A Deep Surrogate Model for Estimating Water Quality Parameters

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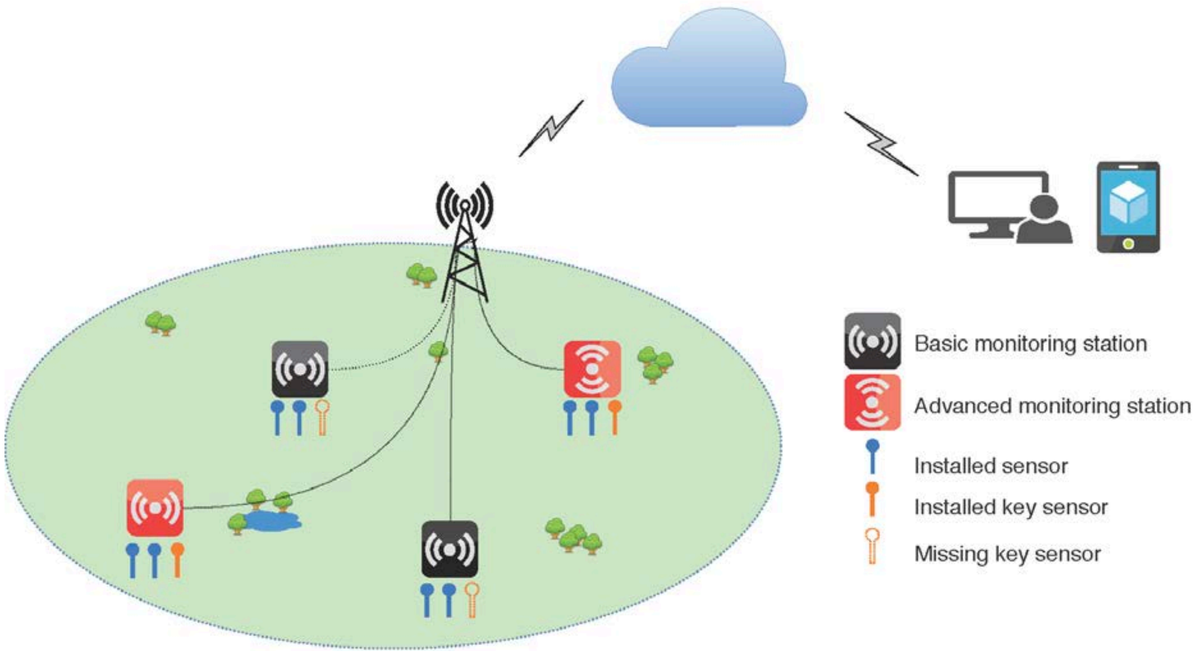
Problems in large-scale water quality monitoring

