

RESEARCH STATEMENT

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1 Overview

Machine learning models serve as a data-driven mechanism for reasoning about real-world problems. Recent advances in deep learning have proven that models can achieve remarkable performance when employing deep neural networks and large amounts of data and computation. Nevertheless, overparameterized deep models can produce overconfident predictions. Moreover, there are many problems where we only have small amount of data or little annotation, in which cases the models can fail to generalize to long-tail cases or unseen tasks.

My research goal is to advance *deep probabilistic programming* as a means of developing interpretable models that uncover structure of problems, reason about uncertainty, and robustly generalize across tasks. This development combines strengths of *deep learning* and *probabilistic programming*. Deep probabilistic programs employ neural networks to parameterize models, thus the models inherit the scalability of deep architectures and benefit from optimization strategies by stochastic gradient descent. Probabilistic programming, on the other hand, allows us to design deep generative models that incorporate necessary domain knowledge as inductive bias if need be. Inductive bias regularizes the models in form of structured priors, which helps to characterize uncertainty and improve generalization, particularly in problems where limited data and little supervision is available. Next I will illustrate my research contributions and propose work in future.

2 Prior Work

2.1 Amortized Inference with Probabilistic Programs

One main challenge in machine learning research is compositionally reasoning about the world as human cognition. My research work tackles this problem by designing deep generative models with more complex and structured priors. As we start to build up these models, we increasingly see limitations of standard inference methods when scaling them up to high-dimensional, correlated (and discrete) latent variables.

A recent insight is that any importance sampling method can be used to define a variational objective. This has inspired me to propose the amortized population Gibbs (APG) samplers [1], which frame variational inference as adaptive importance sampling with amortized proposals. This approach exploits structure priors as inductive bias, which allows us to generate high-quality proposals by decomposing a single high-dimensional inference problem into a sequence of lower-dimensional inference problems. This class of methods have a broad range of applications including models with discrete variables. In my collaboration with Zimmermann et al. we generalized this idea and proposed nested variational inference [2], a class of amortized inference methods that construct proposals with nested importance sampling.

My research efforts further motivate the *inference combinators* [3], where Stites and Zimmermann develop a simple grammar to define importance samplers that can be trained using variational methods. With these *inference combinators*, users can concisely tailor sampling strategies to suite particular probabilistic programs, with the guarantee that the resulting sampler always preserves proper weighting with respect to the desired target density. This work sets in motion a precedent for languages of inference, simplifying the development of inference programming, and making inference methods accessible to the broader research community.

2.2 Learning Structured Representation of Complex Domains

One importance use case of deep generative models is to encode meaningful factors of variation of data in form of latent representations. In the absence of supervision, the models do not naturally learn representations that are associated with interpretable data structure. This has motivated the work that I collaborated with Esmaeili et al., where we designed a variational objective to induce disentangled representations, so that individual dimensions of latent variables represent interpretable factors of variation of data [4].

However, further challenges arise when we move towards problems that have data with complex heterogeneity. Without supervision, uncovering inherent structure of data requires incorporating inductive bias in form of structured priors of models. This inspiration led to my design of APG samplers [1], which tackles such problems where the data consists of a corpus of related tasks, within each there is an individual group of observations. By incorporating structured priors, this approach learns representations for not only individual features at observation level, but also aggregated factors of variation at corpus level and group level.

For the purpose of unsupervised representation learning, generative models may not achieve meaningful abstractions of data. Since the generators learn to reconstruct data examples given latent variables, those variables must encode factors of variation that give rise to large discrepancies in data space, regardless of whether these factors are semantically meaningful. To provide an alternative to learning a generative process, Esmaeili and I jointly developed the conjugate energy-based models [5]. The core idea is to characterize consistency between data and latent variables at compressed representation space, without requiring learning a generator that reconstructs input data. Our models encode image data into more abstract representations that can be used for various downstream tasks such as few-label classification and out-of-domain detection.

3 Proposed Work

3.1 Learning for More Generalization with Less Data

The cutting-edge of machine learning research is to make further strides towards more complex domains, where data is limited and imbalanced-distributed. These constraints pose challenges for models to learn to generalize across tasks and adapt to unseen domains. I believe that deep probabilistic programming is a way to aid robustness and generalization. Structured probabilistic models have presented potential to meta-learn the distribution over unsupervised domains, as incorporating inductive bias can regularize the models and characterize uncertainty, while retain enough flexibility. For this reason I propose to develop new models to tackle unsupervised *few-shot learning* tasks of complex data modalities. To train these models, I will continue to work on inference methods that provide flexible sampling strategies for generating good proposals. In addition, I hope to make efforts in increasing the impact of these inference methods. To do so I will actively collaborate with the researchers in probabilistic programming, where I can contribute to the development of probabilistic programming systems for user-programmable inference methods.

3.2 Contrastive Learning for Structured Representations

Despite of recent success in deep generative modeling, why are we still far from performing compositional reasoning about more complex domains? Because real-world data modalities may exhibit a large number of underlying generative factors that give rise to a combinatorial explosion of possible inputs. This poses challenges when learning abstract representations based on generative processes. Recently we see impressive advances in discriminative approaches, such as *contrastive learning*, that learn representations by the consistency between data and latent variables. This can resolve the issues caused by learning to reconstruct data inputs. Thus I propose to develop hybrid models that combine structured priors with contrastive learning methods. A further step for my research career is to eventually adopt these approaches to more practical domains such as healthcare, autonomous vehicles and biochemistry.

References

- [1] Hao Wu, Heiko Zimmermann, Eli Sennesh, Tuan Anh Le, and Jan-Willem Van De Meent. “Amortized Population Gibbs Samplers with Neural Sufficient Statistics”. In: *International Conference on Machine Learning*. PMLR. 2020, pp. 10421–10431.
- [2] Heiko Zimmermann, Hao Wu, Babak Esmaeili, and Jan-Willem van de Meent. “Nested Variational Inference”. In: *Conference on Neural Information Processing Systems*. 2021.
- [3] Sam Stites, Heiko Zimmermann, Hao Wu, Eli Sennesh, and Jan-Willem van de Meent. “Learning Proposals for Probabilistic Programs with Inference Combinators”. In: *Uncertainty in Artificial Intelligence*. 2021.

- [4] Babak Esmaeili, Hao Wu, Sarthak Jain, Alican Bozkurt, Narayanaswamy Siddharth, Brooks Paige, Dana H Brooks, Jennifer Dy, and Jan-Willem Meent. “Structured disentangled representations”. In: *International Conference on Artificial Intelligence and Statistics*. PMLR. 2019, pp. 2525–2534.
- [5] Hao Wu, Babak Esmaeili, Michael Wick, Jean-Baptiste Tristan, and Jan-Willem van de Meent. “Conjugate Energy-Based Models”. In: *International Conference on Machine Learning*. PMLR. 2021.