Adversarially trained LSTMs on reduced order models of urban air pollution simulations

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[INTRODUCTION]

- **Given the amount of data in Computational Fluid Dynamics (CFD) simulations, data-driven approaches are attractive solutions to produce reduced order models (ROMs) [1].**
- **Forecasts using ROMS can be obtained at a fraction of the cost of the original CFD model solution.**
- **Recurrent neural networks (RNN) have been used to model and predict temporal dependencies between inputs and outputs of ROMs [2].**
- **A way to obtain reliable forecasts comes from adversarial losses via adversarial training. This can add robustness by detecting and rejecting adversarial examples.**

[METHODS]

Our workflow (Fig. 1) is composed of four steps:

1. The model fields **x** are decomposed via Principal Components Analysis (PCA). PCA is an unsupervised learning method that simplifies high-dimensional data by transforming it into fewer dimensions. By truncating these Principal Components (PC) we obtain a reduced order model (ROM).
2. The truncated PCs (**P**) are then used to train a Long Short-term Memory (LSTM) network. This is useful for forecasts, and at lower computational cost given that the LSTM is trained on a ROM. The LSTM network takes N previous time-steps to predict the next one.
3. We proposed training the LSTM using adversarial training (adv). This type of training can add robustness by detecting and rejecting adversarial examples with the addition of a discriminator. To reduce the design space, a mirrored LSTM was used in the discriminator. The losses of the LSTM with adversarial training are:

$$\mathcal{L}_D^{adv}(\mathbf{P}_{t+1}) = \mathcal{L}^{bce}(D(\mathbf{P}_{t+1},1)) + \mathcal{L}^{bce}(D(f^{LSTM}(\mathbf{P}_{t-N},\dots,\mathbf{P}_t),0))$$
$$\mathcal{L}_{fLSTM}^{adv}(\mathbf{P}) = \mathcal{L}^{bce}(D(f^{LSTM}(\mathbf{P}_{t-N},\dots,\mathbf{P}_t),1)) + \mathcal{L}^{mse}(f^{LSTM}(\mathbf{P}_{t-N},\dots,\mathbf{P}_t))$$

where bce is Binary Cross-entropy and mse is mean squared error.

4. Once the forecasts are obtained in the ROM space, they are projected back to the PC space, and then to the Physical Space.

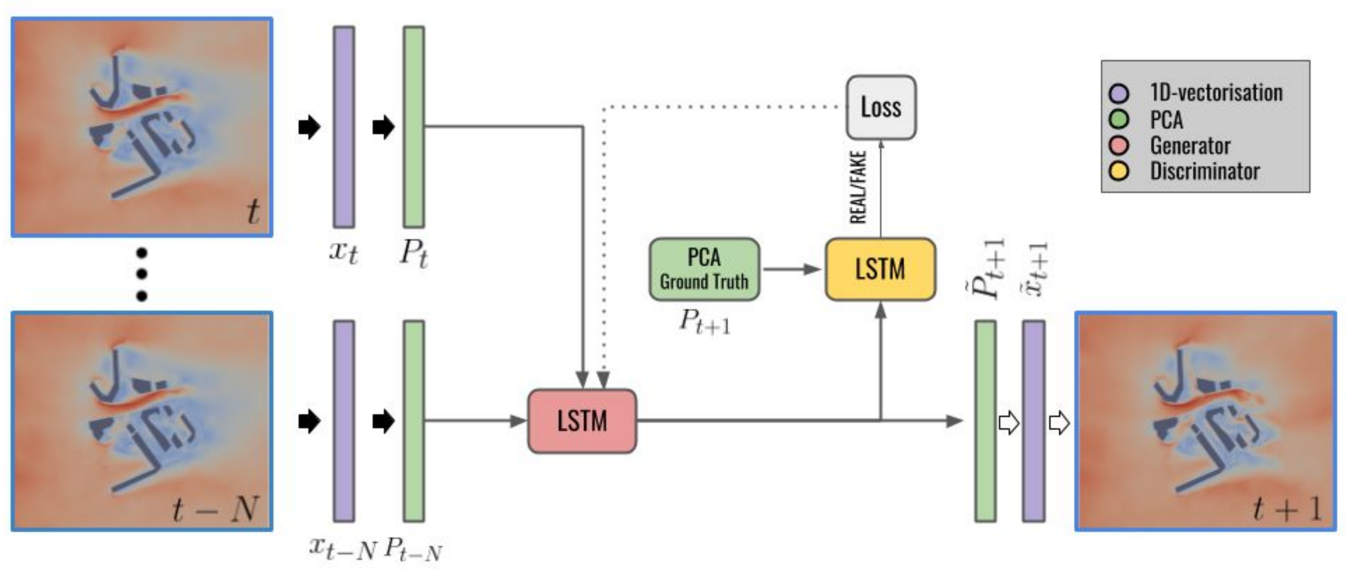

Fig 1. Proposed workflow for adversarial training of LSTM.

