Comparison of Robust Artificial Neural Network and Gaussian Process Model for Interval Regression

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Context

Context

Context

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Context

Context

Real World

Represent

Mathematical World

Mathematical Models

As time passes

Use model to predict future, verify the past

Compare

Observe Future data

Predict Behaviour

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Context

The **big problem** is that the model are expensive to run !!

- Model Complexity.
- The governing equations used to describe the system.
- Computing rare events that exist at the tail of the distribution.

Problem Statement

Surrogate Model

High Fidelity Model

$$f(x)$$

Fast-running Surrogate

$$y = \mu_y(x) + \varepsilon(x)$$

Problem Statement

Surrogate Model

High Fidelity Model

$$f(x)$$

Fast-running surrogate

$$y = \mu_y(x) + \varepsilon(x)$$

Surrogate output

Problem Statement

Surrogate Model

Simulator (Expensive Code)

$$f(x)$$

Fast-running surrogate

$$y = \mu_y(x) + \varepsilon(x)$$

Surrogate output

Mean of surrogate

Problem Statement

Surrogate Model

Simulator (Expensive Code)

$$f(x)$$

Emulator (fast running)

$$y = \mu_y(x) + \varepsilon(x)$$

Simulator Output

Emulator

Noise

Artificial Neural Network as a Surrogate Model

What do we want from an ANN?

Artificial Neural Network as a Surrogate Model

What do we want from an ANN?

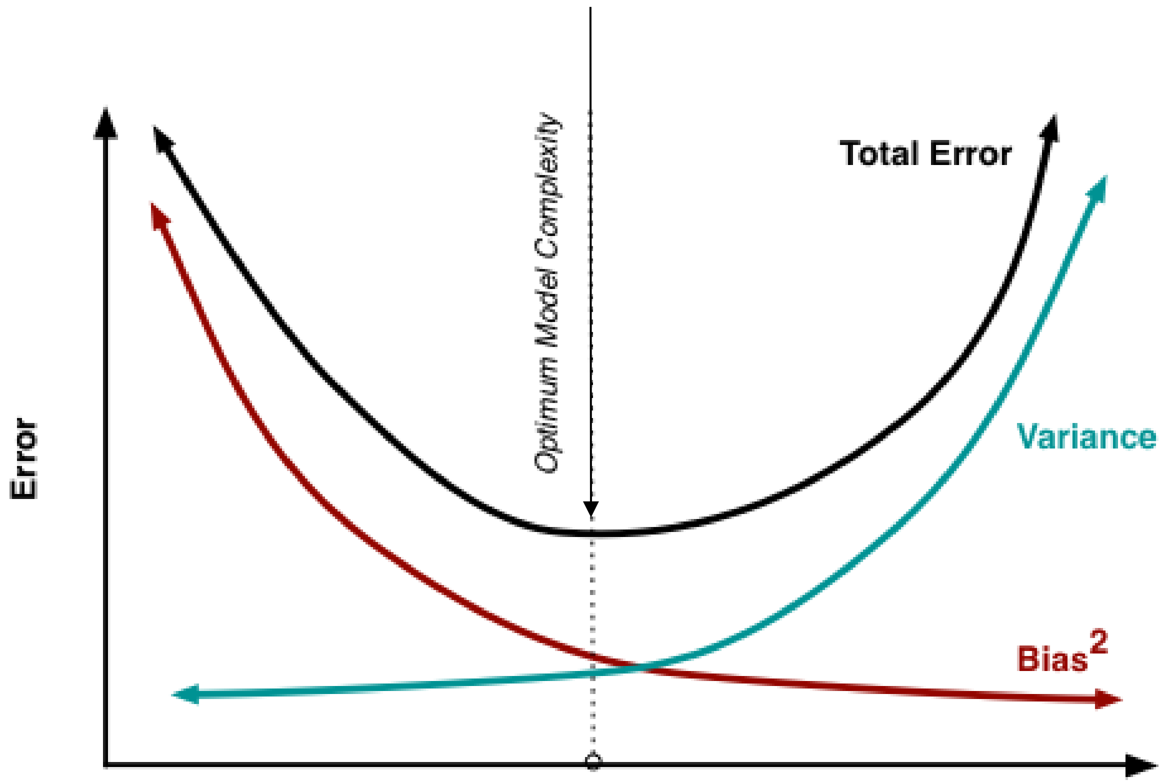
Robustness!!!

