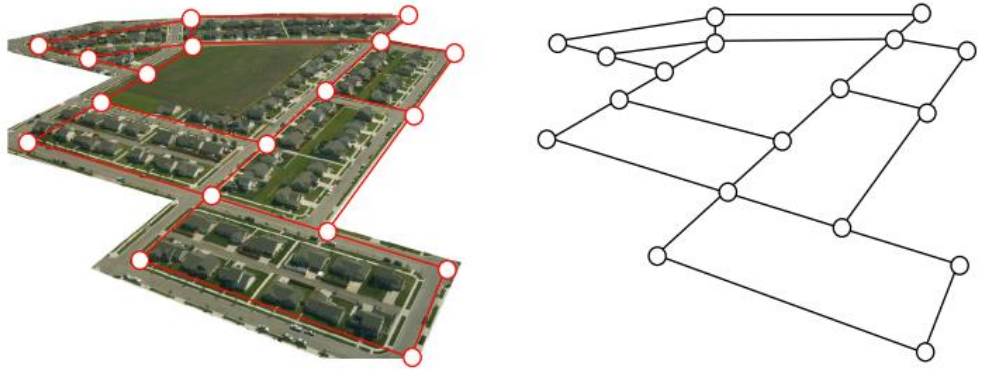
Prototype-enhanced prediction in graph neural networks for climate applications

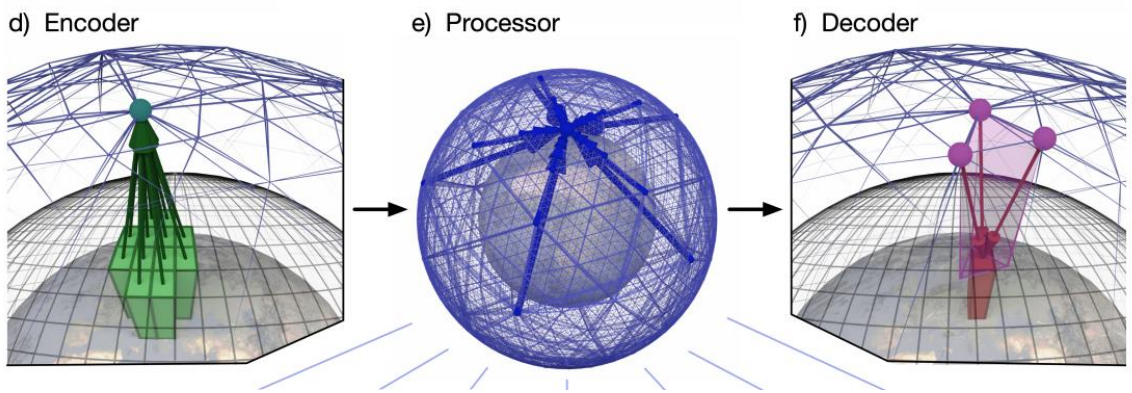
Keshtmand et al. 2025

Overview

- MLJC Website Tour
- FootNet
  - Gaussian Plume informed CNN
- Graph Neural Network
  - Encoder-Process-Decoder
- **Prototype informed GNN**
  - Prototype Selection



Graph Representations



GraphCast, Lam et al. 2023

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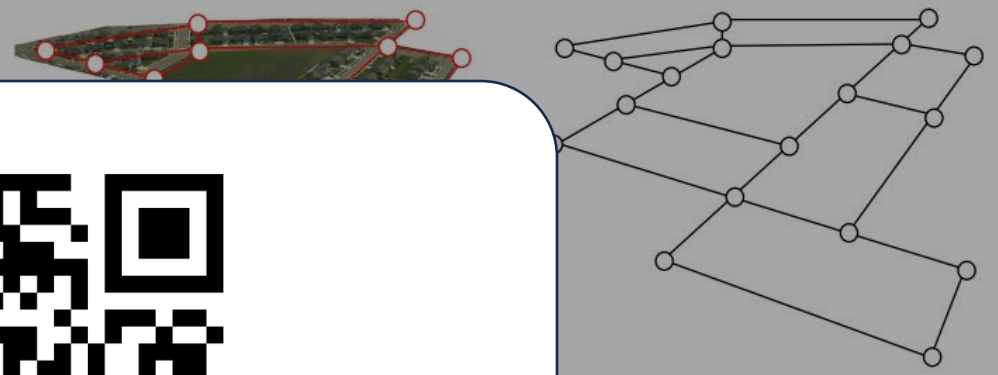

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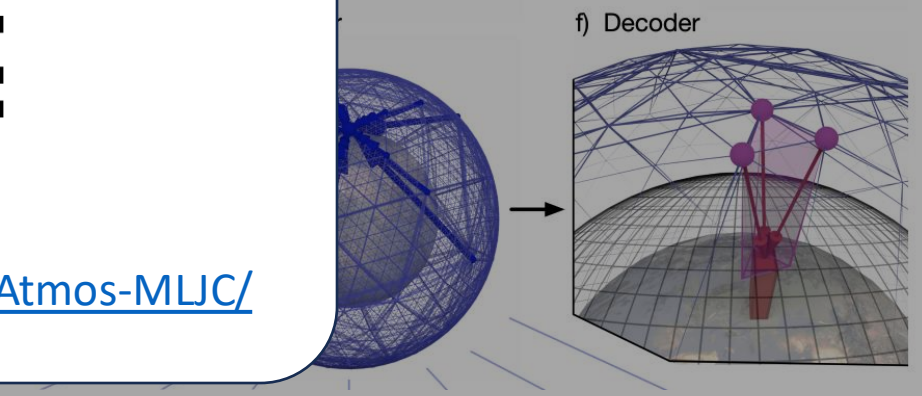

