DEEP NEURAL NETWORK FRAMEWORK FOR INVERTING REMOTELY SENSED CO_2 MEASUREMENTS

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ABSTRACT

We propose a deep learning framework for estimating the CO_2 emissions by inverting the CO_2 concentration measurements from satellites. Our algorithm starts with informed guess of emission distributions of CO_2 and keeps on correcting it till it is consistent with outcome of transport model and CO_2 measurements by satellite. We found that our inversion method is capable of identifying emission sources of CO_2 that are not considered in the prior.

1 INTRODUCTION

Global warming and climate change are the direct effects of air pollutants like CO_2, CH_4, particulate matter and so on. International agreements such as the Kyoto Protocol (kyo (1997)) and the Paris Agreement (par (2015)) have been established to set the emission reduction targets for countries, in the context of global warming. Hence, to assess the effectiveness as well as the adherence by countries to these policies, governments and industries alike are very interested in estimating the distribution of emissions of these pollutants on the surface of the Earth.

For estimating emissions (or fluxes $kg/m^2/s$) broadly there are two classes of methods (McMarrow (2011)). The first, bottom-up methods involve gathering detailed inventory and activity data on individual sources, and the associated emission factors. Bottom-up methods can provide detailed information on the emissions. However, collecting and processing this detailed information can be a complex and costly undertaking. The second, top-down methods involve measuring concentrations (in ppm or similar measure) of the pollutant in the atmosphere and inferring the sources of those concentrations with the help of numerical transport models. Two major frameworks that have been widely used to achieve this are the Ensemble Kalman filter (EnKF) (Peters et al. (2005), van der Laan-Luijkx et al. (2017), Feng et al. (2008)) and the 4-D Variational (4D Var) method (Chevallier et al. (2005), Bergamaschi et al. (2013), Niwa et al. (2017a)).

It is very difficult to prepare and maintain the large amount of data required for inventory based methods. The top-down methods are computationally complex as they often involve running large ensembles of model simulations e.g. in ensemble Kalman filter. Implementing these algorithms require a deep understanding of the underlying physics and computational methods as well. Thus, there is a need for simplified procedure which reduces the complexity. Deep learning (DL) is finding a growing use in the atmospheric and geoscience community (Lauret et al. (2016), Tao et al. (2019), Wang and Qian (2018)) owing to their demonstrated capability in capturing non-linearities in a system.

In the present work, we propose a DL framework for inverting concentrations of a given pollutant and to estimate the distribution of its emissions. The method is generic and can be applied to any pollutant. However, for this work, we predict CO_2 in particular. The choice was determined by the the availability of good quality remotely sensed CO_2 concentrations and its significance to the global warming. Our contributions are:

[1]both authors contributed equally to the research.

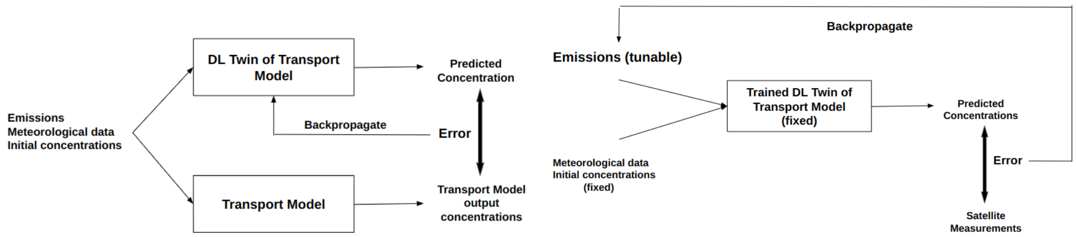

Figure 1: (Left) Part 1 of the proposed framework, (Right) Part 2 of the proposed algorithm

- End-to-end DL framework for inverting concentrations of a given pollutant species using satellite measurements.
- A digital twin of an existing numerical transport model.
- A system that can discover the additional emission sources of the species not included in the prior.

2 Proposed Methodology

2.1 Overview

The two major steps of the method are explained below:

Part 1: Digital twin of a transport model

1. Create a training data set for training a deep learning twin to mimic the results of the transport model. This is achieved by running a transport model with varying meteorological conditions and emission distributions of CO_2.
2. Train the model using the training data as prepared in the first step. Thus, we would have a digital twin of the transport model. It takes as input (i) the emission distribution (ii) meteorological conditions and (iii) initial concentrations and gives as output the future concentrations of the gas (1).

