A Study on Super-Resolution Neural Networks for Anthropogenic Emission Data

Preparatory Project

submitted by

Yuna Katsuyama

Supervisor

Prof. Mihalis Vrekoussis, Dr. Alex Poulidis, Santiago Parraguez Cerda

University of Bremen
Institute of Environmental Physics

Date of Birth: 23.02.2002
Matriculation Number: 6421479

Submission Date: 20.02.26

Abstract

Air pollution remains a major global health and environmental challenge, particularly in rapidly urbanizing regions where high-resolution emission data are scarce. With my proposed project I aim to develop a generalized, transferable framework for downscaling coarse global emission inventories to urban-scale resolution (1 km) using conditional Generative Adversarial Networks (cGANs). By learning spatial patterns from auxiliary data (for example road networks, land use, and night-time lights) the model will enable emission downscaling in any region, even without region-specific training. The downscaled emissions will be integrated into a chemistry transport model (e.g., ICON-ART) to simulate urban air quality, identify key pollution sources, and evaluate mitigation strategies for three main target cities, Tokyo (Japan), Hamburg (Germany), and Bangkok (Thailand). The outcome will be an open-source, globally applicable tool that improves the accuracy of air quality modeling, benefiting both high- and low-income countries. My research will address a critical data gap, support evidence-based policy, and advance equitable access to environmental science.

Contents

1 Introduction

1.1 Air pollution

Air pollution causes serious health problems. In 2019, air pollution caused about 6.7 million deaths. Air pollutants affect the cardiovascular, neurological, respiratory and other organ systems and they increases the risk of death from cardiovascular and respiratory disease, and lung cancer. The major health-damaging air pollutants are particulate matter (PM2.5 and PM10), ozone, nitrogen dioxide, sulfur dioxide and carbon monoxide. (World Health Organization, 2024)

In order to reduce the health impact, WHO published Air Quality Guidelines (AQG) that is the safe levels of pollutant to human health in 1987 and updated them in 2005 and 2021. (World Health Organization, 2021)

In the past, two big air pollution events which are London smog in 1952 and Los angels smog from 1940s to 1970s occurred. Air pollution has been dealt with for centuries and has the air quality has greatly improved.

However, as shown in Figure 1, a large proportion of the population still lives in the regions where air quality is worse than the AQG values.
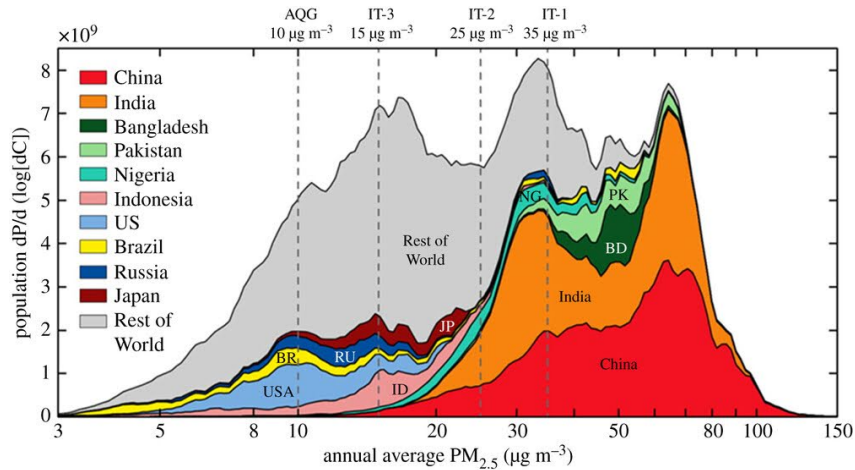

Figure 1: Distributions of the population as a function of annual (2013) average ambient PM2.5 concentration for the world's 10 most populous countries and the rest of the world. Dashed vertical lines indicate World Health Organization Interim Targets (IT) and the Air Quality Guideline (AQG). Reproduced from **Fowler:2020**.

Furthermore, while air quality has improved markedly in high-income countries over this period, it has generally deteriorated in most low- and middle-income countries, in line with large-scale urbanization and economic development. (World Health Organization, 2021) This indicates that addressing air pollution is particularly urgent in developing countries.

(different reason of air pollution , out door , in door) According to Folberth et al., 2015, the 26 largest cities account for significant shares of global emissions of greenhouse gases, 12% of carbon dioxide (CO_2), 7% of methane (CH_4), and large fractions of major air pollutants such as nitrogen oxides (NO_X; 4.6%), sulphur dioxide (SO_2; 5.3%), Black Carbon (BC; 3.8%) and Volatile Organic Compounds (VOCs; 4.8%) Air pollutants can be grouped into two, primary and secondary pollutants. Primary pollutants are emitted from source and secondary pollutants are chemically produced from the primary pollutant.

