



# PREDICTION OF DAILY MAXIMUM OZONE THRESHOLD EXCEEDANCES BY ARTIFICIAL INTELLIGENCE TECHNIQUES IN GERMANY

April 8, 2019 | Bing Gong, Felix Kleinert, Martin Schultz | Jülich Supercomputing Center

# Overview

## 1. Background

- 1.1 Motivation
- 1.2 Research Questions and Objectives
- 1.3 Ground-level ozone

## 2. Methodology

- 2.1 Data selection and preparation
- 2.2 Machine learning mechanism
- 2.3 Imbalanced data solution
- 2.4 Evaluation metrics

## 3. Results

- 3.1 Orig VS. SMOTE
- 3.2 ML VS. CNN
- 3.3 Prediction accuracy on 4 leading days
- 3.4 Deep learning improvement

## 4. Conclusions and Future studies

- 4.1 Conclusions and Future studies

# Motivation

## - Social Impact

### Six common pollutants

**PM**

**O<sub>3</sub>**

**CO**

**SO<sub>2</sub>**

**NO<sub>x</sub>**

**Lead**

### Health Effects



**Asthma**



**Respiratory  
disease**



**Heart  
disease**



**Birth  
defects**



**Intellectual  
disorders**



**Immune system  
damage**



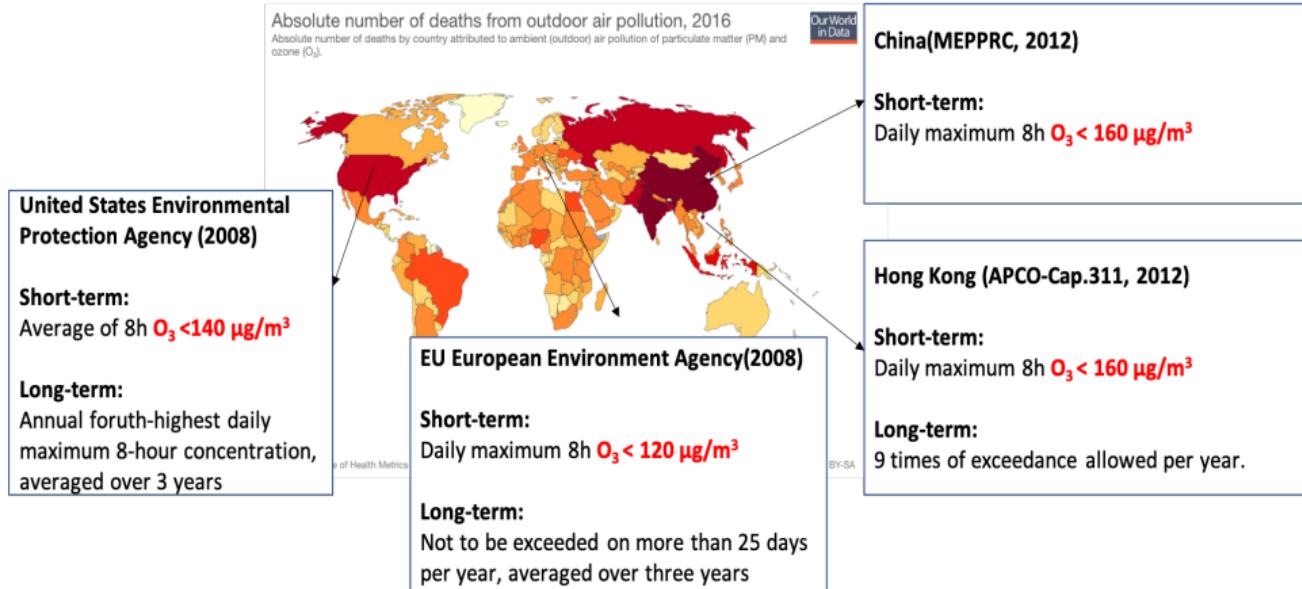
**3 million  
deaths/year**  
(WHO, 2016)

**US \$225  
billion/year**  
(World Bank,  
2016)



# Motivation

## - Regulation and Standard



Normativity of  $O_3$  in United State, European Union, Mainland China, and Hong Kong

