Supplementary material

APPENDIX A
ABBREVIATIONS

Table I shows the abbreviations used in this paper and their meaning. Dataset attribute abbreviations have not been included in this table.

TABLE I: Abbreviations.

Abbreviation	**Meaning**
ANN	Artificial Neural Network
ARIMA	Autoregressive Integrated Moving Average
BMOGW	Binary Multi-Objective Grey Wolf Optimizer
BMOGW-S	Binary Multi-Objective Grey Wolf Optimizer with Sigmoid function
BMOPSO	Binary Multi-Objective Particle Swarm Optimization
CART	Classification And Regression Trees
CC	Correlation Coefficient
CNN	Convolutional Neural Networks
DAL	Deep Air Learning
DeepPINK	Deep Feature Selection using Paired-Input Nonlinear Knockoffs
DNN	Deep Neural Networks
Dropout FR	Dropout Feature Ranking
EML	Extreme Machine Learning
FR	Feature Ranking
FS	Feature Selection
GRU	Gated Recurrent Unit
IBEA	Indicator-Based Evolutionary Algorithm
IGD	Inverted Generational Distance
LASSO	Least Absolute Shrinkage and Selection Operator
LfULG	State Office for Environment, Agriculture and Geology
LSM	Liquid State Machines
LSTM	Long Short Term Memory
MAE	Mean Absolute Error
MAPE	Mean Absolute Percentage Error
MDEFS	Multi-surrogate-assisted Dual-layer Ensemble Feature Selection
MLP	Multilayer Perceptron
MOEA	Multi-Objective Evolutionary Algorithm
MOEA/D	Multi-Objective Evolutionary Algorithm Based on Decomposition
MOPSO	Multi-Objective Particle Swarm Optimization
MSE	Mean Square Error
NAS	Neural Architecture Search
NN	Neural Network
NSGA-II	Nondominated Sorting Genetic Algorithm II
NSGA-III	Nondominated Sorting Genetic Algorithm III
$PM_{2.5}$	Particulate Matter with a diameter of less than 2.5 micrometers
RMSE	Root Mean Square Error
RNN	Recurrent Neural Networks
ROC	Receiver Operating Characteristic
SPEA2	Strength Pareto Evolutionary Algorithm 2
SVM	Support Vector Machine
WS	Window size

APPENDIX B
ARCHITECTURES

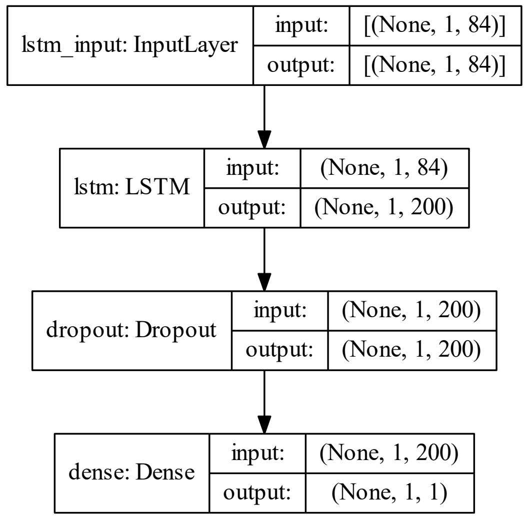


Fig. 1: Architecture of the LSTM neural network used as surrogate model in this paper.

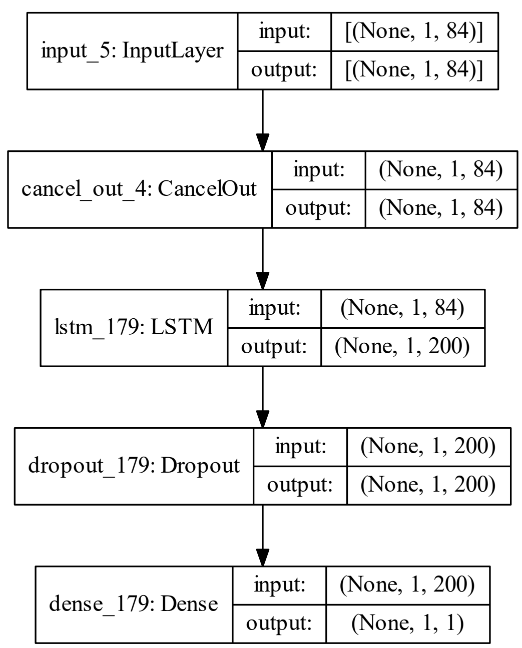


Fig. 2: Architecture of the LSTM neural network with a cancelOut layer.

