TUTORIAL MACHINE LEARNING IN SOLID MECHANICS

TECHNISCHE
UNIVERSITÄT
DARMSTADT

TASK 1: FEED-FORWARD NEURAL NETWORKS

Fabian Roth

TUTORIAL MACHINE LEARNING IN SOLID MECHANICS

SECTIONS

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1 Hyperparameter sweep

2 Input convex neural networks

3 Trainable custom layer

4 Sobolev training

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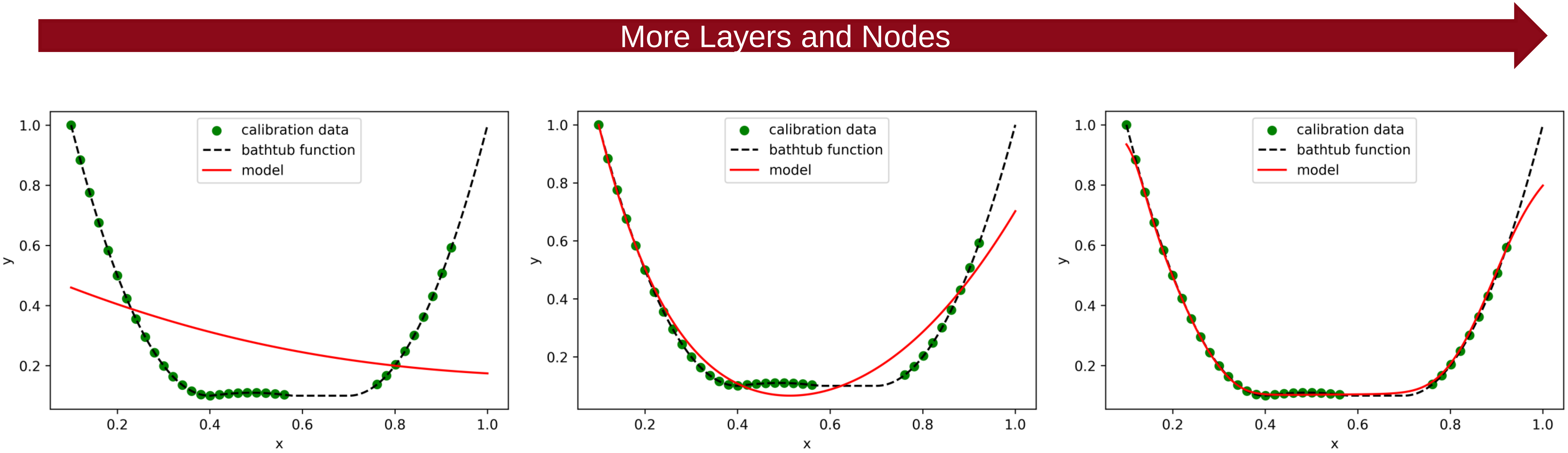
TASK 1 – 1.1

HYPERPARAMETER SWEEP

HYPERPARAMETER SWEEP

MODEL COMPLEXITY



More Layers and Nodes

HYPERPARAMETER SWEEP

MODEL COMPLEXITY... IT’S NOT THAT SIMPLE

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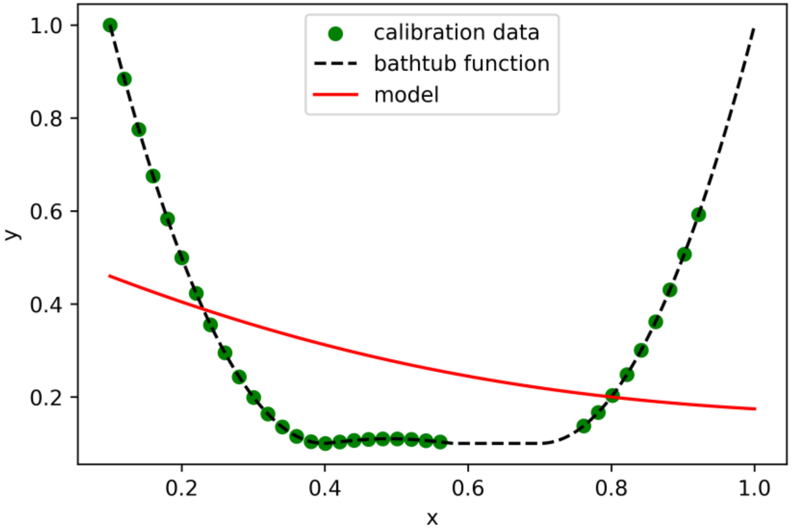
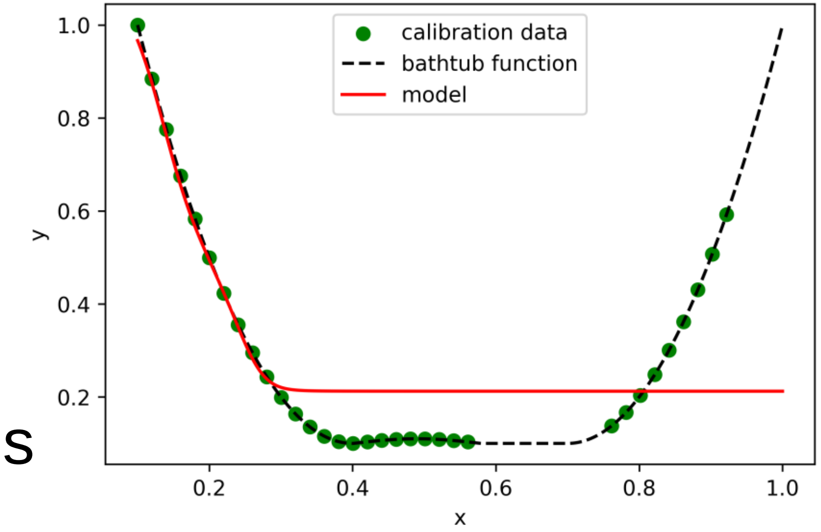


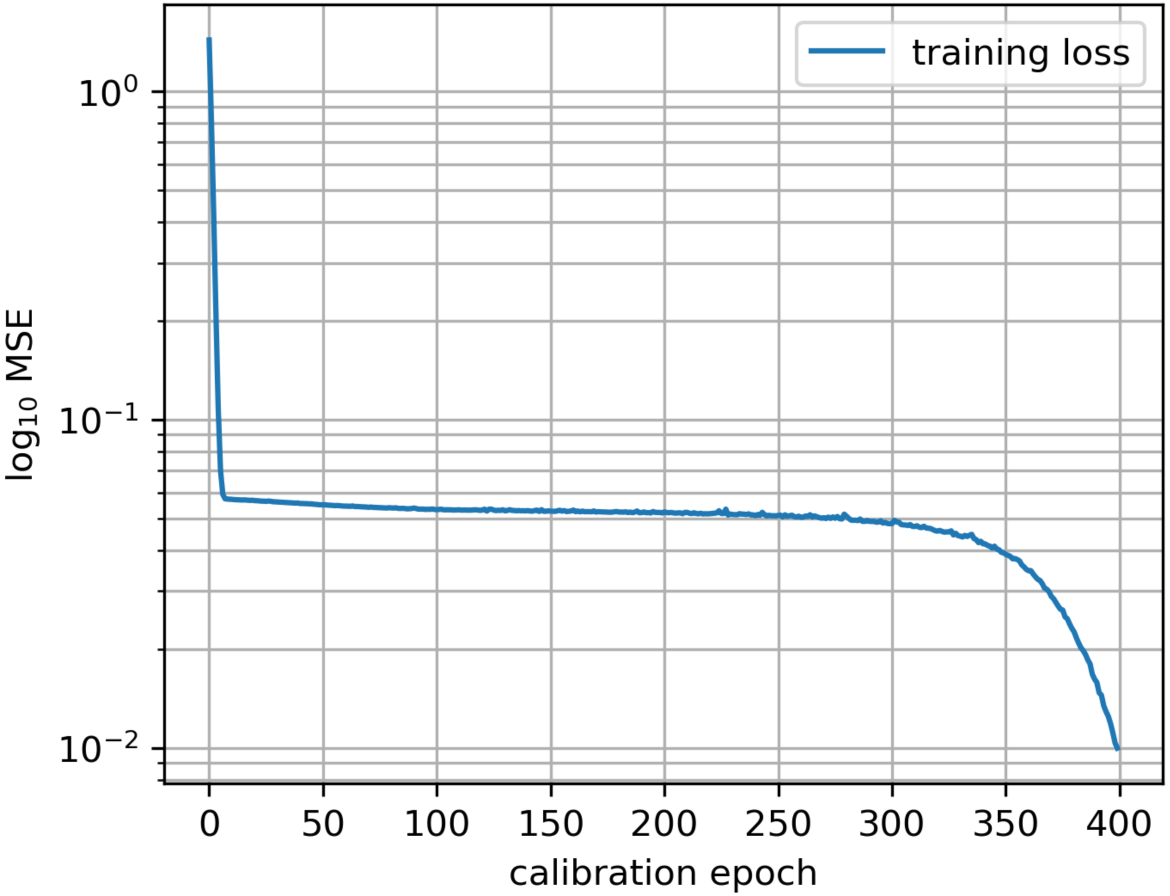
It‘s difficult to underfit on this simple data

