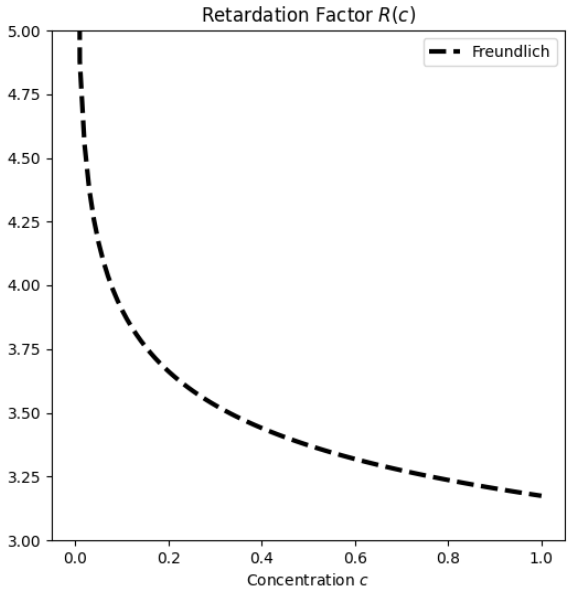
Uncertainty Quantification for Model Constitutive Relations

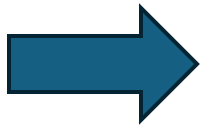
Finite Volume Neural Network (FINN) applied to a Diffusion-Sorption Problem

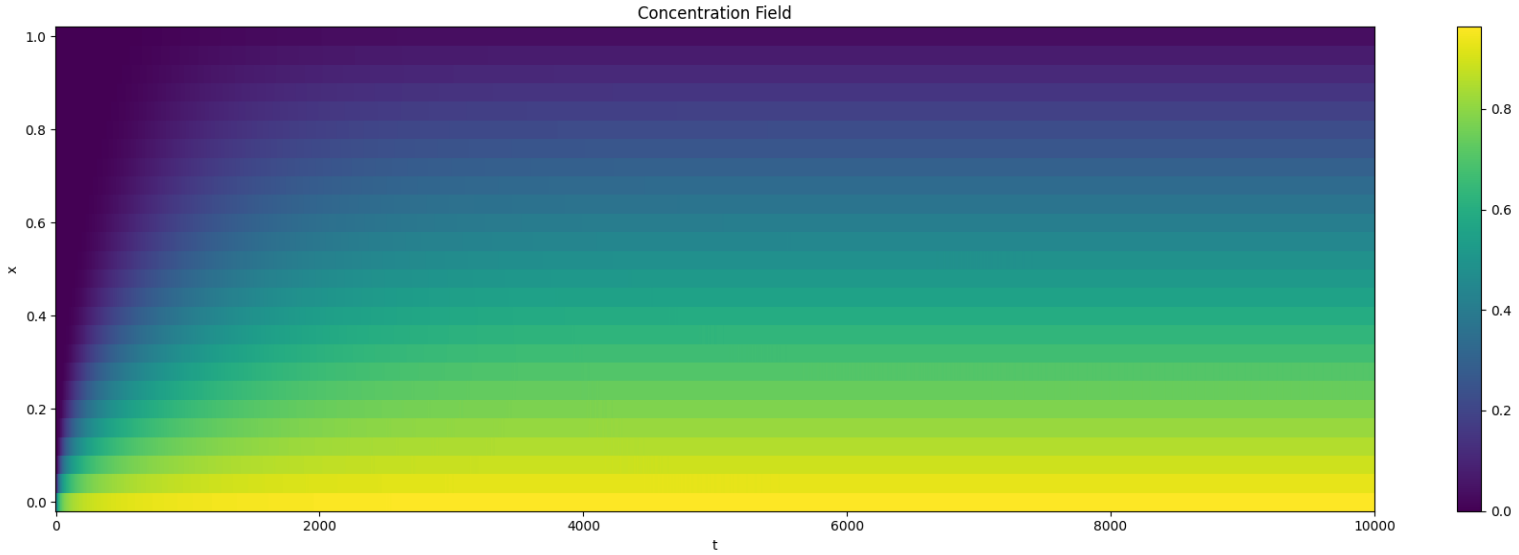
$$\frac{\partial c}{\partial t} = \frac{D}{R(c)} \frac{\partial^2 c}{\partial x^2}$$

Analytical Diffusion-Sorption Solution

$$\frac{\partial c}{\partial t} = \frac{D}{R(c)} \frac{\partial^2 c}{\partial x^2}$$





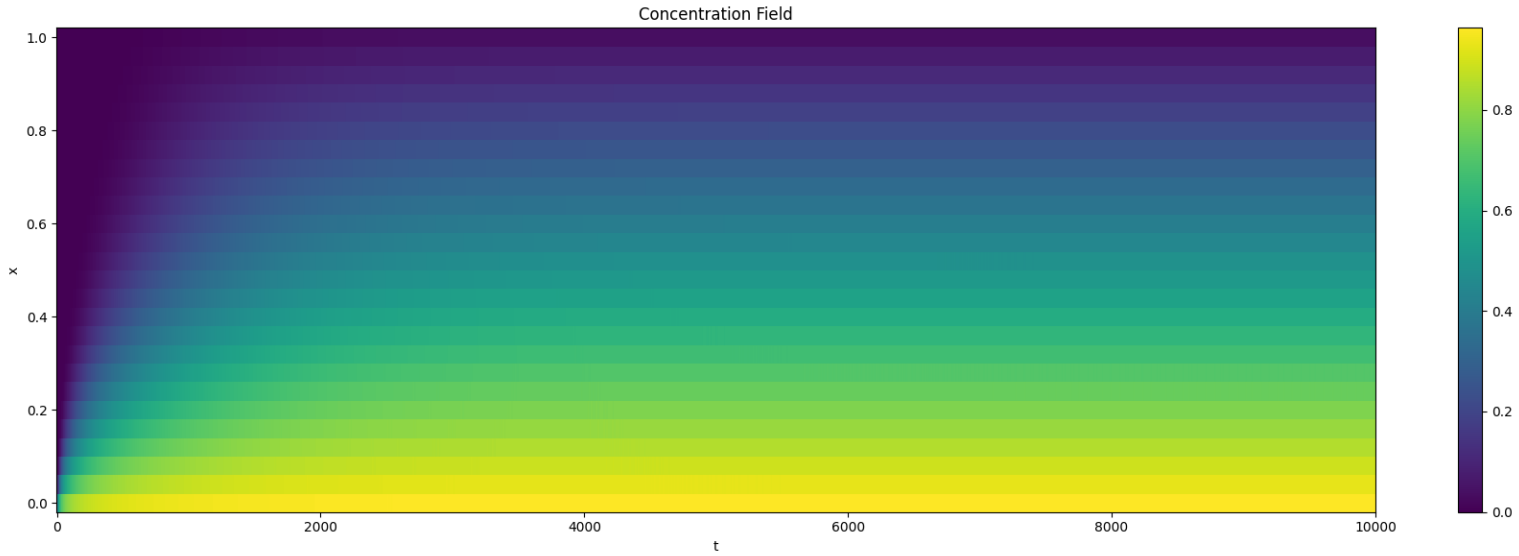


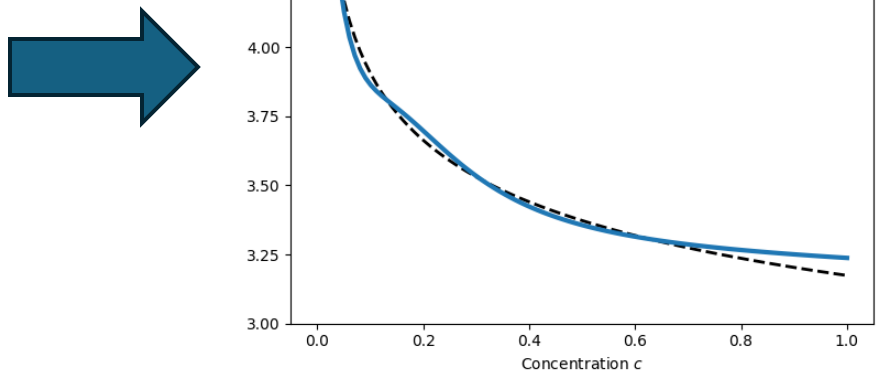
Retardation (given)

Concentration Field (output)

FINN on Diffusion-Sorption Problem

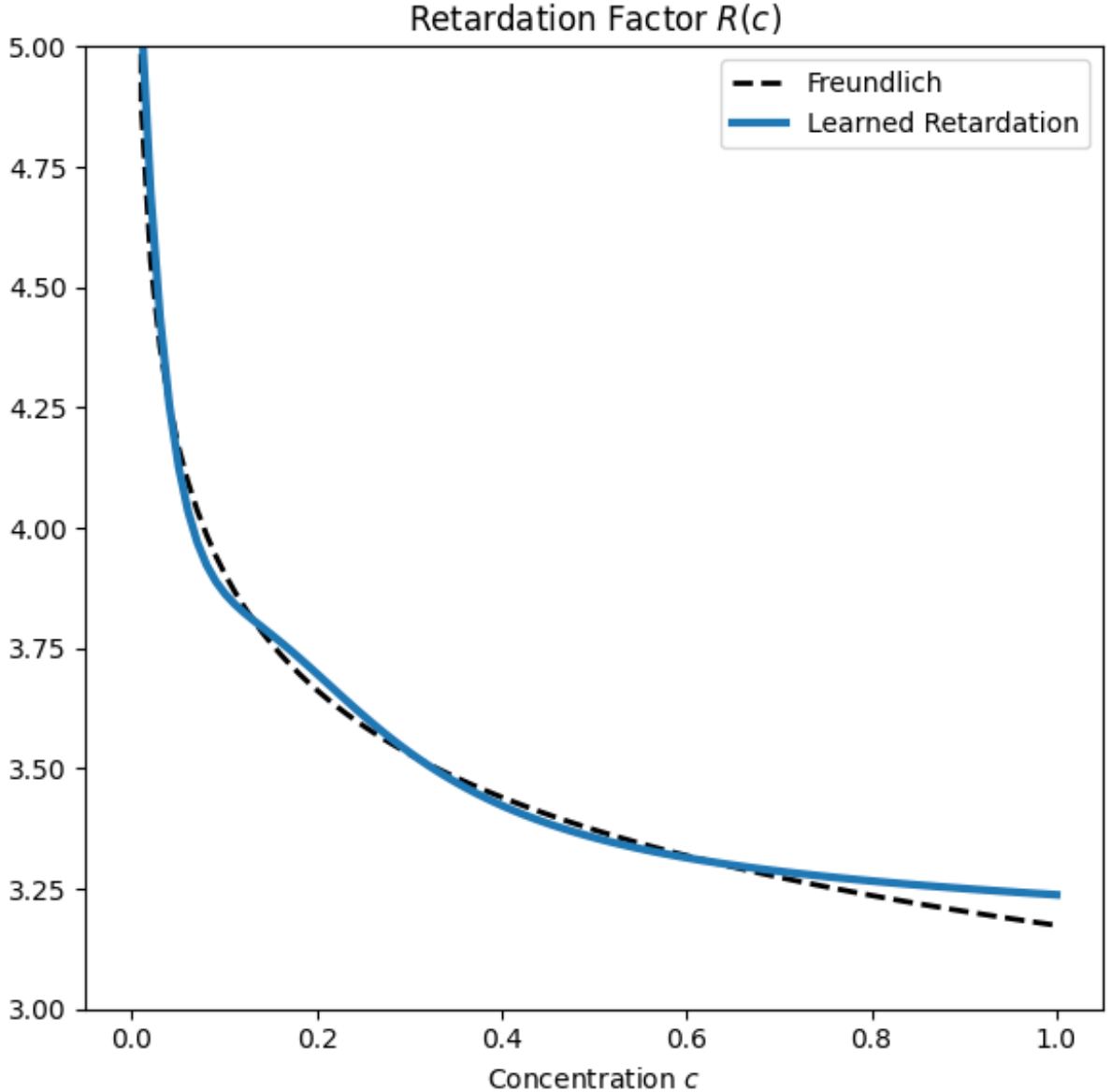
$$\frac{\partial c}{\partial t} = \frac{D}{R(c)} \frac{\partial^2 c}{\partial x^2}$$





Concentration Field
(input, synthetic or measured)

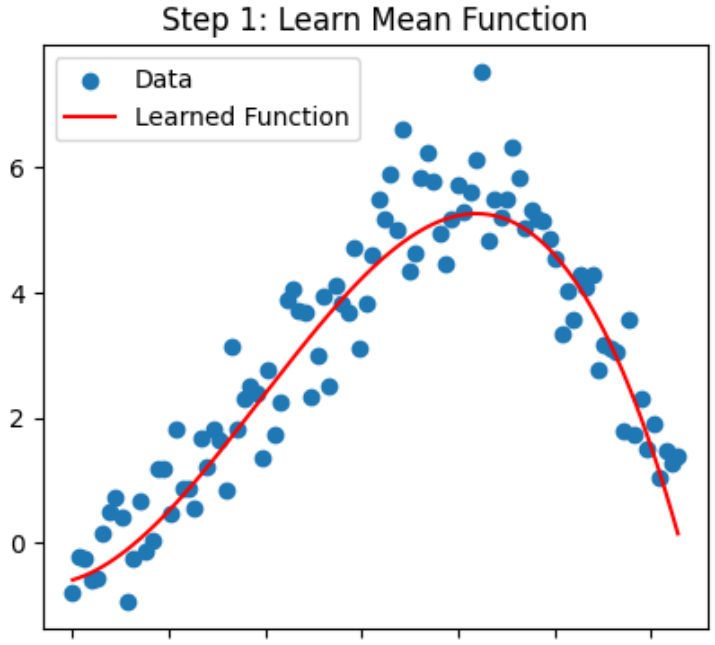
Retardation
(output, learned)

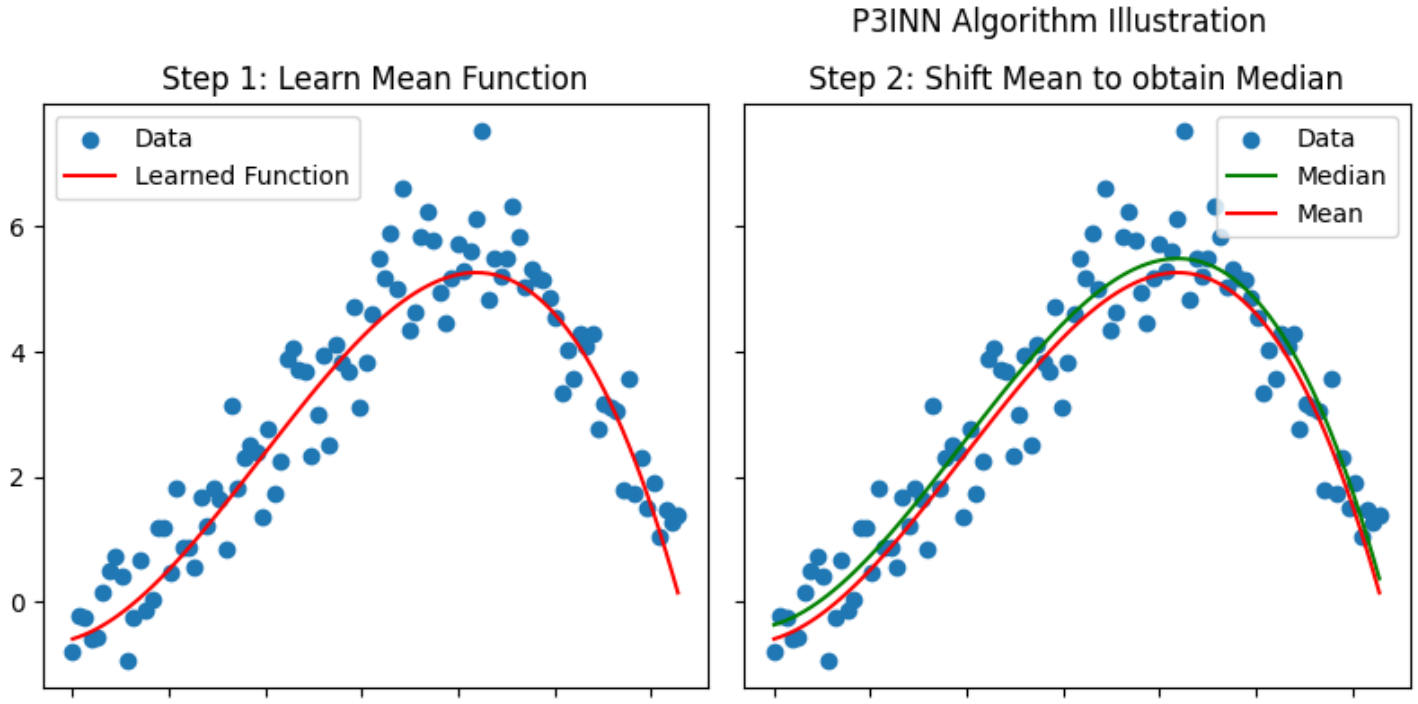

Retardation Factor $R(c)$
Freundlich
Learned Retardation
5.00
4.75
4.50
4.25
4.00
3.75
3.50
3.25
3.00
0.0
0.2
0.4
0.6
0.8
1.0
Concentration c

