
MXFusion

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MXFusion is a library for integrating probabilistic modelling with deep learning.

MXFusion helps you rapidly build and test new methods at scale, by focusing on the modularity of probabilistic models and their integration with modern deep learning techniques.

1.1 Dependencies / Prerequisites

MXFusion's primary dependencies are MXNet ≥ 1.2 and Networkx ≥ 2.1 . See [requirements](#).

1.2 Supported Architectures / Versions

MXFusion is tested on Python 3.5+ on MacOS and Amazon Linux.

1.3 pip

If you just want to use MXFusion and not modify the source, you can install through pip:

```
pip install mxfusion
```

1.4 From source

To install MXFusion from source, after cloning the repository run the following from the top-level directory:

```
pip install .
```


2.1 Topical Guides

Working in MXFusion breaks up into two primary phases. Model definition involves defining the variables, distributions, and functions that make up your model. Inference then takes in real values and learns parameters for your model or gives predictions over the data.

2.1.1 Model Definition

MXFusion is a library for doing probabilistic modelling.

Probabilistic Models can be categorized into directed graphical models (DGM, Bayes Net) and undirected graphical models (UGM). Most popular probabilistic models are DGMs, so MXFusion currently only supports DGMs.

A DGM can be fully defined using 3 basic components: deterministic functions, probabilistic distributions, and random variables. As such, those are the primary ModelComponents in MXFusion.

Model

The primary data structure of MXFusion is the [FactorGraph](#). FactorGraphs contain Variables and Factors. The FactorGraph exposes methods that Inference algorithms call such as drawing samples from the FactorGraph or computing the log pdf of a set of Variables contained in the FactorGraph.

When you want to start modelling, construct a Model object and start attaching ModelComponents to it. You can then see the Model's components by

```
m = Model()
m.v = Variable()
print(m.components)
```

When a ModelComponent is attached to a Model, it is automatically updated in the Model's internal data structures and will be included in any subsequent inference operations over the model.

Model Components

All ModelComponents in MXFusion are identified uniquely by a UUID.

###Variables In a model, there are typically four types of variables: a random variable following a probabilistic distribution, a variable which is the outcome of a deterministic function, a parameter (with no prior distribution), and a constant. The definitions of first two types of variables will be discussed later. The latter two types of variables can be defined with the following statement:

```
m.v = Variable(shape=(10,), constraint=PositiveTransformation())
```

At this stage, you do not need to specify whether v is a parameter or constant, because, if it is a constant, its value will be provided during inference, otherwise it will be treated as a parameter.

A typical example of when a constant would be specified at inference time is the size (shape) of an observed variable, which is known when data is provided. In the above example, we specify the name of the variable, the shape of the variable and the constraint that the variable has. It defines a 10-dimension vector whose values are always positive ($v \geq 0$).

Factors

####Distributions In a probabilistic model, random variables relate to each other through probabilistic distributions.

During model definition, the typical interface to generate a 2 dimensional random variable x from a zero mean unit variance Gaussian distribution looks like:

```
m.x = Normal.generate_variable(mean=0, variance=1, shape=(2,))
```

The two dimensions are independent to each other and both follow the same Gaussian distribution. The parameters or shape of a distribution can also be variables, for example:

```
m.mean = Variable(shape=(2,))
m.y_shape = Variable()
m.y = Normal.generate_variable(mean=m.mean, variance=1, shape=m.y_shape)
```

MXFusion also allows users to specify a prior distribution over pre-existing variables. This is particularly handy for interfacing with neural networks in MXNet because it allows you to set priors over parameters in an existing Gluon Block, such as a neural network implementation. The API for specifying a prior distribution looks like:

```
m.x = Variable(shape=(2,))
m.x.set_prior(Gaussian(mean=0, variance=1))
```

The above code defines a variable x and sets the prior distribution of each dimension of x to be a scalar unit Gaussian distribution.

Because Models are FactorGraphs, it is common to want to know what ModelComponents come before or after a particular component in the graph. These are accessed through the ModelComponent properties `successors` and `predecessors`.

```
m.mean = Variable()
m.var = Variable()
m.y = Normal.generate_variable(mean=m.mean, variance=m.var)
```

####Functions The last building block of probabilistic models are deterministic functions. The ability to define sophisticated functions allows users to build expressive models with a family of standard probabilistic distributions. As MXNet already provides full functionality for defining a function and automatically evaluating its gradients, Functions

in MXFusion are a wrapper over the functions in MXNet's Gluon interface. Functions are defined in standard MXNet syntax and provided to the MXFusion Function wrapper as below.

First we define a function in MXNet Gluon syntax using a Block object:

```
class F(mx.gluon.Block):
    def forward(self, x, y):
        return x*2+y
```

Then we create an MXFusion Function instance by passing in our Gluon function instance:

```
f_gluon = F()
m.f_mf = MXFusionGluonFunction(f_gluon)
```

Then this MXFusion Function can be called using MXFusion variables and its outcome will another variable[s] representing the outcome of the function:

```
m.x = Variable(shape=(2,))
m.y = Variable(shape=(2,))
m.f = f_mf(x, y)
```

FAQ

- Why don't you support undirected graphical models (UGM)?
- A UGM is typically defined in terms of a set of potential functions. Each potential function is a non-negative function that is defined on a subset of variables in a model. The joint probability distribution of an UGM is defined as the product of all the potential functions divided by a normalization term (known as a partition function).
- The notation of a DGM and an UGM can be unified into a factor graph, where a factor can be either a probabilistic distribution or a potential function. **In our implementation, the distribution UI is inherited from the factor abstract class, which enables future extension to support UGM**, although inference algorithms for UGM will be completely different.

2.1.2 Inference

Notes about inference in MXFusion.

Inference Algorithms

MXFusion currently supports stochastic variational inference.

Variational Inference

Variational inference is an approximate inference method that can serve as the inference method over generic models built in MXFusion. The main idea of variational inference is to approximate the (often intractable) posterior distribution of our model with a simpler parametric approximation, referred to as a variational posterior distribution. The goal is then to optimize the parameters of this variational posterior distribution to best approximate our true posterior distribution. This is typically done by minimizing the lower bound of the logarithm of the marginal distribution:

$$\begin{equation} \log p(y|z) = \log \int_x p(y|x) p(x|z) \geq \int_x q(x|y,z) \log \frac{p(y|x) p(x|z)}{q(x|y,z)} = \text{mathcal{L}}(y,z), \quad \text{label{eqn:lower_bound_1}} \end{equation}$$

where $p(y|x)$ forms a probabilistic model with x as a latent variable, $q(x|y)$ is the variational posterior distribution, and the lower bound is denoted as $\mathcal{L}(y,z)$. By then taking a natural exponentiation of $\mathcal{L}(y,z)$, we get a lower bound of the marginal probability denoted as $\tilde{p}(y|z) = e^{\mathcal{L}(y,z)}$.

A technical challenge with VI is that the integral of the lower bound of a probabilistic module with respect to external latent variables may not always be tractable. Stochastic variational inference (SVI) offers an approximated solution to this new intractability by applying Monte Carlo Integration. Monte Carlo Integration is applicable to generic probabilistic distributions and lower bounds as long as we are able to draw samples from the variational posterior.

In this case, the lower bound is approximated as
$$\mathcal{L}(l, z) \approx \frac{1}{N} \sum_i \log \frac{p(l|y_i) e^{\mathcal{L}(y_i, z)}}{q(y_{ilz})}, \quad \mathcal{L}(y_i, z) \approx \frac{1}{M} \sum_j \log \frac{p(y_{ilx_j}) p(x_{jlz})}{q(x_{jly_i}, z)}, \quad \text{end{equation}}$$
 where $y_{ilz} \sim q(y|z)$, $x_{jly_i, z} \sim q(x|y_i, z)$ and N is the number of samples of y and M is the number of samples of x given y . Note that if there is a closed form solution of $\tilde{p}(y_{ilz})$, the calculation of $\mathcal{L}(y_i, z)$ can be replaced with the closed-form solution.

Let's look at a simple model and then see how we apply stochastic variational inference to it in practice using MXFusion.

Creating a Posterior

Examples

Probabilistic PCA Tutorial

This tutorial will demonstrate Probabilistic PCA, a factor analysis technique.

Maths and notation following [Machine Learning: A Probabilistic Perspective](#).

Installation

Follow the installation instructions in the [README](#) file to get setup.

Probabilistic Modeling Introduction

Probabilistic Models can be categorized into directed graphical models (DGM, Bayes Net) and undirected graphical models (UGM). Most popular probabilistic models are DGMs, so MXFusion will only support the definition of DGMs unless there is a strong customer need of UGMs in future.

A DGM can be fully defined using 3 basic components: deterministic functions, probabilistic distributions, and random variables. We show the interface for defining a model using each of the three components below.

First lets import the basic libraries we'll need to train our model and visualize some data.

```
In [1]: import mxfusion as mf
import mxnet as mx
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

```
/Users/erimeiss/.pyenv/versions/jupyter3/lib/python3.6/site-packages/scipy/stats/morestats.py:12: DeprecationWarning:
from numpy.testing.decorators import setastest
```

Data Generation

We'll take as our function to learn components of the `log spiral function` because it's 2-dimensional and easy to visualize.