APPENDIX C
HYPERVOLUME EVOLUTION

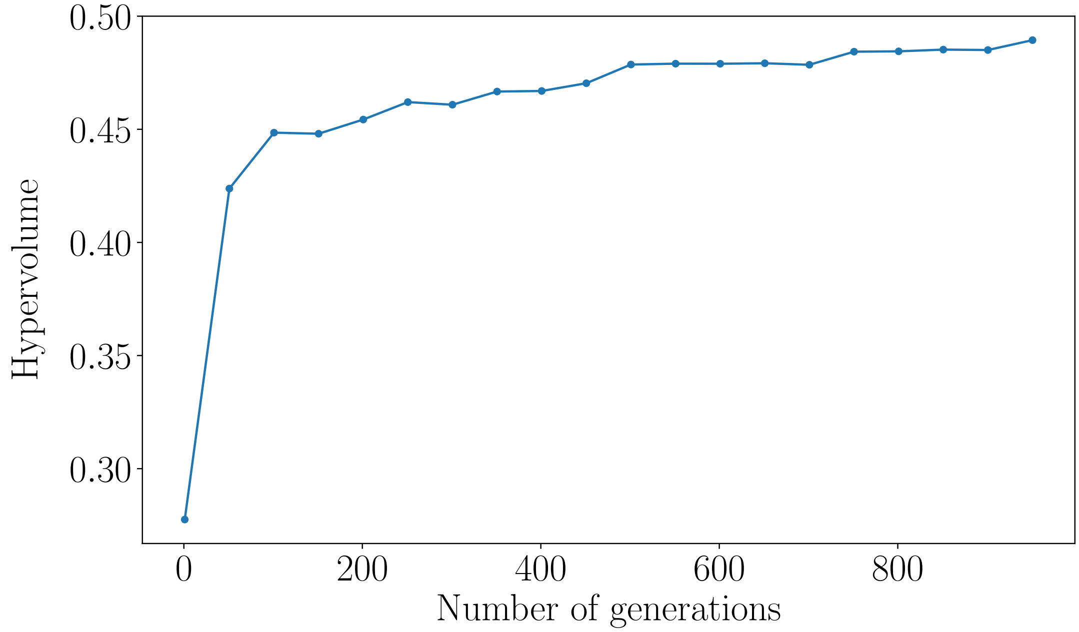


Fig. 3: Hypervolume evolution of *O1O2O3-NSGA-II*, best run, 100,000 evaluations.

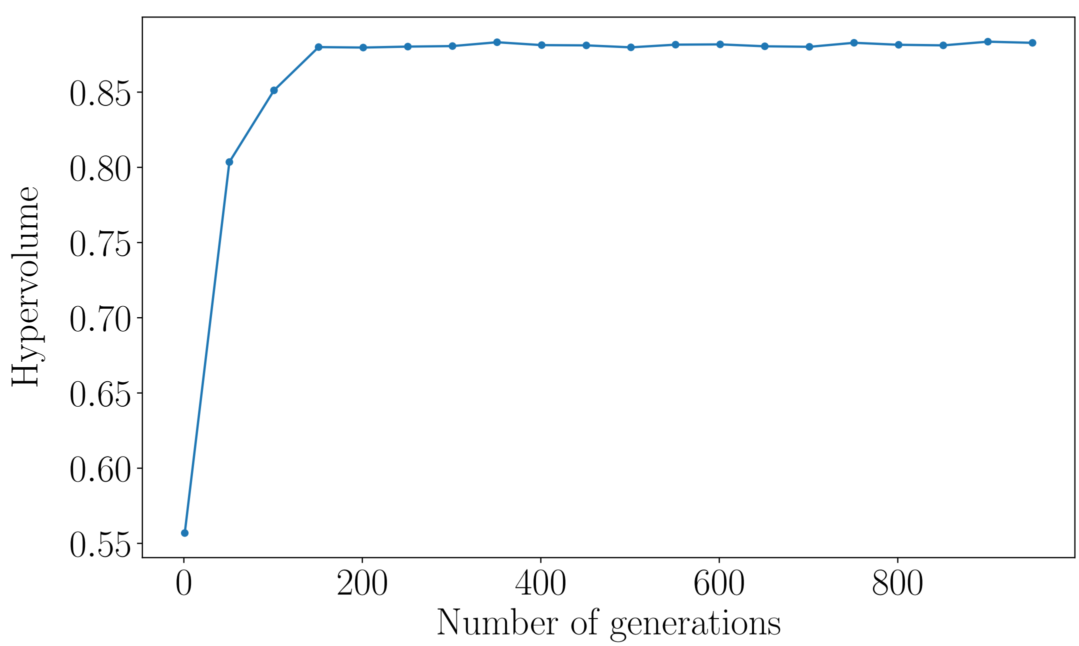
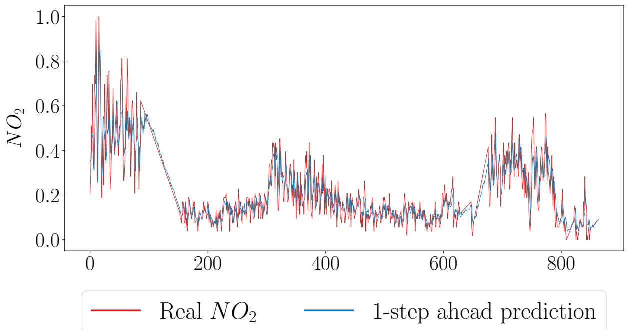
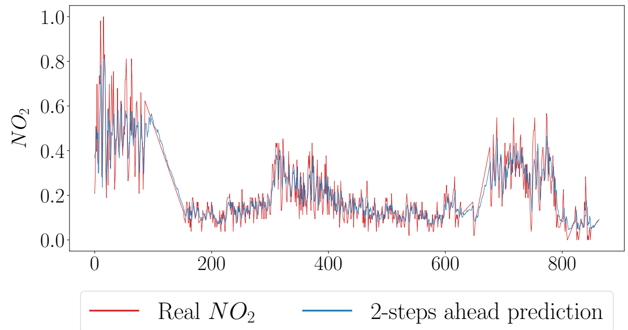


Fig. 4: Hypervolume evolution of *O1O2O3O4-NSGA-II*, best run, 100,000 evaluations.

