Delta Flow-Salinity Modeling using Physics-Informed Neural Networks: Tutorial

Workshop on Delta Flow-Salinity Modeling Using Machine Learning
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Module #4

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Introduction

Fundamentals of PINN

What is Physics-informed Neural Network (PINN) [1,2]?

- The laws of physics described by differential equations
- **Neural network** system for solving such differential equations
  - Inputs as independent variables of the function
  - Differential equation **embedded** into the loss function of the neural network
- Train the neural network to minimize the loss function
- No need for mesh and discretization
  - Data-driven

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[1] Raissi, M.; Perdikaris, P.; Karniadakis, G. E. JCP 2019

[2] Psichogios, D. C; Ungar, L. H. AIChE 1992

Introduction

Advection-Dispersion Equation

- Delta operations and control strategies frequently accessed using **flow-salinity relationships**
- Flow-salinity relations governed by Advection-Dispersion equation [3,4]
- $$A\frac{\partial S}{\partial t} - Q(x,t)\frac{\partial S}{\partial x} = KA\frac{\partial^2 S}{\partial x^2}, \qquad x \in [x_a, x_b], t \in [t_a, t_b]$$
    - A is cross-sectional area (constant)
    - K is longitudinal dispersion coefficient (constant)
    - $Q(x,t)$ is volumetric flowrate
    - $S(x,t)$ is concentration of salt
    - x is longitudinal direction (increasing in upstream)
    - t is time
- 'G-model' [3,4] approach:
    - modified steady-state solution to antecedent outflow-salinity relations at a fixed position

[3] Denton, Richard. ASCE 1993
[4] Denton, R.; Sullivan, G. CCWD 1993

Introduction

Advection-Dispersion Equation: PINN approach

1. Construct a neural network: $\hat{S}(x, t; \theta)$
2. Gather training data points:
   A. Measured/simulated data points $\{(x_i, t_i), S_i^*\}, i = 1,\ldots, N_d$
   B. Collocation points (randomly drawn) $\{(x_i, t_i)\}, i = 1,\ldots, N_c$ within domain
3. Define **physics-informed** loss function:

$$L(\theta) = \omega_F L_F(\theta) + \omega_D L_D(\theta)$$

where

$$L_F(\theta) = \frac{1}{N_d + N_c} \sum_{i=1}^{N_d+N_c} | A\frac{\partial \hat{S}}{\partial t_i} - Q(x_i, t_i)\frac{\partial \hat{S}}{\partial x_i} - KA\frac{\partial^2 \hat{S}}{\partial x_i^2} |^2$$

$$L_D(\theta) = \frac{1}{N_d} \sum_{i=1}^{N_d} | \hat{S}(x_i, t_i; \theta) - S^*(x_i, t_i) |^2$$