Part 2: Inversion

1. Take an initial (prior) estimate of the emission distribution. This estimate can come from bottom-up inventory-based methods or remote sensing observations and analyses (Deshpande et al. (2022); Banolia et al. (2023)).
2. Collect the satellite data of the CO_2 concentrations for the relevant dates. These will be total-column measurements.
3. Use the transport twin trained in part 1 to generate predictions of the concentrations using the relevant meteorological data and initial concentrations. Convert the concentrations over a 3D grid to total-column. The result will be a 2D grid of concentration predicted by the transport twin.
4. Compare the predictions with the satellite data and compute the 'loss'.
5. Hold all the parameters of the transport twin fixed and backpropagate the loss through the whole network to the emission values and update them. The strong assumption is that the measurements and the transport twin are correct.
6. With the updated emission values, repeat steps 3-6 while monitoring the magnitude of the loss between the twin's predictions and satellite measurements. Stop the iteration when the loss stops decreasing (1).

At the end of this step, the result will be the updated emissions that are consistent with the satellite measurements and transport process.

2.2 Digital twin of transport model

We evaluated 10 most well-known transport models (Bey et al. (2001), Lamarque et al. (2012), Grell et al. (2005), Hourdin et al. (2006), Byun and Schere (2006), Pisso et al. (2019), Maksyutov et al. (2008), McGregor and Dix (2008), Niwa et al. (2017b)) and chose the GEOS-Chem (Bey et al.

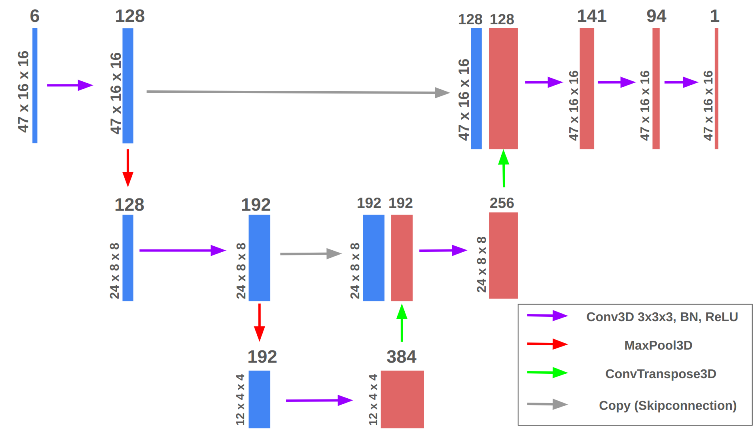

Figure 2: The U-Net architecture used in this work

(2001)) model. GEOS-Chem (Bey et al. (2001)) is widely used popuar transport model (Eastham et al. (2014)).

We used U-Net architecture (Ronneberger et al. (2015)) for deep learning (DL) twin that does the double duty of learning the transport and inversion (2).

DL Twin Model Training: The training data for the DL Twin (which is a neural network) was generated using the GEOS-Chem numerical transport model. The process involved providing the transport model with a wide range of input conditions and recording its output. These input-output pairs contain information about the physical processes that drive atmospheric transport and using these pairs, the DL Twin model would learn the same.

Its common to rescale the input quantities to make NN training more efficient. Hence we normalized the values of the inputs namely emissions, initial concentrations, winds, pressure and temperature to the range of 0 to 1. The values were then re-centered to 0.5 to bring most of the values in the range [0,1]. In order to account for the lack of boundary conditions, we excluded the cells at the edges of the grid for the computation of the loss function and hence for the training. If the correct concentration changes (over the 3D grid and inside the 10×10 horizontal region) are T and the corresponding predicted concentration changes are P, then the loss function we used is:

$$Loss = \frac{\Sigma(T_i - P_i)^2}{\Sigma T_i^2}. \tag{1}$$

.

Other important training parameters were batch size: 4, 3D convolution kernel size: $3 \times 3 \times 3$, model size: $\sim$ 7.6 million parameters, model weights initialisation using *kaiming-normal* (He et al. (2015)), activation function: ReLU, optimiser: `adam`, learning rate: 0.001, number of training epochs: 50.