```
In [2]: def log_spiral(a,b,t):
        x = a * np.exp(b*t) * np.cos(t)
        y = a * np.exp(b*t) * np.sin(t)
        return np.vstack([x,y]).T
```

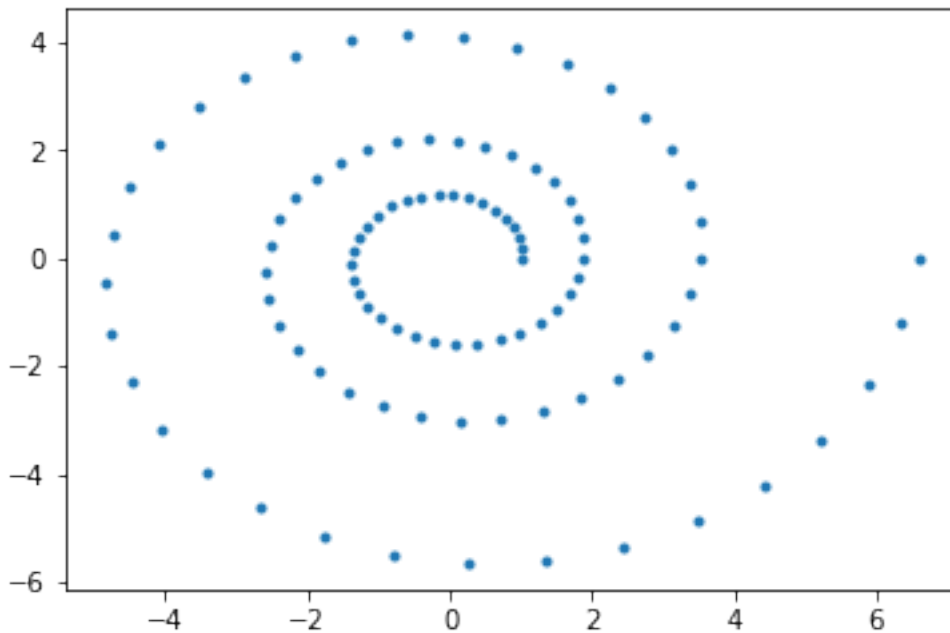
We parameterize the function with 100 data points and plot the resulting function.

```
In [3]: N = 100
        D = 100
        K = 2

        a = 1
        b = 0.1
        t = np.linspace(0,6*np.pi,N)
        r = log_spiral(a,b,t)

In [4]: r.shape
Out[4]: (100, 2)

In [5]: plt.plot(r[:,0], r[:,1],'.')
Out[5]: [<matplotlib.lines.Line2D at 0x11ced7668>]
```



We now project our K dimensional \mathbf{r} into a high-dimensional D space using a random matrix of random weights \mathbf{W} . Now that \mathbf{r} is embedded in a D dimensional space the goal of PPCA will be to recover \mathbf{r} in its original low-dimensional K space.

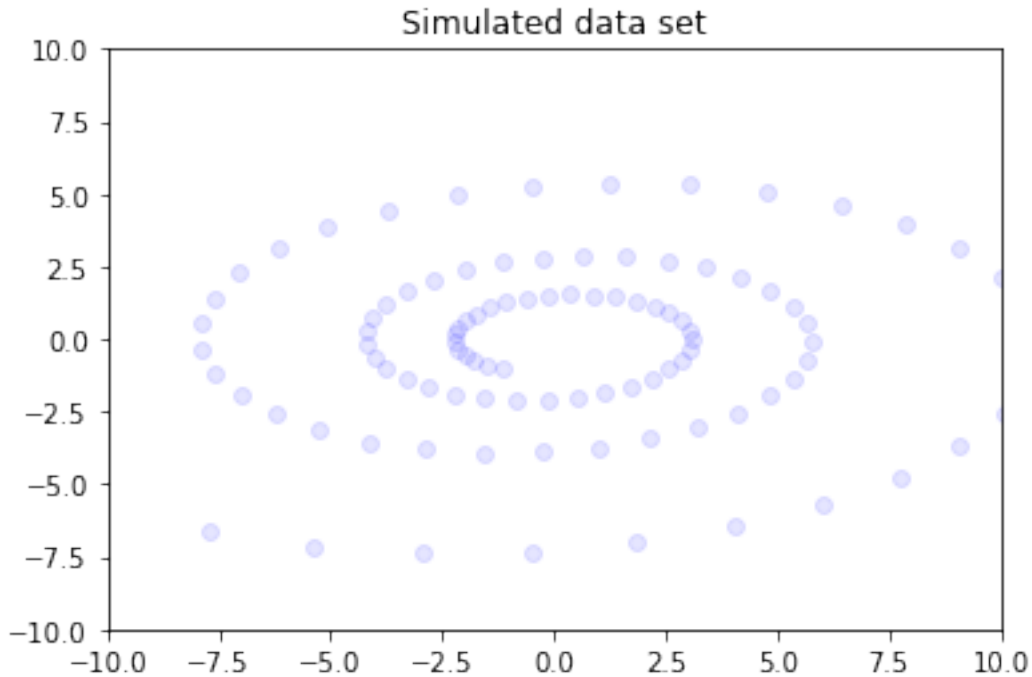
```
In [6]: w = np.random.randn(K,N)
        x_train = np.dot(r,w) + np.random.randn(N,N) * 1e-3

In [7]: # from sklearn.decomposition import PCA
        # pca = PCA(n_components=2)
```

```
# new_r = pca.fit_transform(r_high)
# plt.plot(new_r[:,0], new_r[:,1],'.')
```

You can explore the higher dimensional data manually by changing dim1 and dim2 in the following cell.

```
In [8]: dim1 = 79
        dim2 = 11
        plt.scatter(x_train[:,dim1], x_train[:,dim2], color='blue', alpha=0.1)
        plt.axis([-10, 10, -10, 10])
        plt.title("Simulated data set")
        plt.show()
```



MXFusion Model Definition

Import MXFusion and MXNet modelling components

```
In [9]: from mxfusion.models import Model
        import mxnet.gluon.nn as nn
        from mxfusion.components import Variable
        from mxfusion.components.variables import PositiveTransformation
```

The primary data structure in MXFusion is the Model. Models hold ModelComponents, such as Variables, Distributions, and Functions which are the what define a probabilistic model.

The model we'll be defining for PPCA is:

$$p(z) \sim N(\mu, \Sigma)$$

$$p(x|z, \theta) \sim N(\mathbf{W}\mathbf{z} + \mu, \Psi)$$

where:

$$z \in \mathbb{R}^{NxK}, \mu \in \mathbb{R}^K, \Sigma \in \mathbb{R}^{NxK \times K}, x \in \mathbb{R}^{Nx D}$$

$$\Psi \in \mathbb{R}^{Nx D \times D}, \Psi = [\Psi_0, \dots, \Psi_N], \Psi_i = \sigma^2 \mathbf{I}$$

z here is our latent variable of interest, x is the observed data, and all other variables are parameters or constants of the model.

First we create an MXFusion Model object to build our PPCA model on.

```
In [10]: m = Model()
```

We attach `Variable` objects to our model to collect them in a centralized place. Internally, these are organized into a factor graph which is used during Inference.

```
In [11]: m.w = Variable(shape=(K,D), initial_value=mx.nd.array(np.random.randn(K,D)))
```

Because the mean of x 's distribution is composed of the dot product of z and W , we need to create a dot product function. First we create a dot product function in MXNet and then wrap the function into MXFusion using the `MXFusionGluonFunction` class. `m.dot` can then be called like a normal python function and will apply to the variables it is called on.

```
In [12]: dot = nn.HybridLambda(function='dot')
        m.dot = mf.functions.MXFusionGluonFunction(dot, nOutputs=1, broadcastable=False)
```

Now we define `m.z` which has an identity matrix covariance, `cov`, and zero mean.

`m.z` and `sigma_2` are then used to define `m.x`.

Note that both `sigma_2` and `cov` will be added implicitly into the `Model` because they are inputs to `m.x`.

```
In [13]: cov = mx.nd.broadcast_to(mx.nd.expand_dims(mx.nd.array(np.eye(K,K)), 0), shape=(N,K,K))
        m.z = mf.distributions.MultivariateNormal.define_variable(mean=mx.nd.zeros(shape=(N,K)), cov=cov)
        sigma_2 = Variable(shape=(1,), transformation=PositiveTransformation())
        m.x = mf.distributions.Normal.define_variable(mean=m.dot(m.z, m.w), variance=sigma_2, shape=(N,K))
```

Posterior Definition

Now that we have our model, we need to define a posterior with parameters for the inference algorithm to optimize. When constructing a Posterior, we pass in the `Model` it is defined over and `ModelComponent`'s from the original `Model` are accessible and visible in the Posterior.

The covariance matrix must continue to be positive definite throughout the optimization process in order to succeed in the Cholesky decomposition when drawing samples or computing the log pdf of $q.z$. To satisfy this, we pass the covariance matrix parameters through a Gluon function that forces it into a Symmetric matrix which for suitable initialization values should maintain positive definite-ness throughout the optimization procedure.

```
In [14]: from mxfusion.inference import BatchInferenceLoop, GradBasedInference, StochasticVariationalInference
        class SymmetricMatrix(mx.gluon.HybridBlock):
            def hybrid_forward(self, F, x, *args, **kwargs):
                return F.sum((F.expand_dims(x, 3)*F.expand_dims(x, 2)), axis=-3)
```

While this model has an analytical solution, we will run Variational Inference to find the posterior to demonstrate inference in a setting where the answer is known.

We place a multivariate normal prior over z because that is z 's prior in the model and we don't need to approximate anything in this case. Because the form we're optimizing over is the true model, the optimization is convex and will always converge to the same answer given by classical PCA given enough iterations.

```
In [15]: q = mf.models.Posterior(m)
        sym = mf.components.functions.MXFusionGluonFunction(SymmetricMatrix(), nOutputs=1, broadcastable=False)
        cov = Variable(shape=(N,K,K), initial_value=mx.nd.broadcast_to(mx.nd.expand_dims(mx.nd.array(np.eye(K,K)), 0), shape=(N,K,K)))
        q.post_cov = sym(cov)
        q.post_mean = Variable(shape=(N,K), initial_value=mx.nd.array(np.random.randn(N,K)))
        q.z.set_prior(mf.distributions.MultivariateNormal(mean=q.post_mean, covariance=q.post_cov))
```

We now take our posterior and model, along with an observation pattern (in our case only $m.x$ is observed) and create an inference algorithm. This inference algorithm is combined with a gradient loop to create the Inference method `infr`.

```
In [16]: observed = [m.x]
         alg = StochasticVariationalInference(nSamples=3, model=m, posterior=q, observed=observed)
         infr = GradBasedInference(inference_algorithm=alg, grad_loop=BatchInferenceLoop())
```

The inference method is then initialized with our training data and we run optimization for a while until convergence.