# Research Questions and Objectives

- Predict the exceedances of the maximum 8h ozone concentrations in Germany

## Research Questions:

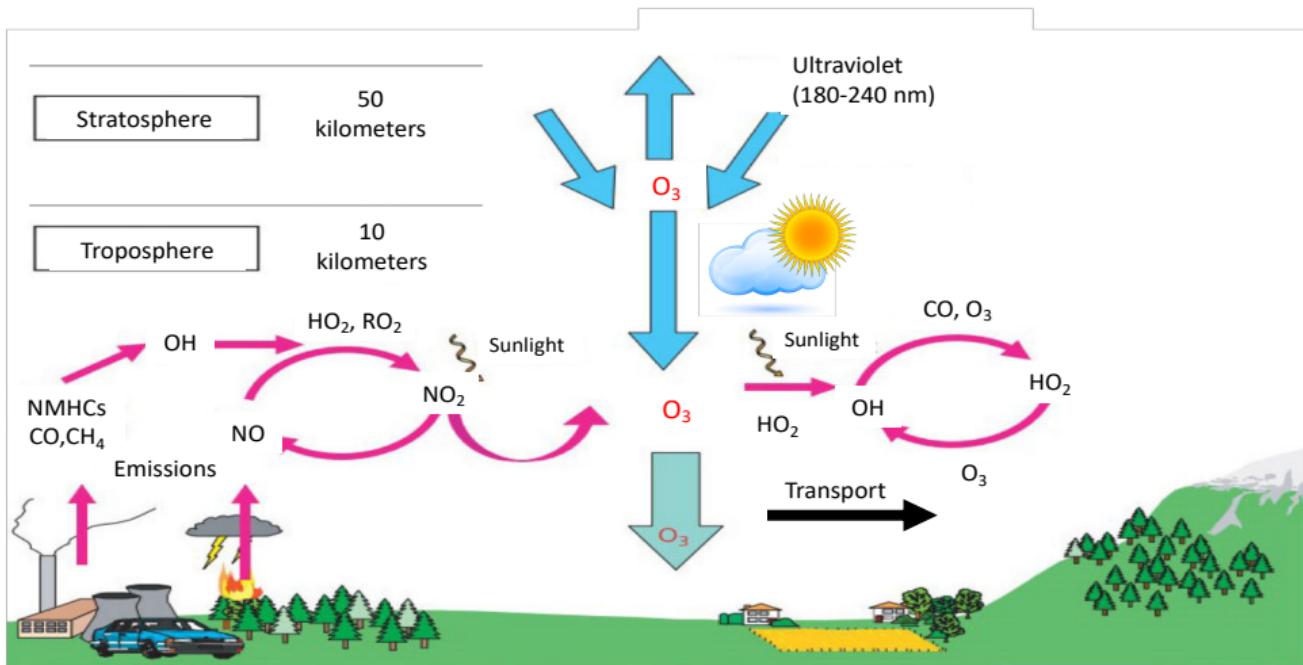
- Can **machine learning** enhance the prediction accuracy for the air quality warning system ?
- How do different machine learning methods perform in the **classification task** of predicting threshold exceedances?
- **How far in the future** can make ozone prediction by machine learning/deep learning?



Map of the study region  
Baden-Württemberg in Germany  
(Source:onTheWorldMap.com)

# Ground-level ozone

## - Factors controlling ozone level



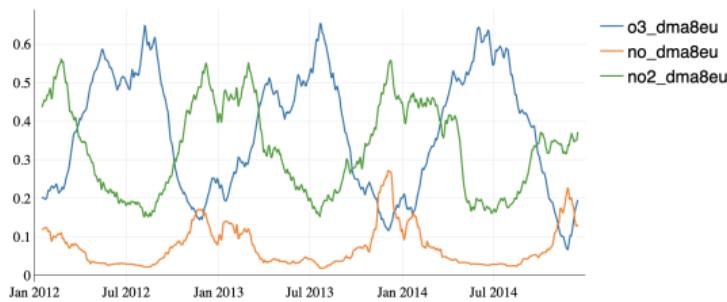
Schematic diagram for ozone formation (Fowler et al., 2008)

# Ground-level ozone

## - Key variables

Table: Pollution variables as inputs for modelling

Variable	Description	Unit
o3_dma8eu	Daily maximum 8-hour average ozone	ppb
no_dma8eu	Daily maximum 8-hour nitrogen monoxide	ppb
no2_dma8eu	Daily maximum 8-hour nitrogen dioxide	ppb



Moving average values of O<sub>3</sub>, no\_dma8eu and no2\_dma8eu from 2012 to 2014 at Station DEBW010