GraphCast, Lam et al. 2023

MLJC Website
https://nightingale-lzh.github.io/UW-Atmos-MLJC/

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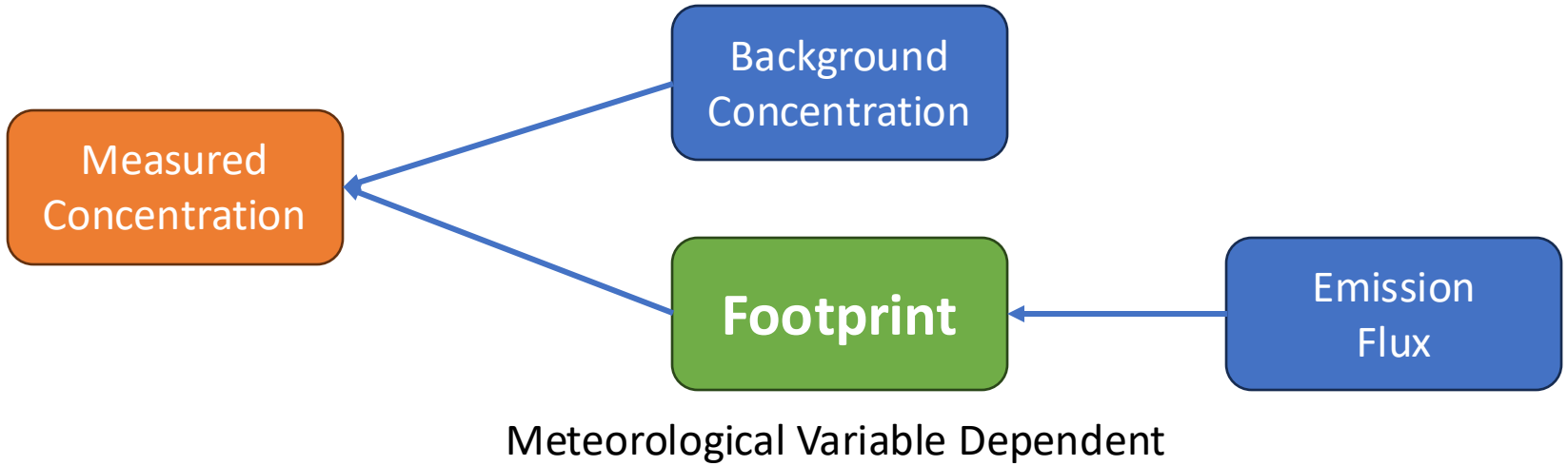
FootNet What is our objective?

- Predicting the **Footprint** of Plume from a GHG Source



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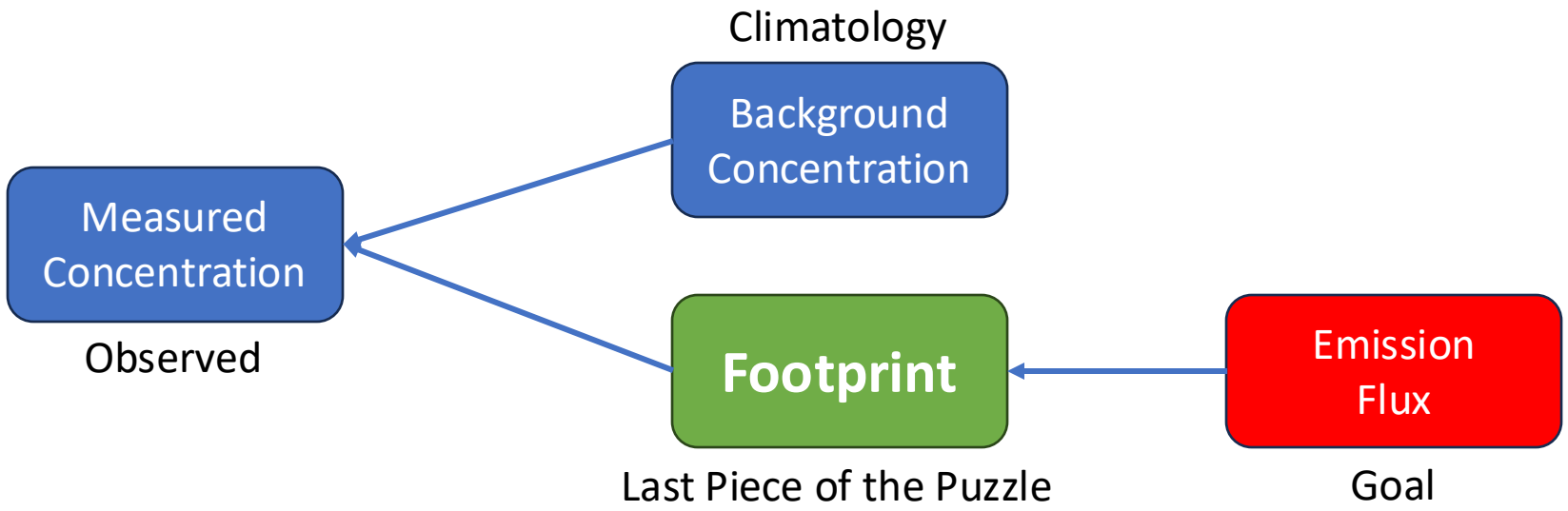