```
In [17]: infr.initialize(x=mx.nd.array(x_train))

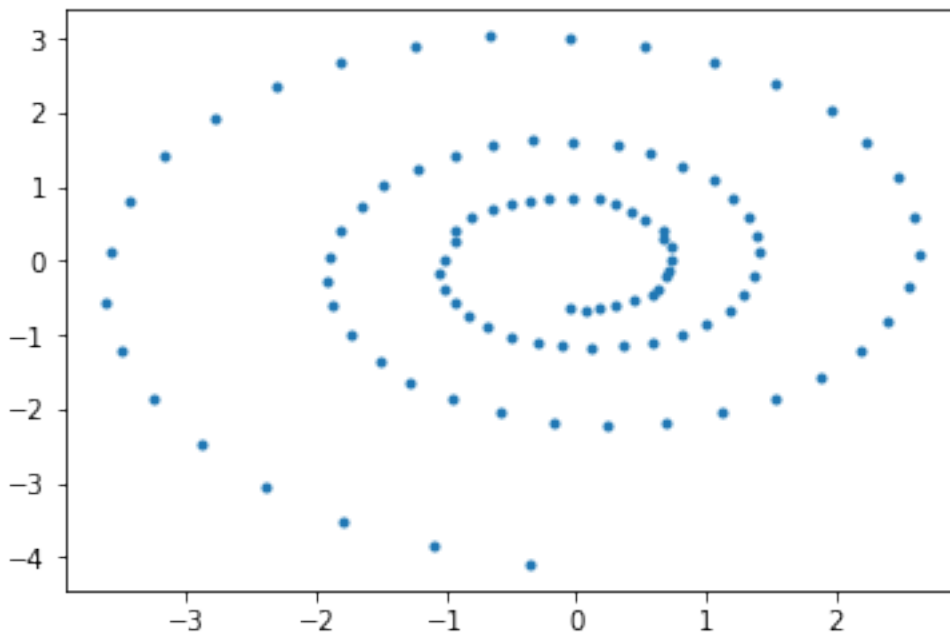
/Users/erimeiss/workspace/MXFusion/src/MXFusion/mxfusion/inference/inference_parameters.py:52: UserWarning: InferenceParameters has already been initialized. The existing one will be overwritten.
  warnings.warn("InferenceParameters has already been initialized. The existing one will be overwritten.")

In [18]: infr.run(max_iter=1000, learning_rate=1e-2, x=mx.nd.array(x_train))

/Users/erimeiss/workspace/MXFusion/src/MXFusion/mxfusion/inference/inference.py:111: UserWarning: Trying to initialize the inference twice, skipping.
  warnings.warn("Trying to initialize the inference twice, skipping.")
/Users/erimeiss/workspace/MXFusion/src/MXFusion/mxfusion/models/factor_graph.py:194: UserWarning: Function evaluation in FactorGraph.compute_log_prob_RT: the outcome variable 'x' is not observed.
  warnings.warn('Function evaluation in FactorGraph.compute_log_prob_RT: the outcome variable ' + str(x) + ' is not observed.')
```

Once training completes, we retrieve the posterior mean (our trained representation for $\mathbf{Wz} + \mu$) from the inference method and plot it. As shown, the plot recovers (up to rotation) the original 2D data quite well.

```
In [19]: post_z_mean = infr.params[q.z.factor.mean].asnumpy()
In [20]: post_z_mean.shape
Out[20]: (100, 2)
In [21]: plt.plot(post_z_mean[:,0], post_z_mean[:,1],'.')
Out[21]: [<matplotlib.lines.Line2D at 0x11d6f3e80>]
```



Saving Inference Results

2.2 Design Choices

2.2.1 CIPs

CIPs are a design proposal mechanism from the Apache Software Foundation.

CHAPTER 3

API Reference

mxfusion

Below is a list of tutorial / example notebooks demonstrating MXFusion's functionality.

4.1 Getting Started

4.2 Example Models

4.2.1 Bayesian Neural Network (VI) for classification (under Development)

```
In [1]: import mxfusion as mf
import mxnet as mx
import numpy as np
import mxnet.gluon.nn as nn
import mxfusion.components
import mxfusion.inference

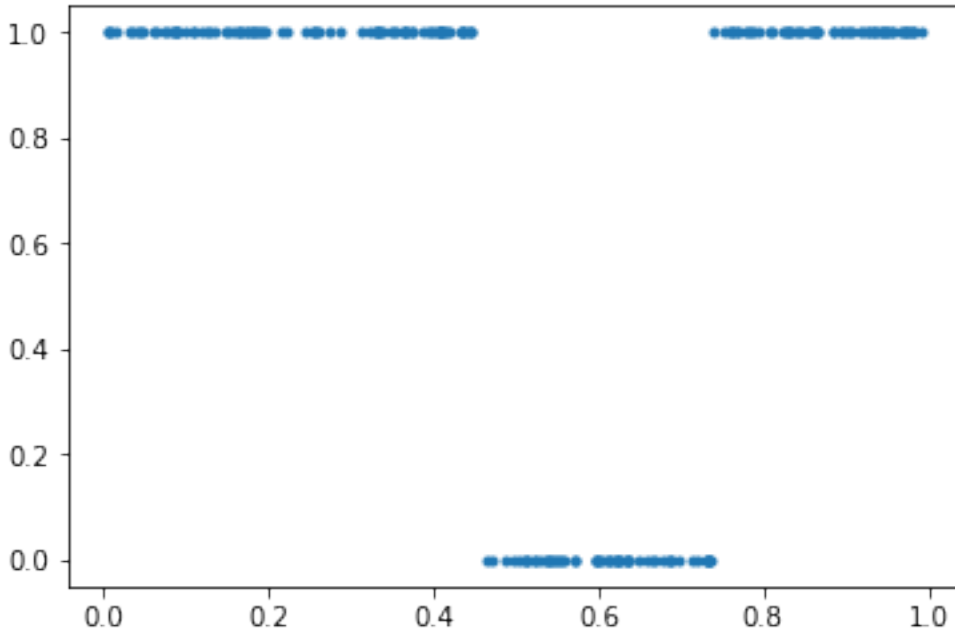
/Users/zhenwend/anaconda3/lib/python3.6/site-packages/h5py/__init__.py:36: FutureWarning: Conversion
from ._conv import register_converters as _register_converters
```

Generate Synthetic Data

```
In [75]: import GPy
import matplotlib inline
from pylab import *

np.random.seed(4)
k = GPy.kern.RBF(1, lengthscale=0.1)
x = np.random.rand(200,1)
y = np.random.multivariate_normal(mean=np.zeros((200,)), cov=k.K(x), size=(1,)).T>0.
plot(x[:,0], y[:,0], '.')

Out[75]: [<matplotlib.lines.Line2D at 0x1a22348898>]
```



```
In [76]: D = 10
net = nn.HybridSequential(prefix='nn_')
with net.name_scope():
    net.add(nn.Dense(D, activation="tanh", flatten=False, in_units=1))
    net.add(nn.Dense(D, activation="tanh", flatten=False, in_units=D))
    net.add(nn.Dense(2, flatten=False, in_units=D))
net.initialize(mx.init.Xavier(magnitude=1))

In [77]: from mxfusion.components.variables.var_trans import PositiveTransformation
from mxfusion.inference import VariationalPosteriorForwardSampling

In [78]: m = mf.components.Model()
m.N = mf.components.Variable()
m.f = mf.components.functions.MXFusionGluonFunction(net, nOutputs=1, broadcastable=False)
m.x = mf.components.Variable(shape=(m.N,1))
m.r = m.f(m.x)
for _,v in m.r.factor.block_variables:
    v.set_prior(mf.components.distributions.Normal(mean=mx.nd.array([0]),variance=mx.nd.array([1])))
m.y = mf.components.distributions.Categorical.define_variable(log_prob=m.r, shape=(m.N,1))
m.show()

Variable(45b58) ~ Normal(mean=Variable(738a7), variance=Variable(9ef9b))
Variable(d7aa2) ~ Normal(mean=Variable(b4564), variance=Variable(02ad0))
Variable(ace48) ~ Normal(mean=Variable(3989f), variance=Variable(49e6a))
Variable(35ae3) ~ Normal(mean=Variable(666b4), variance=Variable(5c0d8))
Variable(7a303) ~ Normal(mean=Variable(9d461), variance=Variable(dd20b))
Variable(28ccc) ~ Normal(mean=Variable(37c47), variance=Variable(a7de6))
r = GluonFunctionEvaluation(nn_dense0_weight=Variable(28ccc), nn_dense0_bias=Variable(7a303), nn_dense0_activation=Variable(45b58))
y ~ Categorical(log_prob=r)

In [79]: from mxfusion.inference import BatchInferenceLoop, create_Gaussian_meanfield, GradBasedInference

In [80]: observed = [m.y, m.x]
q = create_Gaussian_meanfield(model=m, observed=observed)
alg = StochasticVariationalInference(num_samples=5, model=m, posterior=q, observed=observed)
# alg = MAP(model=m, observed=observed)
infr = GradBasedInference(inference_algorithm=alg, grad_loop=BatchInferenceLoop())
```

```

In [81]: infr.initialize(y=mx.nd.array(y), x=mx.nd.array(x))

/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/inference/inference_parameters.py:52: UserWarning:In

In [82]: for v_name, v in m.r.factor.block_variables:
        uuid = v.uuid
        loc_uuid = infr.inference_algorithm.posterior[uuid].factor.variance.uuid
        a = infr.params.param_dict[loc_uuid].data().asnumpy()
        a[:] = 1e-8
        infr.params[infr.inference_algorithm.posterior[uuid].factor.mean] = net.collect_params()
        infr.params[infr.inference_algorithm.posterior[uuid].factor.variance] = mx.nd.array(a)

In [83]: infr.run(max_iter=500, learning_rate=1e-1, y=mx.nd.array(y), x=mx.nd.array(x), verbose=True)

/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/inference/inference.py:111: UserWarning:Trying to in