Table: Meteorological variables as inputs for modelling

Variable	Description	Unit
pbheight_max	Maximum height of planetary boundary layer	m
relhum_max	Daily maximum relative humidity	%
temp_max	Daily maximum temperature	° C
u_mean	Daily mean u-component (zonal) of wind	m/s
v_mean	Daily mean v-component (meridional) of wind	m/s
cloudcover_mean	Daily mean total cloud cover	%

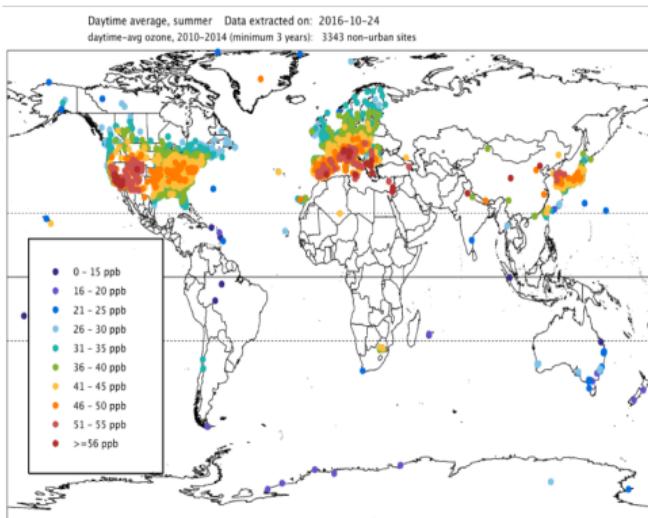


Moving average values of O<sub>3</sub>, cloudcover\_mean, pbheight\_max, relhum\_max, and temp\_max from 2012 to 2014 at Station DEBW010

# Data selection and preparation

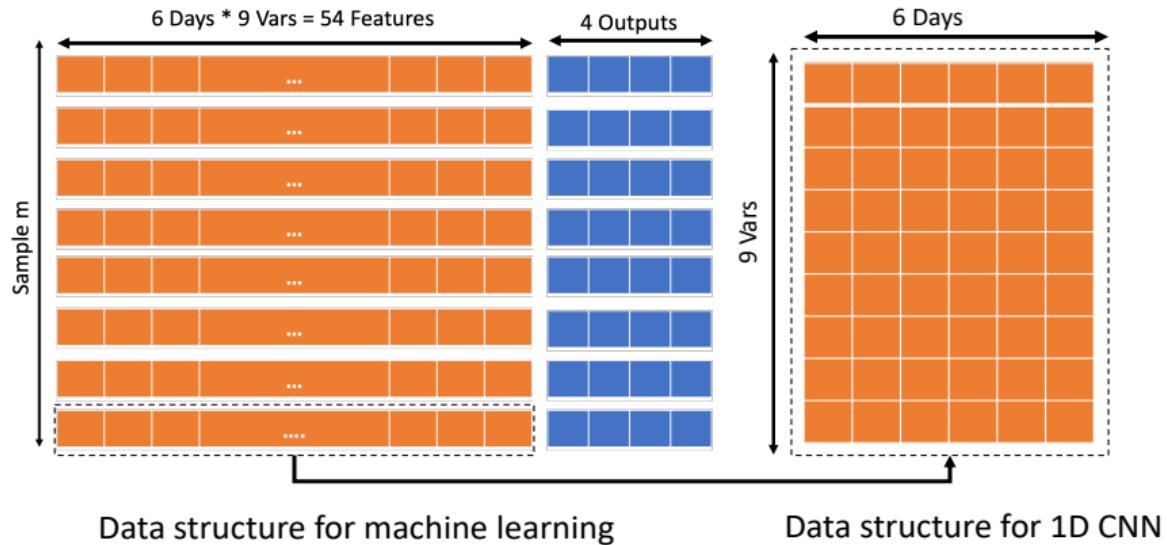
- Tropospheric Ozone Assessment Report (TOAR) Database for variable selection

25 variables, more than 10,000 measurement sites from over 30 different sources around the world