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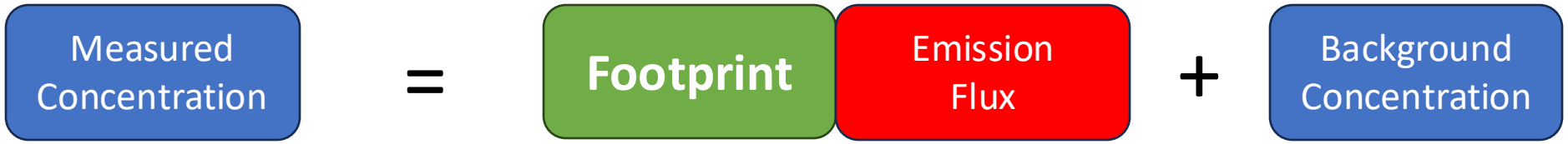

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$$\mathbf{y} = \mathbf{Hx} + \mathbf{b}$$

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$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$$ Jacobian, Sensitivity

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FootNet

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$$\mathbf{y} = \mathbf{Hx} + \mathbf{b}$$

So, Linear Regression? No,

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He et al. 2025

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- Predicting the **Footprint** of Plume from a GHG Source

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So, Linear Regression?

No, ~~Because this is a ML paper~~

Because we are looking for H, not x

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FootNet Predicting Footprint

- Input meteorological variables at **t** and **t - 6h**
- Output **H**
- Model:

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FootNet Predicting Footprint

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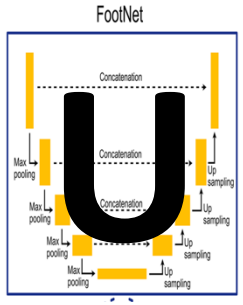
CNN- U Net



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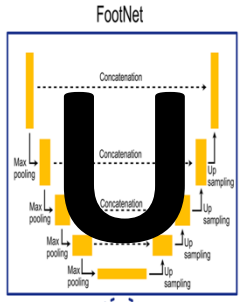

- Validation: Measured Footprint

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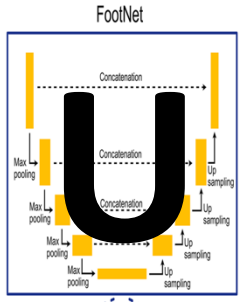
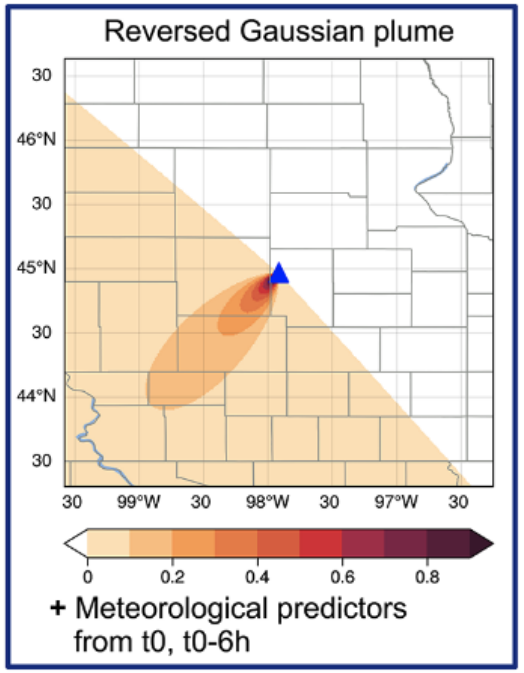


- Validation: Measured Footprint

Improvement, also include



Quick Calculation
under the Gaussian diffusion assumption

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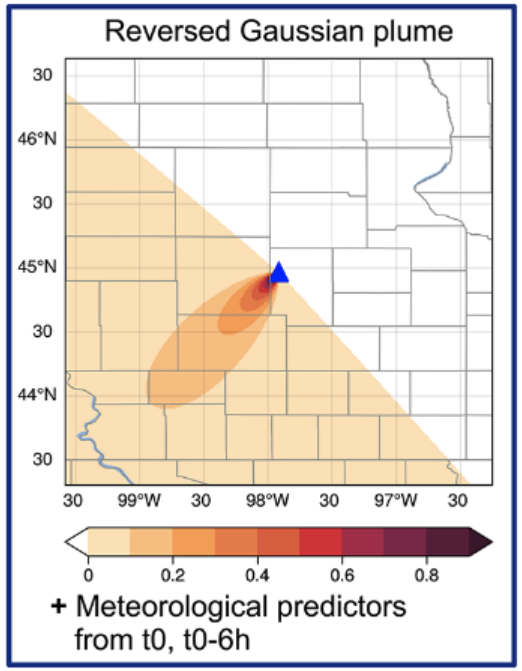
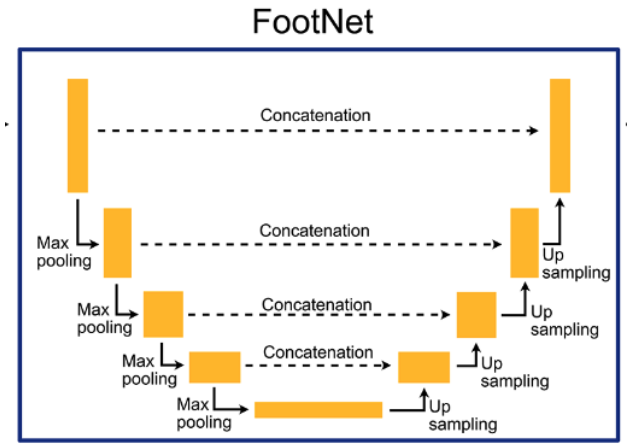
FootNet Predicting Footprint

Therefore, we got



informed **CNN-**



Net

(Wait, Berkeley color theme?)