Iteration 1 logL: -1544.5255126953125
Iteration 2 logL: -1539.4837646484375
Iteration 3 logL: -1511.021484375
Iteration 4 logL: -1505.3983154296875
Iteration 5 logL: -1494.5648193359375
Iteration 6 logL: -1491.2451171875
Iteration 7 logL: -1478.662841796875
Iteration 8 logL: -1478.6864013671875
Iteration 9 logL: -1471.1865234375
Iteration 10 logL: -1452.61962890625
Iteration 11 logL: -1451.615478515625
Iteration 12 logL: -1444.682373046875
Iteration 13 logL: -1445.5955810546875
Iteration 14 logL: -1430.4305419921875
Iteration 15 logL: -1418.5712890625
Iteration 16 logL: -1418.8111572265625
Iteration 17 logL: -1404.1358642578125
Iteration 18 logL: -1400.627685546875
Iteration 19 logL: -1381.745361328125
Iteration 20 logL: -1376.2139892578125
Iteration 21 logL: -1372.777099609375
Iteration 22 logL: -1366.9664306640625
Iteration 23 logL: -1361.6920166015625
Iteration 24 logL: -1342.0687255859375
Iteration 25 logL: -1341.3878173828125
Iteration 26 logL: -1335.53271484375
Iteration 27 logL: -1321.6600341796875
Iteration 28 logL: -1322.144287109375
Iteration 29 logL: -1304.44482421875
Iteration 30 logL: -1296.4647216796875
Iteration 31 logL: -1288.6043701171875
Iteration 32 logL: -1288.419189453125
Iteration 33 logL: -1273.767333984375
Iteration 34 logL: -1261.6514892578125
Iteration 35 logL: -1246.7862548828125
Iteration 36 logL: -1237.2008056640625
Iteration 37 logL: -1230.070556640625
Iteration 38 logL: -1217.3485107421875
Iteration 39 logL: -1210.28466796875
Iteration 40 logL: -1196.698486328125
Iteration 41 logL: -1179.746826171875
Iteration 42 logL: -1172.70556640625
Iteration 43 logL: -1153.209716796875
Iteration 44 logL: -1144.113037109375
Iteration 45 logL: -1131.1912841796875

```

```
Iteration 46 logL: -1122.3773193359375
Iteration 47 logL: -1108.426025390625
Iteration 48 logL: -1095.648193359375
Iteration 49 logL: -1082.5948486328125
Iteration 50 logL: -1079.716552734375
Iteration 51 logL: -1066.1383056640625
Iteration 52 logL: -1065.216064453125
Iteration 53 logL: -1048.493896484375
Iteration 54 logL: -1039.2891845703125
Iteration 55 logL: -1040.451416015625
Iteration 56 logL: -1024.9017333984375
Iteration 57 logL: -1007.782958984375
Iteration 58 logL: -1014.7578125
Iteration 59 logL: -991.4736328125
Iteration 60 logL: -991.7649536132812
Iteration 61 logL: -981.59716796875
Iteration 62 logL: -974.068603515625
Iteration 63 logL: -972.3157958984375
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```

```

In [12]: for uuid, v in infr.inference_algorithm.posterior.variables.items():
         if uuid in infr.params.param_dict:
             print(v.name, infr.params[v])

```

```

In [84]: xt = np.linspace(0,1,100)[: ,None]

```

```

In [85]: infr2 = VariationalPosteriorForwardSampling(10, [m.x], infr, [m.r])
         res = infr2.run(x=mx.nd.array(xt))

```

```

/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/core/factor_graph.py:65: UserWarning:The value N has
/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/core/factor_graph.py:65: UserWarning:The value y has
/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/inference/inference_parameters.py:52: UserWarning:In

```

```

In [86]: yt = res[m.r].asnumpy()

```

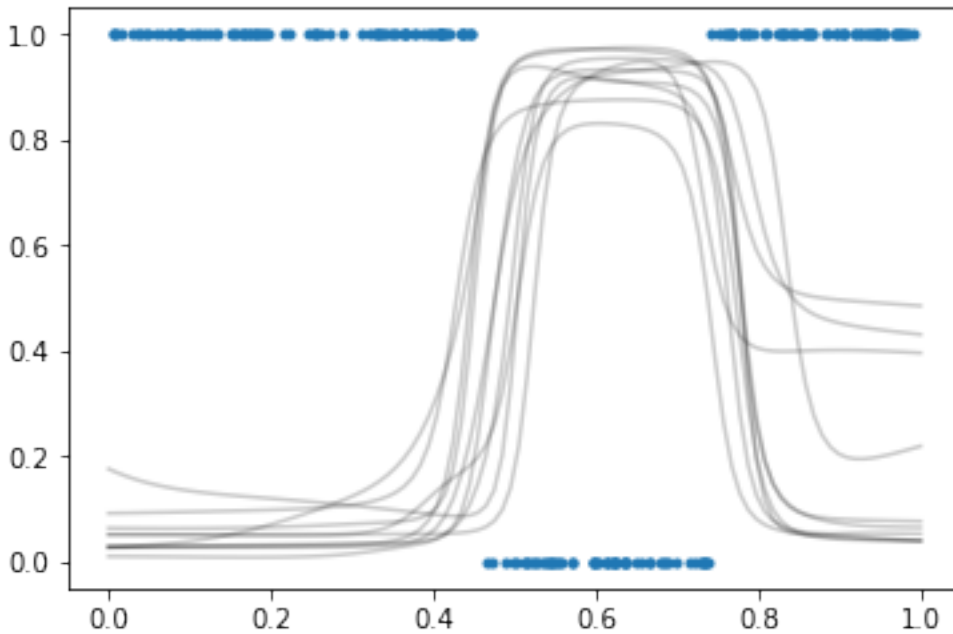
```

In [87]: # plot(xt[:,0],yt[:,0])
         yt_mean = yt.mean(0)
         yt_std = yt.std(0)

```

```
#plot(xt[:,0], yt.mean(0)[:,0])
#errorbar(xt[:,0],y=yt_mean[:,0],yerr=yt_std[:,0]*2)
for i in range(yt.shape[0]):
    plot(xt[:,0],1./(1+np.exp(-yt[i,:,0])), 'k', alpha=0.2)
plot(x[:,0],y[:,0],'.')
```

Out [87]: [<matplotlib.lines.Line2D at 0x1a222e37f0>]



4.2.2 Bayesian Neural Network (VI) for regression

Zhenwen Dai (2018-8-21)

```
In [1]: import mxfusion as mf
import mxnet as mx
import numpy as np
import mxnet.gluon.nn as nn
import mxfusion.components
import mxfusion.inference
```

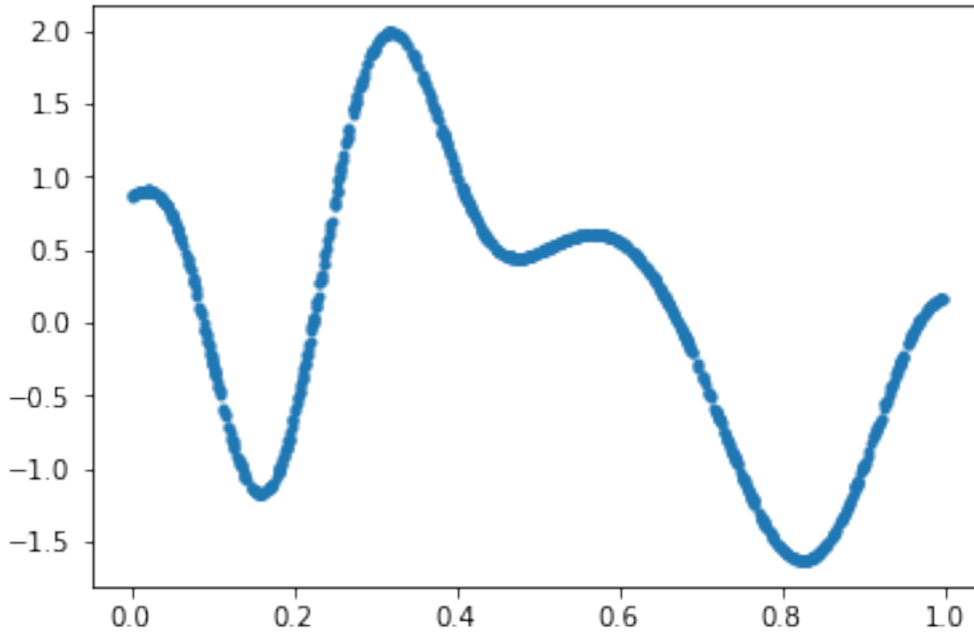
```
/Users/zhenwend/anaconda3/lib/python3.6/site-packages/h5py/__init__.py:36: FutureWarning: Conversion
from ._conv import register_converters as _register_converters
```

Generate Synthetic Data

```
In [2]: import GPy
%matplotlib inline
from pylab import *

k = GPy.kern.RBF(1, lengthscale=0.1)
x = np.random.rand(1000,1)
y = np.random.multivariate_normal(mean=np.zeros((1000,)), cov=k.K(x), size=(1,)).T
plot(x[:,0], y[:,0], '.')
```

Out [2]: [<matplotlib.lines.Line2D at 0x1097ed358>]



Model definition

```
In [3]: D = 50
net = nn.HybridSequential(prefix='nn_')
with net.name_scope():
    net.add(nn.Dense(D, activation="tanh"))
    net.add(nn.Dense(D, activation="tanh"))
    net.add(nn.Dense(1, flatten=True))
net.initialize(mx.init.Xavier(magnitude=3))
_=net(mx.nd.array(x))

In [4]: from mxfusion.components.var_trans import PositiveTransformation
from mxfusion.inference import VariationalPosteriorForwardSampling

In [5]: m = mf.core.Model()
m.N = mf.components.Variable()
m.f = mf.components.functions.MXFusionGluonFunction(net, nOutputs=1,broadcastable=False)
m.x = mf.components.Variable(shape=(m.N,1))
m.v = mf.components.Variable(shape=(1,), transformation=PositiveTransformation(), initial_val=1)
#m.prior_variance = mf.core.Variable(shape=(1,), transformation=PositiveTransformation())
m.r = m.f(m.x)
for _,v in m.r.factor.block_variables:
    v.set_prior(mf.components.distributions.Normal(mean=mx.nd.array([0]),variance=mx.nd.array([1])))
m.y = mf.components.distributions.Normal.define_variable(mean=m.r, variance=m.v, shape=(m.N,1))
m.show()

Variable(24825) ~ Normal(mean=Variable(3706e), variance=Variable(78c3f))
Variable(1f4c5) ~ Normal(mean=Variable(d8e05), variance=Variable(b73d6))
Variable(1dbe9) ~ Normal(mean=Variable(6e428), variance=Variable(ee4e8))
Variable(9abb8) ~ Normal(mean=Variable(f8cb1), variance=Variable(73d44))
Variable(cdf2a) ~ Normal(mean=Variable(b4c6f), variance=Variable(5f593))
Variable(e28f4) ~ Normal(mean=Variable(528e0), variance=Variable(c17f7))
r = GluonFunctionEvaluation(nn_dense0_weight=Variable(e28f4), nn_dense0_bias=Variable(cdf2a), nn_dense0_activation=Variable(e28f4))
y ~ Normal(mean=r, variance=v)
```