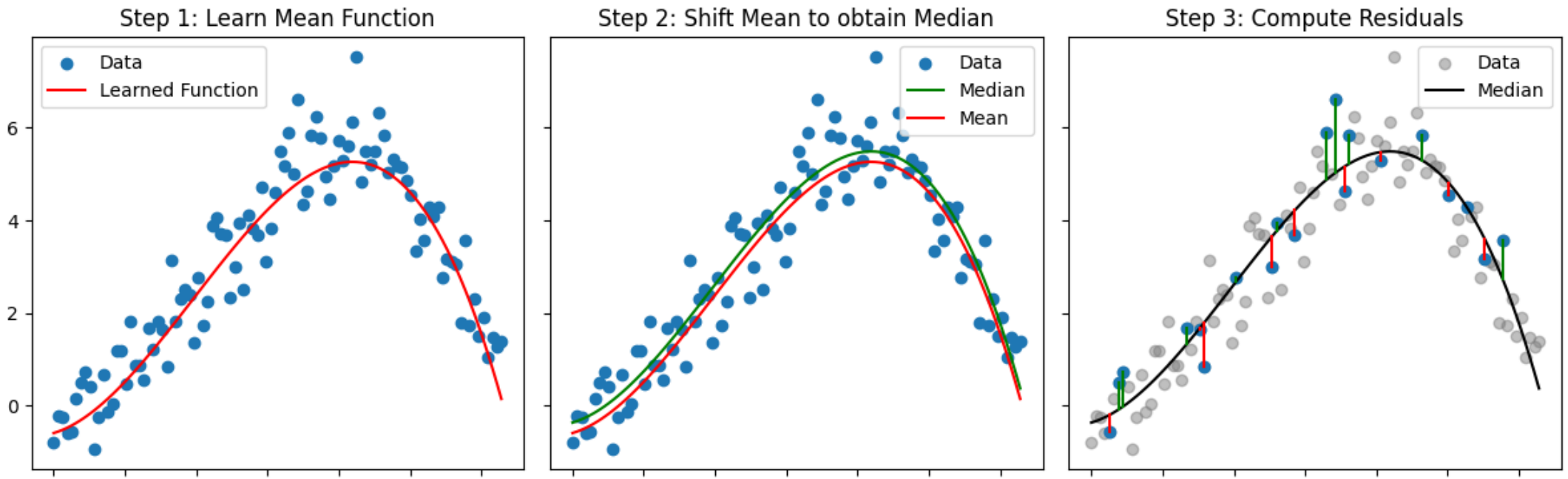
PI3NN Method

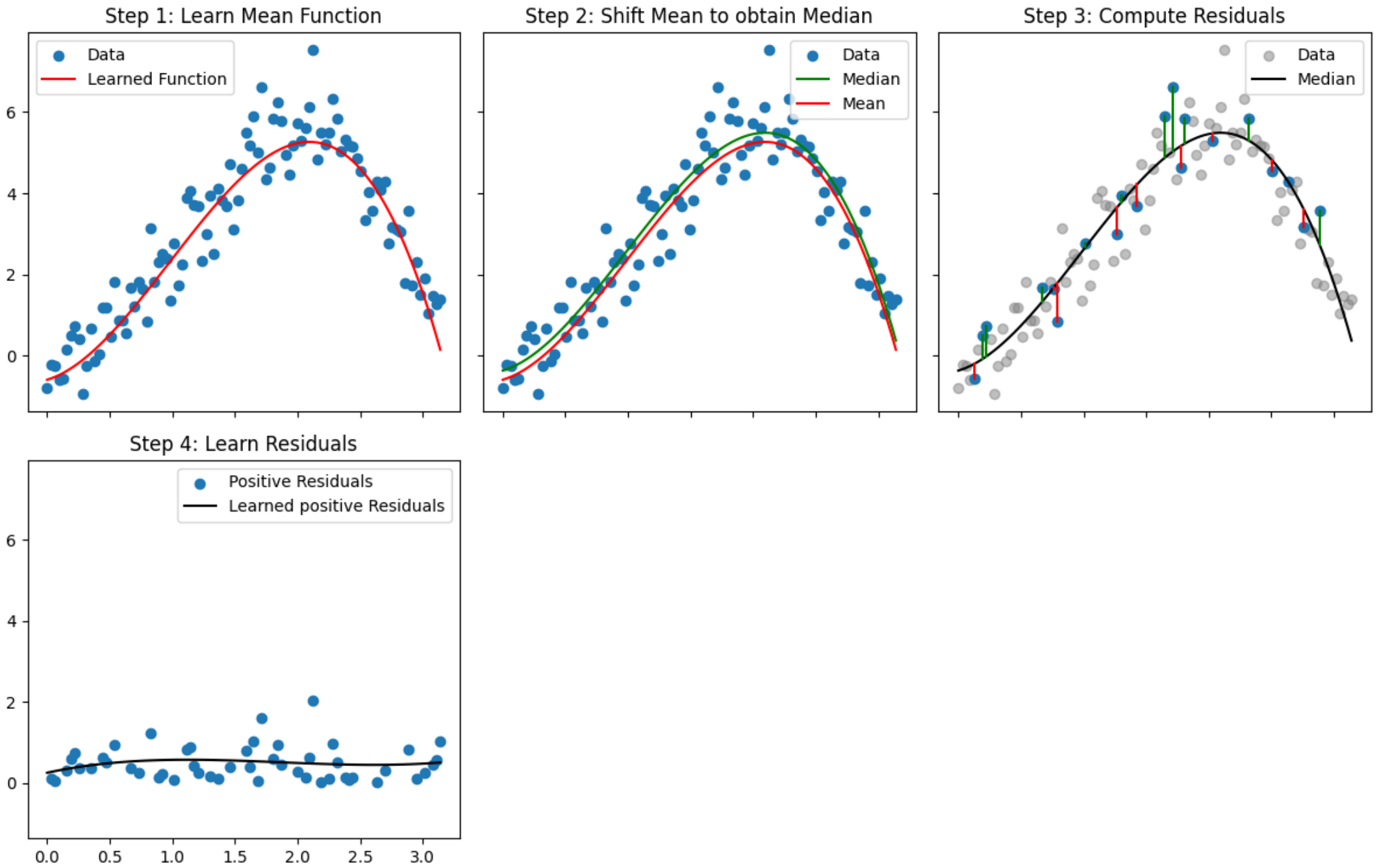
Prediction Intervals from 3 Neural Networks

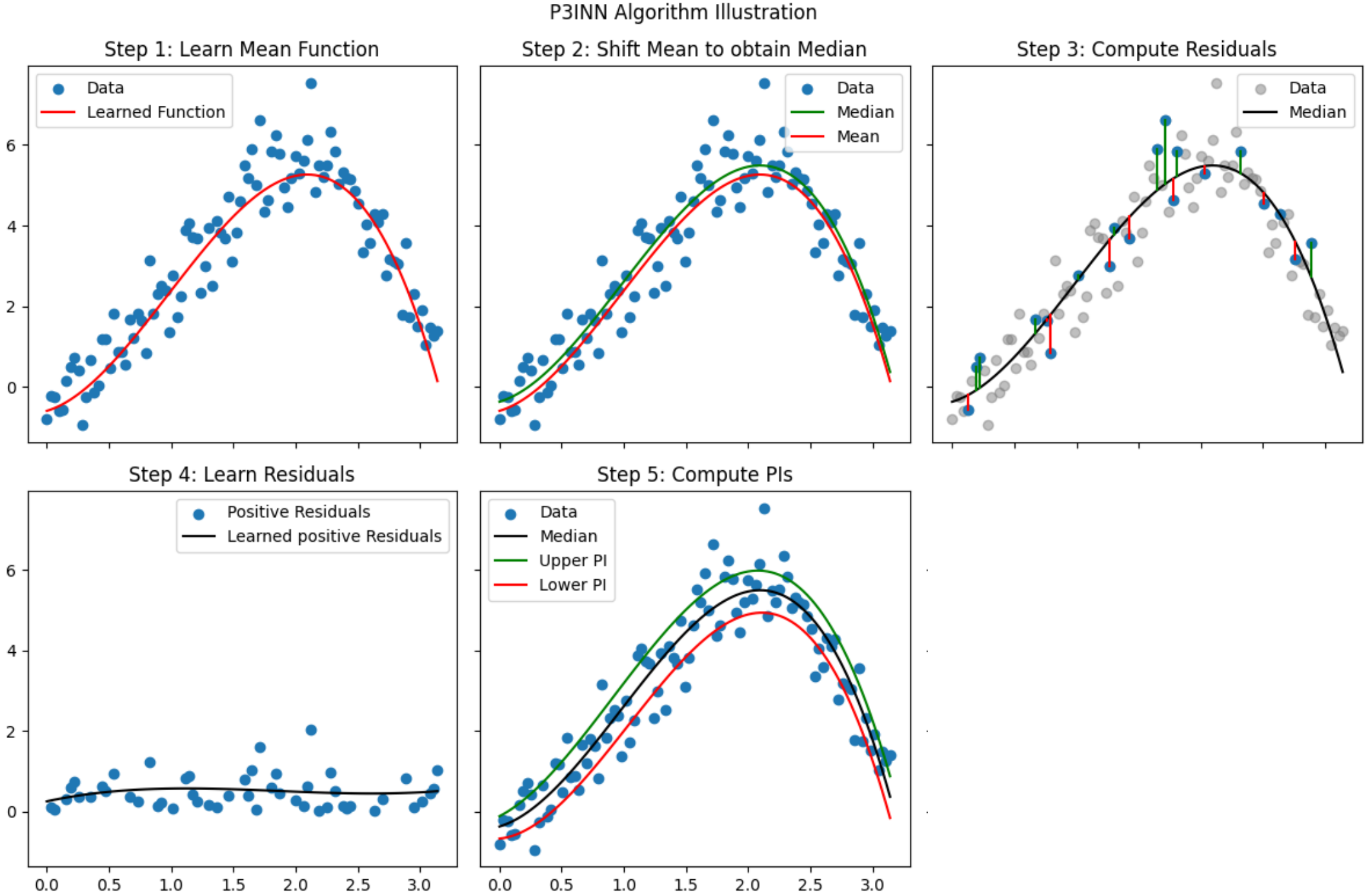
P3INN Algorithm Illustration

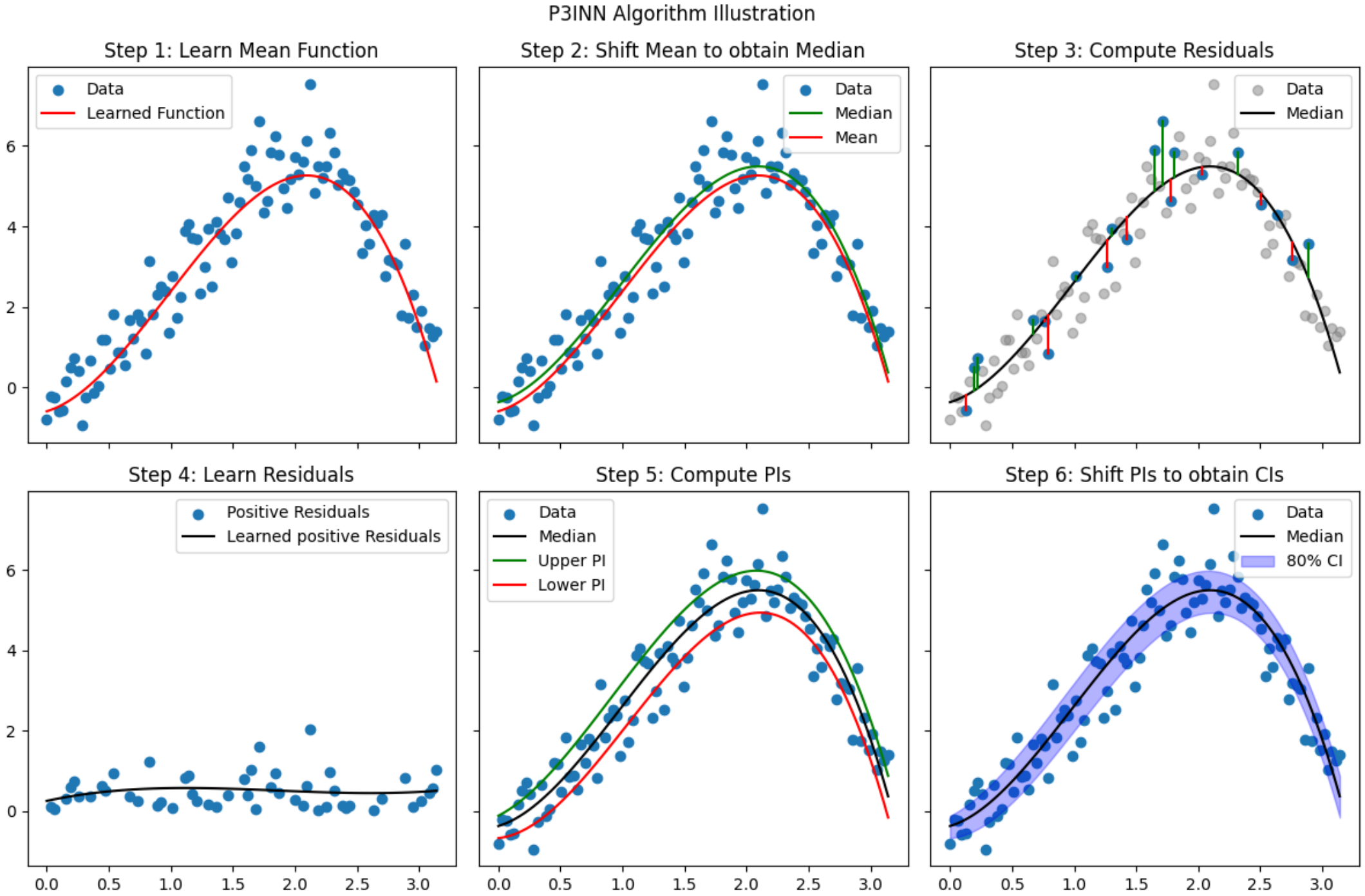



P3INN Algorithm Illustration
Step 1: Learn Mean Function
Data
Learned Function
6
4
2
0
Step 2: Shift Mean to obtain Median
Data
Median
Mean


P3INN Algorithm Illustration
Step 1: Learn Mean Function
Data
Learned Function
6
4
2
0
Step 2: Shift Mean to obtain Median
Data
Median
Mean
Step 3: Compute Residuals
Data
Median


P3INN Algorithm Illustration
Step 1: Learn Mean Function
Data
Learned Function
Step 2: Shift Mean to obtain Median
Data
Median
Mean
Step 3: Compute Residuals
Data
Median
Step 4: Learn Residuals
Positive Residuals
Learned positive Residuals
0
2
4
6
0.0
0.5
1.0
1.5
2.0
2.5
3.0


P3INN Algorithm Illustration
Step 1: Learn Mean Function
Data
Learned Function
Step 2: Shift Mean to obtain Median
Data
Median
Mean
Step 3: Compute Residuals
Data
Median
Step 4: Learn Residuals
Positive Residuals
Learned positive Residuals
Step 5: Compute PIs
Data
Median
Upper PI
Lower PI
0
2
4
6
0.0
0.5
1.0
1.5
2.0
2.5
3.0

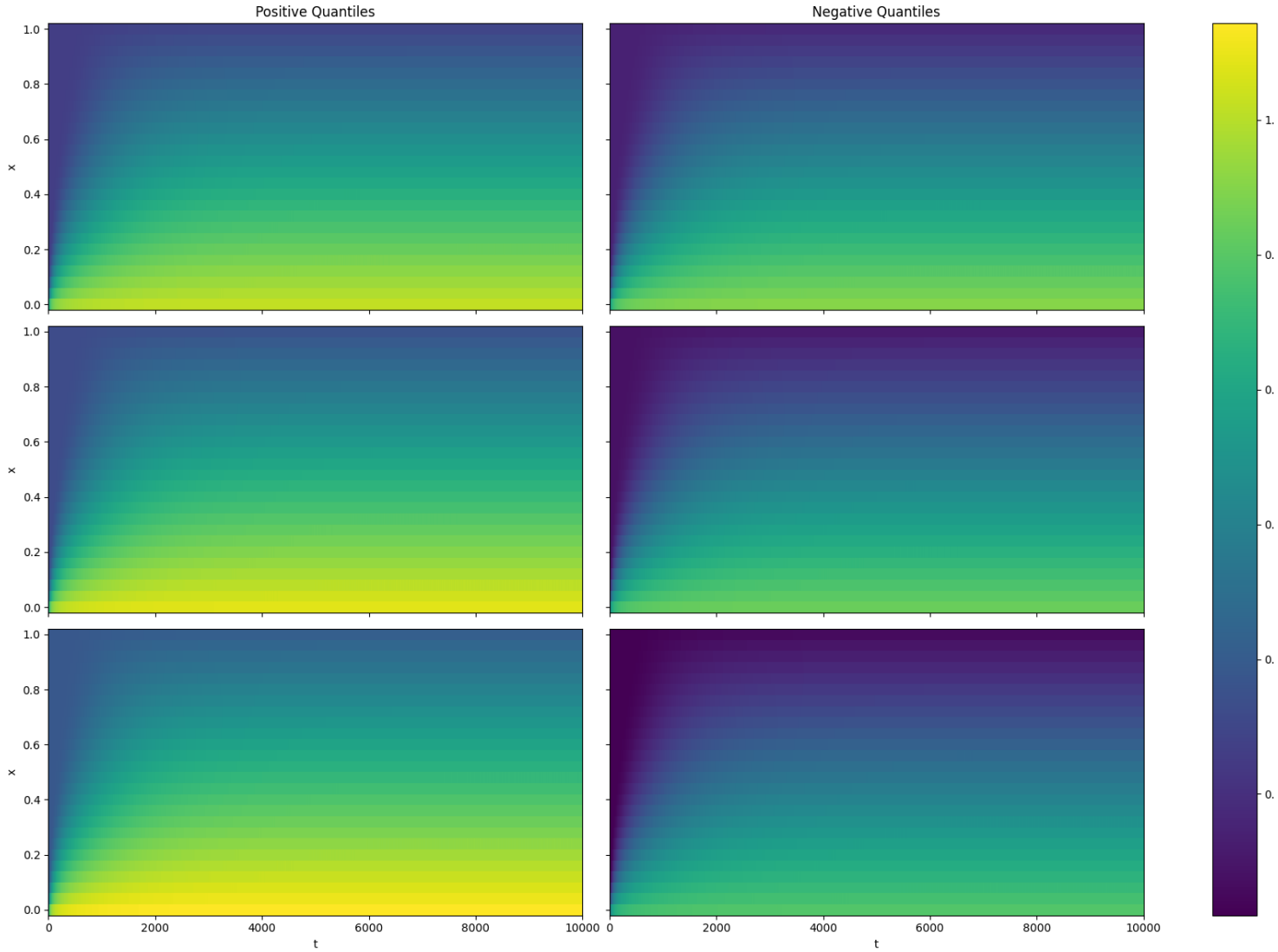

P3INN Algorithm Illustration
Step 1: Learn Mean Function
Data
Learned Function
Step 2: Shift Mean to obtain Median
Data
Median
Mean
Step 3: Compute Residuals
Data
Median
Step 4: Learn Residuals
Positive Residuals
Learned positive Residuals
Step 5: Compute PIs
Data
Median
Upper PI
Lower PI
Step 6: Shift PIs to obtain CIs
Data
Median
80% CI
0
2
4
6
0.0
0.5
1.0
1.5
2.0
2.5
3.0

