Gap Filling of Surface Ocean pCO2, with Uncertainty

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DATA VISUALIZATION

Our project presents a new machine-learning-based method to estimate surface ocean pCO2 and evaluate the uncertainty of estimates. Given the fact that only small percentage (around 1.56%) of our observed data owns pCO2 value, we decide to make use of the simulated data (left) to help us train and test our model. The full-filled “Truth” could also help us evaluate our method performance. From the following two pictures, we could see the simulated data is a good representation of observed data.

Figure 1. Color plot of pCO2 from simulated and observed Dataset

KRIGING SYSTEM

The first conditional distribution of pCO2 given spatial data is estimated by nearby data points. This leverages the kriging mean and variance of simple kriging system using nearby observations to parametrize the conditional Gaussian distribution.

We use GeoStatTools package in Python to conduct the interpolation, which result becomes our estimated mean, and the errors become our variances, which will be used to parametrize the conditional Gaussian distribution.

Figure 2. True distributions and predicted distributions by kriging system.

GMM-EM ALGORITHM

The second conditional distribution of pCO2 given the colocated observed feature is estimated by taking the advantage of Expectation Maximization (EM) algorithm and Gaussian Mixture Model (GMM). To be specific, it is defined as the marginal of the conditional GMM given other features observed at same data location. Therefore, to obtain this conditional distribution, we first implemented GMM to get the soft clustering boundary for simulated data with GMM, then imputed the missing value of pCO2 conditioned on other observed features by using EM algorithm and clustering statistic generated from GMM.

Figure 3. A Demo: GMM-EM for filling missing values in a cluster

As shown in Figure 4, the data points which are closer to each other spatially are more likely to be assigned to the same cluster, even though the spatial information of data points is not used during the training of GMM. Therefore, the clustering result follows our initial assumption about data and GMM and is trustworthy for our cases.

Figure 4. GMM Clustering Result

Conclusions and Recommendations

The ultimate goal for our project is to predict oceanic pCO2 level for unknown regions and get statistical inference for our prediction. The final step is to apply the algorithms to the whole dataset and to evaluate their performance in different clusters.

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References