Borch: A Deep Universal Probabilistic Programming Language

Abstract

Ever since the Multilayered Perceptron was first introduced the connectionist community has struggled with the concept of uncertainty and how this could be represented in these types of models. This past decade has seen a lot of effort in trying to join the principled approach of probabilistic modeling with the scalable nature of deep neural networks. While the theoretical benefits of this consolidation are clear, there are also several important practical aspects of these endeavors; namely to force the models we create to represent, learn, and report uncertainty in every prediction that is made. Many of these efforts have been based on extending existing frameworks with additional structures. We present Borch, a scalable deep universal probabilistic programming language, built on top of PyTorch. The code is available for download and use in our repo.

Keywords uppl • neural networks • uncertainty • pytorch

1 Introduction

The ability to solve a wide variety of challenging real world problems using machine learning has flourished during the course of the past decade. We’ve seen advancements within diverse application areas, e.g., vision (Bojarski et al. 2016), natural language and physics (Bakarji et al. 2022). We’ve also seen the emergence of a new paradigm for machine learning where it is possible to teach a computer how to complete mathematical proofs (Davis 2021; Davies et al. 2021) and even compete in a real-world programming competition (Li et al. 2022). Despite the fact that most of these advances were achieved by neural networks, there are still areas where neural networks are far from being superior to more traditional machine learning methods (Shwartz-Ziv and Armon 2021). The strength in many of these methods lies in that they are easier to interpret and reason about. However, despite these recent success, most of the models
developed and in use today lack the ability to adequately quantify the confidence in the predictions given (Ghahramani 2015).

This is especially problematic for models that are exposed to out of distribution (OOD) examples. When it comes to deploying neural networks in real world applications, OOD data will inevitably be an issue (Henriksson et al. 2021). Elaborate data augmentation processes and larger training datasets can help make the networks more robust (Zheng et al. 2016), but will never cover the entire spectrum of possible scenarios. This is the most significant reason to model and report the uncertainty in model parameters as well as the data.

With the ambition to understand uncertainty in predictions it is natural to turn to a Bayesian treatment of model parameters, likelihood and data (Dasgupta et al. 2020).

2 About Uncertainties

One of the most important concepts in modeling any system is to know what you do not know (Kläs and Vollmer 2018). That may sound like an impossible situation to resolve, but it’s really quite simple. We don’t need to know why we don’t know something, we only need to quantify the degree of our ignorance. As such, it is important to categorize different uncertainties to help us reason about where our lack of knowledge resides.

For most practical purposes in machine learning we categorize uncertainties into Epistemic and Aleatoric uncertainty (Kiureghian and Ditlevsen 2009). They are shown in Figure 1.

Epistemic uncertainty encapsulates the uncertainty the model has about its own representation of the problem at hand. It represents all things the model doesn’t know but in principle could. Examples of this can be data left out of the training set. Another example is structural limitations of the model itself.

Aleatoric uncertainty on the other hand encapsulates the uncertainty that happens as a consequence of running an experiment multiple times. It’s basically the innate uncertainty that we cannot model our way out of. This particular type of uncertainty comes in two flavors. Homoskedastic Aleatoric Uncertainty is the uncertainty or variance observed across the entire dataset, i.e., one value. Heteroskedastic Aleatoric Uncertainty on the other hand changes as a function of each observation. This means that you can have a rather high “data uncertainty” for observation A, while having a low uncertainty for observation B.

![Figure 1: A classification of common uncertainties that are useful to consider in machine learning models.](image-url)
2.1 Probabilistic Programming

Universal Deep Probabilistic programming languages unify techniques for formal description of computation with the representation and use of uncertain knowledge (Goodman and Stuhlmüller 2014). These languages have seen recent interest from artificial intelligence, programming languages, cognitive science, and natural languages communities (Gawlikowski et al. 2021).

Implementing probabilistic models from scratch is highly error-prone and requires a high degree of expertise (Goodman and Stuhlmüller 2014; Tolpin et al. 2016). This results in models that are very hard to develop, extend and to reuse. To combat these issues practitioners usually revert to using a probabilistic programming language (PPL) which enables the expression of probabilistic programs and performing inference on those programs.