Inference with Meanfield

```
In [7]: from mxfusion.inference import BatchInferenceLoop, create_Gaussian_meanfield, GradBasedInference

In [9]: observed = [m.y, m.x]
        q = create_Gaussian_meanfield(model=m, observed=observed)
        alg = StochasticVariationalInference(num_samples=3, model=m, posterior=q, observed=observed)
        infr = GradBasedInference(inference_algorithm=alg, grad_loop=BatchInferenceLoop())

In [10]: infr.initialize(y=mx.nd.array(y), x=mx.nd.array(x))

/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/inference/inference_parameters.py:52: UserWarning:Inference
algorithm is not supported for this model.

In [13]: for v_name, v in m.r.factor.block_variables:
        uuid = v.uuid
        loc_uuid = infr.inference_algorithm.posterior[uuid].factor.variance.uuid
        a = infr.params.param_dict[loc_uuid].data().asnumpy()
        a[:] = 1e-6
        infr.params[infr.inference_algorithm.posterior[uuid].factor.mean] = net.collect_params('mean')
        infr.params[infr.inference_algorithm.posterior[uuid].factor.variance] = mx.nd.array(a)

In [14]: infr.run(max_iter=2000, learning_rate=1e-2, y=mx.nd.array(y), x=mx.nd.array(x), verbose=True)

/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/inference/inference.py:111: UserWarning:Trying to infer
with a model that is not supported by the inference algorithm.

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Iteration 4 logL: -18668.005859375
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Iteration 1849 logL: -1119.8642578125
Iteration 1850 logL: -1010.772216796875
Iteration 1851 logL: -1057.302734375
Iteration 1852 logL: -1090.306884765625
Iteration 1853 logL: -1407.312255859375
Iteration 1854 logL: -1477.843505859375
Iteration 1855 logL: -1237.176025390625
Iteration 1856 logL: -1005.63037109375
Iteration 1857 logL: -1027.980224609375
Iteration 1858 logL: -1343.48583984375
Iteration 1859 logL: -1054.12548828125
Iteration 1860 logL: -1100.2314453125
Iteration 1861 logL: -940.71484375
Iteration 1862 logL: -1200.455322265625
Iteration 1863 logL: -1142.964111328125
Iteration 1864 logL: -905.65185546875
Iteration 1865 logL: -1021.826416015625
```

```
Iteration 1866 logL: -1014.808349609375
Iteration 1867 logL: -1071.56103515625
Iteration 1868 logL: -1333.482177734375
Iteration 1869 logL: -963.418701171875
Iteration 1870 logL: -1064.89697265625
Iteration 1871 logL: -1108.72900390625
Iteration 1872 logL: -1067.771484375
Iteration 1873 logL: -1127.8828125
Iteration 1874 logL: -1081.60302734375
Iteration 1875 logL: -965.2626953125
Iteration 1876 logL: -988.87255859375
Iteration 1877 logL: -1065.111083984375
Iteration 1878 logL: -998.36376953125
Iteration 1879 logL: -987.1142578125
Iteration 1880 logL: -1086.422119140625
Iteration 1881 logL: -1011.31591796875
Iteration 1882 logL: -1096.4521484375
Iteration 1883 logL: -1229.218994140625
Iteration 1884 logL: -1258.369873046875
Iteration 1885 logL: -1353.3291015625
Iteration 1886 logL: -857.21875
Iteration 1887 logL: -1257.5390625
Iteration 1888 logL: -983.54736328125
Iteration 1889 logL: -1463.050048828125
Iteration 1890 logL: -902.812255859375
Iteration 1891 logL: -1015.60205078125
Iteration 1892 logL: -937.58642578125
Iteration 1893 logL: -973.899169921875
Iteration 1894 logL: -1120.499755859375
Iteration 1895 logL: -1576.31640625
Iteration 1896 logL: -1102.259521484375
Iteration 1897 logL: -1324.40478515625
Iteration 1898 logL: -1041.040771484375
Iteration 1899 logL: -1416.749267578125
Iteration 1900 logL: -1493.891357421875
Iteration 1901 logL: -1039.11279296875
Iteration 1902 logL: -1012.100341796875
Iteration 1903 logL: -1212.315673828125
Iteration 1904 logL: -1539.478515625
Iteration 1905 logL: -1077.4384765625
Iteration 1906 logL: -992.618408203125
Iteration 1907 logL: -979.22802734375
Iteration 1908 logL: -1281.15771484375
Iteration 1909 logL: -1554.8798828125
Iteration 1910 logL: -1005.364990234375
Iteration 1911 logL: -899.75537109375
Iteration 1912 logL: -1055.173095703125
Iteration 1913 logL: -1163.792724609375
Iteration 1914 logL: -1157.046142578125
Iteration 1915 logL: -1776.942626953125
Iteration 1916 logL: -1032.344970703125
Iteration 1917 logL: -1102.173095703125
Iteration 1918 logL: -1496.106201171875
Iteration 1919 logL: -1098.893310546875
Iteration 1920 logL: -1040.317138671875
Iteration 1921 logL: -1673.8388671875
Iteration 1922 logL: -1684.88623046875
Iteration 1923 logL: -1116.3251953125
Iteration 1924 logL: -1416.927001953125
```

```
Iteration 1925 logL: -987.152587890625
Iteration 1926 logL: -1066.673095703125
Iteration 1927 logL: -1040.917724609375
Iteration 1928 logL: -1074.169921875
Iteration 1929 logL: -1119.952880859375
Iteration 1930 logL: -1414.101806640625
Iteration 1931 logL: -876.994384765625
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Iteration 1936 logL: -991.05908203125
Iteration 1937 logL: -1131.446044921875
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Iteration 1941 logL: -1233.37841796875
Iteration 1942 logL: -1017.934814453125
Iteration 1943 logL: -832.17529296875
Iteration 1944 logL: -989.371826171875
Iteration 1945 logL: -1345.60302734375
Iteration 1946 logL: -1143.80224609375
Iteration 1947 logL: -1175.467041015625
Iteration 1948 logL: -1102.8701171875
Iteration 1949 logL: -1056.500244140625
Iteration 1950 logL: -951.403564453125
Iteration 1951 logL: -856.87353515625
Iteration 1952 logL: -1007.120849609375
Iteration 1953 logL: -896.989013671875
Iteration 1954 logL: -1194.041259765625
Iteration 1955 logL: -1053.199462890625
Iteration 1956 logL: -865.03466796875
Iteration 1957 logL: -1246.1025390625
Iteration 1958 logL: -1341.726318359375
Iteration 1959 logL: -889.03857421875
Iteration 1960 logL: -1292.580322265625
Iteration 1961 logL: -921.563232421875
Iteration 1962 logL: -1567.103759765625
Iteration 1963 logL: -1208.059814453125
Iteration 1964 logL: -921.08056640625
Iteration 1965 logL: -1033.3154296875
Iteration 1966 logL: -1243.2275390625
Iteration 1967 logL: -1147.265380859375
Iteration 1968 logL: -1195.745361328125
Iteration 1969 logL: -827.04443359375
Iteration 1970 logL: -1138.609375
Iteration 1971 logL: -975.8818359375
Iteration 1972 logL: -1208.3505859375
Iteration 1973 logL: -855.1357421875
Iteration 1974 logL: -957.8818359375
Iteration 1975 logL: -963.307373046875
Iteration 1976 logL: -1086.295166015625
Iteration 1977 logL: -902.845703125
Iteration 1978 logL: -1262.313232421875
Iteration 1979 logL: -1039.027587890625
Iteration 1980 logL: -892.798095703125
Iteration 1981 logL: -943.1220703125
Iteration 1982 logL: -1156.06591796875
Iteration 1983 logL: -1353.580078125
```

```
Iteration 1984 logL: -856.92529296875
Iteration 1985 logL: -1020.078857421875
Iteration 1986 logL: -1095.52685546875
Iteration 1987 logL: -1237.697265625
Iteration 1988 logL: -998.10693359375
Iteration 1989 logL: -1152.889892578125
Iteration 1990 logL: -963.375732421875
Iteration 1991 logL: -925.7431640625
Iteration 1992 logL: -906.114013671875
Iteration 1993 logL: -1085.943359375
Iteration 1994 logL: -1247.585693359375
Iteration 1995 logL: -931.400146484375
Iteration 1996 logL: -993.2607421875
Iteration 1997 logL: -1423.531005859375
Iteration 1998 logL: -968.134521484375
Iteration 1999 logL: -927.2412109375
Iteration 2000 logL: -987.966064453125
```