[STUDY AREA]

The study area is a 3D realistic representation of a part of Southeast London. And the data comes from a CFD simulation including velocities, and tracer fields. The tracer field mimics a busy traffic junction. The dispersion of the pollution is described by the classic advection-diffusion. Our workflow is general enough to represent any other CFD model solution in different locations given that enough data is available.

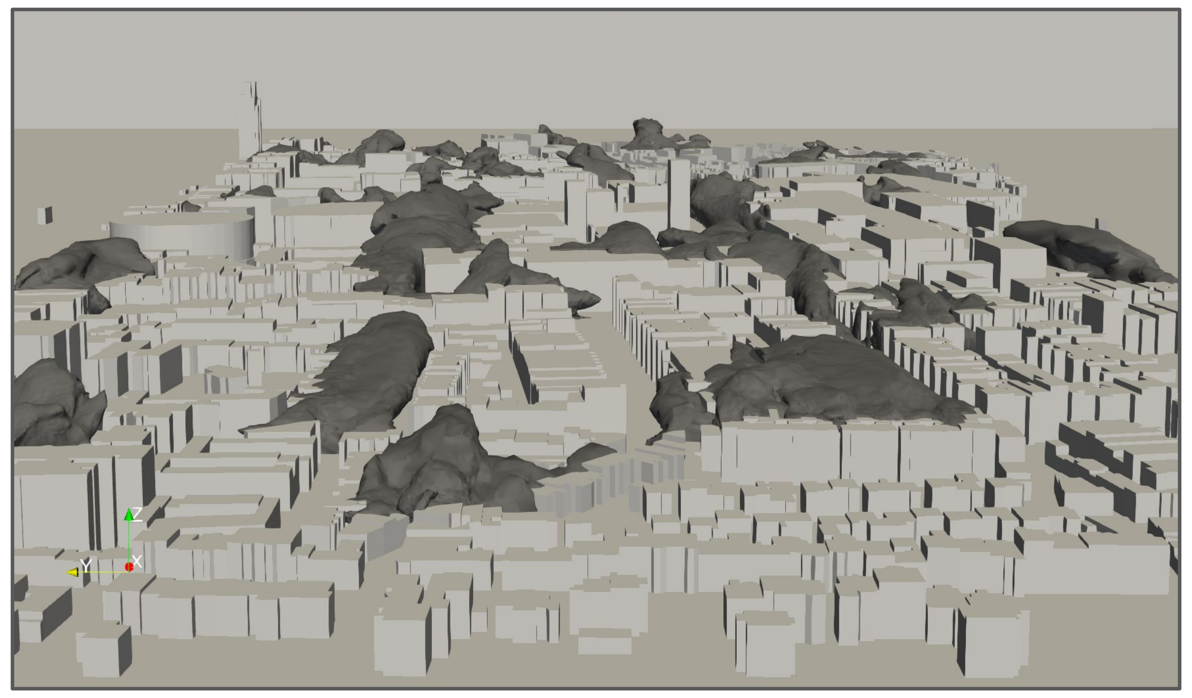

Fig 2: CFD simulation, with different tracers, of South Kensington, London, UK. This is a potential, more complex, domain that could be used to scale our workflow.

[RESULTS]

Four experiments were set up to assess the improved forecast of the adversarially trained LSTM ($LSTM^{adv}$). A PCA was applied to two output fields from the CFD simulation: Tracer (1-dimensional, unitless), and Velocity (3-dimensional, ms−1). To each of these set of PCs, a truncation of 64 and 128 PCs was applied which explains over 90% of variance in each case. The truncation to 64 PCs and 128 PCs reduces the size of the dataset by 4 and 3 orders of magnitude, respectively. Only 90% of the data is used for training, and 10% is used for validation.

