InferPy: Probabilistic Modeling with Deep Neural Networks Made Easy

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Abstract

InferPy is a Python package for probabilistic modeling with deep neural networks. InferPy defines a user-friendly API which trades-off model complexity with ease of use, unlike other libraries whose focus is on dealing with very general probabilistic models at the cost of having a more complex API. In particular, Inferpy allows to define, learn and evaluate general hierarchical probabilistic models containing deep neural networks in a compact and simple way. InferPy is built on top of Tensorflow, Edward2 and Keras.

Keywords: Deep Probabilistic modeling, Hierarchical probabilistic models, Neural networks, Latent variables, Tensorflow, User-friendly

1. Introduction

Recent advances in variational methods [1] have made possible the development of a new formalism, namely deep probabilistic modeling [2], which combines probabilistic models within neural networks (NNs) to capture complex non-linear relationships among random variables. The release of multiple libraries for deep probabilistic modelling [3, 4] are greatly expanding the adoption of these powerful probabilistic modeling techniques. However, these libraries are usually difficult to use, especially when defining distributions containing NNs, which requires explicitly dealing with multidimensional matrices (i.e. tensors).

This paper presents a new version of InferPy as a high-level Python API for probabilistic modeling with deep NNs with a strong focus on ease of
use. The main differences with the previous version \cite{5} are the following ones. Models can now contain deep NNs to model non-linear relationships among random variables. The API has been significantly changed to make it compatible with the use of deep NNs. Moreover, InferPy relies now on Tensorflow Probability (TFP) and Edward2 \cite{3} (we previously relied on the first version of Edward, but this library is no longer under development).

2. Background

Probabilistic models with deep NNs are usually found in the literature under the name of deep generative models \cite{6}. These can generate data samples using probabilistic constructs that include NNs. This has provoked a strong impact within the deep learning community as it allowed dealing with many unsupervised learning problems. See \cite{2} for a recent review of these models. Along these lines, a new set of software tools have appeared, building on top of standard deep learning frameworks, in order to accommodate probabilistic models containing NNs \cite{5,3,4}. These tools usually fall under the umbrella term probabilistic programming languages (PPLs) \cite{7}, and provide support for methods for reasoning about complex probabilistic models. Some examples are Edward2/TFP \cite{8,3}, Pyro \cite{4}, etc.

3. Software Framework

The main features of InferPy are: (i) Its simple API allows easy prototyping of probabilistic models including NNs; (ii) Unlike Edward2/TFP, it is not require to have a strong background in the inference methods available (Variational Inference \cite{1,2} and Monte Carlo methods \cite{9}) as many details are hidden to the user; (iii) Parallelization details are also hidden to the user: InferPy runs seamlessly on CPUs and GPUs. InferPy can be seen as an upper layer for working with Edward2/TFP. Thus, models that can be defined in InferPy are those that can be defined using Edward2/TFP. InferPy is distributed as open-software (Apache-2.0) using Pypi and its source code is available at GitHub (see Tab. 1 and 2).

4. Illustrative Example

For illustrating the usage of InferPy, we will consider a variational autoencoder (VAE) \cite{10}, as it is one of the most widely used probabilistic models containing deep NNs. In a VAE, every object has a unknown latent representation (a code), modeled with a multivariate Gaussian (a distribution over
possible codes). This latent representation gives rise to a multivariate Gaussian distribution over the observed representation (the decoded observation of this object) by passing the latent representation through a NN called the decoder. This part of the model is defined in Fig. 1 (lines 1 to 9) and the creation of an instance (line 10), which is an object of class inf.models.probmodel. A probabilistic model in InferPy is defined as a function with the decorator @inf.probmodel. Following the statistical inference terminology, we refer to this part of the model as the p model.