Reasons for Uncertainty

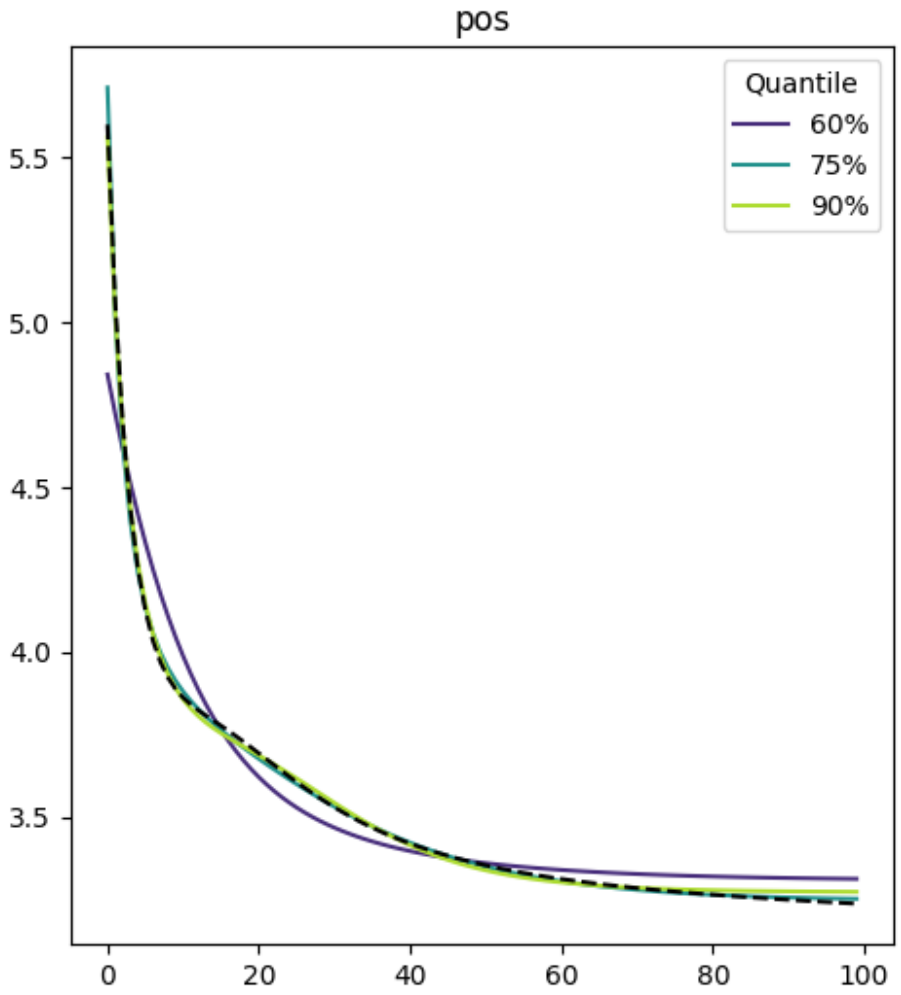
1. Data Uncertainty
2. Model Uncertainty

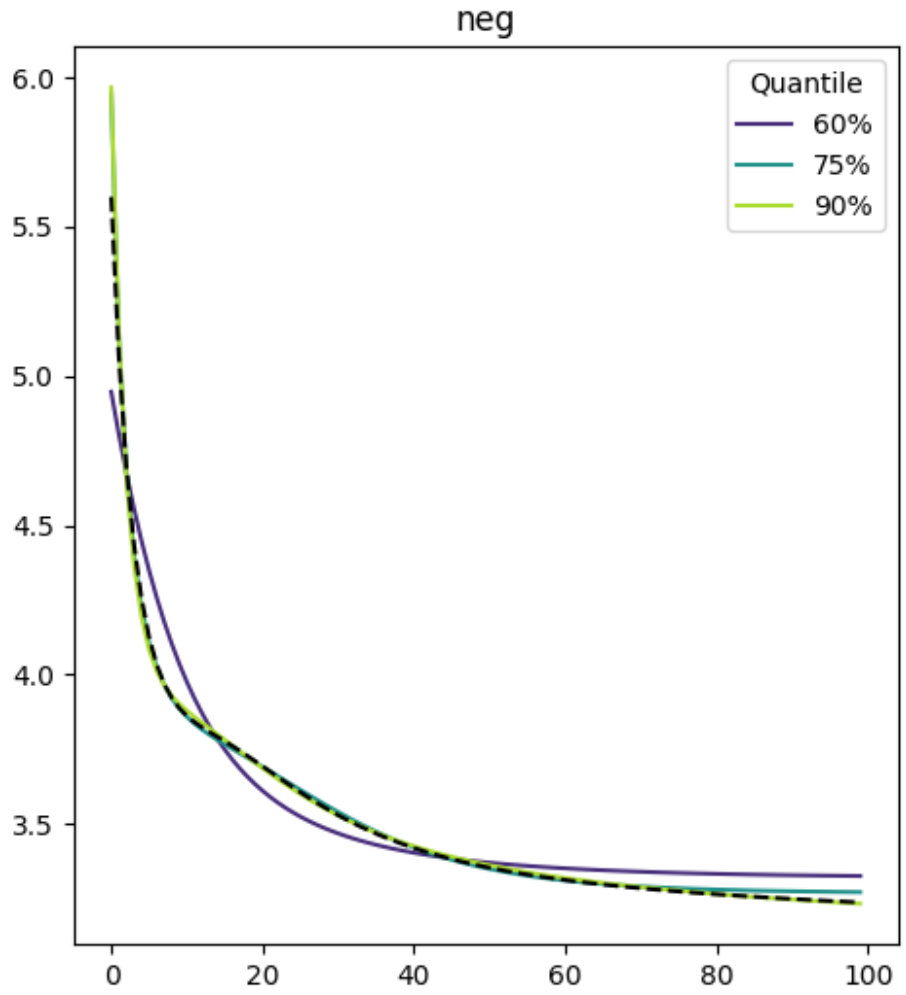
1. Data Uncertainty

PIs from Data Uncertainty

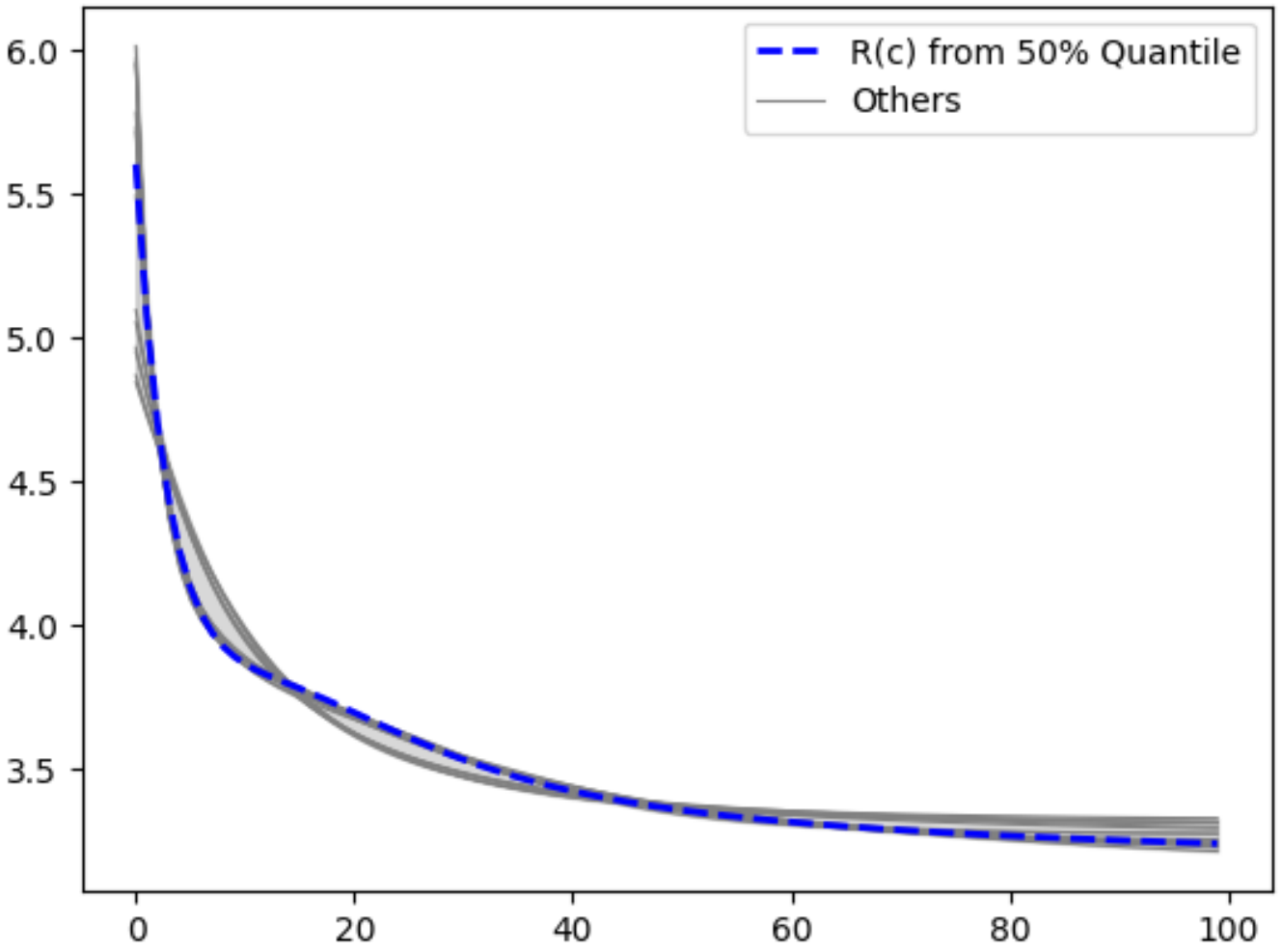


PIs from Data Uncertainty





PIs from Data Uncertainty

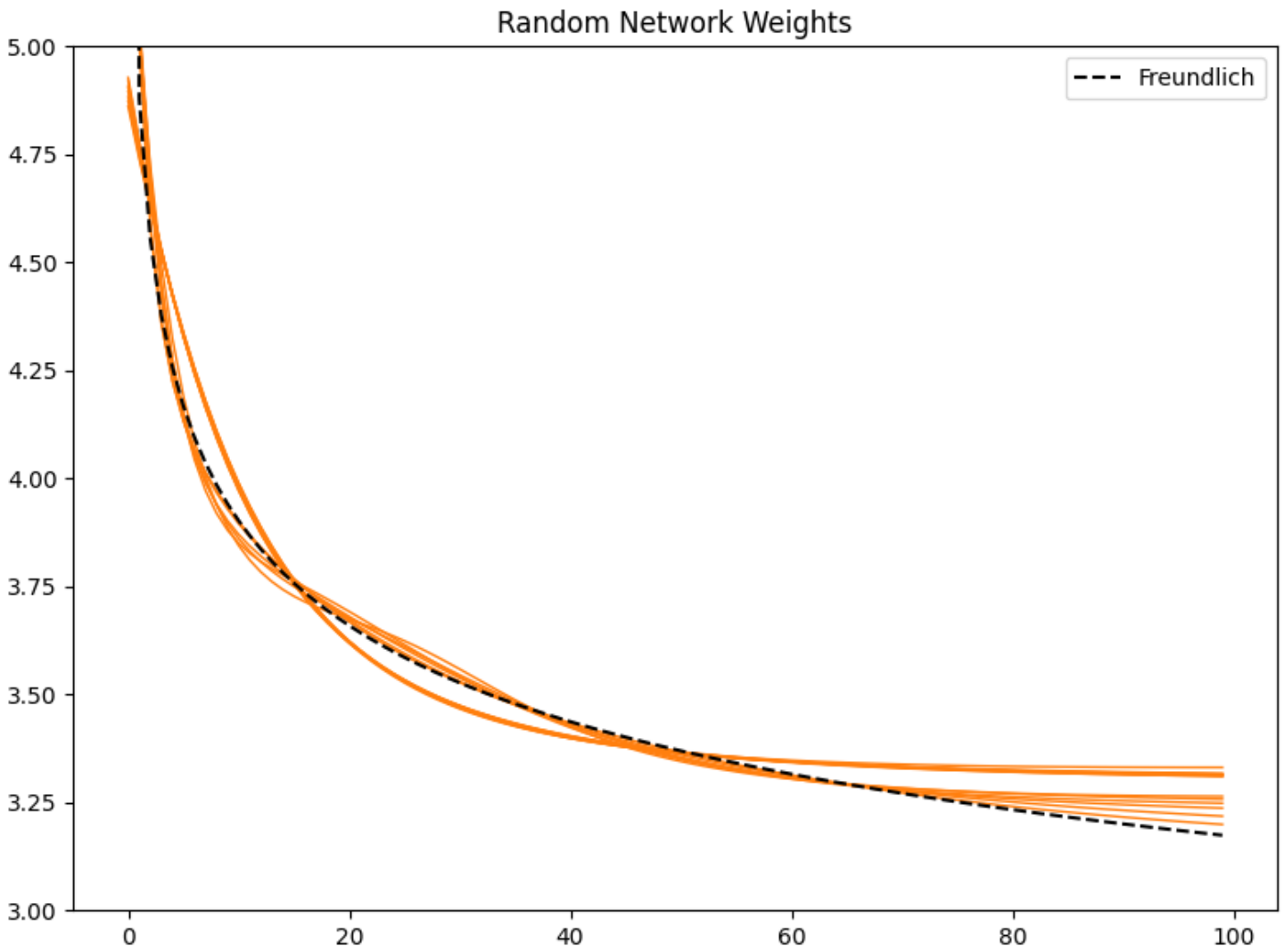


2. Model Uncertainty

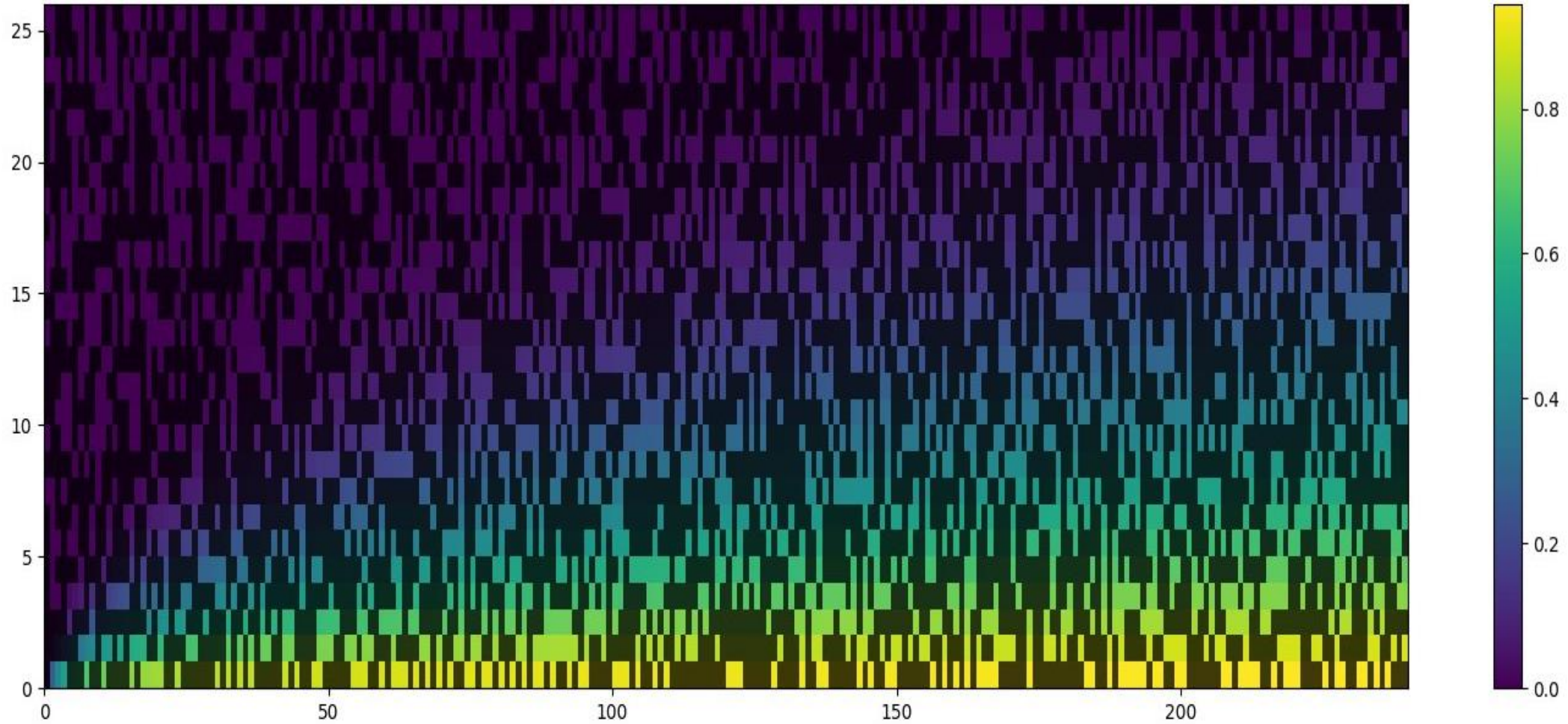
Model Uncertainty of FINN

1. Randomly initialized neural network weights
2. "Information extraction" from incomplete data
    - "Noisy Concentration Mask"
    - "Time Interval Subset"