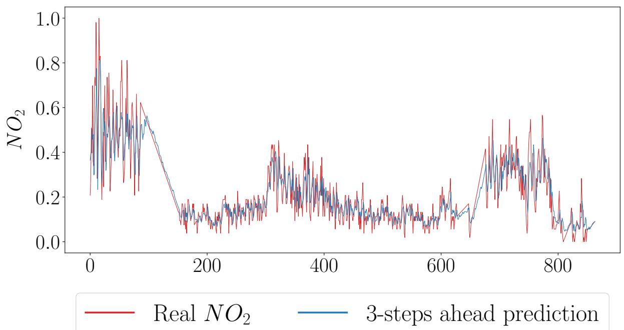
Appendix D
Graphic results of the best prediction models found in this research



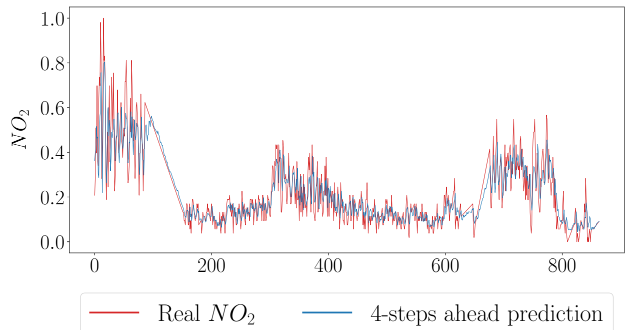
(a) 1-step ahead



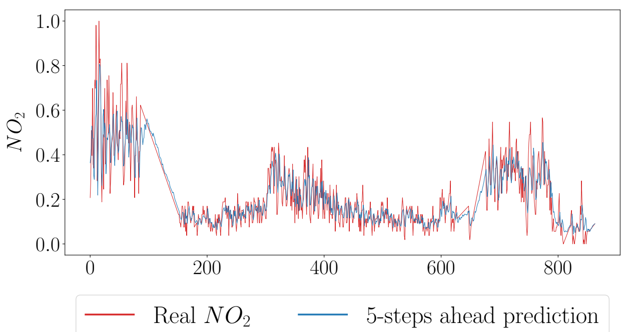
(b) 2-steps ahead



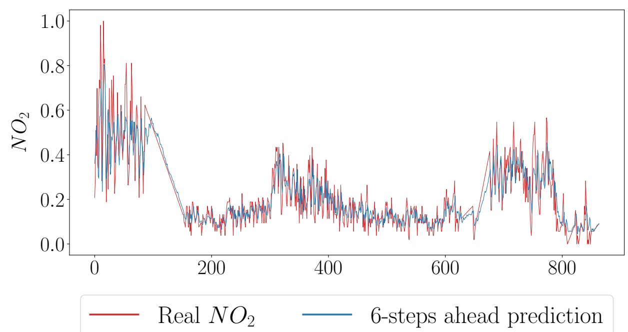
(c) 3-steps ahead



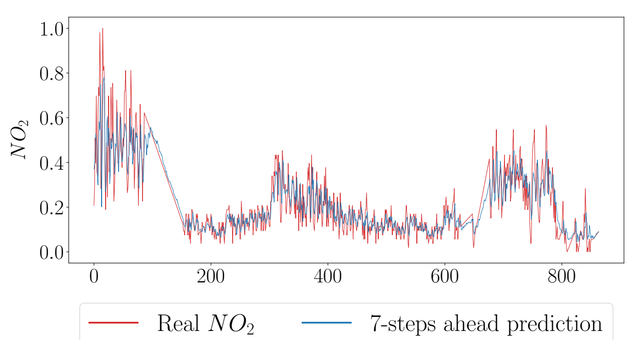
(d) 4-steps ahead



(e) 5-steps ahead

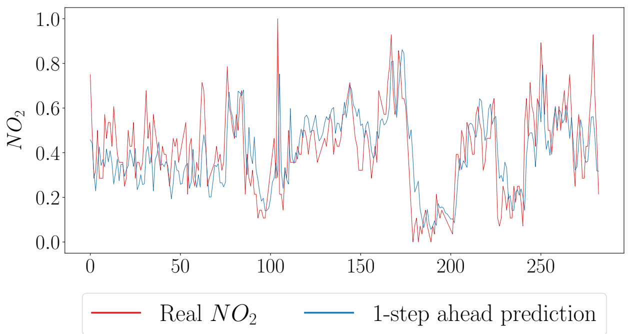


(f) 6-steps ahead

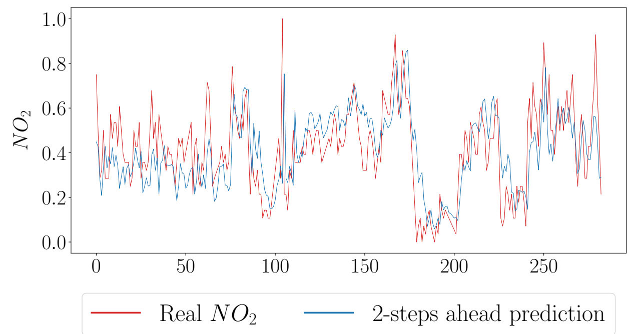


(g) 7-steps ahead

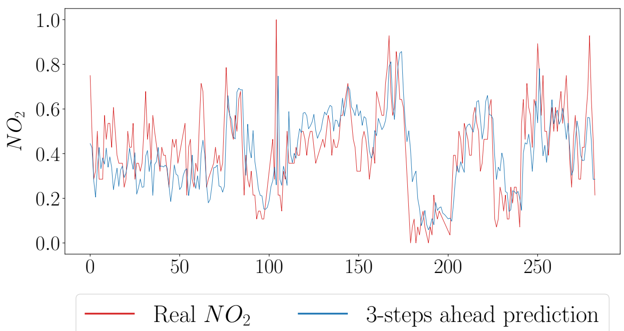
Fig. 5: Times series of the 7-steps ahead predictions for NO_2 evaluated on training dataset R of the prediction model obtained with *O1O2O3-NSGA-II* (air quality problem).



