Structural Machine Learning Models and Their Applications

期末報告　資科一高哲凱

Introduction

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

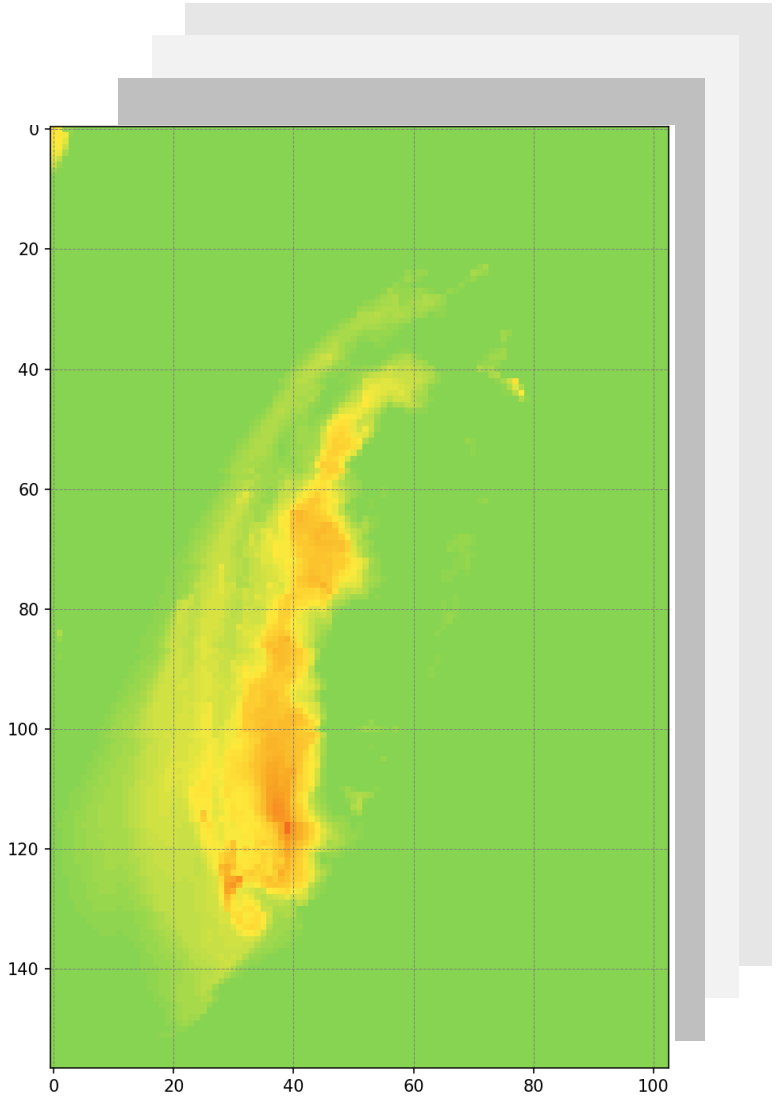
二、資料來源：中研院高解析度空氣品質擬預報資料

三、訓練資料：2020, 2021, 2022 年份，共26,304筆 (shape: 157x103)

四、測試資料：2023 年份，共8,760筆筆 (shape: 157x103)

https://history.colife.org.tw/?cd=%E7%A9%BA%E6%B0%A3%E5%93%81%E8%B3%AA/%E4%B8%AD%E7%A0%94%E9%99%A2_%E7%A9%BA%E5%93%81%E9%A0%90%E5%A0%B1%E6%A8%A1%E6%93%AC%E8%B3%87%E6%96%99#/