Artificial Neural Network as a Surrogate Model

What do we want from an ANN?

Robustness!!!

Low bias and variance



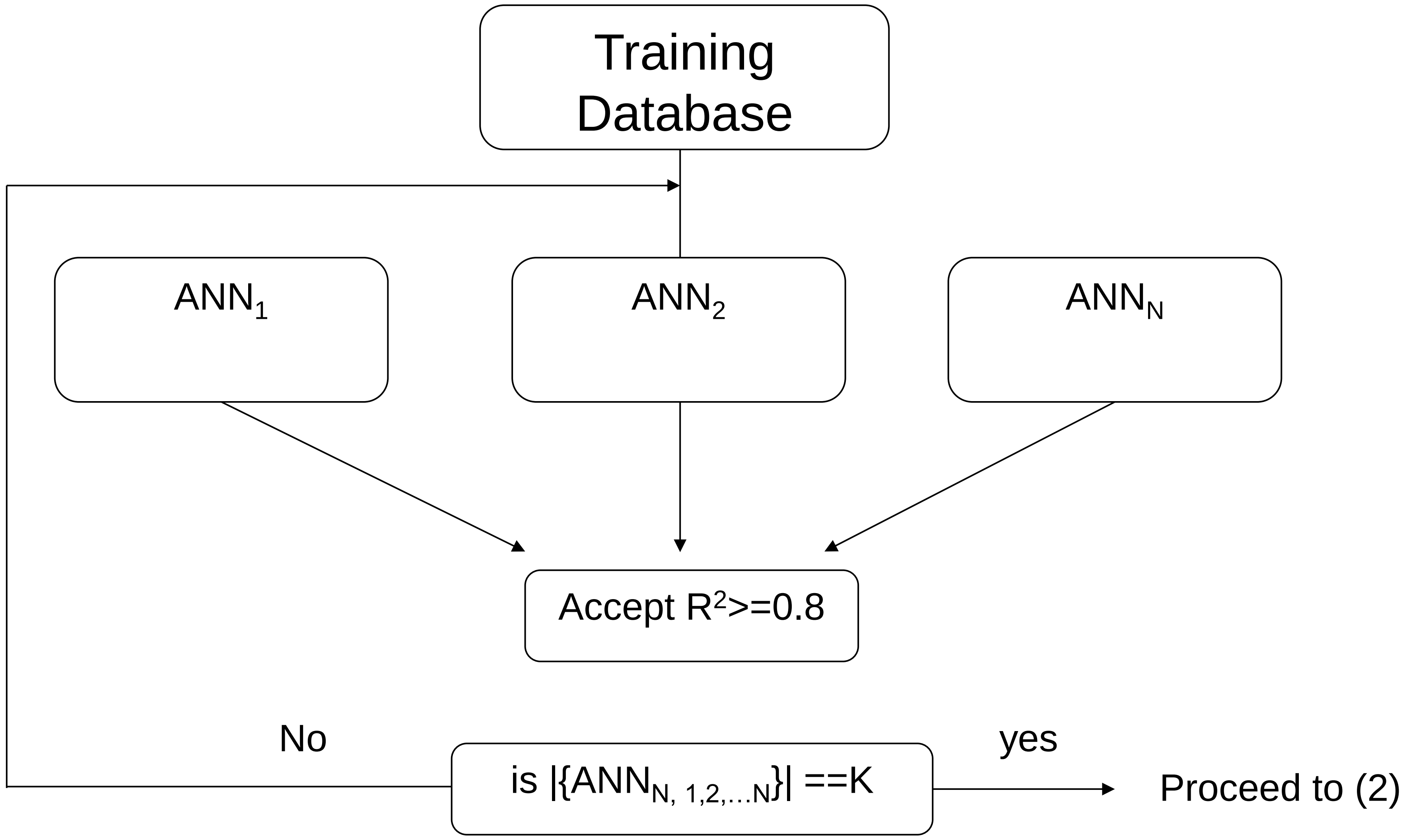
Artificial Neural Network as a Surrogate Model

The big problem are the **uncertainties** introduces on top of the surrogate model

- Random model parameters.
  - Train a large set of models,
  - Select the best model based on a performance metric (i.e. R^2).
  - Noise in data could falsify results.

