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AI4Urban project website

Machine-learning based variational data assimilation for unknown emission source identification in urban environments

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Introduction

Urban pollutants transport affected by:
- Urban boundary layer flow
- Emission sources

To identify emission sources, inversion method (data assimilation) is used
- Given observed mixing ratio at locations
- Given (or modelling) meteorological conditions
- Find emission location and rate

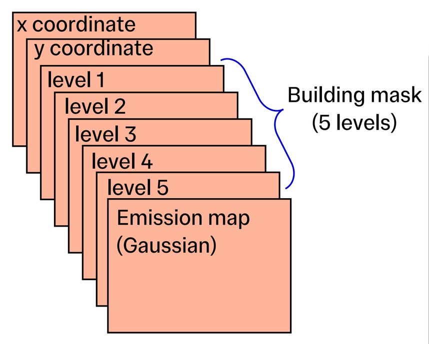
Physics-based methods:
- Based on numerical methods;
- Obeying physical conservations;
- Can be slow

Data-driven method:
- Fast
- Automatic-differentiation (no need to code adjoint)

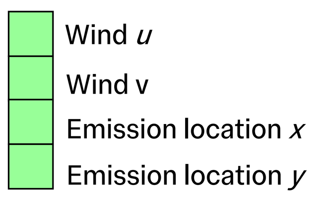
Forward model

U-Net with FiLM condition modulation

Input: (B, 8, 200, 200)



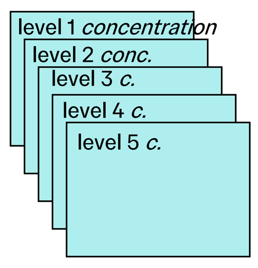
Condition: (B, 4)



U-Net Architecture

Stage	Layer	Output shape	Params
Input	–	$8 \times 200 \times 200$	–
Encoder	DoubleConv (32)	$32 \times 200 \times 200$	16,064
	MaxPool2d	$32 \times 100 \times 100$	–
	DoubleConv (64)	$64 \times 100 \times 100$	64,064
	MaxPool2d	$64 \times 50 \times 50$	–
Bottleneck	DoubleConv (128)	$128 \times 50 \times 50$	238,400
Decoder	ConvTranspose2d (64)	$64 \times 100 \times 100$	32,832
	DoubleConv (64)	$64 \times 100 \times 100$	119,360
	ConvTranspose2d (32)	$32 \times 200 \times 200$	8,224
	DoubleConv (32)	$32 \times 200 \times 200$	32,192
Output	Conv2d (1×1)	$5 \times 200 \times 200$	165

Each DoubleConv consists of:
- 1st convolution (in_ch , out_ch , kernel_size=3, padding=1)
- A FiLM modulating layer to inject condition — *FiLM: **F**eature-w**i**se **L**inear **M**odulation*
  - MLP: 4 -> 64 -> 2 * out_ch
  - Then apply to each channel: $\alpha \cdot x + \beta$
- 2nd convolution (out_ch , out_ch , kernel_size=3, padding=1)



Output: (B, 5, 200, 200)

Concentration fields on five layers

Loss function (weighted MSE loss) (weighted inversely with pixel value frequency)

Ground truth concentration fields

Training for 20,000 epochs: Training MSE error ~7e-5, Validation MSE error ~3e-4 (normalised log10 ppm)