4. Train $\hat{S}(x, t; \theta)$ by minimizing the loss function $L(\theta)$

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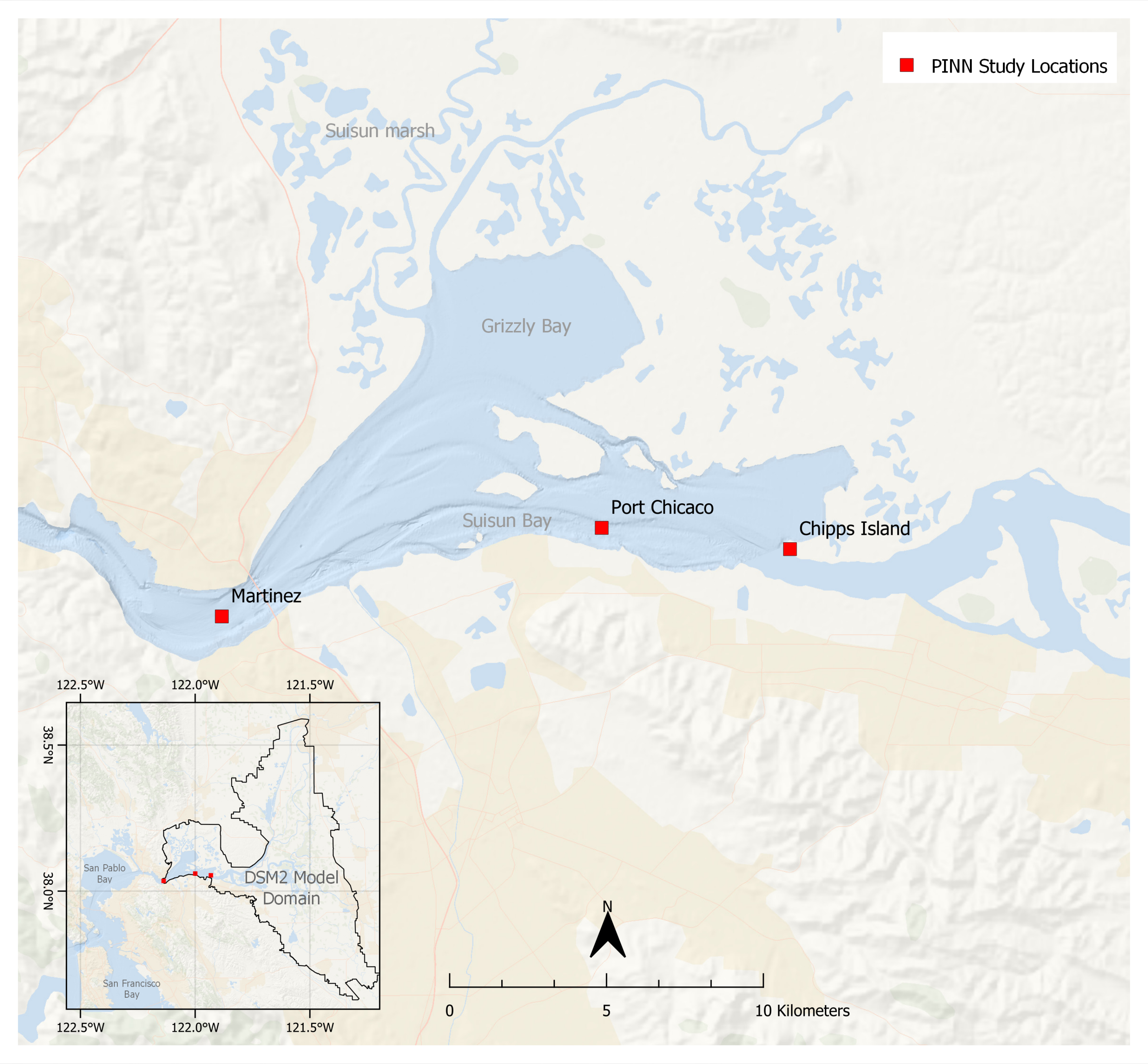
PINN for salinity transport

Problem Setup & Dataset



- **Daily DSM2 simulated** data (outflow and EC) from **1991 to 2015** at **3 Stations:** Martinez, Port Chicago, Chipps Island

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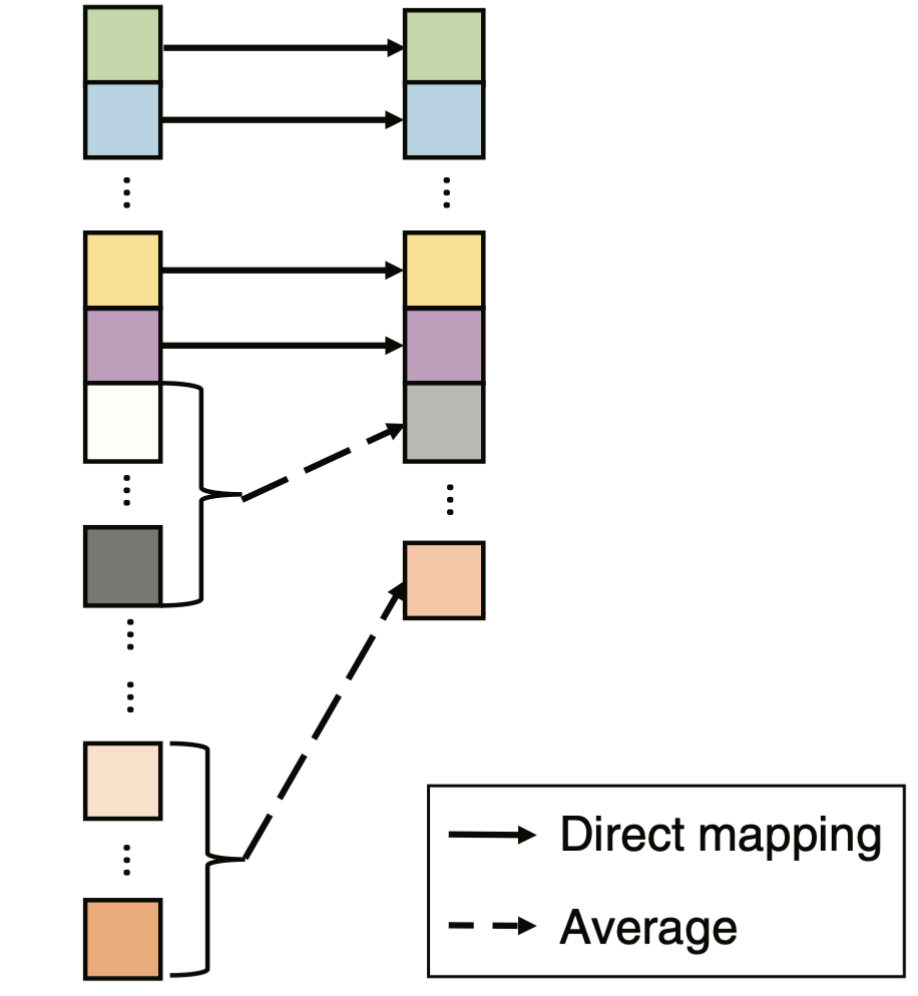
PINN for salinity transport

