Can neural networks be explained using polynomial regression and Taylor series?

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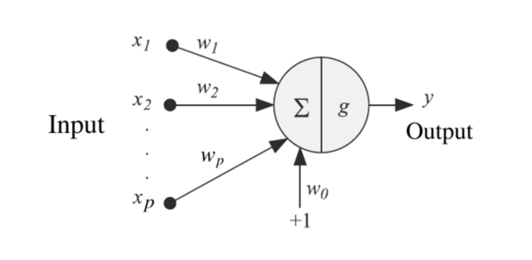
- Neural Networks (NN) are one of the most widely used tools in Machine Learning.



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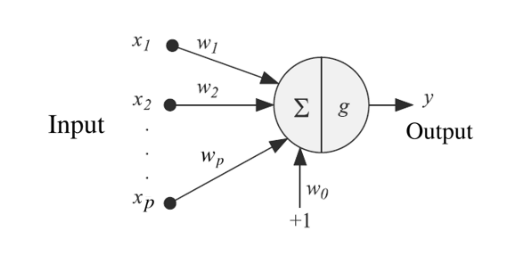

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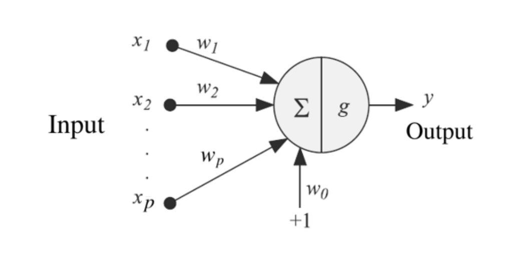

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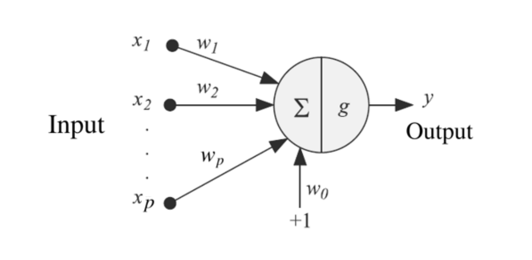

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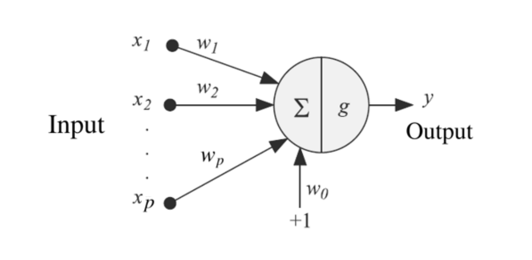

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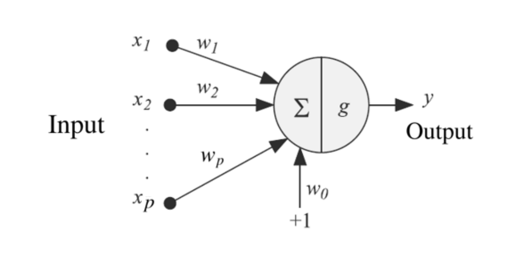

- However, NNs present some limitations:
  - Considered "black boxes".
  - Hyperparameter tuning.
  - Assessing the uncertainty and error in their predictions.
- A new perspective: the authors of Cheng et al., 2019 conjectured that NNs are equivalent to Polynomial Regression (PR).

Motivation: Proposed equivalence in Cheng et al., 2019

Publication

Cheng, X., Khomtchouk, B., Matloff, N., & Mohanty, P. (2019). Polynomial Regression As an Alternative to Neural Nets. *arXiv:1806.06850 [cs, stat]*

They present the following ideas:

- NNs are a form of PR.
- The degree of the polynomial increases with each hidden layer.
- PR properties can be used to study and even solve NN problems.
- Experimental results: PR performs as good as NNs in the used datasets.
- Using PR instead of NNs: R package (polyreg).

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However...

The relation between PR and NNs is not explicitly proven.

Our contribution

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Main objectives:

- Find an explicit expression to build a PR from the weights of a given NN, using Taylor expansion.
  - First, for a single hidden layer NN, then extending it to deeper layers.
- Study through simulations the validity of the proposed method.

