BayesPy: Variational Bayesian Inference in Python

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Abstract

BayesPy is an open-source Python software package for performing variational Bayesian inference. It is based on the variational message passing framework and supports conjugate exponential family models. By removing the tedious task of implementing the variational Bayesian update equations, the user can construct models faster and in a less error-prone way. Simple syntax, flexible model construction and efficient inference make BayesPy suitable for both average and expert Bayesian users. It also supports some advanced methods such as stochastic and collapsed variational inference.

Keywords: Variational Bayes, probabilistic programming, Python

1. Introduction

Bayesian framework provides a theoretically solid and consistent way to construct models and perform inference. In practice, however, the inference is usually analytically intractable and is therefore based on approximation methods such as variational Bayes (VB), expectation propagation (EP) and Markov chain Monte Carlo (MCMC) (Bishop, 2006). Deriving and implementing the formulas for an approximation method is often straightforward but tedious, time consuming and error prone.

BayesPy is a Python 3 package providing tools for constructing conjugate exponential family models and performing VB inference easily and efficiently. It is based on the variational message passing (VMP) framework which defines a simple message passing protocol (Winn and Bishop, 2005). This enables implementation of small general nodes that can be used as building blocks for large complex models. BayesPy offers a comprehensive collection of built-in nodes that can be used to build a wide range of models and a simple interface for implementing custom nodes. The package is released under the MIT license.

Several other projects have similar goals for making Bayesian inference easier and faster to apply. VB inference is available in Bayes Blocks (Raiko et al., 2007), VIBES (Bishop et al., 2002) and Infer.NET (Minka et al., 2014). Bayes Blocks is an open-source C++/Python package but limited to scalar Gaussian nodes and a few deterministic functions, thus making it very limited. VIBES is an old software package for Java, released under the revised BSD license, but it is no longer actively developed. VIBES has been replaced by Infer.NET, which is partly closed source and licensed for non-commercial use only. Instead of VB inference, mainly MCMC is supported by other projects such as PyMC (Patil et al., 2010), OpenBUGS (Thomas et al., 2006), Dimple (Hershey et al., 2012) and Stan (Stan Development Team, 2014). Thus, there is a need for an open-source and maintained VB software package.

2. Features

BayesPy can be used to construct conjugate exponential family models. The documentation provides detailed examples of how to construct a variety of models, including principal component analysis models, linear state-space models, mixture models and hidden Markov models. BayesPy has also been used in two publications about parameter expansion and time-varying dynamics for linear state-space models (Luttinen, 2013; Luttinen et al., 2014).

Using BayesPy for Bayesian inference consists of four main steps: constructing the model, providing data, finding the posterior approximation and examining the results. The user constructs the model from small modular blocks called nodes. Roughly, each node corresponds to a latent variable, a set of observations or a deterministic function. The inference engine is used to run the message passing algorithm in order to obtain the posterior approximation. The resulting posterior can be examined, for instance, by using a few built-in plotting functions or printing the parameters of the posterior distributions.

Nodes are the primary building blocks for models in BayesPy. There are two types of nodes: stochastic and deterministic. Stochastic nodes correspond to probability distributions and deterministic nodes correspond to functions. Built-in stochastic nodes include all common exponential family distributions (e.g., Gaussian, gamma and Dirichlet distributions), a general mixture distribution and a few complex nodes for dynamic variables (e.g., discrete and Gaussian Markov chains). Built-in deterministic nodes include a gating node and a general sum-product node. In case a model cannot be constructed using the built-in nodes, the documentation provides instructions for implementing new nodes.

BayesPy is designed to be simple enough for non-expert users but flexible and efficient enough for expert users. One goal is to keep the syntax easy and intuitive to read and write by making it similar to the mathematical formulation of the model. Missing values are easy to handle and the variables can be monitored by plotting the posterior distributions during the learning. BayesPy has also preliminary support for some advanced VB methods such as stochastic variational inference (Hoffman et al., 2013), deterministic annealing (Katahira et al., 2008), collapsed inference (Hensman et al., 2012), Riemannian conjugate gradient learning (Honkela et al., 2010), parameter expansions (Qi and Jaakkola, 2007) and pattern searches (Honkela et al., 2003). For developers, the unit testing framework helps in finding bugs, making changes and implementing new features in a robust manner.

BayesPy can be installed similarly to other Python packages. It requires Python 3 and a few popular packages: NumPy, SciPy, matplotlib and h5py. The latest release can be installed from Python Package Index (PyPI) and detailed instructions can be found from the comprehensive online documentation[1]. The latest development version is available at GitHub[2], which is also the platform used for reporting bugs and making pull requests.