Underfitting might have different causes



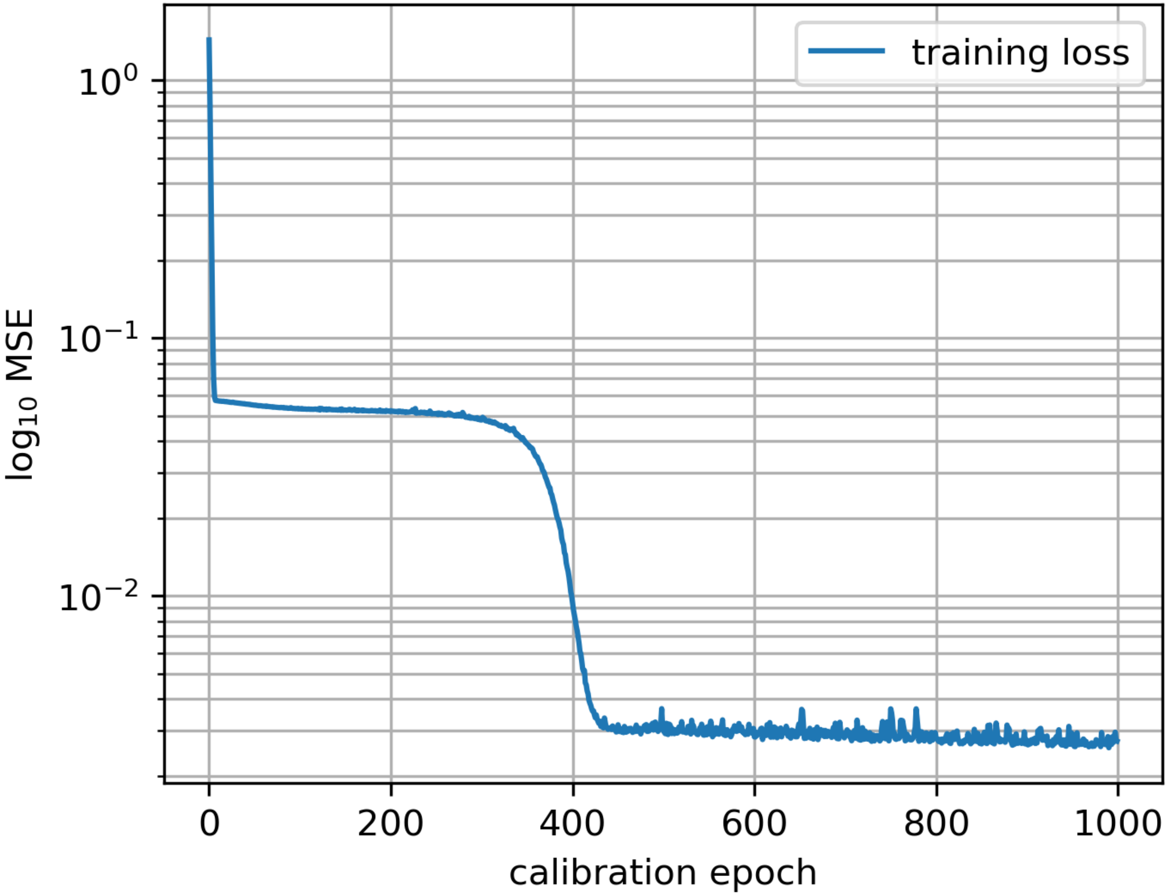
HYPERPARAMETER SWEEP

NUMBER OF EPOCHS



HYPERPARAMETER SWEEP

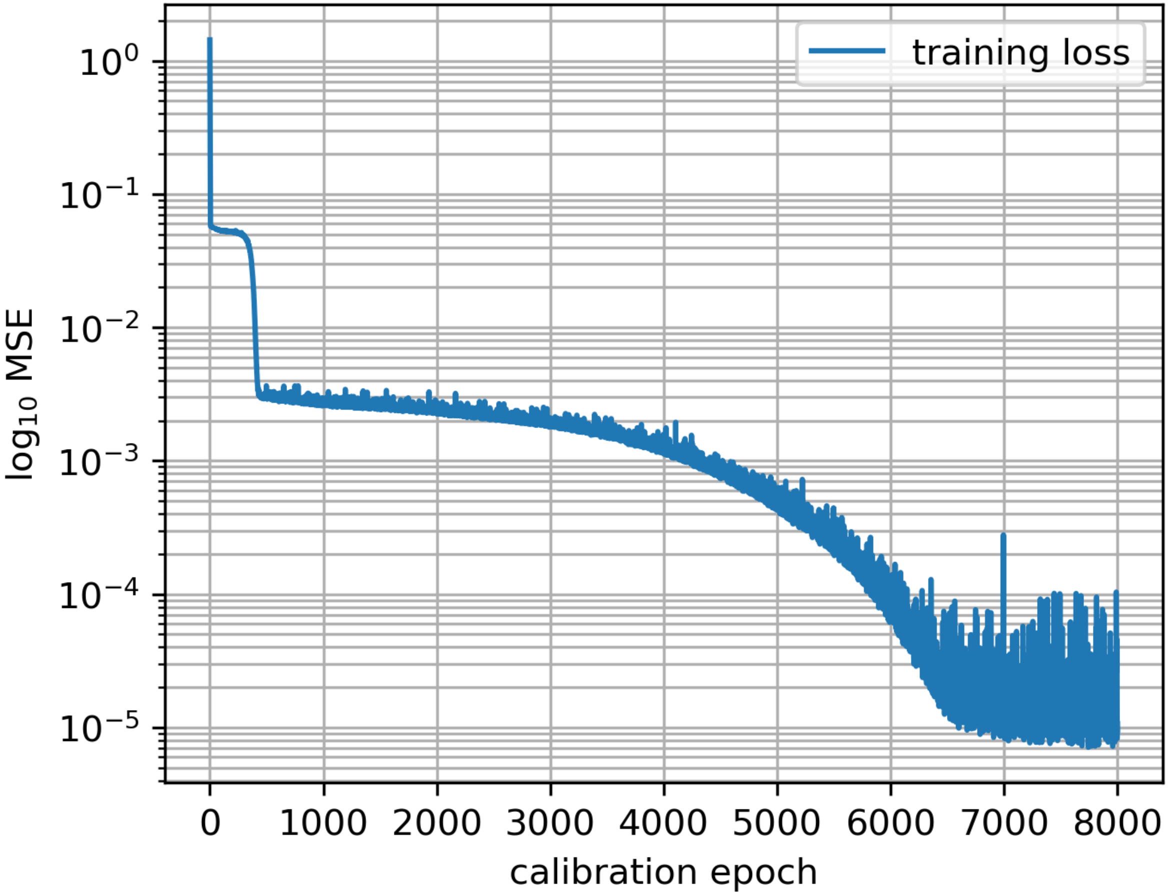
NUMBER OF EPOCHS



- Train until convergence

HYPERPARAMETER SWEEP

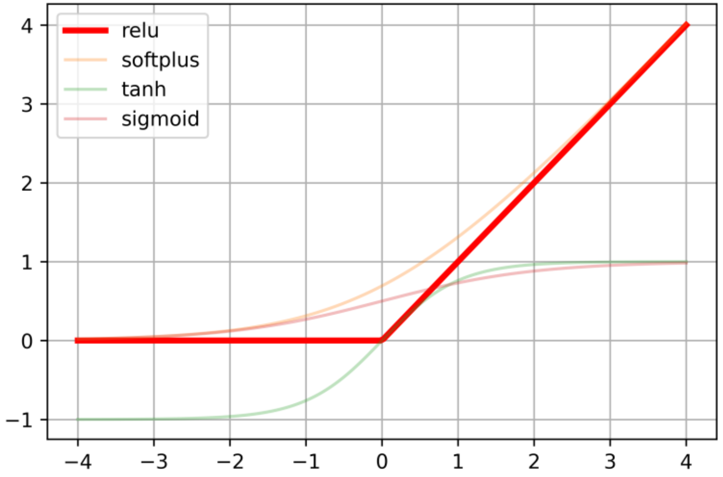
NUMBER OF EPOCHS

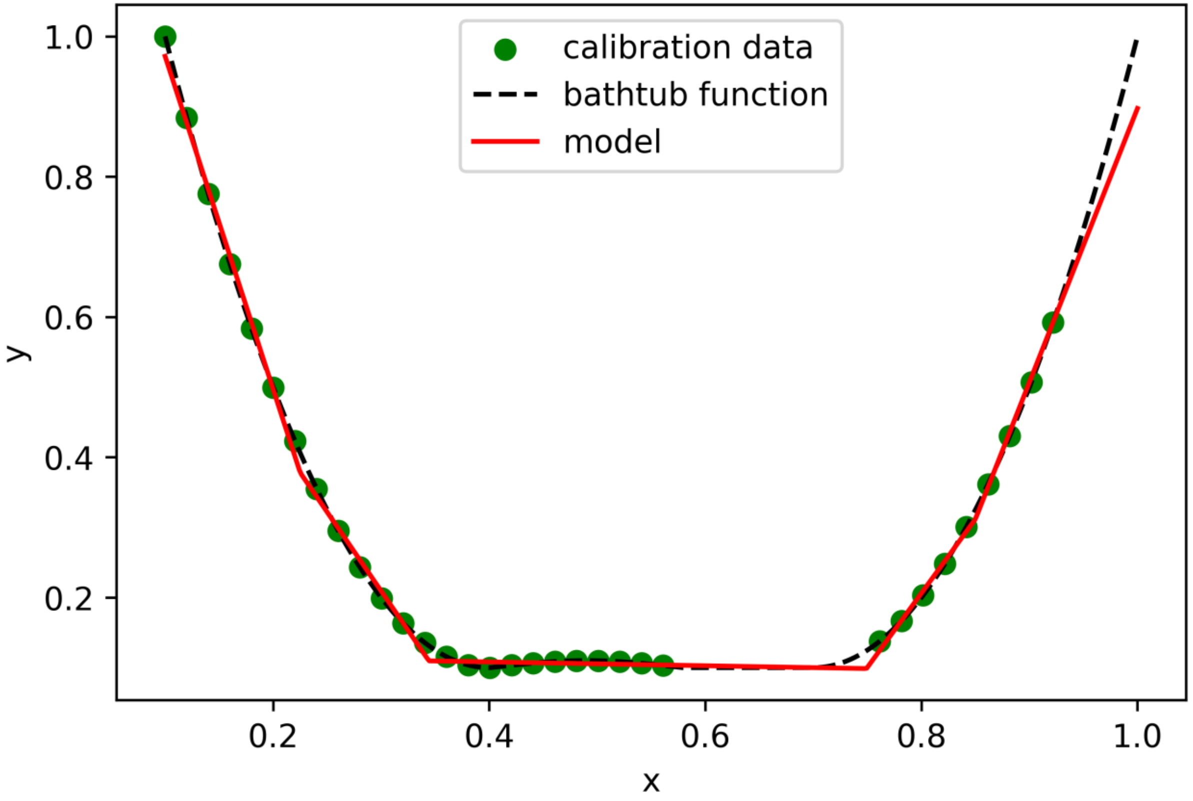


- Train until convergence
- “False“ convergence

HYPERPARAMETER SWEEP