Proposed Method

(1) Construction of a set of K Identical Networks



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Proposed Method

(2) Rank the ANNs in the set

$$P(N_k|D_{train}) = \frac{P(D_{train}\{x,y\}|N_k)P(N_k)}{\sum_{q=1}^{M} P\left(D_{train}\{x,y\}\middle|N_q\right)P(N_q)}$$

$P(D_{train}\{x,y\}|N_k)$ ← Likelihood of the *k^th^* network in the set

$P(N_k)$ ← Prior Probability of *k^th^* network in the set

$P(N_k|D_{train})$ ← Posterior Probability of *k^th^* network in the set

- Due to the difficulty of estimating $P(N_k)$ uniform probability *1/M* is assigned

$$\sigma_k^2 = \frac{1}{N}\sum_{i=1}^{N} \varepsilon_{ki}^2 \qquad \varepsilon_{ki} = D_{train}\{y_i\} - \hat{y}_i, \varepsilon_{ki} \sim N\left(0, \sigma_k^2\right), i = 1, \ldots, \mathrm{N}$$

Maximum Likelihood Estimation Approach

$$P(D_{train}|N_k) \approx \frac{1}{\sqrt{2\pi\sigma_k^2}} \frac{1}{N}\sum_{i=1}^{N} exp\left\{\frac{-[y_i - \hat{y}_{ki}]^2}{2\sigma_k^2}\right\}$$

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Proposed Method

(3) Device Robust prediction and quantify of model uncertainties

$$y_{robust} = \hat{y}^* + A_f$$

y_{robust} ⟵ robust prediction (i.e. best prediction considering model uncertainties)

$\hat{y}^*$ ⟵ Prediction from best Neural Network

A_f ⟵ Adjustment factor assumed to be a normally distributed *N(μ, σ)*

$$E[A_f] = \sum_{i=1}^{M} P(N_i|D_{train})(\hat{y}_i - \hat{y}^*)$$

$$Var[A_f] = \sum_{i=1}^{M} P(N_i|D_{train})\,(\hat{y}_i - E[y_{robust}])^2$$

$$E[y_{robust}] = \hat{y}^* + E[A_f]$$

$$Var[y_{robust}] = Var[A_f]$$

Confidence Interval ⟶ $[\overline{y}_{robust}, \quad \underline{y}_{robust}]$

$$\bar{y}_{robust} = E(y_{robust}) + 1.96\sqrt{Var(y_{robust})}$$

$$\underline{y}_{robust} = E(y_{adj}) - 1.96\sqrt{Var(y_{robust})}$$

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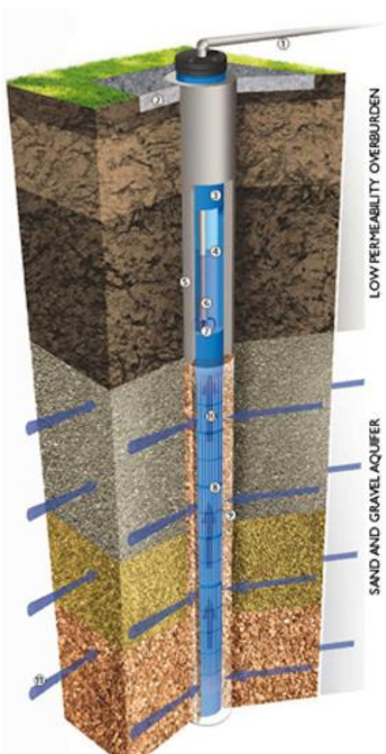
Simulation of water through a bore hole