(a) 1-step ahead



(b) 2-steps ahead



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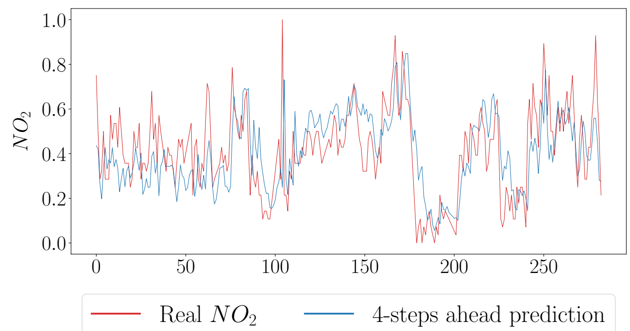

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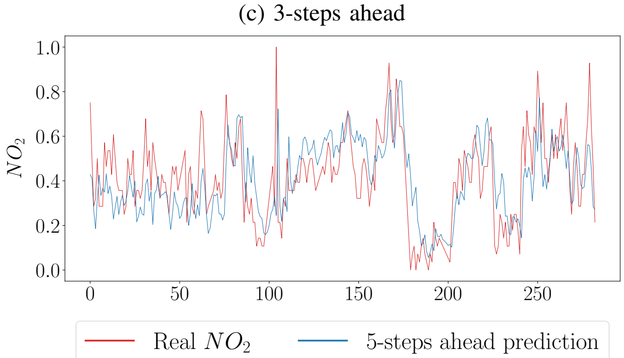
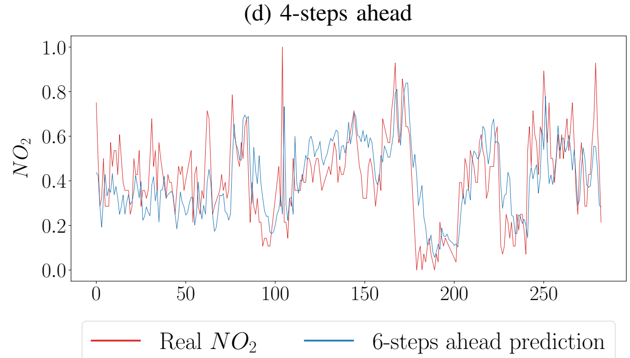
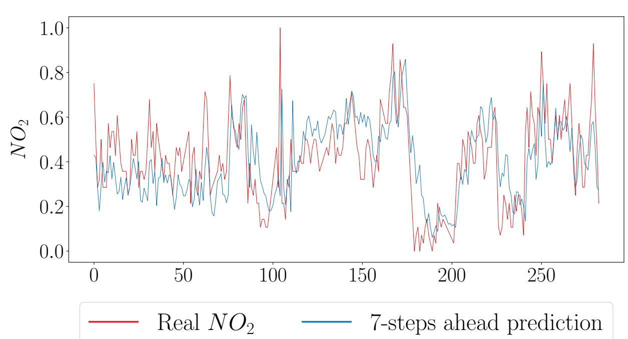


(e) 5-steps ahead

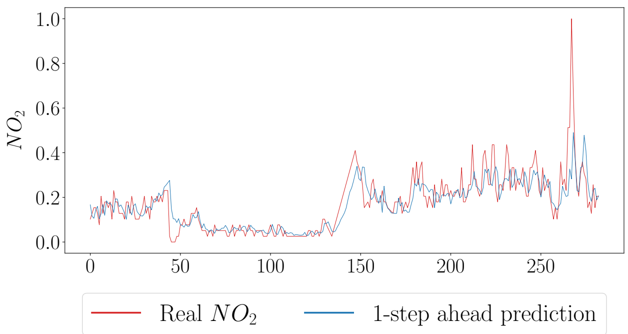


(f) 6-steps ahead

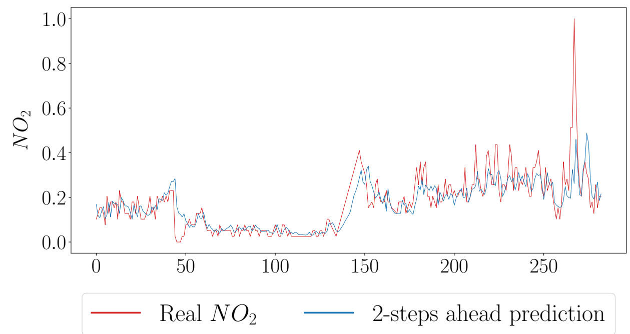


(g) 7-steps ahead

Fig. 6: Times series of the 7-steps ahead predictions for NO_2 evaluated on validation dataset V of the prediction model obtained with *O1O2O3-NSGA-II* (air quality problem).