Proposed method

Notation: Polynomial Regression

- Polynomial Regression:

$$Y = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + \cdots + \\ \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \cdots + \beta_{1p\ldots p} x_1 x_p^{k-1} + \beta_{p\ldots p} x_p^k.$$

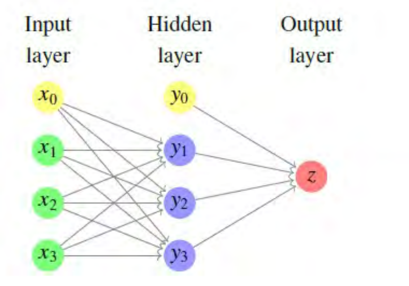
Notation: Neural Network

- Hidden layer neurons:

$$y_j = g\left(\sum_{i=0}^{p} w_{i,j} x_i\right).$$

- Final output:

$$z = \sum_{j=0}^{h_1} v_j y_j = \sum_{j=0}^{h_1} v_j g\left(\sum_{i=0}^{p} w_{i,j} x_i\right).$$



Proposed method: Necessary tools

Taylor expansion

$$y_j = g\left(\sum_{i=0}^{p}(w_{i,j}x_i)\right) = \sum_{n=0}^{\infty}\frac{g^{(n)}(a)}{n!}\left(\sum_{i=0}^{p}(w_{i,j}x_i) - a\right)^n$$

↓

Binomial Theorem

$$\left(\sum_{i=0}^{p} w_{i,j}x_i - a\right)^n = \sum_{k=0}^{n}\binom{n}{k}(-a)^{n-k}\left(\sum_{i=0}^{p}(w_{i,j}x_i)\right)^k$$

↓

Multinomial Theorem

$$\left(\sum_{i=0}^{p} w_{i,j}x_i\right)^k = \sum_{m_0+\cdots+m_p=k}\binom{k}{m_0,\ldots,m_p}(w_{0,j}x_0)^{m_0}\cdots(w_{p,j}x_p)^{m_p}$$

Proposed Method: Building the coefficients formula

- Combining all of the previous steps to obtain the output of the NN, setting the Taylor expansion at $a = 0$ and truncating the series at a given degree q:

$$z = v_0 + \sum_{j=1}^{h_1} v_j \sum_{n=0}^{q} \frac{g^{(n)}(0)}{n!} \times$$

$$\times \left[\sum_{m_0+\cdots+m_p=n} \binom{n}{m_0, \ldots, m_p} (w_{0,j}x_0)^{m_0} \cdots (w_{p,j}x_p)^{m_p} \right]$$

Proposed Method: Building the coefficients formula

The following PR coefficients are obtained:

- Intercept:

$$\beta_0 = v_0 + \sum_{j=1}^{h_1} v_j \left(\sum_{n=0}^{q} \frac{g^{(n)}(0)}{n!} (w_{0,j})^n \right)$$

- Rest of the coefficients:

$$\beta_{l_1 l_2 \ldots l_t} = \sum_{j=1}^{h_1} v_j \left(\sum_{n=t}^{q} \frac{g^{(n)}(0)}{(n-t)! \cdot m_1! \cdots m_p!} (w_{0,j})^{n-t} (w_{1,j})^{m_1} \ldots (w_{p,j})^{m_p} \right)$$

Taylor expansion validity for some activation functions

Activation Functions considered:

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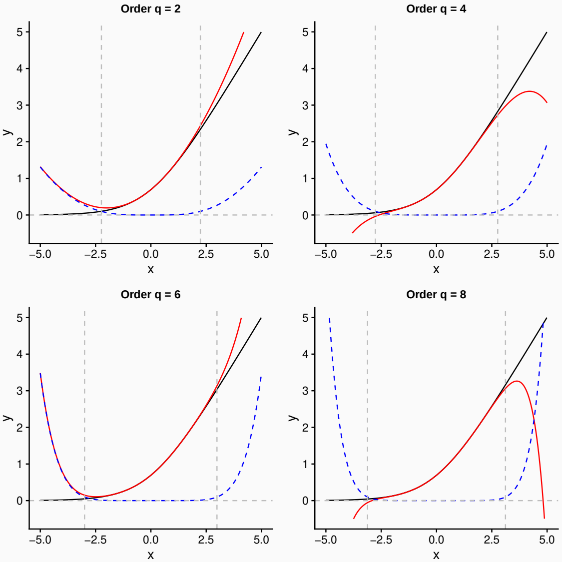
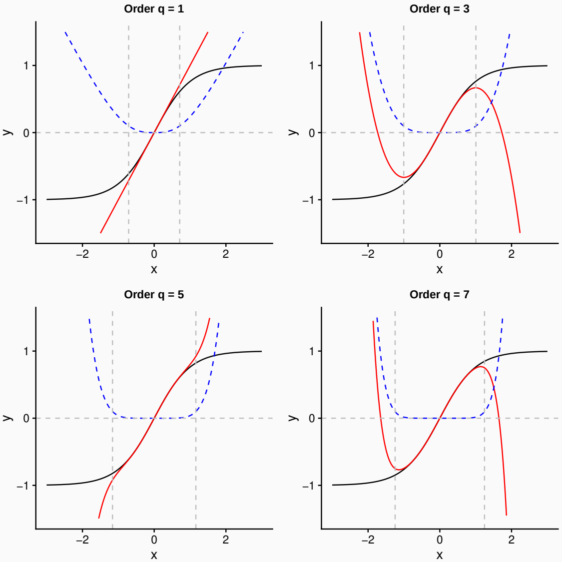
- **Sigmoid:**

