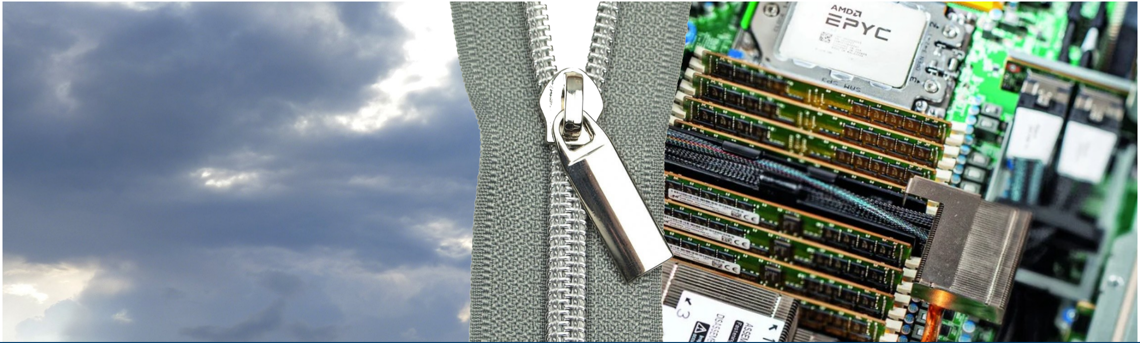

Representing chemical history of ozone

a method development study for deep learning models

30-04-2021 | Felix Kleinert[FZJ, BN], Lukas H. Leufen[FZJ, BN], Aurelia Lupascu[IASS], Tim Butler[IASS], and Martin G. Schultz[FZJ] | f.kleinert@fz-juelich.de | vEGU 2021 ITS4.4/AS4.1

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Outline

Overall goal

Improve quality of station based near-surface ozone predictions

Goal of this method development study

- Design different concepts of representing chemical history of air parcel (capturing transport)
- Benchmark concepts against baseline model which is not aware of chemical history
- Compare the change in prediction quality

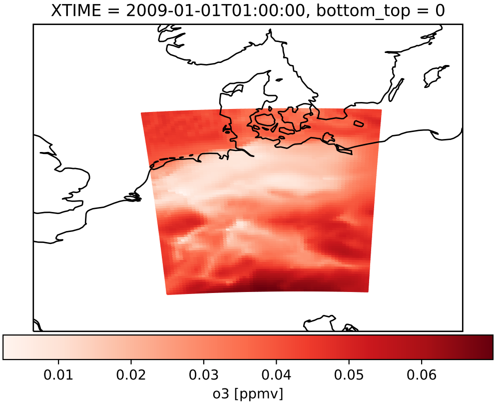
General prediction task

”Use chemical and meteorological model data of the past few hours to predict near-surface ozone concentrations for a lead time of up to two hours”

Data: WRF-Chem simulation

Model data

- We use WRF-Chem data as the gridded model data provides an internally consistent dataset with complete spatial coverage and no missing values
- Changes in forecasting performance can be attributed to concepts rather than a change in data availability (irregular distribution of measurement stations)
- Short period where advection is dominant (Jan to Mar 2009)



Info

In this study, we use model data (see also [3]) to train neural networks. Later on, we will apply the best working concept to measurement data of the Tropospheric Ozone Assessment Report (TOAR) database [6], e.g. to improve the IntelliO3-ts model [2].

Supervised machine learning

Supervised machine learning approach

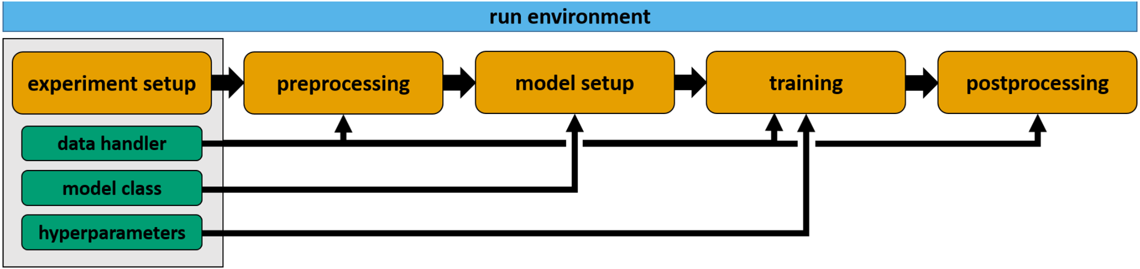
- Task: Find unknown function f which maps input pattern ($\mathbf{X}$) to corresponding labels/ ground truth ($\mathbf{y}$)
- Machine learning model is estimator ($\hat{f}$) which maps $\mathbf{X}$ to an estimate $\hat{\mathbf{y}}$ of the ground truth
- Goodness of estimate quantified by error/ loss function
- Generally ground truth and estimates differ $f(\mathbf{X}) = \mathbf{y} \neq \hat{\mathbf{y}} = \hat{f}(\mathbf{X})$