1. Random Network Weights

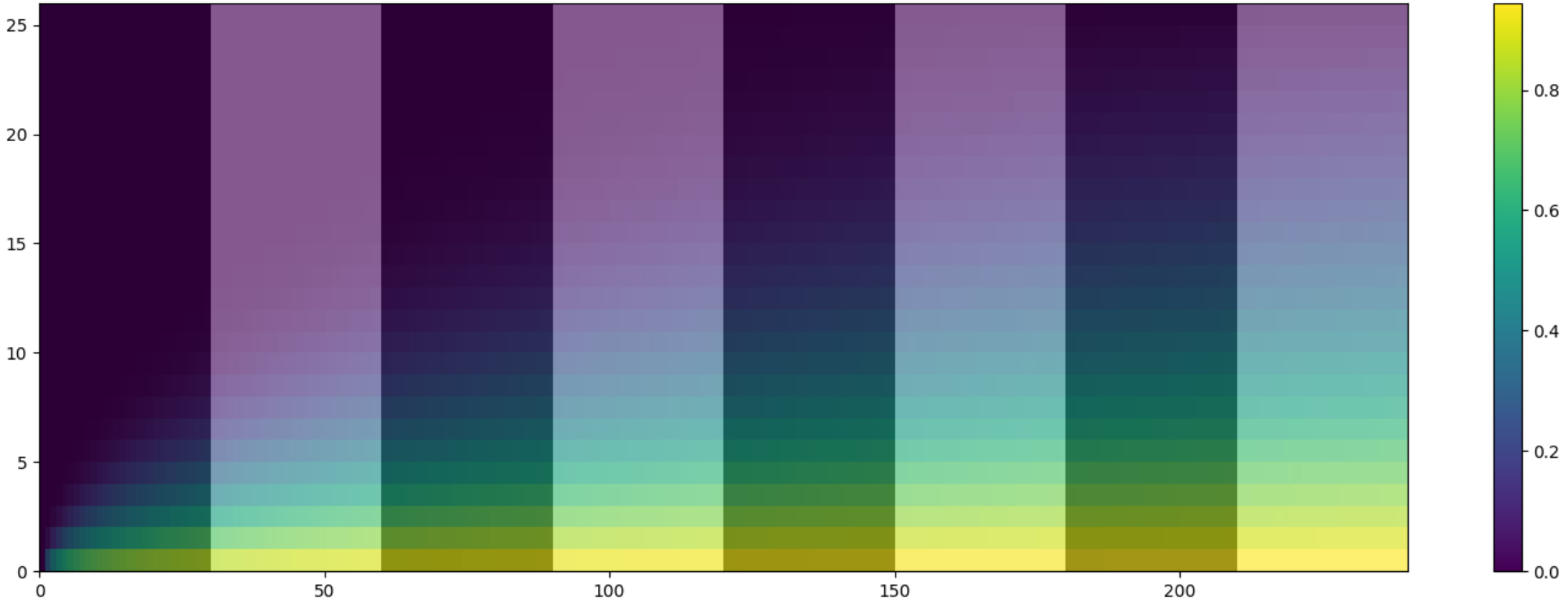


2a. Noisy Concentration Mask

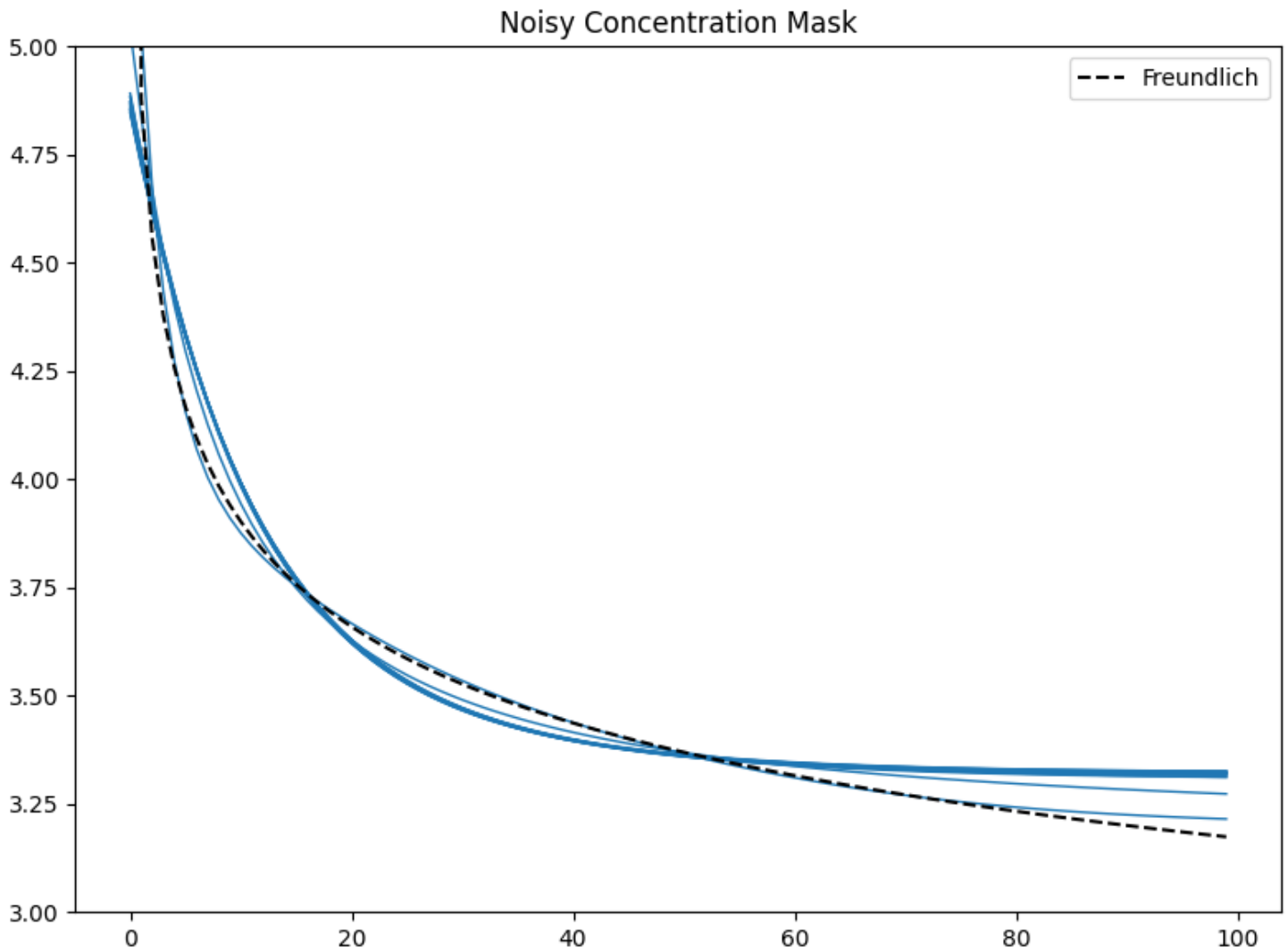


2b. Time Interval Subsets

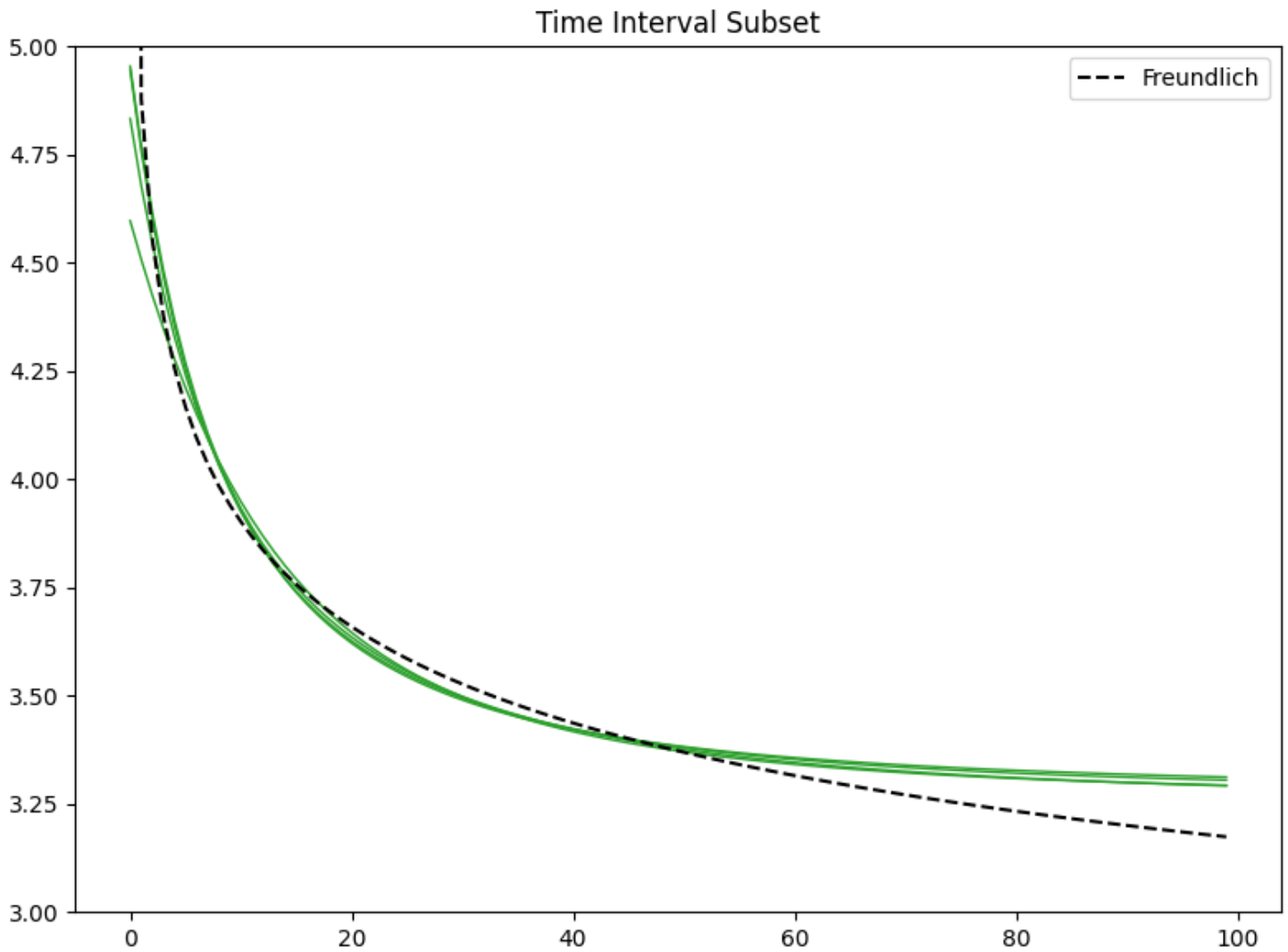
FINN on each Time Interval separately



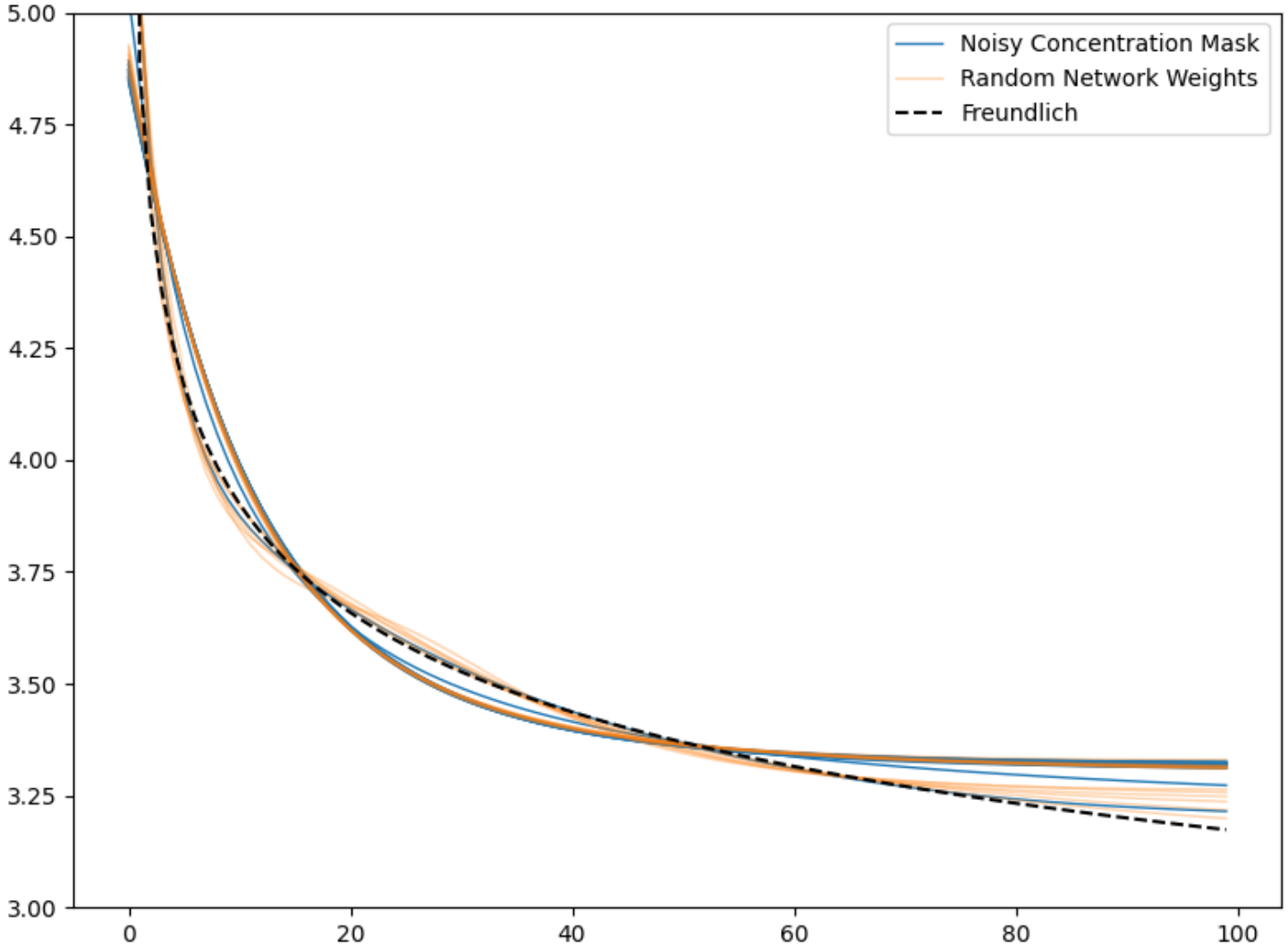
2a. Noisy Concentration Mask



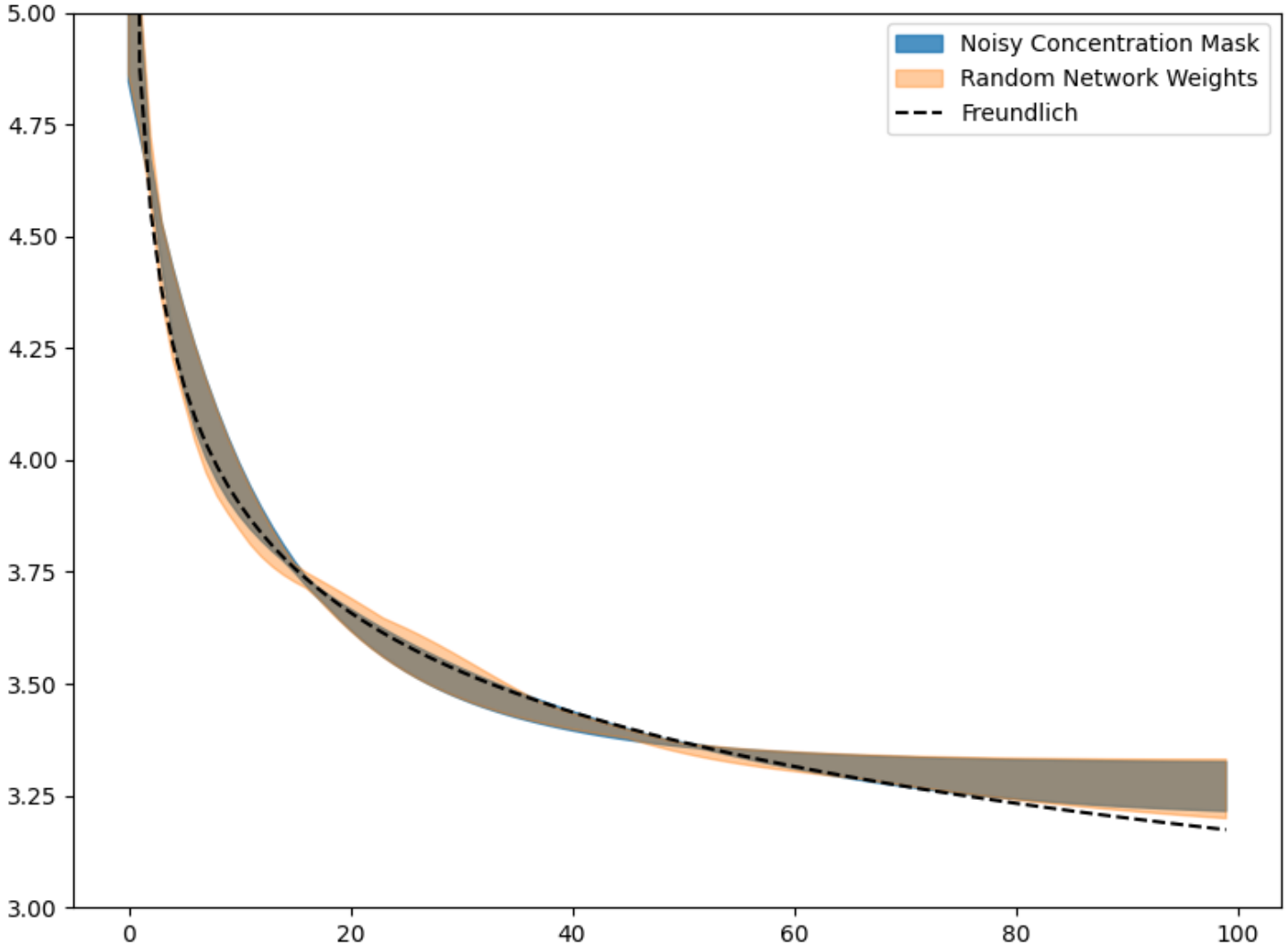
