Programming Languages for Deep Probabilistic Programming

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ABSTRACT

Probabilistic programming is an approach to adopt probabilistic models and inference as first-class citizens of a programming language. Its main goal is lowering the entry barrier into the field of probabilistic modeling and allow easier and faster prototyping in research.

In recent years, a new class of these languages has risen: Deep probabilistic programming languages. Their focus is on unifying probabilistic programming languages with the modeling power, efficiency, and composability of deep neural networks in the field of machine learning. We focus on Edward, a Turing-complete deep probabilistic programming language, and compare it to prior, as well as future work. Edward makes probabilistic programming as flexible and computationally efficient as deep learning and allows for rich compositions of probabilistic models and inference procedures.

KEYWORDS

machine learning, programming language, systems, probabilistic programming

1 INTRODUCTION

Probabilistic modeling is the task of describing the state of the world by using the mathematics of probability theory. With this, we can express all forms of uncertainty and noise associated with the model. We can make use of the inverse probability, or Bayes' rule, to answer questions about specific states in our world, given that we observe either everything else or only partial states from the rest of the world — this is called *probabilistic inference*. Using probabilistic modeling we can e.g. model the relationships between the time of the day, the day of the week, the traffic status between two cities and the weather conditions. This means we can now answer queries like *"What is the probability that there is a traffic jam on a Monday between 8 and 9 o'clock when it's rainy on my road to work?"* or *"At what time on Thursdays is the traffic the lowest?"*. We can either infer the probability of some state or use these probabilities to find the most likely state, given some observations of the world (called most probable explanation inference or *MPE*). Often, computing these probabilities exactly in probabilistic models is intractable (though there is a whole subclass of probabilistic models that focuses on tractable inference, such as Sum-Product Networks (Poon and Domingos, 2012) or Cutset Networks (Rahman et al., 2014)). Therefore, methods of approximate inference such as Markov Chain Monte Carlo, Variation Bayesian methods or expectation propagation have been developed, achieving a trade-off between computation time and accuracy.

Probabilistic programming concerns the syntax and semantics for programming languages, describing inference problems and constructing solvers that computationally characterize denoted probability distributions (van de Meent et al., 2018). Probabilistic programming is at the intersection and draws the attention of the machine learning, statistics and programming languages community. The last two decades have shown that the need for probabilistic programming languages (PPL) has increased and is long not satisfied as the following (incomplete) list of PPLs in chronological order shows: BUGS (Spiegelhalter et al., 1996), BNT (Murphy, 2001), IBAL (Pfeffer, 2001), JAGS (Plummer, 2003), BLOG (Milch et al., 2005), Figaro (Pfeffer, 2009), Church (Goodman et al., 2012), Augur (Tristan et al., 2013), LibBi (Murray, 2013), Venture (Mansinghka et al., 2014), Probabilistic-C (Paige and Wood, 2014), webPPL (Goodman and Stuhlmüller, 2014), PyMC (Salvatier et al., 2015), Anglican (Tolpin et al., 2015), BayesDB (Mansinghka et al., 2015), Hakaru (Narayanan et al., 2016), PSI (Gehr et al., 2016), CPProb (Casado et al., 2017), Stan (Carpenter et al., 2017), Birch (Murray and Schön, 2018), Touring.jl (Ge et al., 2018).

In recent years, the emerging field of deep learning has shown the importance of well established programming frameworks that back the foundations of the field. The nature of deep neural networks is compositional, that is, we can connect layers in creative ways and do neither need to worry about the actual forward propagation, nor about the backward propagation details based on gradient-based optimizations. Frameworks such as PyTorch (Paszke et al., 2019), TensorFlow (Abadi et al., 2015), CNTK (Seide and Agarwal, 2016) and MXNET (Chen et al., 2015) have accelerated the development of new successful deep learning architectures. With the rise of deep learning, new probabilistic modeling approaches, using deep neural networks as their building blocks, such as Variational Auto-Encoder (VAE) (Diederik et al., 2014), Normalizing Flows (Rezende and Mohamed, 2015) or Bayesian Recurrent Neural Networks (Fortunato et al., 2017) have surfaced. Since then, the next wave of PPLs has materialized: Deep probabilistic programming languages. These are built on top of already well established deep learning frameworks that are developed around a single key concept: computational graphs. Deep probabilistic programming languages use and extend this concept by introducing stochastic nodes representing probability distributions defined conditionally on their parent nodes. Tran et al. (2017) have leveraged these concepts in their novel deep probabilistic programming framework called Edward. Its main goal is to achieve the same composability and computational efficiency of deep learning for probabilistic modeling and probabilistic inference.

