blue dots), and GPR (green dots).

Since the variations of nutrients primarily occur in the upper water column, we focused on the nutrient reconstruction in the upper 300 m at Station ALOHA. Overall, the models reproduced the profiles of NO_x^- from 1988 to 2021 well (Fig. 9a-d). To evaluate models' ability to reconstruct nutrient variations in time, the nutrient concentrations were averaged monthly over the upper 300 m. As compared to

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observations, RF, LightGBM, and GPR all well reconstructed the interannual variations of NO_x^-, DIP and $Si(OH)_4$ at Station ALOHA (Figs. 9e, S6, and S7).

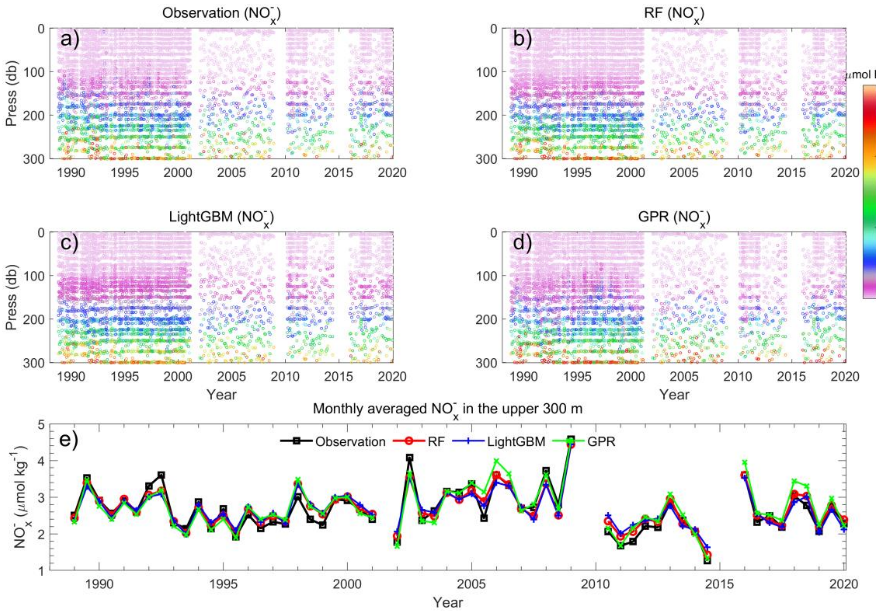

Figure 9. Temporal variations of NO_x^- concentrations in the upper 300 m at Station ALOHA from 1988 to 2021 for observed (a) and reconstructed NO_x^- by Random Forest (RF; b), LightGBM (c), and Gaussian Process Regression (GPR; d). (e) Time series of monthly averaged NO_x^- concentrations in the upper 300 m from observations, and reconstructions by RF, LightGBM, and GPR.

3.2 Reconstructed nutrients and their distributions

The final reconstructed nutrient dataset aligns with the spatiotemporal coverage of the quality-controlled WOD hydrographic dataset, comprising 472,652,680 data points for each nutrient (NO_x^-, NO_2^-, DIP, and $Si(OH)_4$) from 1,920,634 stations across 35,744 cruises, spanning from 1895 to 2024 (Table 2). Most data points are located above 2,000 m, with fewer observations at greater depths due to observational platform limitations. Since the distribution patterns of NO_x^-, DIP, and $Si(OH)_4$ are consistent across the different methods (Figs. 10–13, S8–S16), we focus on the reconstructed NO_x^- from RF model in this section unless stated otherwise.

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Figs. 10–13 present the monthly climatology of NO_x^- at 5 m, 100 m, 500 m, and 1,000 m in the North Pacific. At 5 m, the reconstructed NO_x^- accurately captures the established spatial patterns, with elevated concentrations in the subpolar gyre, Bering Sea, and equatorial regions, and depleted concentrations in the North Pacific Subtropical Gyre (NPSG). Seasonally, the basin-averaged surface NO_x^- concentrations display the highest value of 3.50 μmol kg^{-1} in March, in contrast to the lowest value of 1.82 μmol kg^{-1} in September. These results agree with Yasunaka et al. (2014, 2021), who, using extensive surface nutrient observations (up to 14,000 for nitrate) in the North Pacific, reported similar spatial and seasonal patterns.