2b. Time Interval Subset



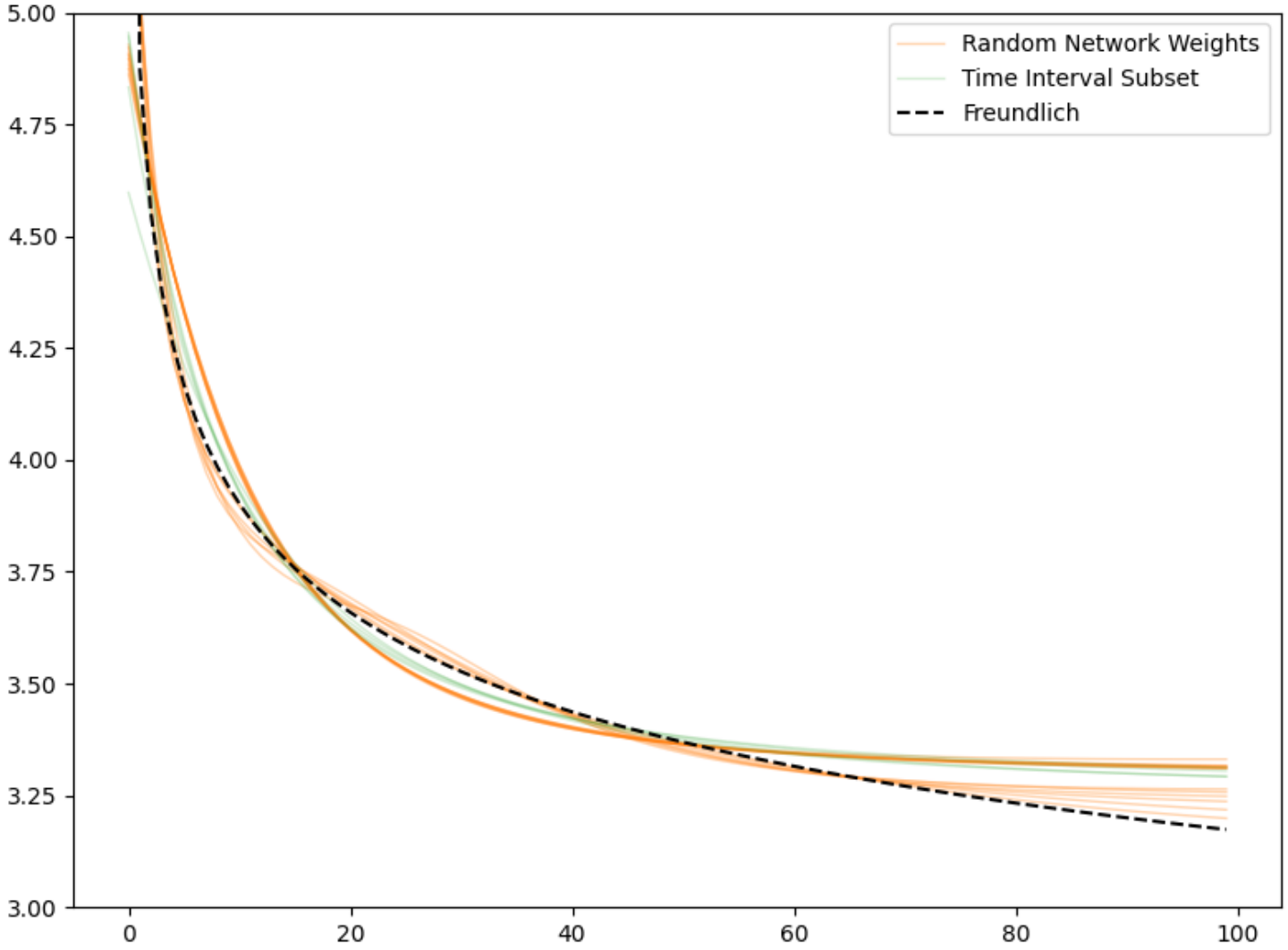
Comparison: Weights – Concentration Mask



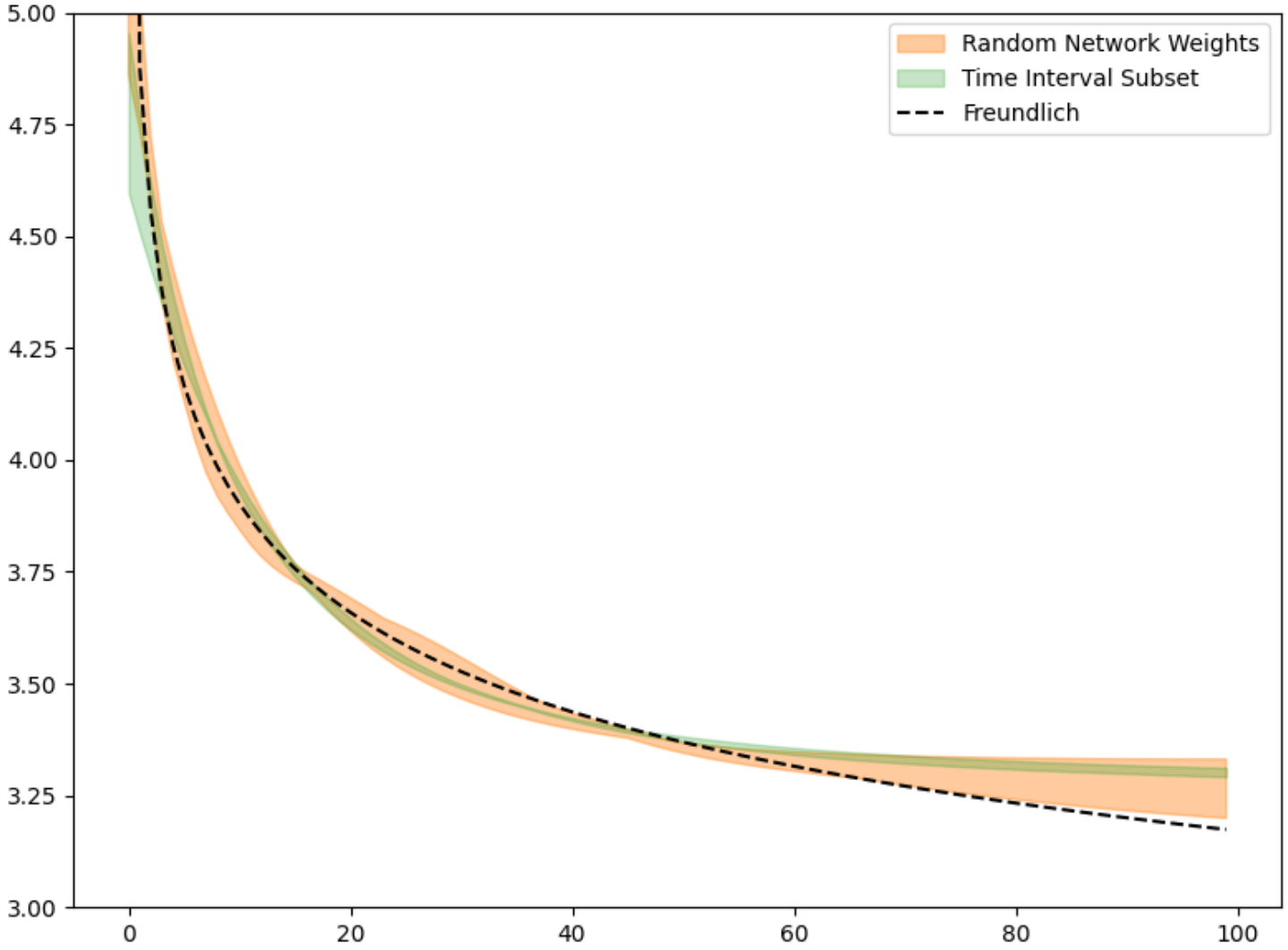
Comparison: Weights – Concentration Mask



Comparison: Weights – Time Interval Subset



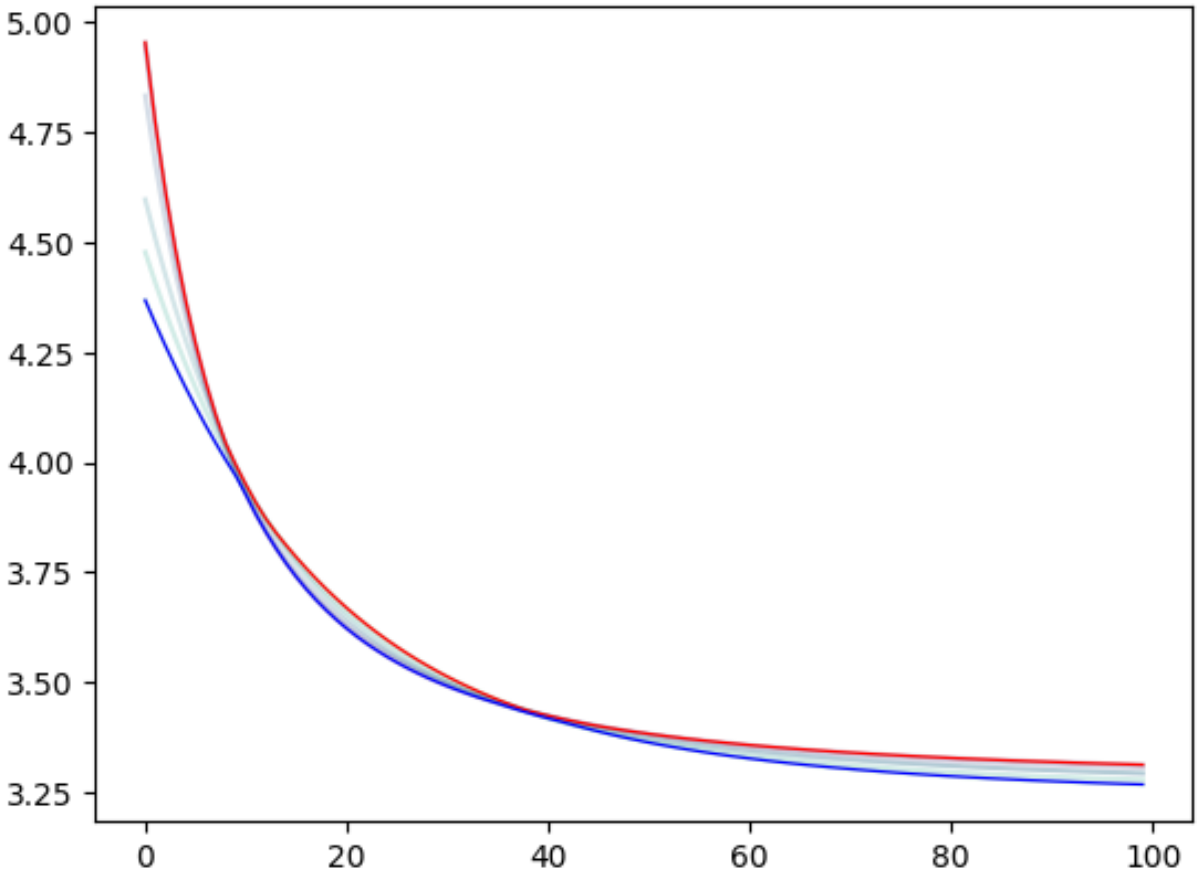
Comparison: Weights – Time Interval Subset