This paper is structured as follows: Section 2 mentions related work and the main trade-offs in deep probabilistic programming languages. Section 3 covers the contributions of Edward while Section 4 gives a critical view on its paper. Finally, Section 5 gives a short conclusion and outlook in the field of deep PPLs.

2 RELATED WORK

Probabilistic programming languages typically face the division into two groups, stemming from the trade-off between efficiency and expressiveness. PPLs such as BUGS (Spiegelhalter et al., 1996), BNT (Murphy, 2001), JAGS (Plummer, 2003), PyMC (Salvatier et al.,

2015) or Stan (Carpenter et al., 2017) are restricted to a niche class of probabilistic models and focus on optimizing the inference procedures for this specific subclass, gaining computational efficiency. Others like IBALAP (Pfeffer, 2001), Figaro (Pfeffer, 2009), BLOG (Milch et al., 2005) or Church (Goodman et al., 2012) are able to represent rich classes of graphical models, emphasizing expressiveness but suffer from more general inference procedure implementations and therefore do not scale well with increasing model or data size. Edward makes an effort to be the first PPL to bridge this gap: it is Turing-complete, supporting any computable probability distribution while implementing efficient inference algorithms, leveraging model structure and the computational graph.

Since then, deep probabilistic programming has also attracted large companies that support its development such as Pyro (Bingham et al., 2019) from Uber based on PyTorch and TensorFlow Probability (Dillon et al., 2017) from Google based on TensorFlow.

3 EDWARD: DEEP PROBABILISTIC PROGRAMMING

Edward is a deep probabilistic programming language. Probabilistic programming lets users specify probabilistic models as programs and compile those models down into inference procedures. At its core are two compositional representations as first-class citizens: random variables and inference. Edward allows fitting the same model using a variety of composable inference methods such as point estimation, variational inference, and Markov Chain Monte Carlo. Its key concept is to make no distinction between a model or an inference block, that is, models are simply a composition or collection of random variables while inference is the way of modifying parameters in this collection, subject to another.

To stay computationally efficient, Edward is based on TensorFlow and uses its computational graph. Therefore, it uses all benefits from TensorFlow like distributed model training, model parallelism, parameter vectorization and easy GPU support.

3.1 Compositional Representations for Models

One of Edward's focus is on the compositionality of probabilistic models. Therefore, Tran et al. have posed two main criteria on the compositional representation for probabilistic models. Firstly, Edward requires tight integration with computational graphs such that nodes can represent operations on the data while edges can represent data that is being communicated between the nodes. The second necessity is the invariance of model representations under the computational graph such that the graph can be reused during inference time. With these design principles, it becomes easy to develop probabilistic programs in a computational graph framework. It allows the composition of random variables to build arbitrary complex structures while still representing all operations in the computational graph itself.

To illustrate the power of Edward's compositionality, we demonstrate a simple Beta-Bernoulli model in Figure 1 which is described by the following joint probability distribution:

$$p\left(\mathbf{x}, \theta\right) = \text{Beta}\left(\theta \mid 1, 1\right) \prod_{n=1}^{50} \text{Bernoulli}\left(\mathbf{x} \mid \theta\right) \quad ,$$

Figure 1: The computational graph for a Beta-Bernoulli program. $\mathbf{x}^*$ is sampled from a Bernoulli distribution with $p = \theta^*$ and θ^* is sampled from a Beta distribution with parameters $a = 1, b = 1$.