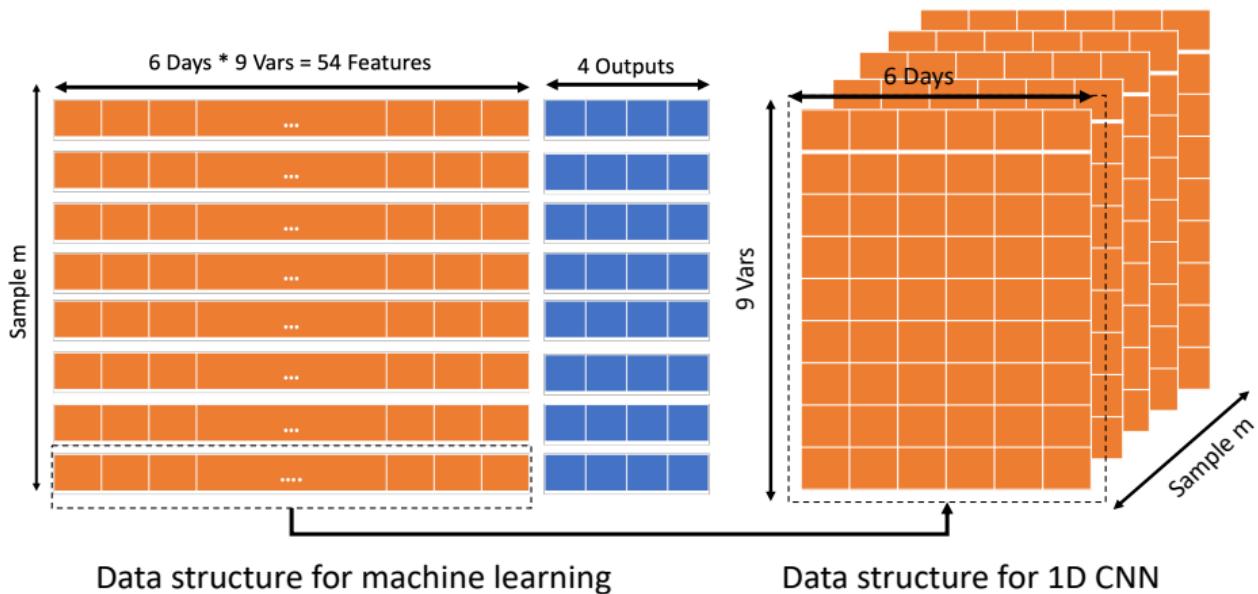
# Data selection and preparation

## - Dataset structure for machine learning and Convolutional Neural Network



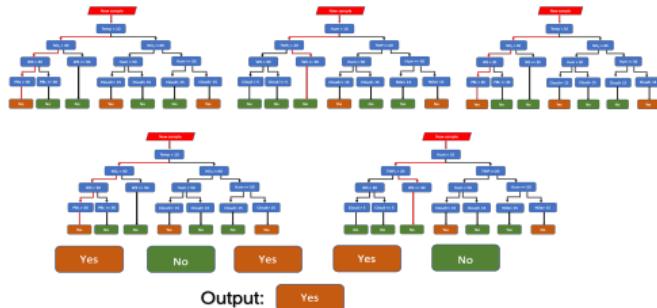
# Data selection and preparation

## - Dataset structure for machine learning and Convolutional Neural Network

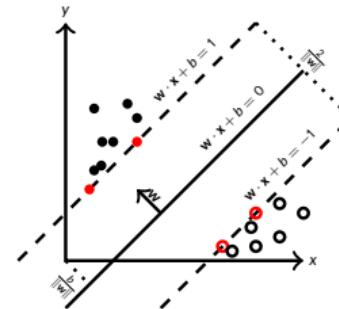


# Machine learning mechanism

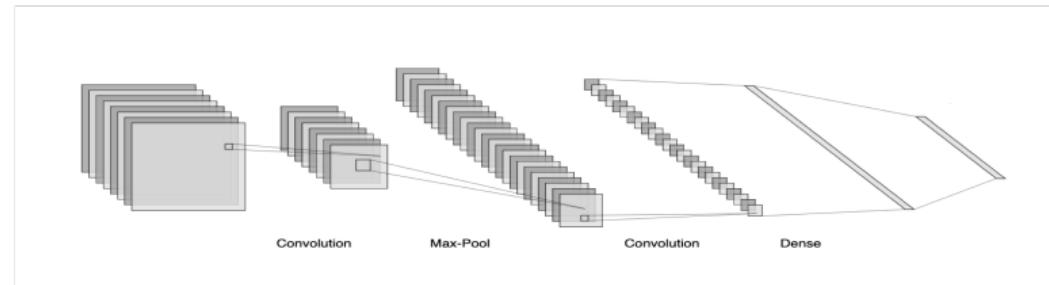
- Random Forest, Support Vector Machine, and Convolutional Neural Network



