Adversarial autoencoders and adversarial LSTM for improved forecasts of urban air pollution simulations

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BACKGROUND

- Given the amount of data in Computational Fluid Dynamics (CFD) simulations, data-driven approaches are attractive solutions to produce reduced order models (ROMs).
- 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 **[1]**.
- A way to obtain reliable forecasts comes from adversarial losses via adversarial training. This can add robustness by detecting and rejecting adversarial examples **[2]**.

STUDY AREA

The study area is a 3D case including 14 buildings representing a real urban area located near Elephant and Castle, South London, UK. The 3D case is 720m x 676m x 250m is composed of an unstructured mesh including m = 100,040 nodes per dimension and n = 1000 time-steps

The tracer field mimics a busy traffic junction. A log-profile velocity (representing the wind profile of the atmospheric boundary layer) is used in the 3D case. The building facades and bottom surface have no-slip boundary conditions. Whilst, top and sides of the domain have a free-slip boundary condition.

METHODS

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

1. The model fields $\mathbf{x}$ are decomposed via Principal Components Analysis (PCA). PCA is an unsupervised learning method that simplifies high-dimensional data by transforming it into fewer dimensions.

2. The truncated PCs ($\mathbf{P}$) are then used to train an adversarial auto encoder (PC-AAE). This produces matches the latent space to an arbitrary prior:

$$\mathcal{L}^{adv}_{\mathcal{D}^A}(\mathbf{P}) = \mathcal{L}^{bce}_{\hat{\mathbf{z}}\sim p(\mathbf{z})}(\mathcal{D}^A(\hat{\mathbf{z}}),1)) + \mathcal{L}^{bce}_{\mathbf{z}\sim q(\mathbf{z})}(\mathcal{D}^A(\mathbf{z}),0))$$
$$\mathcal{L}^{adv}_{f PC-AAE}(\mathbf{P}) = \mathcal{L}^{bce}_{\mathbf{z}\sim q(\mathbf{z})}(\mathcal{D}^A(\mathbf{z}),1)) + \mathcal{L}^{mse}(\tilde{\mathbf{P}},\mathbf{P})$$

3. The latent space $\mathbf{z}$, is then trained using an adversarial LSTM (ALSTM). This type of training can add robustness by detecting and rejecting adversarial examples with the addition of a discriminator. Since $\mathbf{z}$ is sampled from a normal distribution this gives ALSTM a constraint and reduces the possibility to land on out-of-distribution data:

$$\mathcal{L}^{adv}_{\mathcal{D}^B}(\Delta\mathbf{z}) = \mathcal{L}^{bce}(\mathcal{D}^B(\Delta\mathbf{z},1)) + \mathcal{L}^{bce}(\mathcal{D}^B(\Delta\tilde{\mathbf{z}},0))$$
$$\mathcal{L}^{adv}_{f ALSTM}(\Delta\mathbf{z}) = \mathcal{L}^{bce}(\mathcal{D}^B(\Delta\tilde{\mathbf{z}},1)) + \mathcal{L}^{mse}(\Delta\tilde{\mathbf{z}},\Delta\mathbf{z})$$

where bce is binary cross-entropy and mse is mean squared error.