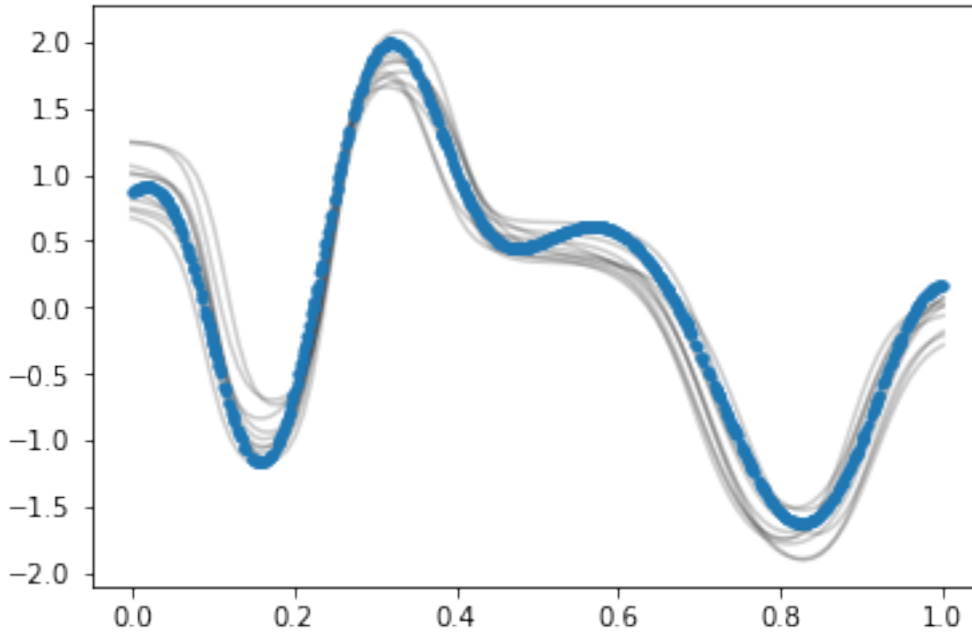
Use prediction to visualize the resulting BNN

```
In [15]: xt = np.linspace(0,1,100)[: ,None]
In [16]: infr2 = VariationalPosteriorForwardSampling(10, [m.x], infr, [m.r])
         res = infr2.run(x=mx.nd.array(xt))

/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/core/factor_graph.py:65: UserWarning:The value N has
/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/core/factor_graph.py:65: UserWarning:The value y has
/Users/zhenwend/mxfusion/src/MXFusion/mxfusion/inference/inference_parameters.py:52: UserWarning:In

In [17]: yt = res[m.r].asnumpy()
In [18]: # plot(xt[:,0],yt[:,0])
         yt_mean = yt.mean(0)
         yt_std = yt.std(0)
         #plot(xt[:,0], yt.mean(0)[: ,0])
         #errorbar(xt[:,0],y=yt_mean[:,0],yerr=yt_std[:,0]*2)
         for i in range(yt.shape[0]):
             plot(xt[:,0],yt[i,:,0], 'k', alpha=0.2)
         plot(x[:,0],y[:,0], '.')

Out[18]: [<matplotlib.lines.Line2D at 0x1a26059b00>]
```



4.2.3 Variational Auto-Encoder (VAE)

Zhenwen Dai (2018-8-21)

```
In [1]: import mxfusion as mf
import mxnet as mx
import numpy as np
import mxnet.gluon.nn as nn
import mxfusion.components
import mxfusion.inference
%matplotlib inline
from pylab import *
```

```
/Users/zhenwend/anaconda3/lib/python3.6/site-packages/h5py/__init__.py:36: FutureWarning: Conversion
from ._conv import register_converters as _register_converters
```

Load a toy dataset

```
In [2]: import GPy
data = GPy.util.datasets.oil_100()
Y = data['X']
label = data['Y'].argmax(1)
```

```
In [3]: N, D = Y.shape
```

Model Defintion

```
In [4]: Q = 2
```

```
In [5]: H = 50
encoder = nn.HybridSequential(prefix='encoder_')
with encoder.name_scope():
```



```
/Users/zhenwend/anaconda3/lib/python3.6/site-packages/mxnet/gluon/parameter.py:689: UserWarning:Para
/Users/zhenwend/anaconda3/lib/python3.6/site-packages/mxnet/gluon/parameter.py:689: UserWarning:Para

Iteration 1 logL: -1460.925048828125
Iteration 2 logL: -1562.58935546875
Iteration 3 logL: -1281.037109375
Iteration 4 logL: -1202.09814453125
Iteration 5 logL: -1215.446533203125
Iteration 6 logL: -1242.7581787109375
Iteration 7 logL: -1206.203125
Iteration 8 logL: -1193.624755859375
Iteration 9 logL: -1133.6195068359375
Iteration 10 logL: -1112.78466796875
Iteration 11 logL: -1098.210205078125
Iteration 12 logL: -1090.024169921875
Iteration 13 logL: -1077.6949462890625
Iteration 14 logL: -1074.197021484375
Iteration 15 logL: -1060.966796875
Iteration 16 logL: -1047.22314453125
Iteration 17 logL: -1042.4344482421875
Iteration 18 logL: -1035.609619140625
Iteration 19 logL: -1028.633544921875
Iteration 20 logL: -1029.137939453125
Iteration 21 logL: -1024.3011474609375
Iteration 22 logL: -1023.6302490234375
Iteration 23 logL: -1019.930908203125
Iteration 24 logL: -1010.139892578125
Iteration 25 logL: -1006.3385009765625
Iteration 26 logL: -1000.4537353515625
Iteration 27 logL: -994.9822998046875
Iteration 28 logL: -989.8155517578125
Iteration 29 logL: -982.1632080078125
Iteration 30 logL: -977.3480834960938
Iteration 31 logL: -974.651123046875
Iteration 32 logL: -974.5823364257812
Iteration 33 logL: -967.2603759765625
Iteration 34 logL: -963.084716796875
Iteration 35 logL: -957.8111572265625
Iteration 36 logL: -956.9771118164062
Iteration 37 logL: -947.5377807617188
Iteration 38 logL: -945.8042602539062
Iteration 39 logL: -944.1073608398438
Iteration 40 logL: -938.4964599609375
Iteration 41 logL: -930.6653442382812
Iteration 42 logL: -925.6103515625
Iteration 43 logL: -924.9813842773438
Iteration 44 logL: -924.310302734375
Iteration 45 logL: -916.4560546875
Iteration 46 logL: -917.2510375976562
Iteration 47 logL: -910.7885131835938
Iteration 48 logL: -908.1454467773438
Iteration 49 logL: -902.584716796875
Iteration 50 logL: -900.215087890625
Iteration 51 logL: -894.9979248046875
Iteration 52 logL: -892.5367431640625
Iteration 53 logL: -890.0333251953125
Iteration 54 logL: -885.6333618164062
Iteration 55 logL: -880.012451171875
Iteration 56 logL: -876.5682373046875
```

```
Iteration 57 logL: -872.11328125
Iteration 58 logL: -874.2131958007812
Iteration 59 logL: -866.4677734375
Iteration 60 logL: -862.5056762695312
Iteration 61 logL: -860.6942138671875
Iteration 62 logL: -859.4818115234375
Iteration 63 logL: -851.3370971679688
Iteration 64 logL: -846.3784790039062
Iteration 65 logL: -844.3232421875
Iteration 66 logL: -841.620361328125
Iteration 67 logL: -839.131591796875
Iteration 68 logL: -835.3382568359375
Iteration 69 logL: -831.16259765625
Iteration 70 logL: -828.3026123046875
Iteration 71 logL: -823.78564453125
Iteration 72 logL: -819.6796875
Iteration 73 logL: -816.356201171875
Iteration 74 logL: -812.4974365234375
Iteration 75 logL: -807.6212768554688
Iteration 76 logL: -804.9386596679688
Iteration 77 logL: -804.6951293945312
Iteration 78 logL: -796.6724243164062
Iteration 79 logL: -793.4720458984375
Iteration 80 logL: -790.3905029296875
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Iteration 84 logL: -779.7852783203125
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Iteration 89 logL: -761.1930541992188
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Iteration 93 logL: -742.4610595703125
Iteration 94 logL: -745.5780639648438
Iteration 95 logL: -739.9026489257812
Iteration 96 logL: -735.1586303710938
Iteration 97 logL: -729.9743041992188
Iteration 98 logL: -727.3143920898438
Iteration 99 logL: -721.768798828125
Iteration 100 logL: -721.2698974609375
Iteration 101 logL: -714.2559204101562
Iteration 102 logL: -707.76318359375
Iteration 103 logL: -709.2598876953125
Iteration 104 logL: -706.3348999023438
Iteration 105 logL: -707.056884765625
Iteration 106 logL: -698.32958984375
Iteration 107 logL: -692.884765625
Iteration 108 logL: -688.1893310546875
Iteration 109 logL: -683.2183837890625
Iteration 110 logL: -684.6583251953125
Iteration 111 logL: -674.1200561523438
Iteration 112 logL: -674.0984497070312
Iteration 113 logL: -671.21533203125
Iteration 114 logL: -664.57421875
Iteration 115 logL: -666.19140625
```

```
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Iteration 118 logL: -658.775146484375
Iteration 119 logL: -650.1072998046875
Iteration 120 logL: -645.4615478515625
Iteration 121 logL: -648.34326171875
Iteration 122 logL: -640.14599609375
Iteration 123 logL: -636.5962524414062
Iteration 124 logL: -639.0338134765625
Iteration 125 logL: -626.3507080078125
Iteration 126 logL: -624.8009643554688
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Iteration 129 logL: -613.326171875
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Iteration 133 logL: -601.2283325195312
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Iteration 135 logL: -592.0599975585938
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Iteration 139 logL: -578.5697631835938
Iteration 140 logL: -578.210205078125
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Iteration 142 logL: -573.1090087890625
Iteration 143 logL: -569.6796875
Iteration 144 logL: -568.4530029296875
Iteration 145 logL: -567.4485473632812
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Iteration 148 logL: -553.80126953125
Iteration 149 logL: -548.371826171875
Iteration 150 logL: -546.1668090820312
Iteration 151 logL: -536.4398193359375
Iteration 152 logL: -532.5432739257812
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Iteration 160 logL: -513.127197265625
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Iteration 172 logL: -482.5163269042969
Iteration 173 logL: -472.4610595703125
Iteration 174 logL: -484.8624267578125
```

```
Iteration 175 logL: -470.081298828125
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```

