NOMU: Neural Optimization-based Model Uncertainty

ICML 2022

Jakob Heiss*, Jakob Weissteiner*, Hanna Wutte*, Sven Seuken, Josef Teichmann

July 10, 2022

What is (good) model uncertainty?

Model Uncertainty (Epistemic Uncertainty) vs Data Noise (Aleatoric Uncertainty)

Bayesian Uncertainty Framework:
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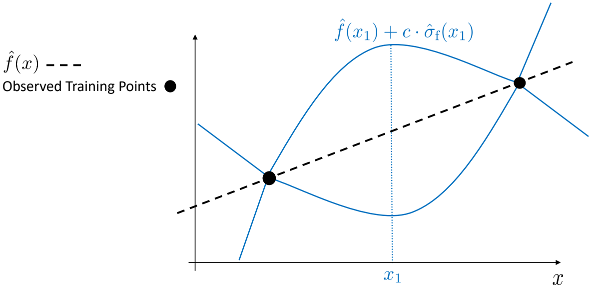

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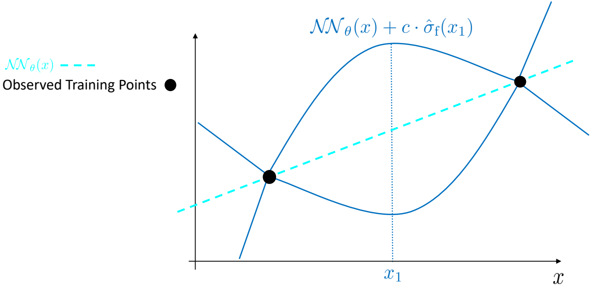

Prior Work. Capturing Model Uncertainty for Neural Networks

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We introduce NOMU to address these limitations.

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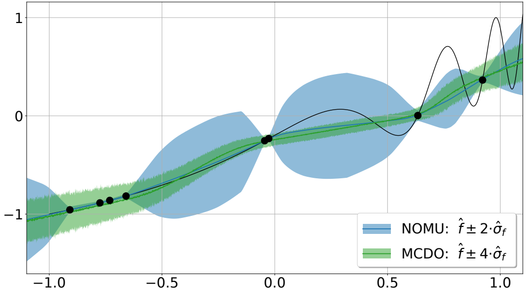
D1. Non-negativity of MU, i.e., $\hat{\sigma}_f \geq 0$.



NOMU and a benchmark MC dropout. Shaded areas are MU bounds. The unknown true function is shown as black solid line, training points as black dots.

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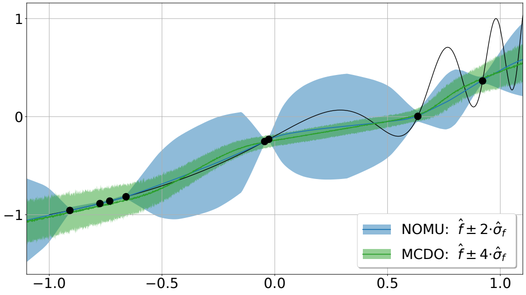

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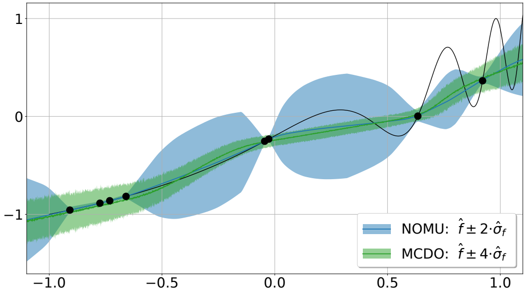

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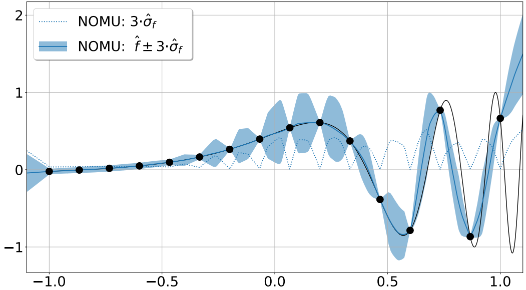

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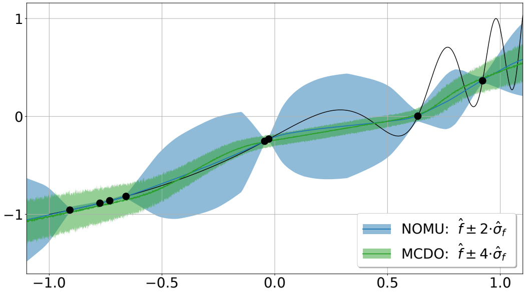
D5. MU vanishes for training data to infinity, i.e., $\lim_{n^{\text{train}} \to \infty} \hat{\sigma}_f \equiv 0$.