Outflow Data Preprocessing

- Important to use antecedent outflow information [3,4,5]
- For each daily outflow Q_n, create a 18-dimensional data vector $\overrightarrow{Q}_n = [Q_{n,1}, \ldots, Q_{n,18}]$ containing information of previous 118 days' outflow values:

$$Q_{n,i} = Q_{n-i+1}, \quad \text{for } i \in \{1, \ldots, 8\}$$

$$Q_{n,i+8} = \frac{1}{11}\sum_{j=1}^{11} Q_{n-11i-j+4}, \quad \text{for } i \in \{1, \ldots, 10\}$$



From [5]

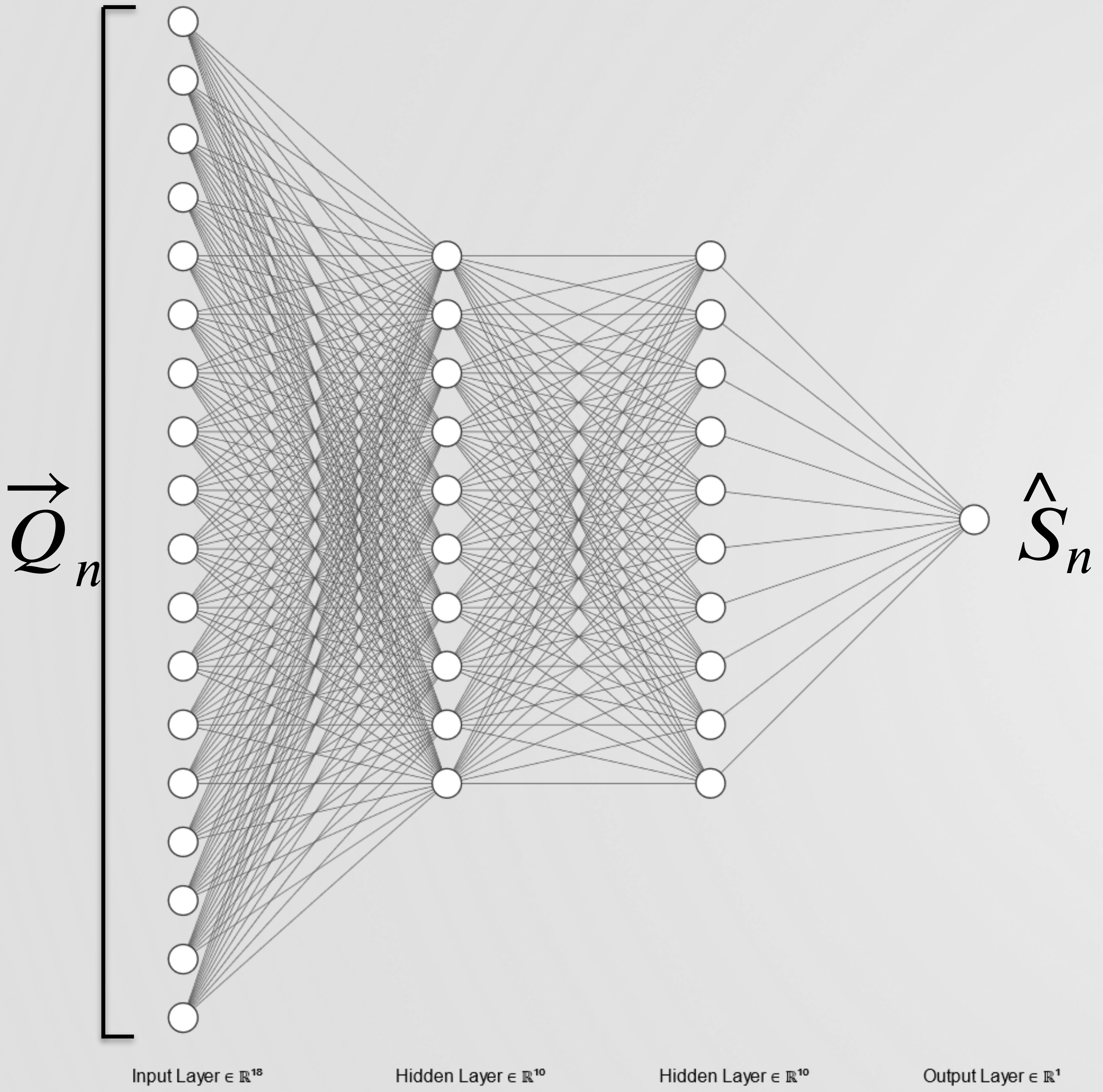