Training

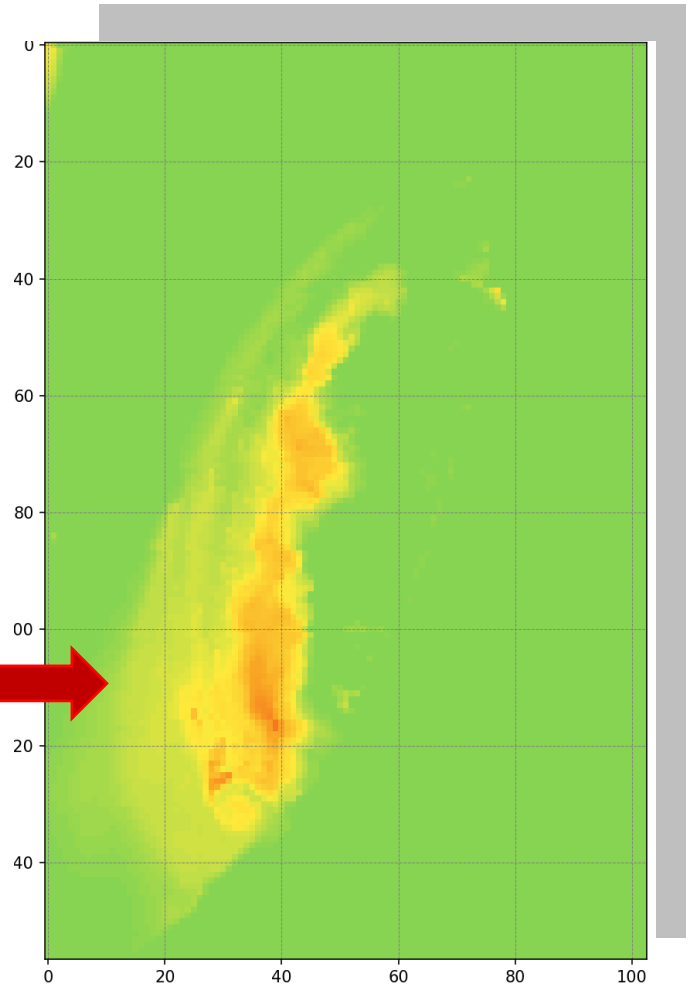


INPUT

5/1 00小時的

- PM2.5場
- 溫度場(K)
- 風速場
- 風向場
- 濕度場
- 經度
- 緯度

一小時後



OUTPUT

5/1 01小時的

- PM2.5場
- 溫度場(K)
- 風速場
- 風向場
- 濕度場

5/1 01小時的 Ground Truth → MSE Loss

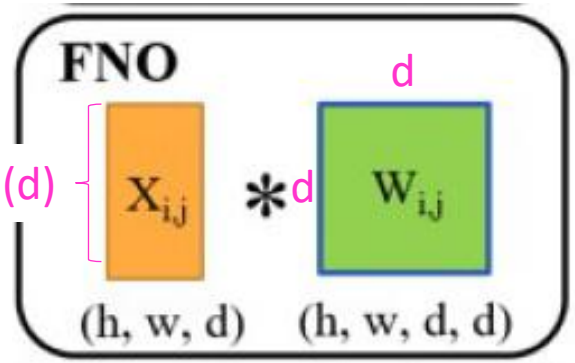
Model

1. UNet (本報告的 UNet 架構基於 segmentation_models.pytorch 套件實作)

```
model = smp.Unet(
    encoder_name="resnet34",
    encoder_depth=3,    # 下採樣次數
    decoder_channels=(128, 64, 32),   # 各層通道數
    in_channels=7,
    classes=5)
```

Yakubovskiy, P. (2019). *Segmentation Models Pytorch*. GitHub repository: https://github.com/qubvel/segmentation_models.pytorch

2. FNO (Fourier Neural Operator)



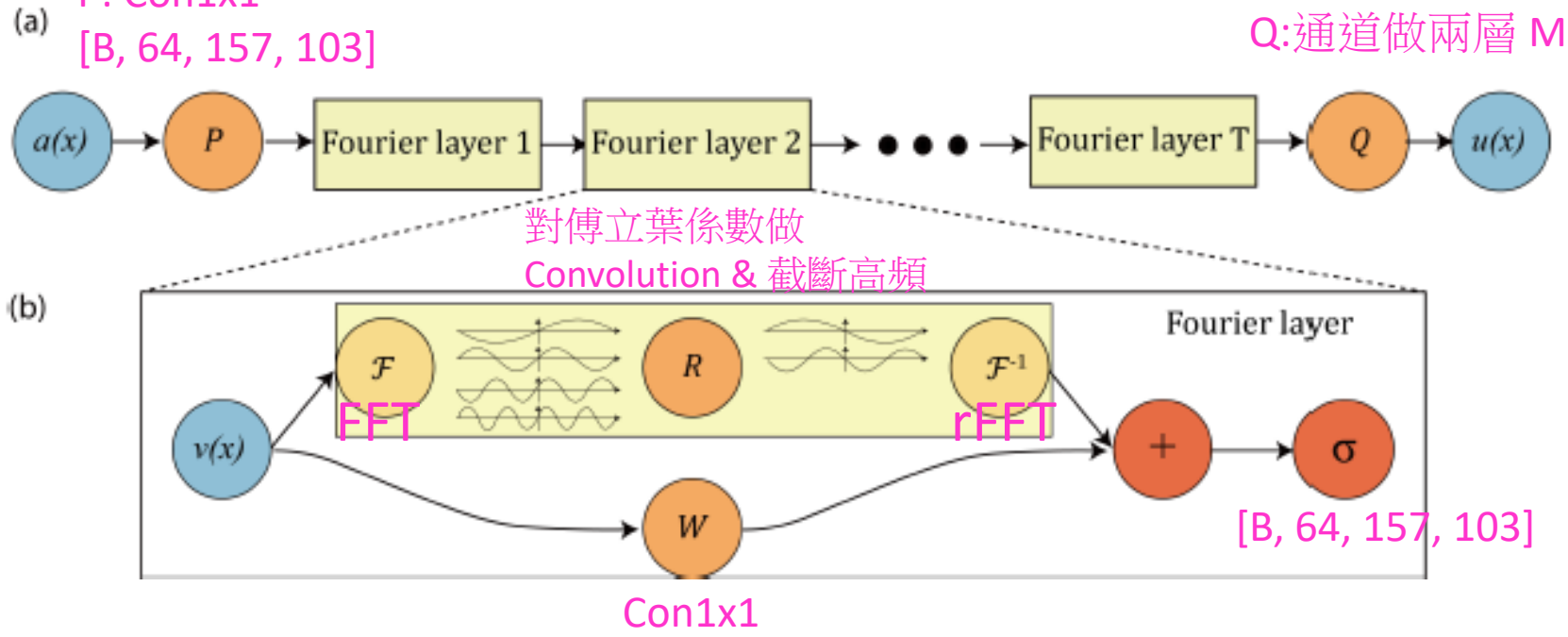
B: batch size=32

P: Con1x1
[B, 64, 157, 103]