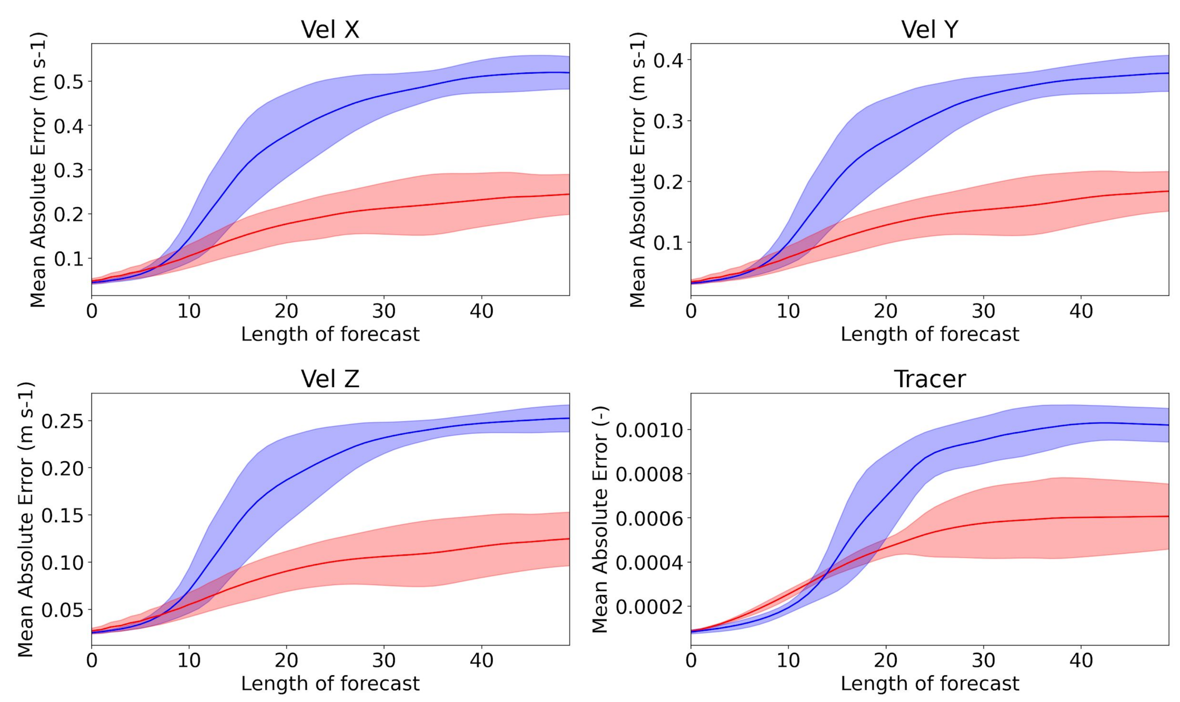

Fig 3. Comparison of $LSTM^{classic}$ (blue) and $LSTM^{adv}$ (red). The shaded areas show an ensemble of errors of 50 time-step long forecast from different starting points within training data) with 128 PCs. The solid line is the mean and the shaded area is one standard deviation from the mean.

The forecasts are created by using previous time-steps from data and producing a forecast. This forecast is subsequently used as an input for the prediction of the next time-step. After a set observation period (iterations), it is very clear that the LSTM with adversarial training outperforms the LSTM trained in a "classic" way. The forecasts are 4 orders of magnitude faster than the CFD simulation.