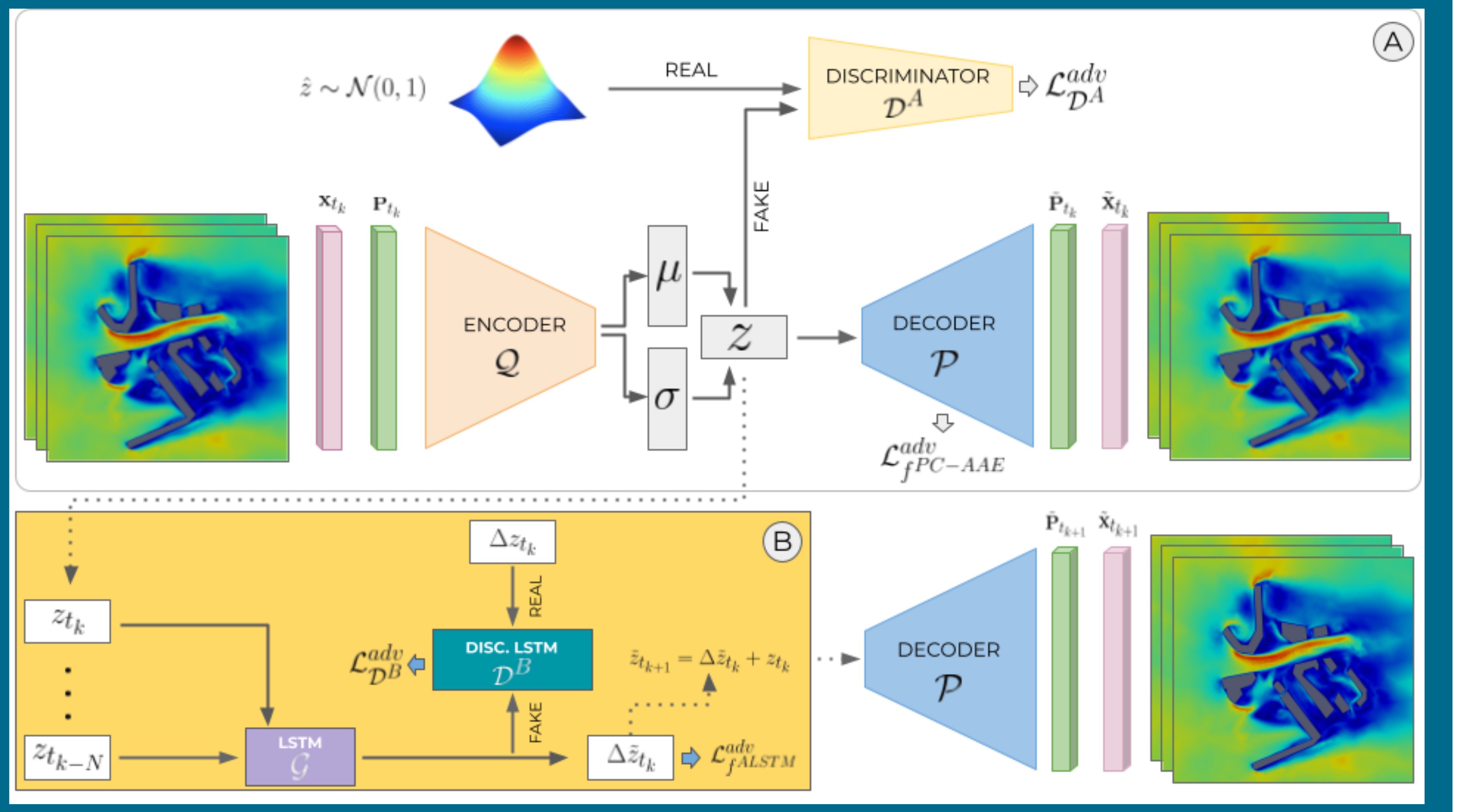

Fig. 1. Network A: PC-based adversarial AE. Network B: Adversarial LSTM. Solid lines input within the same network, dashed lines input to another network.

4. Once these networks are trained, we are able to return to the physical space with:

$$\tilde{\mathbf{z}}_{t_{k+1}} = \Delta\tilde{\mathbf{z}}_{t_k} + \mathbf{z}_{t_k}$$
$$\tilde{\mathbf{x}}_{t_{k+1}} = \mathcal{P}(\tilde{\mathbf{z}}_{t_{k+1}}) + \bar{\mathbf{x}}$$

Our workflow is general enough to represent any other CFD model solution in different locations given that enough data is available.

