Zagatti_HW05

May 31, 2022

1 Homework 05 - Sebastiano Zagatti

[2]:
```
!pip install pyro-ppl

import os
import sys
import json
import numpy as np
import torch
torch.set_default_dtype(torch.float64)

import sklearn
from sklearn.datasets import make_circles
from sklearn.gaussian_process import GaussianProcessClassifier
import sklearn.gaussian_process as gp_sklearn

import pyro
import pyro.distributions as dist
from pyro.infer import MCMC, HMC, NUTS
from pyro.infer import SVI, Trace_ELBO, TraceEnum_ELBO
from pyro.contrib.autoguide import AutoDiagonalNormal
from pyro.optim import Adam
import pyro.contrib.gp as gp

import matplotlib.pyplot as plt
import seaborn as sns
```

```
Looking in indexes: https://pypi.org/simple, https://us-python.pkg.dev/colab-
wheels/public/simple/
Requirement already satisfied: pyro-ppl in /usr/local/lib/python3.7/dist-
packages (1.8.1)
Requirement already satisfied: numpy>=1.7 in /usr/local/lib/python3.7/dist-
packages (from pyro-ppl) (1.21.6)
Requirement already satisfied: pyro-api>=0.1.1 in /usr/local/lib/python3.7/dist-
packages (from pyro-ppl) (0.1.2)
Requirement already satisfied: torch>=1.11.0 in /usr/local/lib/python3.7/dist-
packages (from pyro-ppl) (1.11.0+cu113)
Requirement already satisfied: opt-einsum>=2.3.2 in
```

```
/usr/local/lib/python3.7/dist-packages (from pyro-ppl) (3.3.0)
Requirement already satisfied: tqdm>=4.36 in /usr/local/lib/python3.7/dist-
packages (from pyro-ppl) (4.64.0)
Requirement already satisfied: typing-extensions in
/usr/local/lib/python3.7/dist-packages (from torch>=1.11.0->pyro-ppl) (4.2.0)
```

Let's consider a binary classification problem on Circles dataset. The input is two-dimensional and the response is binary $(0, 1)$.

We observe 1000 points x from this dataset and their labels y:

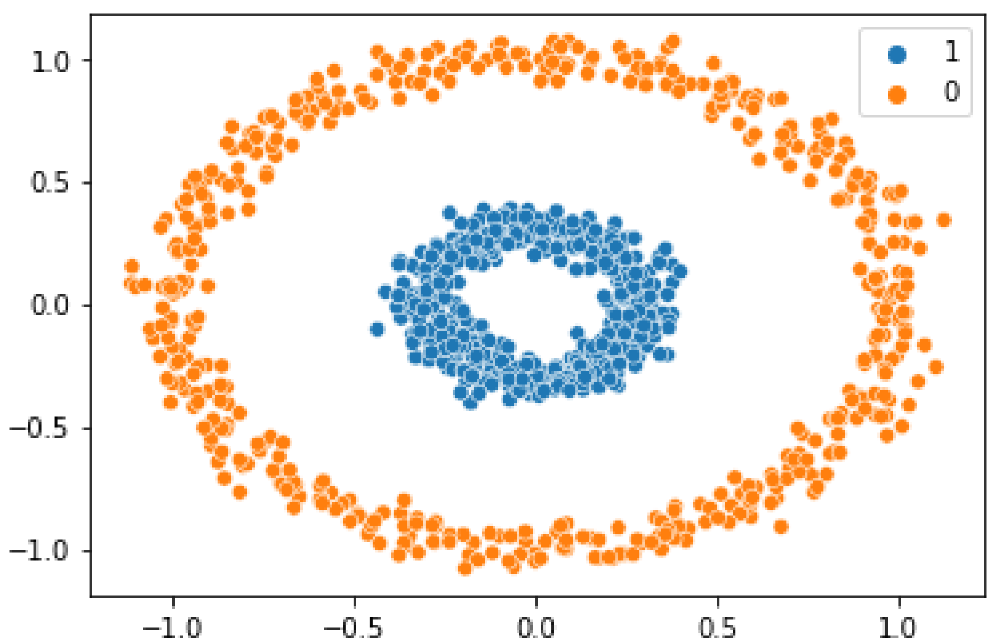
[3]:

```
x, y = make_circles(n_samples=1000, factor=0.3, noise=0.05, random_state=0)
x = torch.from_numpy(x)
y = torch.from_numpy(y).double()

def scatterplot(x, y):
    colors = np.array(['0', '1'])
    sns.scatterplot(x[:, 0], x[:, 1], hue=colors[y.int()])

scatterplot(x, y)
```

```
/usr/local/lib/python3.7/dist-packages/seaborn/_decorators.py:43: FutureWarning:
Pass the following variables as keyword args: x, y. From version 0.12, the only
valid positional argument will be `data`, and passing other arguments without an
explicit keyword will result in an error or misinterpretation.
  FutureWarning
```



1.1 scikit-learn: GaussianProcessClassifier

1. `GaussianProcessClassifier` from scikit-learn library approximates the non-Gaussian posterior by a Gaussian using Laplace approximation. Define an RBF kernel `gp_sklearn.kernels.RBF` with lenghtscale parameter = 1 and fit a Gaussian Process classifier to the observed data (x, y).