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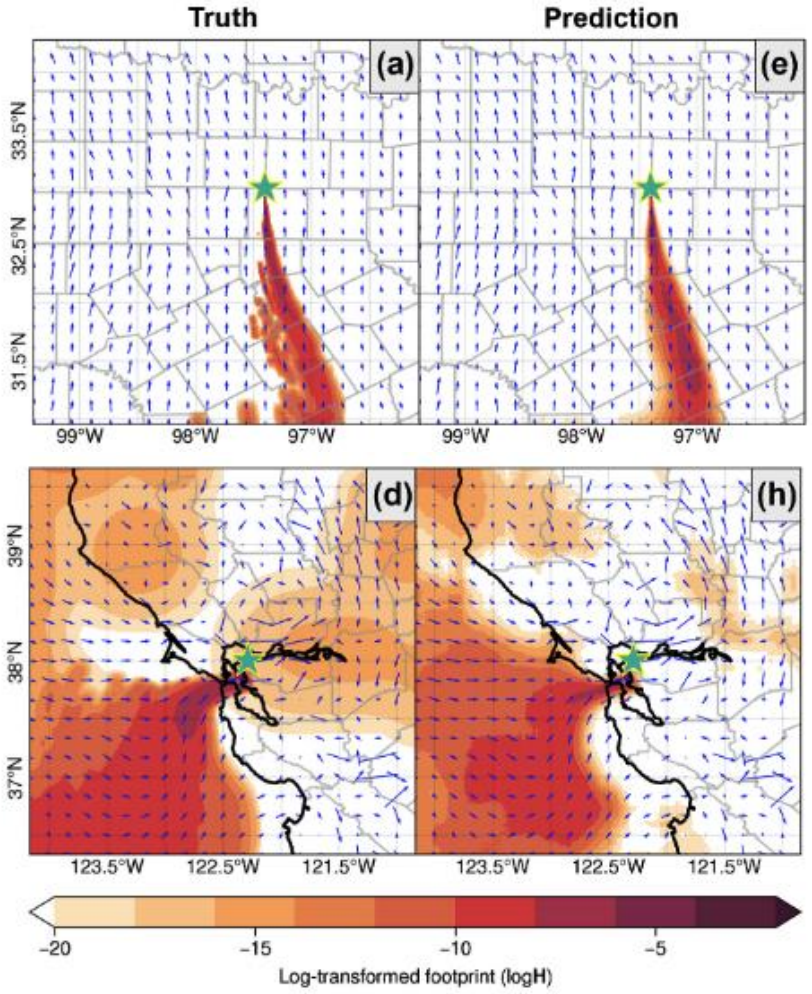
FootNet

Predicting Footprint

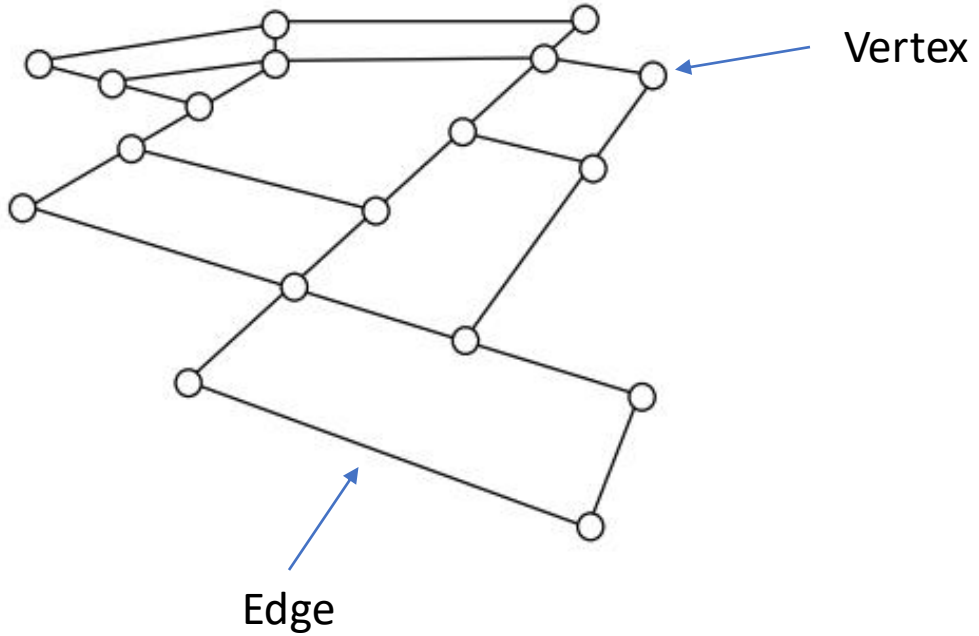


Now, GNN Chaos

1. Keisler 2022	GNN Architecture
2. Fillola et al, 2023b	Using GNN Predicting Footprint
3. Keshtmand et al. 2025	Adding Prototype Enhancement

What is Graph

- Collection of {(V, E)}
  - Vertices (or nodes, or points)
  - Edges (or links, or lines)



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Graphs can be represented as Matrices

What is Graph

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  - Vertices (or nodes, or points)
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- The most important thing:

Graphs can be represented as Matrices

Note: CS people will shove any matrix into neural network

What is Graph

- Behold

  - Graph → MLP = **Graph** Neural Network
  - Graph → CNN = **Graph** Convolutional Network
  - Graph → Transformer = **Graph** Attention Network
  - Graph → GRU = Gated **Graph** Sequence Neural Network

- Now, Graph + anything has a new name: **Message Passing Layer**

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- Now, Graph + anything has a new name: **Message Passing Layer**