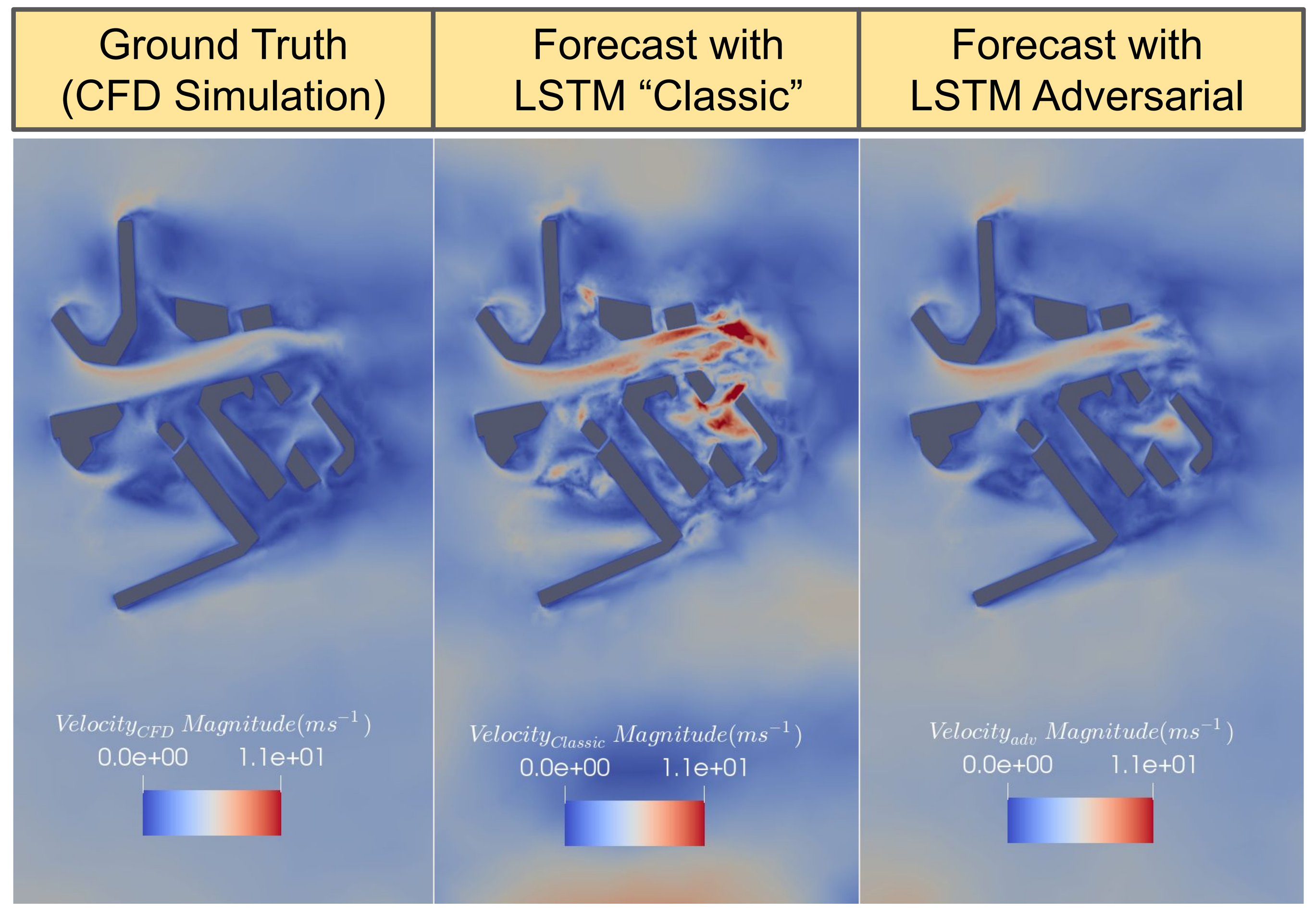

Fig 4. Comparison of forecasted velocity in ms^{-1} (magnitude) fields by LSTM without adversarial training and LSTM with adversarial training with 64 PCs. This is a 25 time-step forecast starting from *t=350*.

[CONCLUSIONS]

- **We presented an adversarially trained LSTM that improves the forecast of a LSTM trained in a "classical" way.**
- **This is important when accurate near real-time predictions are needed and not enough data is available. It can be observed that adversarially trained LSTM does not diverge greatly from the underlying physical model given the constraint of the discriminator network.**
- **The replacement of the CFD solution by these models will speed up the forecast process towards a real-time solution. The robustness of the adversarial training could produce more physically realistic flows.**
- **Future work will apply the same methodology to different dimension reduction schemes. Furthermore, this framework is data-agnostic and could be applied to different CFD models of larger complexity where enough data is available.**

REFERENCES

[1] Quilodrán Casas C., Arcucci, R., & Guo, Y. (2020, February). Urban air pollution forecasts generated from latent space representation. In *ICLR 2020 Workshop on Integration of Deep Neural Models and Differential Equations.*

[2] Quilodrán Casas, C., Arcucci, R., Wu, P., Pain, C., & Guo, Y. K. (2020). A Reduced Order Deep Data Assimilation model. *Physica D: Nonlinear Phenomena*, *412*, 132615.