[4]:
```
RBF = gp_sklearn.kernels.RBF(length_scale = 1.0)
GPC = GaussianProcessClassifier(kernel = RBF, random_state = 0)

fitted_GPC = GPC.fit(x, y)
```

2. Use `plot_sklearn_predictions` function defined below to plot the posterior predictive mean function over a finite grid of points. You should pass as inputs the learned GP classifier `sklearn_gp_classifier` , the observed points x and their labels y.

[5]:
```
def meshgrid(x, n, eps=0.1):
    x0, x1 = np.meshgrid(np.linspace(x[:, 0].min()-eps, x[:, 0].max()+eps, n),
                         np.linspace(x[:, 1].min()-eps, x[:, 1].max()+eps, n))
    x_grid = np.stack([x0.ravel(), x1.ravel()], axis=-1)
    return x0, x1, x_grid

def plot_sklearn_predictions(sklearn_gp_classifier, x, y):
    x0, x1, x_grid = meshgrid(x, 30)
    preds = sklearn_gp_classifier.predict_proba(x_grid)
    preds_0 = preds[:,0].reshape(x0.shape)
    preds_1 = preds[:,1].reshape(x0.shape)
    plt.figure(figsize=(10,6))
    plt.contourf(x0, x1, preds_0, 101, cmap=plt.get_cmap('bwr'), vmin=0, vmax=1)
    plt.contourf(x0, x1, preds_1, 101, cmap=plt.get_cmap('bwr'), vmin=0, vmax=1)
    plt.title(f'Posterior Mean')
    plt.xticks([]); plt.yticks([])
    plt.colorbar()
    scatterplot(x, y)
```

[6]:
```
plot_sklearn_predictions(GPC, x, y)
```

```
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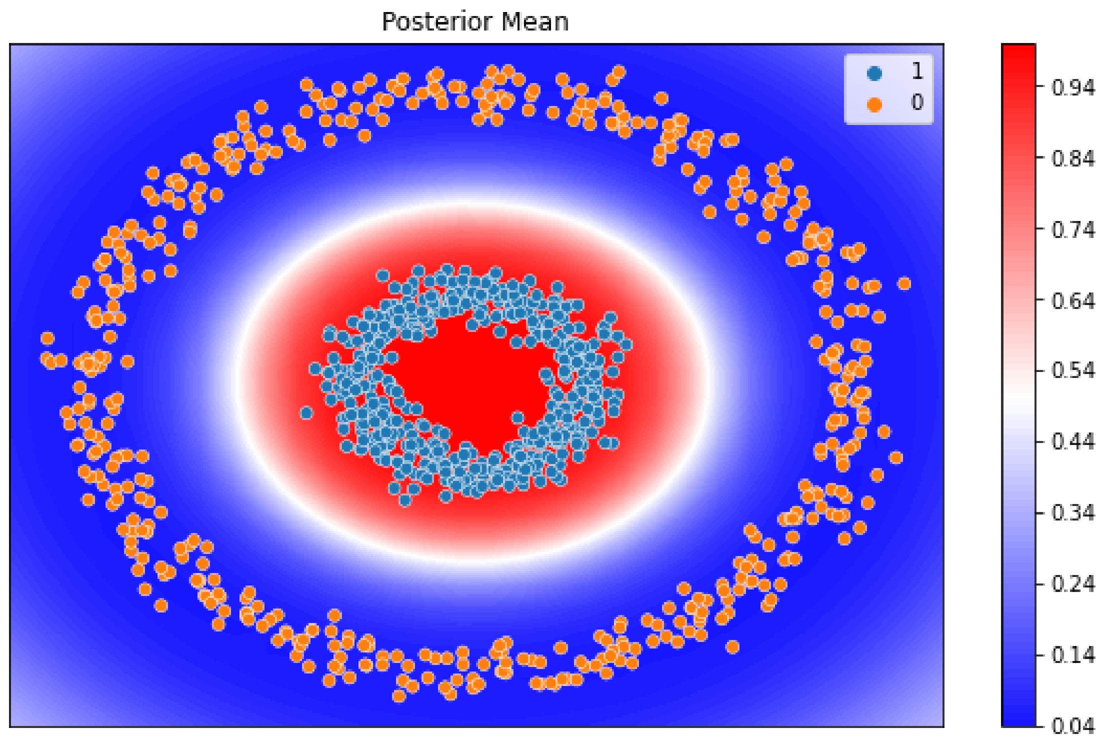

1.2 scikit-learn: GaussianProcessClassifier

Consider the following generative model:

$$y_n | p_n \sim \text{Bernoulli}(p_n) \qquad n = 1, \dots, N$$
$$\mu \sim \mathcal{N}(0, 1)$$
$$\sigma, l \sim LogNormal(0, 1)$$
$$\text{logit}(\mathbf{p}) | \mu, \sigma, l \sim \mathcal{GP}\left(\mu, K_{\sigma,t}(x_n)\right)$$

We model the binary response variable with a Bernoulli likelihood. The logit of the probability is a Gaussian Process with predictors x_n and kernel matrix $K_{\sigma,l}$, parametrized by variance σ and lengthscale l.

We want to solve this binary classification problem by means of HMC inference, so we need to reparametrize the multivariate Gaussian $\mathcal{GP}\left(\mu, K_{\sigma,l}(x_n)\right)$ in order to ensure computational efficiency. Specifically, we model the logit probability as:

$$\text{logit}(\mathbf{p}) = \mu \cdot \mathbf{1}_N + \eta \cdot L$$

where L is the Cholesky factor of $K_{\sigma,l}$ and $\eta_n \sim \mathcal{N}(0, 1)$. This relationship is implemented by the `get_logits` function below.

[7]:
```python
def get_logits(x, mu, sigma, l, eta):
    kernel = gp.kernels.RBF(input_dim=2, variance=torch.tensor(sigma),␣
 ↪lengthscale = torch.tensor(l))
    K = kernel.forward(x, x) + torch.eye(x.shape[0]) * 1e-6
    L = K.cholesky()
    return mu+torch.mv(L,eta)
```

3. Write a pyro model `gp_classifier(x,y)` that implements the reparametrized generative model, using `get_logits` function and `pyro.plate` on independent observations y_n.

[8]:
```python
def gp_classifier(x, y):
    mu = pyro.sample("mu", dist.Normal(0, 1))
    sigma = pyro.sample("sigma", dist.LogNormal(0, 1))
    l = pyro.sample("l", dist.LogNormal(0, 1))
    with pyro.plate('i', len(x)):
        eta = pyro.sample("eta", dist.Normal(0, 1))
        logit_p = get_logits(x, mu, sigma, l, eta)
        y = pyro.sample("y", dist.Bernoulli(torch.sigmoid(logit_p)), obs = y)
```

4. Use pyro `NUTS` on the `gp_classifier` model to infer the posterior distribution of its parameters. Set `num_samples=10` and `warmup_steps=50` . Then extract the posterior samples using pyro `.get_samples()` and print the keys of this dictionary using `.keys()` method.

[10]:
```python
kernel = NUTS(gp_classifier)
mcmc = MCMC(kernel, warmup_steps=50, num_samples=10, num_chains = 3)
mcmc.run(x, y)
```