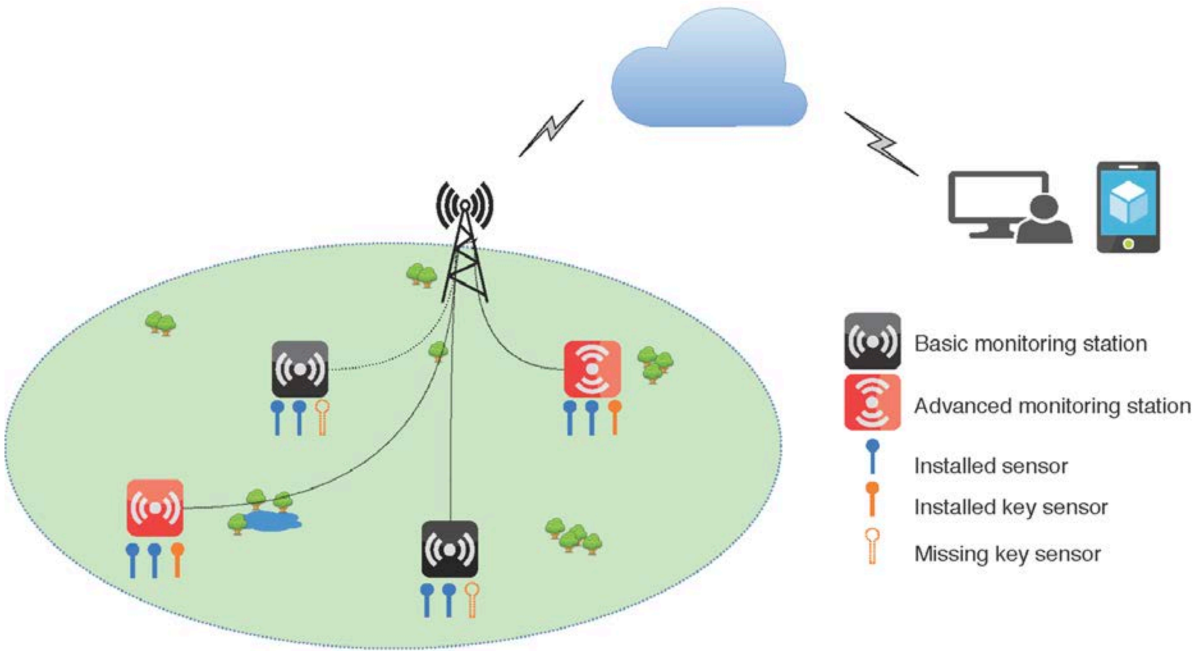


Only few monitoring stations have key sensor installed.

Reasons:

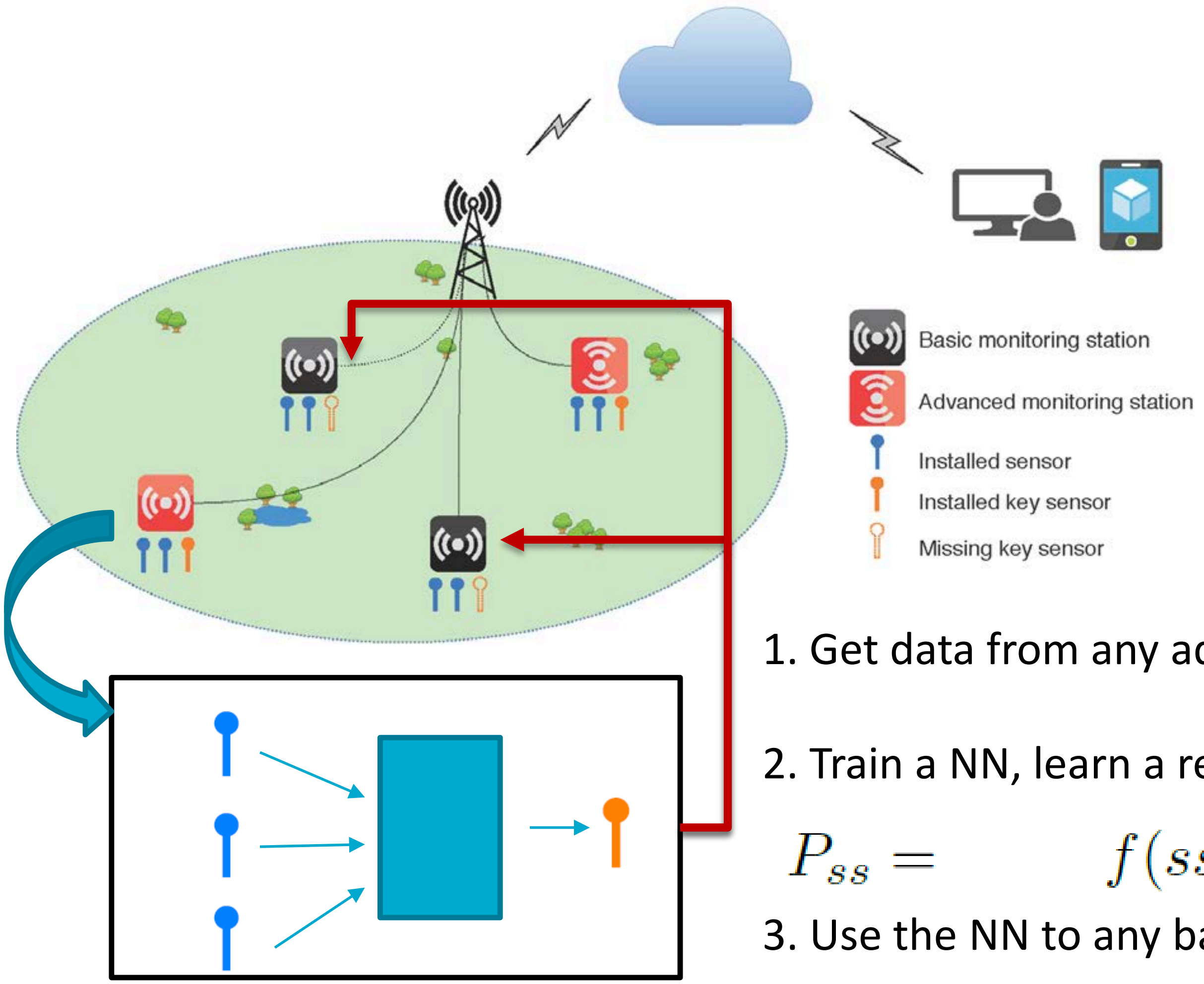
- **The cost of the key sensor is prohibitive**
- **The deployment is restricted by the environmental conditions**
- **Some parameter is physically impractical to be measured directly**