We introduce Borch, a universal probabilistic programming language built on PyTorch (Paszke et al. 2019). Throughout the paper we illustrate code\(^1\) to show the expressiveness of the language.

3 Design Principles

3.1 Basic Syntax

Borch is built around a few core primitives. (i) Distributions that provide standard features such as generation of samples and calculation of log probabilities of distributions etc. (ii) Random Variables (RV) which unify distributions with tensors. (iii) Posteriors that handle how the inference algorithm creates samples. (iv) A Module which is the object used to keep track of RVs and the inference algorithm.

We recommend two different coding patterns, functional and object-oriented depending on the type of model used. The functional syntax is straightforward and easy to understand. The forward pass of a simple linear regression model can be implemented as follows:

```python
def forward(bm, x):
    bm.b = Normal(0, 3)
    bm.a = Normal(0, 3)
    bm.sigma = HalfNormal(1)
    mu = bm.b * x + bm.a
    bm.y = Normal(mu, bm.sigma)
    return bm.y
```

The functional programming paradigm has the benefit of being more similar to the actual mathematics of neural networks in flow and execution order.

In some cases the object-oriented paradigm is more natural and the corresponding code for the forward pass of the simple linear regression model would look like below:

```python
class Model(Module):
    def __init__(self):
        super().__init__()
        self.b = Normal(0, 3)
        self.a = Normal(0, 3)
        self.sigma = HalfNormal(1)

    def forward(self, x):
        mu = self.b * x + self.a
        self.y = Normal(mu, self.sigma)
        return self.y
```

For users of torch.nn (Paszke et al. 2019) and tensorflow.keras (Chollet et al. 2015) this should look familiar.

As illustrated in the code snippets above, Borch supports both formalisms which enables flexibility in the model expression. Thus, one can choose the most suitable approach for the model at hand. When working with hierarchical models a functional style tends to produce cleaner code (Buitléir, Russell, and Daly 2013) as there is a lot of code that needs to be executed on each pass. When following the object-oriented approach, the hierarchy should be expressed

\(^1\)The code snippets shown in the paper are just excerpts. Full examples are available at https://gitlab.com/desupervised/research/borch-paper and more elaborate tutorials are available at https://borch.readthedocs.io.
in the forward pass, and only isolated random variables should be put in the __init__ function. This is a common pattern for neural networks and thus the object-oriented paradigm is more compatible with many existing tutorials and applications for neural networks.

In order to be an effective PPL it is important to have the ability to condition on any random variable in the model. Further, being able to fit a model while conditioning on an arbitrary set of random variables is key. Also, un-conditioning a subset of those variables such the same model can be used to generate predictions allows for the expression of a wide variety of models. This is done in Borch using the observe method on the Module object.

```python
model.observe(y=y)
forward(model, x) == y
```

Then in order to stop observing and be able to generate predictions from the model one can use:

```python
model.observe(None)
forward(model, x) != y
```

This way of conditioning on data enables us to move from a generative state to a discriminatory state in one line of code.

### 3.2 Scaling

In order to handle the ever-growing size of models and data, a PPL needs to be scalable. This means handling everything from a simple linear regression model to a billion parameter image classification neural network trained on a graphics processing unit (GPU). At the same time it needs to be flexible enough to express a wide range of models and that these models can be fit with a multitude of inference methods. Borch is composable such that models can be fit by the method most suitable to a given problem. As such, any model can be conditioned on data through diverse methods, e.g., Markov Chain Monte Carlo (MCMC) (Brooks et al. 2011), Variational Inference (VI) (Blei, Kucukelbir, and McAuliffe 2017) and Maximum a Posteriori (MAP) (Bassett and Deride 2018).