Random variables are objects of class inf.models.RandomVariable. Variables composing a probabilistic model are those instantiated during the execution of its decorated function. The with inf.datamodel() syntaxis is used to indicate the random variables contained within this construct are replicated for every data sample. Every replicated variable is conditionally independent given the previous random variables (if any) defined outside this with statement. This construct enormously simplify the code of the model.

```
@inf.probmodel
def vae(k, d0, d, decoder):
    with inf.datamodel():
        z = inf.Normal(tf.ones(k), 1, name="z")
        x = inf.Normal(decoder(z, d0, d), 1, name="x")
    def decoder(z, d0, d):
        h0 = tf.keras.layers.Dense(d0, activation=tf.nn.relu)
        h1 = tf.keras.layers.Dense(d)
        return h1(h0(z))
    p = vae(k=2, d0=100, d=28*28, decoder=decoder)
```

Figure 1: p-model and decoder

The encoder part of a VAE defines the inference part of the model: given the observed representation of an object we need to find the posterior probability over possible latent representations (codes) of this object, in the form a multivariate Gaussian. In a VAE, this inference part is defined using an amortized variational inference [1, 2] scheme, which relies on an encoder network. Following the variational inference terminology, we call this part of the model as the q model. As shown in Fig. 2 this part is similarly defined with the same decorator. The correspondence between the variables in the

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1 In contrast to other libraries, the number of replications will be automatically calculated just before the inference.
decoder part and the encoder part of the model is done by the argument name, i.e., they should be the same. In this case, the input arguments are the same but the last one, which corresponds with the decoder/encoder NN.

```
@inf.probmodel
def qmodel(k, d0, d, encoder):
    with inf.datamodel():
        x = inf.Normal(tf.ones(d), 1, name="x")
        output = encoder(x, d0, k)
        qz_loc = output[:, :k]
        qz_scale = tf.nn.softplus(output[:, k:])+0.01
        qz = inf.Normal(qz_loc, qz_scale, name="z")

    def encoder(x, d0, k):
        h0 = tf.keras.layers.Dense(d0, activation=tf.nn.relu)
        h1 = tf.keras.layers.Dense(2*k)
        return h1(h0(x))

    q = qmodel(k=2, d0=100, d=28*28, encoder=encoder)
```

Figure 2: q-model and encode

A minimal example using (stochastic) variational inference [1, 2] as a learning engine is given in Fig. 3. Even though the learning algorithm can be further configured. In this case, an object of class `inf.inference.SVI` is created with the q-model, the epochs (number of iterations) and batch_size as input arguments. The optimization starts when the method fit() is invoked. Finally, we might sample from the posterior of z (latent representation) or from the posterior predictive (generating new samples).

```
SVI = inf.inference.SVI(q, epochs=1000, batch_size=100)
p.fit(\{"x": x_train\}, SVI)
postz = p.posterior("z", data=\{"x": x_train[100:,:]\}).sample()
x_gen = p.posterior_predictive("x", data=\{"z": postz\}).sample()
```

Figure 3: Inference of the posterior distributions

The analogous Edward2/TFP for this model is far more complex. This can be found in the online documentation (see Tab. [1 and 2], together with other examples and a complete user manual.

5. Conclusions

We have briefly presented how InferPy allows simple probabilistic modeling with deep NNs. As most of the inference details are hidden, this package can be used for users without a strong probabilistic background.
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## Metadata

### Current executable software version

| Nr. | (executable) Software metadata description |   |
|-----|--------------------------------------------|---|
| S1  | Current software version | 1.2.0 |
| S2  | Permanent link to executables of this version | https://pypi.org/project/inferpy/ |
| S3  | Legal Software License | Apache 2.0 |
| S4  | Computing platform/Operating System | Linux, OS X, Microsoft Windows, Unix-like |
| S5  | Installation requirements & dependencies | Pip, Python 3.5-3.6, tensorflow 1.12.1-2.0 tensorflow-probability 0.5.0-1.0, networkx 2.2.0-3.0 |
| S6  | Link to user manual | https://inferpy.readthedocs.io/ |
| S7  | Support email for questions | inferpy.api@gmail.com |

Table 1: Software metadata

### Current code version

| Nr. | Code metadata description |   |
|-----|----------------------------|---|
| C1  | Current code version | 1.2.0 |
| C2  | Permanent link to code/repository used of this code version | https://github.com/PGM-Lab/InferPy/ |
| C3  | Legal Code License | Apache 2.0 |
| C4  | Code versioning system used | github |
| C5  | Software code languages, tools, and services used | Python |
| C6  | Compilation requirements, operating environments | Python 3.5-3.6, tensorflow 1.12.1-2.0 tensorflow-probability 0.5.0-1.0, networkx 2.2.0-3.0 |
| C7  | Link to developer documentation/manual | https://inferpy.readthedocs.io/ |
| C8  | Support email for questions | inferpy.api@gmail.com |

Table 2: Code metadata