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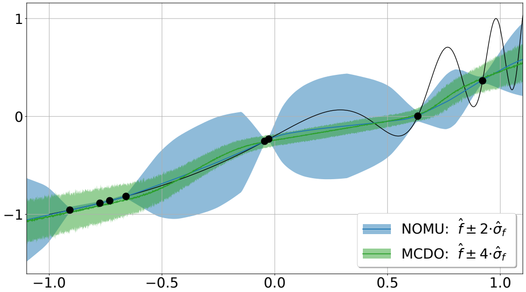

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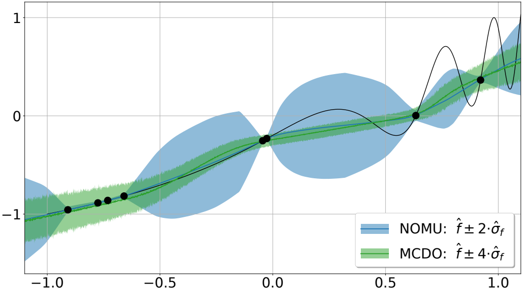

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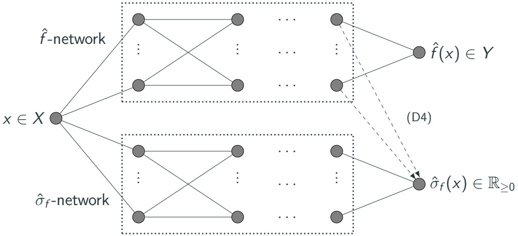
2. Loss function (output dim $q = 1$)

$$\mathcal{NN}_\theta \colon X \to Y \times \mathbb{R}_{\geq 0}$$
$$x \mapsto \mathcal{NN}_\theta(x) := (\hat{f}(x), \hat{\sigma}_f(x))$$



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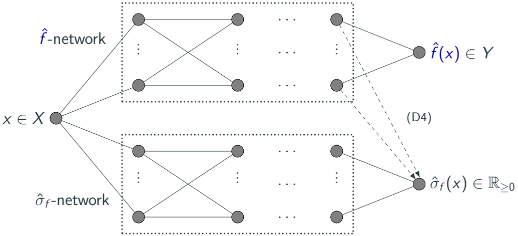

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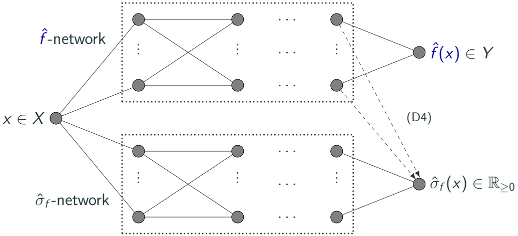

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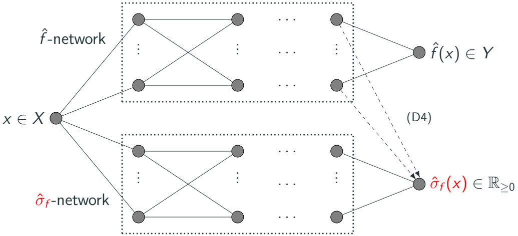

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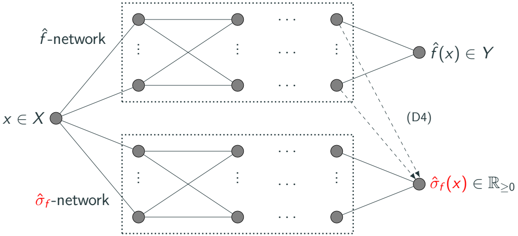

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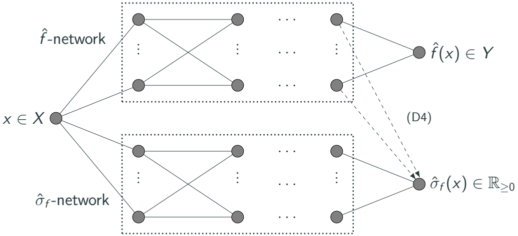

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- NOMU's Uncertainty bounds: $\hat{f}(x) \pm c\hat{\sigma}_f(x)$, for input $x \in X$.
- NOMU's Hyperparameters: $(\mu_{sqr}, \mu_{exp}, c_{exp})$

Experiments

Regression: BNN Test Bed and UCI Data Sets.

BNN Test Bed: Noiseless Regression.

Table 1: Average NLL and a 95% CI over 200 BNN samples. Winners are marked in gray.

Function	NOMU	GP	MCDO	DE	HDE
BNN1D	-1.65±0.10	-1.08±0.22	-0.34±0.23	-0.38±0.36	8.47±1.00
BNN2D	-1.16±0.05	-0.52±0.11	-0.33±0.13	-0.77±0.07	9.11±0.39
BNN5D	-0.37±0.02	-0.33±0.02	-0.05±0.04	-0.13±0.03	8.41±1.00

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UCI Data Sets: Noisy Regression.