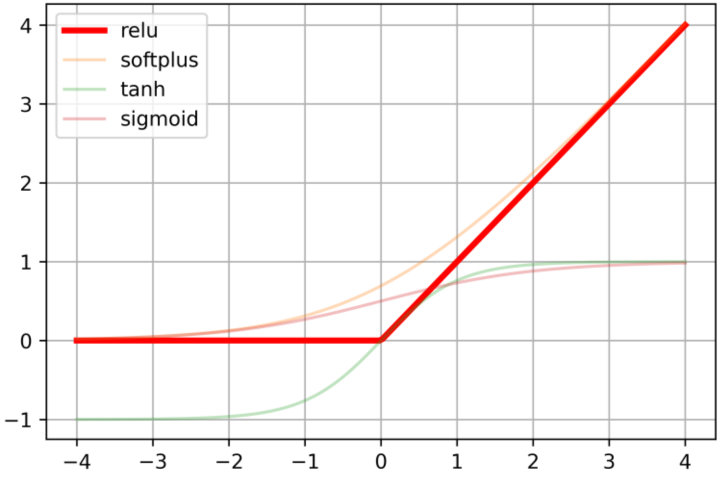
ACTIVATION FUNCTIONS - RELU

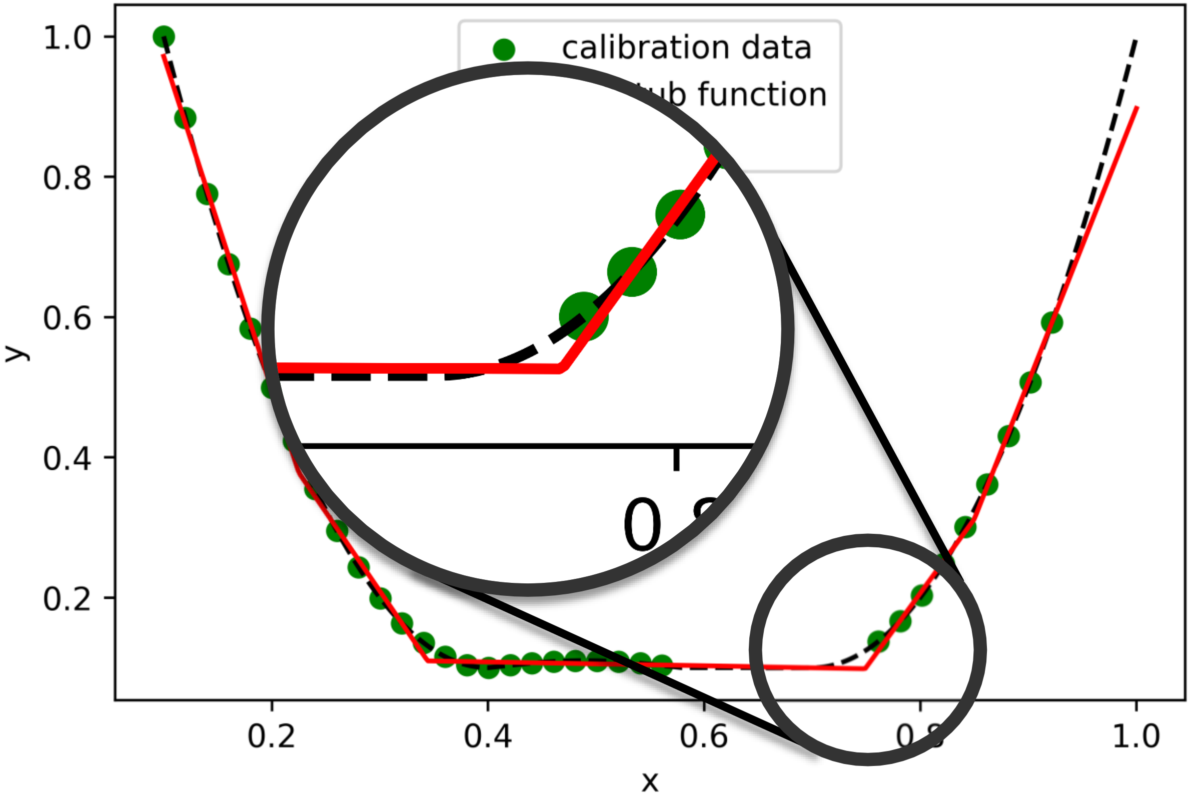




HYPERPARAMETER SWEEP

ACTIVATION FUNCTIONS - RELU

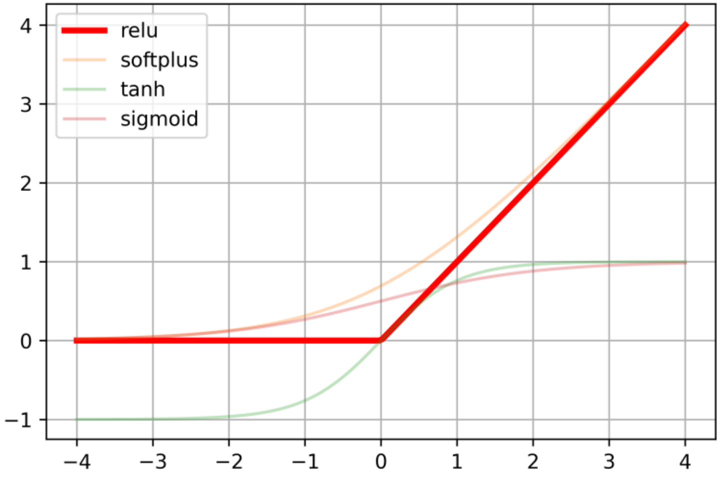


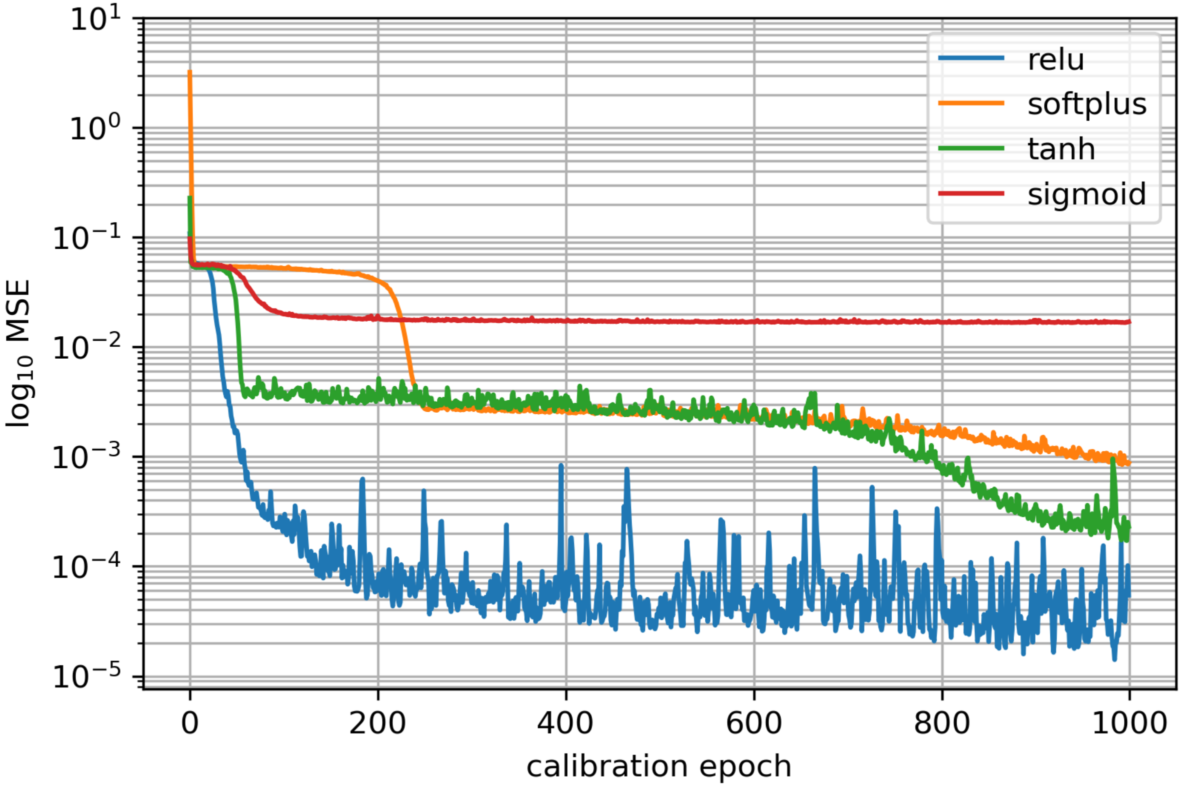


- Not continuously differentiable

HYPERPARAMETER SWEEP

ACTIVATION FUNCTIONS - RELU

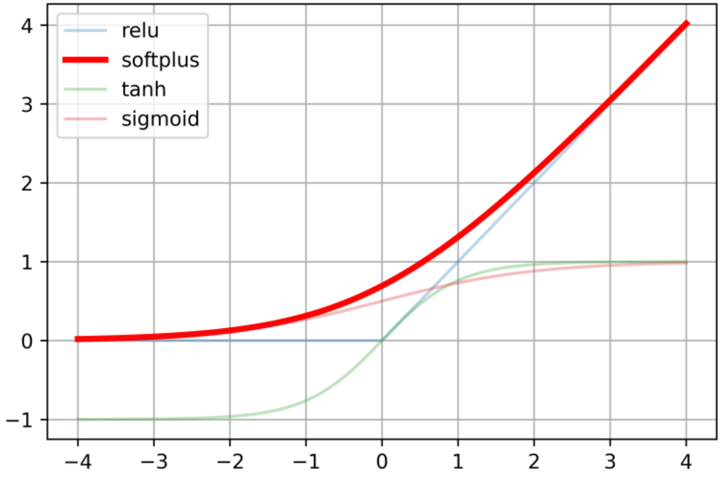


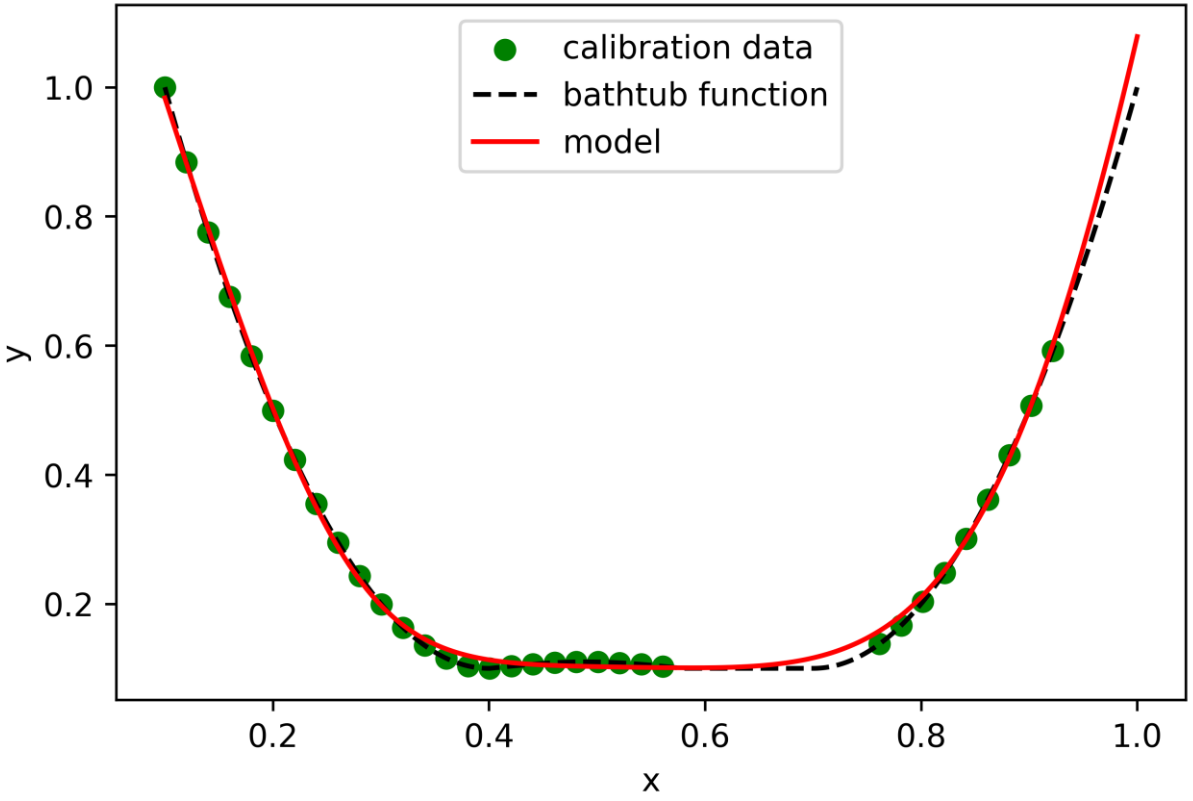


- Not continuously differentiable