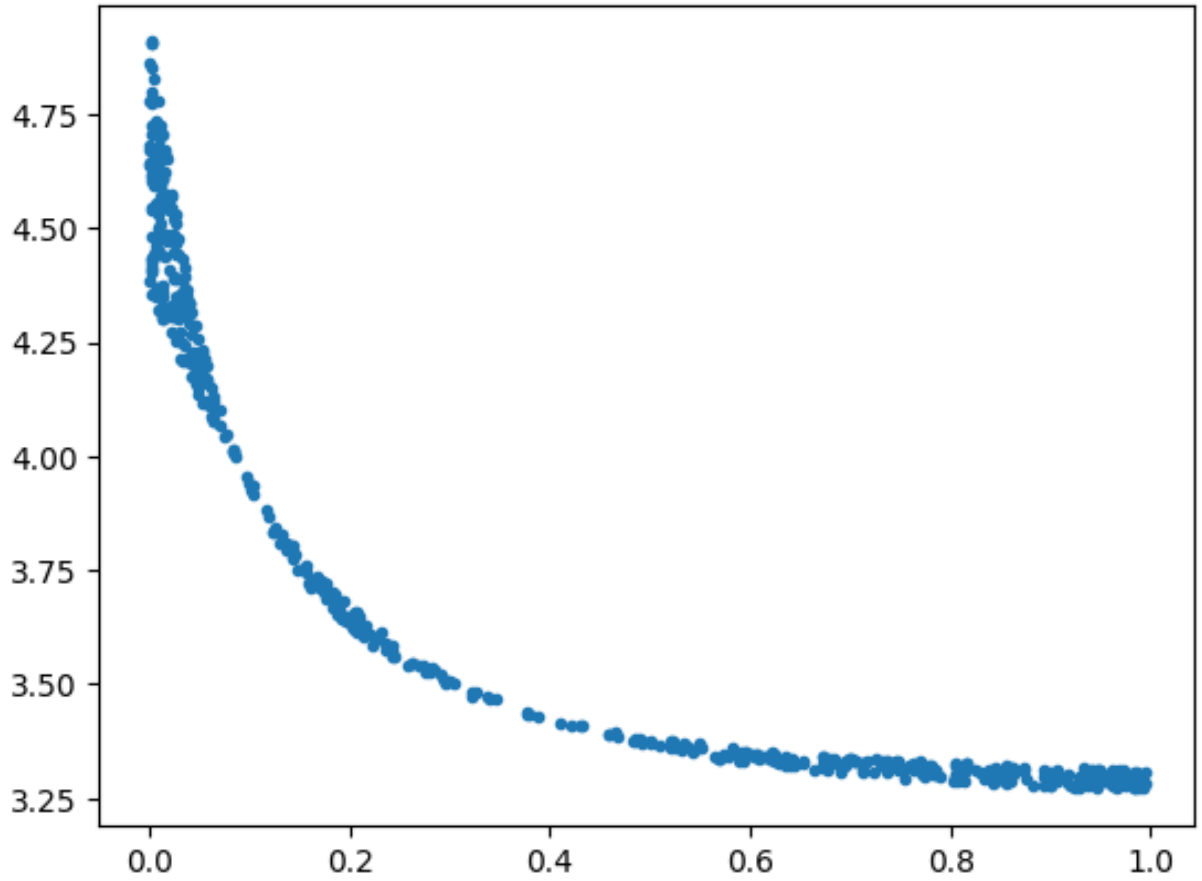


Application of PI3NN

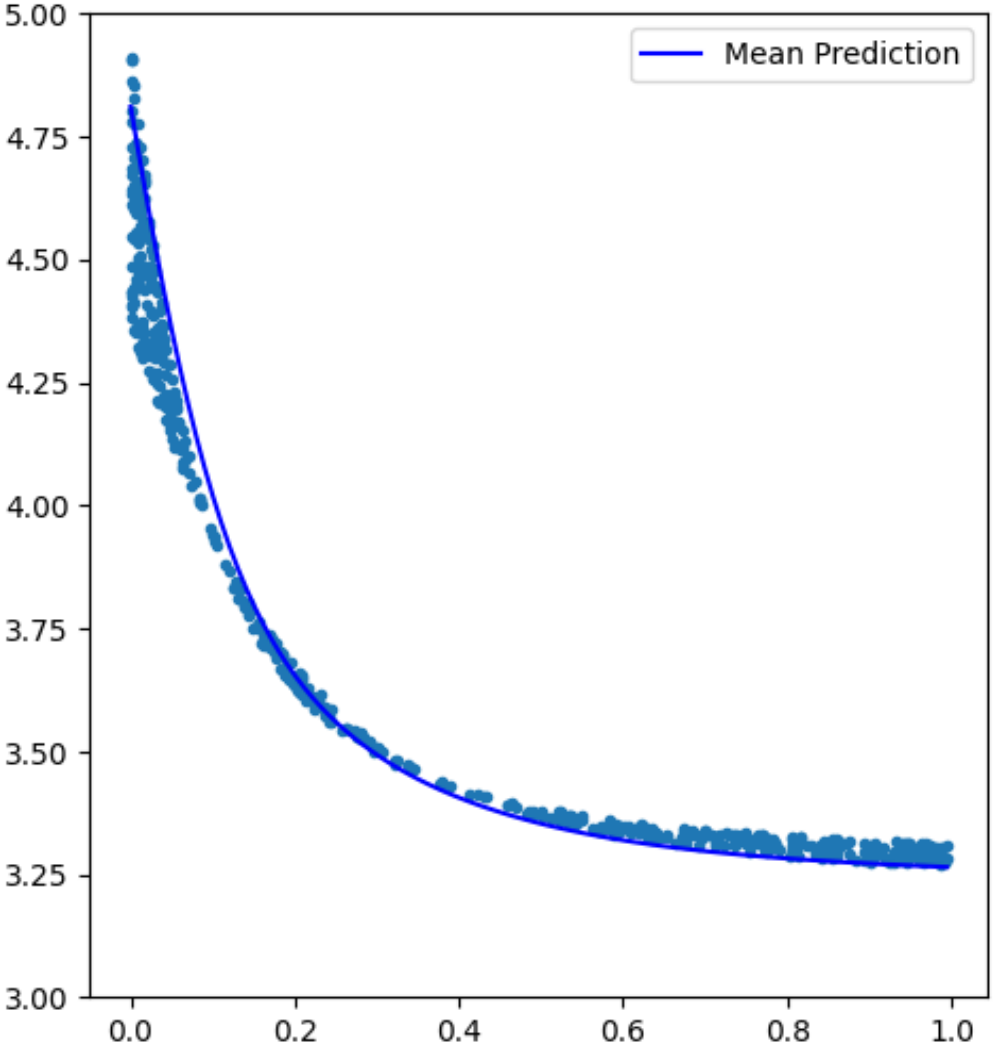
- PI3NN Advantage:
  - Computationally inexpensive computation of Quantiles
- Idea:
  - Sample points for PI3NN from enveloping curves

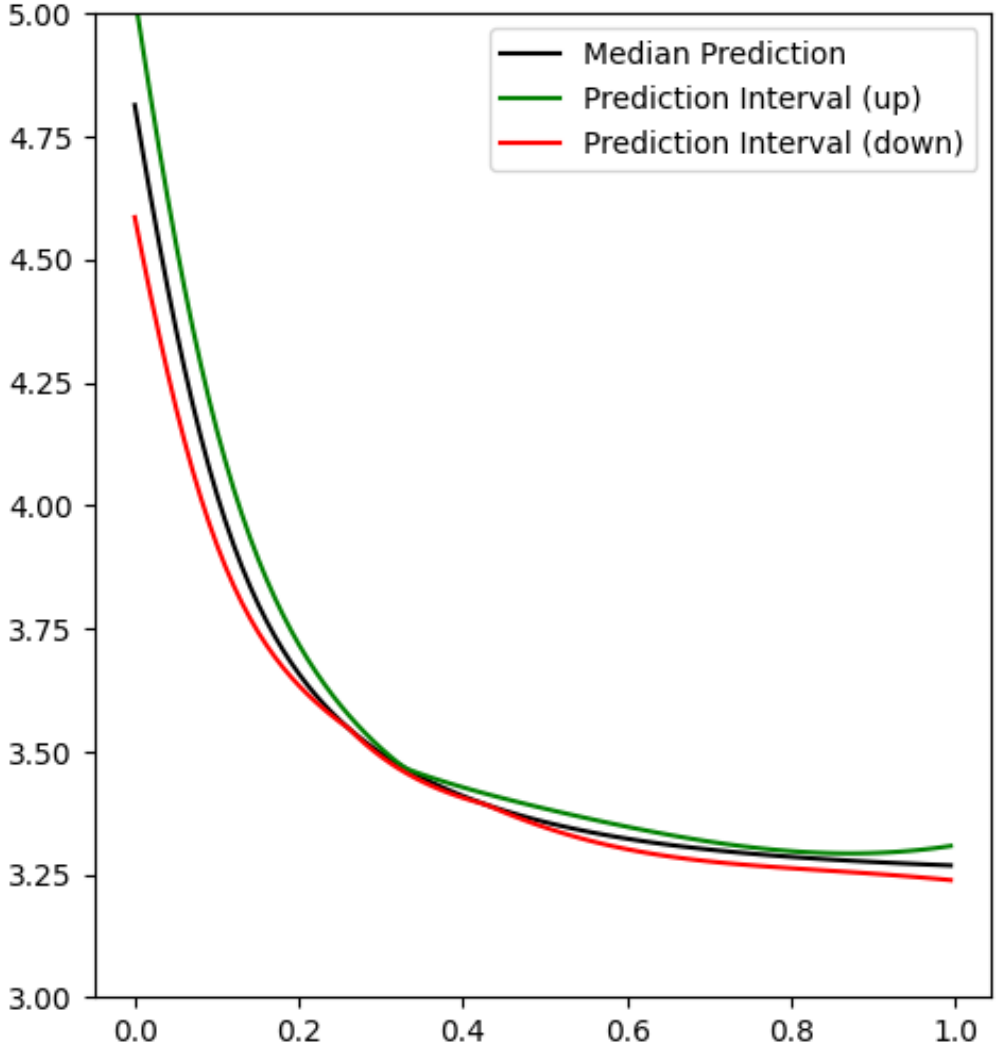
Application of PI3NN – Dataset Generation



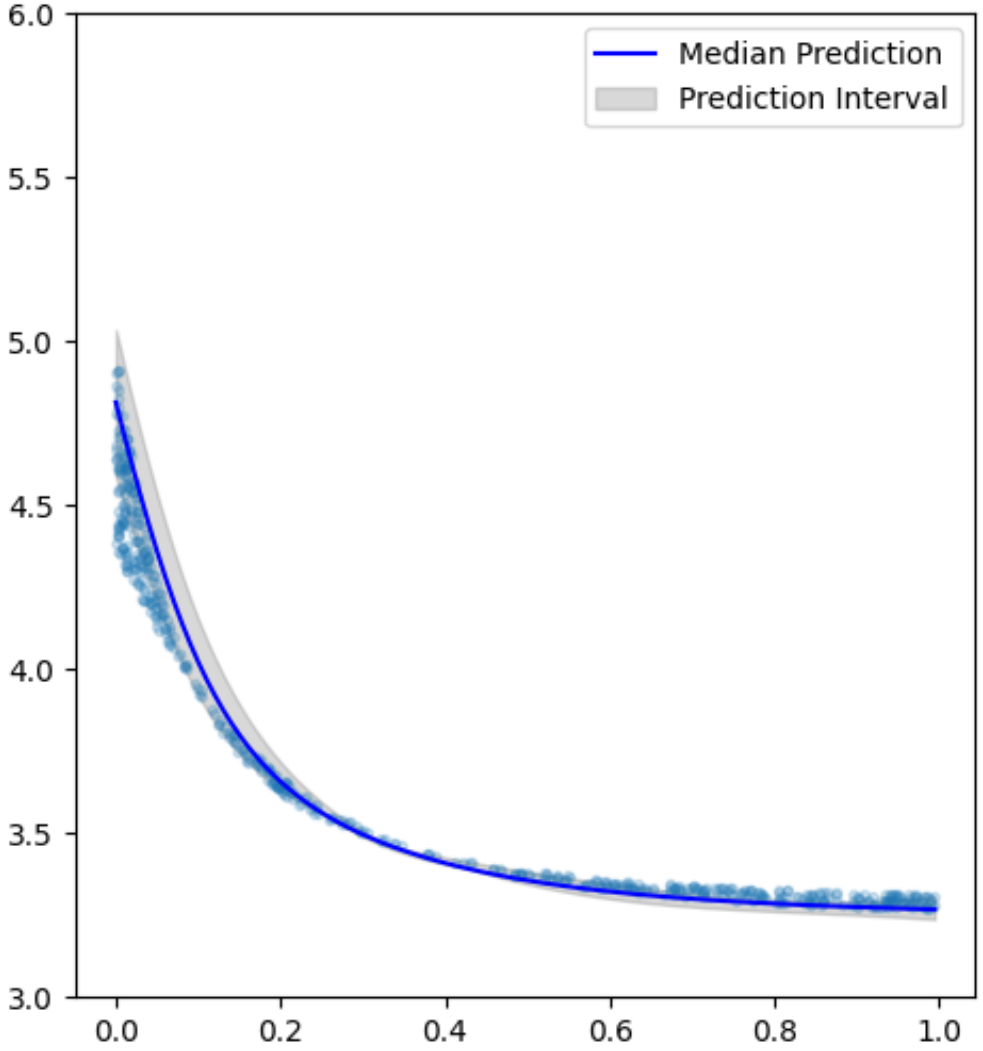


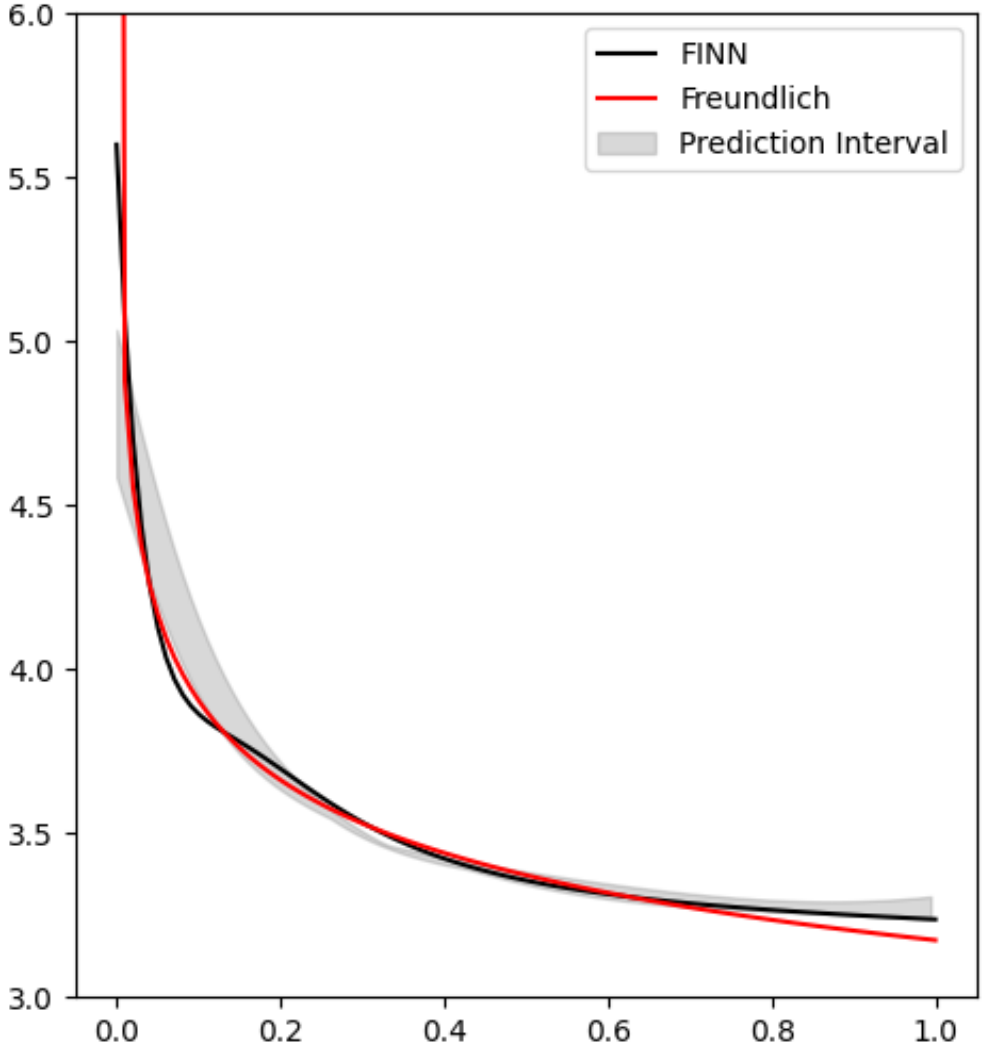
Application of PI3NN - Training





Application of PI3NN - Training





TODOs

- Issues near 0:
  - PI3NN struggels
  - Large errors for Rs of time intervals method
- Which method to choose to sample points for PI3NN

Extra Slides

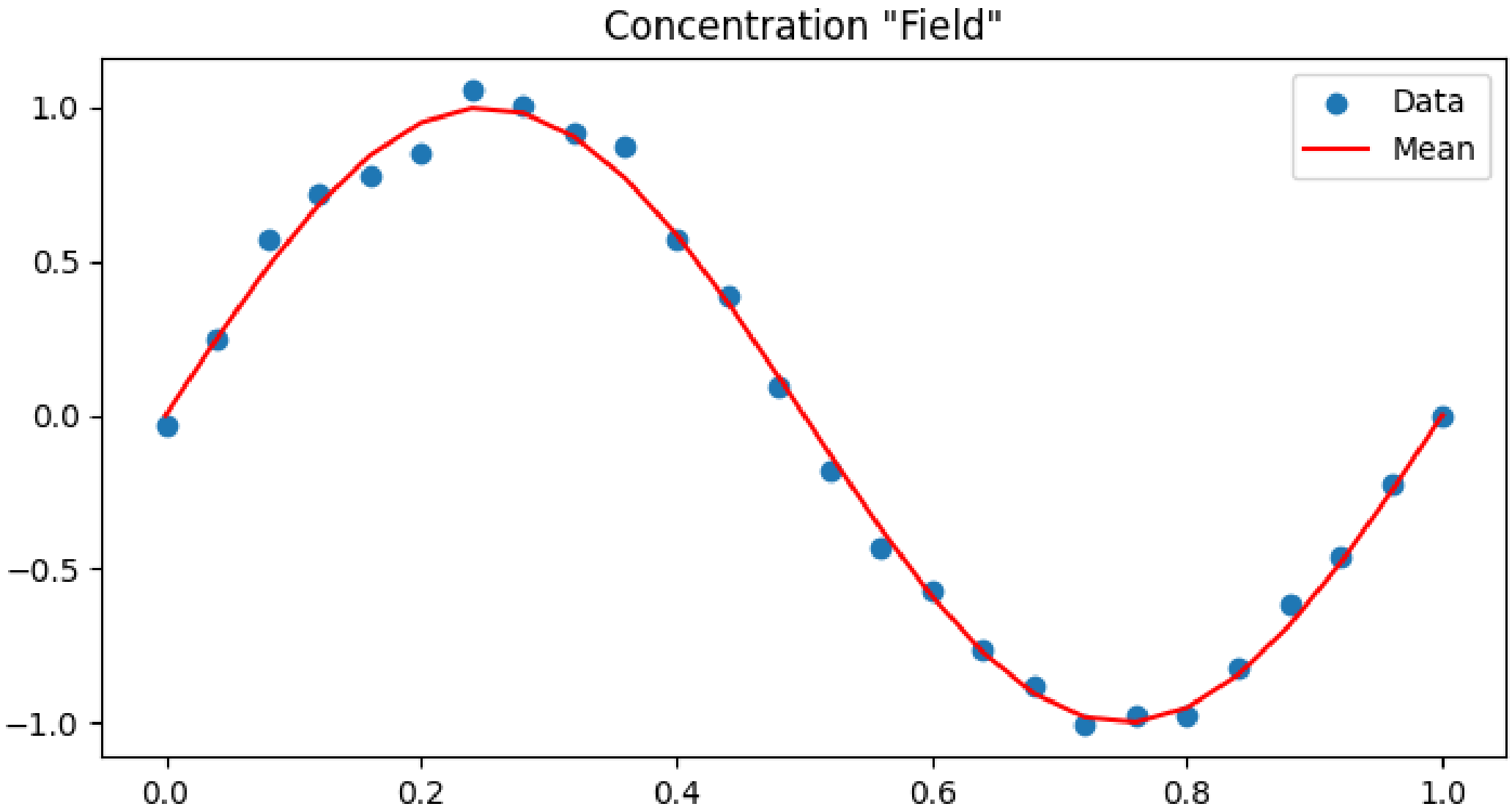
FINN Method

$$\frac{\partial c}{\partial t} = \frac{D}{R(c)} \frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial c_i}{\partial t} v_i = A_{i-1} \frac{D_i}{R(c_i)} \frac{c_{i-1} - c_i}{\Delta x} - A_{i+1} \frac{D_i}{R(c_i)} \frac{c_i - c_{i+1}}{\Delta x}$$

