

Structural Machine Learning Models and Their Applications

期末報告 資料一高哲凱

Introduction

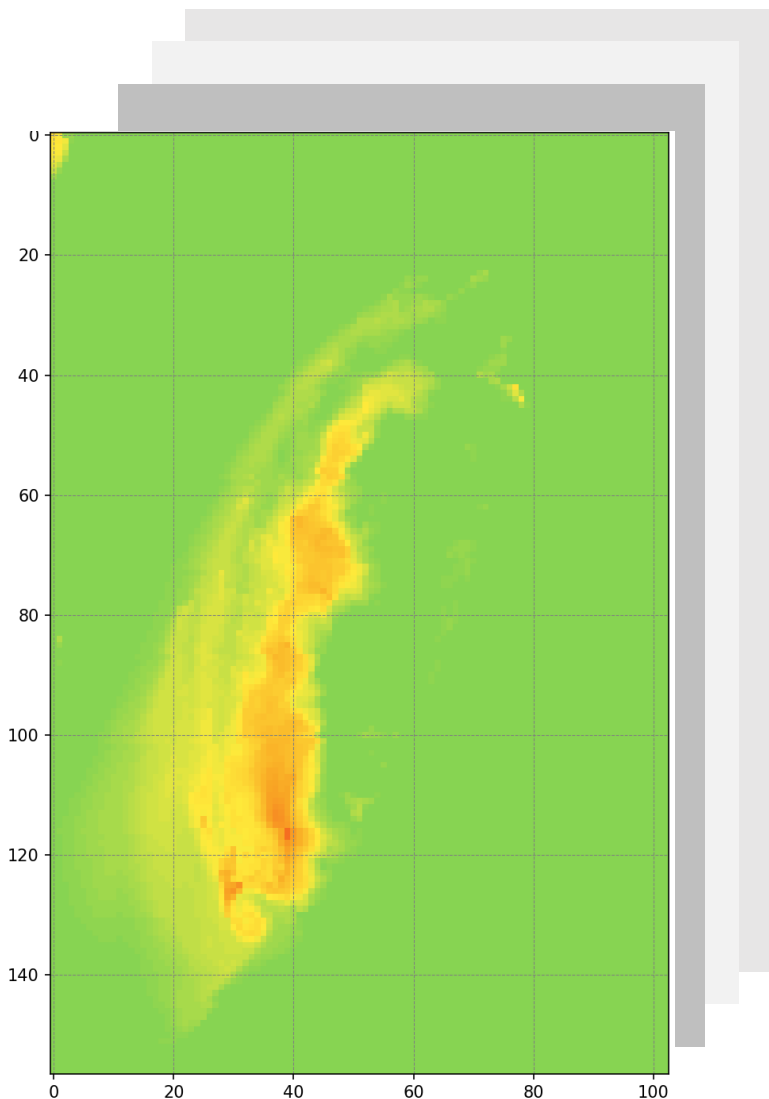
一、任務：使用前一小時PM2.5，並給定其他輔助資料，預測未來一小時的PM2.5。

二、資料來源：[中研院高解析度空氣品質擬預報資料](#)

三、訓練資料：2020, 2021, 2022 年份，共12,771筆 (shape: 157x103)

四、測試資料：2023 年份，共4,340筆 (shape: 157x103)