[3] Denton, Richard. ASCE 1993

[4] Denton, R.; Sullivan, G. CCWD 1993

[5] Qi S.; Bai Z.; Ding Z.; Jayasundara N.; He M.; Sandhu P.; Seneviratne S.; Kadir T. JWRPM 2021

PINN for salinity transport

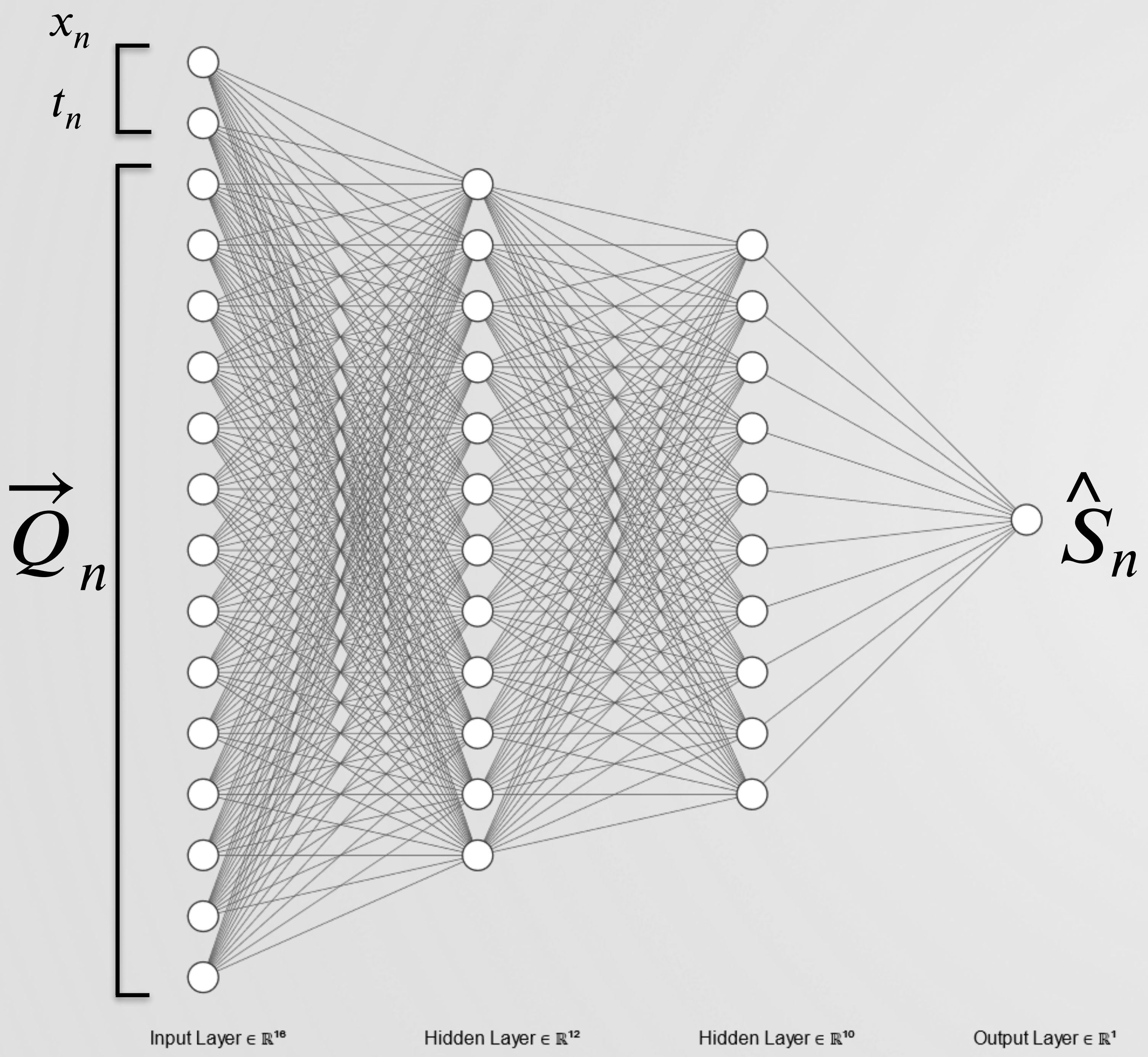
ANN Architecture



- Feed-forward, fully-connected (MLP)
- Input: outflow data vector $\overrightarrow{Q}_n$
- Output: estimated EC $\hat{S}_n$
- Train by minimizing mean square error $\sum_n \|\hat{S}_n - S_n\|^2$

