



Supplement of

Estimation of ground-level NO_2 and its spatiotemporal variations in China using GEMS measurements and a nested machine learning model

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Figure S1: Spatial distributions of station-based correction factor between 8:00 AM and 3:00 PM (UTC+8) for 2021.



Figure S2: Spatial distributions of interpolated correction factor from individual hours between 8:00 AM and 3:00 PM (UTC+8) for 2021.



Figure S3: Spatial distributions of (a-d) station-based and (e-h) interpolated correction factors for estimating seasonal mean of NO₂ concentration for 2021.



Figure S4: Spatial distribution of (a) station-based and (b) interpolated correction factors for estimating annual mean NO₂ concentration for 2021.



Figure S5: Hour-by-hour 10-fold cross-validation of satellite-estimated ground-level NO₂ concentrations for basic Model I without considering the NMH. The red dotted line represents a 1:1 relationship. The solid black line is the line of best fit between the ground-measured NO₂ and the satellite-estimated NO₂. The scattered dots represent the individual NO₂ values for each ground measurement and satellite-based estimation. The color scale ranging from red to blue represents the density of the NO₂ values, with red indicating high density and blue representing low density.



Figure S6: Hour-by-hour 10-fold cross-validation of satellite-estimated ground-level NO₂ concentrations for nested Model II after considering the NMH. The red dotted line represents a 1:1 relationship. The solid black line is the line of best fit between the ground-measured NO₂ and the satellite-estimated NO₂. The scattered dots represent the individual NO₂ values for each ground measurement and satellite-based estimation. The color scale ranging from red to blue represents the density of the NO₂ values, with red indicating high density and blue representing low density.



Figure S7: 10-fold cross-validation for different population categories: lightly populated (LP, first column), moderately populated (MP, second column), highly populated (HP, third column), and supremely highly populated (SHP, last column). (a-d) for basic Model I without considering the NMH. (e-h) for nested Model II after considering the NMH. The red dotted line represents a 1:1 relationship. The solid black line is the line of best fit between the ground-measured NO₂ and the satellite-estimated NO₂. The scattered dots represent the individual NO₂ values for each ground measurement and satellite-based estimation. The color scale ranging from red to blue represents the density of the NO₂ values, with red indicating high density and blue representing low density.



Figure S8: Grid-based 10-fold cross-validation where ground-based observations are available. (a-b) for basic Model I without considering the NMH. (c-d) for nested Model II after considering NMH. Each circle on the map represents a grid point for which ground-based observations are available.