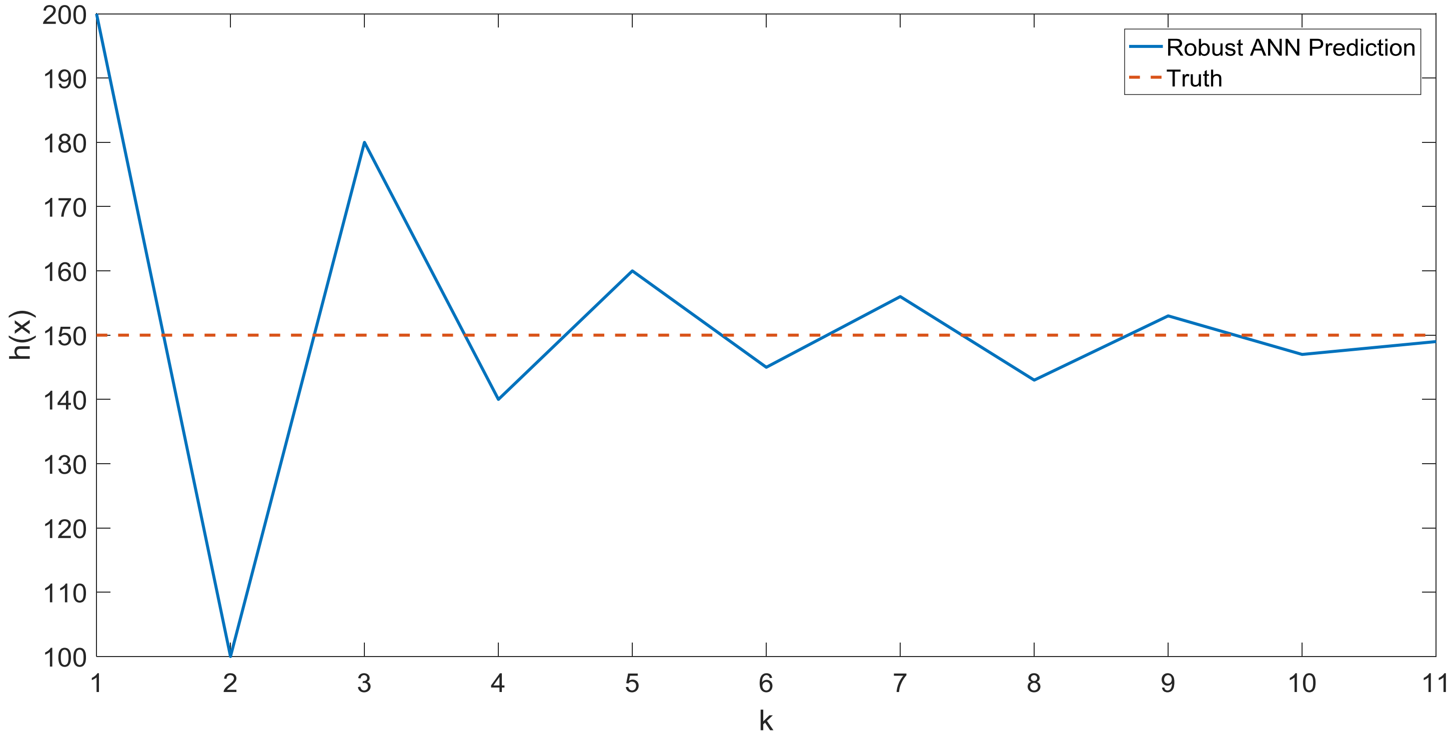
$$h(x) = \frac{2\pi T_u (H_u - H_l)}{\ln(r/r_w)\left(1 + \frac{2LT_u}{\ln(r/r_w) r_w^2 K_w} + \frac{T_u}{T_l}\right)}$$



Parameters	Distribution	Values
r_w	Uniform	[0.05 0.15]
r	Log-Normal	[7.71 1.0056]
T_u	Uniform	[63070 115600]
H_u	Uniform	[990 1110]
T_l	Uniform	[63.1 116]
H_l	Uniform	[700 820]
L	Uniform	[1120 1680]
K_w	Uniform	[9855 12045]