The Magic of GNN is not GNN itself; it is how to make a graph

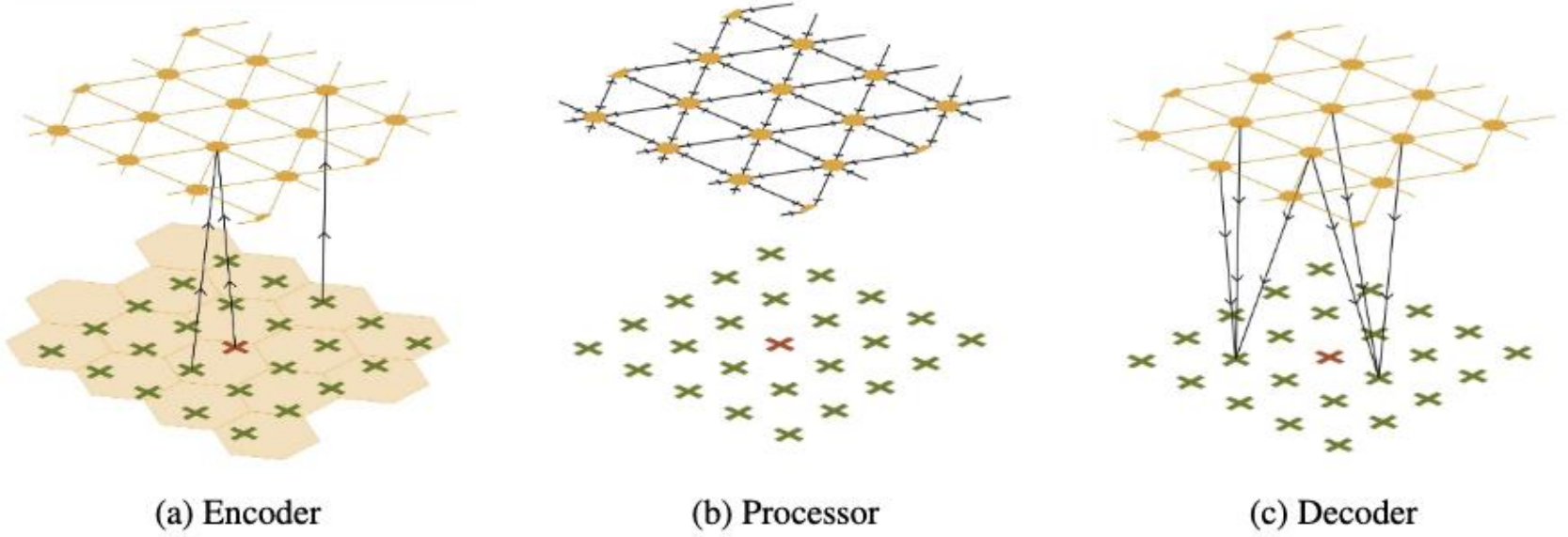
Overview: (1) Keisler 2022

Encoder-Process-Decoder

Fillola et al, 2023b

H3 Mesh

Lat-Lon Grid



(a) Encoder (b) Processor (c) Decoder

Convert Grid into Mesh
(Distance Weighted Average)

Fix Edge Matrix…
Pass Vertices into MLP
(Multiple times)

Convert Mesh to Grid
(Distance Weighted Average)

Overview: (1) Keisler 2022

Encoder-Process-Decoder

Fillola et al, 2023b

H3 Mesh

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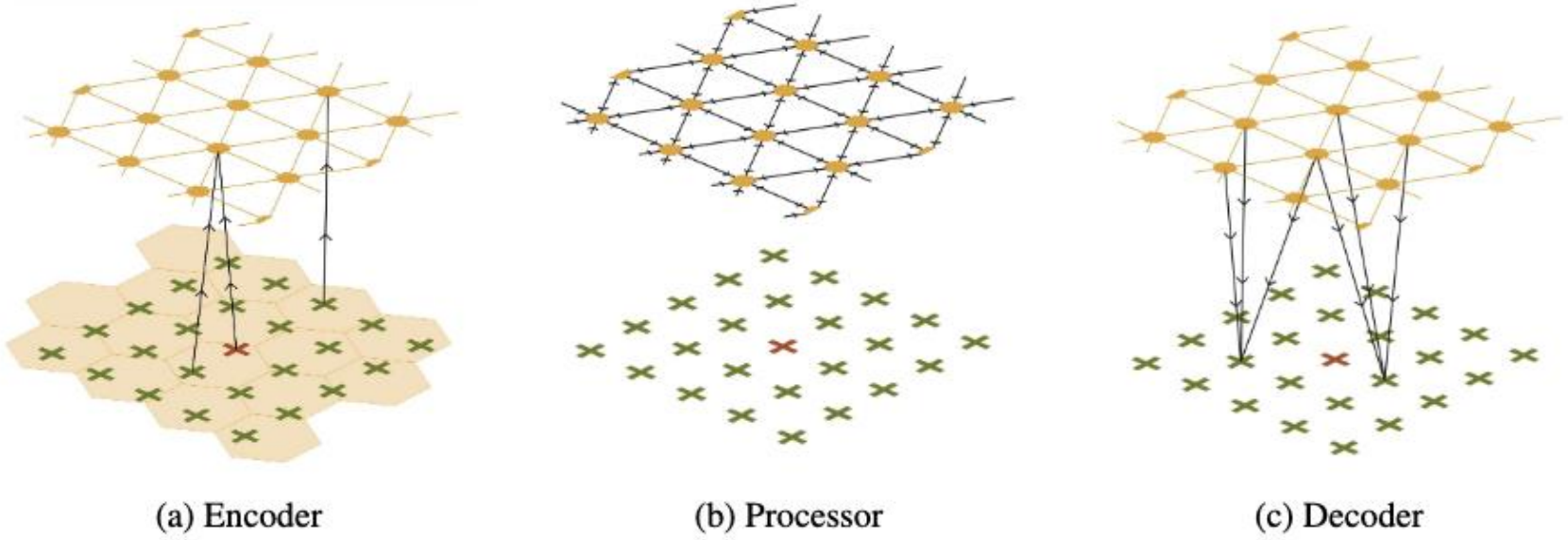