```
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Iteration 235 logL: -268.1728210449219
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Iteration 245 logL: -262.0987243652344
Iteration 246 logL: -233.15167236328125
Iteration 247 logL: -229.3694305419922
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Iteration 250 logL: -253.81594848632812
Iteration 251 logL: -189.490966796875
Iteration 252 logL: -224.66537475585938
Iteration 253 logL: -199.2983856201172
Iteration 254 logL: -214.942626953125
Iteration 255 logL: -180.802734375
Iteration 256 logL: -218.85873413085938
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Iteration 258 logL: -189.5235137939453
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Iteration 260 logL: -180.61697387695312
Iteration 261 logL: -166.8021697998047
Iteration 262 logL: -156.7022705078125
Iteration 263 logL: -162.89773559570312
Iteration 264 logL: -166.24488830566406
Iteration 265 logL: -160.3469696044922
Iteration 266 logL: -153.28945922851562
Iteration 267 logL: -157.59815979003906
Iteration 268 logL: -167.51414489746094
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Iteration 819 logL: 805.5083618164062
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Iteration 821 logL: 788.1103515625
Iteration 822 logL: 784.2445068359375
Iteration 823 logL: 800.9007568359375
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Iteration 1295 logL: 1051.98876953125
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Iteration 1733 logL: 1155.8565673828125
Iteration 1734 logL: 1141.1715087890625
Iteration 1735 logL: 1088.83837890625
Iteration 1736 logL: 1172.6944580078125
Iteration 1737 logL: 1180.142333984375
Iteration 1738 logL: 1113.2823486328125
Iteration 1739 logL: 1139.8388671875
Iteration 1740 logL: 1173.06201171875
Iteration 1741 logL: 1120.55126953125
Iteration 1742 logL: 1149.968505859375
Iteration 1743 logL: 1187.1422119140625
Iteration 1744 logL: 1172.948974609375
Iteration 1745 logL: 1146.9542236328125
Iteration 1746 logL: 1195.833251953125
Iteration 1747 logL: 1197.7987060546875
Iteration 1748 logL: 1190.53515625
Iteration 1749 logL: 1200.8770751953125
Iteration 1750 logL: 1202.64404296875
Iteration 1751 logL: 1176.536376953125
Iteration 1752 logL: 1204.62353515625
Iteration 1753 logL: 1171.98046875
Iteration 1754 logL: 1138.4837646484375
Iteration 1755 logL: 1168.888671875
Iteration 1756 logL: 1123.74951171875
Iteration 1757 logL: 1099.937744140625
Iteration 1758 logL: 1099.6246337890625
Iteration 1759 logL: 1095.86669921875
Iteration 1760 logL: 1129.895263671875
Iteration 1761 logL: 1061.75341796875
Iteration 1762 logL: 981.8104248046875
Iteration 1763 logL: 1072.3914794921875
Iteration 1764 logL: 1060.898193359375
Iteration 1765 logL: 1064.474365234375
Iteration 1766 logL: 1071.06640625
Iteration 1767 logL: 1029.953369140625
```

```
Iteration 1768 logL: 1157.8651123046875
Iteration 1769 logL: 1072.356201171875
Iteration 1770 logL: 1094.0537109375
Iteration 1771 logL: 1134.451416015625
Iteration 1772 logL: 1059.017822265625
Iteration 1773 logL: 1029.544189453125
Iteration 1774 logL: 1103.8106689453125
Iteration 1775 logL: 1160.5919189453125
Iteration 1776 logL: 1131.671142578125
Iteration 1777 logL: 1128.98046875
Iteration 1778 logL: 1189.90185546875
Iteration 1779 logL: 1136.0472412109375
Iteration 1780 logL: 1103.69775390625
Iteration 1781 logL: 1176.66650390625
Iteration 1782 logL: 1156.9439697265625
Iteration 1783 logL: 1018.382568359375
Iteration 1784 logL: 1121.1993408203125
Iteration 1785 logL: 1174.5164794921875
Iteration 1786 logL: 1138.939697265625
Iteration 1787 logL: 1201.796630859375
Iteration 1788 logL: 1161.7603759765625
Iteration 1789 logL: 1155.3951416015625
Iteration 1790 logL: 1175.95263671875
Iteration 1791 logL: 1190.130126953125
Iteration 1792 logL: 1173.4368896484375
Iteration 1793 logL: 1192.296875
Iteration 1794 logL: 1189.837646484375
Iteration 1795 logL: 1180.27734375
Iteration 1796 logL: 1200.889892578125
Iteration 1797 logL: 1175.4337158203125
Iteration 1798 logL: 1159.1953125
Iteration 1799 logL: 1195.88671875
Iteration 1800 logL: 1186.492919921875
Iteration 1801 logL: 1154.389404296875
Iteration 1802 logL: 1210.261474609375
Iteration 1803 logL: 1188.316162109375
Iteration 1804 logL: 1147.332275390625
Iteration 1805 logL: 1172.823974609375
Iteration 1806 logL: 1190.45556640625
Iteration 1807 logL: 1187.948974609375
Iteration 1808 logL: 1190.2025146484375
Iteration 1809 logL: 1163.7408447265625
Iteration 1810 logL: 1209.648681640625
Iteration 1811 logL: 1209.9573974609375
Iteration 1812 logL: 1181.302734375
Iteration 1813 logL: 1199.8917236328125
Iteration 1814 logL: 1229.9256591796875
Iteration 1815 logL: 1146.1197509765625
Iteration 1816 logL: 1150.55810546875
Iteration 1817 logL: 1197.42919921875
Iteration 1818 logL: 1208.4410400390625
Iteration 1819 logL: 1229.9888916015625
Iteration 1820 logL: 1191.4019775390625
Iteration 1821 logL: 1202.1630859375
Iteration 1822 logL: 1183.2589111328125
Iteration 1823 logL: 1184.36865234375
Iteration 1824 logL: 1179.5299072265625
Iteration 1825 logL: 1195.7923583984375
Iteration 1826 logL: 1207.087890625
```

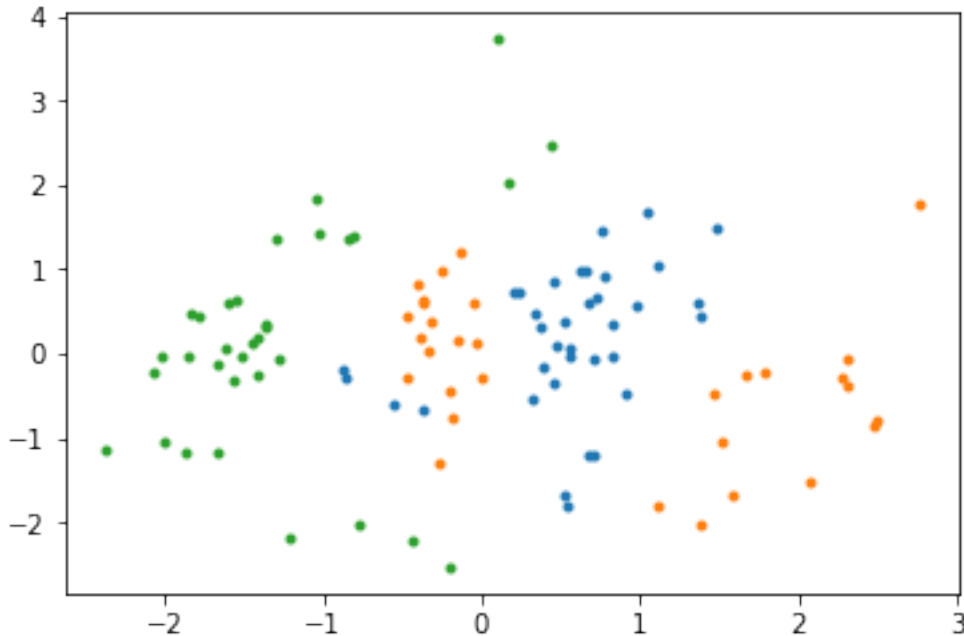
```
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Iteration 1828 logL: 1137.027587890625
Iteration 1829 logL: 1150.9666748046875
Iteration 1830 logL: 1153.437255859375
Iteration 1831 logL: 1195.476318359375
Iteration 1832 logL: 1201.533935546875
Iteration 1833 logL: 1209.5994873046875
Iteration 1834 logL: 1133.618896484375
Iteration 1835 logL: 1119.32373046875
Iteration 1836 logL: 1163.4991455078125
Iteration 1837 logL: 1176.7540283203125
Iteration 1838 logL: 1182.48046875
Iteration 1839 logL: 1180.406982421875
Iteration 1840 logL: 1139.6094970703125
Iteration 1841 logL: 1161.464599609375
Iteration 1842 logL: 1150.23486328125
Iteration 1843 logL: 1201.280517578125
Iteration 1844 logL: 1171.5853271484375
Iteration 1845 logL: 1145.40234375
Iteration 1846 logL: 1153.2955322265625
Iteration 1847 logL: 1182.4085693359375
Iteration 1848 logL: 1182.6571044921875
Iteration 1849 logL: 1121.10498046875
Iteration 1850 logL: 1168.7552490234375
Iteration 1851 logL: 1215.7532958984375
Iteration 1852 logL: 1168.606201171875
Iteration 1853 logL: 1156.6822509765625
Iteration 1854 logL: 1185.0814208984375
Iteration 1855 logL: 1208.6463623046875
Iteration 1856 logL: 1177.5478515625
Iteration 1857 logL: 1141.1156005859375
Iteration 1858 logL: 1191.260498046875
Iteration 1859 logL: 1197.61767578125
Iteration 1860 logL: 1227.127197265625
Iteration 1861 logL: 1163.735107421875
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Iteration 1864 logL: 1213.536865234375
Iteration 1865 logL: 1185.064453125
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Iteration 1867 logL: 1200.761962890625
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Iteration 1872 logL: 1214.810791015625
Iteration 1873 logL: 1194.4130859375
Iteration 1874 logL: 1198.478515625
Iteration 1875 logL: 1210.9346923828125
Iteration 1876 logL: 1211.574462890625
Iteration 1877 logL: 1205.450439453125
Iteration 1878 logL: 1172.6024169921875
Iteration 1879 logL: 1174.087646484375
Iteration 1880 logL: 1203.639892578125
Iteration 1881 logL: 1190.721435546875
Iteration 1882 logL: 1192.437744140625
Iteration 1883 logL: 1220.7801513671875
Iteration 1884 logL: 1226.697509765625
Iteration 1885 logL: 1211.2330322265625
```

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Iteration 1889 logL: 1082.3958740234375
Iteration 1890 logL: 1176.63623046875
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Iteration 1897 logL: 1107.7596435546875
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Iteration 1899 logL: 1192.389404296875
Iteration 1900 logL: 1214.0885009765625
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Iteration 1902 logL: 1143.033447265625
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Iteration 1905 logL: 1183.93896484375
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Iteration 1908 logL: 1223.955810546875
Iteration 1909 logL: 1210.2122802734375
Iteration 1910 logL: 1181.78759765625
Iteration 1911 logL: 1210.9541015625
Iteration 1912 logL: 1204.458984375
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Iteration 1915 logL: 1198.698974609375
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Iteration 1918 logL: 1186.60546875
Iteration 1919 logL: 1183.64013671875
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Iteration 1922 logL: 1123.248779296875
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Iteration 1926 logL: 1157.0389404296875
Iteration 1927 logL: 1124.8778076171875
Iteration 1928 logL: 1168.7947998046875
Iteration 1929 logL: 1134.8958740234375
Iteration 1930 logL: 1171.053955078125
Iteration 1931 logL: 1164.15185546875
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Iteration 1940 logL: 1184.2755126953125
Iteration 1941 logL: 1211.376708984375
Iteration 1942 logL: 1223.527587890625
Iteration 1943 logL: 1248.0943603515625
Iteration 1944 logL: 1256.9500732421875
```