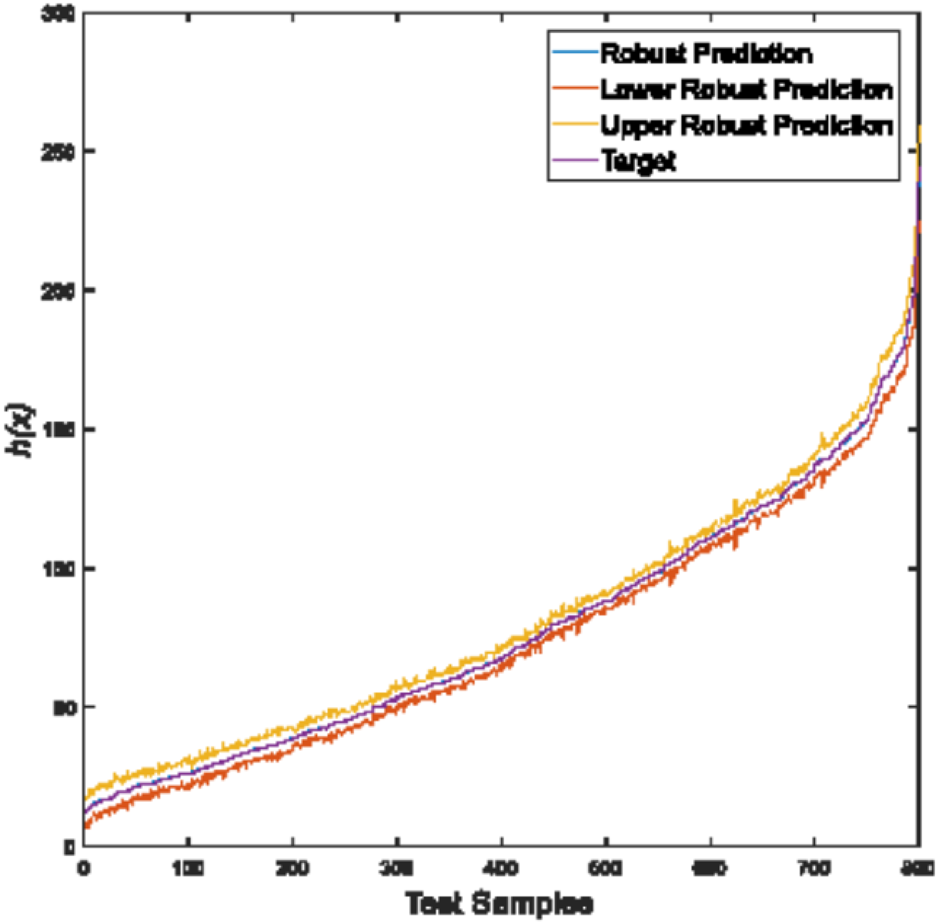
Case Study: Experimental settings

- Design of experiment via LHS (1000 training samples)
- Train ANN
  - 1 hidden layer ANN architecture [8 5 1]
  - Adam optimizer (Tensorflow)