RESULTS

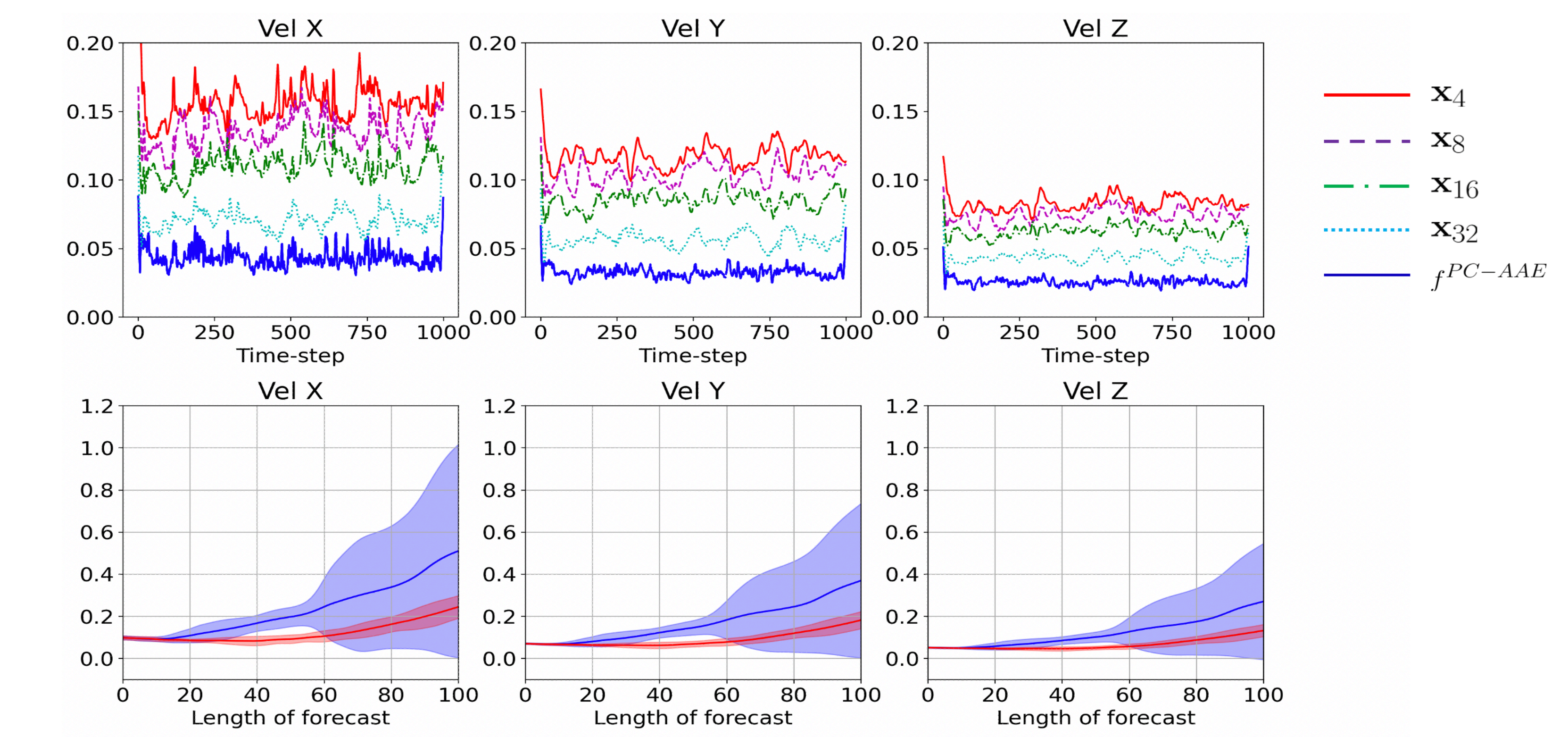

Fig. 2. Mean absolute error in m s-1. Top: $f^{PC\text{-}AAE}$ and reconstruction $\mathbf{x}_\tau$ with τ = {4, 8, 16, 32} principal components. Bottom: Ensemble of forecast errors with LSTM without adversarial training (blue) and Adversarial LSTM (red) from 50 different starting points using 8 dimensions in the latent space. The solid line is the mean and the shaded area is one standard deviation.