$$g(x) = \frac{1}{1 + e^{-x}}$$

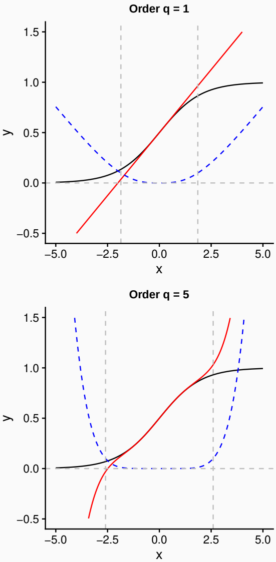
Taylor expansion: softplus



Taylor expansion: hyperbolic tangent

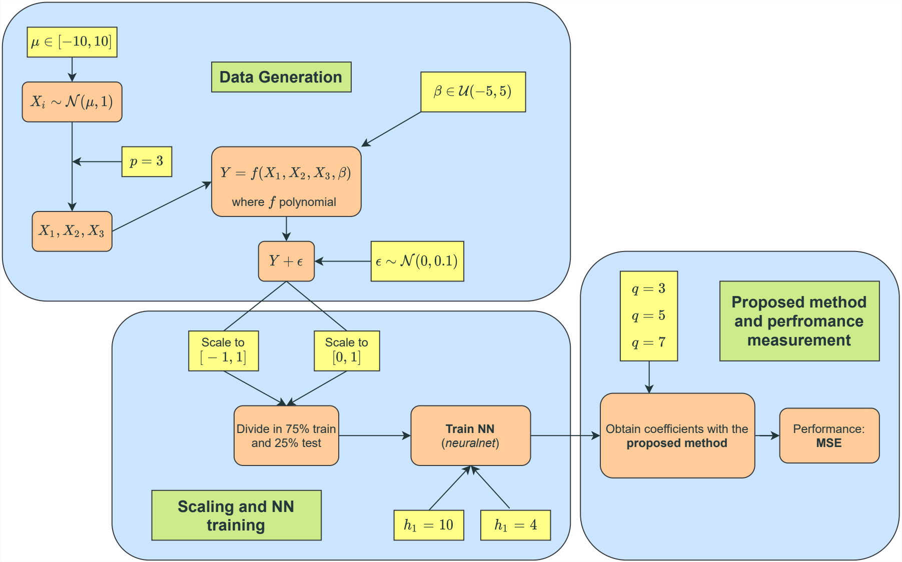


Taylor expansion: sigmoid

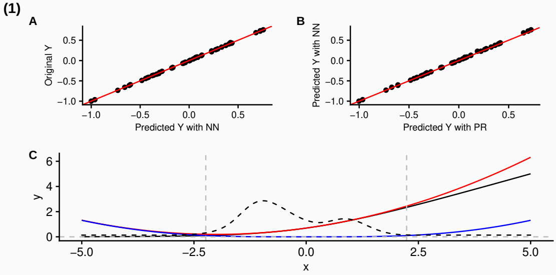


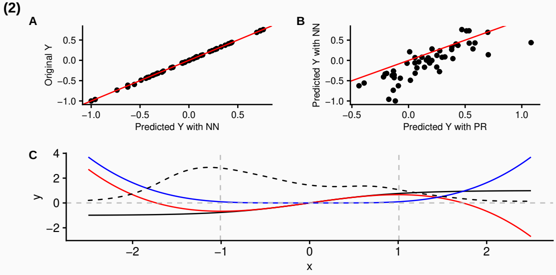
Simulation study (without restrictions)