(a) Encoder (b) Processor (c) Decoder

Convert Grid into Mesh
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Fix Edge Matrix…
Pass Vertices into MLP

Convert Mesh to Grid
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I am disappointed
Be honest, I think the magic of a graph is the edges, not only the vertices
Just check Adaptive Mesh CFD

Overview: (1) Keisler 2022

Encoder-Process-Decoder

- Mesh: h3 from h3geo
- Equal representation of neighbors on Earth
- Decoupled Grid space and Mesh space
  - Mixed resolution

All six neighbors of a hexagon (ring 1)

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Encoder-Process-Decoder

- Mesh: h3 from h3geo
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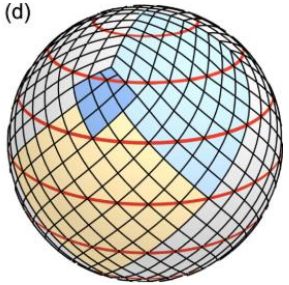
Also, What if we
use HEALPix mesh
(Edges are fixed anyway)



arXiv > physics > arXiv:2311.06253v2

Physics > Atmospheric and Oceanic Physics

[Submitted on 11 Sep 2023 (v1), last revised 19 Jun 2024 (this version, v2)]

Advancing Parsimonious Deep Learning Weather Prediction using the HEALPix Mesh

Matthias Karlbauer, Nathaniel Cresswell-Clay, Dale R. Durran, Raul A. Moreno, Thorsten Kurth, Boris Bonev, Noah Brenowitz, Martin V. Butz

We present a parsimonious deep learning weather prediction model to forecast seven atmospheric variables with 3-h time resolution for up to one-year lead times
Pixelization (HEALPix). In comparison to state-of-the-art (SOTA) machine learning (ML) weather forecast models, such as Pangu-Weather and GraphCast, our DLWP-

Overview: (2) Fillola et al, 2023b

GNN → Footprint

- Grid Size: 0.352x0.234 (Much Coarser than FootNet)
- A lot of Meteorological Variables
- Over Brazil
- Measurement: Particle Simulation (NAME) from Met Office
- Result: (What is this?)

Table 1: Performance metrics of footprint emulator with current setup. See A for metric definitions

Pixel-level metrics	Footprint-level metrics		Concentration-level metrics		
MAE	Dice similarity	Accuracy	R2	NMAE	Mean Bias Error
$1.1 \cdot 10^{-4}$	$57.2\% \pm 18\%$	$65.8\% \pm 9\%$	0.448	0.3829	6.43

Overview: (2) Fillola et al, 2023b

GNN → Footprint

- **Result:** (Oh, this one)

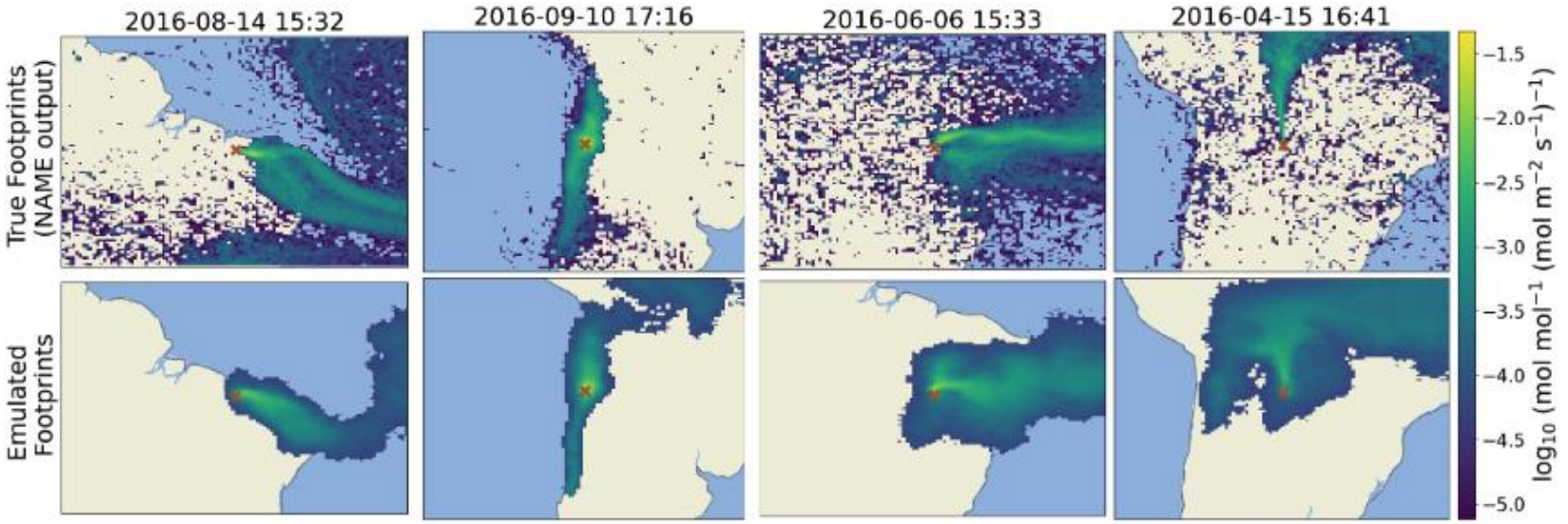


Figure 1: Samples of LPDM-generated footprints (top row) and the corresponding emulated footprints (bottom row), for an area of size ≈ 3300×2500 km over Brazil. The date in each column and the red cross in the centre of each image show when and where the satellite measurement was taken, and the footprint indicates the area to which that particular measurement is sensitive to. Note the $\log_{10}$ scale.