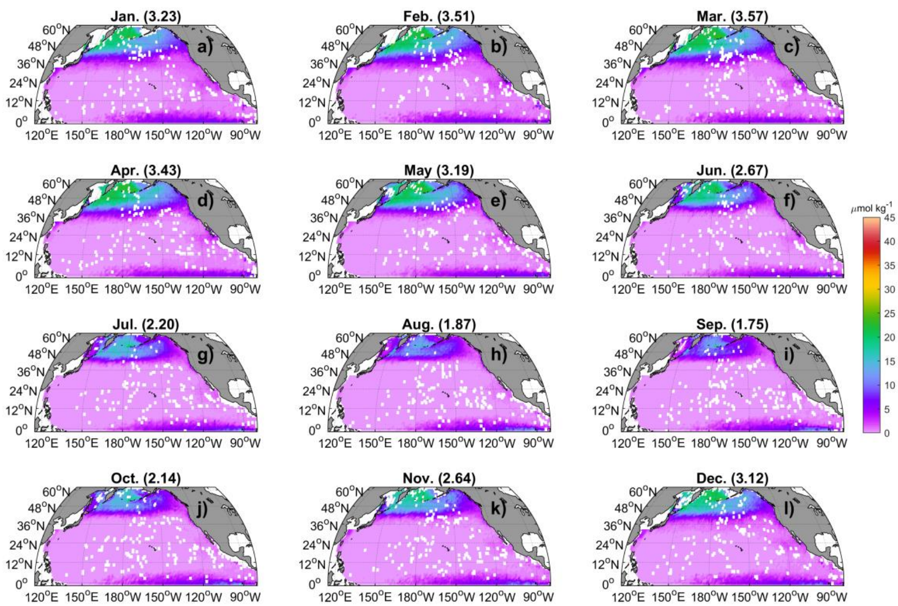

Figure 10. The monthly climatology of NO_x^- at 5 m in the North Pacific. Data are binned and averaged within 1×1° grid cells. The values in the title represent the spatial mean values.

At 100 m, NO_x^- concentrations are elevated particularly in the subarctic gyre, north of the Equator, and the eastern North Pacific, while the central regions, particularly the NPSG, exhibit lower values. At 500 m, NO_x^- concentrations display patterns similar to those at 100 m, except that the NO_x^- concentrations in the western NPSG are evidently

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lower than those in other regions (Fig. 13). At 1000 m, concentrations in the southwestern North Pacific Ocean are markedly lower than those in other regions (Fig. 12). Below 100 m depth, seasonal variability in NO_x^- is minimal (Figs. 11–13). Compared to the World Ocean Atlas (WOA23) climatology (Figs. S17–S25), although the seasonal patterns are similar in the surface layer, the reconstructed NO_x^- concentrations are lower than those in WOA23. In addition, our reconstructions capture finer spatial detail, exhibit less oversmoothing, and avoid artificial "bull's-eye" patterns. It should be noted that our climatology is derived from the mean of existing data, which heavily relies on the spatiotemporal distribution of those data and may not represent the true climatological mean.