3. Example

This section demonstrates the key steps in using BayesPy. An artificial Gaussian mixture dataset is created by drawing 500 samples from two 2-dimensional Gaussian distributions. 200 samples have mean $[2, 2]$ and 300 samples have mean $[0, 0]$:

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1. `http://bayespy.org`
2. `https://github.com/bayespy/bayespy`

```
1  import numpy as np
2  N = 500; D = 2
3  data = np.random.randn(N, D)
4  data[:200,:] += 2*np.ones(D)
```

We construct a mixture model for the data and assume that the parameters, the cluster assignments and the true number of clusters are unknown. The model uses a maximum number of five clusters but the effective number of clusters will be determined automatically:

```
5  K = 5
```

The unknown cluster means and precision matrices are given Gaussian and Wishart prior distributions:

```
6  from bayespy import nodes
7  mu = nodes.Gaussian(np.zeros(D), 0.01*np.identity(D), plates=(K,))
8  Lambda = nodes.Wishart(D, D*np.identity(D), plates=(K,))
```

The `plates` keyword argument is used to define repetitions similarly to the plate notation in graphical models. The cluster assignments are categorical variables, and the cluster probabilities are given a Dirichlet prior distribution:

```
9   alpha = nodes.Dirichlet(0.01*np.ones(K))
10  z = nodes.Categorical(alpha, plates=(N,))
```

The observations are from a Gaussian mixture distribution:

```
11  y = nodes.Mixture(z, nodes.Gaussian, mu, Lambda)
```

The second argument for the `Mixture` node defines the type of the mixture distribution, in this case Gaussian. The variable is marked as observed by providing the data:

```
12  y.observe(data)
```

Next, we want to find the posterior approximation for our latent variables. We create the variational Bayesian inference engine:

```
13  from bayespy.inference import VB
14  Q = VB(y, mu, z, Lambda, alpha)
```

Before running the VMP algorithm, the symmetry in the model is broken by a random initialization of the cluster assignments:

```
15  z.initialize_from_random()
```

Without the random initialization, the clusters would not be separated. The VMP algorithm updates the variables in turns and is run for 200 iterations or until convergence:

```
16  Q.update(repeat=200)
```

The results can be examined visually by using `bayespy.plot` module:

```
17  import bayespy.plot as bpplt
18  bpplt.gaussian_mixture_2d(y, alpha=alpha)
19  bpplt.pyplot.show()
```

It is also possible to print the parameters of the approximate posterior distributions:

```
20  print(alpha)
```

The `bayespy.plot` module contains also other functions for visually examining the distributions.

Table 1: The average CPU time in milliseconds per iteration for each dataset. The results in parentheses have the following meanings: a) BayesPy without using broadcasting. b) Infer.NET using the same factorization as in BayesPy.

	Small GMM	Large GMM	Small PCA	Large PCA
BayesPy	6	90	7 (60)	400 (1 500)
Infer.NET	25	4 600	37 (350)	2 200 (210 000)

4. Comparison with Infer.NET

This section provides a brief comparison with Infer.NET because it is another active project implementing the variational message passing algorithm, whereas the other related active projects implement MCMC. The main advantages of Infer.NET over BayesPy are its support for non-conjugate models (e.g., logistic regression) and other inference engines (EP and Gibbs sampling). On the other hand, BayesPy is open-source software and supports several advanced VB methods (e.g., stochastic variational inference and collapsed inference).

The speed of the packages were compared by using two widely used models: a Gaussian mixture model (GMM) and principal component analysis (PCA).[3] Both models were run for small and large artificial datasets. For GMM, the small model used 10 clusters for 200 observations with 2 dimensions, and the large model used 40 clusters for 2000 observations with 10 dimensions. For PCA, the small model used 10-dimensional latent space for 500 observations with 20 dimensions, and the large model used 40-dimensional latent space for 2000 observations with 100 dimensions. For the PCA model, Infer.NET used both a fully factorizing approximation and also the same approximation as in BayesPy which did not factorize with respect to the latent space dimensions. The experiments were run on a quad-core (i7-4702MQ) Linux computer. Because the packages run practically identical algorithms and thus converged to similar solutions in a similar number of iterations (50–100 iterations depending on the dataset), we compared the average CPU time per iteration.

The results are summarized in Table 1. For all datasets, BayesPy is faster probably because it uses highly optimized numerical libraries (BLAS and LAPACK). For PCA, BayesPy also automatically avoids redundant computations which arise because latent variables have equal posterior covariance matrices. However, such broadcasting is not always possible (e.g., if there are missing values in the PCA data). Thus, the table also presents the results when BayesPy is forced to not use broadcasting: BayesPy is slower than Infer.NET on the smaller PCA dataset but faster on the larger PCA dataset. If Infer.NET used the same factorization for PCA as BayesPy, Infer.NET may be orders of magnitude slower.

5. Conclusions

BayesPy provides a simple and efficient way to construct conjugate exponential family models and to find the variational Bayesian posterior approximation in Python. In addition to the standard variational message passing, it supports several advanced methods such as stochastic and collapsed variational inference. Future plans include support for non-conjugate models and non-parametric models (e.g., Gaussian and Dirichlet processes).

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3. The scripts for running the experiments are available as supplementary material.

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