- Fast convergence

HYPERPARAMETER SWEEP

ACTIVATION FUNCTIONS - SOFTPLUS

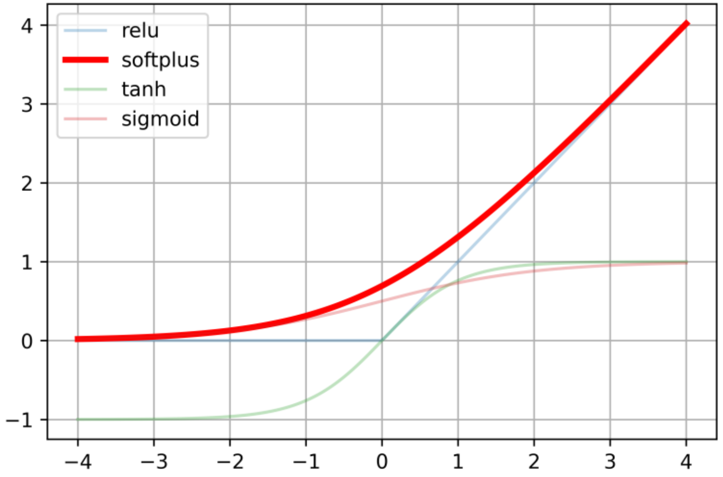


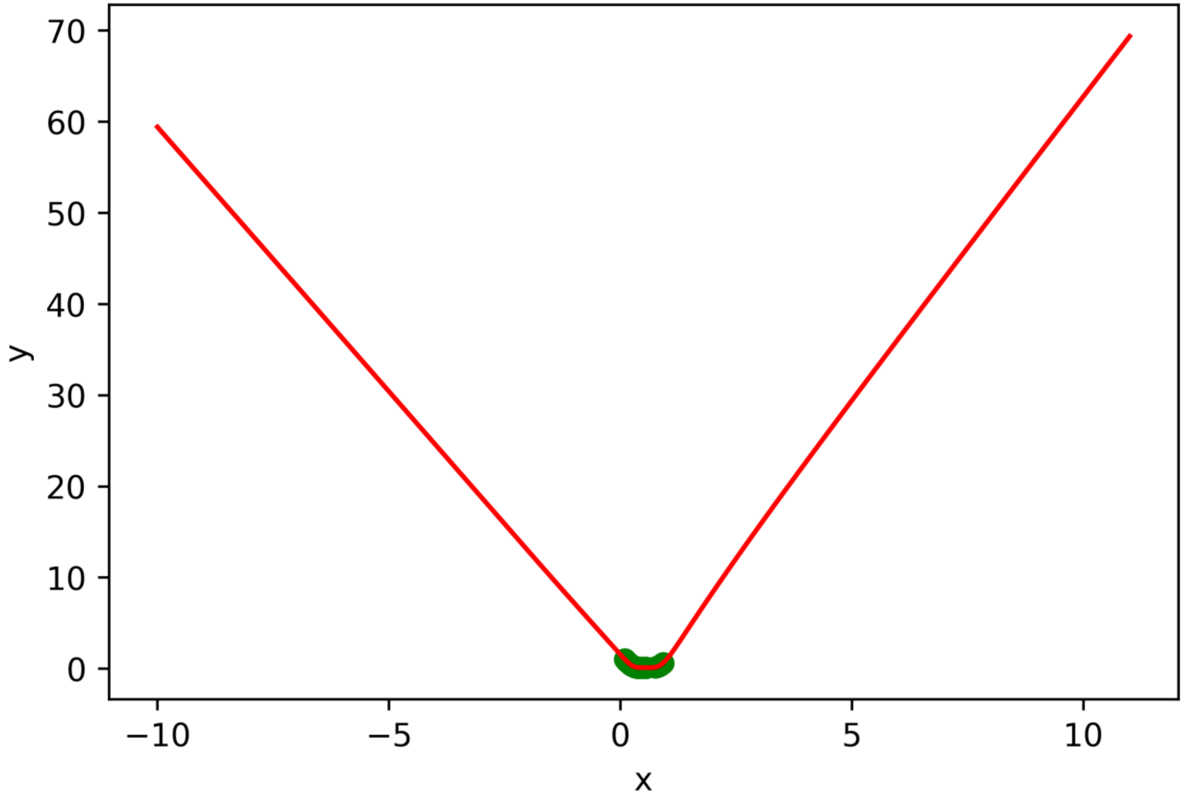


- Infinitely differentiable

HYPERPARAMETER SWEEP

ACTIVATION FUNCTIONS - SOFTPLUS

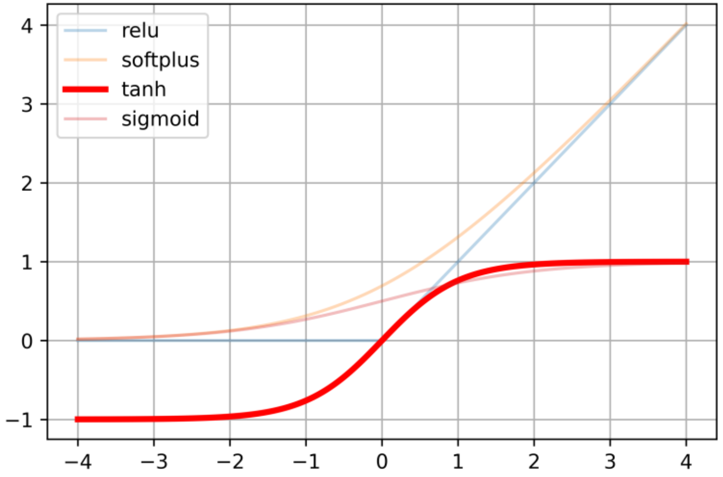




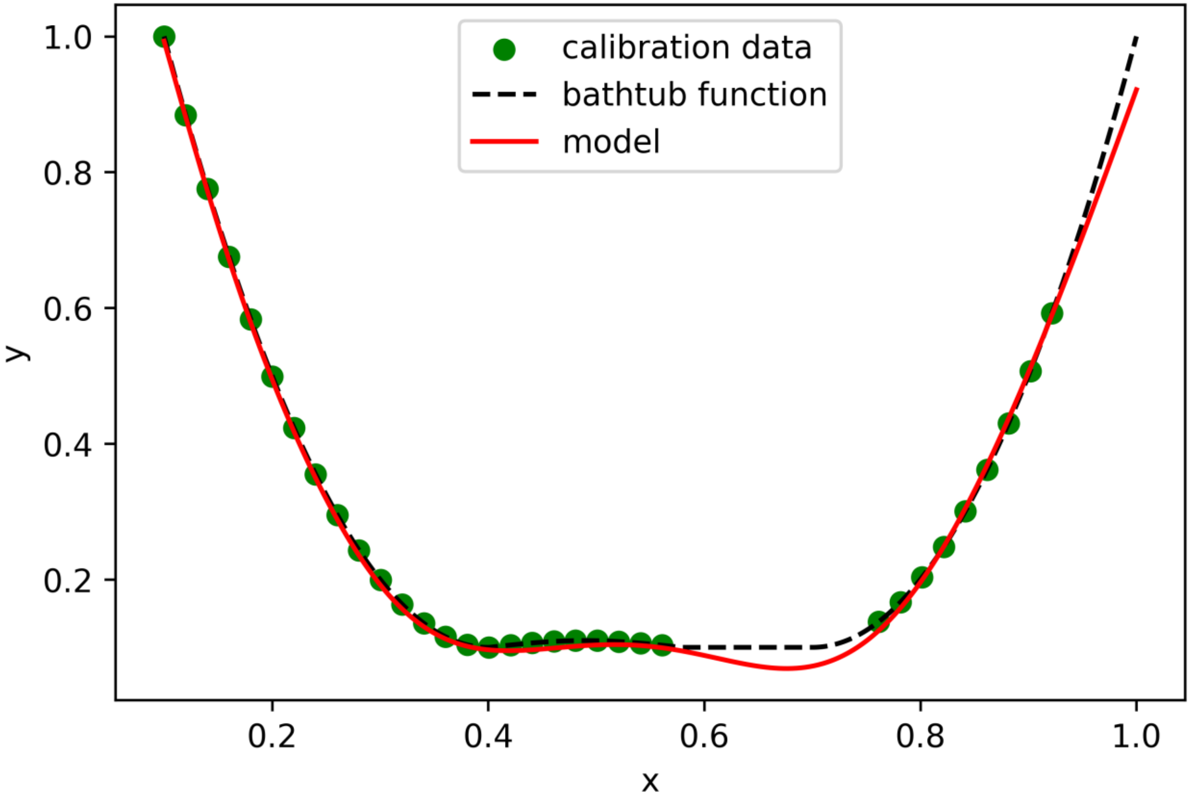
- Infinitely differentiable
- Unbounded

HYPERPARAMETER SWEEP

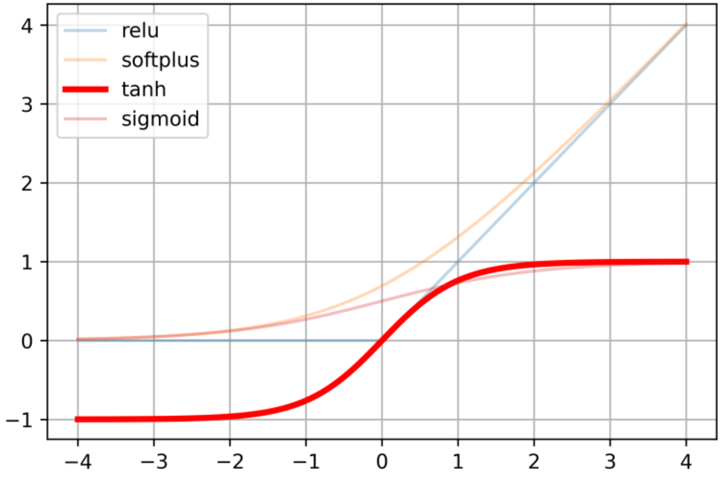