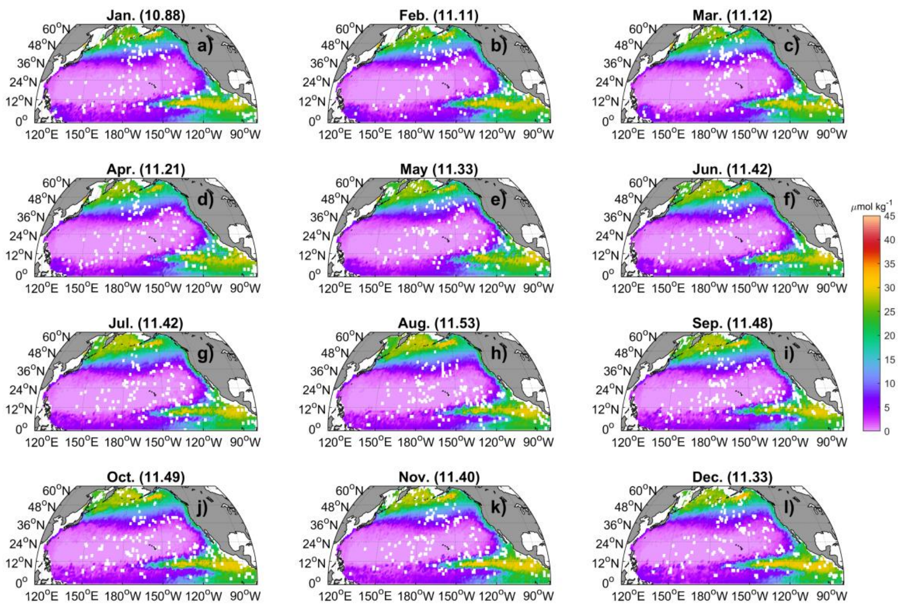

Figure 11. The monthly climatology of NO_x^- at 100 m in the North Pacific. Data are binned and averaged within 1×1° grid cells. The values in the title represent the spatial mean values.

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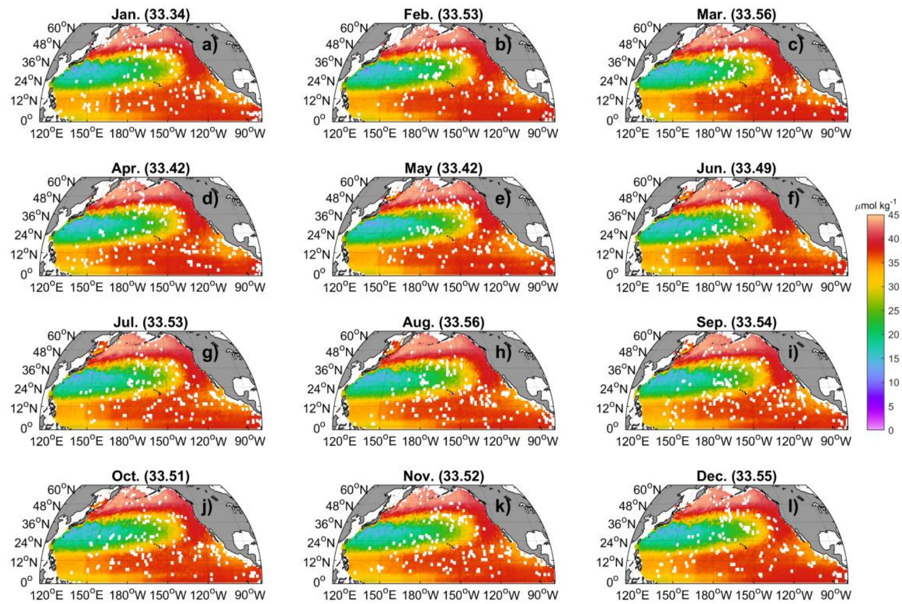

Figure 12. The monthly climatology of NO_x^- at 500 m in the North Pacific. Data are binned and averaged within 1×1° grid cells. The values in the title represent the spatial mean values.