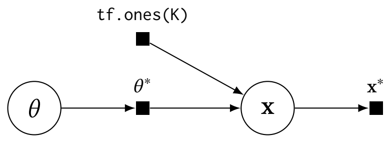
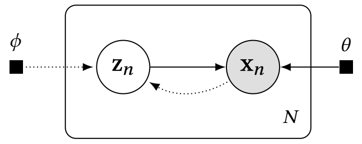


Figure 2: A Variational Auto-Encoder implementation constructed in Edward, with dotted lines for the inference model.



where $\mathbf{x} \in \mathbb{R}^{50}$ are 50 datapoints which all share the same latent variable θ, sampled from a beta distribution. The equivalent code in Edward is as simple as the following two lines:

```python
theta = Beta(a=1, b=1)
x = Bernoulli(p=tf.ones(50) * theta)
```

Evaluating the above snippet will evaluate the computational graph in Figure 1 at its root node: the sampling operation $\mathbf{x}^*$ from the specified Bernoulli distribution. For this operation to be evaluated, its parent must first be retrieved, that is, creating a 50-dimensional vector of ones using `tf.ones(50)` and performing the sampling operation on the beta distribution node to obtain a single θ value. Both of these operations have no dependencies and can thus be immediately computed. Finally, the sampling of $\mathbf{x}$ can be performed with θ and `tf.ones(50)` as input to obtain 50 Beta-Bernoulli distributed samples.

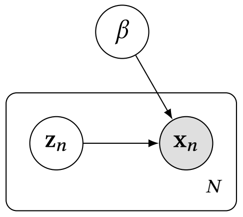
As an additional example, we want to highlight an implementation of Variational Auto-Encoder in Edward, visualized in Figure 2. The model is composed of a probabilistic model over the data distribution and a variational model to approximate the former's posterior.

```python
# Probabilistic model
z = Normal(mu=tf.zeros([N, d]), sigma=tf.ones([N, d]))
h = Dense(256, activation='relu')(z)
x = Bernoulli(logits=Dense(28 * 28, activation=None)(h))

# Variational model
qx = tf.placeholder(tf.float32, [N, 28 * 28])
qh = Dense(256, activation='relu')(qx)
qz = Normal(mu=Dense(d, activation=None)(qh),
            sigma=Dense(d, activation='softplus')(qh))
```

The program covers N data points $x_n \in \{0, 1\}^{28x28}$ with d latent variables $z_n \in \mathbb{R}^d$ each. Two densely connected layers with 256 hidden units using the ReLU activation function compose the probabilistic model, generating 28×28 binary pixel images. The second part defines the variational model with the same hidden layer architecture, producing output parameters of the normal posterior approximation. It becomes clear, that Edward allows for crisp and concise probabilistic programs: the probabilistic model, as well

Figure 3: Hierarchical model with local variables $\mathbf{z}_n$ and global variables β modeling the graph representation of Equation (1)



as the variational model can be easily extended, their probabilistic assumptions adapted.

Edward uses the higher-level framework Keras (Chollet et al., 2015) to include neural network building blocks such as the `Dense` layer used above.

3.2 Compositional Representations for Inference

To bridge the gap between the two groups of PPLs, Tran et al. pose two criteria on the compositional representation for inference. On the one hand, Edward shall support a large collection of different inference classes where the form of the inferred posterior depends on the inference algorithm. On the other hand, invariance of inference under the computational graph is desired, meaning the posterior can be composed as part of another model. This can be simply illustrated with the example in Figure 3 that represents a joint distribution over the data $\mathbf{x}$, local variables $\mathbf{z}$, and global variables β:

$$p(\mathbf{x}, \mathbf{z}, \beta) = p(\beta) \prod_{n=1}^{N} p(z_n \mid \beta)\, p(x_n \mid z_n, \beta) \quad . \tag{1}$$