Training



INPUT

5/1 00小時的

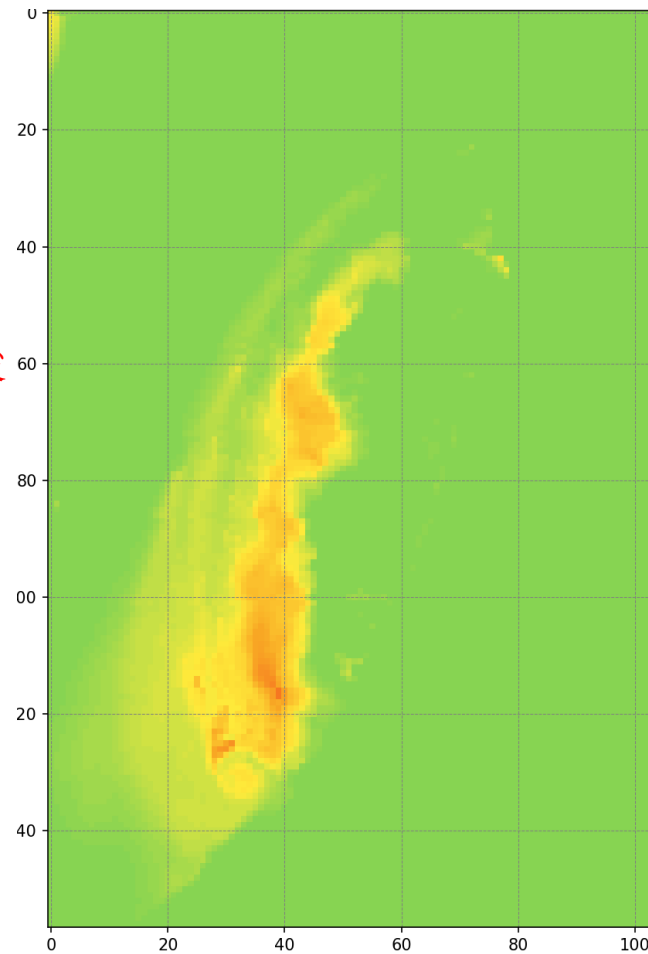
- PM2.5場



5/1 01小時的

- 溫度場(K)
- 風速場
- 風向場
- 濕度場
- 經度
- 緯度

5/1 01小時的 Ground Truth



OUTPUT

5/1 01小時的

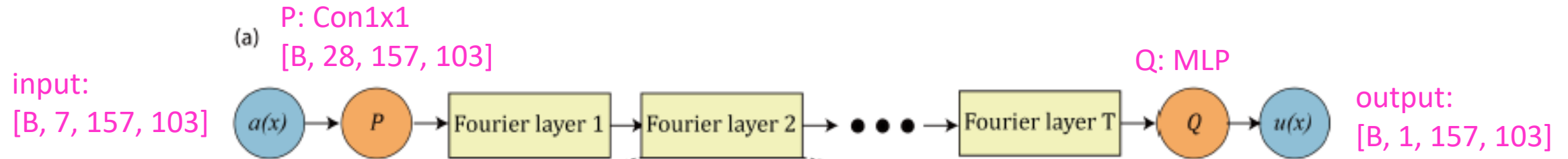
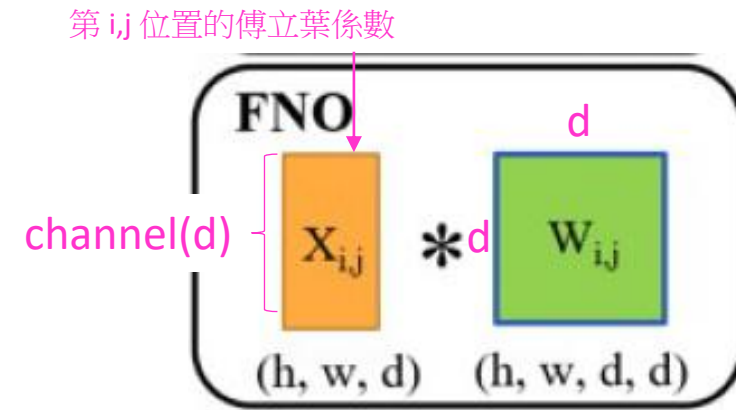
- PM2.5場