Data generation

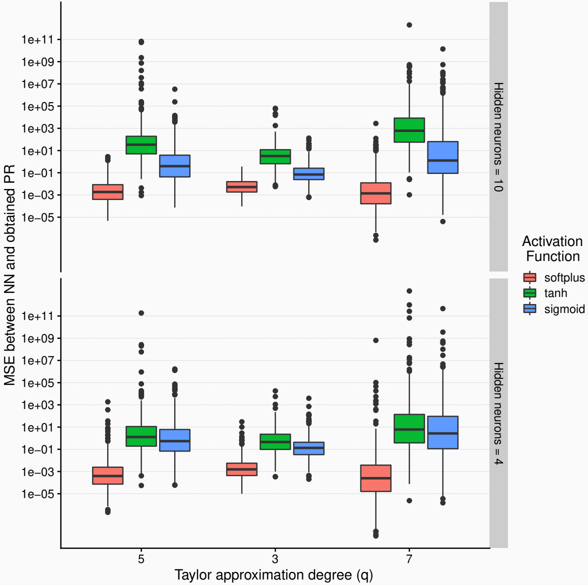


Performance examples

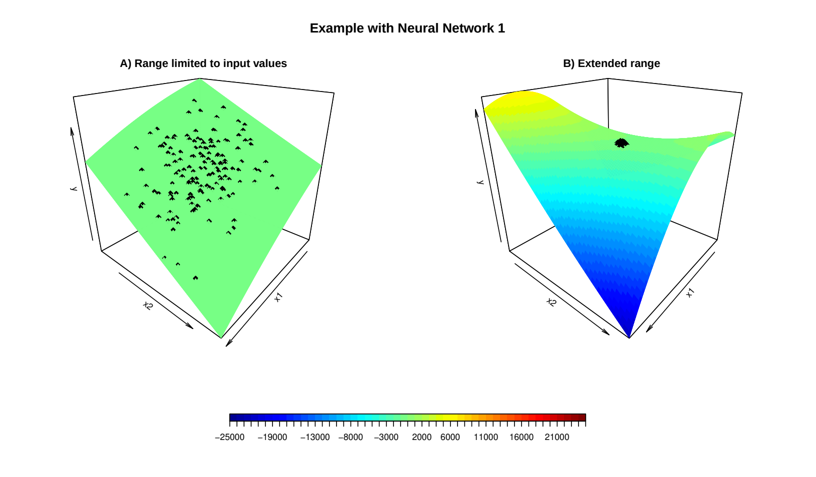




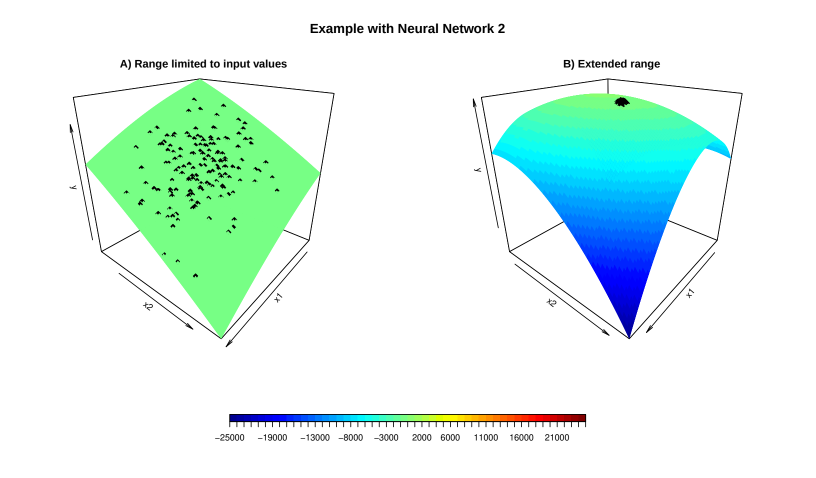
500 MSE simulations scaling to [-1,1]