Q:通道做兩層 MLP

input:
[B, 7, 157, 103]

output:
[B, 5, 157, 103]



Model

2. FNO (Fourier Neural Operator)

- 在頻域學習 (低頻主導，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

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)*.

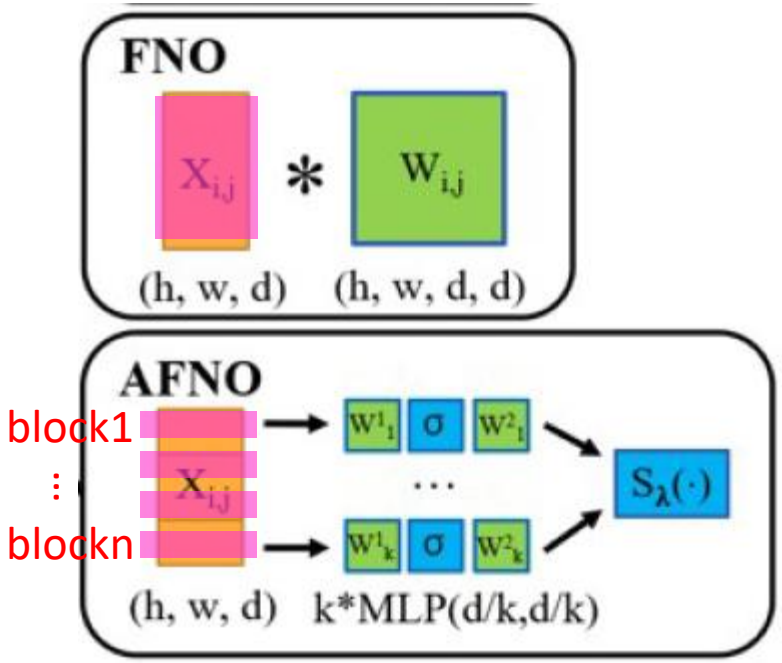
2. FNO (Fourier Neural Operator)報告中的 FNO 基於 neuralop.models 套件實作。

```
model = FNO(
    n_modes=(38, 26),    # number of modes to keep in Fourier Layer
    hidden_channels=32,
    n_layers=4,    # number of block
    in_channels=7,
    out_channels=5,
    positional_embedding=None,
    domain_padding=0.1,
    norm="group_norm")
```

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.

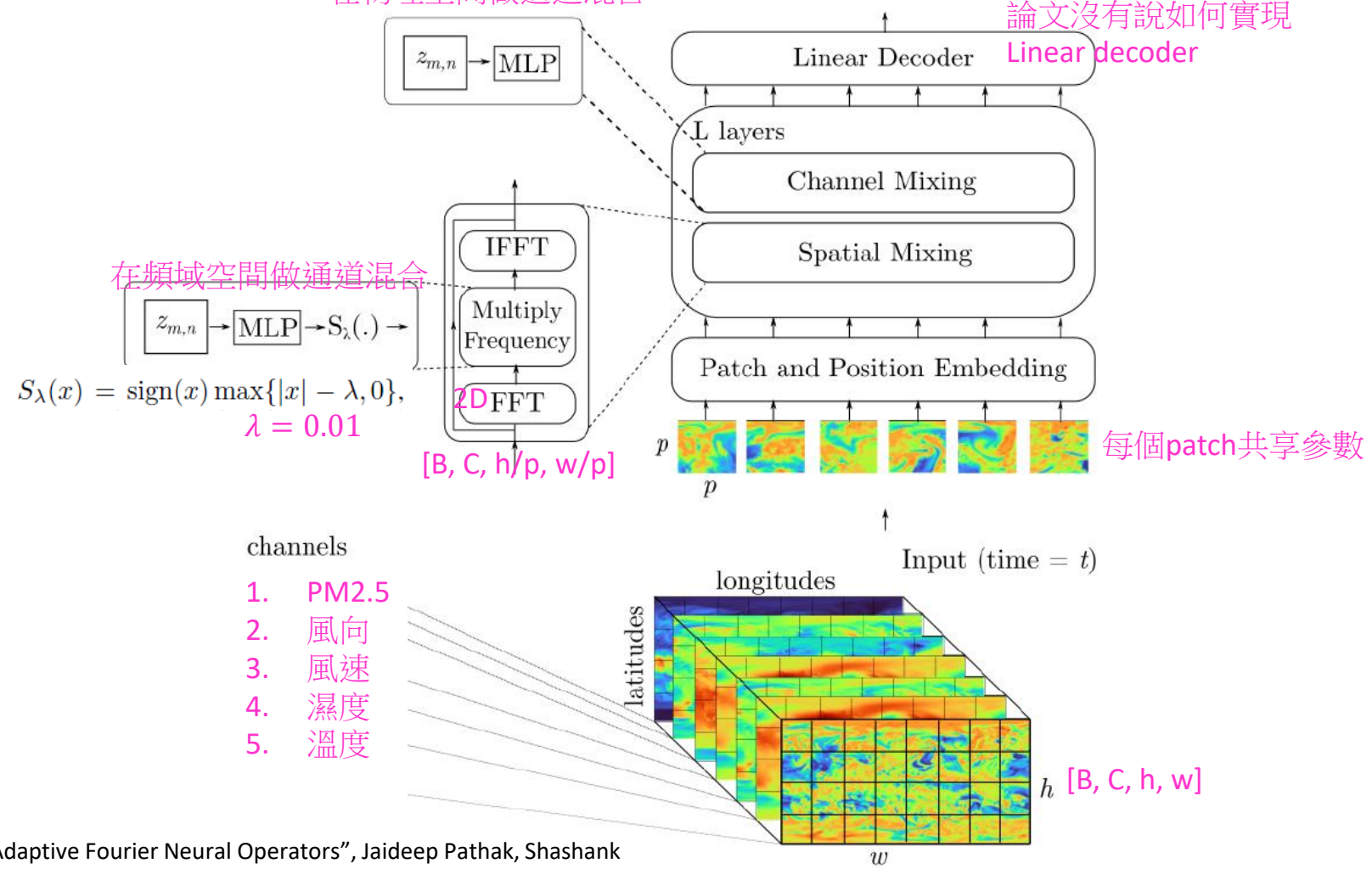
3. AFNO (Adaptive Fourier Neural Operator)改良transformer的mixing strategy