In inference, we want to obtain the posterior distribution $p(\mathbf{z}, \beta \mid \mathbf{x}_{train}; \boldsymbol{\theta})$ with training data $\mathbf{x}_{train}$ and model parameters $\boldsymbol{\theta}$. This can be formulated as an optimization problem:

$$\min_{\boldsymbol{\lambda}, \boldsymbol{\theta}} \mathcal{L}\left(p(\mathbf{z}, \beta \mid \mathbf{x}_{train}; \boldsymbol{\theta}),\ q(\mathbf{z}, \beta; \boldsymbol{\lambda})\right) \quad , \tag{2}$$

where $q(\mathbf{z}, \beta; \boldsymbol{\lambda})$ is the distribution that approximates the true posterior $p(\mathbf{z}, \beta \mid \mathbf{x}_{train}; \boldsymbol{\theta})$, $\boldsymbol{\lambda}$ are model parameters of the posterior approximation, and $\mathcal{L}$ is a loss function between the true posterior p and its approximation q. The inference algorithm will determine the form of q, L and the rules to update the model parameters $\{\boldsymbol{\theta}, \boldsymbol{\lambda}\}$.

In Edward, this problem statement translates to the following code which defines and solves the optimization in Equation (2):

```
# Create inference with reference to variables
inference = ed.Inference(latent_vars={beta: qbeta, z: qz},
                         data={x: x_train})

# Build computational graph
inference.initialize()

# Run computations to update parameters
while condition:
    inference.update()
```

Table 1: Benchmarks comparing Edward against handwritten NumPy, Stan, PyMC3 and handwritten TensorFlow on logistic regression using Hamiltonian Monte Carlo iterations.

Probabilistic programming system	Runtime (s)
Handwritten NumPy (1 CPU)	534
Stan (1 CPU)	171
PyMC3 (12 CPU)	30.0
Edward (12 CPU)	**8.2**
Handwritten TensorFlow (GPU)	5.0
Edward (GPU)	**4.9**

where `qbeta` and `qz` are posterior variables and `x_train` are observed variables. With this design principle, Edward supports multiple sub-classes of inference procedures such as *Variational inference*, which uses a group of distributions to find a close approximation of the true posterior, *Monte Carlo inference*, which approximates the posterior using samples, and *Generative Adversarial Network inference*, mapping random points in a latent space to points in the data distribution.

Edward further allows posing inference as a collection of separate inference programs. As an example, the following code implements variational Estimation-Maximization (EM) inference (Neal and Hinton, 1993), using an approximate E-step (variational inference) over local and an M-step (MAP inference) over global variables:

```
# Define global and local variables
qbeta = PointMass(params=tf.Variable(tf.zeros([K, D])))
qz = Categorical(logits=tf.Variable(tf.zeros([N, K])))

# E-Step over local variables
inf_e = ed.VariationalInference(latent_vars={z: qz},
                                data={x: x_train, beta: qbeta})
# M-Step over global variables
inf_m = ed.MAP(latent_vars={beta: qbeta},
               data={x: x_train, z: qz})

# Expectation-Maximization loop
while not_converged:
  inf_e.update()  # Run E-Step
  inf_m.update()  # Run M-Step
```

3.3 Experiments

Tran et al. have benchmarked the runtime of Edward, Stan, PyMC, handwritten TensorFlow and handwritten NumPy using logistic regression on the Covertype dataset ($N = 581012, D = 54$) by performing a fixed number of Hamiltonian Monte Carlo (Neal, 2012) iterations. The benchmark results (see Table 1) show that Edward (GPU) delivers a 35x speedup over Stan (1 CPU) and a 6x speedup over PyMC3 (12 CPU). Moreover, Edward is as fast as handwritten TensorFlow code, implying, that no overhead is produced.

The hardware was a 12-core Intel i7-5930K CPU at 3.50GHz and an NVIDIA Titan X (Maxwell) GPU. It is important to note that the Stan implementation at the time of Tran et al.'s (2017) publication was only capable of using a single CPU. Starting with version `2.18` of Stan (`stan-math`), threading support can be switched on during compile-time (but is experimental and tagged unsafe). Furthermore,

Table 2: Different inference procedures for a probabilistic encoder-decoder architecture evaluating the negative log-likelihood on the binarized MNIST dataset, showing that Edward makes it easy to develop and experiment with a large pool of inference algorithms.