None neural network competitor models

- Ordinary least-squares (ols)
- Persistence (persi)

Learning Framework: MLAir

- We carry out our experiments with MLAir [5]
- We extended the code to represent chemical history (`DataHandlers`)

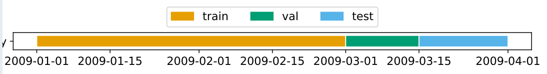


Visualization of the MLAir standard setup (from [5, Fig. 1])

Baseline model ($\hat{f}_b$)

Data

- Data from 8 surface grid boxes
- Input (**X**)
  - Variables: O_3, NO, NO_2, CO, T2, wdir10, wspd10, PSFC, PBLH, CLDFRA
  - Time: t_{-6} to t_0, hourly
  - Shape: (# samples, # prev time steps, 1, # vars)
- Target variable (**y**): O_3 for t_1 to t_2



Data split

Model

- 2× CNN layers [4] where vars are used as channels
- 3 × 1 kernel, 16 and 32 filters
- Symmetric padding, ELU activation [1]
- 2× FC layer, ELU and linear activation

Baseline prediction task

"Use chemical and meteorological model data of the past few hours **at a specific grid box** to predict near-surface ozone concentrations for a lead time of up to two hours **at that particular grid box.**"

Representing chemical history

- The ozone concentration at a particular point in space and time depends on the chemical history of an air parcel (where it has been before).
- The baseline model only captures the history of the fixed grid box rather than the air parcel.

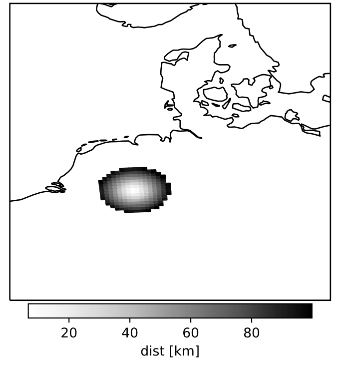
$\rightarrow$ Ideally we would use backward trajectories

- Backward trajectories require full field of model data (not directly available when using measurement data)

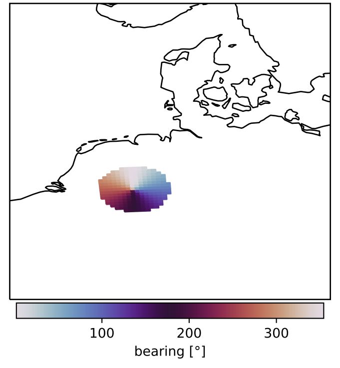
$\Rightarrow$ Approximation by wind sector

Sectorial preprocessing

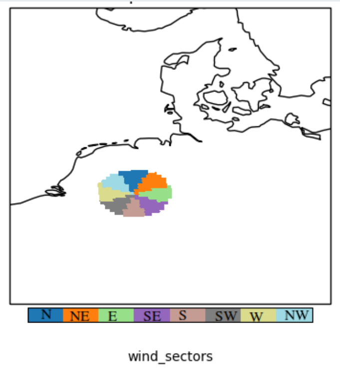
Exemplary point of interest (POI)



- Distance from POI to neighbouring grid boxes (here max. 100 km)



- Bearing from POI to neighbouring grid boxes



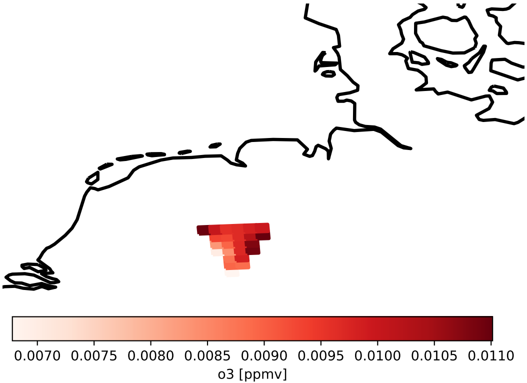
- Assign each grid box to a sector used for aggregation

Sector model ($\hat{f}_s$)

Data preprocessing

- Data of Baseline Model
- \+ Aggregated (mean) data of each var from upstream sector determined by wind direction at t_0 e.g. mean over N sector (see right figure as an example for O_3)
- Used as additional variables (channels in neural network) $\rightarrow$ 20 variables (10 (grid box) +10 (sector))

$\rightarrow$ Additional variables represent sector



Sector prediction task

"Use chemical and meteorological model data of the past few hours at a specific grid box **and spatially aggregated sector data of the current wind direction (upstream)** to predict near-surface ozone concentrations for a lead time of up to two hours at that particular grid box."