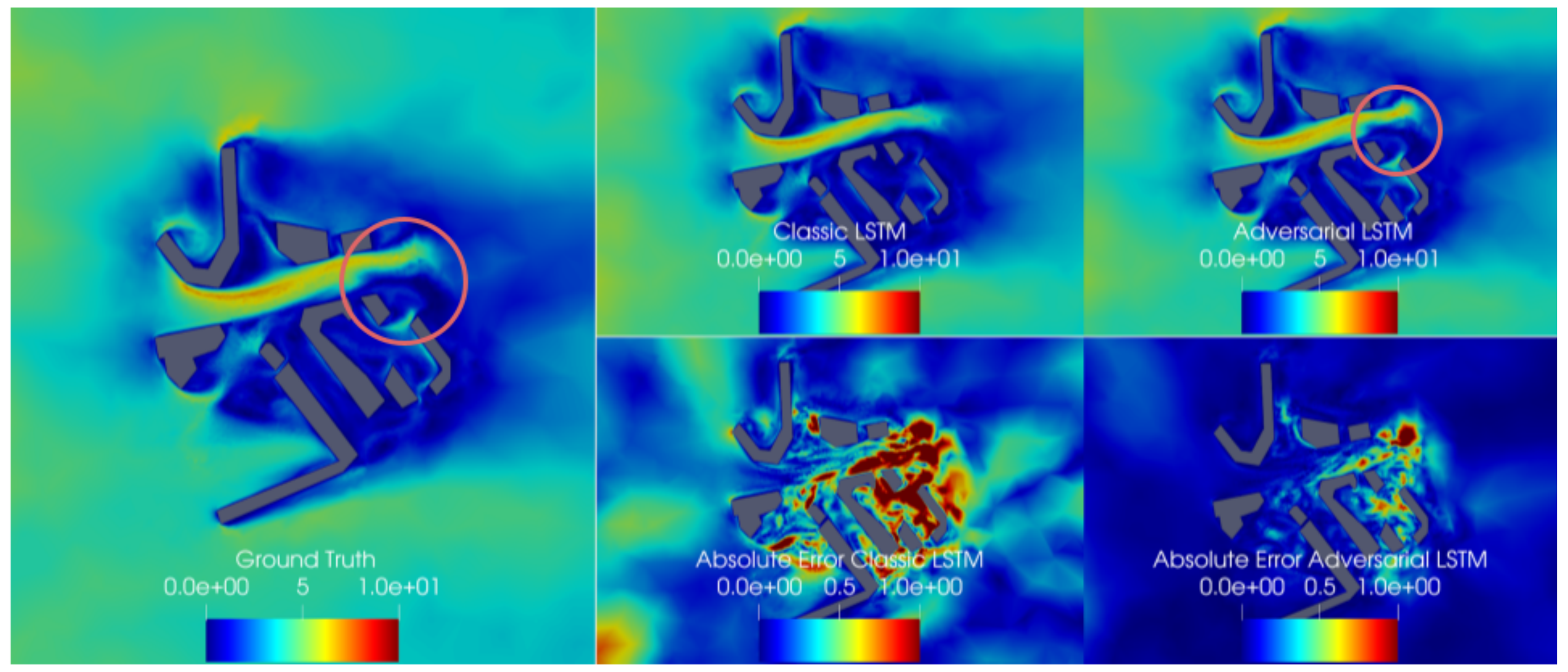

Fig. 3. Comparison of forecasted velocity in m s-1 (magnitude) fields by LSTM without adversarial training and the adversarial LSTM and the absolute error with respect to the ground truth. This is a 80 time-step forecast starting from t=200. This is a horizontal slice normal to the Z-axis 10 m above ground.

SUMMARY

We have presented for adversarial training add robustness to forecast CFD simulations in the latent space. Our general workflow allow us to produce real-time and realistic flow forecast up to 4 orders of magnitude faster than the original CFD simulation.

REFERENCES

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[2] Quilodrán-Casas, C., Arcucci, R., Pain, C., & Guo, Y. (2021). Adversarially trained LSTMs on reduced order models of urban air pollution simulations. *Machine Learning and the Physical Sciences NeurIPS 2020 workshop.*

Paper and code

Inhale project