MSE Loss

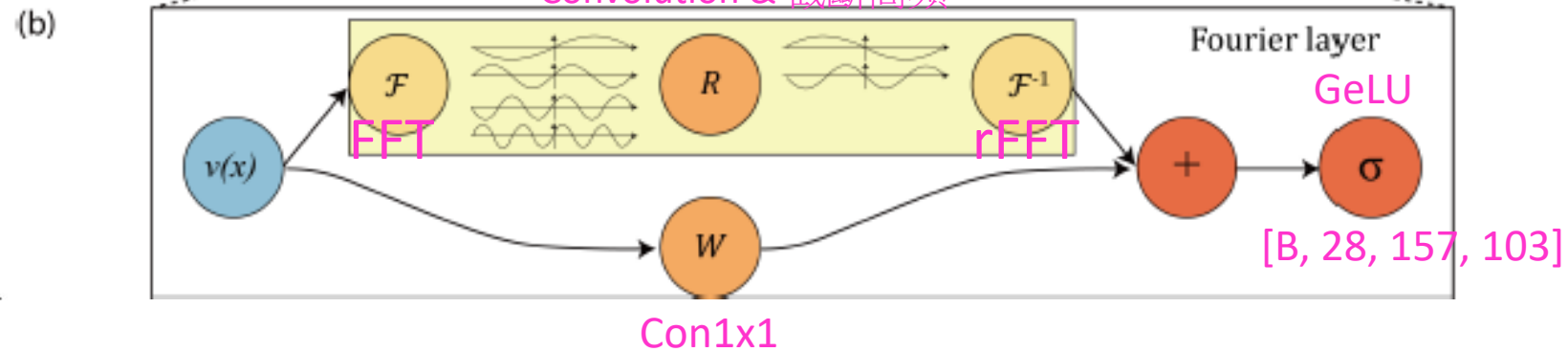
Model

1. FNO (Fourier Neural Operator)

B: batch size=32



對傅立葉係數做
Convolution & 截斷高頻



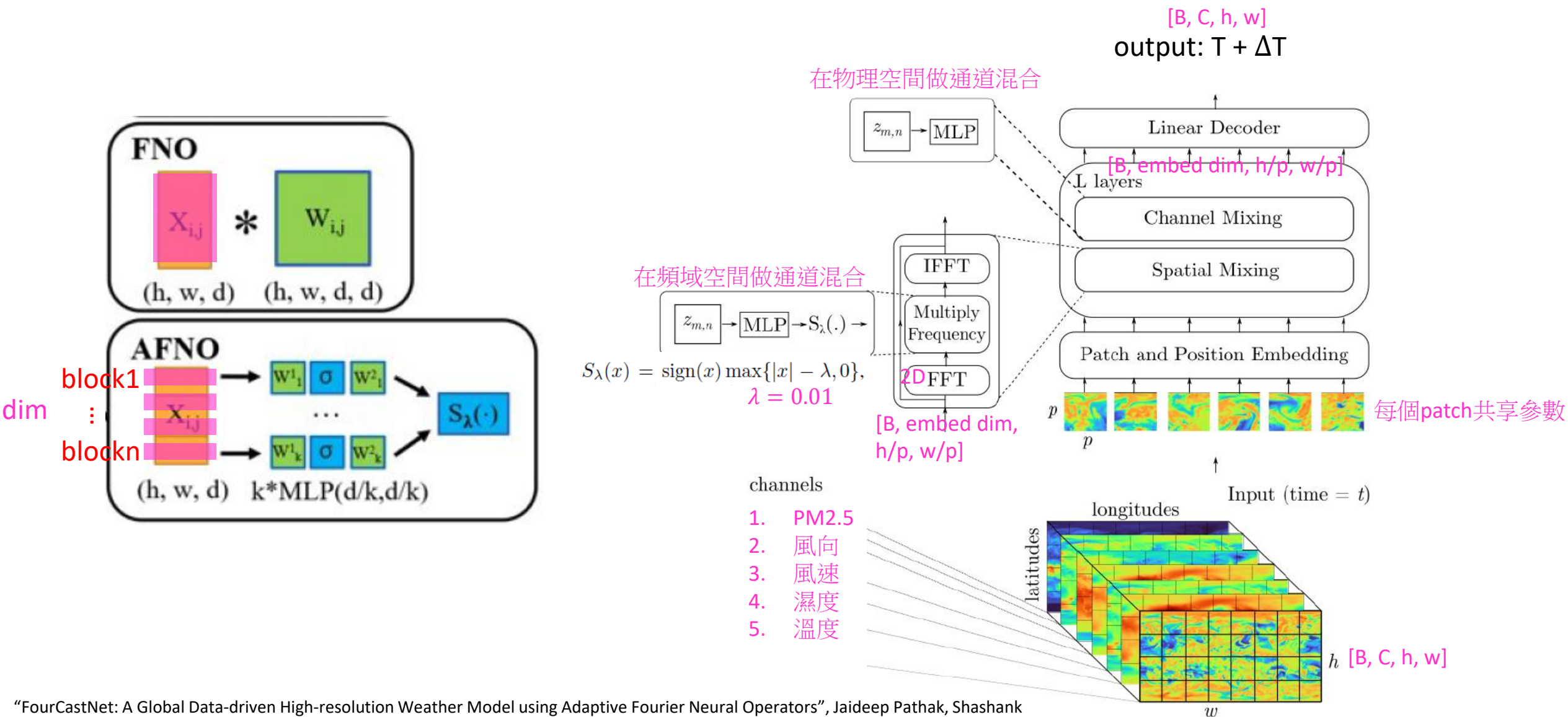
Li, Z., Kovachki, N., Azizzadenesheli, K., Liu, B., Bhattacharya, K., Stuart, A., & Anandkumar, A. (2021). *Fourier Neural Operator for Parametric Partial Differential Equations*. In *International Conference on Learning Representations (ICLR)*.

Model

2. FNO (Fourier Neural Operator)

- 在頻域學習 (傾向低頻，截斷高頻，可能捨棄細節)
- 可將輸入輸出視為連續函數
- 全局視野
- 難捕捉局部特徵
- 擅長解 PDE

2. AFNO (Adaptive Fourier Neural Operator)改良transformer的mixing strategy



3. Comparison of AFNO and FNO

項目	Adaptive Fourier Neural Operator	Fourier Neural Operator
頻域通道混合方式	使用 MLP 混合每個通道	使用單一線性轉換混合所有通道
通道分組策略	將通道劃分為多個 block，分別處理（類似 Multi-head）	所有通道一次處理，無分組
頻域濾波方式	對傅立葉係數執行 soft-thresholding	截斷固定數量的高頻傅立葉係數（使用手動設定的 cut-off 超參數）
有無共享參數	each patch share params	每個頻率分量間不存在參數共享

Experiment

- learning rate = 0.001
- epochs = 100
- CosineAnnealingLR
- loss: MSE
- optimizer: Adam

1. FNO (Fourier Neural Operator) 報告中的 FNO 基於 neuralop.models 套件實作。

```
model = FNO(  
    n_modes=(28, 18),    # number of modes to keep in Fourier Layer  
    hidden_channels=28,  
    n_layers=3,    # number of block  
    in_channels=7,  
    out_channels=1,  
    domain_padding=0.1)
```



Kossaifi, J., Kovachki, N., Li, Z., Pitt, D., Liu-Schiaffini, M., George, R., Bonev, B., Azizzadenesheli, K., Berner, J., and Anandkumar, A. , "A Library for Learning Neural Operators", ArXiv, 2024.

