Table S1. Comparison of improved UniSO-N with MLP and with in-context Transformer neural processes (TNP; Nguyen & Grover, 2022) on unconstrained tasks from Design-Bench and SOO-Bench, where the best and runner-up results on each task are **Blue** and **Violet**. $\mathcal{D}$(best) denotes the best score in the offline dataset. Here, UniSO-N + TNP-UCB maximizes the UCB acquisition function for one epoch on trained TNP to obtain final candidates, following Nguyen et al. (2024), and UniSO-N + TNP-ED directly regresses the score values and maximizes the model output, following Section 3.2.2 in Nguyen et al. (2023).

Task	$\mathcal{D}$(best)	UniSO-N + MLP	UniSO-N + TNP-UCB	UniSO-N + TNP-ED
Ant	165.326	**269.691 ± 77.425**	110.143 ± 229.571	**292.098 ± 229.171**
D'Kitty	**199.363**	**173.911 ± 46.662**	-226.316 ± 317.276	129.005 ± 41.107
Superconductor	**74.000**	**67.333 ± 10.838**	58.653 ± 20.171	64.544 ± 2.888
TF Bind 8	0.439	**0.833 ± 0.005**	0.638 ± 0.000	**0.713 ± 0.000**
TF Bind 10	0.005	**0.959 ± 0.115**	**0.674 ± 0.000**	0.397 ± 0.000
GTOPX 2	-195.586	**-124.995 ± 56.170**	-183.413 ± 81.862	**-181.144 ± 11.685**
GTOPX 3	-151.190	**-62.622 ± 22.261**	-180.053 ± 93.678	**-99.735 ± 2.637**
GTOPX 4	-215.716	**-110.284 ± 17.559**	**-130.988 ± 38.336**	-178.791 ± 79.623
GTOPX 6	-112.599	**-57.435 ± 18.832**	**-108.859 ± 25.493**	-195.184 ± 40.626
Avg. Rank	N/A	**1.111 ± 0.314**	2.667 ± 0.471	**2.222 ± 0.629**

Table S2. Few-shot experimental results of improved UniSO-N with MLP and with in-context TNP (Nguyen & Grover, 2022) on RobotPush, Rover, and LunarLander, where the best and runner-up results on each task are **Blue** and **Violet**. $\mathcal{D}$(best) denotes the best score in the offline dataset. Here, UniSO-N + TNP-UCB maximizes the UCB acquisition function for one epoch on trained TNP to obtain final candidates, following Nguyen et al. (2024), and UniSO-N + TNP-ED directly regresses the score values and maximizes the model output, following Section 3.2.2 in Nguyen et al. (2023). UniSO-N + MLP utilizes few-shot data to fine-tune MLP regressor, while UniSO-N + TNP-UCB and UniSO-N + TNP-ED directly view the few-shot data as context points.

Task	$\mathcal{D}$(best)	UniSO-N + MLP	UniSO-N + TNP-UCB	UniSO-N + TNP-ED
RobotPush	0.102	**7.014 ± 0.000**	**3.769 ± 1.969**	0.877 ± 1.041
Rover	-16.148	**-8.488 ± 0.003**	-12.593 ± 1.891	**-12.038 ± 1.142**
LunarLander	**7.038**	**287.038 ± 0.000**	-113.493 ± 129.223	-79.885 ± 91.442
Avg. Rank	N/A	**1.000 ± 0.000**	2.667 ± 0.471	**2.333 ± 0.471**