(a) 1-step ahead



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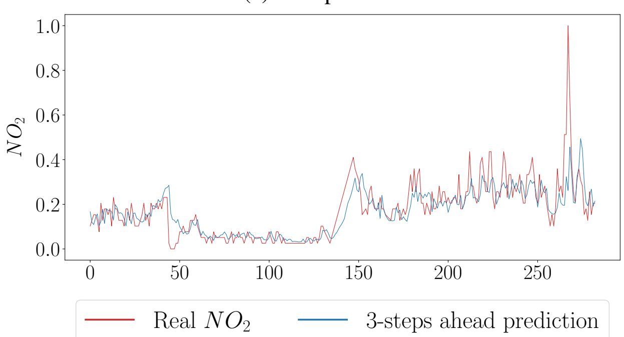
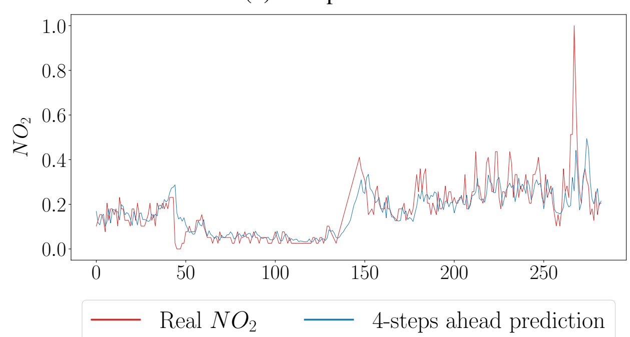
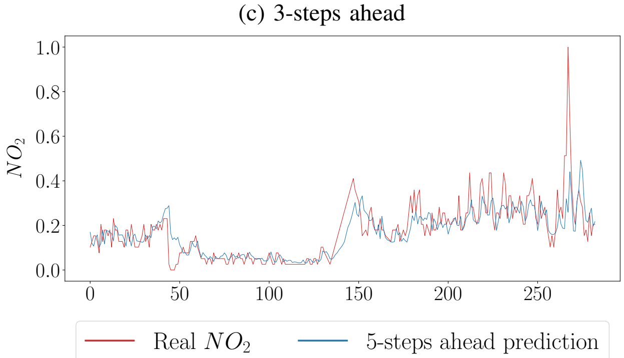