output: T + ΔT

在物理空間做通道混合

論文沒有說如何實現
Linear decoder



channels

1. PM2.5
2. 風向
3. 風速
4. 濕度
5. 溫度

"FourCastNet: A Global Data-driven High-resolution Weather Model using Adaptive Fourier Neural Operators", Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, Zongyi Li, Kamyar Azizzadenesheli, Pedram Hassanzadeh, Karthik Kashinath, Animashree Anandkumar https://arxiv.org/abs/2202.11214

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

1. 使用 FNO 實現transformer中的 token mixing。
2. 在頻域，使用 mlp 混合每個通道。
3. 將通道分為數個blocks，每個block各自混合，以至於節省計算量。

   (類似multi-head的概念)
4. 混合後，對傅立葉係數做 soft-thresholding

   (假設PDE方程式通常由低頻主導)

"FourCastNet: A Global Data-driven High-resolution Weather Model using Adaptive Fourier Neural Operators", Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, Zongyi Li, Kamyar Azizzadenesheli, Pedram Hassanzadeh, Karthik Kashinath, Animashree Anandkumar https://arxiv.org/abs/2202.11214

3. AFNO (Adaptive Fourier Neural Operator)

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

patch size=(4, 4)

number of input channels=7

number of output channels=5

embed dim=112　　# 每個token的長度

depth=6　　# 總共做六次傅立葉轉換　https://github.com/NVlabs/AFNO-transformer

Guibas, John and Mardani, Morteza and Li, Zongyi and Tao, Andrew and Anandkumar, Anima and Catanzaro, Bryan.(2021) “Efficient Token Mixing for Transformers via Adaptive Fourier Neural Operators”. In International Conference on Learning Representations(ICLR). https://arxiv.org/abs/2111.13587

Experiment

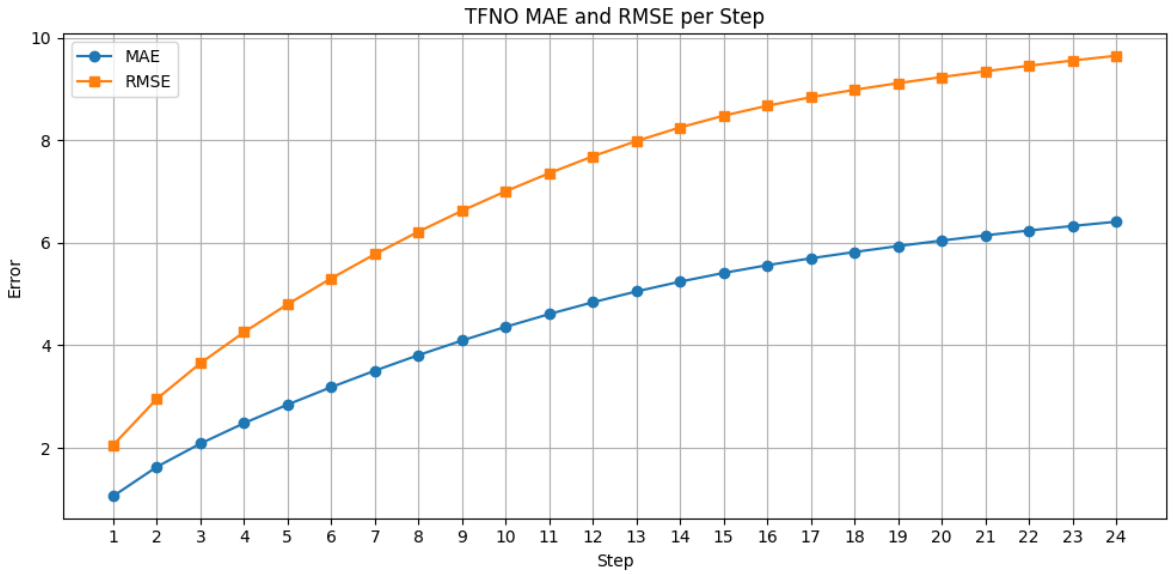
- learning_rate = 0.001
- epochs = 200
- CosineAnnealingLR
- loss: MSE
- optimizer: Adam (weight_decay=1e-4)