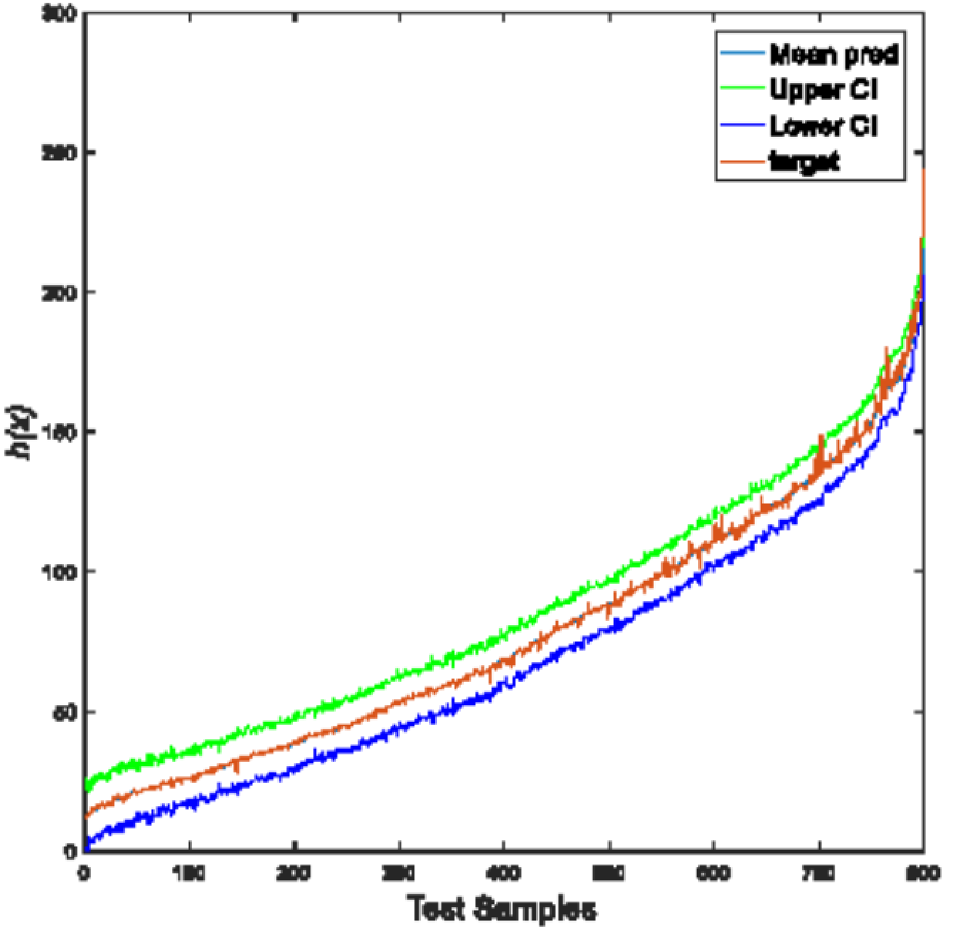


Results

Robust ANN Prediction



Prediction from GP Model

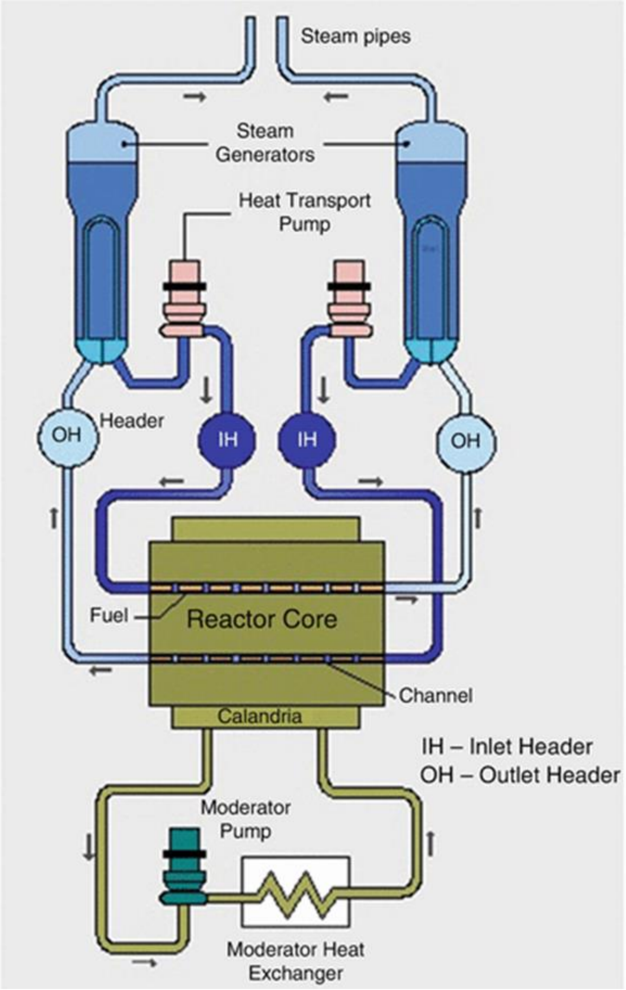


Case Study 2

- ➢ Presents a Nuclear Engineering problem (T V Santhosh, et al (2011)
- ➢ Task is to predict the break size
  - ▪ Pipe transporting fluid
  - ▪ Loss of coolant accident
  - ▪ Pattern recognition tool

Experimental settings

- ➢ Adopting an architecture [37 19 26 1] for k=10 iterations



TV Santhosh, et al. A diagnostic system for identifying accident conditions in
a nuclear reactor. Nuclear engineering and design, 241(1):177{184, 2011.