Inversion model

Bayesian formulation and MAP estimation

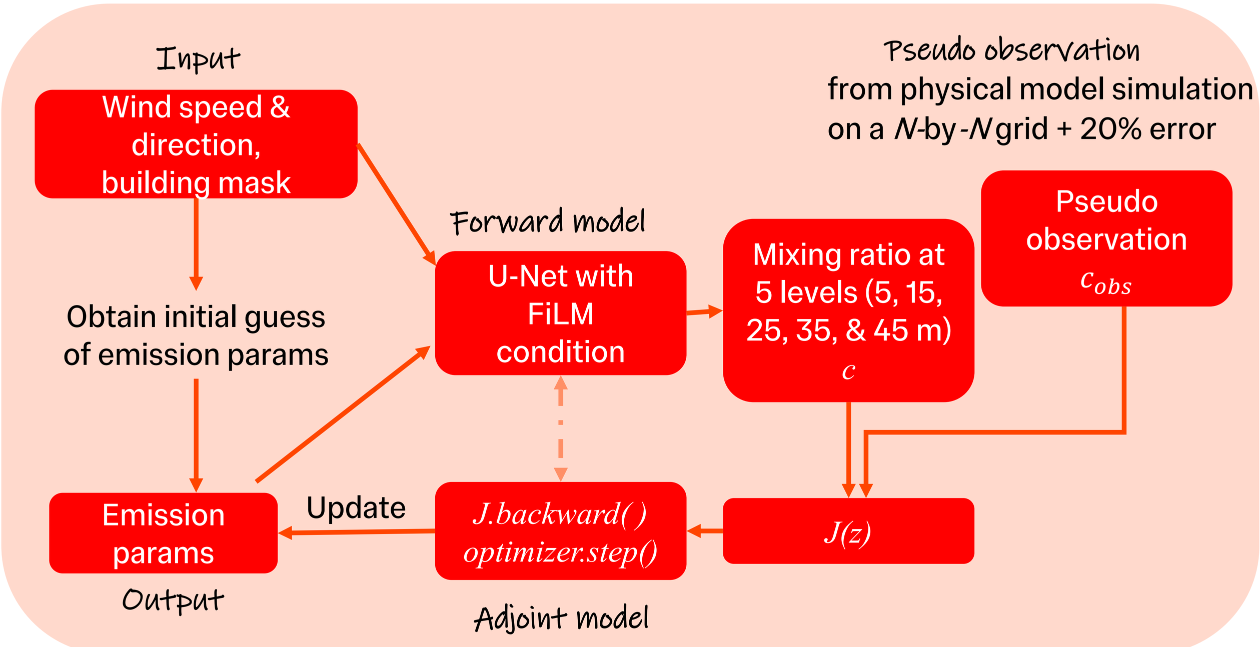
- Background error: uniform distribution
  - Assuming no prior information
- Observation error: Gaussian distribution
  - Assuming all obs points' errors are independent and at same level (20% ppm)
- Using max a posterior estimation, **cost function**

$$J(z) = \frac{1}{2}\left(\log_{10}(c_{obs}) - \log_{10}\left(\boldsymbol{H}(\boldsymbol{M}(z))\right)\right)^T \mathbf{R}^{-1}\left(\log_{10}(c_{obs}) - \boldsymbol{H}(\boldsymbol{M}(z))\right)$$

where $z = [x_e, y_e, r_e]^T$ $\boldsymbol{M}$: forward model $\boldsymbol{H}$: obs operator

Inversion process

- Selection of pseudo-observations:
  - A grid of N-by-N obs points on 35-m level
  - 20% random perturbation (error) added to pseudo-obs.
- Initial guess of z : (x_e, y_e, r_e)
  - Trial of a series of candidates
  - select the one with minimal J as initial guess
- Optimisation method:
  - `torch.optim.Adam`
  - Learning rate = 1
  - Call `J.backward()` for gradient
  - `optimizer.step()` for updating parameters