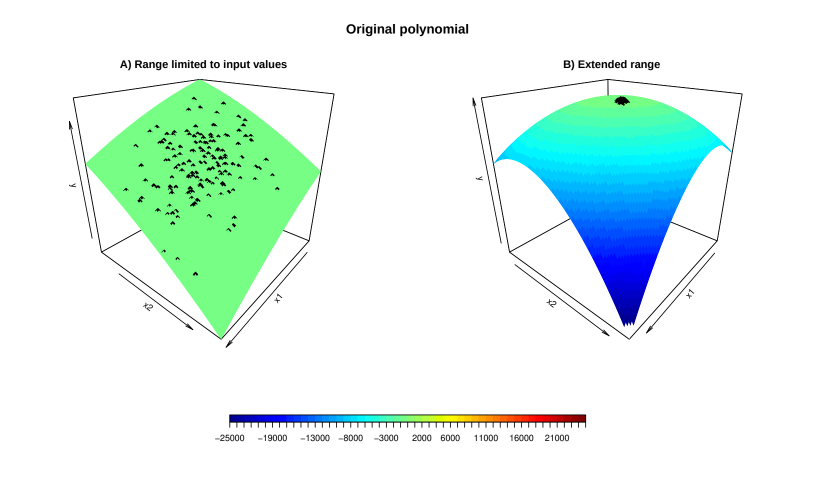
Same data, different NNs (1)



Same data, different NNs (2)



Same data, 4 different NNs: Original surface



Simulation study (with restriction)

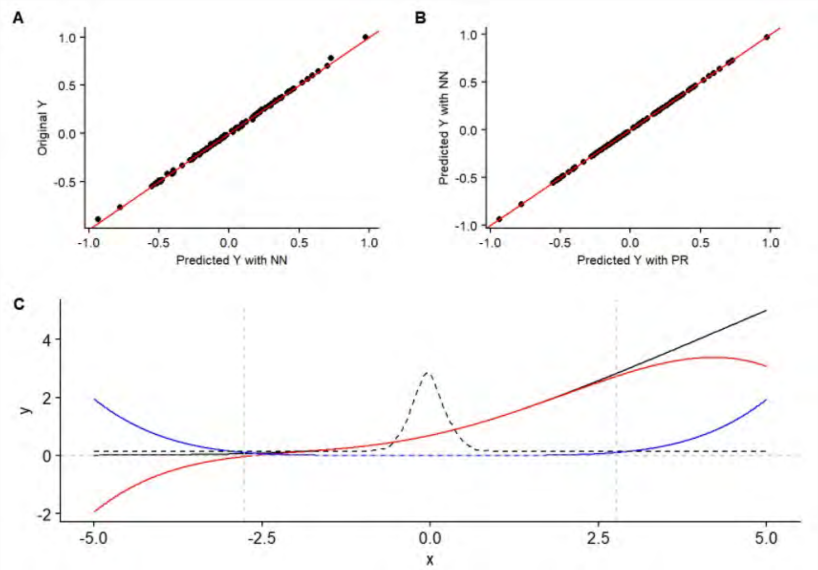
Constraining the weights in the hidden layers

- Limited region where Taylor expansion is accurate.
  - Impose an ℓ_1-norm equal to one for the hidden layer weights: $||\vec{w}_j||_1 = \sum_{i=0}^{p} |w_{i,j}| = 1$ for all j.
  - Then the synaptic potentials u_j are also constrained by 1 in absolute value:

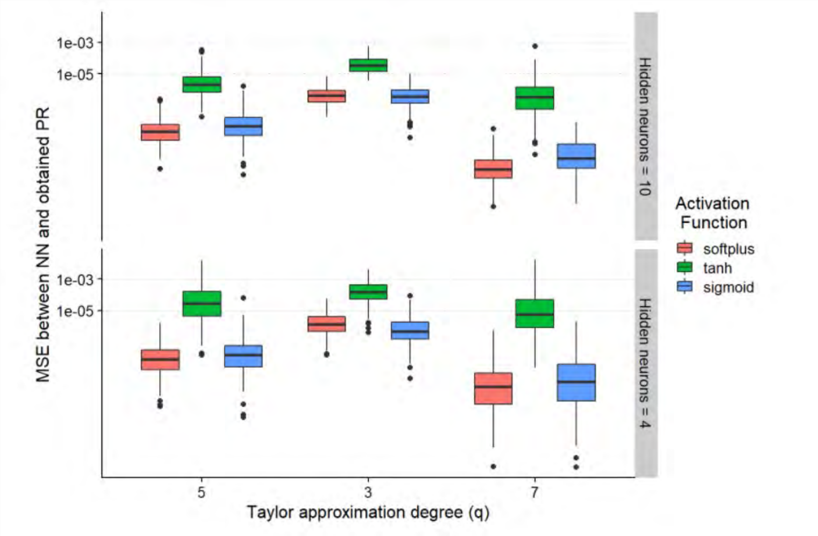
$$|u_j| = \left|\sum_{i=0}^{p} w_{i,j} x_i\right| \leq \sum_{i=0}^{p} |w_{i,j} x_i| \leq \sum_{i=0}^{p} |w_{i,j}| = ||\vec{w}_j||_1 = 1,$$