Overview: (3) Keshtmand et al. 2025

Prototype → GNN → Footprint

- Setup: Same as before, but adding prototype
- How to select prototype?
  - Expert-Driven Method

How?

  - Random Method
  - Data-Driven Method
    - K-mean Cluster

Overview: (3) Keshtmand et al. 2025

Prototype → GNN → Footprint

- Setup: Same as before, but adding prototype
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  - Expert-Driven Method

and a data-driven approach. An atmospheric dispersion expert chooses manually n footprints, aiming to cover a wide range of different conditions, such as where the upwind areas of the footprint are one of the four main cardinal directions (Fig. 1a). For comparison, we also train a

  - Random Method
  - Data-Driven Method
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Overview: (3) Keshtmand et al. 2025

Prototype → GNN → Footprint

- Setup: Same as before, but adding prototype
- How to assign a prototype
  - Shortest L2 distance of the PCA-64 space

$$L_2(\vec{x}) = \|\vec{x}\|_2 := \sqrt{\sum_i |x_i|^2}$$

Overview: (3) Keshtmand et al. 2025

Prototype → GNN → Footprint

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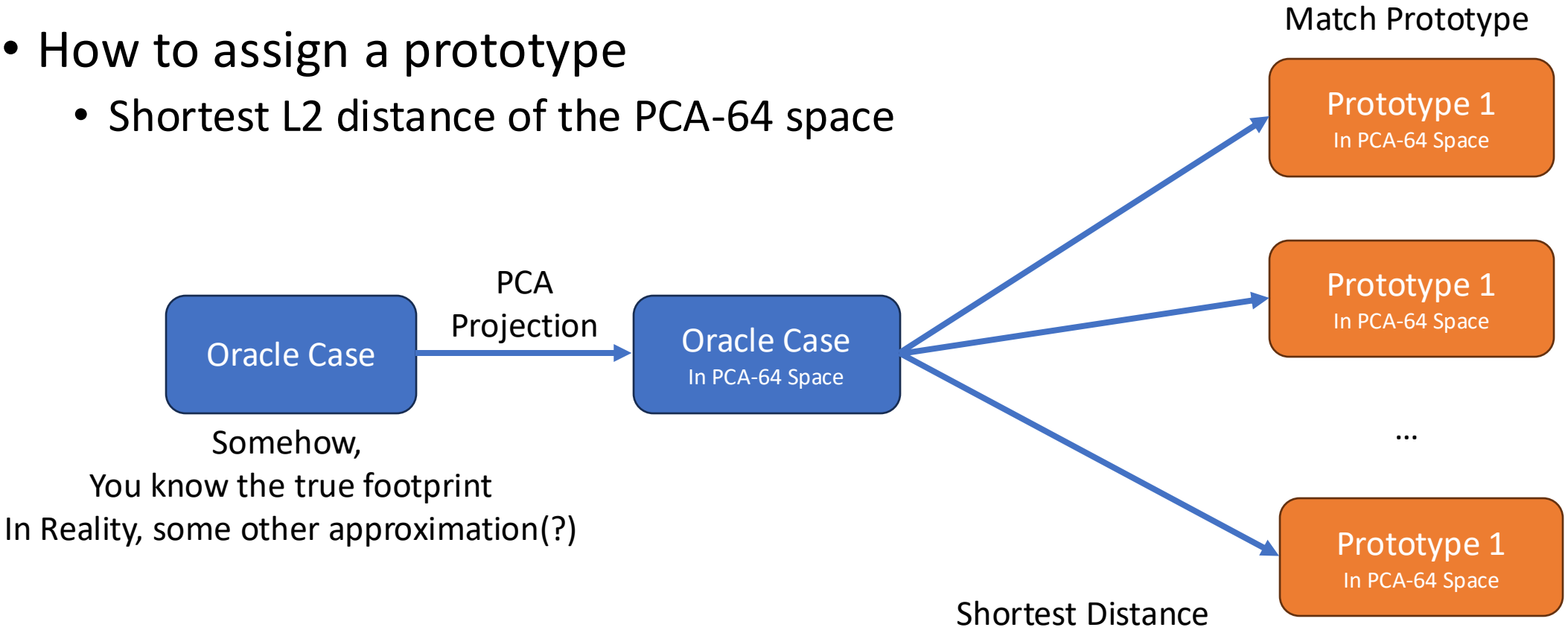