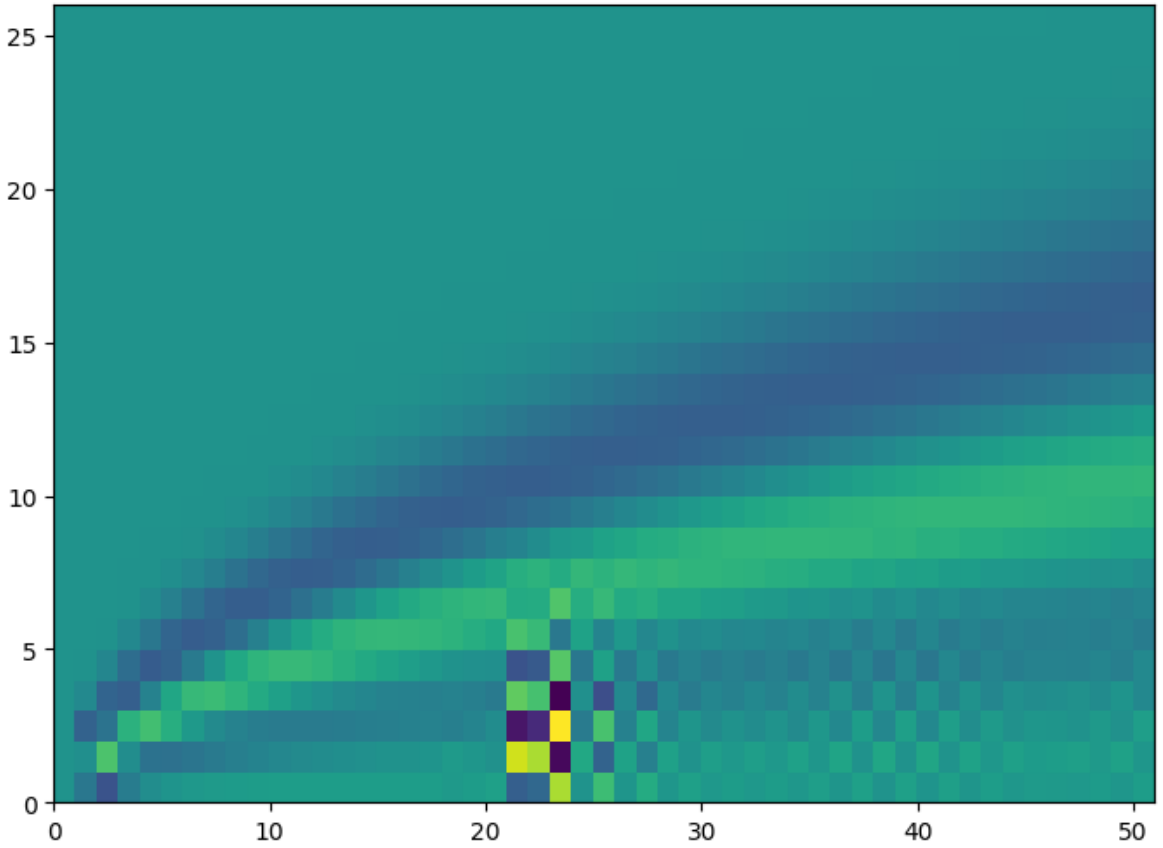
Approach 1: PIs for Concentration Field

Diffusion-Sorption Residual Field

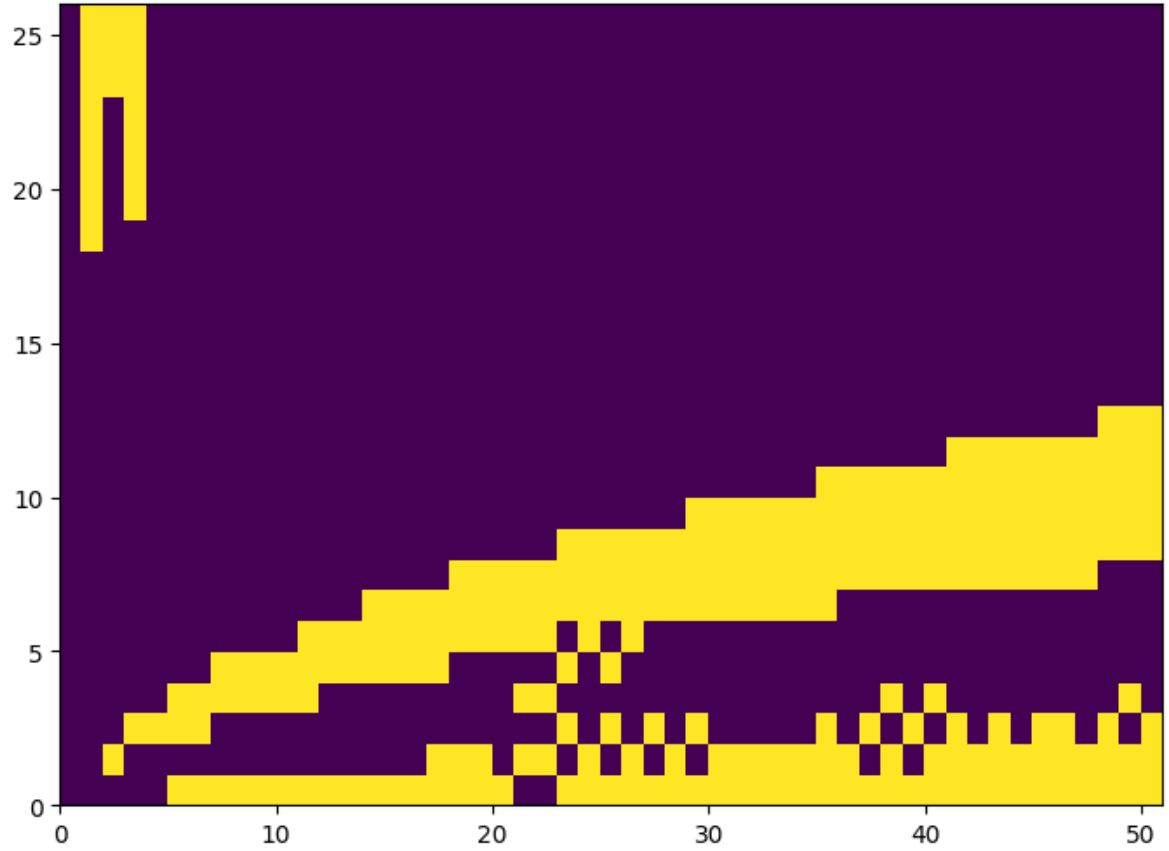


Diffusion-Sorption Residual Field

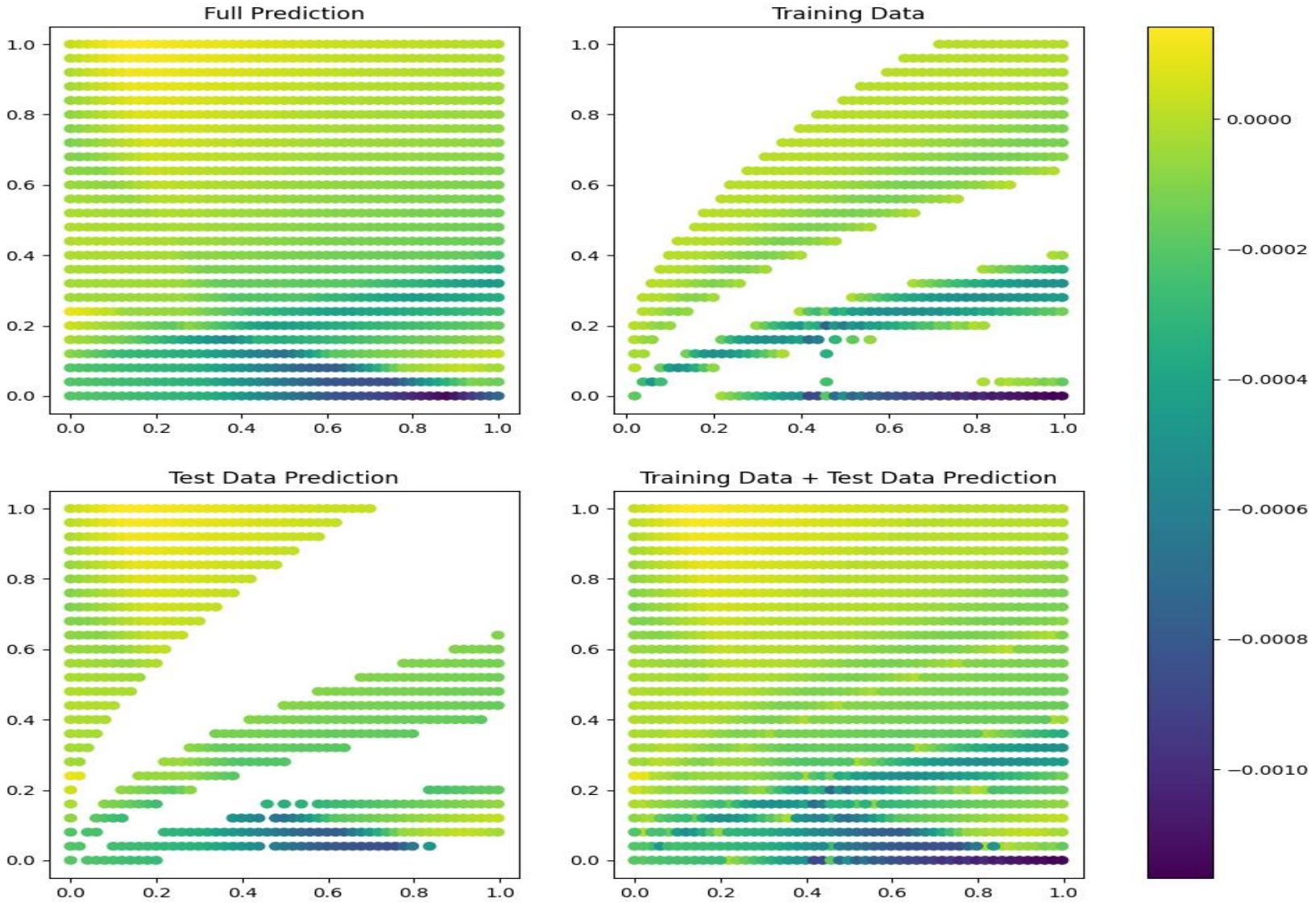
Residual Values (max 0.002)



