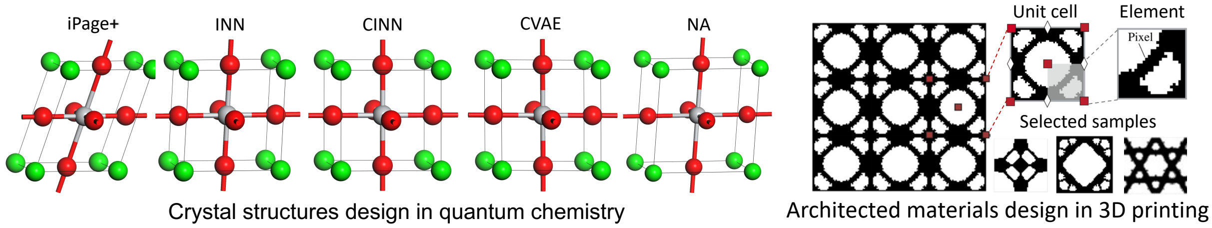

Figure 6: Two real-world design applications: (Left) Crystal structure design problem in quantum chemistry and (Right) Architected materials design problem in additive manufacturing.

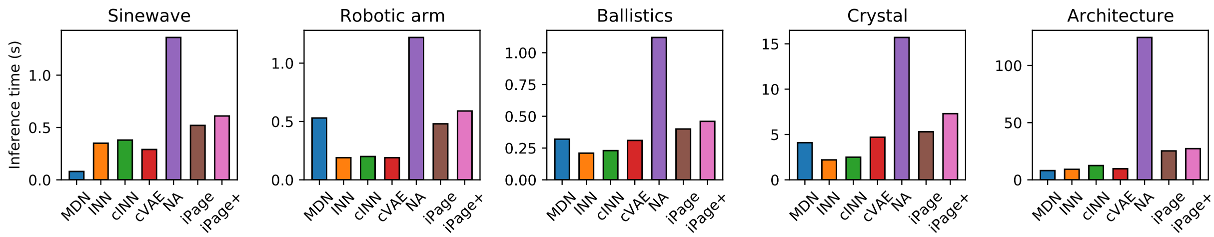

Figure 7: Total time cost (inference and localization) for 1000 solutions. The time-to-solution using iPage with other baselines on three benchmarks are compared side-by-side.

Table 3: Performance comparison of tested methods on five tasks for 1000 solutions conditioned on a specific observation $\mathbf{y}^*$. We repeat 50 times to obtain the standard deviation for each case.

Method	Sinewave	Robotic Arm	Ballistics	Crystal Design	Architecture Design
Mixture density networks (MDN)	0.22 ± 5.1e-4	0.023 ± 2.3e-5	0.041 ± 2.9e-5	0.84 ± 3.3e-2	1.81 ± 2.0e-1
Invertible neural network (INN)	0.19 ± 9.3e-5	0.015 ± 4.7e-5	0.024 ± 1.9e-5	0.57 ± 4.7e-2	0.83 ± 9.1e-2
conditional INN (cINN)	0.16 ± 5.0e-4	0.032 ± 3.1e-5	0.652 ± 4.3e-5	0.42 ± 8.8e-2	0.82 ± 8.5e-2
conditional VAE (cVAE)	0.25 ± 7.0e-4	0.021 ± 5.6e-5	0.912 ± 3.2e-5	0.70 ± 9.0e-2	1.20 ± 1.7e-1
Neural-Adjoint (NA)	0.011 ± 9.1e-6	0.012 ± 4.8e-5	0.031 ± 4.7e-5	0.15 ± 6.6e-3	0.79 ± 9.3e-2
iPage (with maximin LHS)	**0.004 ± 2.1e-6**	**0.008 ± 7.6e-6**	**0.023 ± 8.9e-6**	**0.14 ± 2.2e-3**	**0.22 ± 1.2e-2**

method has advantages in learning accuracy but shows an obvious drawback of large computational costs compared to the other models. Fig. 7 shows the total time cost including the inference and localization process on five tasks using one NVIDIA V100 GPU. Due to the invertible architecture, INN and cINN are efficient at sampling the posterior distributions. The time cost of iPage is slightly higher than INN, cINN and cVAE but still significantly lower than NA even though gradient descent is employed (few steps in local search).

Conclusion

In this work, we develop an efficient inverse learning approach that utilizes posterior samples to accelerate the localization of all inverse solutions via gradient descent. To fully explore the parameter space, variance-reduced sampling strategies are imposed on the latent space to improve space-filling capability. Multiple experiments demonstrate that our approach outperforms the baselines and significantly improves the accuracy, efficiency, and robustness for solving inverse problems, specifically in complex natural science and engineering design applications. One current limitation is the efficiency of space-filling sampling in high-dimensional spaces. Future work will aim to improve sampling efficiency by leveraging scalable numerical algorithms. Also, we plan to apply the iPage method to broader topics in safe and robust AI, e.g., safe decision-making with Bayesian optimal experimental design (**?**), and privacy defense in federated learning (**?**).

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