Overview: (3) Keshtmand et al. 2025

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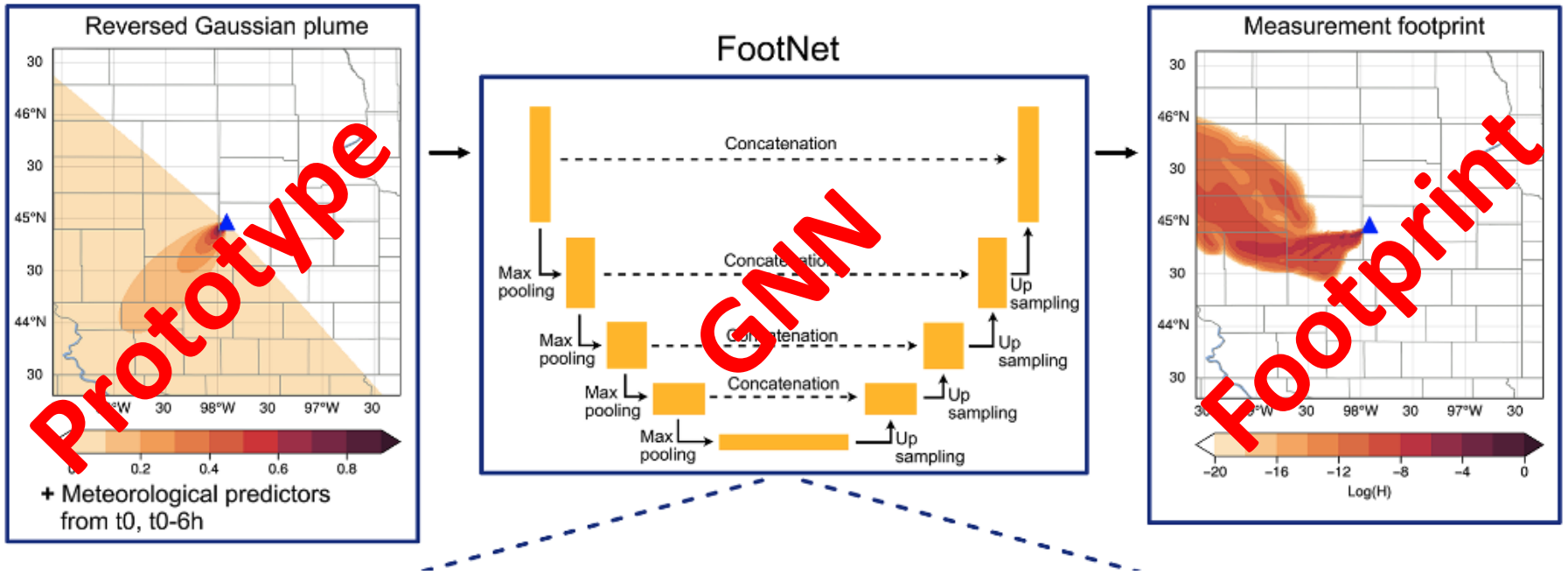


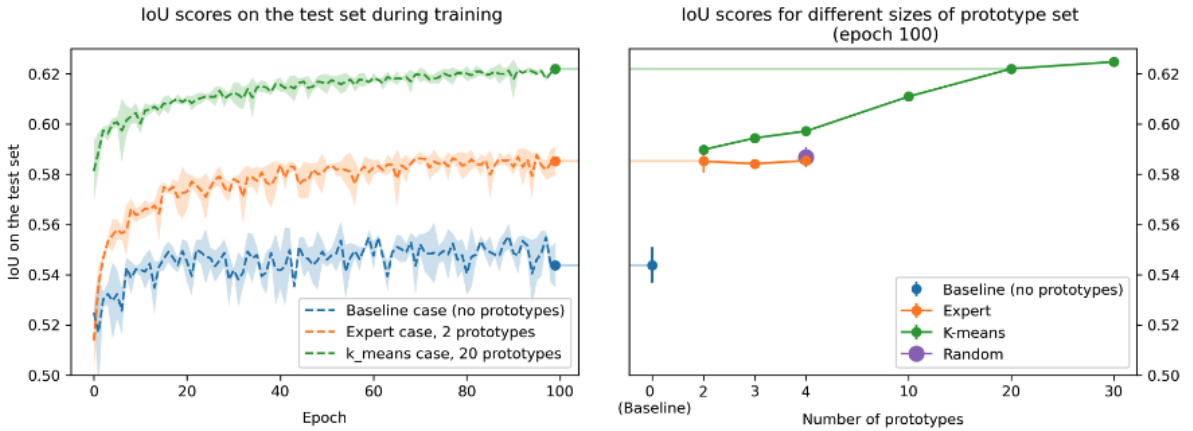
And other Met-Vars

Overview: (3) Keshtmand et al. 2025

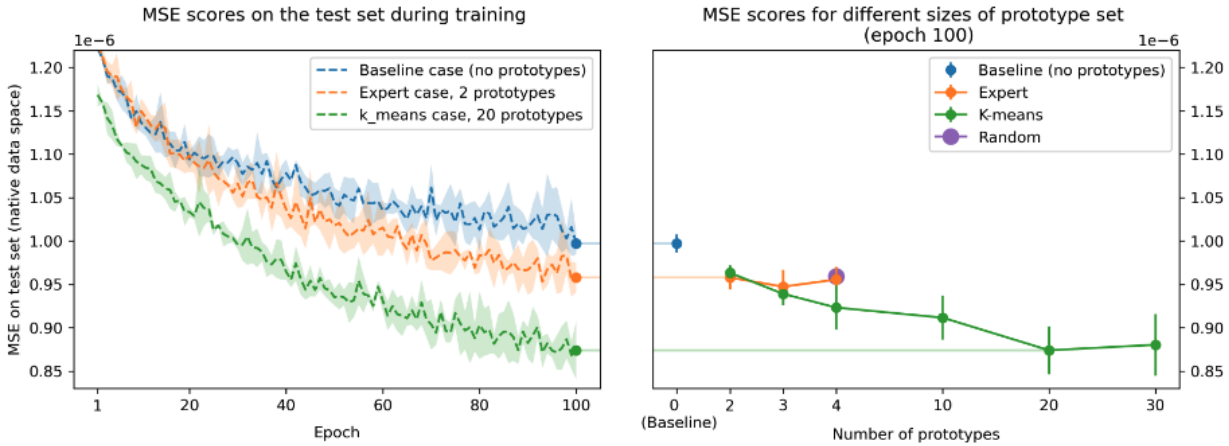
Prototype → GNN → Footprint

- Result Discussion:

(a) Intersection over Union (IoU) score for different prototype sets (Higher is better)



(b) Mean Squared Error (MSE) score for different prototype sets (Lower is better)



Overview: (3) Keshtmand et al. 2025

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