Extended sector model ($\hat{f}_{es}$)

Data preprocessing

- Data of Baseline model
- Data of Sector model

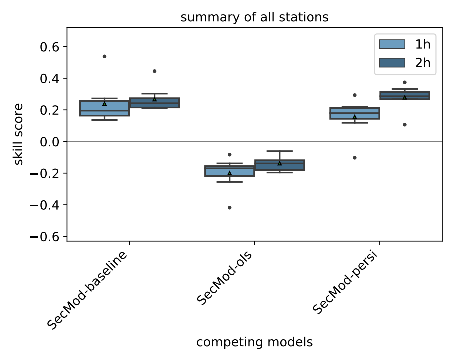
\+ Sector data of the two adjacent sectors
  - Aggregated (mean) data of each variable from adjacent sectors of wind direction at t_0 (left and right sectors, e.g. NW, and NE if main sector is N)
  - Used as additional variables (channels in neural network) $\rightarrow$ 40 variables (10 (grid box) +10 (main sector) +10 (left sector) +10 (right sector))

Extended sector prediction task

"Use chemical and meteorological model data of the past few hours at a specific grid box, spatially aggregated sector data of the current wind direction (upstream) **and spatially aggregated sector data of the two adjacent sectors** to predict near-surface ozone concentrations for a lead time of up to two hours at that particular grid box."

Results: Model comparison

Sector model

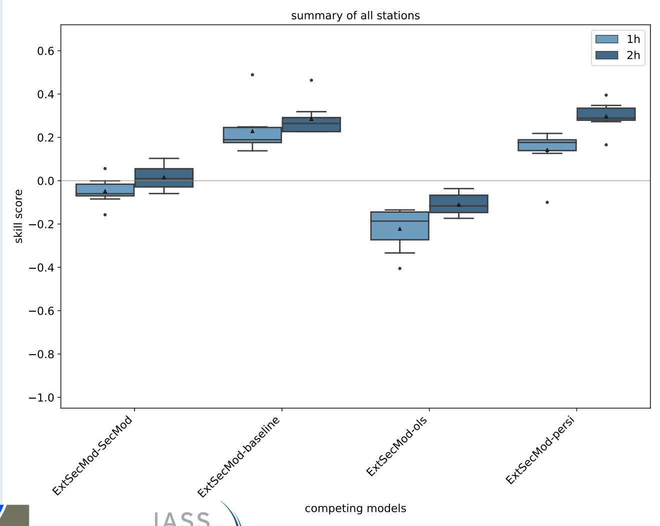


$\Rightarrow$ 20% improvement over baseline

Skill score

$$SS \begin{cases} >0, & \text{first model outperforms second,} \\ =0, & \text{first model as good as second,} \\ <0, & \text{second model outperforms first.} \end{cases}$$