<https://arxiv.org/abs/2412.10354>.

Kovachki, N., Li, Z., Liu, B., Azizzadenesheli, K., Bhattacharya, K., Stuart, A., and Anandkumar A. , "Neural Operator: Learning Maps Between Function Spaces", , JMLR, 2021.

<https://arxiv.org/abs/2108.08481>.

2. AFNO (Adaptive Fourier Neural Operator) <https://github.com/NVlabs/AFNO-transformer>

input image (157, 103) pad to (160, 120) # 因為要切patch

patch size=(4, 4)

number of input channels=7

number of output channels=1

number of blocks=4 # 把通道切多少塊

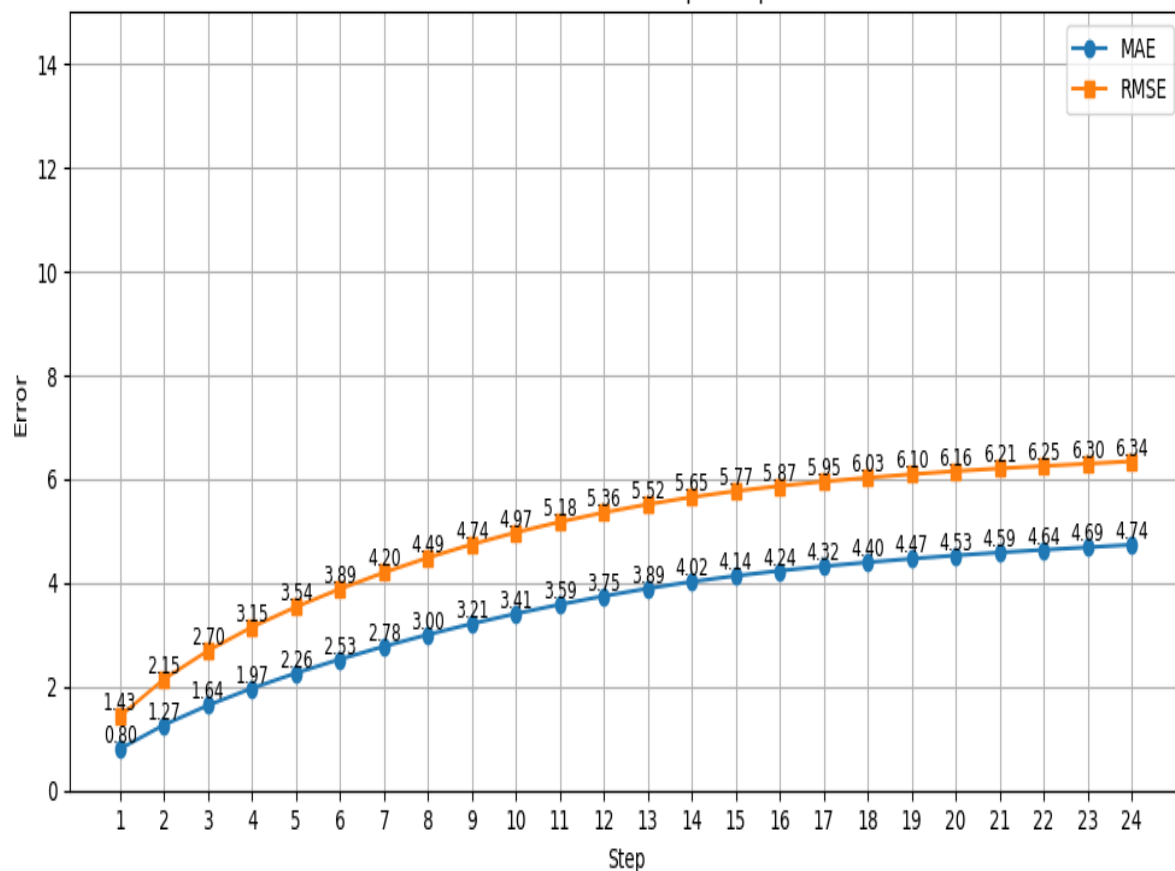