Problems in large-scale water quality monitoring



How to get the key parameter from the basic monitoring stations?

Current approach



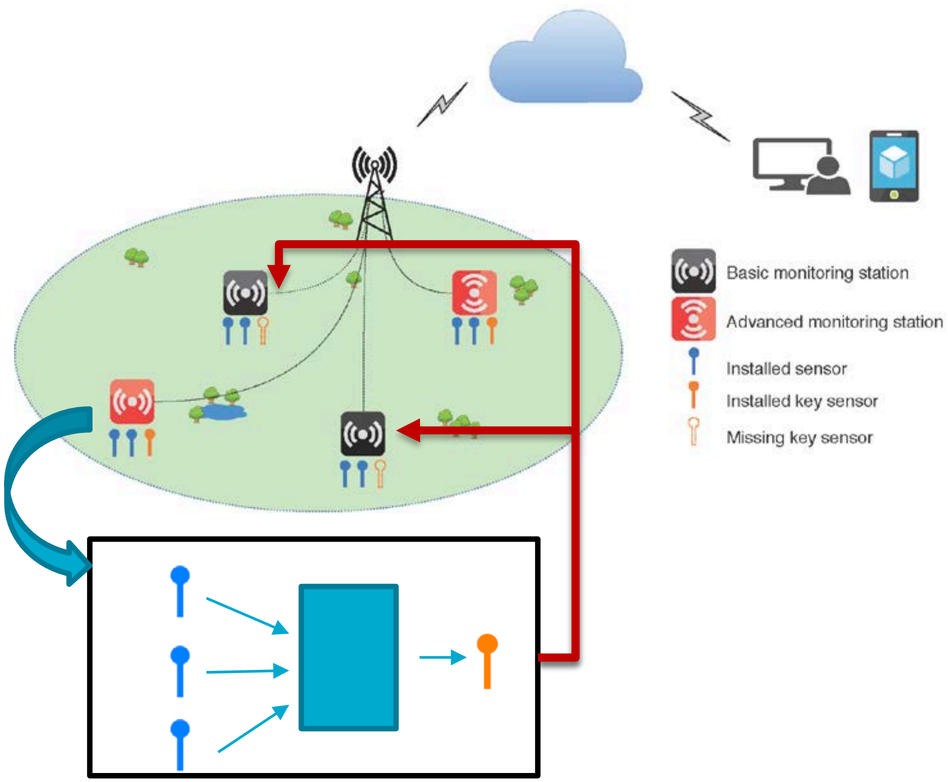
1. Get data from any advanced stations

2. Train a NN, learn a regression relationship:

$$P_{ss} = f(ss_1, ss_2, ..., ss_k)$$

3. Use the NN to any basic stations to get estimated P

Limitations about current solutions



In large-scale environmental monitoring:

1. The surrogate relationship f() are considered to be temporal-varying.

2. The key observation is influenced by the weather condition, biochemical reaction.

3. Monitoring stations are deployed over broad geographical areas, diverse environmental perturbations between stations can have a negative impact.

This work

A deep transferring learning based solution:

Denoising Autoencoder + transfer learning + temporal feature encoding

1. **Stacked Denoising AE to abstract water quality features**

Pre-training a WQ feature learner

2. Encode temporal and environmental information to the surrogate model

Not use LSTM or other recurrent architecture, but encode temporal info

3. A regressor with the domain adaptation layer to capture the data
distribution deviation between different monitoring stations

