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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. It defines a user-friendly API that 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, this package 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 Probability and Keras.

Keywords: Deep Probabilistic modeling, Hierarchical probabilistic models, Neural networks, Bayesian layers, Tensorflow, User-friendly

1. Introduction

Advances in variational methods [1] have made possible the development of a new formalism, namely *deep probabilistic modeling* [2], which combines probabilistic models within deep neural networks (DNNs) to capture complex non-linear relationships among random variables. The release of multiple libraries for deep probabilistic modeling [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 dealing with multidimensional matrices (i.e. tensors).

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This paper presents a new version of InferPy as a high-level Python API for probabilistic modeling with DNNs with a strong focus on ease of use. (A major release of the code has been performed: from 0.2.x to 1.2.x.) The main differences with the previous version [5] are the following ones. Models can now contain DNNs to model non-linear relationships among random variables. The API has been significantly changed to make it compatible with the use of DNNs. Inferpy relies now on Tensorflow Probability (TFP) [3] (Inferpy’s previous version relied on Edward [6], which is deprecated).

2. Background

Probabilistic models with DNNs are usually found in the literature under the name of *deep generative models* or *Bayesian deep learning* [7]. The former focuses on density estimation using DNNs, while the latter focuses on treating the parameters of a DNN as random variables to capture the model uncertainty. See [2] for a recent review of all these models. Along these lines, new software tools have appeared to deal with probabilistic models containing DNNs [5, 3, 4]. These tools usually fall under the umbrella term *probabilistic programming languages* (PPLs) [8], and provide support for methods for reasoning about complex probabilistic models. Some examples are TFP [3], Pyro [4], etc.

3. Software Framework

The main features of InferPy are: (i) Its simple API allows easy prototyping of probabilistic models including DNNs; (ii) Unlike TFP, it is not required to have a strong background in the inference methods available (Variational Inference [1, 2] and Monte Carlo methods [9]) as many details are hidden to the user; (iii) InferPy runs seamlessly on CPUs and GPUs. InferPy can be seen as an upper layer for working with TFP. Thus, models that can be defined in InferPy are those that can be defined using 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) [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 8) and the creation of an instance (line 9), 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()` syntax is used to indicate the InferPy 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` statement¹. This construct enormously simplify the code of the model.

```

1  @inf.probmodel
2  def vae(k, d0, d):
3      with inf.datamodel():
4          z = inf.Normal(tf.ones(k), 1, name="z")
5          decoder = inf.layers.Sequential([
6              tfp.layers.DenseFlipout(d0, activation=tf.nn.relu),
7              tf.keras.layers.Dense(d)])
8          x = inf.Normal(decoder(z), 1, name="x")
9  p = vae(k=2, d0=100, d=28*28)

```

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 *decoder* part and the *encoder* part of the model is done by the argument `name`, i.e.,

¹In contrast to other libraries, the number of replications will be automatically calculated just before the inference.

they should be the same. For the NNs definition, standard Keras code can be used. However, in case of Bayesian NNs (e.g., `tfp.layers.DenseFlipout` defines a *Bayesian layer*), the `Sequential` model provided by InferPy must be used. This provides a Bayesian treatment of the *decoder network*.

```

1  @inf.probmodel
2  def qmodel(k, d0, d):
3      with inf.datamodel():
4          x = inf.Normal(tf.ones(d), 1, name="x")
5          encoder = tf.keras.Sequential([
6              tf.keras.layers.Dense(d0, activation=tf.nn.relu),
7              tf.keras.layers.Dense(2 * k)])
8          output = encoder(x)
9          qz_loc = output[:, :k]
10         qz_scale = tf.nn.softplus(output[:, k:])+0.01
11         qz = inf.Normal(qz_loc, qz_scale, name="z")
12         q = qmodel(k=2, d0=100, d=28*28)

```

Figure 2: q-model and encoder

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).

```

1  SVI = inf.inference.SVI(q, epochs=1000, batch_size=100)
2  p.fit({"x": x_train}, SVI)
3  postz = p.posterior("z", data={"x": x_train[:M, :]}).sample()
4  x_gen = p.posterior_predictive('x', data={"z": postz}).sample()

```

Figure 3: Inference from the posterior distributions

The analogous TFP code 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

InferPy can now represent probabilistic models containing DNNs using a simple and compact API. 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	1.3.0
S2	Permanent link to executables of this version	https://pypi.org/project/inferpy/1.3.0/
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 3.5-3.7, tensorflow 1.12.1-1.15.0 tensorflow-probability 0.7.0, 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	1.3.0
C2	Permanent link to code/repository used of this code version	https://github.com/PGM-Lab/InferPy/tree/1.3.0
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 3.5-3.7, tensorflow 1.12.1-1.15.0 tensorflow-probability 0.7.0, 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