embedding dim=112 # 每個token的長度

depth=3 # 3 layers

Results

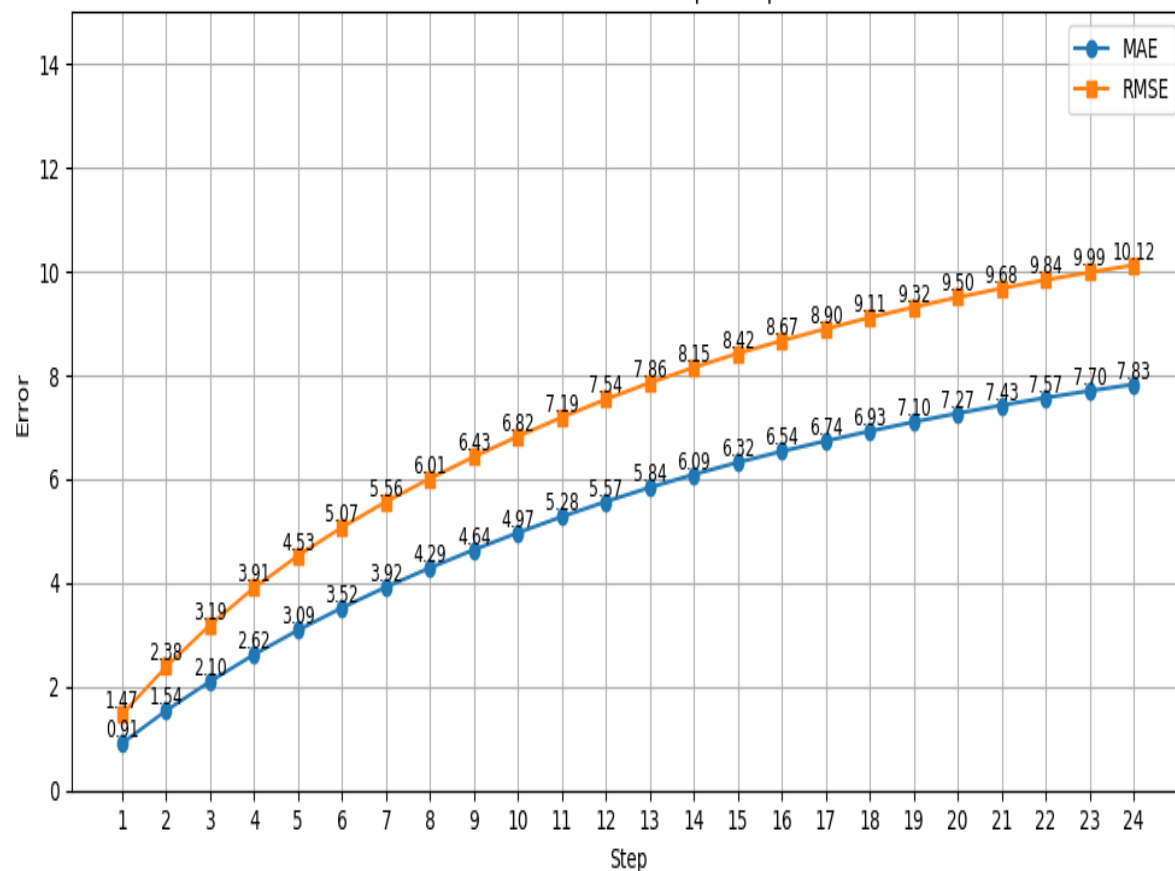
以自回歸方式，推論未來 24hr 的平均 PM2.5 濃度。

FNO MAE and RMSE per Step



FNO

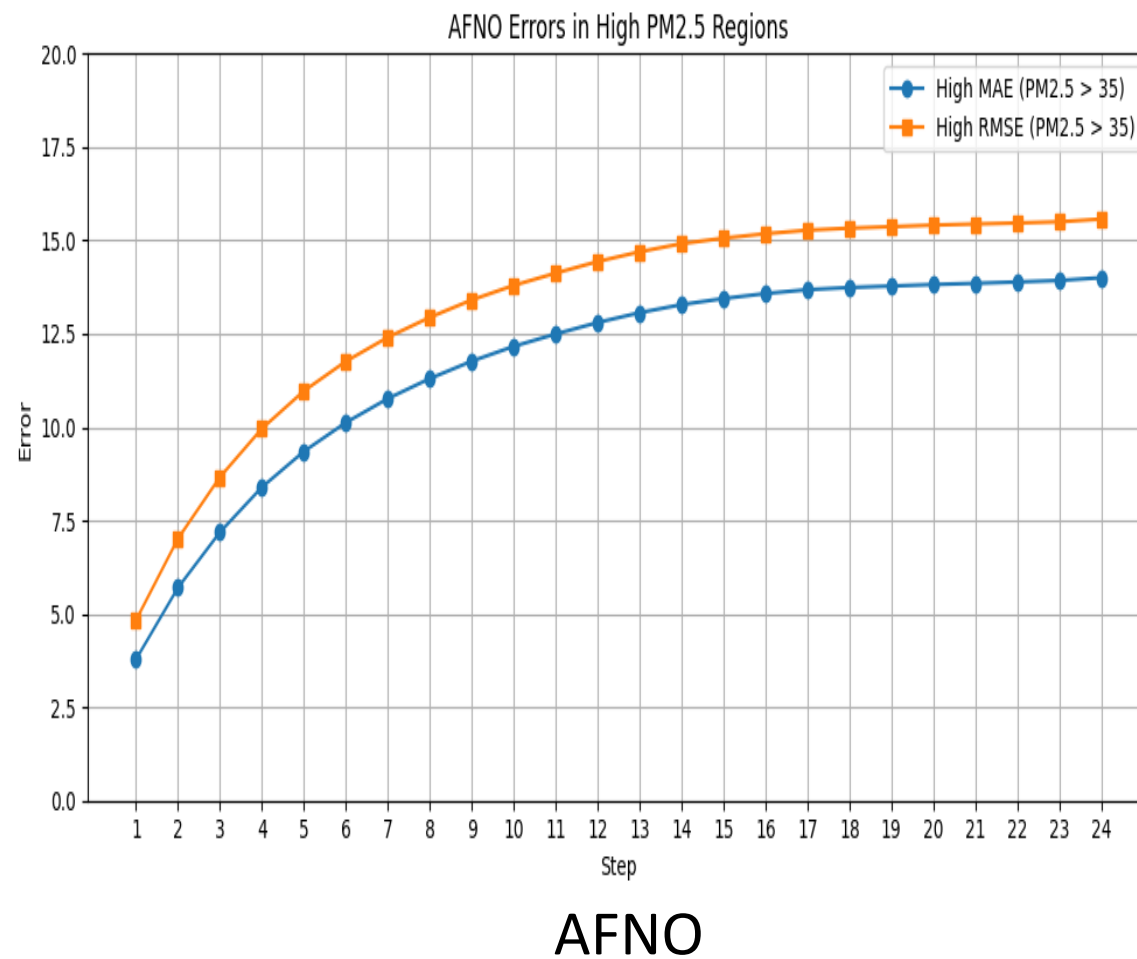
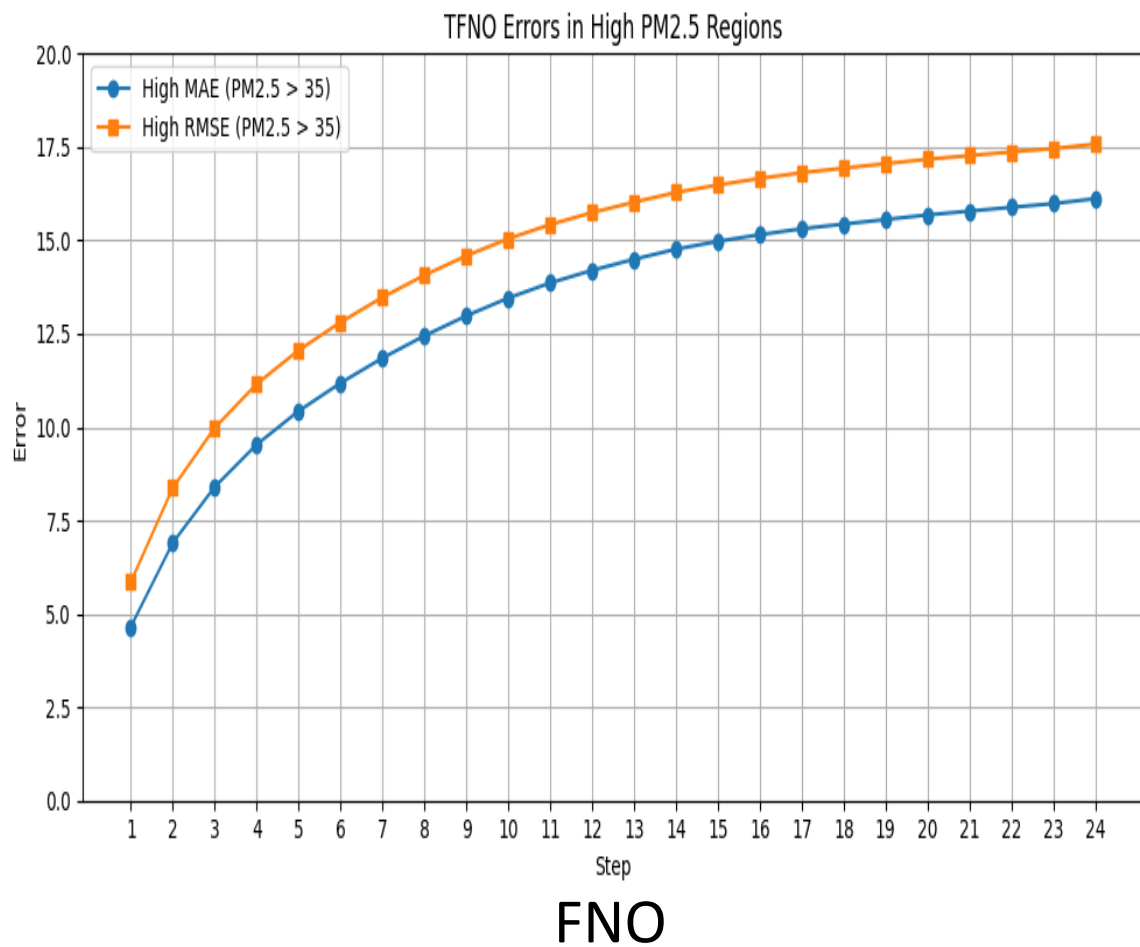
AFNO MAE and RMSE per Step