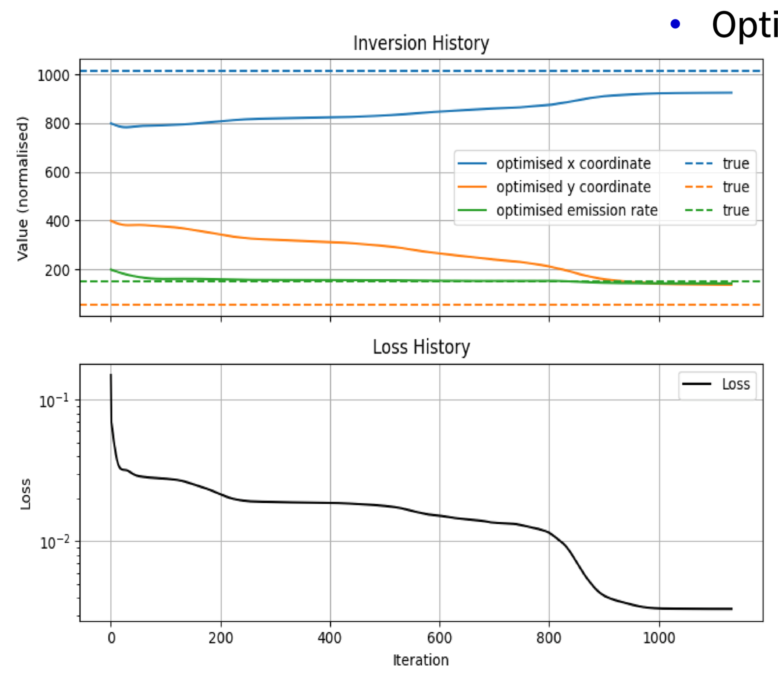
Results

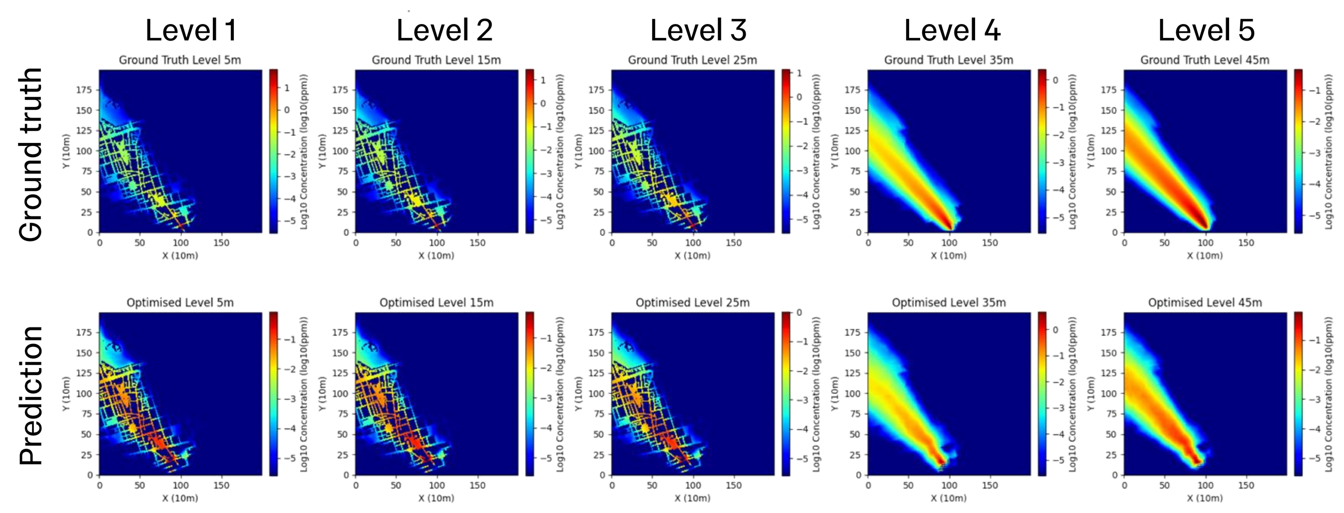
Inversion history of a particular case

Single emission source

- 10 m/s SE wind, single emission location
- Ground truth: location (1015, 55), 150 ton/yr
- Optimised: location (925.1, 137.3), 142.0 ton/yr

Using 16 ob pnts (on a 4x4 grid)



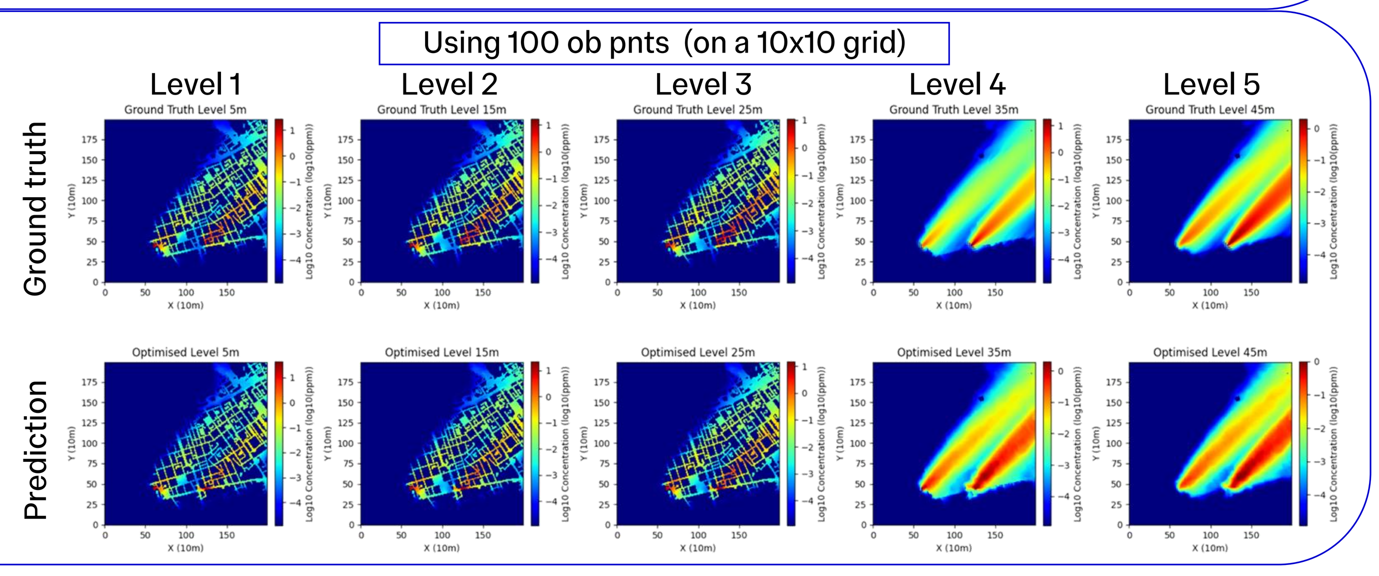


- Predicted concentration using optimised emission parameters
- All colour-bar using log10 (ppm) scale.