where $|x_i| \leq 1$ because of the $[-1, 1]$ scaling. Therefore, $|u_j| \leq 1$.

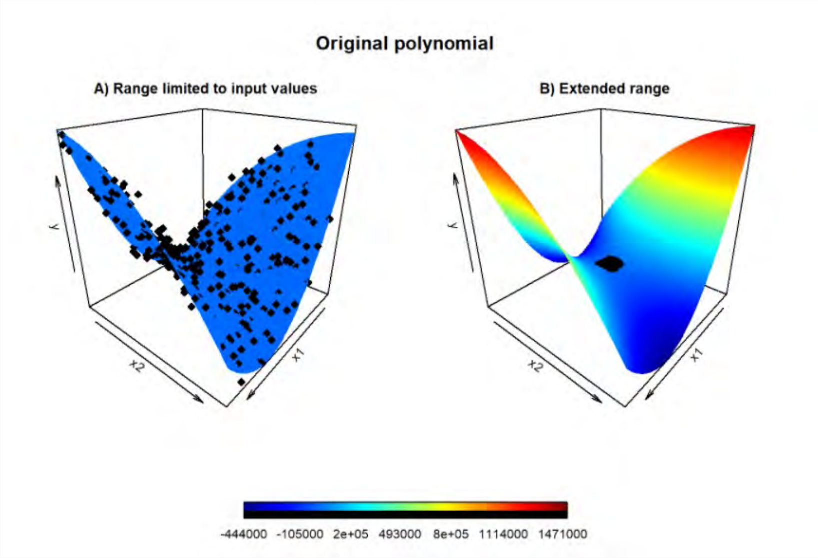
Example using weight constraints



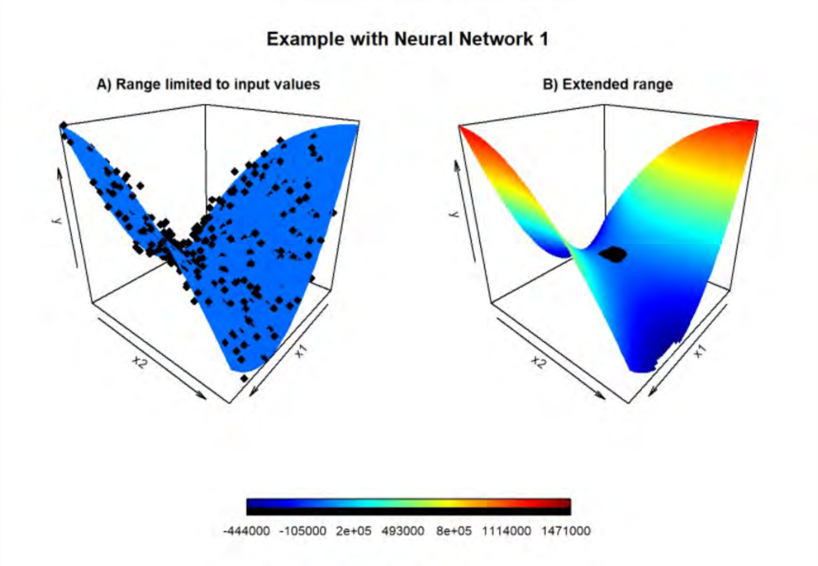
MSE simulations (restricted weights)



Surface example: Original Polynomial



Surface example: PR obtained from a NN



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- Implement the proposed method in a package (R/Python).

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  - Model NNs error and uncertainty using PR.

Main References

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Thanks for your attention!

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