A machine learning approach to estimate surface $p$CO$_2$ from satellite measurements


**Background:**
Surface seawater partial pressure of CO$_2$ ($p$CO$_2$) is a critical parameter in the quantification of air-sea CO$_2$ flux, which plays an important role in quantifying the global carbon budget and understanding ocean acidification, yet no unified model exists to remotely estimate surface $p$CO$_2$ in complex regions.

**Methods:**
This study evaluates different approaches of $p$CO$_2$ measurement in the Gulf of Mexico (GOM), including multi-linear regression (MLR), multi-nonlinear regression (MNR), principle component regression (PCR), decision tree, supporting vector machines (SVMs), multilayer perceptron neural network (MPNN), and random forest based regression ensemble (RFRE). The machine learning model (RFRE) was then applied to the Gulf of Maine (G. Maine) using local model training.

**Results:**
- The RFRE model showed significant improvement over other models in the GOM as well as improved results in the G. Maine.
- Uncertainties in the estimated surface $p$CO$_2$ are within 10 μatm for a large range.

**Significance:**
The results suggest that the RFRE may serve as a robust approach for other regions once sufficient field-measured $p$CO$_2$ data are available for model training.

RFRE surface $p$CO$_2$ model performance in the Mississippi River delta and offshore regions, evaluated with independent underway $p$CO$_2$ data collected from cruise GU1703_Leg2 (Table 2). (a) MODIS surface $p$CO$_2$ composite map for the cruise period (Jul. 22–Aug. 05, 2017), with field-measured $p$CO$_2$ along the cruise track overlaid and color coded in the same way as the MODIS image; (b) Comparison between field-measured $p$CO$_2$ and contemporaneous ($\pm$ 24 h) MODIS-derived $p$CO$_2$; (c) Comparison between field-measured $p$CO$_2$ and MODIS-derived $p$CO$_2$ extracted from the MODIS composite map for the cruise period (a). The red dots with values of 0 on the X-axis in (b) and (c) indicate that there are no contemporaneous MODIS-derived $p$CO$_2$ due to various non-optimal satellite observing conditions, and 'P1' and 'P2' in each panel represent the start and end of the cruise, respectively. (For interpretation of the references to color and tables in this figure legend, the reader is referred to the web version of this article.)