PINN for salinity transport

PINN Architecture



- Feed-forward, fully-connected (MLP)
- Input: outflow data vector $\vec{Q}_n$ **and** location x_n and time t_n
  - x_n ranging between Martinez and Chipps Island
  - t_n ranging between 1991 and 2015
- Output: estimated EC $\hat{S}_n$
- Train by minimizing mean squared error **and** PDE (Advection-Dispersion) loss

$$\sum_n \|\hat{S}_n - S_n\|^2 + \sum_n \left\| A\frac{\partial \hat{S}}{\partial t}\bigg|_{(x_n,t_n)} - Q_{n,1}\frac{\partial \hat{S}}{\partial x}\bigg|_{(x_n,t_n)} - KA\frac{\partial^2 \hat{S}}{\partial x^2}\bigg|_{(x_n,t_n)} \right\|^2$$

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Experimental Results

5-fold Cross-Validation

- K-fold cross-validation
- 5-fold on 25 years of DSM2-simulated data from 1991-2015
  - 80% training, 20% testing
- For each fold: best hyper-parameters each for ANN and PINN
- Evaluation metrics: Bias, Nash-Sutcliffe Efficiency (NSE)

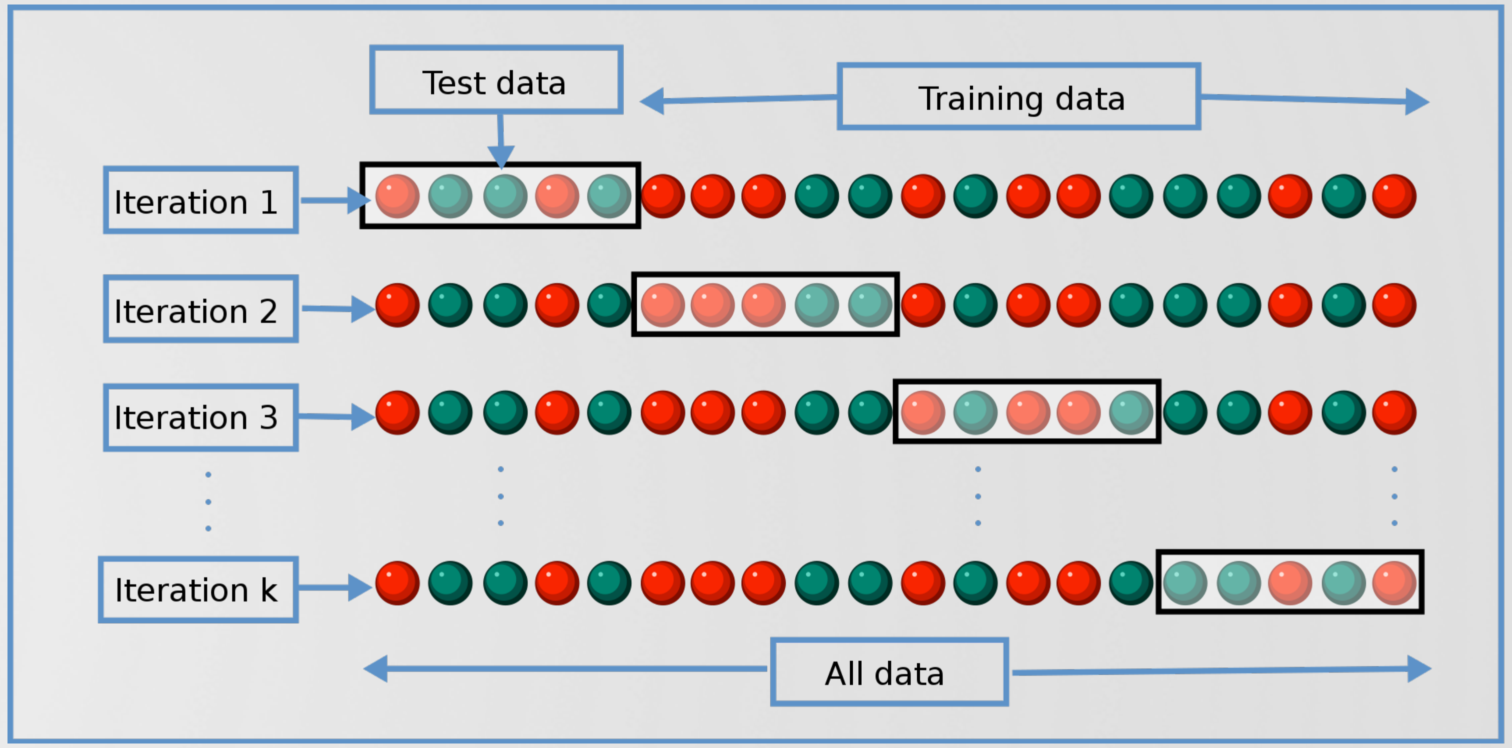
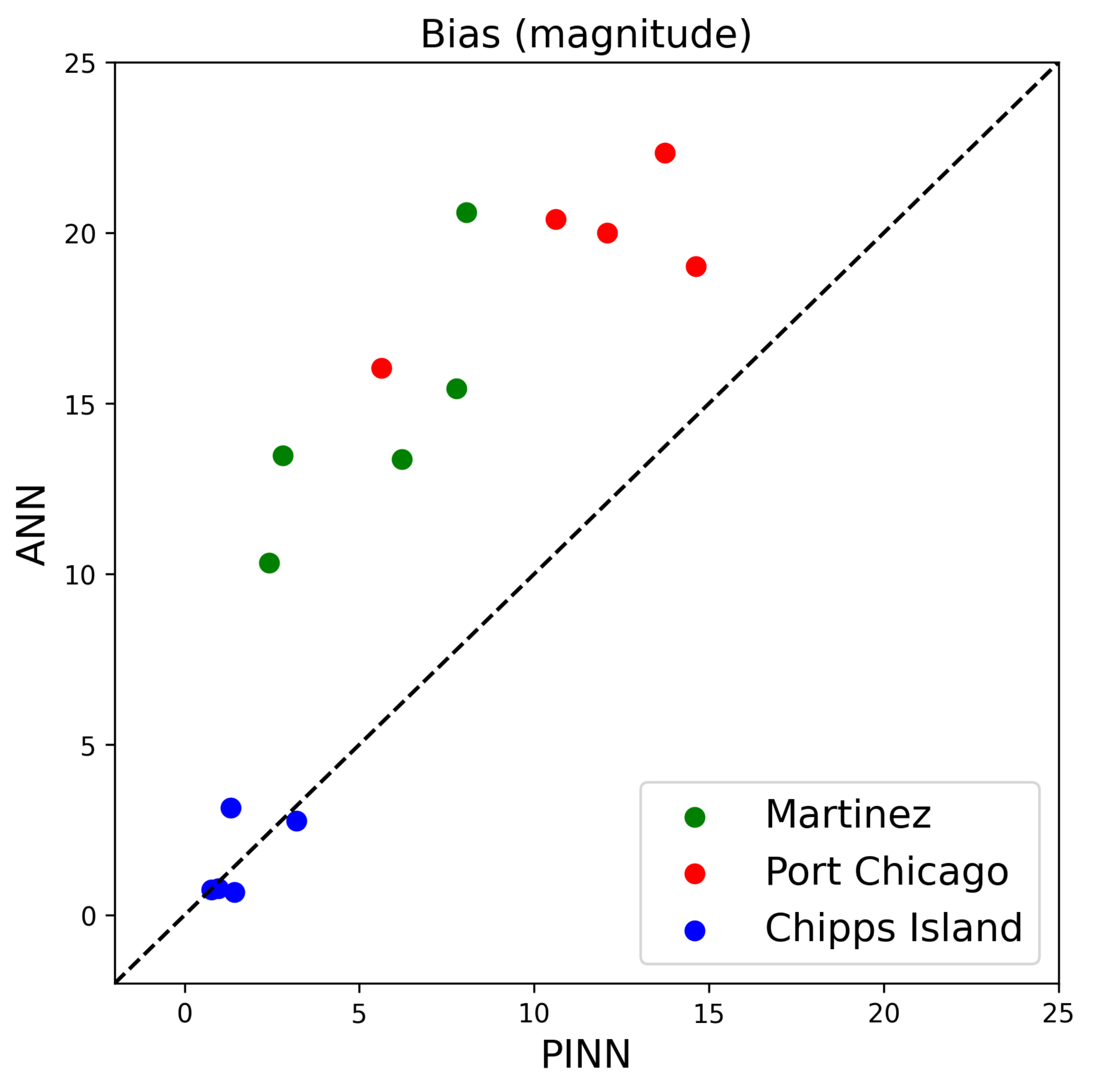


