Team: Wunderpus Octopus

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> Modeling the relationship between biogeochemical layers and chlorophyll density





Modeling the relationship between biogeochemical layers and chlorophyll density

Select Ocean Regions:

Shallow regions are significant due to their enhanced light availability, nutrient recycling, and diverse ecosystems, supporting higher primary productivity and biodiversity.

We selected region of interest:

• North Sea

Select time frame : Sep 1997 - Dec 2021

Research questions

- What are the primary biogeochemical and physical factors influencing chlorophyll density in various shallow sea regions?
- How can these factors be quantitatively integrated into a robust predictive model for chlorophyll density?





Combining observation data with simulated data

Copernicus Marine Datasets included

- Dataset 1: Global Ocean Color (satellite observations)
 - Chlorophyll
- Dataset 2: Global Ocean Biochemistry (simulated)
 - 02; NO3; PO4; Si; Fe
- Dataset 3: Global Ocean OSTIA (using in-situ & satellite data)
 - Sea Surface Temperature
- Dataset 4: Multi Observation Global Ocean (using in-situ & satellite data)
 - Sea Surface Salinity and Sea Surface Density
- Dataset 5: Global Ocean Surface Carbon (From model based on in-situ data)
 - Dissolved inorganic carbon; Total alkalinity; Surface partial pressure of CO2 Sea water pH; Calcite saturation state; Aragonite saturation state; Surface downward flux of CO2



XGBoost Modeling Approach

Extract data from **Copernicus Mariner** Datasets

Data Preprocessing

- Match resolution between datasets
- Keep chlorophyll values within 99 percentile

421801 data points and 19 features

Evaluation Metric for model comparison: Root Mean Square Error (RMSE) and Mean Absolute Percentage Error (MAPE) on the validation set

- Baseline model:
 - Chlorophyll prediction = average value of chlorophyll in the training set
- Regression models: XGBoost
 - Bayesian hyperparameter tuning to minimize 5-0 fold CV RMSE on training set



XGBoost Results

Keep only one of the features among corr > 0.8

Final feature set: ['latitude', 'longitude', 'year, 'month', 'fgco2', 'omega_ca', 'ph', 'fe', 'no3', 'si', 'o2', 'sos']

Model performance on validation set after hyperparameter optimization

Model	RMSE	MAPE
Baseline	1.03	1.08
XGBoost	0.32	0.17



SHAP-based feature importance using XGBoost model on the test set

ConvLSTM

- Goal: Incorporate both time and space into the neural network architecture
- Strategy: combine a CNN (which handles spatial data) and LSTM (for time)



Image and idea found in "A time series image prediction method combining a CNN and LSTM and its application in typhoon track" prediction"









ConvLSTM: Results

- Utilized a ConvLSTM model to capture spatial and temporal dependencies in the chlorophyll concentration data.
- The model was trained for 20 epochs using an Adam optimizer and mixed precision training to speed up the process.
- Evaluated the model using RMSE, which showed some discrepancies between predicted and actual values, particularly in high-concentration areas







CNN models

- In addition to normalizing training data to have zero mean and unit std, we also process the NaN values as follows:
 - Flatten each feature tensor, find and save the positions of NaNs and drop them out.
 - Train the model on the data without NaNs.
 - After prediction plug back the NaNs and get final plot.



Original tensor of 93 x 117 = 10881 is reduced to 83 x 116 = 9628.







CNN models

Loss/ Epoch plots for each model:



loss_fn = nn.MSELoss()

model_resnet_list = training.training_loop($n_{epochs} = n_{epochs}$, optimizer = optimizer, model = model_resnet, loss_fn = loss_fn, batchsize = batch, train_loader = train_loader, val_loader = val_loader



```
model_resnet = models.NetResDeep(n_chans1=32, ten_size= reduced_tensors.redten_size
                            , poolten_size=reduced_tensors.poolsize).to(device = device)
optimizer = optim.SGD(params=model_resnet.parameters(), lr=learning_rate)
```

• We have used ['fe','no3','o2','si','ph'] as features with 288 images (months) for training and 72 images for the validation set.

TS



Conclusions



Iron fertilization can enhance fishery ecosystem

RMSE		
0.32		
0.22		
0.89		