Random Forest



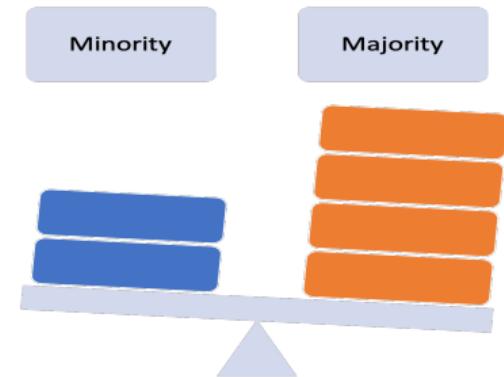
Support Vector Machine



1D CNN

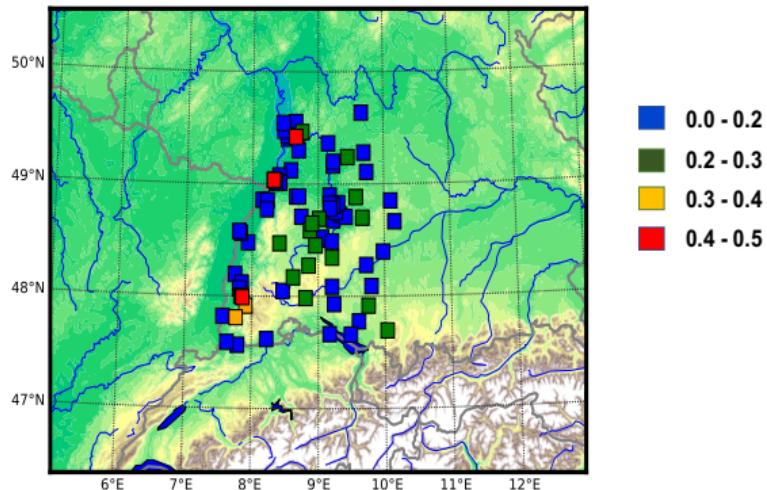
# Imbalanced data solution

## - Imbalanced data issue



$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

		Observed	
		Minority	Majority
Predicted	Minority	TP	FP
	Majority	FN	TN

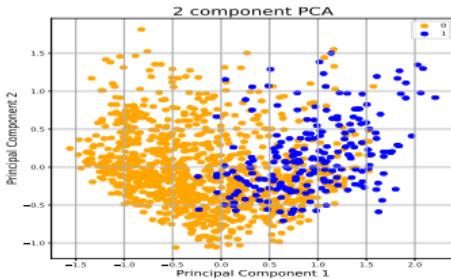
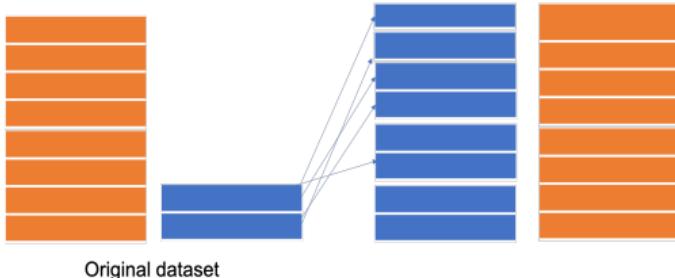


Exceedance frequency ( $\frac{\text{No.of Exceedances}}{\text{No.of samples}}$ ) for all the monitoring stations in BW state

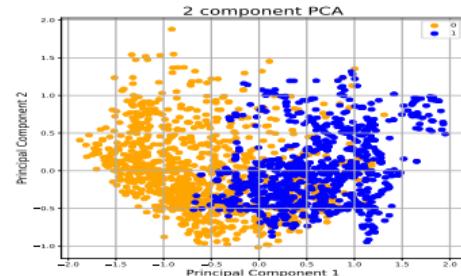
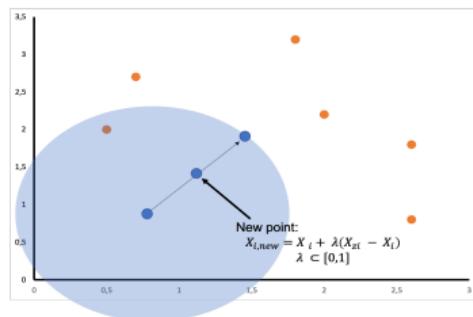
# Imbalanced data solution