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Iteration 1990 logL: 1222.82470703125
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Iteration 1992 logL: 1195.4183349609375
Iteration 1993 logL: 1223.42919921875
Iteration 1994 logL: 1202.7012939453125
Iteration 1995 logL: 1181.566650390625
Iteration 1996 logL: 1211.32568359375
Iteration 1997 logL: 1247.471435546875
Iteration 1998 logL: 1243.31005859375
Iteration 1999 logL: 1203.407470703125
Iteration 2000 logL: 1221.434326171875
```


Plot the training data in the latent space

```
In [13]: q_x_mean = q.encoder.block(mx.nd.array(Y)).asnumpy()
In [14]: for i in range(3):
           plot(q_x_mean[label==i,0], q_x_mean[label==i,1], '.')
           plot(q_x_mean[label==i,0], q_x_mean[label==i,1], '.')
```



4.3 Developer Tutorials

4.3.1 Writing a new Distribution

To write and use a new Distribution class in MXFusion, fill out the Distribution interface and either the Univariate or Multivariate interface, depending on the type of distribution you are creating.

There are 4 primary methods to fill out for a Distribution in MXFusion: * `__init__` - This is the constructor for the Distribution. It takes in any parameters the distribution needs. It also defines names for the input variable[s] that the distribution takes and the output variable[s] it produces. * `log_pdf` - This method returns the logarithm of probabilistic density function for the distribution. This is called during Inference time as necessary to perform the Inference algorithm. * `draw_samples` - This method returns drawn samples from the distribution. This is called during Inference time as necessary to perform the Inference algorithm. * `define_variable` - This is used to generate random variables drawn from the Distribution used during model definition.

`log_pdf` and `draw_samples` are implemented using MXNet functions to compute on the input variables, which at Inference time are MXNet arrays or MXNet symbolic variables.

This notebook will take the Normal distribution as a reference.

File Structure

Code for distributions lives in the `mxfusion/components/distributions` directory.

If you're implementing the *FancyNew* distribution then you should create a file called `mxfusion/components/distributions/fancy_new.py` for the class to live in.

Interface Implementation

Since this example is for a Univariate Normal distribution, our class extends the `UnivariateDistribution` class.

The Normal distribution's constructor takes in objects for its `mean` and `variance`, specifications for data type and context, and a random number generator if not the default.

In addition, a distribution can take in additional parameters used for calculating that aren't inputs. We refer to these additional parameters as the Distribution's `attributes`. The difference between an input and an attribute is primarily that inputs are dynamic at inference time, while attributes are static throughout a given inference run.

In this case, `minibatch_ratio` is a static attribute, as it doesn't change for a given minibatch size during inference.

The mean and variance can be either `Variables` or `MXNet` arrays if they are constants.

As mentioned above, you define names for the input and output variable[s] for the distribution here. These names are used when printing and generally inspecting the model, so give meaningful names. We prefer names like `mean` and `variance` to ones like `location` and `scale` or greek letters like `mew` and `sigma`.

```
In [ ]: class Normal(UnivariateDistribution):
        """
        The one-dimensional normal distribution. The normal distribution can be defined over a scalar.

        :param mean: Mean of the normal distribution.
        :type mean: Variable
        :param variance: Variance of the normal distribution.
        :type variance: Variable
        :param rand_gen: the random generator (default: MXNetRandomGenerator)
        :type rand_gen: RandomGenerator
        :param dtype: the data type for float point numbers
        :type dtype: numpy.float32 or numpy.float64
        :param ctx: the mxnet context (default: None/current context)
        :type ctx: None or mxnet.cpu or mxnet.gpu
        """
        def __init__(self, mean, variance, rand_gen=None, minibatch_ratio=1.,
                      dtype=None, ctx=None):
            self.minibatch_ratio = minibatch_ratio
            if not isinstance(mean, Variable):
                mean = Variable(value=mean)
            if not isinstance(variance, Variable):
                variance = Variable(value=variance)

            inputs = [('mean', mean), ('variance', variance)]
            input_names = ['mean', 'variance']
            output_names = ['random_variable']
            super(Normal, self).__init__(inputs=inputs, outputs=None,
                                         input_names=input_names,
                                         output_names=output_names,
                                         rand_gen=rand_gen, dtype=dtype, ctx=ctx)
```

If your distribution's `__init__` function only takes in parameters that get passed onto its super constructor, you don't need to implement `replicate_self`. If it does take additional parameters (as the Normal distribution does for `minibatch_ratio`), those parameters need to be copied over to the replicant Distribution before returning, as below.

```
In [ ]: def replicate_self(self, attribute_map=None):
        """
        Replicates this Factor, using new inputs, outputs, and a new uuid.
```

```

Used during model replication to functionally replicate a factor into a new graph.
:param inputs: new input variables of the factor
:type inputs: a dict of {'name' : Variable} or None
:param outputs: new output variables of the factor.
:type outputs: a dict of {'name' : Variable} or None
"""
replicant = super(Normal, self).replicate_self(attribute_map)
replicant.minibatch_ratio = self.minibatch_ratio
return replicant

```

`log_pdf` and `draw_samples` are relatively straightforward for implementation. These are the meaningful parts of the Distribution that you're implementing, putting the math into code using MXNet operators for the compute.

If it's a distribution that isn't well documented on Wikipedia, please add a link to a paper or other resource that explains what it's doing and why.

```

In [ ]: def log_pdf(self, mean, variance, random_variable, F=None):
        """
        Computes the logarithm of the probability density function (PDF) of the normal distribution.

        :param mean: the mean of the normal distribution
        :type mean: MXNet NDArray or MXNet Symbol
        :param variance: the variance of the normal distributions
        :type variance: MXNet NDArray or MXNet Symbol
        :param random_variable: the random variable of the normal distribution
        :type random_variable: MXNet NDArray or MXNet Symbol
        :param F: the MXNet computation mode (mxnet.symbol or mxnet.ndarray)
        :returns: log pdf of the distribution
        :rtype: MXNet NDArray or MXNet Symbol
        """
        F = get_default_MXNet_mode() if F is None else F
        logvar = np.log(2 * np.pi) / -2 + F.log(variance) / -2
        logL = F.broadcast_add(logvar, F.broadcast_div(F.square(
            F.broadcast_minus(random_variable, mean)), -2 * variance))
        return logL

In [ ]: def draw_samples(self, mean, variance, rv_shape, num_samples=1, F=None):
        """
        Draw samples from the normal distribution.

        :param mean: the mean of the normal distribution
        :type mean: MXNet NDArray or MXNet Symbol
        :param variance: the variance of the normal distributions
        :type variance: MXNet NDArray or MXNet Symbol
        :param rv_shape: the shape of each sample
        :type rv_shape: tuple
        :param num_samples: the number of drawn samples (default: one)
        :int num_samples: int
        :param F: the MXNet computation mode (mxnet.symbol or mxnet.ndarray)
        :returns: a set samples of the normal distribution
        :rtype: MXNet NDArray or MXNet Symbol
        """
        F = get_default_MXNet_mode() if F is None else F
        out_shape = (num_samples,) + rv_shape
        return F.broadcast_add(F.broadcast_mul(self._rand_gen.sample_normal(
            shape=out_shape, dtype=self.dtype, ctx=self.ctx,
            F.sqrt(variance))), mean)

```

`define_variable` is just a helper function for end users. All it does is take in parameters for the distribution, create a distribution based on those parameters, then return the output variables of that distribution.

```
In [ ]: @staticmethod
def define_variable(mean=0., variance=1., shape=None, rand_gen=None,
                    minibatch_ratio=1., dtype=None, ctx=None):
    """
    Creates and returns a random variable drawn from a normal distribution.

    :param mean: Mean of the distribution.
    :param variance: Variance of the distribution.
    :param shape: the shape of the random variable(s)
    :type shape: tuple or [tuple]
    :param rand_gen: the random generator (default: MXNetRandomGenerator)
    :type rand_gen: RandomGenerator
    :param dtype: the data type for float point numbers
    :type dtype: numpy.float32 or numpy.float64
    :param ctx: the mxnet context (default: None/current context)
    :type ctx: None or mxnet.cpu or mxnet.gpu
    :returns: the random variables drawn from the normal distribution.
    :rtype: Variable
    """
    normal = Normal(mean=mean, variance=variance, rand_gen=rand_gen,
                    dtype=dtype, ctx=ctx)
    normal._generate_outputs(shape=shape)
    return normal.random_variable
```

Using your new distribution

At this point, you should be ready to start testing your new Distribution's functionality by importing it like any other MXFusion component.

Testing

Before submitting your new code as a pull request, please write unit tests that verify it works as expected. This should include numerical checks against edge cases. See the existing test cases for the Normal or Categorical distributions for example tests.

CHAPTER 5

Indices and tables

- `genindex`
- `modindex`
- `search`