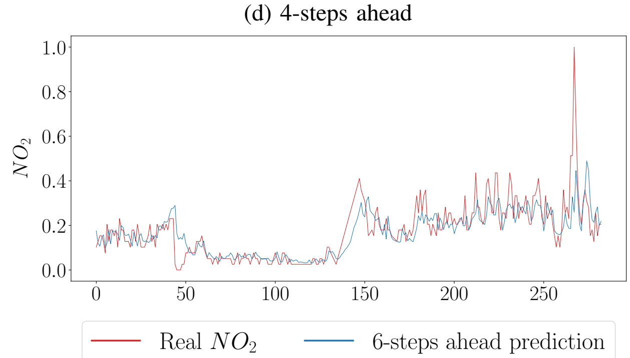
(c) 3-steps ahead



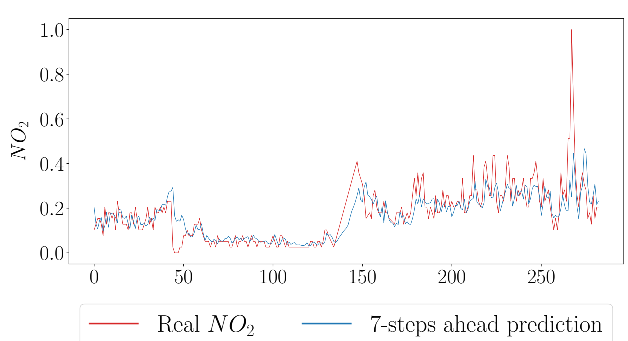
(d) 4-steps ahead



(e) 5-steps ahead

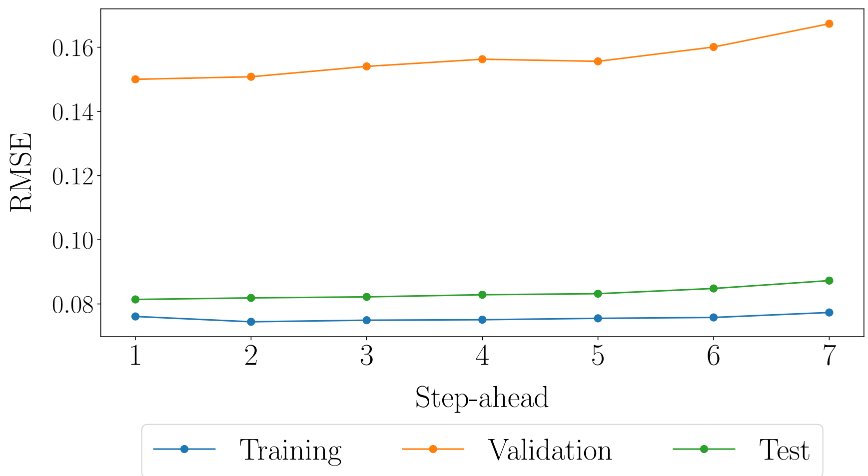


(f) 6-steps ahead

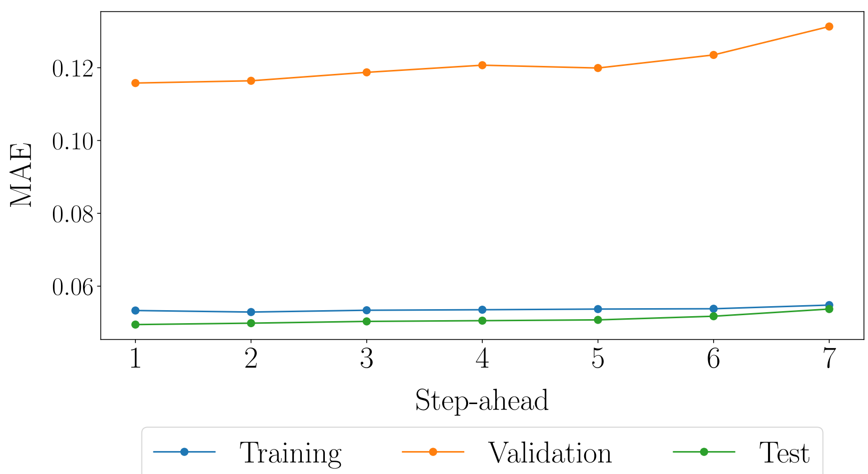


(g) 7-steps ahead

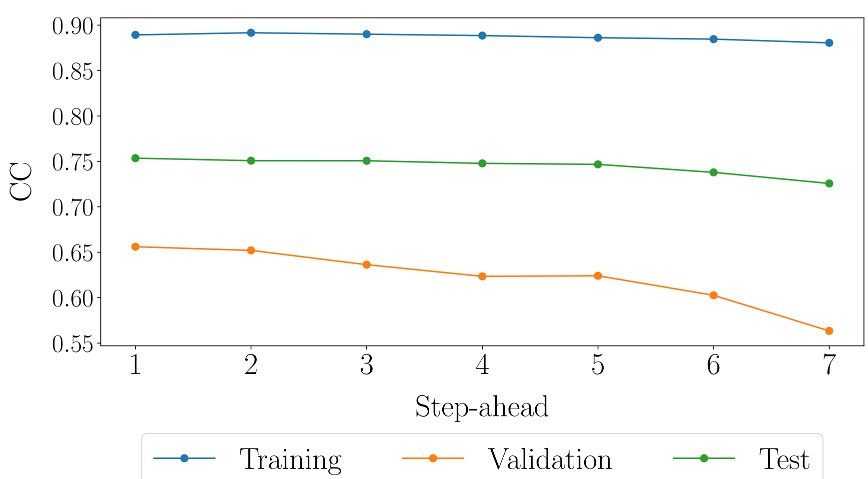
Fig. 7: Times series of the 7-steps ahead predictions for NO_2 evaluated on test dataset T of the prediction model obtained with *O1O2O3-NSGA-II* (air quality problem).



(a) RMSE



(b) MAE



(c) CC

Fig. 8: RMSE, MAE and CC of the 7-steps ahead predictions evaluated on R, V and T datasets of the prediction model obtained with *O1O2O3-NSGA-II* (air quality problem).

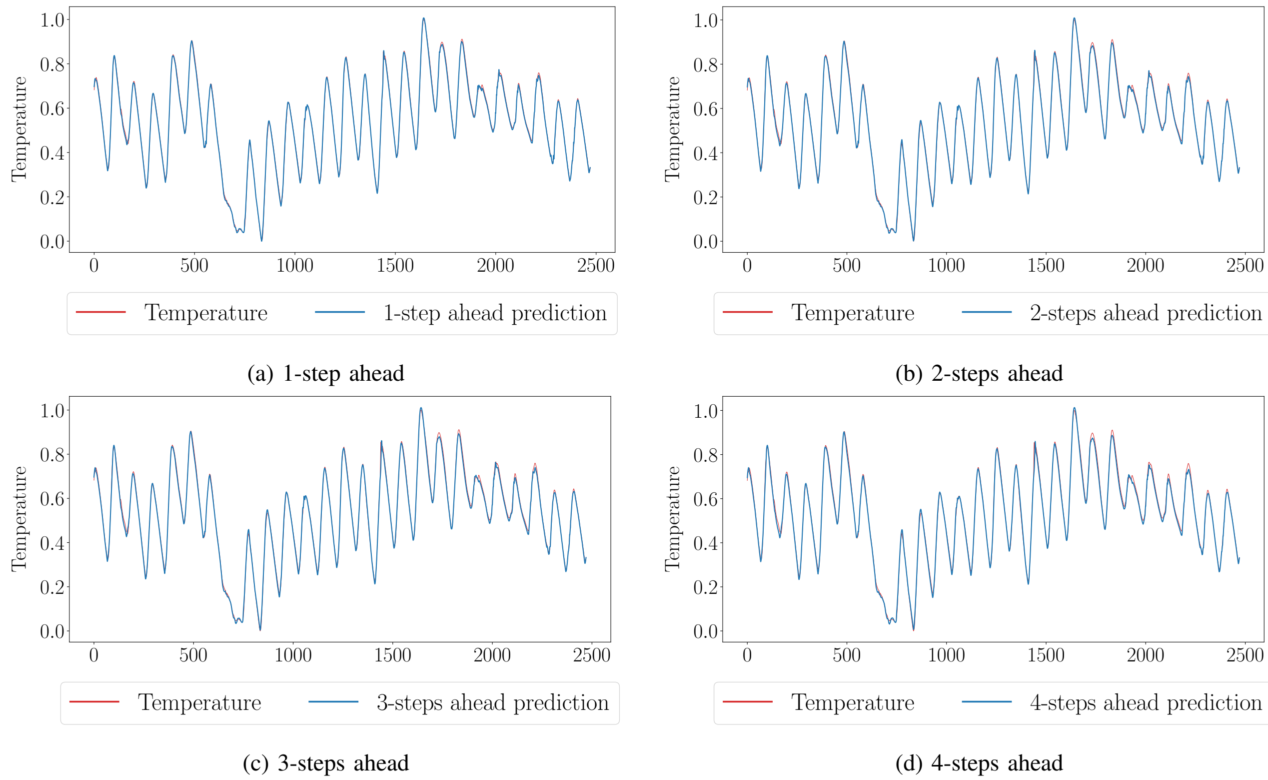


Fig. 9: Times series of the 4-steps ahead predictions for *IT* evaluated on training dataset R of the prediction model obtained with *O1O2O3O4-NSGA-II* (indoor temperature problem).