SDAE

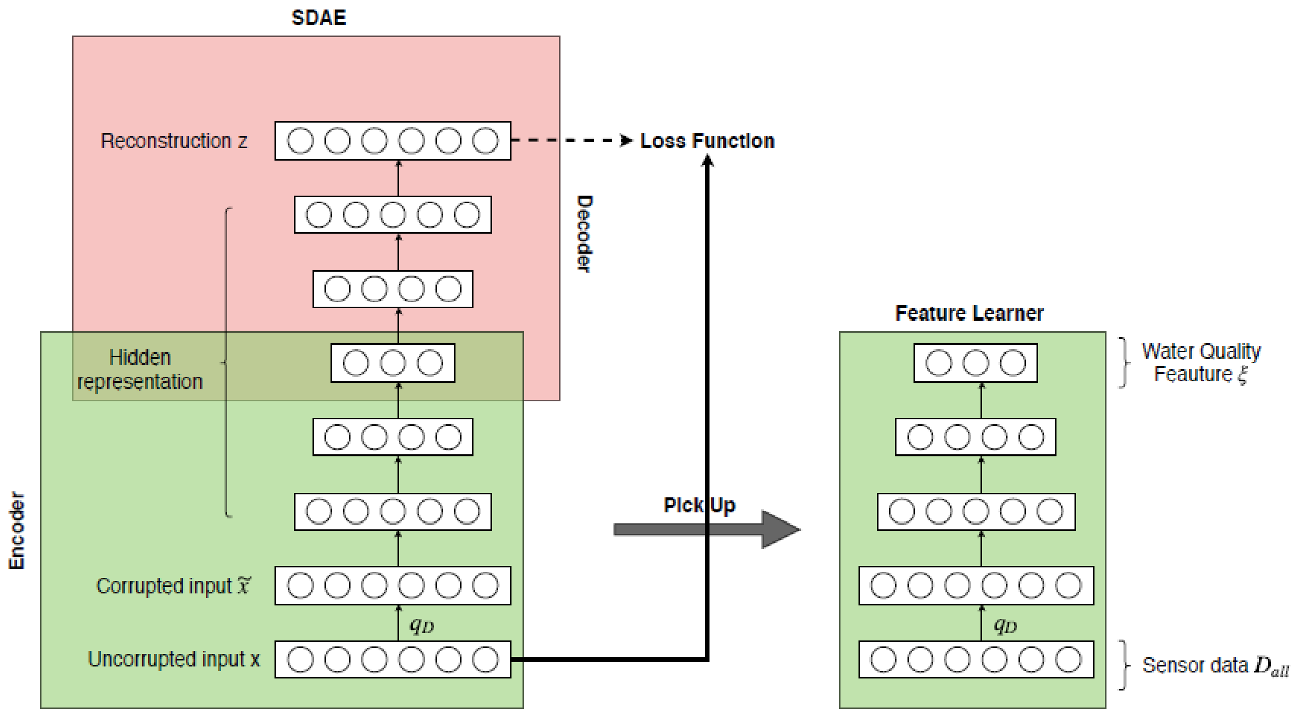


Fig. 2: A SDAE for water quality feature learning. After pre-training, the encoder of SDAE is picked to extract the latent features from D_{all}.