ACTIVATION FUNCTIONS - TANH

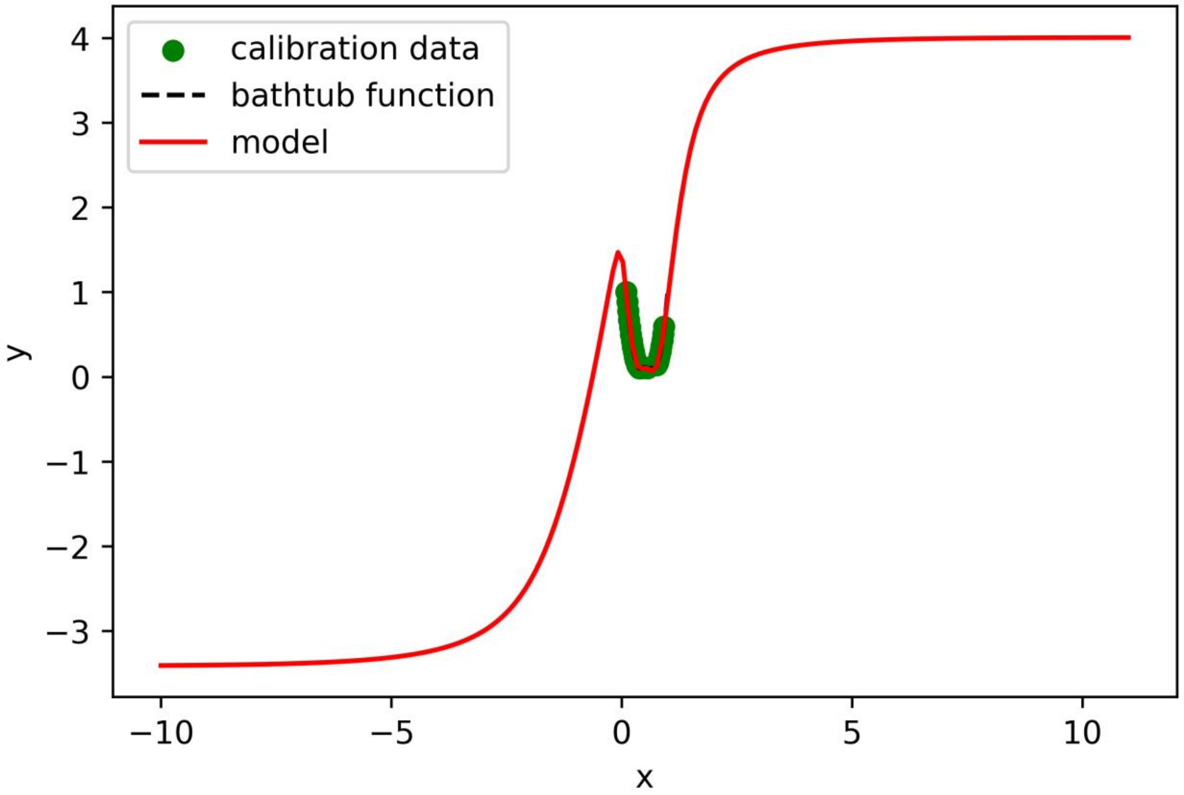


- Infinitely differentiable



ACTIVATION FUNCTIONS - TANH

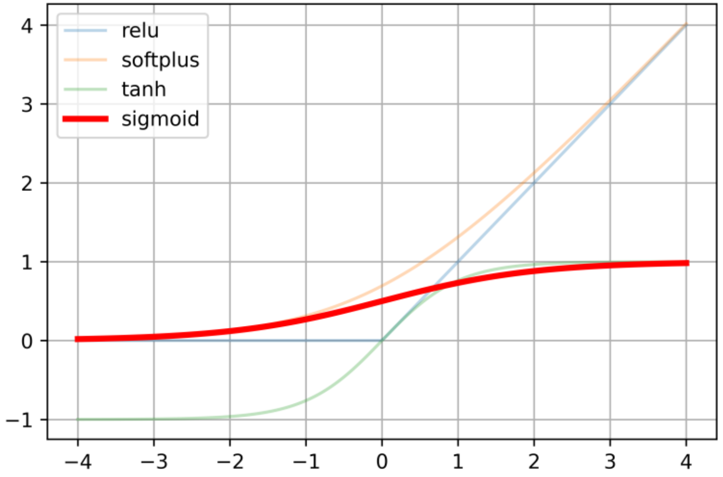


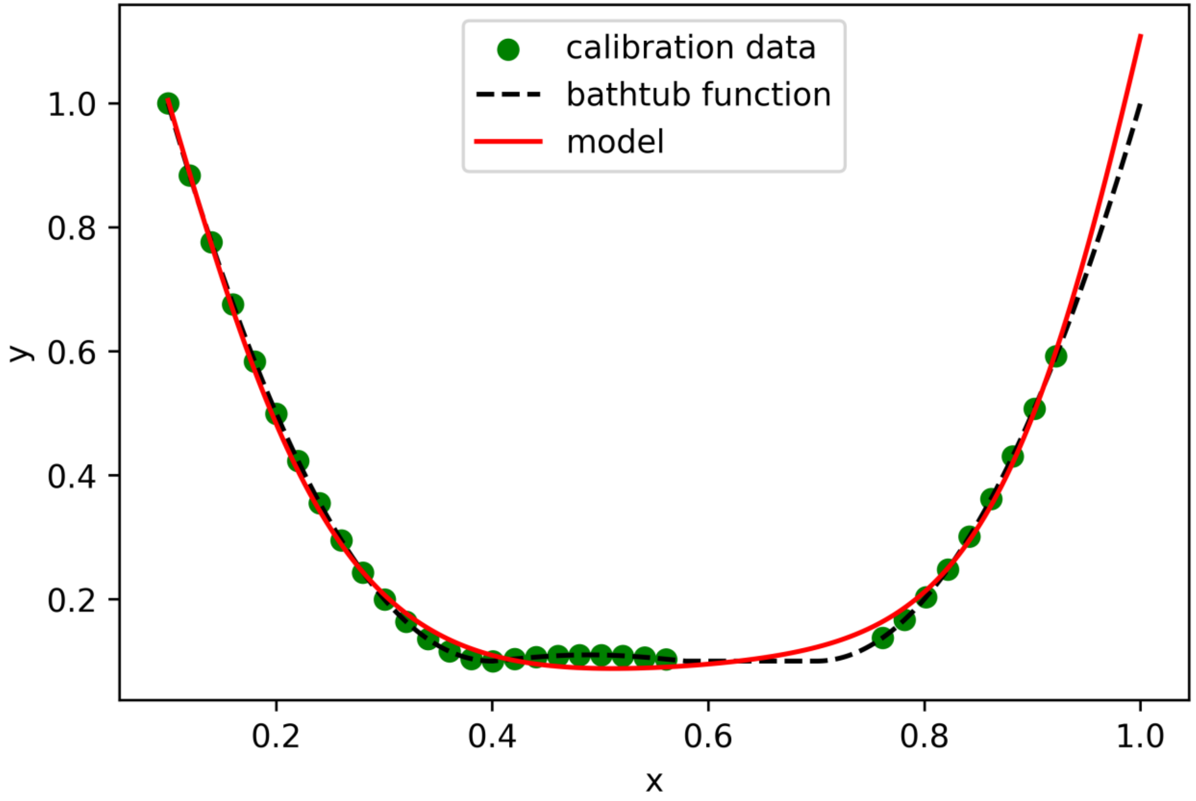


- Infinitely differentiable
- Bounded

HYPERPARAMETER SWEEP

ACTIVATION FUNCTIONS - SIGMOID

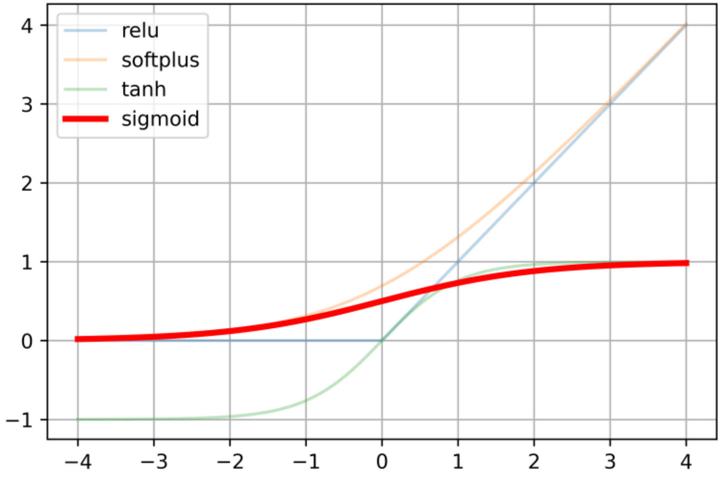




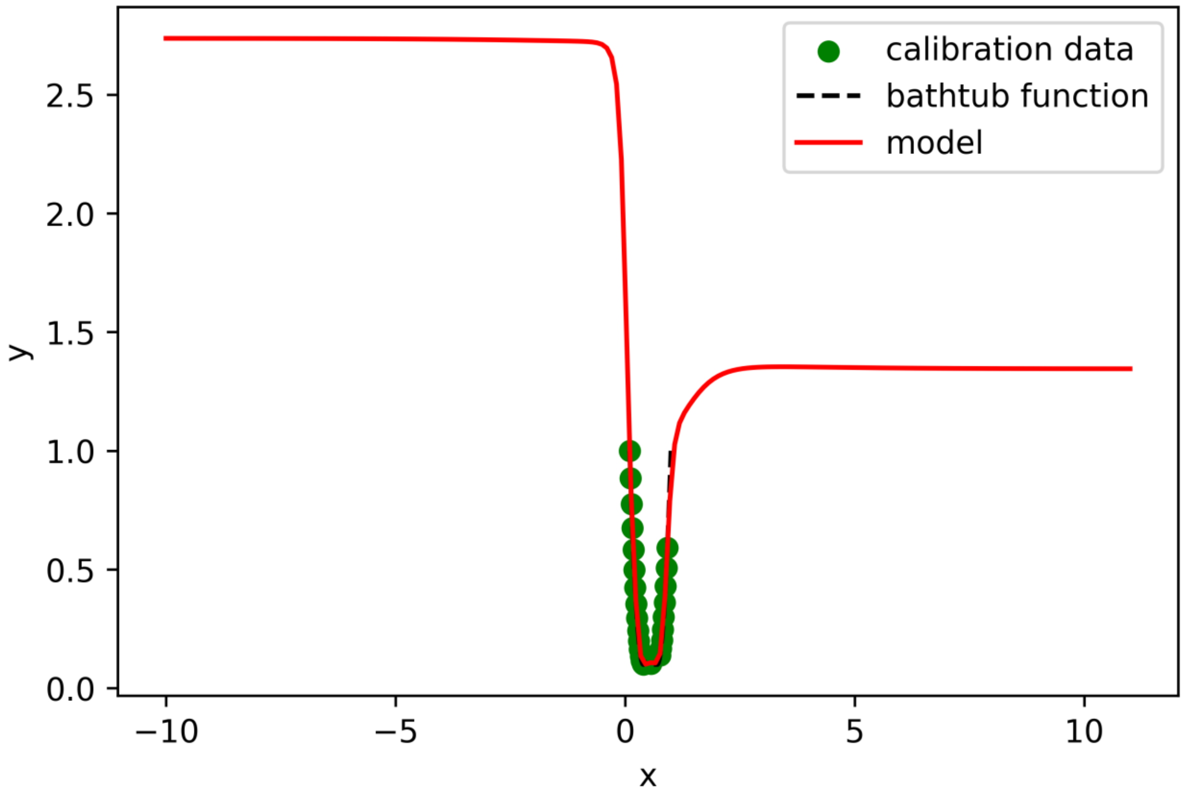
- Infinitely differentiable

HYPERPARAMETER SWEEP

