



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

Introduction2.pdf

Motivation

- Regulation and Standard

Regulations.png

Normativity of O₃ 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?

BW_locations.jpg

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

Ground-level ozone

- Factors controlling ozone level

OzoneFormation4.pdf

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

pollu_corr.png

Moving average values of O₃, no_dma8eu and no2_dma8eu from 2012 to 2014 at Station DEBW010

Table: Meteorological variables as inputs for modelling

Variable	Description	Unit
pblheight_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	%

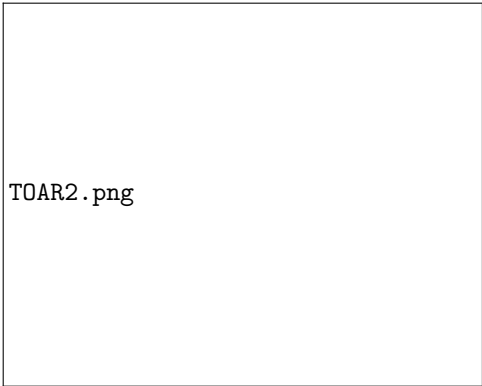
meteo_corr.png

Moving average values of O₃, cloudcover_mean, pblheight_max, relhum_max, and temp_max from 2012 to 2014 at Station DEBW010

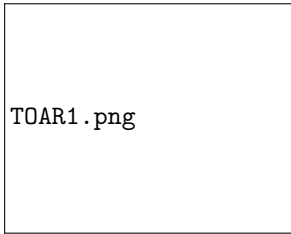
Data selection and preparation

- 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



TOAR2 .png



TOAR1 .png

Data selection and preparation

- Dataset structure for machine learning and Convolutional Neural Network

DataSetStructure1.pdf

Data selection and preparation

- Dataset structure for machine learning and Convolutional Neural Network

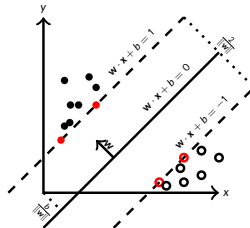
DataSetStructure2.pdf

Machine learning mechanism

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

RF . png

Random Forest



Support Vector Machine

DL . png

1D CNN

Imbalanced data solution

- Imbalanced data issue

imbalanceDataIssue.png

ImbalancAccuracy.png

		Observed	
		Minority	Majority
Predicted	Minority	TP	FP
	Majority	FN	TN

ExceedanceRate2.pdf

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.png

SMOTE.png

DEBW048X_train_pca2.pdf

Scatter plot of raw data in 2 Dimensions

DEBW048X_res_pca2.pdf

Scatter plot of SMOTE data in 2 Dimensions

Synthetic Minority Over-sampling Technique(SMOTE)

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 = $\frac{a \cdot d}{(d + c) \cdot (a + c)}$

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?

SVM_RF_DL_SMOTE_V4.png

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?

SVM_RF_DL_SMOTE_AbsValues3.png

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

Prediction accuracy on 4 leading days

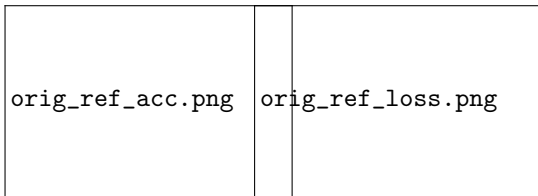
- Forecasting 4 leading days

SMOTE_CNN_DAYS1_4.png

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

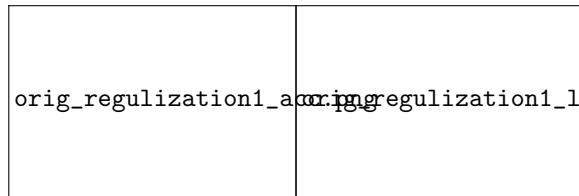
Deep learning improvement

- Deep Learning diagnosis



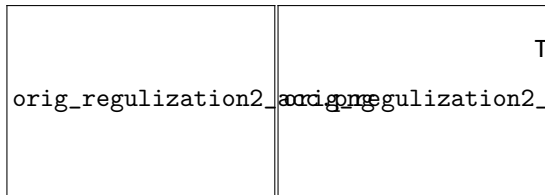
Accuracy-M1

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 diagnosis as:

- Overfitting
- Local minimal

Conclusions and Future studies

- Preliminary conclusions and Future studies

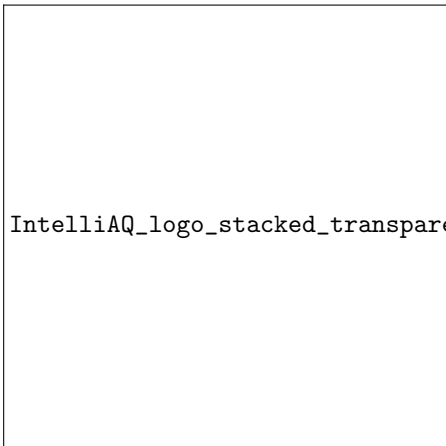
■ Preliminary conclusions:

- 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:

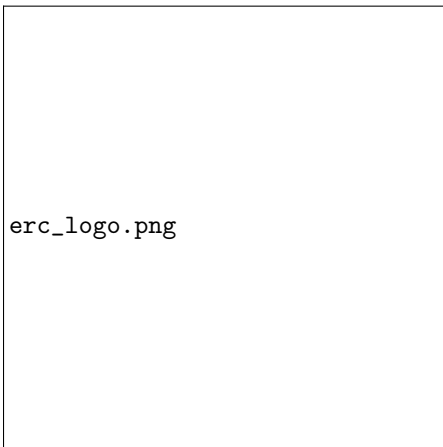
- Deep learning structure
 - Cost-sensitive CNN for imbalanced data
 - Universal network for all the stations
 - LSTM
- Data Level
 - Size of variables (Feature engineering, spatial factors etc.)
 - Heterogeneous data sources

Acknowledgement



IntelliAQ_logo_stacked_transparent.png

<http://www.IntelliAQ.eu>



erc_logo.png

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

Thank You!

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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).