NO$_X$ is a mixture of NO and NO$_2$. It is a primary pollutant and it mainly emitted from human activities. High-temperature combustion such as transportation, power plants and industry produces ozone from N$_2$ and O$_2$. NO$_X$ has a short life time from one day to few days. PM is classified two PM$_2$.5 and PM$_1$0 by its particle size. Example of VOCs are benzen, toluene and formaldehyde. 80$\tilde{9}$0 % of VOCs are emitted from natural sources such as trees, plants and soil. Anthropogenic emission sources are solvent (paint and cleaning product), fuel and gas.

Chemistry transport models (CTMs) are the best tool for assessing air-pollution mitigation strategies. They simulate the emission, transport, and chemical transformation of key pollutants (e.g. NO$_X$, SO$_2$, CO, VOCs, and PM) to generate time-dependent, three-dimensional concentration and deposition fields (Seinfeld and Pandis, 2016). Pollutant lifetimes depend on meteorology (through wind, temperature, precipitation) and chemical interactions and are further complicated by secondary pollutant formation such as O$_3$, and secondary organic aerosols (SOA). By simulating these processes, CTMs reproduce atmospheric conditions and surface pollutant levels and enable scenario-based analyses (for example for emission reductions) to project air quality changes with potential mitigation strategies (Seinfeld and Pandis, 2016).

1.2 Importance of emission inventories

1.3 Emission downscaling

1.3.1 Rule-based downscaling

1.3.2 Machine learning-based downscaling

1.4 Purposes

In my master project, I aim to develop a downscale method of emission inventories by using machine learning. Implementation of auxiliary data (for example road networks, population distribution, land use and night-time lights) will be expected to improve the downscale accuracy. And city-scale analysis of downscaled emission inventories will enable to investigate the cause of air pollution. In my preparatory project, I aim to make initial result of emission downscaling using machine learning. The project consists of 3 main tasks, air quality data manipulation, neural network development and diagnosis with the sample dataset, and initial test with actual air quality data manipulation.

2 Methods

2.1 Machine learning models

Machine learning is a method to make computers learn from data without explicit programming. Basement of machine learning is linear regression. Neural network is a machine learning architecture. Convolutional neural networks (CNNs) are a supervised machine learning method, which were originally developed for images (2D data). They consist of a neural network with additional layers called convolution layers and pooling layers. A convolution layer extracts patterns from an image by applying a 2D filter (kernel) whose values are learnable parameters. The pooling layer then reduces the spatial dimensions of the resulting feature maps, which helps retain the most important

information while improving robustness against slight translations, rotations, and small distortions in the input image. Super-resolution CNNs (SRCNNs) represents the mapping function that takes the low-resolution image as the input and outputs the high-resolution one. It consists of three operations: patch extraction and representation, non-linear mapping and reconstruction. These three operators are modeled by the same form of a convolutional layer. (Dong et al., 2016).

train, validation and test Optimizer (Adam, SGDs) Epoch Actuivate function back error propoagation learning rate Loss function is an index of the model performance and it is calculated by the difference between the model result and target values. Loss function is also used to train the models by back error propagation. Two major ways are by mean square error (MSE, Eq. 1) and cross entropy (CE, Eq. 2). Suitable adaptation of loss function is important for the effective training. MSE is for prediction and BCE is for classification task.

$$\mathcal{L}_{\text{MSE}} = \frac{1}{N} \sum_{n=1}^{N} \sum_{i=1}^{C} (y_{n,i} - \hat{y}_{n,i})^2 \tag{1}$$

$$\mathcal{L}_{\text{CE}} = -\frac{1}{N} \sum_{n=1}^{N} \sum_{i=1}^{C} y_{n,i} \log (\hat{y}_{n,i}) \tag{2}$$

2.2 Experiment1: Hand written digits classification

As a preliminary test of convolutional neural networks (CNNs), I performed handwritten digit classification. This experiment was conducted to construct a basic CNN model and evaluate its performance. For this work, the MNIST dataset was used, which is available via the GitHub repository by **sunsided_minist**. The MNIST dataset consists of handwritten digits (0–9) and is commonly used for evaluating classification algorithms in machine learning. The implementation of the classification model was based on the example code by Khattak, 2022. This code utilizes PyTorch to create and train a neural network on the MNIST dataset. Modifications were made to reproduce and validate the results within the scope of this work. Cross entropy is used for loss function. The network consists of three convolutional layer and one fully connected layer. The filter size was 3×3 and number of filter in each convolutional layer was 32, 64 and 64. Stochastic gradient descent (SDG) was used for optimizer and the learning rate was 1e-4. As the number of dataset and the size of dataset were small. Batch learning was applied instead of mini-batch learning. Train dataset 1000 and validation dataset was 100. In this experiment, test has not done. CPU and GPU

2.3 Experiment2: Image super resolution

2.4 Experiment3: Emission super resolution

Global emission inventories typically have coarse spatial resolutions, over 0.1° ($\sim 10 \ km$). The Copernicus Atmosphere Monitoring Service global anthropogenic dataset (CAMS-GLOB-ANT; Kuenen et al., 2022) is the current state of the art, covering the globe with a 0.1° resolution.