### 3.3 Variable Scoping

In many Python-based PPLs there is a lack of reflectiveness in the model expression resulting in model specifications that require explicit naming of the variables instantiated. For example in PyMC3 (Salvatier, Wiecki, and Fonnesbeck 2016) it looks like this:

```python
with pm.Model() as linear_model:
  weights = pm.Normal("weights", mu=0, sigma=1)
```

and in Pyro (Bingham et al. 2019) it is written as below.

```python
weights = pyro.sample("weights", dist.Normal(0, 1))
```

This results in the variable weights which will be shared across the model and thus does not enable scoping using the standard Python syntax but has to be handled manually or with custom primitives. This lack of scoping results in a source of potential bugs, it is easy to deal with for small models but as the model grows in complexity it becomes more problematic. In Borch we strived to make probabilistic programming as easy as we possibly could. That’s why we can simply write the following and avoid the verbose syntax present in, e.g., Pyro, NumPyro and PyMC3.

```python
module.weights = Normal(0, 1)
```

### 3.4 Native Feel

We aim to allow the full expressiveness of normal Python code and ease of integration with other tools. Since PyTorch (Paszke et al. 2019) offers auto differentiation for dynamic computational graphs, GPU support and native integration with Python primitives the same holds true for Borch since it builds on top of PyTorch. Thus, we support features like stochastic control flow out of the box.

```python
def forward(module, data):
  if random(1) > 0:
    module.weight = Normal(-1, 1)
  else:
    module.weight = Normal(1, 10)
  return data*torch.exp(module.weight)
```
3.5 Neural Networks

We set out to keep the feel of how PyTorch expresses neural networks and make it a seamless experience to do Bayesian inference using Borch for anyone with PyTorch experience. Thus, we wanted it to be fully compatible with normal Python functions. We also wanted a tight integration with PyTorch such that one gets dynamic control flow and the same type of user experience when creating models in Borch.

To enable this for neural networks we provide an interface almost identical to the torch.nn modules and in most cases it is possible to just switch from `import torch.nn as nn` to `import borch.nn as nn`. This makes a network defined in PyTorch probabilistic, without any other changes in the model specification. Thus, a simple MNIST (Deng 2012) image classification model can be written like below.

```python
import torch.nn.functional as F
from borch import nn

class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 6, 5)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1 = nn.Linear(16 * 5 * 5, 120)
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)

    def forward(self, x):
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(1, -1)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x

Changing an entire neural network to be Bayesian is not always required though. Often it makes sense to only make specific parts or layers of the neural network Bayesian. Using the MNIST example above we can easily compose Borch and PyTorch such that only the two last layers are Bayesian. This means that the last decision layers will learn uncertainty while the earlier layers of the network will have point parameters. We write the adapted MNIST model as below.

```python
import torch
import borch
import torch.nn.functional as F

class Net(borch.nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = torch.nn.Conv2d(1, 6, 5)
        self.conv2 = torch.nn.Conv2d(6, 16, 5)
        self.fc1 = torch.nn.Linear(16 * 5 * 5, 120)
        self.fc2 = borch.nn.Linear(120, 84)
        self.fc3 = borch.nn.Linear(84, 10)

    def forward(self, x):
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(1, -1)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```
The signature for PyTorch `nn` modules has also been extended to support the ability to set priors for the weights of an `nn` module. Thus, to use the priors in Figure 2 for the fully connected dense layer `fc3` in the Bayesian MNIST model, it is as simple as

```python
self.fc3 = nn.Linear(84, 10, weight=Normal(0, 1e-2), bias=Normal(0, 1))
```

where the weight and bias arguments are broadcast to the shape of each tensor in the `nn.Linear` module.

Figure 2: Illustration of the histograms of the two prior distributions broadcast to the weights and the biases of the dense layer `fc3` in the MNIST model. In this example the biases and weights are given by $b \sim \mathcal{N}(0, 1)$ and $\omega \sim \mathcal{N}(0, 0.01)$ respectively.

### 3.6 Transforming Networks to Become Bayesian

Transfer learning (Farahani et al. 2021) is commonly used to take a network trained on one problem as a starting point and train it to solve a different problem. In the same way Borch allows taking a `torch.nn` network and converting the whole or a part of it to be Bayesian. This makes it possible to quickly introduce uncertainty to a full scale model.