## - Imbalanced data solution: Modifying class distribution

Oversampling



Scatter plot of raw data in 2 Dimensions



Scatter plot of SMOTE data in 2 Dimensions

### Synthetic Minority Over-sampling Technique(SMOTE)

Member of the Helmholtz Association

April 8, 2019

Slide 12

# Evaluation metrics

## - Classification evaluation metrics

### Generic evaluation metric

		Observed		Total
		Positive	Negative	
Predicted	Positive	a	b	$a + b$
	Negative	c	d	$c + d$
Total		$a + c$	$b + d$	N

- Accuracy =  $\frac{a + d}{a + b + c + d}$
- Precision =  $\frac{a}{a + b}$
- Recall =  $\frac{a}{a + c}$

### Evaluation metric for imbalanced data

- F1 - Score =  $\frac{2 \cdot \text{Recall} \cdot \text{Precision}}{\text{Recall} + \text{Precision}}$
- G-means =  $\sqrt{\frac{a \cdot d}{(d + c) \cdot (a + c)}}$

$y_i$  are the prediction values, and  $\hat{y}_i$  are the observed values.

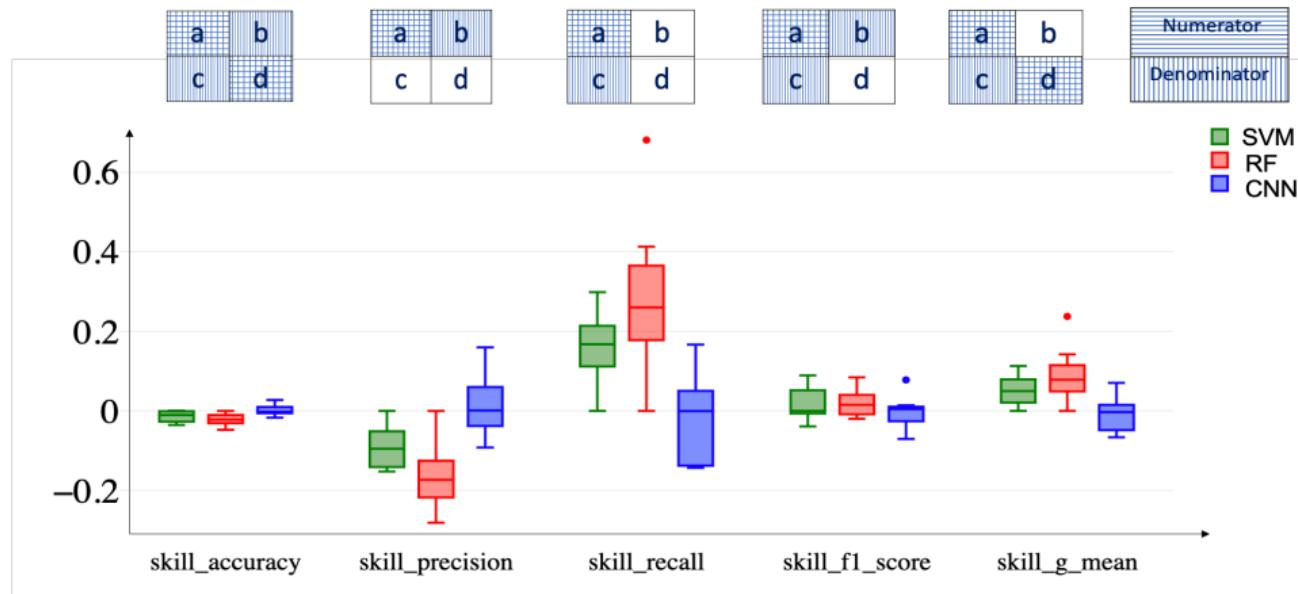
### Skill score

Use the skill score for comparing the target model  $t$  and reference model  $ref$  based on measurement  $m$ .