Supplementary Information Encoding

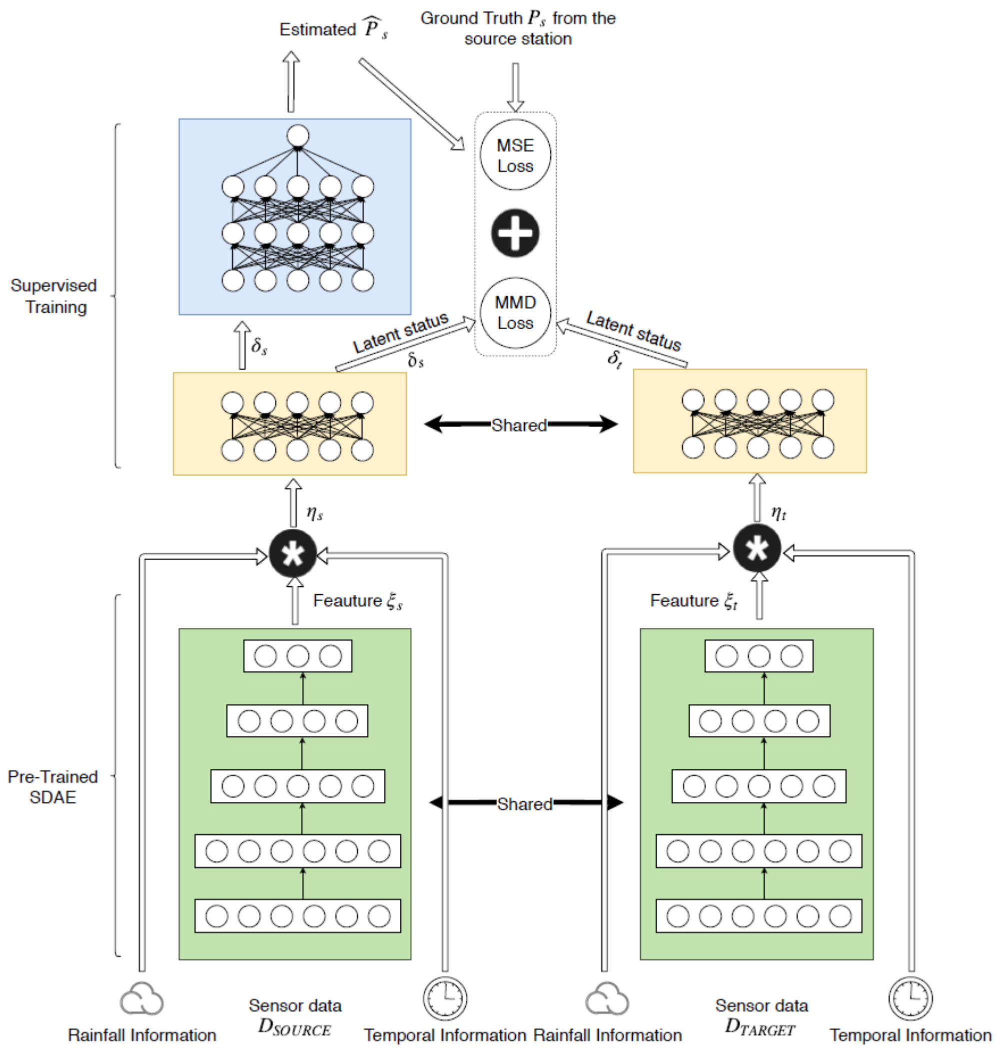
TABLE I: Supplementary Information.

Type	Features	Range
Temporal:		
	Hour of the day	0-23
	Day of the week	0-6
	Month of the year	0-11
Climate:		
	Rainfall	0mm-200mm

- Capture the hourly, daily and monthly pattern
- Rainfall is another important information

These features are not processed by the SDAE

Deep Transfer Learning-based Surrogate Model



Deep Transfer Learning-based Surrogate Model

1. The Loss includes both MSE and MMD,
   - MSE for regression accuracy
   - MMD for minimizing the data distance between stations

$$L = \mathrm{R}_{\mathrm{loss}}(P_s, \hat{P}_s) + \mathrm{MMD}_{\mathrm{loss}}(\delta_s, \delta_t) \qquad (11)$$

where $\mathrm{R}_{\mathrm{loss}}$ and $\mathrm{MMD}_{\mathrm{loss}}$ represent the regression loss and the MMD loss.

2. This model also utilises the information from target stations to train the model.
   - Not only apply a trained model to the target station.

3. WQ data from all the stations are utilized. (SDAE pertaining part)

Experiments
Monitoring stations

Fig. 4: Queensland Government's water quality monitoring network in the Great Barrier Reef region (part). The black and red icon represents the basic and advanced water quality monitoring station. Four water quality monitoring stations are illustrated in Table II.

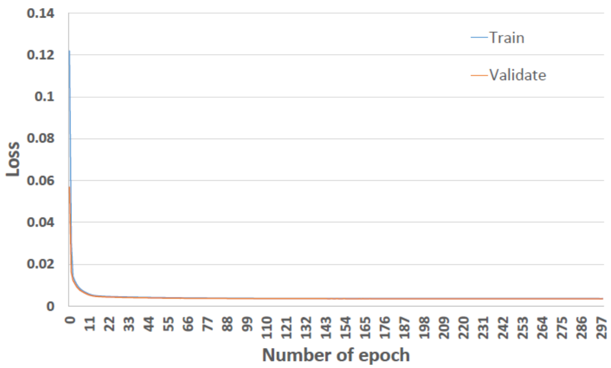
Experiments
WQ Data

TABLE III: Water quality and climate data from 1/1/2017 to 31/8/2018.