Here we show how to create a Bayesian MobileNetV3 (Howard et al. 2019) network in just a few lines of code.

```python
import torchvision
import borch
import torch

mobilenet = borch.nn.borchify_network(
    torchvision.models.mobilenet_v3_small(pretrained=True),
)
# Now it can be used to predict
borch.sample(mobilenet)
mobilenet(torch.randn(3, 3, 224, 224))
```

However, we do not need to make the entire network Bayesian. Instead, we can make parts of the network Bayesian and the process is the same.

```python
mobilenet = models.mobilenet_v3_small(pretrained=True)
mobilenet.classifier = borchify_network(mobilenet.classifier)
borch.sample(mobilenet)
mobilenet(torch.randn(3, 3, 224, 224))
```

A couple of notable differences compared to PyTorch are:

1. We need to `borchify` or `lift` the network up to a probabilistic network.
2. We need to sample the posterior weights before generating a prediction. Without the sample statement we will reuse the same weights over and over again.

Note that it makes no difference whether we call `torch.sample` on only the classifier (`torch.sample(mobilenet.classifier)`) or on the entire network (`torch.sample(mobilenet)`) as the operation is applied recursively and only affects the segments of the network which are constructed with Borch.

### 3.7 Inference

The primary focus in the development of Borch has been to ensure that one can actually create and train state of the art neural networks. In order to achieve this a lot of attention has been focused on variational inference (Paisley, Blei, and Jordan 2012) as an inference method, as it, together with MAP, are the fitting methods that can scale to big neural networks.

To this end we wanted to make it easy to control the approximating distribution for different parts of the network. This is done by the concept of a posterior, that guides the approximating distribution. In order to offer full control of the approximating distribution we have Manual posterior. Below is a minimal example where we simply infer the location and scale of a normal distribution.

```python
def forward(mod):
    mod.test = Normal(5, 1)
```

The posterior is specified in the same way. In order for the parameters to be learnable we need to define them as `torch.nn.Parameter`s. The `Parameter` wrapper for tensors just lets the framework know that it should be returned when calling `model.parameters()` in the same way `torch` does it. Thus, this is a convenient way to pass them to an optimizer.

```python
man_posterior = posterior.Manual()
man_posterior.mean = torch.nn.Parameter(torch.ones(1))
man_posterior.sd = torch.nn.Parameter(torch.ones(1))

def forward_posterior(posterior):
    scale = torch.exp(posterior.sd)+0.01
    mean = posterior.mean.abs()
    posterior.test = dist.Normal(mean, scale)
```

While we support the manual expression of the posterior using the `torch.posterior.Manual`, we found that in the case of large neural networks it was simply easier to automatically create the appropriate approximate posterior. This still allows control over what posterior is used where in the network. It is done by simply specifying the posterior for each module.

```python
class Net(nn.Module):
    def __init__(self, posterior=borch.posterior.Automatic())
        self.conv1 = Conv2d(1, 6, 5, posterior=borch.posterior.Normal(log_scale=-3))
        self.conv2 = Conv2d(6, 16, 5, posterior=borch.posterior.Normal(log_scale=-3))
        self.fc1 = Linear(16 * 5 * 5, 120, posterior=borch.posterior.ScaledNormal(scaling=1e-2))
        self.fc2 = Linear(120, 10, posterior=borch.posterior.ScaledNormal(scaling=1e-2))
    def forward(self, x):
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(1, -1)
        x = F.relu(self.fc1(x))
        x = self.fc2(x)
        self.classification = Categorical(logits=x)
        return x
```
In this example we used the Automatic posterior for the top level module as it will automatically detect that the `x` in `self.classification = Categorical(logits=x)` will be updated in each forward. Thus, it will not create a parameter for `logits` that would be optimized. For the layers `conv1` and `conv2` the `Normal` posterior was used, creating a normal distribution as an approximating distribution where the scale goes through a `exp` transform. We can control at what value the unconstrained scale is initialized at. This is different to the `ScaledNormal` used for `fc1` and `fc2` which creates a Normal distribution as the approximating distribution but scales the width of the initialization point based on the prior.