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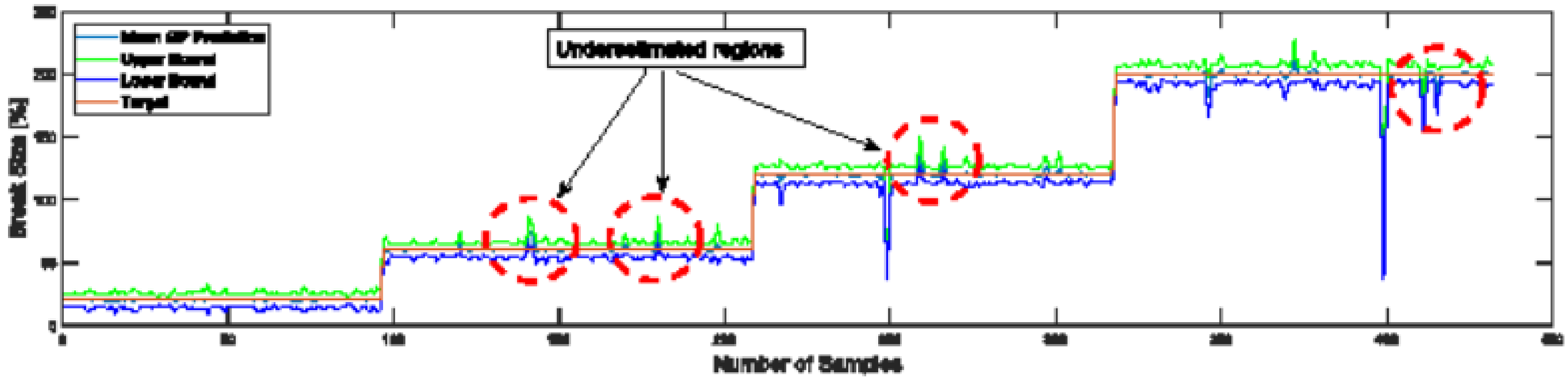
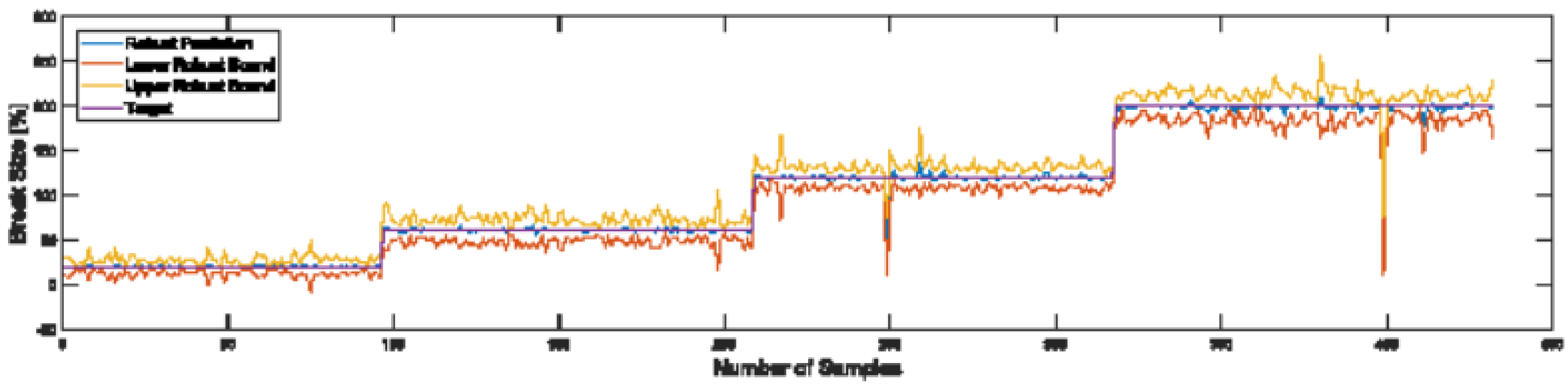
Results





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Conclusion

- Robust ANN performed better than GP model in terms of predicting tighter confidence bounds.

- Although for some cases the confidence bounds produced by robust ANN are larger than the bounds GP model, the reliability of robust ANN bounds is usually higher.

- For big data set, robust ANN will always perform better than GP model.