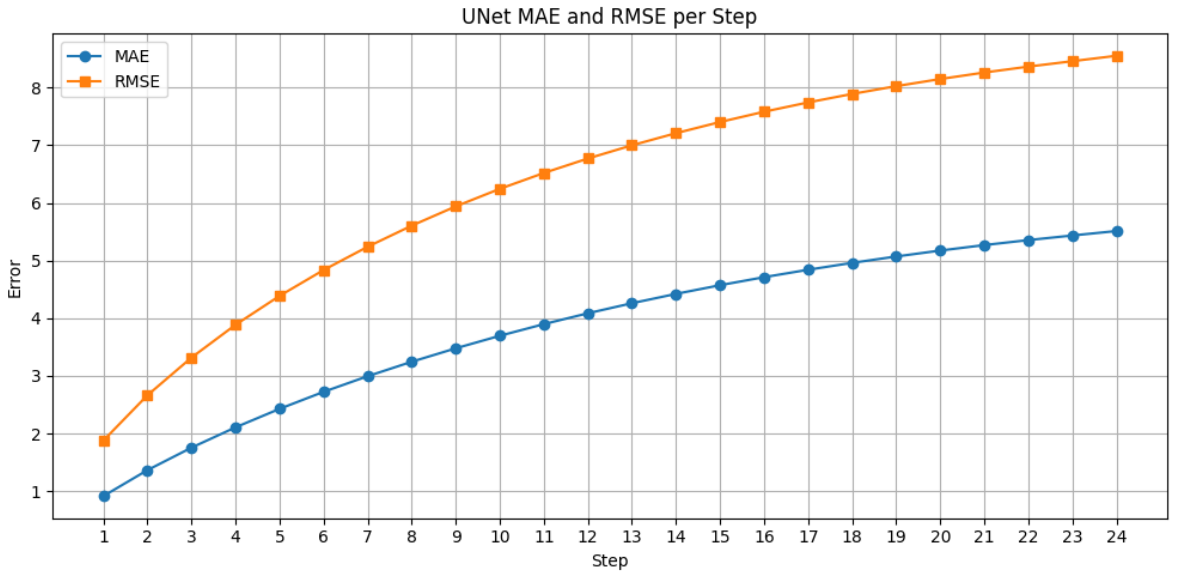
Results

評估未來8小時的預估誤差

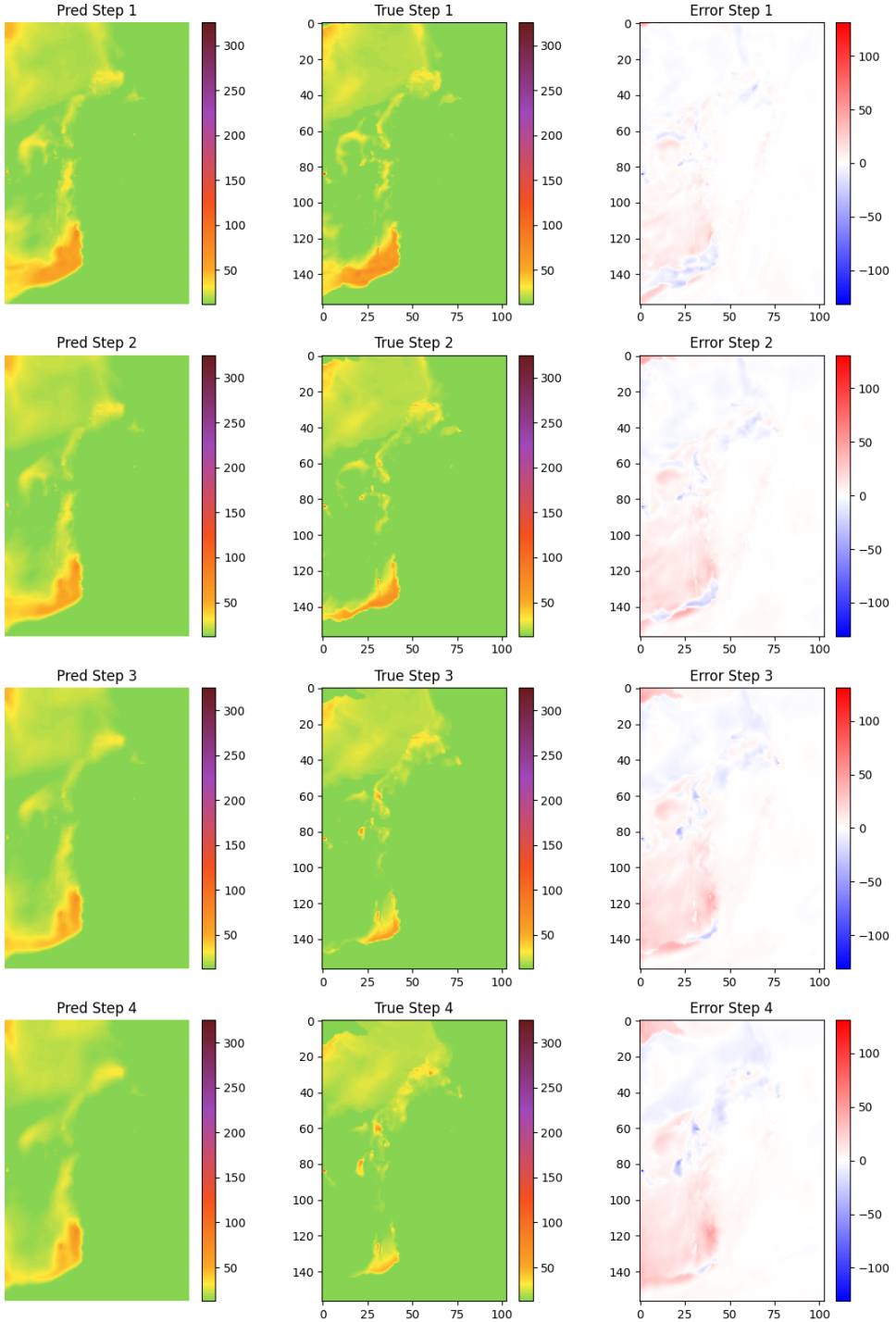
推論方式：使用第k-1小時的預測結果，推論第k小時，直到第24小時。