We picked 61 days in the year at random and used all samples belonging to those days for the *validation* of our model. Samples belonging to the rest of the days were used for training. To prevent over-fitting the training was stopped when the validation loss stopped decreasing for some epochs.

2.3 Inversion

Prior Emissions For the prior emissions, we used the Open-source Data Inventory for Anthropogenic CO_2 (ODIAC) dataset (Oda and Maksyutov (2011)), which provides high-resolution global maps of fossil fuel CO_2 emissions. We obtained the satellite measurements of CO_2 concentrations from the OCO2_L2_Lite_FP data product of NASA's OCO-2 satellite. From this we mainly extracted the total-column CO_2 concentration measurements and the vertical averaging kernels corresponding to the relevant dates.

Inversion Procedure: With the trained DL twin model, we carried out the inversion step. We took the monthly averaged ODIAC CO_2 emissions for July 2018 over our Asia region, aggregated it to working resolution $4^\circ \times 5^\circ$ and took these emissions as the prior for 1st July 2018. The transport twin predicts the 3D concentrations (in ppm) for 2^{nd} July 2018. The 3D concentrations are converted to total-column concentrations using the OCO-2 averaging kernels corresponding to 2^{nd} July 2018. The predicted total-column concentrations are compared with the OCO-2 measurements for 2^{nd} July 2018 and the error is back-propagated to the emission values. Based on the corrected emissions, the twin model again predicts the 3D concentrations for 2^{nd} July and so on. 200 such iterations are performed.

3 Results and Discussion

Digital twin validation: The digital twin showed a low validation loss for concentrations. The correlation between the target and predicted values was high (0.885); the model was able to explain 75.1% of the variance in the data. In addition, we prepared samples from the year 2020 and computed the outputs and the loss. The loss averaged over all the 365 days is about 0.4921 which is not too far from the original validation loss, 0.4794. This is a positive indication of the model's generalization ability.

Inversion validation: After running inversion for 200 iterations with no constraints (first experiment) on the emission values from each individual ground cell, the value of the loss is 0.091495, which implies that with the corrected emissions the RMS error with satellite data is about 9%. To consider more realistic situation, we assumed ocean cell to be carbon neutral, and the land cells to show under 10% variability in the prior and posterior emissions. and ran these iterations as a second experiment. RMS error did not show any appreciable change in second experiment.

In addition to observing the loss, we also attempted to compare the results with other benchmark reports such as EDGAR 2022 report (Crippa and Vignati (2022)). For this, we aggregated the reported emissions for each country in Asia region for the year 2018. The first and second experiments gave annual emissions as $\sim$185 Gt and $\sim$60 Gt. respectively. The total emissions according to the EDGAR report were 17.811 Gt for 2018, thus the more realistic model compares well with the EDGAR report.

3.1 Limitations

We faced many limitations in this initial stage of our work, the foremost being limited GPU resources. A total GPU memory of 15 GB restricted the DL twin model size which in turn limited the (i) prediction timescale to 1 day, (ii) transport process to only advection and (iii) transport region to 7200 km $\times$ 9000 km, instead of global. Due to limited CPU resources as well, we used the coarsest resolution available for the transport grid. For inversion, the satellite (OCO-2) data for one day was very sparse; less than 20% out of the 256 cells had data. This could be resolved with a longer prediction timescale. We also faced difficulty in separating anthropogenic emissions from all emission sources that are taken into account by satellite data.

4 Conclusion and Future Work

In this work, we have proposed and implemented a novel algorithm for performing inversion of atmospheric concentrations of a pollutant such as CO_2 to estimate its emission distribution. We got some interesting results that need to be further investigated, particularly the ability to identify sources of the pollutant not included in the prior emissions.

In future, we intend to build a more robust DL transport twin model for more reliable inversion. Particularly, the architecture of the network and the feature engineering in the input data will be important directions to work on. For inversion, the prior emissions should ideally account for the same sources as the satellite measurements. Moreover, it will be helpful to take into account the uncertainties in the satellite measurements. Finally, our grid resolution of $4^\circ \times 5^\circ$ is too coarse for any practical application. Implementing our algorithm on a much higher resolution will provide us more insights but at the same time will be computationally expensive.

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