- $skill_m = (m - m_{ref}) / m_{ref}$

# Orig VS. SMOTE

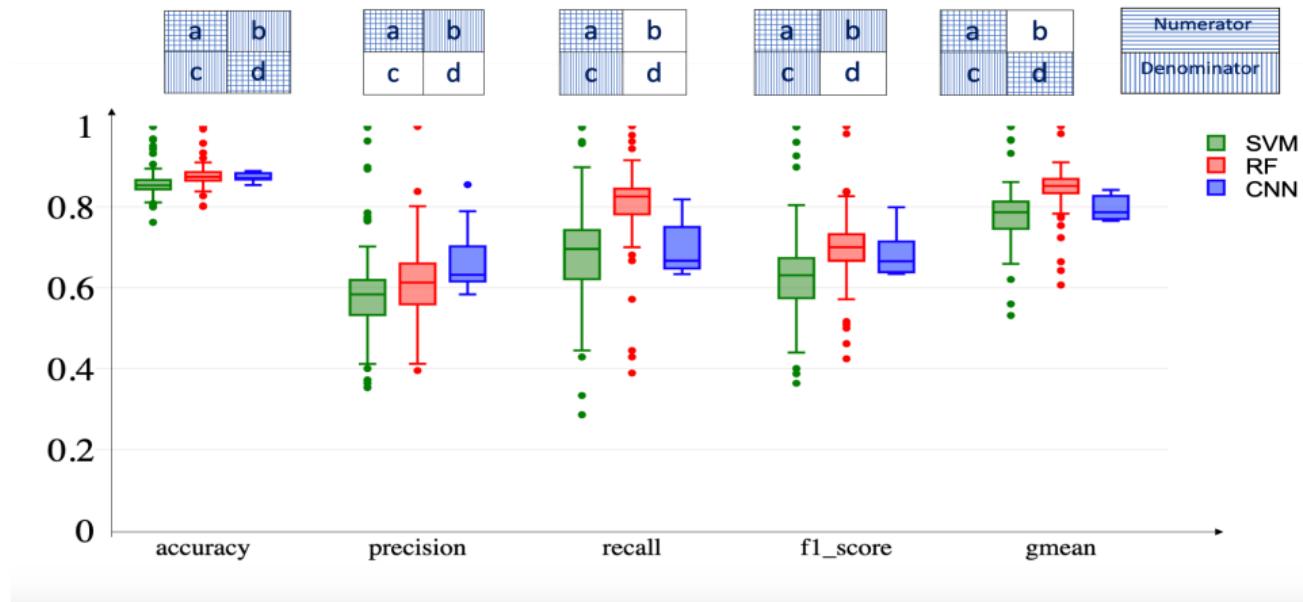
- Does the SMOTE improve the model performance?



Skill scores ( $skill_{SMOTE} = (m_{SMOTE} - m_{orig})/m_{orig}$ ) corresponding to different evaluation metrics for comparing on raw data and SMOTE data from all the monitoring stations

# ML VS. CNN

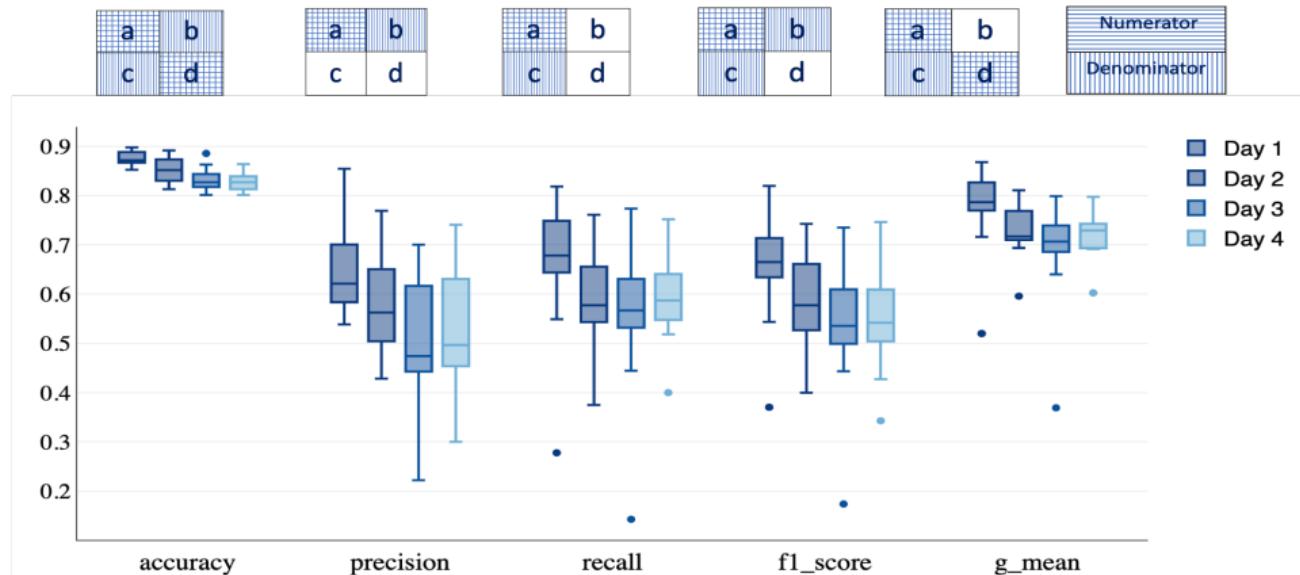
- Does CNN improves the prediction accuracy?