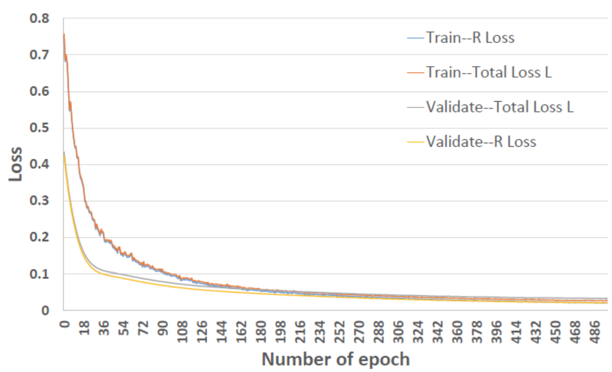
Parameters	Unit	Min	Max	Mean	Std Dev	Sensor Installation
Water quality (4 hourly)						
Water Level	m	7.5	18.7	12.3	3.4	Advanced & Basic stations
Temperature	°C	19.9	33.9	26.8	2.7	Advanced & Basic stations
Conductivity	μS / cm	0.2	47036.1	7392.3	11763.7	Advanced & Basic stations
Water Discharge	m^3/s	-45.8	1686.8	64.4	111.1	Advanced & Basic stations
Turbidity	NTU	0.5	224.6	13.6	24.3	Advanced & Basic stations
Nitrate	mg / L	0.2	30.5	15.9	4.7	Advanced stations
Climate (Daily)						
Rainfall	mm	0	164.8	8.5	19.5	Advanced & Basic stations

Experiments

Training



(a) The training and testing loss for the SDAE (During the first 300th epochs). The loss of the SDAE finally converges after 24000 training epochs in this experiment.



(b) The training and validating loss for the regressor in the DTLSM (During the first 500th epochs). R Loss represents the regression loss. The difference between the R loss and the total loss L is the MMD loss. The well-trained regressor is obtained after 5000 training epochs in this experiment.

TABLE IV: Hyperparameters of the DTLSM.

Hyperparameters	Value
SDAE	
No. of Hidden Layers for Encoder	3
No. of Hidden Units for Encoder	56, 28, 14
Activation Function for Encoder	Tanh
No. of Hidden Layers for Decoder	3
No. of Hidden Units for Decoder	14, 28, 56
Activation Function for Decoder	Linear
Optimizer	Nadam
Loss Function	MSE
Noise Factor v	0.1
Regressor	
No. of Hidden Units for Each Hidden Layer	14
No. of Regression Layers	2
No. of Domain Adaptation Layers	1
Dropout	0.6
Activation Function	Tanh
Optimizer	Nadam
Loss Function	L in Equation 11

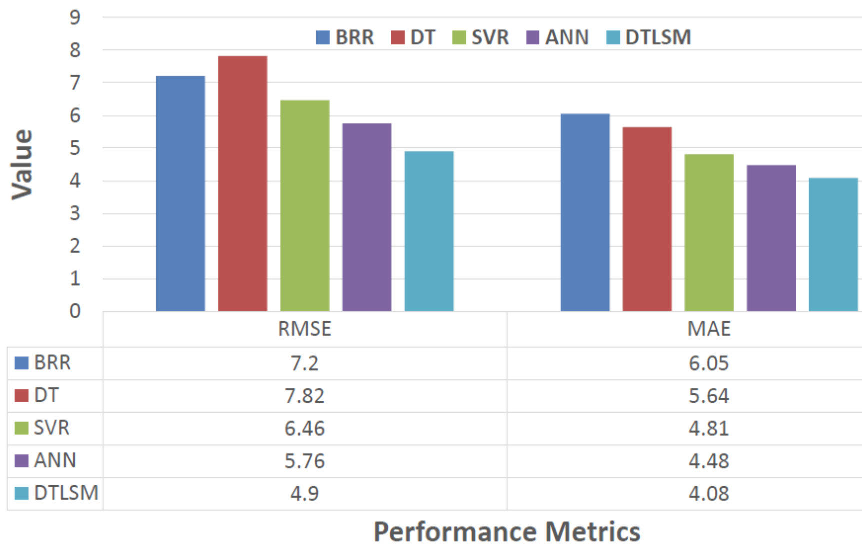
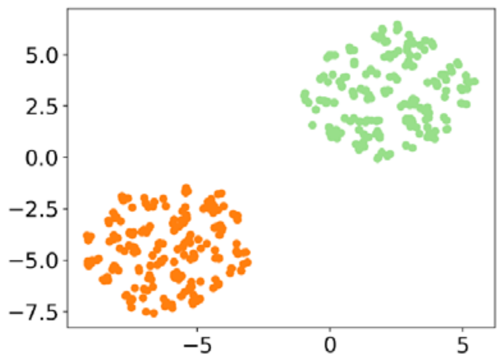