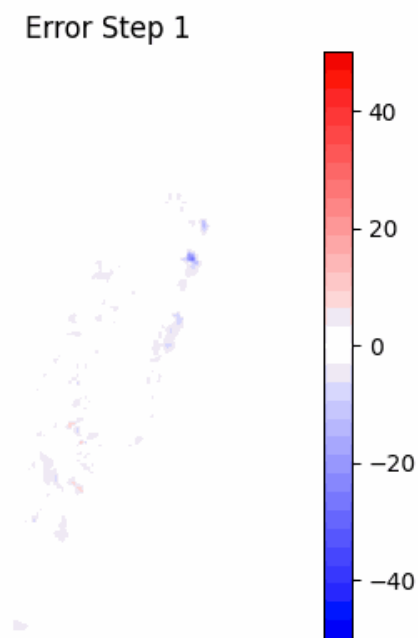
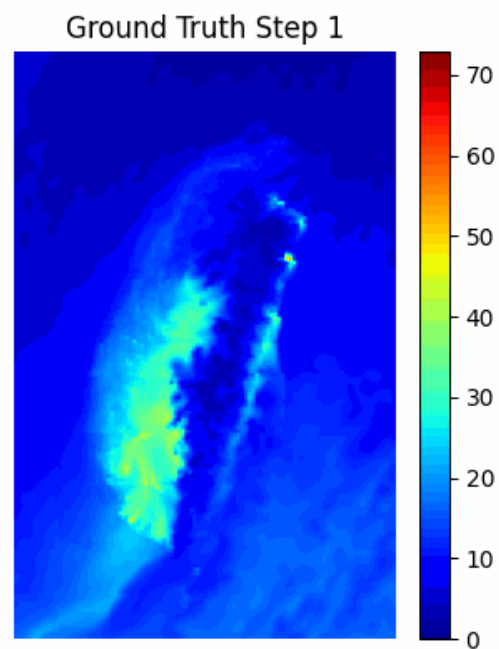
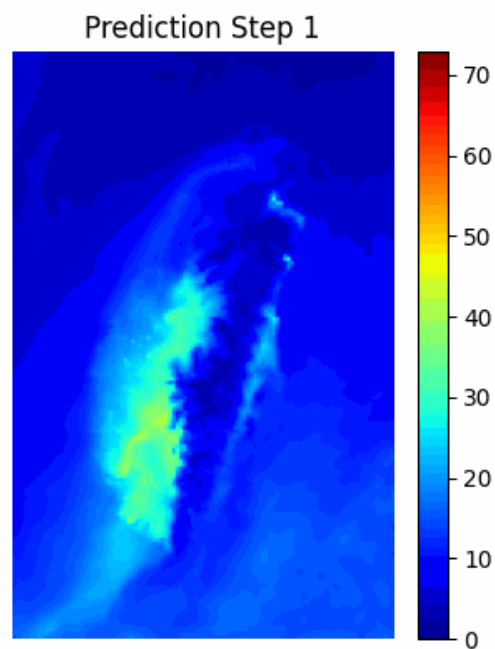
AFNO