Illustration of k-fold cross-validation methodology [6]

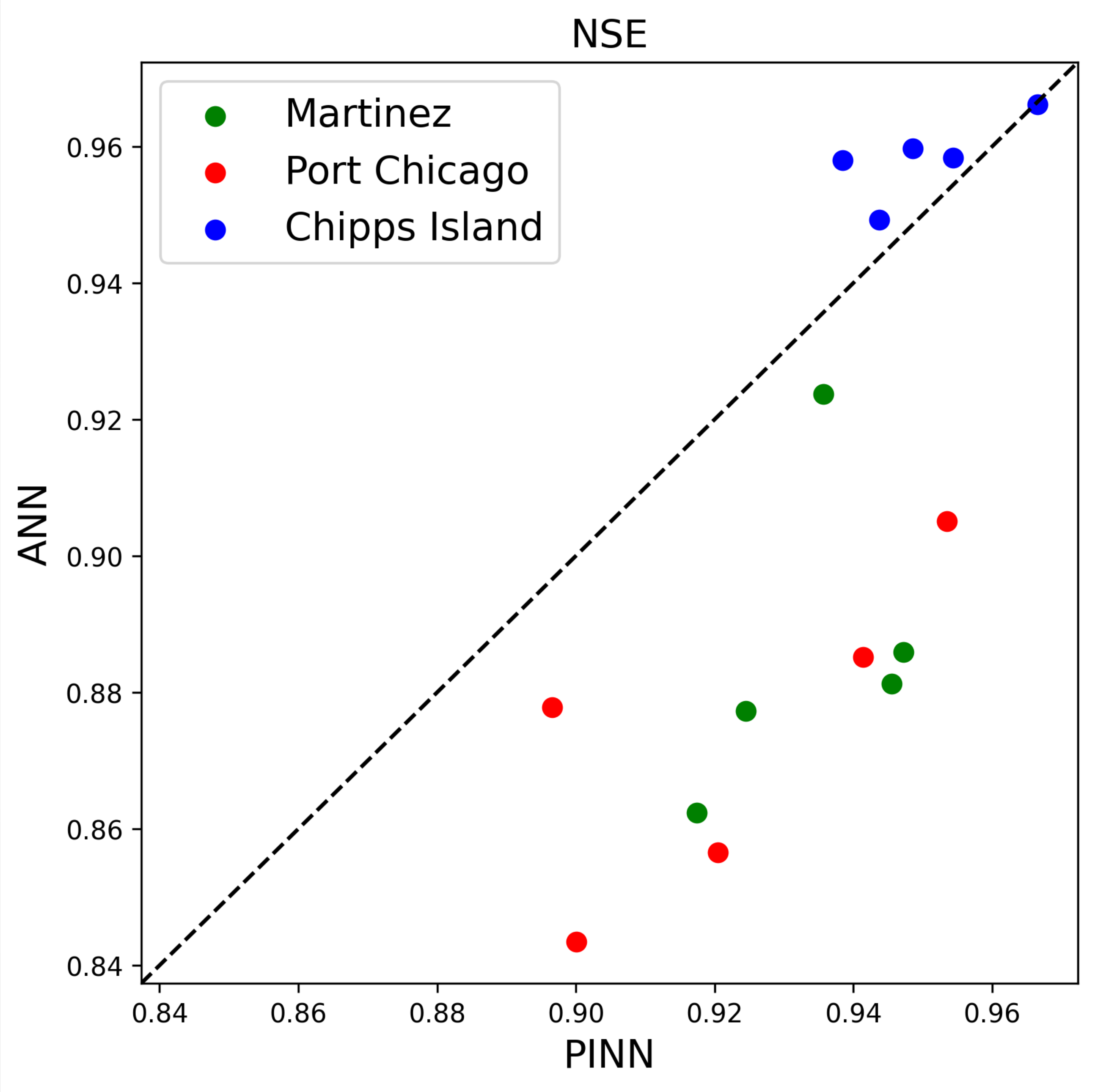
[6] https://commons.wikimedia.org/w/index.php?curid=82298768