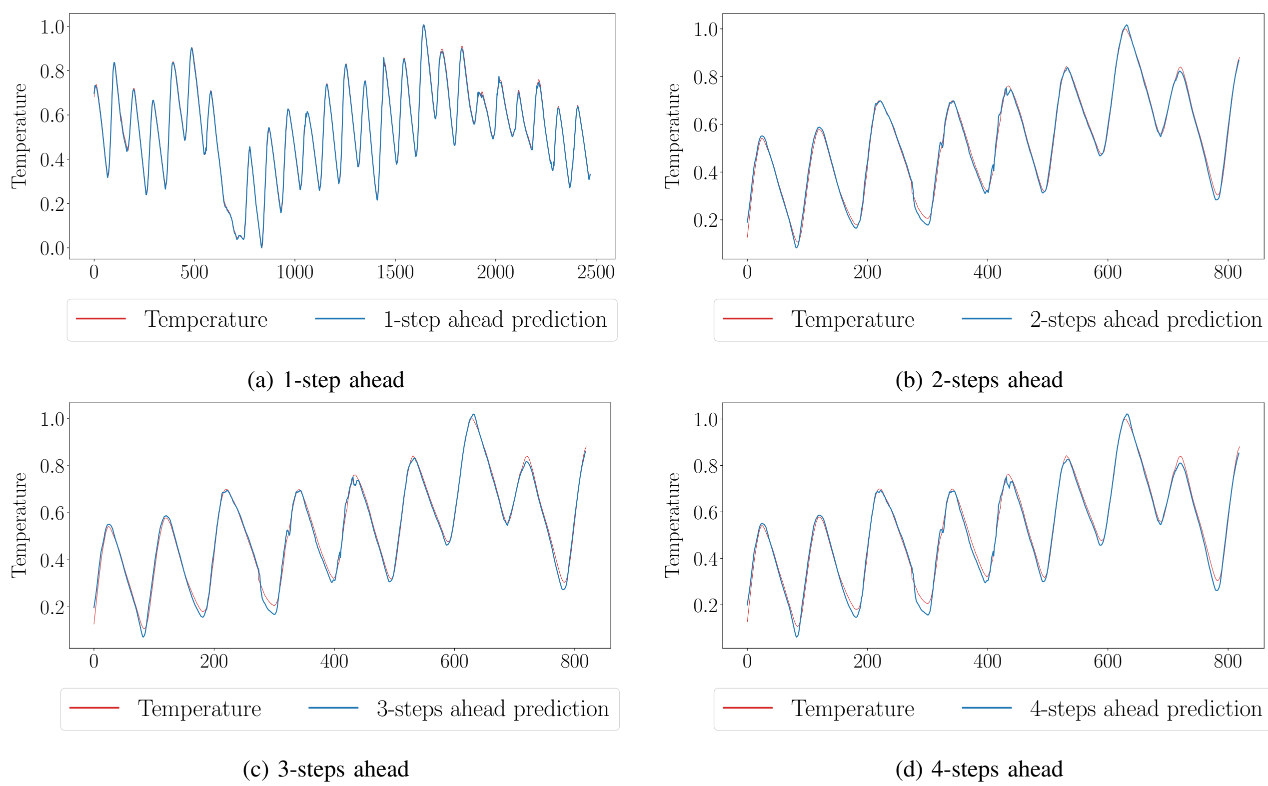
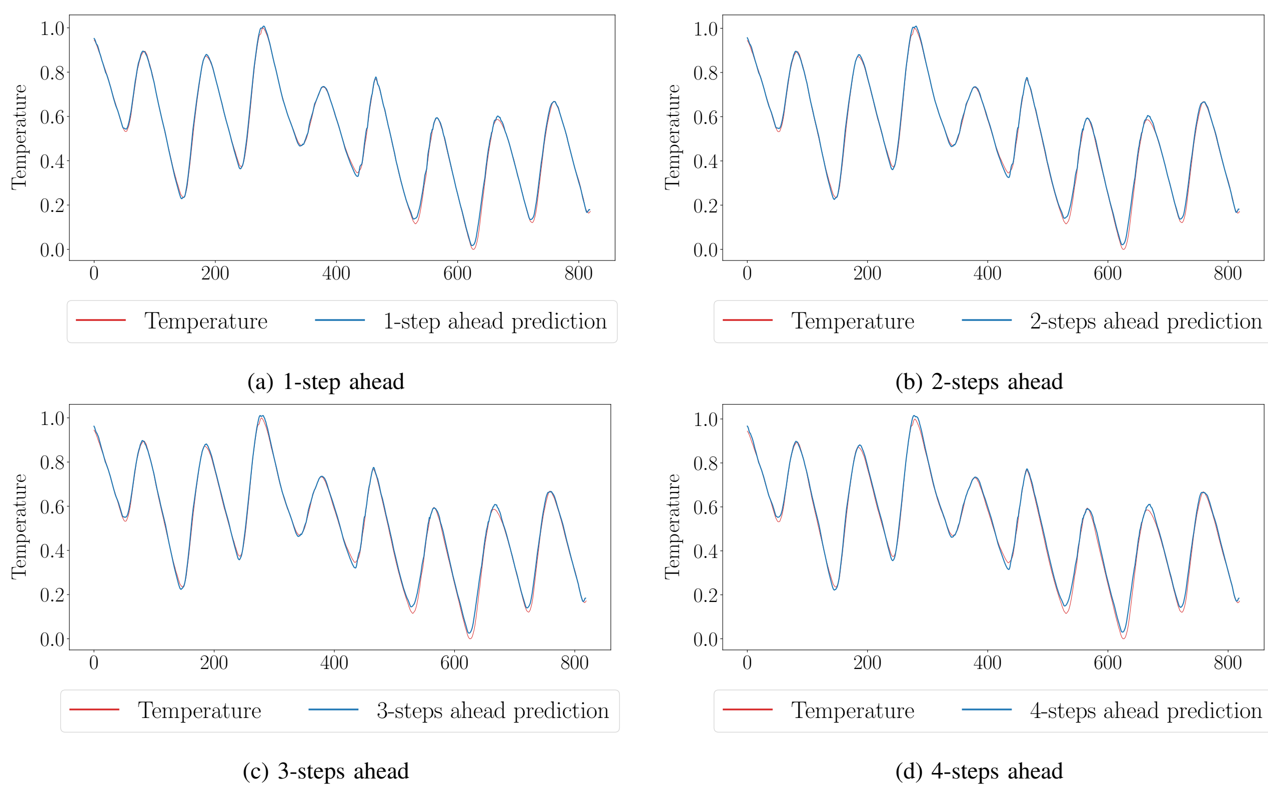


Fig. 10: Times series of the 4-steps ahead predictions for *IT* evaluated on validation dataset V of the prediction model obtained with *O1O2O3O4-NSGA-II* (indoor temperature problem).