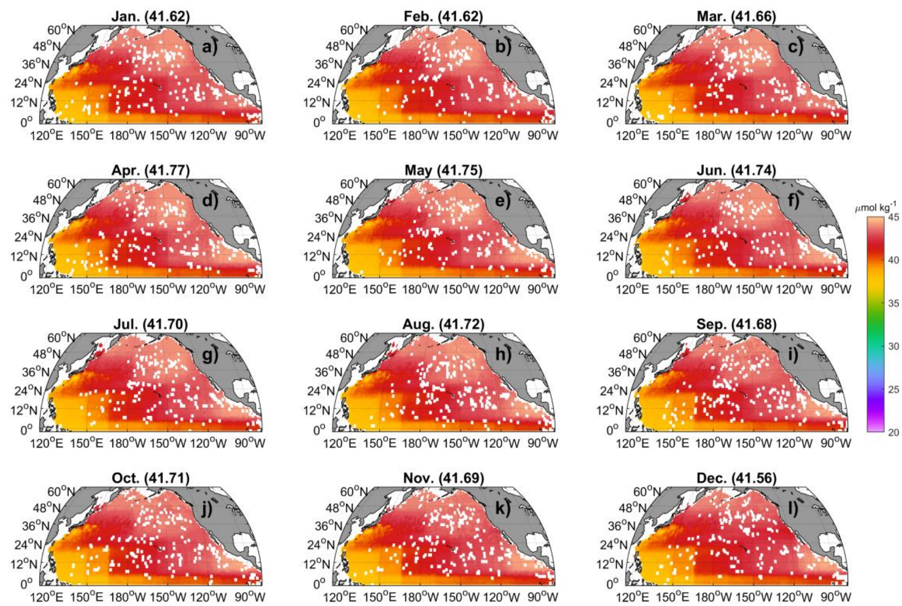

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Figure 13. The monthly climatology of NO_x^- at 1000 m in the North Pacific. Data are binned and averaged within 1×1º grid cells. The values in the title represent the spatial mean values.

Sectional distributions of NO_x^- in the upper 2000 m along 10° N and 180° E were used as examples to illustrate the vertical profile distributions of nutrients within the North Pacific. At 10° N, NO_x^- concentrations increase from ~0.0 µmol kg^{-1} at the surface to ~45.0 µmol kg^{-1} at ~1000 m, followed by a decrease to ~38.0 µmol kg^{-1} at 2000 m. NO_x^- concentrations increase from west to the east in the North Pacific in the upper 300 m (Fig. 14). At 180° E, in the upper 500 m, meridional NO_x^- concentrations increase from the equator to the North Equatorial Current (~10° N), decline within the subtropical gyre, and then increase toward the subarctic region (Fig. 15). Generally, seasonal differences of NO_x^- concentrations along both sections are not evident.

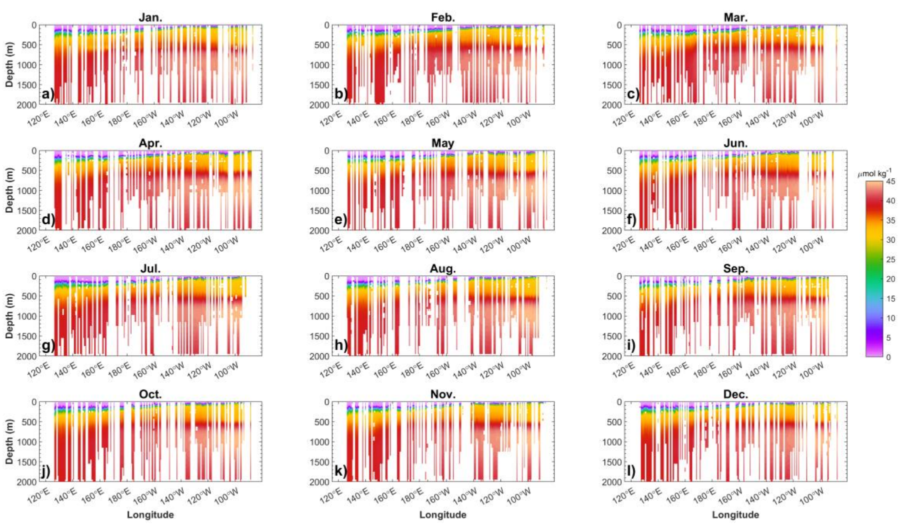

Figure 14. Zonal and monthly climatology of NO_x^- in the upper 2000 m at 10 ºN in the North Pacific. Data were binned and averaged within 1°×1° grid cells.