Extended sector model



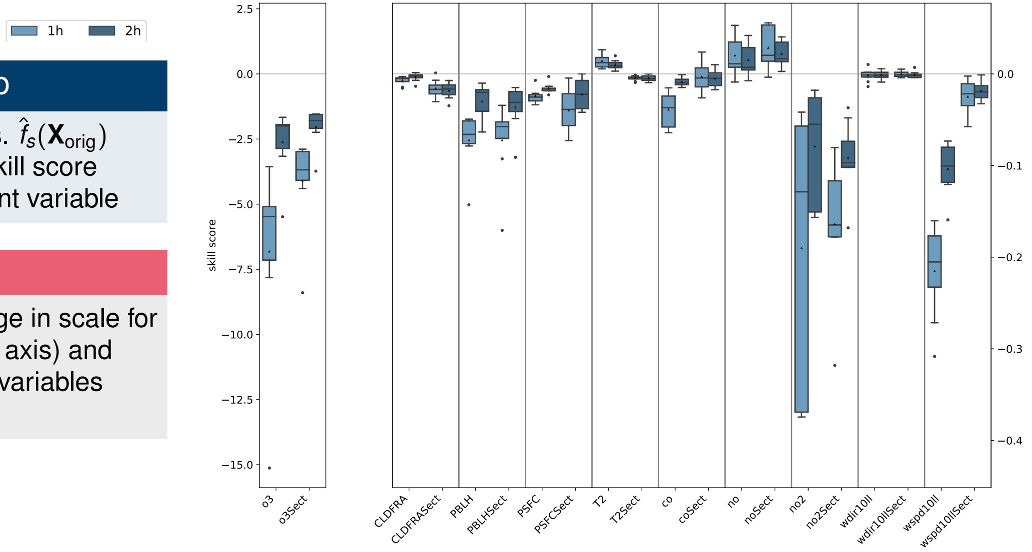
Sector model - importance of variables

Bootstrap

$\hat{f}_s(\mathbf{X}_{\mathrm{boot}})$ vs. $\hat{f}_s(\mathbf{X}_{\mathrm{orig}})$
negative skill score
$\Rightarrow$ important variable

Info

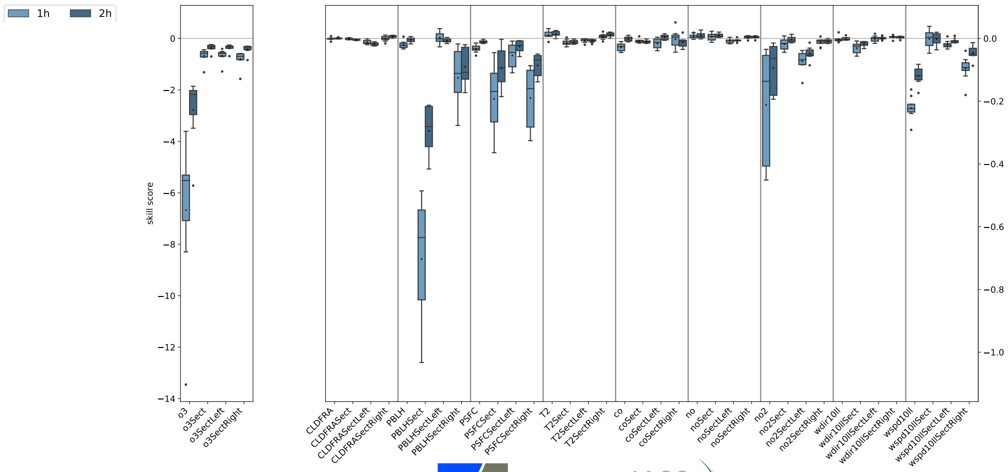
Note change in scale for ozone (left axis) and remaining variables (right axis)



Extended sector model - importance of variables

Bootstrap

$\hat{f}_{es}(\mathbf{X}_{\text{boot}})$ vs. $\hat{f}_{es}(\mathbf{X}_{\text{orig}})$: negative skill score $\Rightarrow$ important variable



Summary & Outlook

Summary

- Including aggregated information of one sector improves the forecast
- Including neighbouring sectors do not further improve the forecasts
- Influence of sector variables differ

⇒ Adding information of one sector seems to be promising also for larger networks

Outlook and further steps

- Increase of lead time
- Perform experiments on larger data set (expected to beat ols)
- Implement spatial interpolation as proposed by [7]
- Integration of best working method into IntelliO3-ts [2]

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http://www.intelliaq.eu

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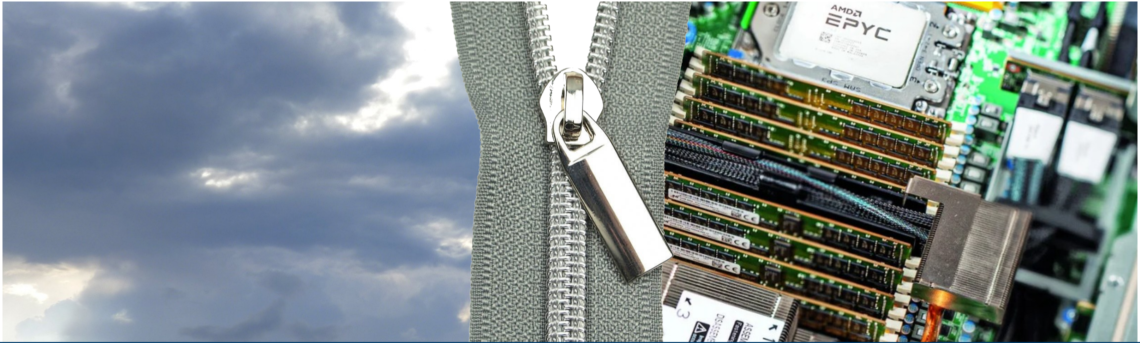

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