Evaluation metrics for SVM, RF, and CNN models on SMOTE dataset for all the monitoring stations

# Prediction accuracy on 4 leading days

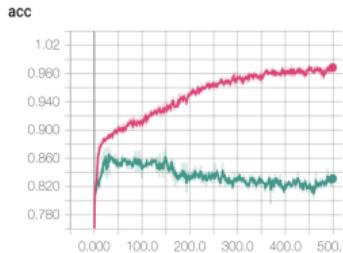
- Forecasting 4 leading days



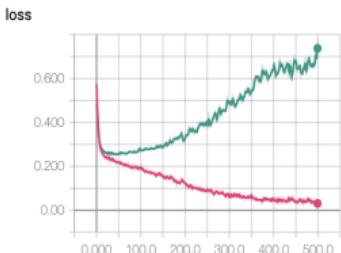
Evaluation metrics of CNN model on SMOTE to predict 4 days ahead for all the monitoring stations

# Deep learning improvement

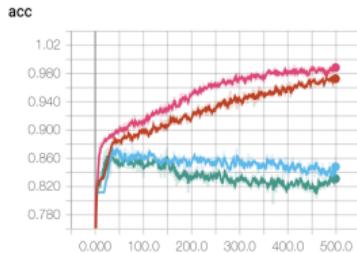
## - Deep Learning diagnosis



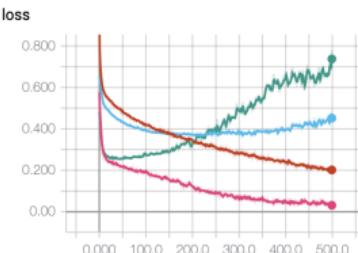
Accuracy-M1



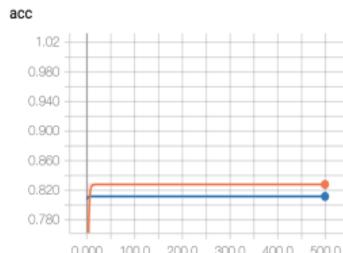
Loss-M1



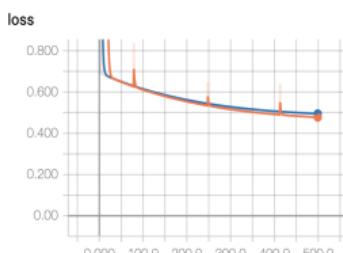
Accuracy-M1-Reg1-l-0.1



Loss-M1-Reg1-l-0.1



Accuracy-M1-Reg1-l-10



Loss-M1-Reg1-l-10

The reference 1D CNN was diagnosed as:

- Over-fitting
- Local minimal

# Conclusions and Future studies

## - Preliminary conclusions and Future studies

### ■ Preliminary conclusions:

- SMOTE can improve the classification performance for model SVM and RF.
- With current set-up CNN is not better than traditional ML techniques; RF wins.
- The prediction accuracy decrease significantly from 1 leading day to 2 day prediction.

### ■ Future studies:

- Deep learning structure
  - Cost-sensitive CNN for imbalanced data
  - Universal network for all the stations
  - LSTM
- Data Level
  - Size of variables (Feature engineering, spatial factors etc.)
  - Heterogeneous data sources

# Acknowledgement

**Intelli  
AQ**

<http://www.IntelliAQ.eu>



**European Research Council**

Established by the European Commission

Funding is provided through  
ERC Advanced grant  
ERC-2017-ADG #787576  
by Martin Schultz

# Thank You!

contact me: [b.gong@fz-juelich.de](mailto:b.gong@fz-juelich.de)

# References I

## - References:

Fowler, D., Amann, M., Anderson, F., Ashmore, M., Cox, P., Depledge, M., ... others (2008). Ground-level ozone in the 21st century: future trends, impacts and policy implications. [Royal Society Science Policy Report, 15\(08\)](#).