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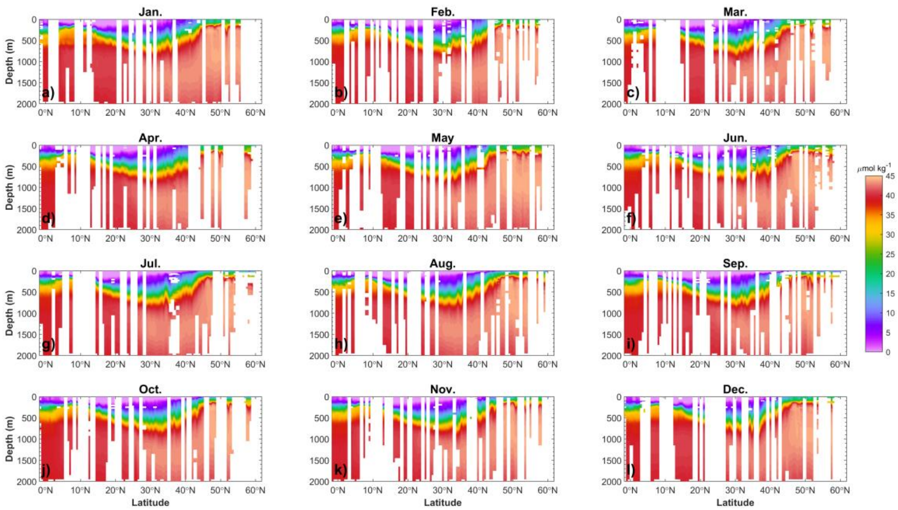

Figure 15. The monthly climatology of NO_x^- in the upper 2000 m at 170 ºE section in the North Pacific. Data were binned and averaged within 1°×1° grid cells.

4 Data availability

The database is available in a data repository (Du et al., 2025; https://zenodo.org/records/17140658). Although the reconstruction results from RF, LightGBM, and GPR are generally consistent, RF yields the best performance. To avoid redundancy and minimize storage requirements—given the large volume of the data files—only the nutrient data reconstructed by RF have been uploaded. Researchers may contact the corresponding authors to request the reconstructions generated by LightGBM and GPR.

5 Conclusion

In this study, we applied rigorous quality control procedures to clean hydrographic and nutrient observations from CCHDO and WOD datasets. The cleaned CCHDO data were then used to train three machine-learning models to relate nutrient concentrations to spatial, temporal, and water-mass predictors. The models were applied to reconstruct nutrient concentrations from hydrographic observations collected from WOD, though most of which lack direct nutrient measurements. We assessed the model performance using four data-partition strategies, and found that all models reproduced held-out data with low RMSE values. RF and GPR slightly outperformed LightGBM. The application of these models to WOD hydrography yielded 472,652,680 reconstructed nutrient concentrations across 1,920,634 stations and 35,744 cruises, spanning from 1895 to 2024. This represents a 2,127– to 2,393-fold increase compared to the original volume of CCHDO nutrient data. The reconstruction captured the spatial, seasonal, and interannual variations of water column nutrients in the North Pacific Ocean well. Compared to the WOA23 climatology, the reconstruction-based nutrient climatology exhibited more realistic spatial structures than WOA23. This high-quality nutrient dataset enables historical nutrient estimation for locations and times with only hydrographic measurements. It also supports studies of climatological and long-term nutrient variability under climate change and anthropogenic impacts, and provides transient boundary conditions for ocean biogeochemical models in the Pacific Ocean.

Author contributions

CD and XL designed the study and dataset. CD, SK, MD, ZC, DS, and XL conceived the project and secured the funding. CD, NZ, QL, and HW collected and processed the data, developed the code, and performed the analysis. SK, MD, ZC, and DS provided methodological guidance and advice. CD and NZ wrote the original draft. All authors reviewed, edited the manuscript.

Competing interests

The contact author has declared that none of the authors has any competing interests.

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Declaration of generative AI and AI-assisted technologies in the writing process: During the preparation of this work the authors used deepseek to check the spelling and grammar. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the publication.

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