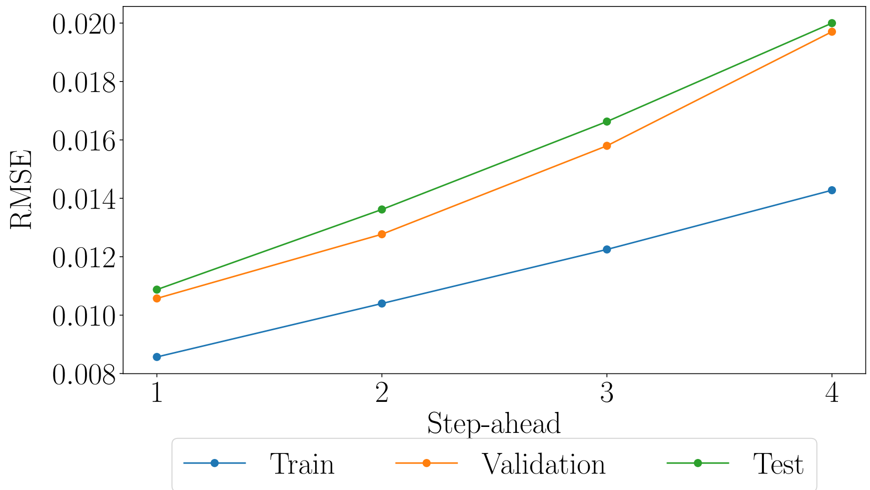
(a) 1-step ahead

(b) 2-steps ahead

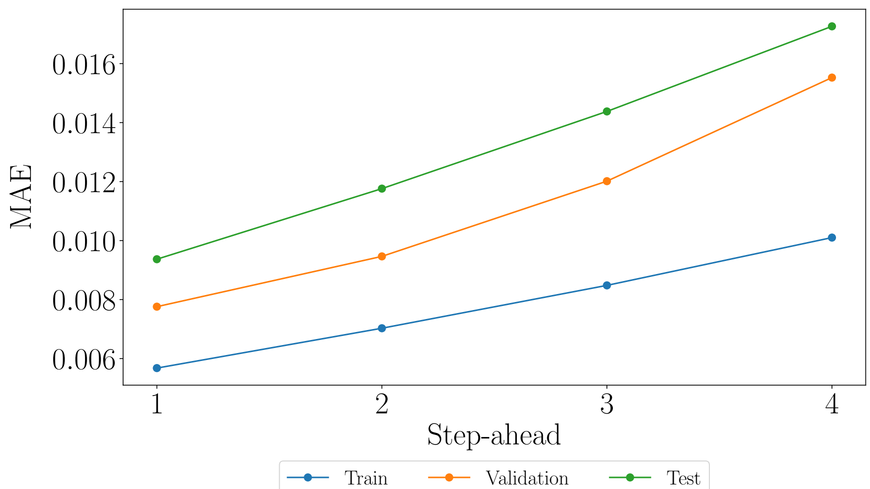
(c) 3-steps ahead

(d) 4-steps ahead

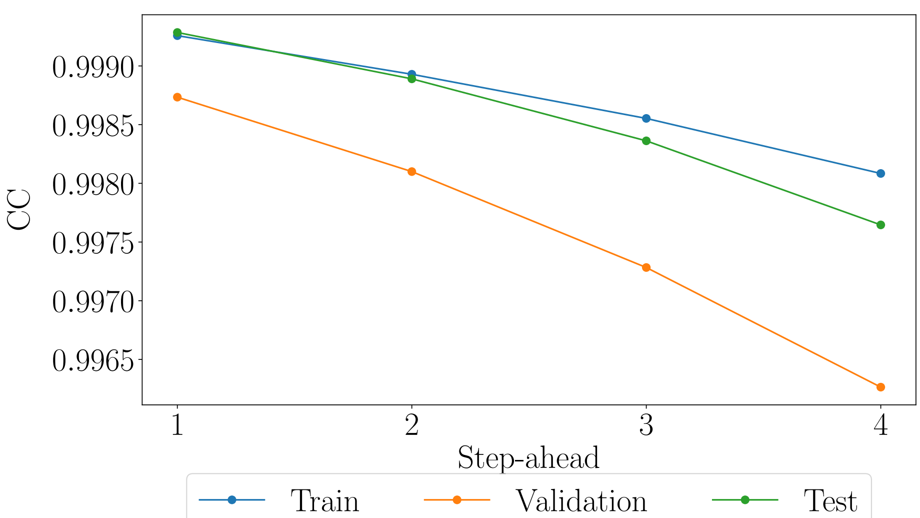
Fig. 11: Times series of the 4-steps ahead predictions for *IT* evaluated on test dataset T of the prediction model obtained with *O1O2O3O4-NSGA-II* (indoor temperature problem).



(a) RMSE



(b) MAE



(c) CC

Fig. 12: RMSE, MAE and CC of the 4-steps ahead predictions evaluated on R, V and T datasets of the prediction model obtained with *O1O2O3O4-NSGA-II* (air quality problem).