ACTIVATION FUNCTIONS - SIGMOID

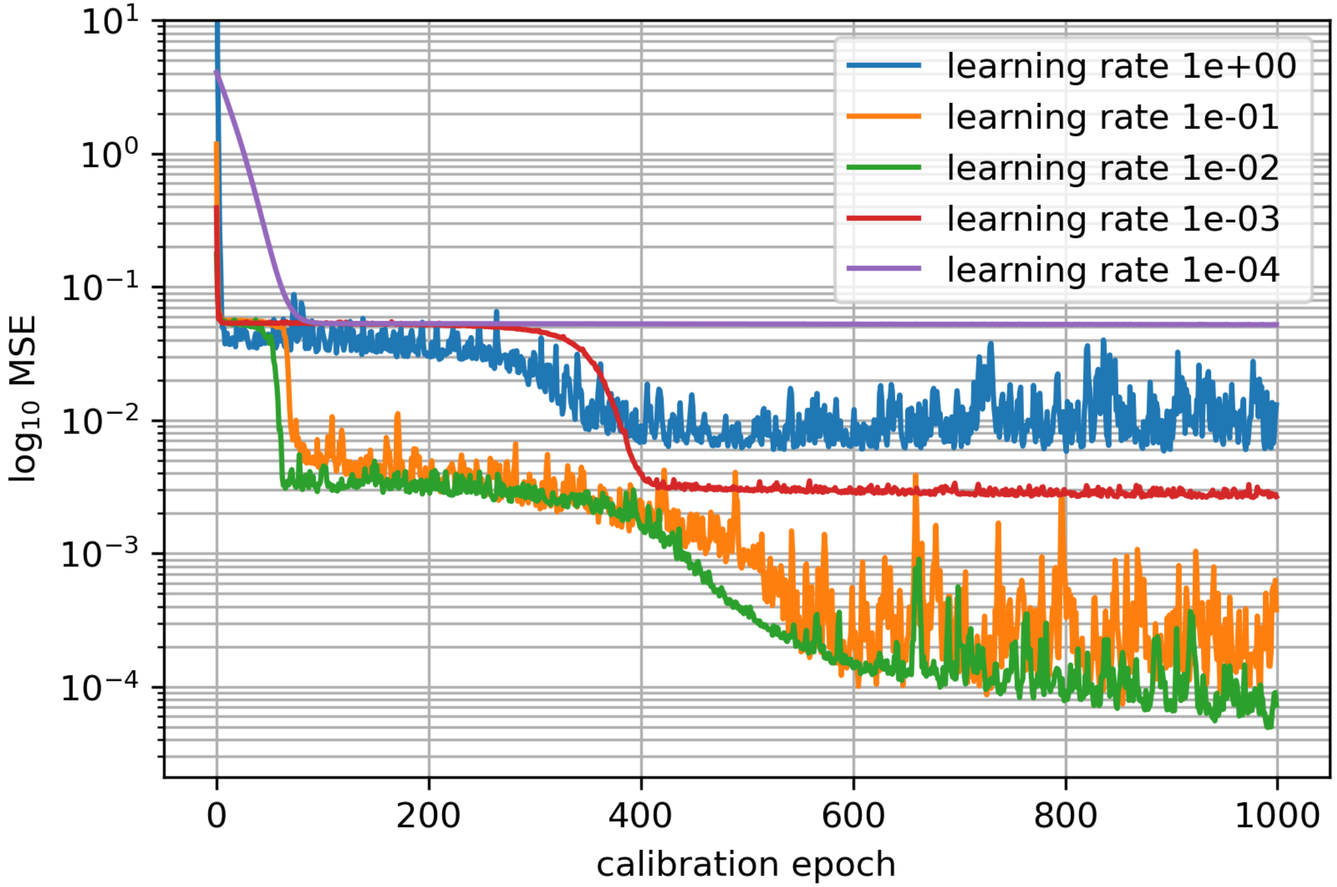


- Infinitely differentiable
- Bounded



HYPERPARAMETER SWEEP

LEARNING RATE



- Problem specific optimal learning rate
- Larger models require smaller learning rates

CONCLUSION

- **Model Complexity:** Complex “enough”
- **Number of epochs:** “Enough” to converge
- **Activation function:** Depends on use case. Differentiability, boundedness, convexity, …