左圖為 FNO 的預測誤差，右圖為 UNet 的預測誤差。

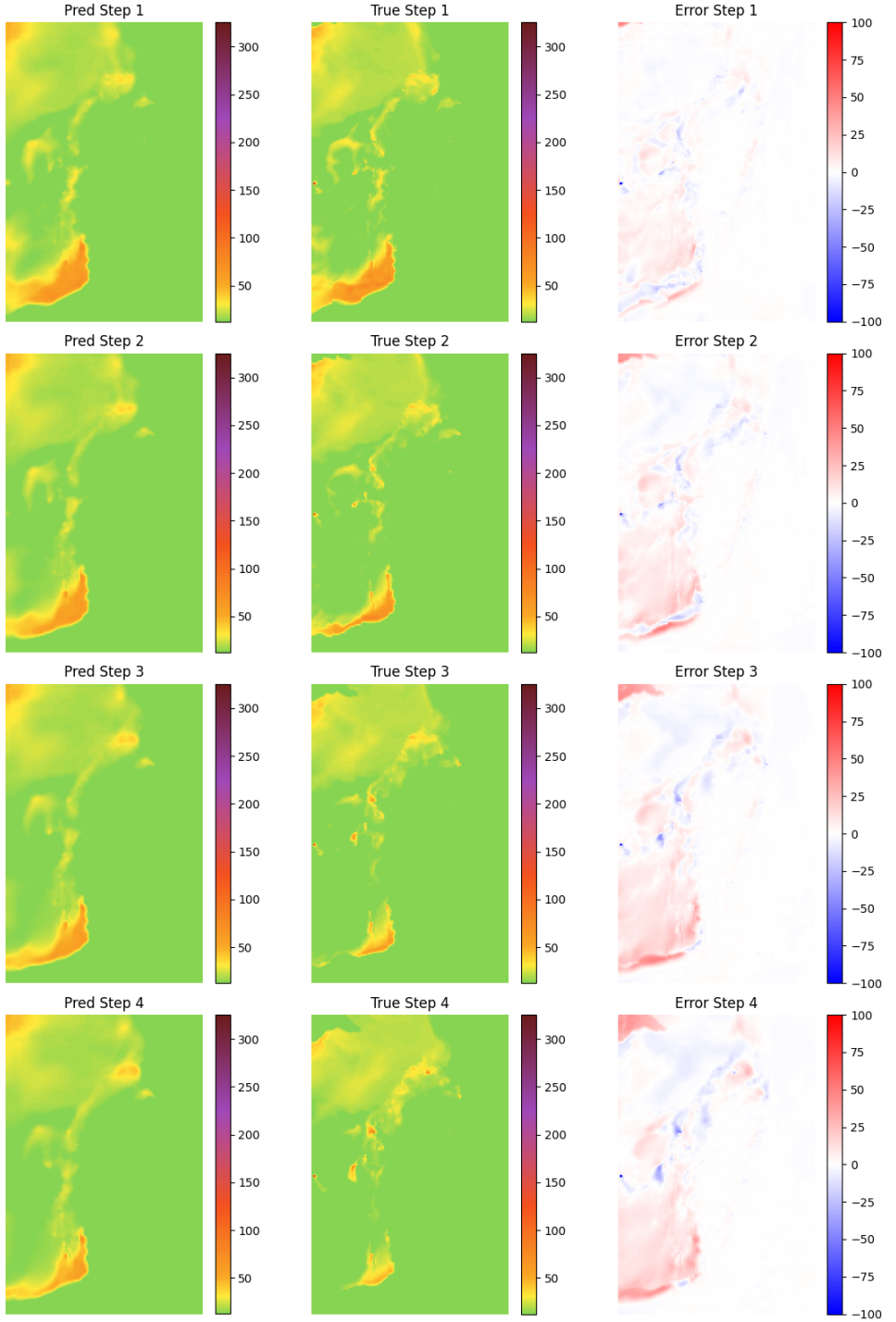




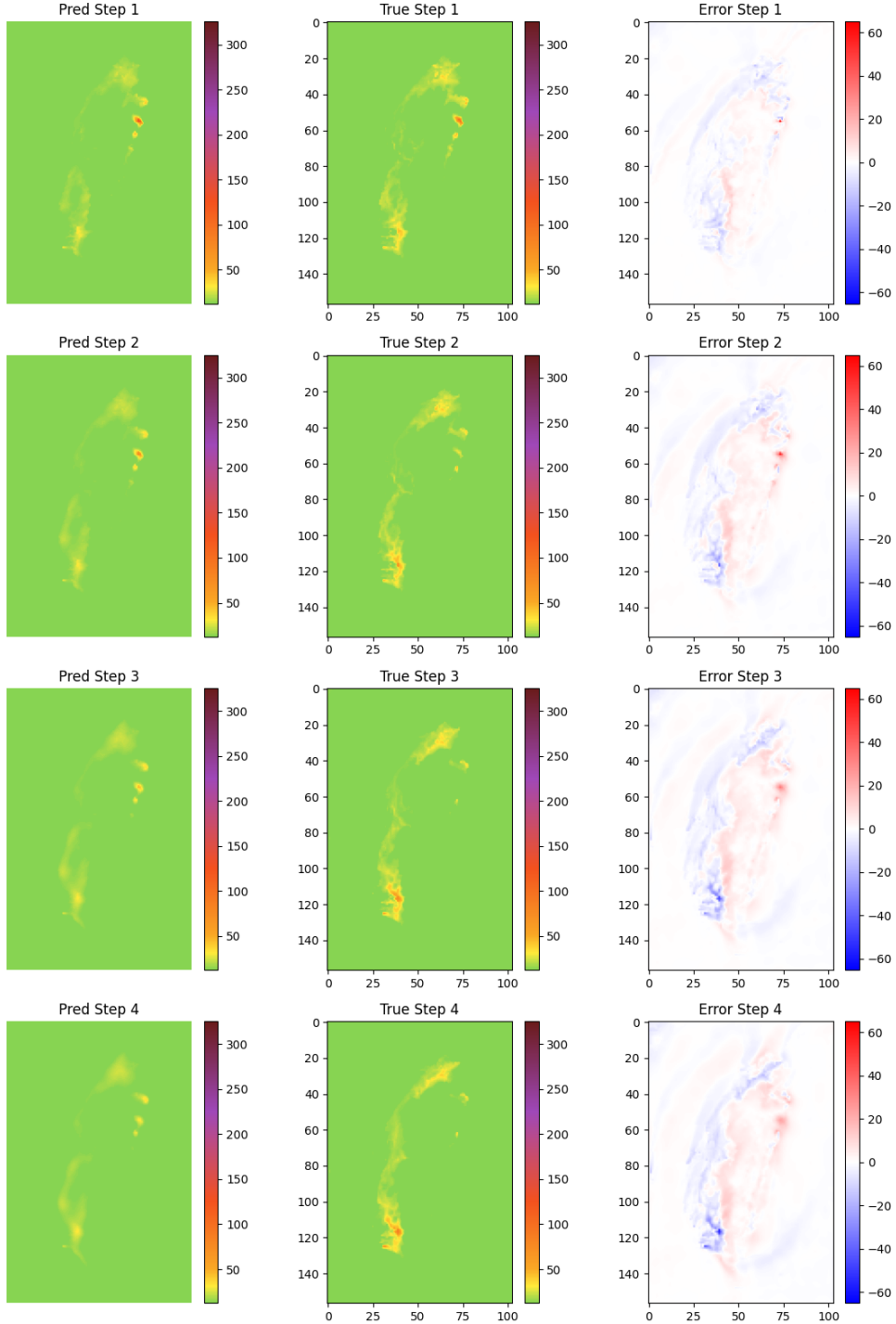
FNO


Pred Step 1
True Step 1
Error Step 1
Pred Step 2
True Step 2
Error Step 2
Pred Step 3
True Step 3
Error Step 3
Pred Step 4
True Step 4
Error Step 4