Double emission sources

Using 100 ob pnts (on a 10x10 grid)

- 10 m/s SW wind, two emission locations
- Ground truth:
  - location #1: (615, 455), 150 ton/yr
  - location #2: (1215, 455), 564 ton/yr
- Optimised:
  - location #1: (615.5, 453.8), 159.8 ton/yr
  - location #2: (1207.6, 431.5), 497.3 ton/yr



Statistics of all inversion test cases

Single source inversion

Statistics	Location error (m)	Emission rate error (%)
mean	242.94	4.53
std	283.23	12.17
min	0.12	0
25%	48.14	0.02
50%	160.26	0.82
75%	335.11	4.33
max	2401.35	145.88

Total number of test cases: 824

Double sources inversion

Statistics	Source 1 Location error (m)	Source 1 Location error (m)	Source 2 Location error (m)	Source 2 Location error (m)
mean	137.28	31.05	147.39	30.63
std	260.86	38.04	278.35	37.61
min	0.26	0	0.33	0.04
25%	25.95	7.48	26.27	6.90
50%	49.43	18.09	51.35	17.81
75%	144.16	41.23	146.97	41.23
max	2196.48	458.69	2360.80	364.14

Total number of test cases: 2000

Data used in this study

Simulated data is used in this study
- Study region: 2 km by 2 km by 500 m around BT tower in Camden, London
- Using urban LES model PALM
- Varying building height based on real OpenStreetMap data
- Releasing 1 single point source at each case
- 4-hr simulation (steady turbulence)
- a total of 4000 cases.

Wind direction
S, SW, W, NW, N, NE, E, SE

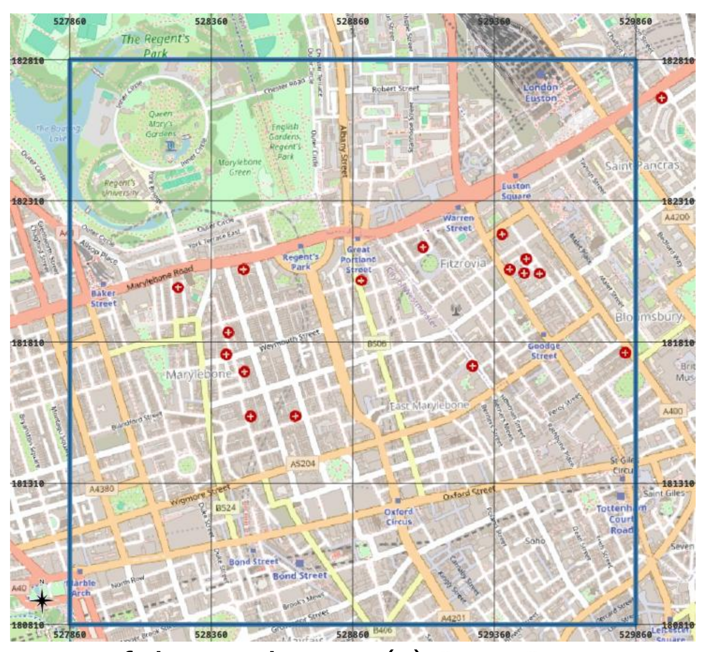
Wind speed
4, 6, 8, 10, 12 m/s

(Log profile is used, numbers here is wind speed at 190 m height)

Emission location
x = 15, 215, ..., 1815
y = 55, 255, ..., 1855
A total of 100 locations

Emission rate
Fixed at 564 ton/yr

(For other emission rates, linearity of transport eq. can be used to derive concentration)



Map of the study area (c) OpenStreetMap

Reference:
- (C) OpenStreetMap Distributed under the Open Data Commons Open Database License (ODbL) v1.0 (for further information, please see https://www.openstreetmap.org/copyright/en)]
- PALM: Maronga, B., et al. (2020). "Overview of the PALM model system 6.0." Geosci. Model Dev. 13(3): 1335-1372.
- U-Net: Ronneberger, Olaf, Philipp Fischer, and Thomas Brox. "U-net: Convolutional networks for biomedical image segmentation." International Conference on Medical image computing and computer-assisted intervention. Cham: Springer international publishing, 2015.
- FiLM: Perez, E., et al. "Visual reasoning with a general conditioning layer, Courville." In Proceedings of the AAAI Conference on Artificial Intelligence. 2017.

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