All parameters affect each other.
Experimentation/parameter studies necessary

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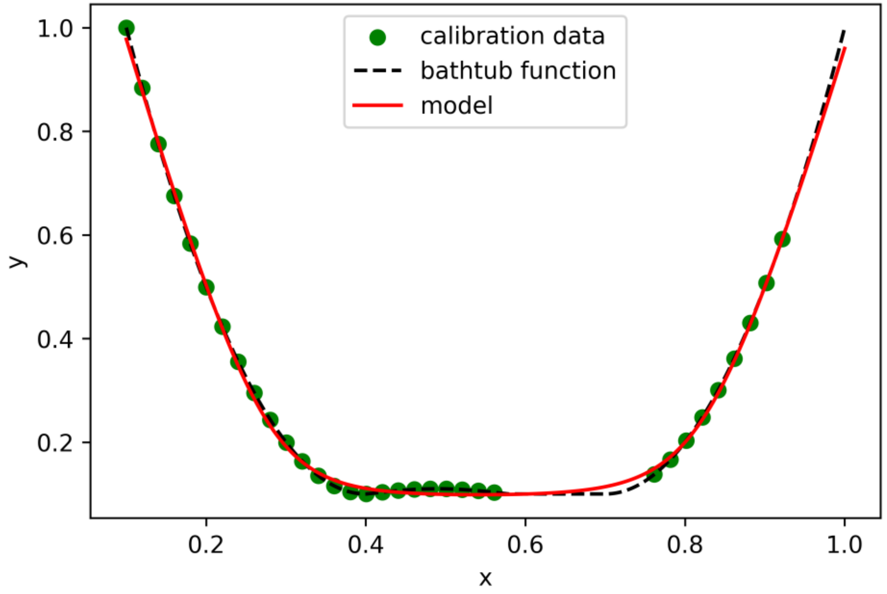
TASK 1 – 1.2

INPUT CONVEX NEURAL NETWORKS

INPUT CONVEX NEURAL NETWORKS

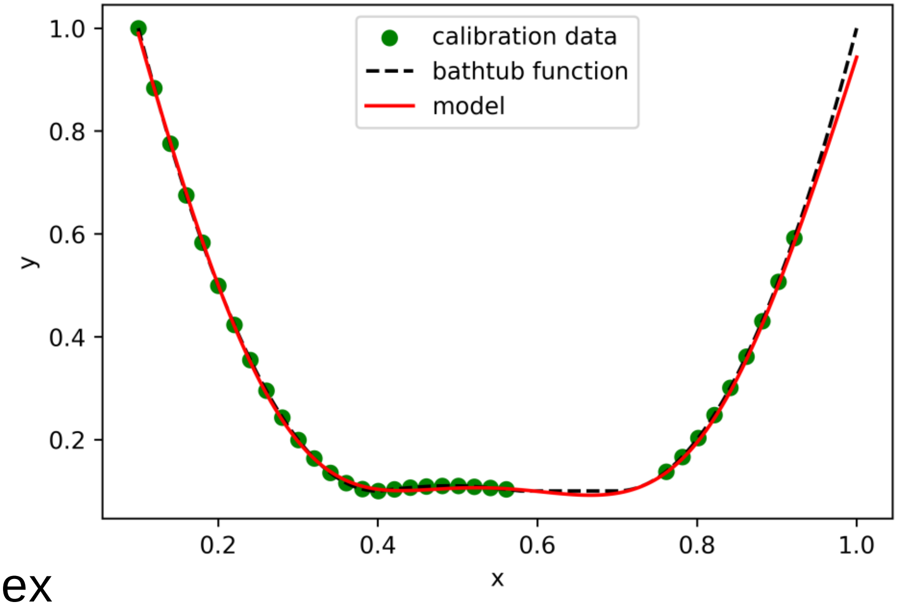
COMPARISON

ICNN



- Convex
- Slower convergence
- Up to 50% zero-weights
- Physically sensible inter- and extrapolation

FFNN

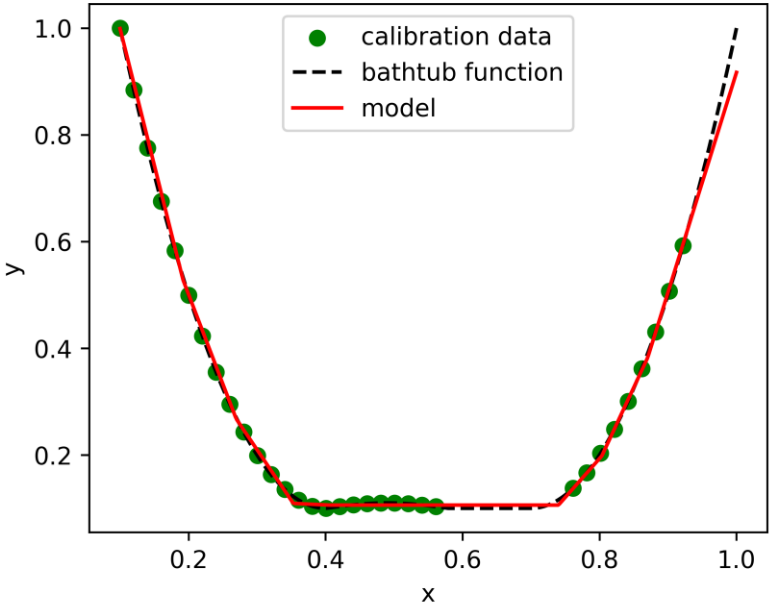


- Not convex
- Faster convergence
- Usually no zero-weights
- Unpredictable inter- and extrapolation behavior

