Supplementary Materials

# Walk-forward cross-validation

Walk-forward cross-validation is a technique to evaluate time-series data. For this, the models are first trained with the 2017 dataset and then used to predict O3 for the first day of the 2018 dataset, which is May 1st, 2018. Then the May 1st, 2018 data is included in the training dataset, and the models are re-trained and used to predict O3 for May 2nd, 2018. This process is repeated for each successive day of the 2018 – 2020 ozone seasons (May to September).

When a new day’s MDA8 O3 is predicted by the ML models, the NMB is recomputed by including the new prediction. The temporal evolution of NMB in **Supplementary Figure 1** shows that the ML models and AIRPACT experience a large variation initially but then tend to somewhat converge. AIRPACT under-predicts the MDA8 O3, and the NMB of AIRPACT is decreasing in 2018. However, the model performance of AIRPACT is improved, and its NMB starts to increase after 2018. There is a jump of AIRPACT NMB in the late 2020, which is because of the large over-prediction of some days in September 2020. Both ML1 and ML2 over-predict the MDA8 O3, and the NMB of ML1 is higher than ML2. The variation of the NMB from ML models is smaller than AIRPACT, so their performance is more stable by year.

# Supplementary Figures and Tables

## Supplementary Figures



Supplementary Figure 1. Evolutions of the NMB from the walk-forward cross-validation. The black dashed lines mark each year.

## Supplementary Tables

Supplementary Table 1. Statistics and forecast verifications from the walk-forward cross-validations.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | | AIRPACT | AIRPACT (w/o 4 extreme values) | ML1 | ML2 |
| R2 | | 0.15 | 0.35 | 0.4 | 0.51 |
| NMB | | 1.9 | 0.36 | 7.8 | 4.5 |
| NME | | 15 | 13 | 16 | 12 |
| HSS | | 0.34 | 0.31 | 0.35 | 0.47 |
| KSS | | 0.30 | 0.30 | 0.65 | 0.45 |
| CSI | 1 | 0.87 | 0.85 | 0.71 | 0.89 |
| 2 | 0.24 | 0.23 | 0.28 | 0.34 |
| 3 | 0 | 0 | 0.22 | 0 |

Although the statistics in **Supplementary Table 1** cover three years (2018 – 2020), it generally agrees with the results of the 10-time, 10-fold cross-validation in **Table 4**, which covers four years (2017 – 2020).

# Data Availability Statement

The AQS observation data are available from US EPA[[1]](#footnote-1). The AIRPACT simulation data are available from Laboratory for Atmospheric Research, Washington State University[[2]](#footnote-2). We acknowledge the WRF database from University of Washington[[3]](#footnote-3).

# Code availability

The code discussed in this paper can be found at https://doi.org/10.5281/zenodo.4745320. The GitHub repository, where future updates will be uploaded can be found at https://github.com/kaifan88/ml\_kennewick.git.

1. https://aqs.epa.gov/ [↑](#footnote-ref-1)
2. http://lar.wsu.edu/R\_apps/ [↑](#footnote-ref-2)
3. https://a.atmos.washington.edu/mm5rt/ [↑](#footnote-ref-3)