Experimental Results

Evaluation metrics



Dots **above** the line indicates better PINN performance



Dots **below** the line indicates better PINN performance

Greater Performance indicator
- Smaller Bias
- Larger NSE

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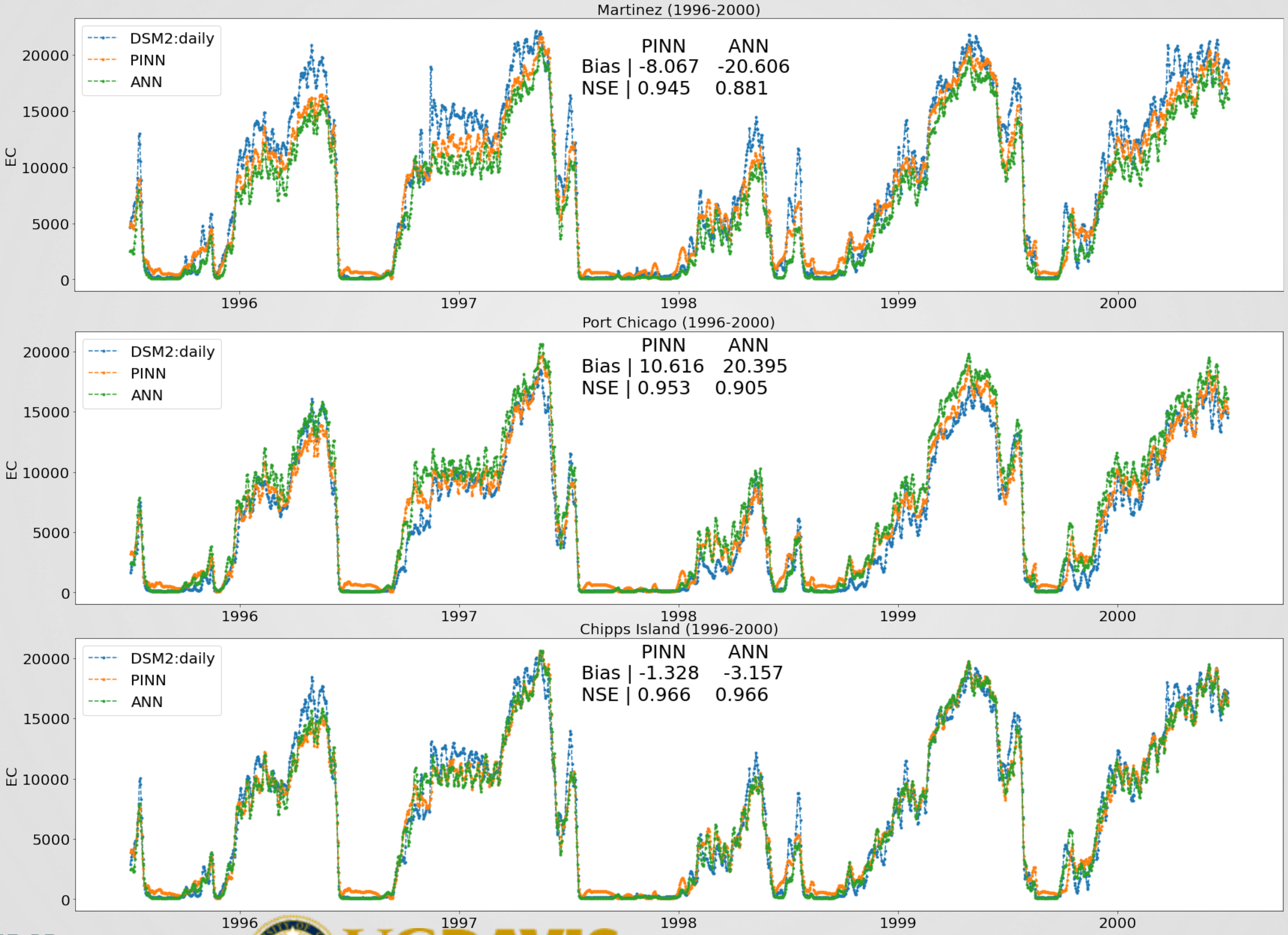
Experimental Results

Time series plots



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References

[1] Raissi, M., Perdikaris, P., and Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational physics, 378:686–707.

[2] Psichogios, D. C. and Ungar, L. H. (1992). A hybrid neural network-first principles approach to process modeling. AIChE Journal, 38(10):1499–1511.

[3] Richard A Denton. Accounting for antecedent conditions in seawater intrusion modeling—Applications for the San Francisco Bay-Delta. In Hydraulic engineering, pages 448–453. ASCE, 1993.

[4] Denton, R. and Sullivan, G. (1993). Antecedent flow-salinity relations: Application to delta planning models. Contra Costa Water District. Concord, California.

[5] Siyu Qi, Zhaojun Bai, Zhi Ding, Nimal Jayasundara, Minxue He, Prabhjot Sandhu, Sanjaya Seneviratne, and Tariq Kadir. Enhanced artificial neural networks for salinity estimation and forecasting in the sacramento-san joaquin delta of california. Journal of Water Resources Planning and Management, 147(10):04021069, 2021.

[6] By Gufosowa - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=82298768


QUESTIONS