Results

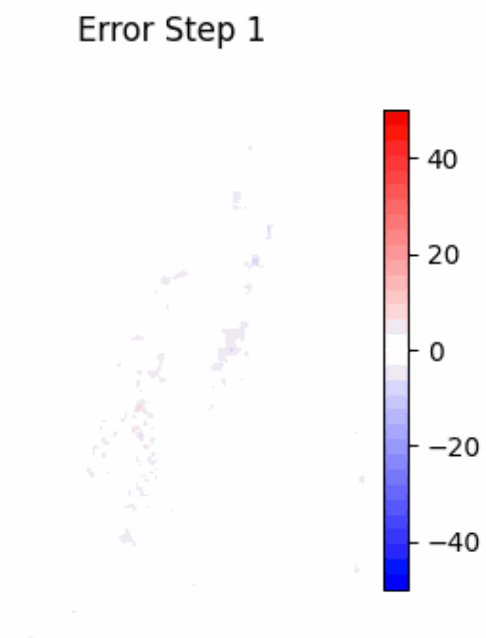
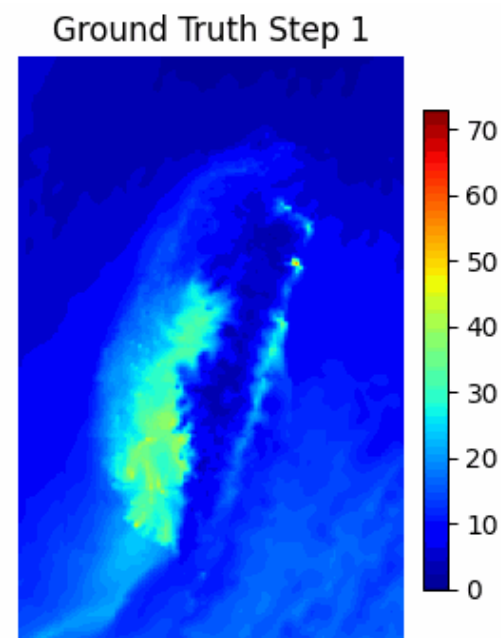
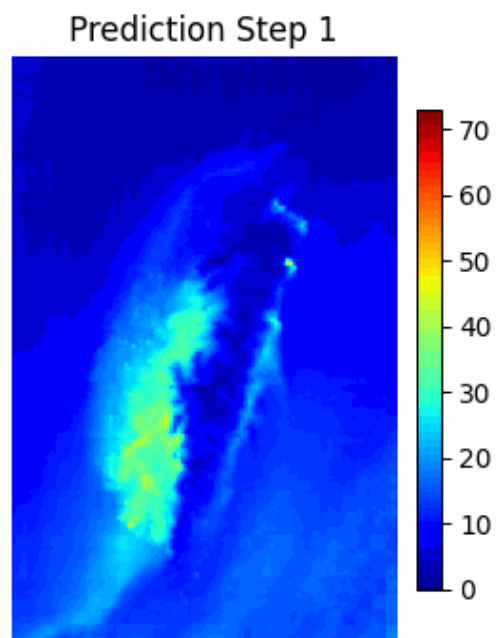
評估高濃度區域 ($>35\mu\text{g}/\text{m}^3$) 的平均誤差



FNO

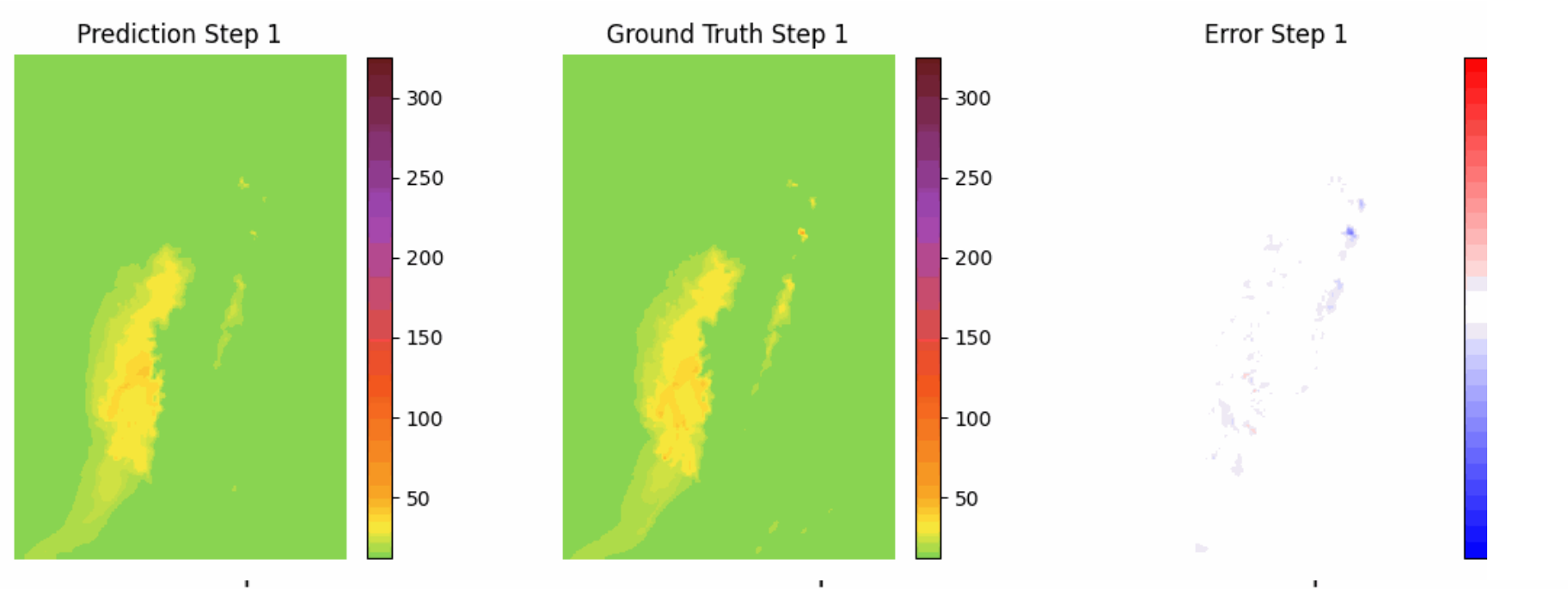


AFNO



用不同的視覺化方式，強化高濃度區域的變化。

FNO



AFNO