Inference method	Negative log-likelihood
VAE (Diederik et al., 2014)	≤ 88.2
VAE without analytic KL	≤ 89.4
VAE with analytic entropy	≤ 88.1
VAE with score function gradient	≤ 87.9
Normalizing flows (Rezende and Mohamed, 2015)	≤ 85.8
Hierarchical variational model (Ranganath et al., 2015)	≤ 85.4
Importance-weighted auto-encoders ($K = 50$) (Burda et al., 2015)	≤ 86.3
HVM with IWAE objective ($K = 5$)	≤ 85.2
Rényi divergence ($\alpha = -1$) (Li and Turner, 2016)	≤ 140.5

even though PyMC3 uses Theano (Al-Rfou et al., 2016) as a backend, its GPU version was slower than the 12-CPU version, largely due to communication overhead with NumPy.

To demonstrate Edward's flexibility, Tran et al. have implemented an array of experiments of complex inference algorithms (see Table 2) with a probabilistic encoder-decoder architecture and evaluated them using held-out log-likelihoods on the binarized MNIST dataset (Salakhutdinov and Murray, 2008).

4 DISCUSSION

With Edward being a programming framework and its paper delivering many code examples, it was natural to go forth and try it out ourselves. Unfortunately, the development of Edward has stopped in July 2018. This resulted in issues such as incompatible dependencies with Edward, as well as conflicting dependencies. Neither code examples from the paper Appendix, nor tutorial Jupyter notebooks from Edward's GitHub repository [1] continue to work. Therefore, no kind of reproducibility could be achieved in our experiments. Edward was dropped in favor of Edward2 (Tran et al., 2018), its direct successor, which was adopted by Google. Edward2 has further achieved inclusion as a sub-module into TensorFlow Probability, a successor of the earlier work on TensorFlow Distributions (Dillon et al., 2017).

Tran et al. (2017) suggest in their related work section, that Edward bridges the gap between PPLs which focus on efficiency but sacrifice generality and PPLs which focus a rich class of covered models but come with decreased performance that does not scale well. In the following sections the author make good points on how they have achieved the covering of a broad range of possible models due to their model and inference composability. Unfortunately, the scaling with respect to model size, as well as data size and complexity has not been empirically shown and is therefore only proposed.

Similar to PyTorch and TensorFlow, Edward has also promised a so-called "model zoo" with its release[2]. A model zoo in the field of deep learning is known as a repository of parametric model architectures with fixed parameters provided that have been extensively optimized on a specific problem statement. The idea is that other users can then simply download and skip the expensive optimization process to use the model in a plug-and-play fashion and compose it with other parts of their own modeling structure. As of this time (February 2020), the Zoo still seems to be unavailable without any redirection or information on alternatives. It seems that this has been a problem in the past, mentioned by reviewers on OpenReview[3]. The associated GitHub issue regarding Edward's roadmap has an item for its model zoo which to this day still states that it is not yet complete.

Furthermore, code examples in Edward were hard to comprehend and follow since they were only snippets extracted from a larger codebase. The amount of code left out remained was not clear. Therefore, even though code examples were provided with good intentions, they have further confused the reader due to being out of context snippets.

Another important criterion for new PPLs (and serious programming languages in general) is their applicability in real-world use-cases. Code samples were mostly given but not empirically evaluated and compared against previous implementations in other frameworks. The authors have reduced their empirical study to an evaluation of Variational Auto-Encoder with a set of different inferences techniques that were already easily accessible in pure TensorFlow.

5 CONCLUSION AND OUTLOOK

The Edward library offers a large collection of probabilistic models and inference procedures in an easily usable form. Its main contributions are the power of compositional representations of probabilistic models and probabilistic inference procedures. To bridge the gap between efficient and general-purpose PPLs, Edward is based on TensorFlow's static computation graph and therefore leverages the advantages of fast, parallelizable computations and GPU support, which in theory should scale to large model and data sizes. A major drawback of Edward is the lack of support for dynamically changing computation graphs that have recently been adopted in TensorFlow, starting with version 2. This has been acknowledged by the authors and addressed in its successor, Edward2.

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[2]http://edwardlib.org/zoo
[3]https://openreview.net/forum?id=Hy6b4Pqee&noteId=Sy0_4dsGl

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