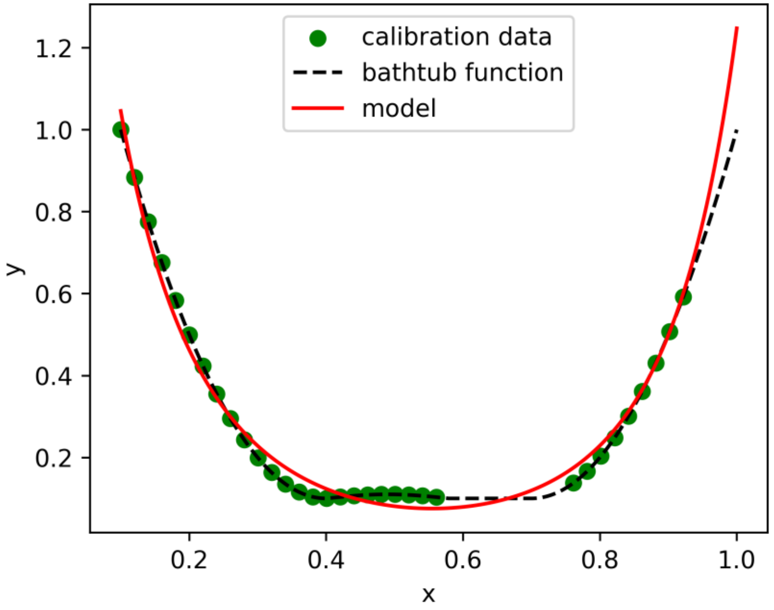
INPUT CONVEX NEURAL NETWORKS

ALTERNATIVE ICNN ACTIVATION FUNCTIONS

All f such that $\frac{d^2 f}{dx^2} > 0, \frac{df}{dx} > 0$. E.g.,



Relu $f(\boldsymbol{x}) = \max(0, \boldsymbol{x})$



Exp $f(\boldsymbol{x}) = e^{\boldsymbol{x}}$

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TASK 1 – 2.2

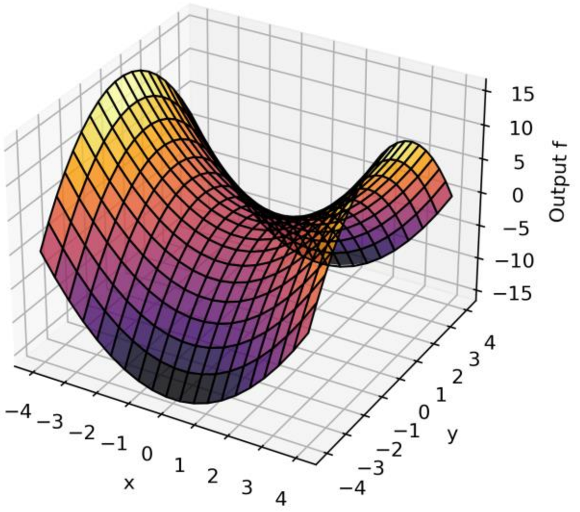
TRAINABLE CUSTOM LAYER

TRAINABLE CUSTOM LAYER

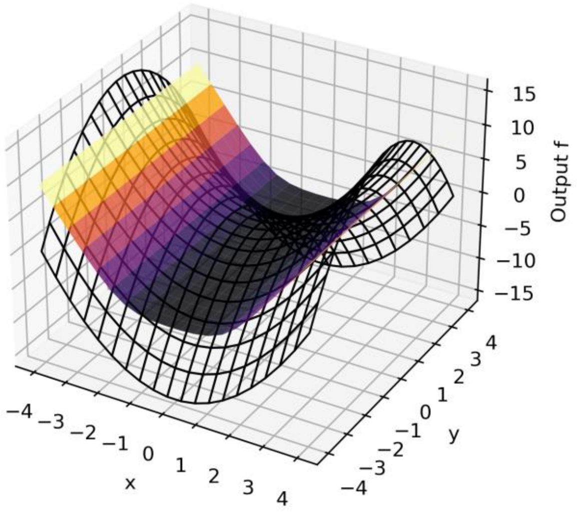
COMPARISON

NON-CONVEX DATA

FFNN

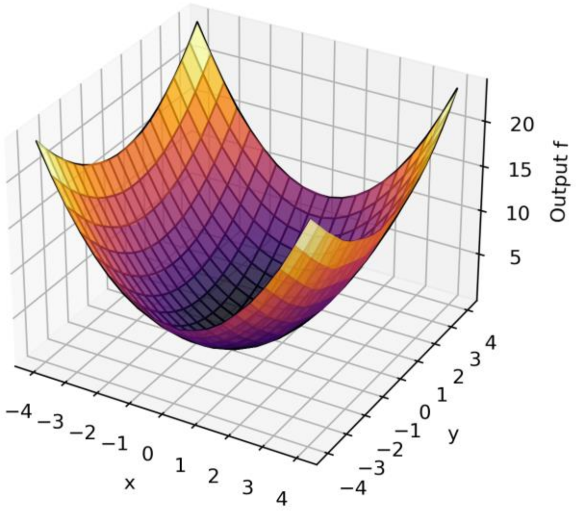


ICNN

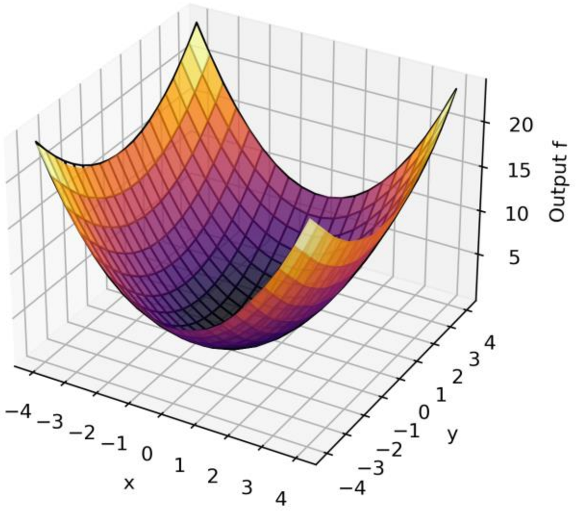


CONVEX DATA

FFNN



ICNN



TASK 1 - 2.3

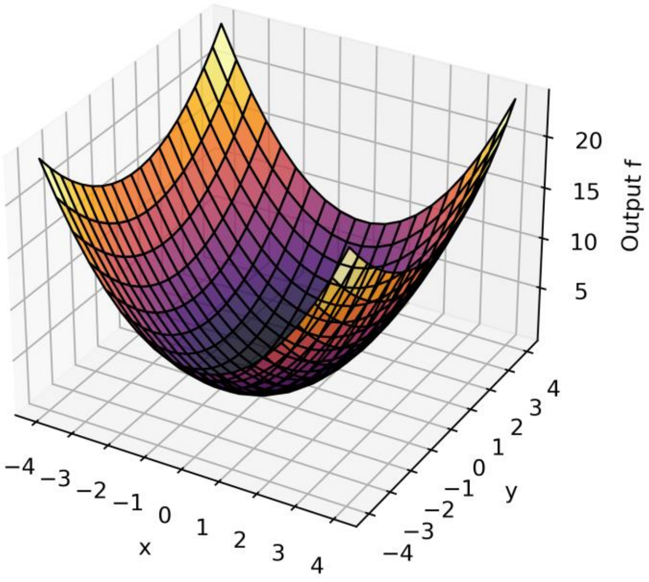
SOBOLEV TRAINING

SOBOLEV TRAINING

PREDICTION

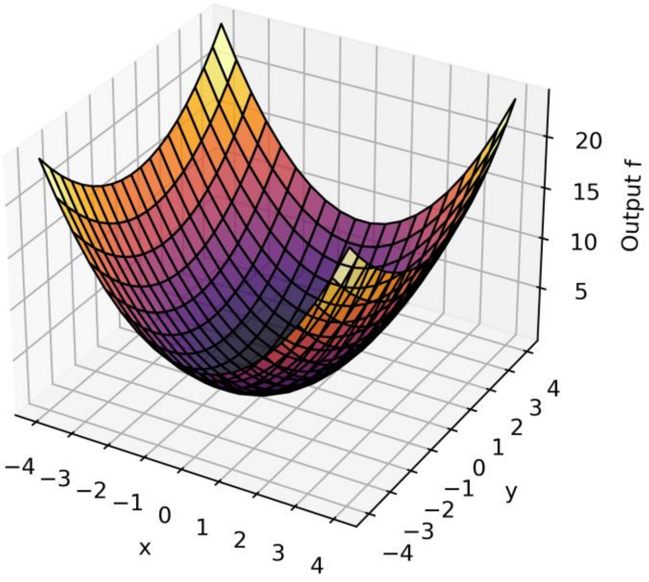
FUNCTION ONLY

Loss 1.343e-02



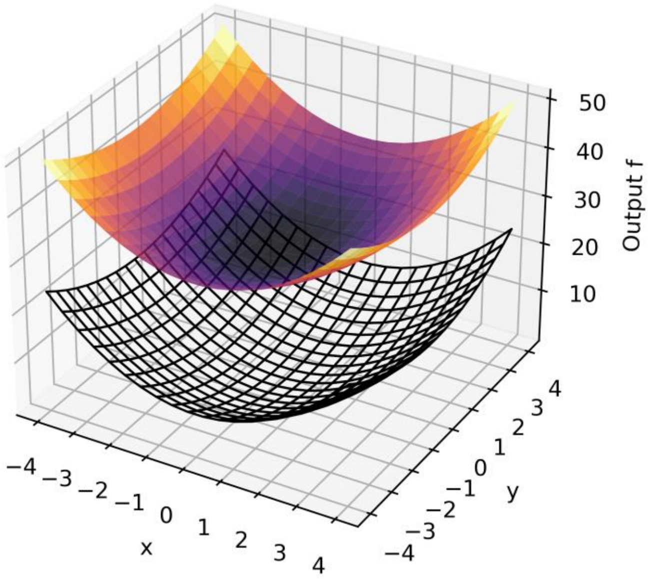
FUNCTION AND GRADIENT

Loss 1.437e-03



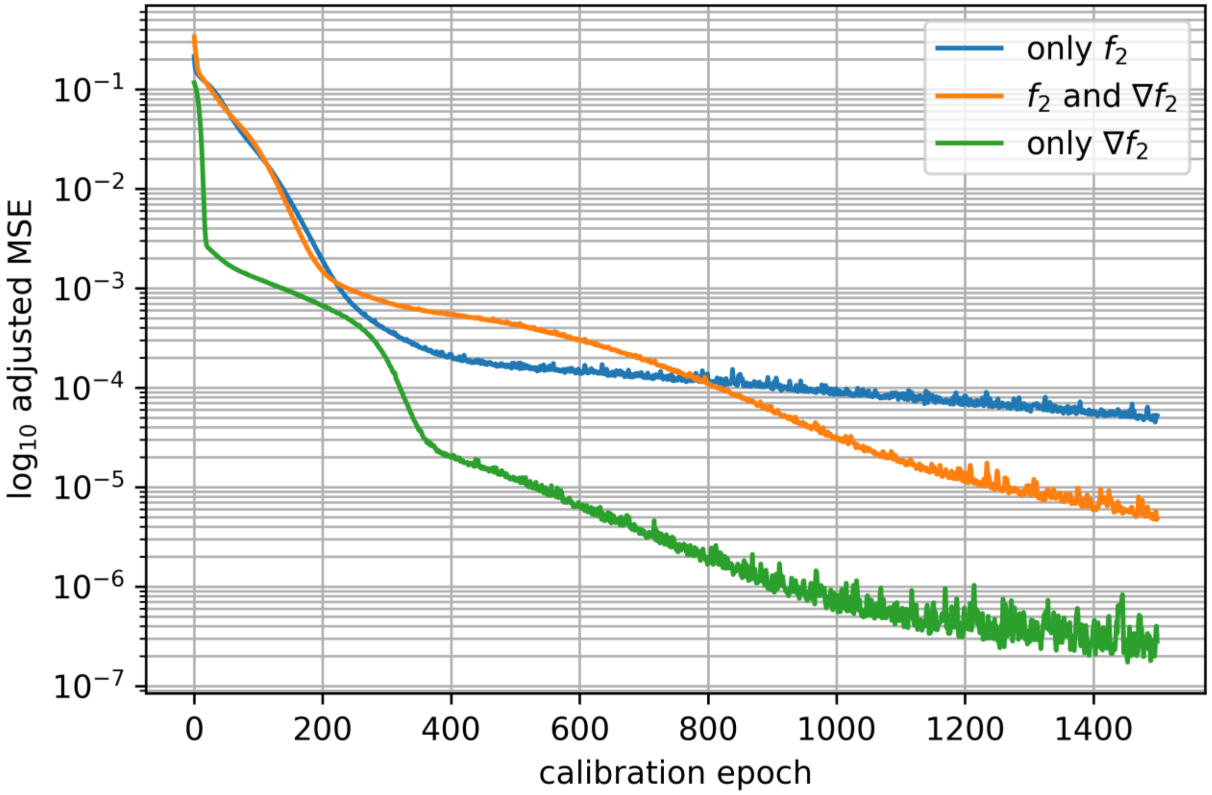
GRADIENT ONLY

Loss 1.045e-04

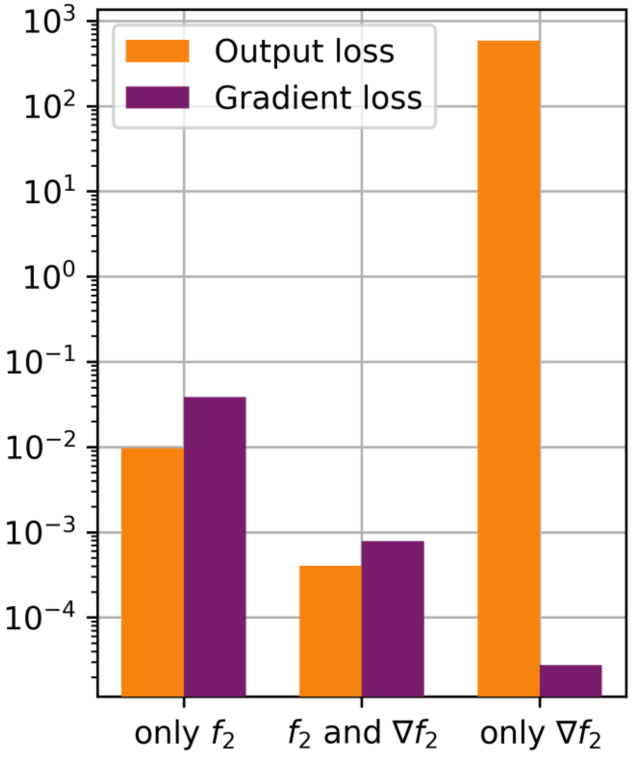


LOSS COMPARISON

TRAINING LOSS



EVALUATION LOSS



DISCUSSION