When using a PPL, depending on the model, one will be interested in using different inference methods. For high confidence in the accuracy of the fit posteriors MCMC methods like The No-U-Turn Sampler (Hoffman and Gelman 2011) are preferred. For bigger models that are more data hungry like a neural network, MCMC methods do not scale well and also suffer from sampling issues (Blei, Kucukelbir, and McAuliffe 2017; Jospin et al. 2022) due to a massively degenerate energy landscape. Here, we need to use some other method like MAP or VI (Blei, Kucukelbir, and McAuliffe 2017).

Borch enables this by tying inference methods to a specific posterior. Thus, if we want to fit a model with MCMC even though the model set a posterior tied to VI at creation, we can simply replace the posterior on all the modules in a model like this:

```python
net = Net()
net.apply(set_posteriors(PointMass))
```

This facilitates the ability to encode the desired posterior when expressing the model. It also allows us to quickly alter the posterior on an instantiated object in order to use a different inference method, or simply to test the effect of a different posterior guide. The use of the term `PointMass` can be confusing but here it refers to a single sample, since each forward pass produces a set of values. It is the distribution of many forward passes that will eventually make up the posterior in this case.

## 4 Comparison to Existing PPLs

The development of Borch started in 2018 out of a necessity to build robust deep learning models that perform well on OOD data. The models developed at Desupervised were required to perform in critical environments where the consequence of a bad decision could be devastating. With this particular need, we realized that a Bayesian formalism made the most sense, but we were unhappy with the performance and coding style of existing frameworks. So we wanted to build large and deep neural networks while still maintaining a standard PPL interface. Thus, Borch is by no means the first PPL of its kind since there has been active development in this area for a long time. The landscape today is also different from when Borch was first developed.

Today, in our point of view, the two main alternatives are Pyro (Bingham et al. 2019) and Tensorflow probability (Dillon et al. 2017). Pyro offers a very solid PPL but very little tooling for neural networks. Tensorflow probability integrates with the Tensorflow Keras api that allows the creation of neural networks in a similar fashion as one can do with Borch.

Borch offers a wider range of Neural Network modules and an interface as a universal PPL that is more intuitive and does not require manual creation of the joint distribution of the model. Several PPLs that influenced the design of Borch were Stan (Stan Development Team 2018), Edward (Tran et al. 2016), PyMC3 (Salvatier, Wiecki, and Fonnesbeck 2016) and ProbTorch (Siddharth et al. 2017).

## 5 Conclusion

In order for deep neural networks to be deployed and used at scale across safety critical industries, e.g., healthcare, pharma, and construction they need the ability to report uncertainty for every prediction made. The importance does not reside in the pursuit of statistical excellence but rather in the necessity for the end user to know how much confidence should be put into the prediction at hand. The likelihood is of little help here since it’s uncalibrated, unnormalized and cannot easily be interpreted. A full Bayesian treatment of a model is required to produce useful, normalized and calibrated probabilities for each prediction.

Many interesting models do not have a closed form expression for the posterior distributions from which predictions are drawn. This predicament often leads practitioners to turn to powerful MCMC techniques like NUTS (Hoffman and Gelman 2011). While NUTS creates good approximations of the posteriors it’s limited in terms of parameter and data scale, making its application to neural networks suboptimal. Several attempts have been made to create languages which extend modern deep learning libraries with a probabilistic framework, e.g. Pyro and Tensorflow Probability. While powerful, we feel that these languages are verbose and put extra mental burden onto the practitioner.
We introduce Borch, a deep universal probabilistic programming language built on PyTorch. It provides a true Pythonic look and feel and can easily enable deep learning practitioners to include uncertainty estimates into their models. A process we call borchify turns a standard PyTorch model into its Bayesian counterpart. This process can operate on the entire network or be constrained to parts of it. This allows the practitioner to choose which pieces of a neural network that make the most sense to make Bayesian.

With this work we aim to remove the obstacles deep learning practitioners have in implementing Bayesian models by providing a language that looks and feels exactly like PyTorch. We hope that the community will build upon this and focus more on OOD predictive quality in all application areas.

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