2.5 Regrid method

area weighted average

3   Preliminary Results

3.1   Result1: Hand written digits classification

Fig. **??** shows the variation of loss function during training. It suggested that after approxiamately 100 epoch, the loss of train and validation was converged. Validation loss was more that 7 times higher than train loss after 200 epoch. Fig. **??** shows the recall of train and test data after 200 times of training (epoch). Recall is defined by the fraction of true positive to actual positive. Thus, the recall is calculated by average of true positive for $0\tilde{9}$ digit. The value is corrected across predicted. While train data prediction 100% correct with the target value(given label), it failed sometimes with the validation dataset. When the input image is 1, it is predicted as 1 every time, and when the input image is 9, approximately 80% are predicted as 9, while 10% predicted as 4 and 10% predicted as 7.
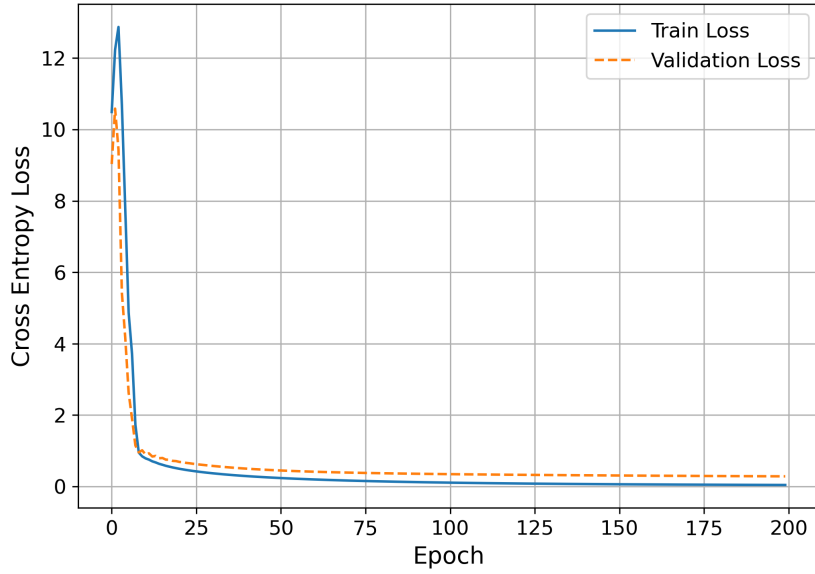

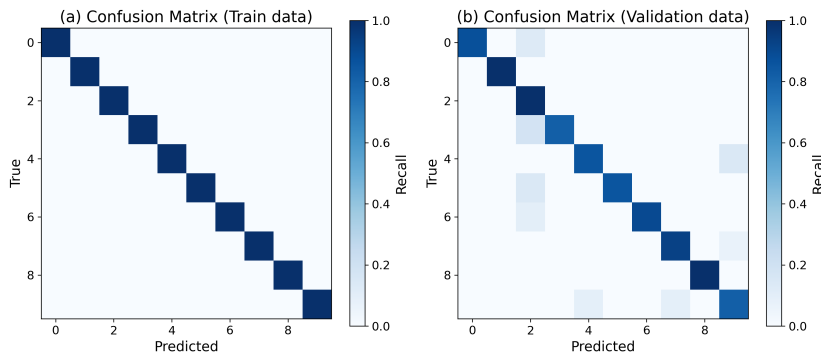Figure 2: Loss function vs. epoch.

Figure 3: Confusion matrix of the classification. (a) is a train data. (b) is a test data. X axis shows predicted value and Y axis shows target value. Color bar shows recall.

Total recall (average of $0\ \tilde{9}$) of train data and validation data were 1.0 and 0.91. The final loss of train and validation were 0.039 and 0.28. Runtime was approximately 6 min

with CPU.

3.2 Image super resolution

3.3 Emission super resolution

4 Discussion

5 Conclusion

6 Future Steps

References

Dong, C., Loy, C. C., He, K., & Tang, X. (2016). Learning a deep convolutional network for image super-resolution. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, *38*(2), 295–307. https://doi.org/10.1109/TPAMI.2015.2439281

Folberth, G. A., Butler, T. M., Collins, W. J., & Rumbold, S. T. (2015). Megacities and climate change–a brief overview. *Environmental pollution*, *203*, 235–242.

Khattak, R. (2022). Digit-classification-pytorch [Accessed: 30-01-2026].

Kuenen, J., Dellaert, S., Visschedijk, A., Jalkanen, J.-P., Super, I., & Denier van der Gon, H. (2022). Cams-reg-v4: A state-of-the-art high-resolution european emission inventory for air quality modelling. *Earth System Science Data*, *14*, 491–515. https://doi.org/10.5194/essd-14-491-2022

Seinfeld, J. H., & Pandis, S. N. (2016). *Atmospheric chemistry and physics: From air pollution to climate change*. John Wiley & Sons.

World Health Organization. (2021). Who global air quality guidelines.

World Health Organization. (2024). What are the health consequences of air pollution on populations? Retrieved August 20, 2025, from https://www.who.int/news/item/25-06-2024-what-are-health-consequences-of-air-pollution-on-populations