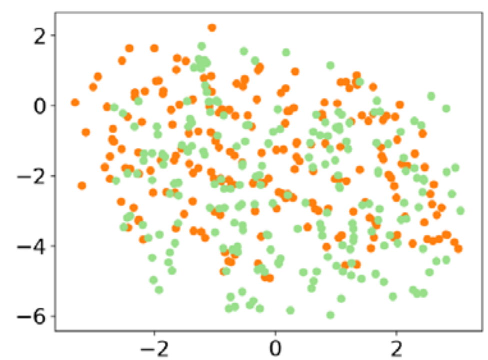
Fig. 8: Evaluation of estimating nitrate concentration by using RMSE and MAE.

Experiments

Latent Status Analysis:



(a) Data distribution of the input vectors η_s and η_t.



(b) Data distribution of the output vectors δ_s and δ_t.

Fig. 9: Visualization of the data distribution for the domain regression layer's inputs and outputs.

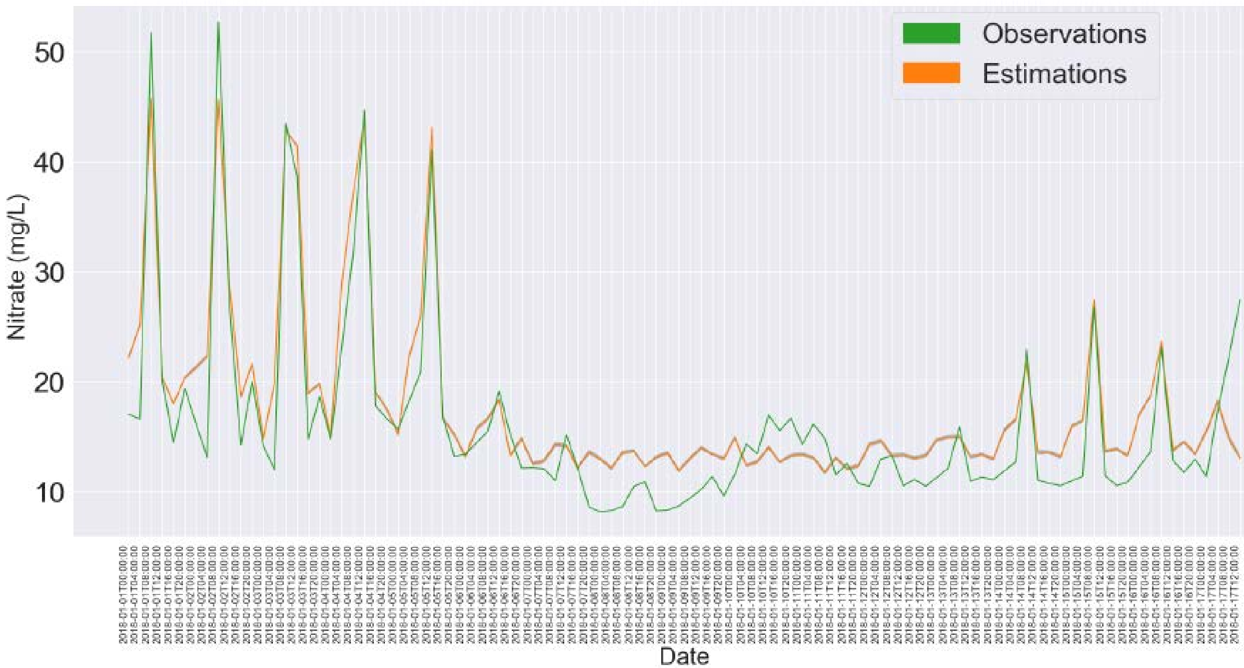
T-SNE is used for data visualization

Experiments

Uncertainty Analysis:

TABLE V: Uncertainty Measurement.

Model Architecture		Model No.	RMSE	MAE
SDAE	Regressor			
56-28-14	14-14-14-1	No. 1	4.90	4.08
		No. 2	5.01	4.01
		No. 3	5.41	4.25
		No. 4	5.42	4.30
		No. 5	5.10	4.20
		No. 6	5.46	4.43
		No. 7	5.27	4.12
		No. 8	5.25	4.33
		No. 9	5.15	4.34
		No. 10	5.18	4.25



Thanks