Table 2: Average NLL and a 95% normal-CI over 20 runs for UCI data sets. Winners are marked in gray.

Dataset	NOMU	DE	MCDO	MCDO2	LL	NLM-HPO	NLM
Boston	2.68 ±0.11	2.41 ±0.49	2.46 ±0.11	2.40 ±0.07	2.57 ±0.09	2.58 ±0.17	3.63 ±0.39
Concrete	3.05 ±0.06	3.06 ±0.35	3.04 ±0.03	2.97 ±0.03	3.05 ±0.07	3.11 ±0.09	3.12 ±0.09
Energy	0.77 ±0.06	1.38 ±0.43	1.99 ±0.03	1.72 ±0.01	0.82 ±0.05	0.69 ±0.05	0.69 ±0.05
Kin8nm	-1.08 ±0.01	-1.20 ±0.03	-0.95 ±0.01	-0.97 ±0.00	-1.23 ±0.01	-1.12 ±0.01	-1.13 ±0.01
Naval	-5.63 ±0.39	-5.63 ±0.09	-3.80 ±0.01	-3.91 ±0.01	-6.40 ±0.11	-7.36 ±0.15	-7.35 ±0.01
CCPP	2.79 ±0.01	2.79 ±0.07	2.80 ±0.01	2.79 ±0.01	2.83 ±0.01	2.79 ±0.01	2.79 ±0.01
Protein	2.79 ±0.01	2.83 ±0.03	2.89 ±0.00	2.87 ±0.00	2.89 ±0.00	2.78 ±0.01	2.81 ±0.00
Wine	1.08 ±0.04	0.94 ±0.23	0.93 ±0.01	0.92 ±0.01	0.97 ±0.03	0.96 ±0.01	1.48 ±0.09
Yacht	1.38 ±0.28	1.18 ±0.41	1.55 ±0.05	1.38 ±0.01	1.01 ±0.09	1.17 ±0.13	1.13 ±0.09

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. . . repeat for a number of seeds.

Table 3: BO results: average final regrets per dimension and ranks for each individual function (1=best to 7=worst).

Function	NOMU	GP	MCDO	DE	HDE	pGP	RAND
Levy5D	1	1	6	3	3	4	7
Rosenbrock5D	1	1	1	1	2	5	7
G-Function5D	2	3	1	4	2	3	7
Perm5D	3	1	1	5	7	2	4
BNN5D	1	1	4	1	4	1	7
Average Regret 5D	2.87×10^{-2}	5.03×10^{-2}	4.70×10^{-2}	5.18×10^{-2}	7.13×10^{-2}	4.14×10^{-2}	1.93×10^{-1}
Levy10D	1	3	5	6	1	1	6
Rosenbrock10D	1	1	2	6	3	2	7
G-Function10D	2	5	1	3	2	5	7
Perm10D	2	1	2	6	2	2	1
BNN10D	1	2	1	1	3	1	7
Average Regret 10D	8.40×10^{-2}	1.17×10^{-1}	6.96×10^{-2}	1.15×10^{-1}	9.32×10^{-2}	9.46×10^{-2}	2.35×10^{-1}
Levy20D	1	1	5	7	1	1	6
Rosenbrock20D	2	2	2	6	1	4	6
G-Function20D	1	4	5	1	1	3	7
Perm20D	3	5	3	2	3	3	1
BNN20D	1	2	2	2	6	1	7
Average Regret 20D	1.12×10^{-1}	1.33×10^{-1}	1.39×10^{-1}	1.71×10^{-1}	1.37×10^{-1}	1.17×10^{-1}	2.80×10^{-1}

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Thank you for your time :)

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D4 "Metric Learning" Step Function

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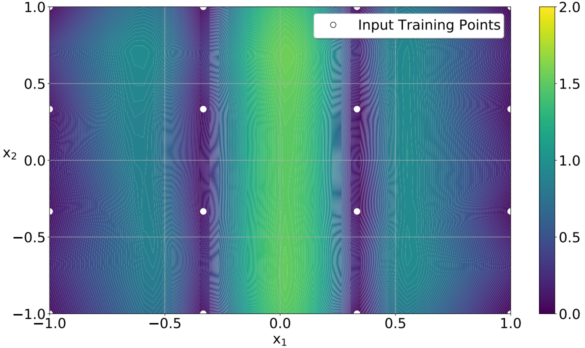
- Step function:

$$f = \mathbb{R}^2 \to \mathbb{R} : (x_1, x_2) \mapsto \begin{cases} -1 & \text{if } x_1 < 0 \\ 1 & \text{if } x_1 \geq 0. \end{cases}$$

- Important feature is x_1.
- Output is independent of x_2.

NOMU's model uncertainty.



Bayesian Optimization Motivation