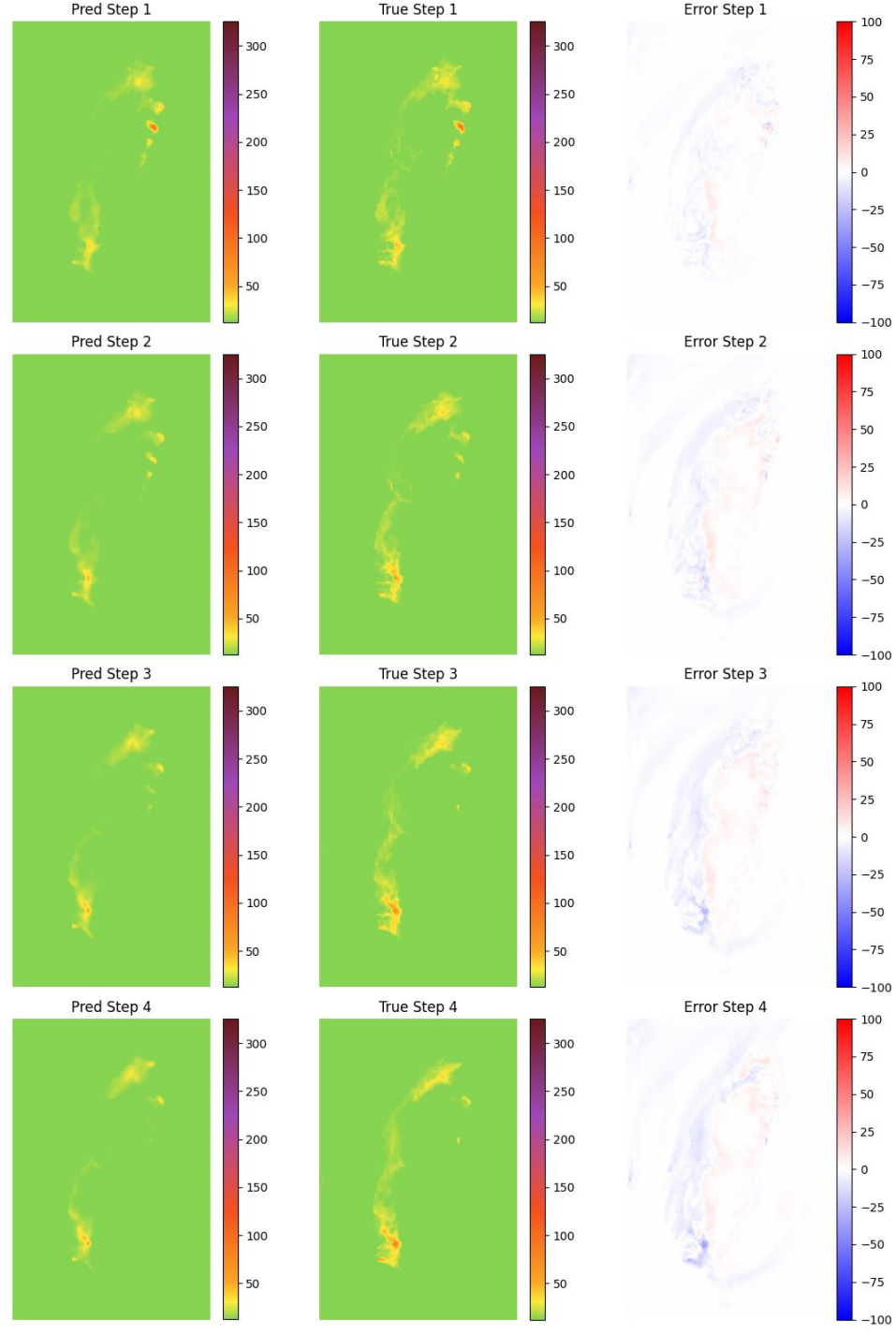
UNet


Pred Step 1
True Step 1
Error Step 1
Pred Step 2
True Step 2
Error Step 2
Pred Step 3
True Step 3
Error Step 3
Pred Step 4
True Step 4
Error Step 4

FNO


Pred Step 1
True Step 1
Error Step 1
Pred Step 2
True Step 2
Error Step 2
Pred Step 3
True Step 3
Error Step 3
Pred Step 4
True Step 4
Error Step 4

UNet


Pred Step 1
True Step 1
Error Step 1
Pred Step 2
True Step 2
Error Step 2
Pred Step 3
True Step 3
Error Step 3
Pred Step 4
True Step 4
Error Step 4

Discussion

1. 氣象資料需要學習局部特徵
2. FNO 計算速度慢，可能還沒完全收斂