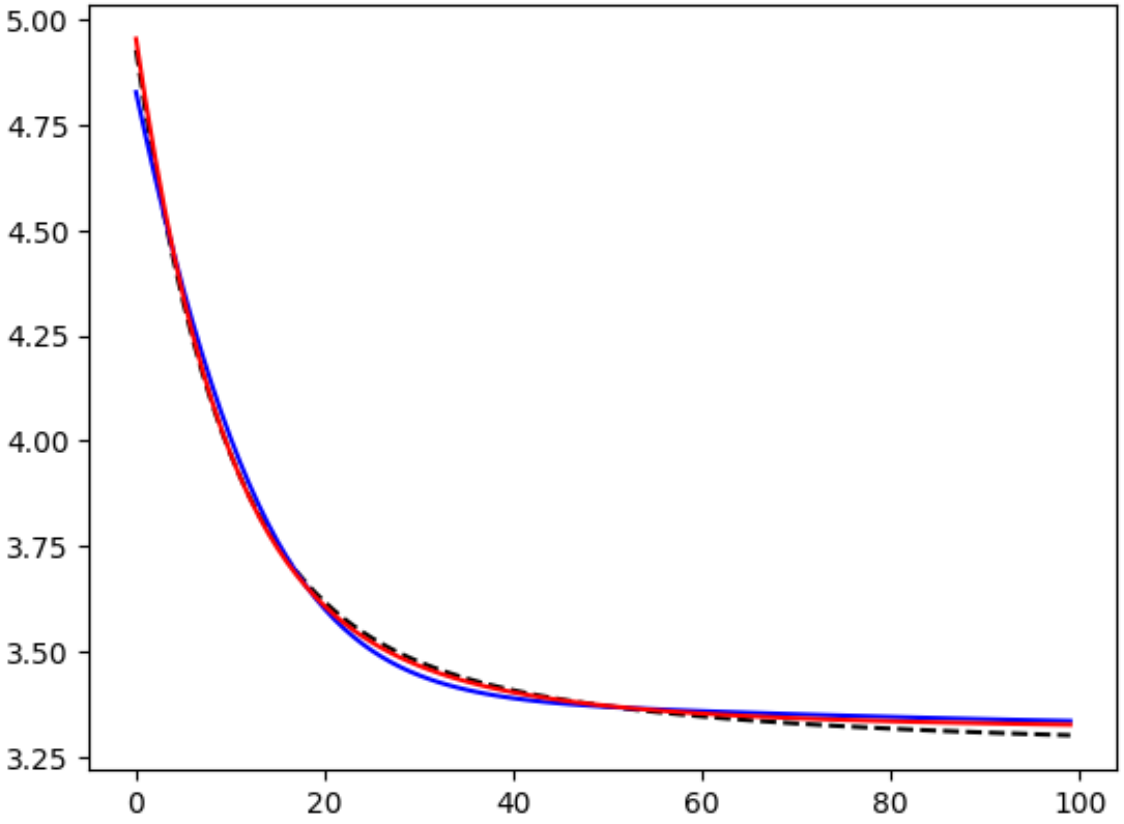
Residual Signs



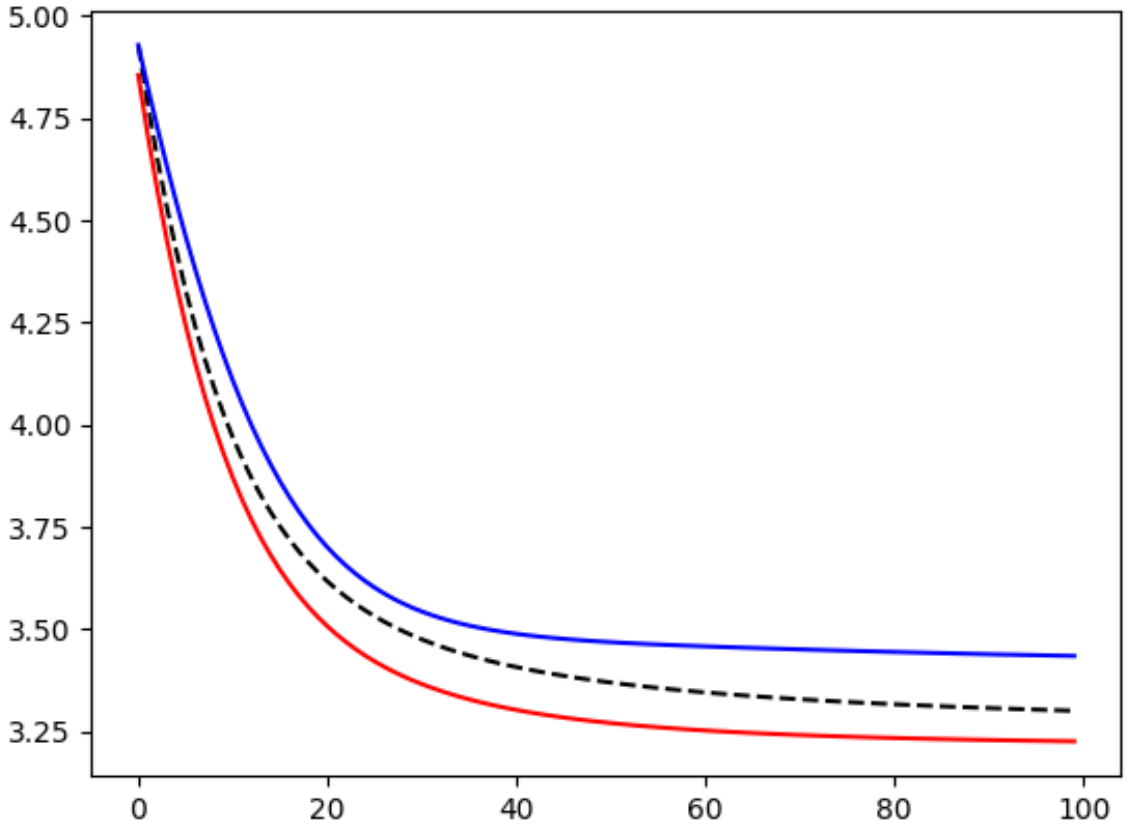
Residual Predictions



Isotherms from Mean and PI Networks

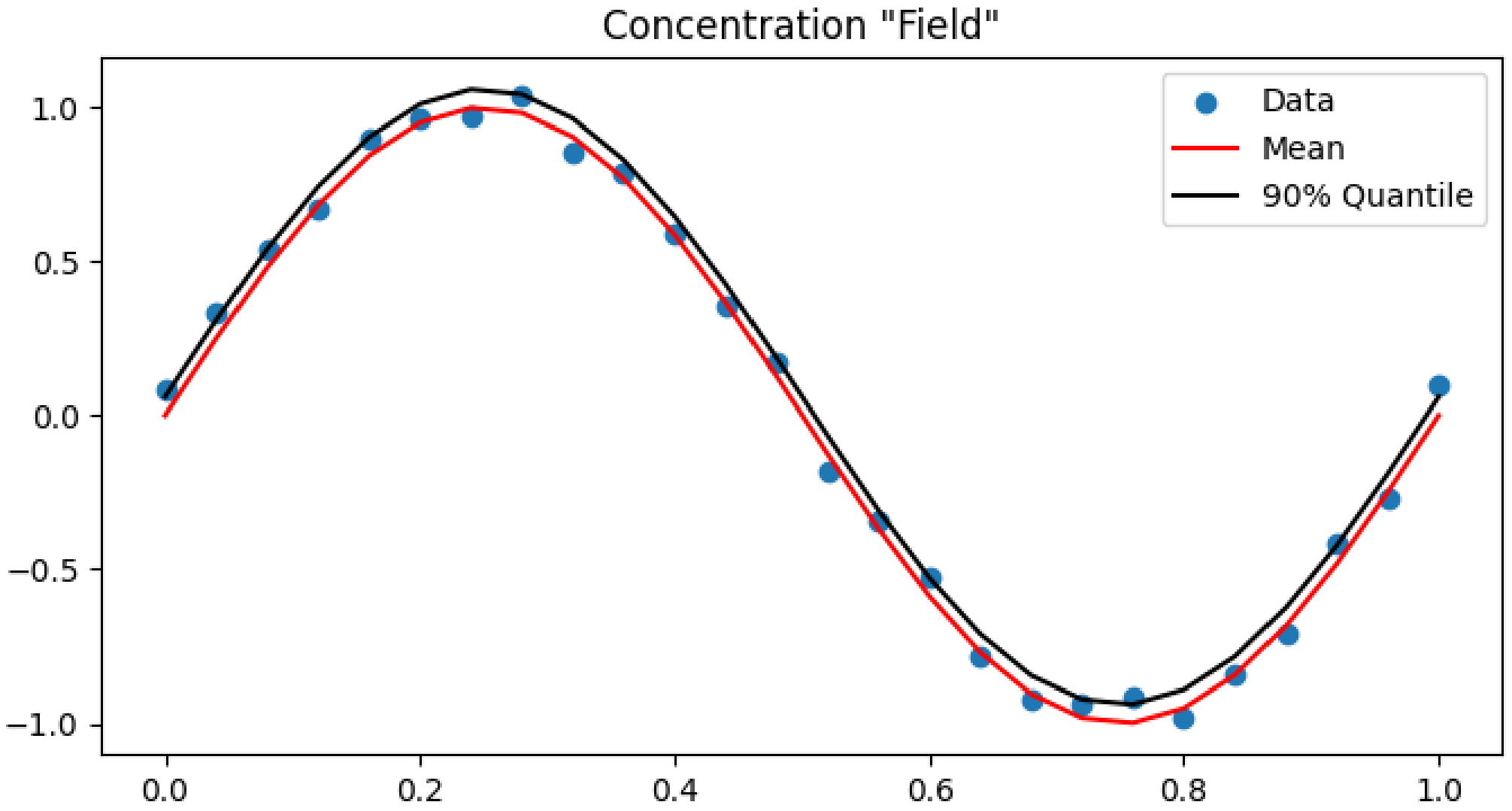


Learned mean and +/- Isotherms

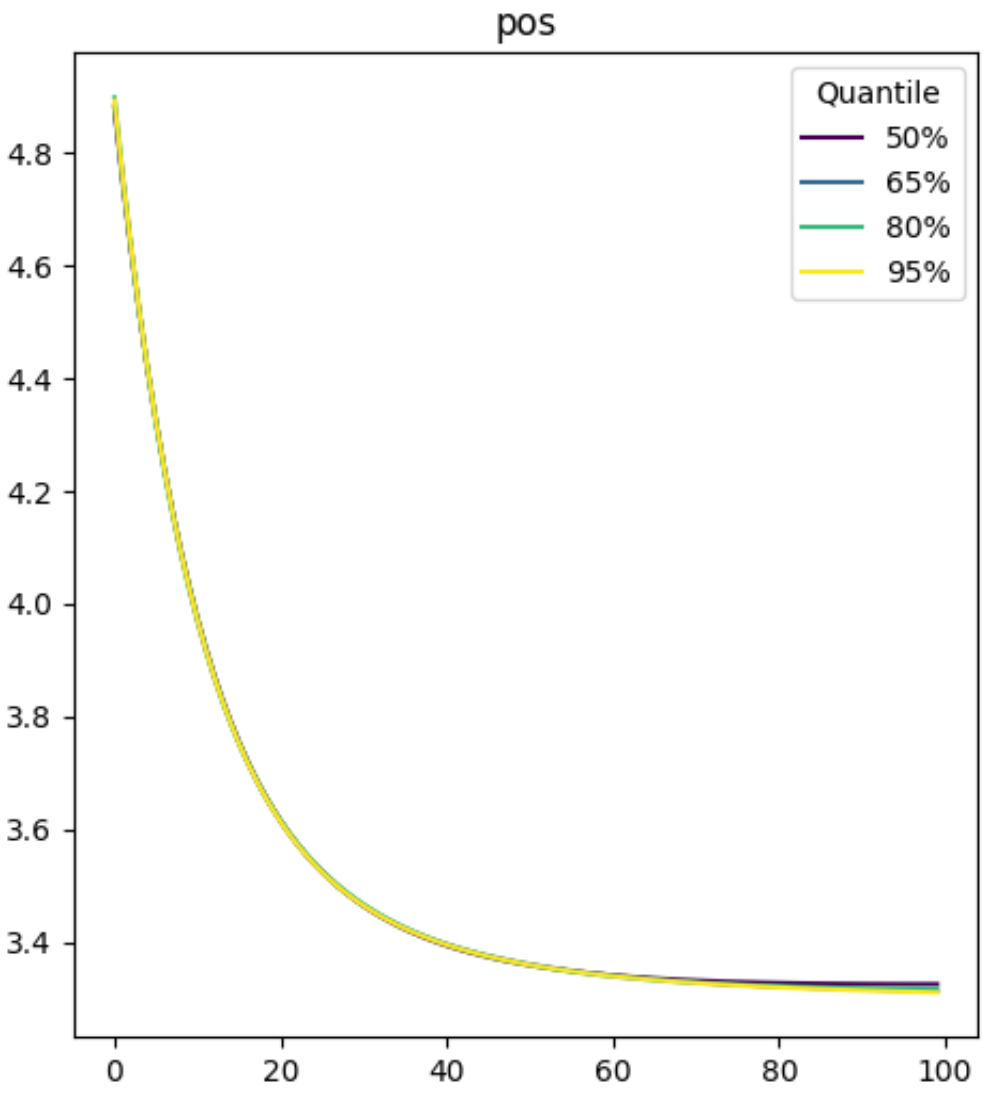


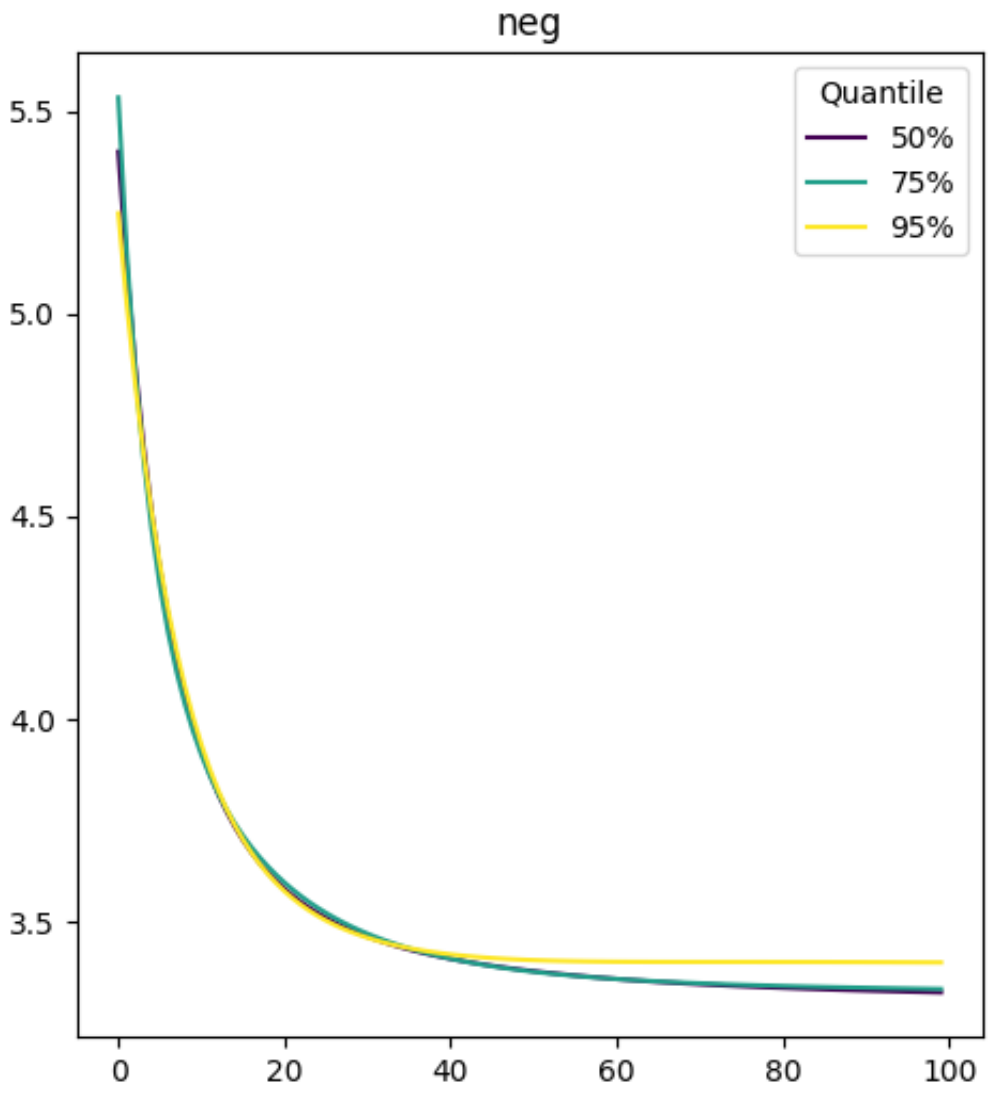
Manually shifted

Isotherm PIs for different Quantiles

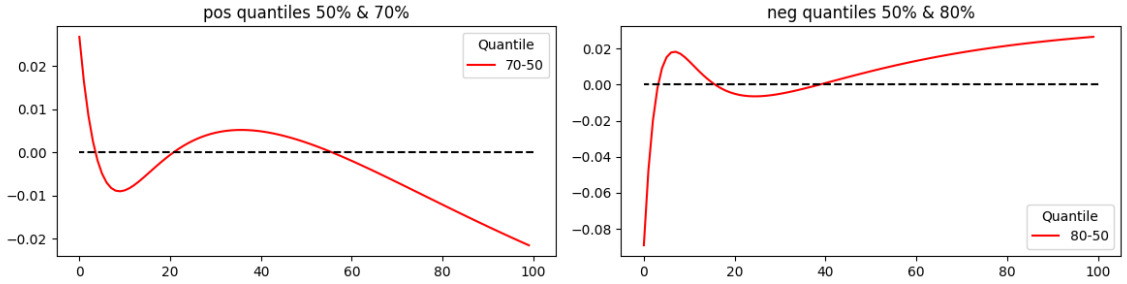


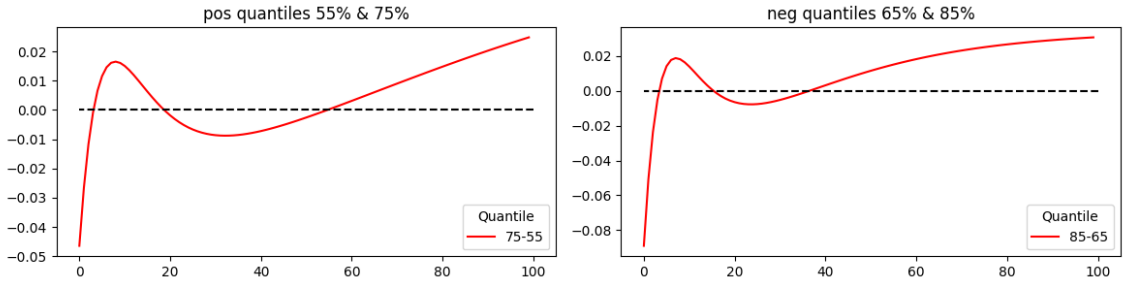
Isotherm PIs for different Quantiles

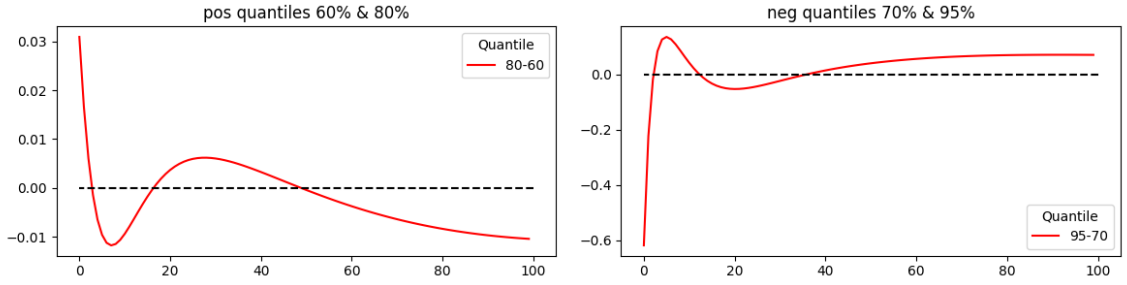


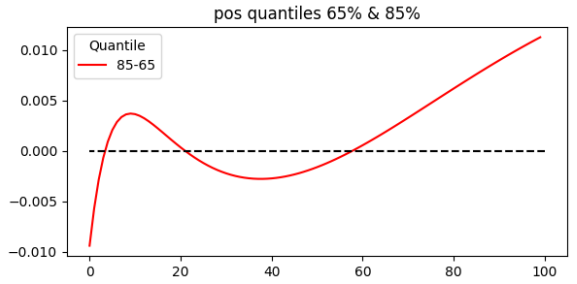


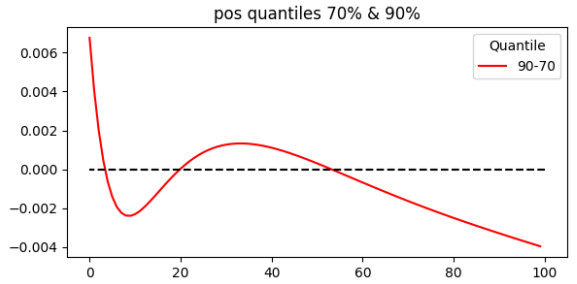
Isotherm PIs for different Quantiles

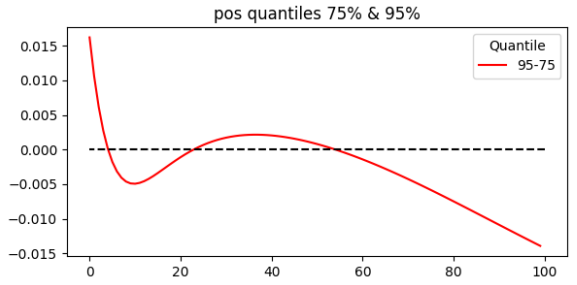




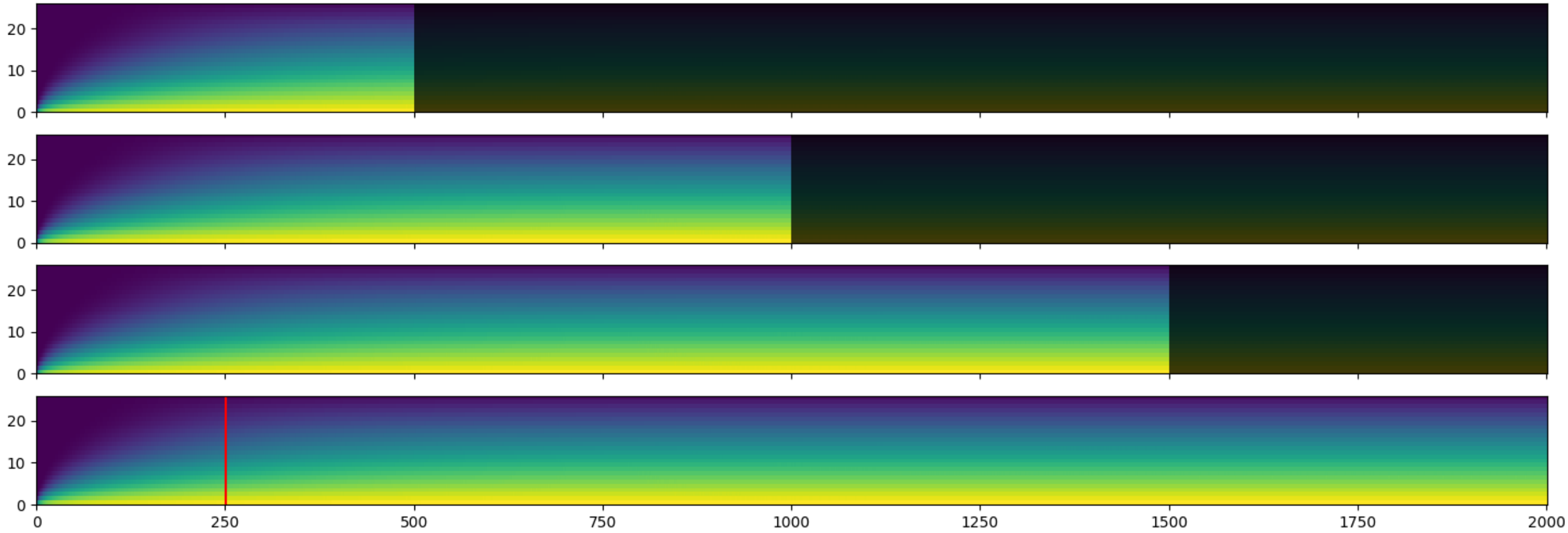








Do Isotherms converge with increasing Dataset



Do Isotherms converge with increasing Dataset