```
/usr/local/lib/python3.7/dist-packages/pyro/infer/mcmc/api.py:500: UserWarning:
num_chains=3 is more than available_cpu=1. Chains will be drawn sequentially.
  num_chains, available_cpu
Warmup:   0%|          | 0/60 [00:00, ?it/s]/usr/local/lib/python3.7/dist-
packages/ipykernel_launcher.py:2: UserWarning: To copy construct from a tensor,
it is recommended to use sourceTensor.clone().detach() or
sourceTensor.clone().detach().requires_grad_(True), rather than
torch.tensor(sourceTensor).

Sample [0]: 100%|     | 60/60 [57:22, 57.37s/it, step size=6.84e-02, acc.
prob=0.204]
Sample [1]: 100%|     | 60/60 [54:28, 54.47s/it, step size=3.56e-02, acc.
prob=0.412]
Sample [2]: 100%|     | 60/60 [58:09, 58.15s/it, step size=2.22e-03, acc.
prob=0.665]
```

[11]:
```python
samples = mcmc.get_samples()
samples.keys()
```

[11]:
```
dict_keys(['eta', 'l', 'mu', 'sigma'])
```

The `posterior_predictive` function below outputs the prediction corresponding to the i-th sample from the posterior distribution. `plot_pyro_predictions` calls this method to compute the average prediction on each input point and plots the posterior predictive mean function over a finite grid of points.

[12]:
```
def posterior_predictive(samples, i, x, x_grid):
  kernel = gp.kernels.RBF(input_dim=2, variance=samples['sigma'][i],
                          lengthscale=samples['l'][i])
  N_grid = x_grid.shape[0]

  y = get_logits(x, samples['mu'][i], samples['sigma'][i],
                 samples['l'][i], samples['eta'][i])

  with torch.no_grad():
    gpr = gp.models.GPRegression(x, y, kernel=kernel)
    mean, cov = gpr(x_grid, full_cov=True)

    yhat = dist.MultivariateNormal(mean, cov + torch.eye(N_grid) * 1e-6).
 ↪sample()
    return yhat.sigmoid().numpy()

def plot_pyro_predictions(posterior_samples, x):
  n_samples = posterior_samples['sigma'].shape[0]
  x0, x1, x_grid = meshgrid(x, 30)
  x_grid = torch.from_numpy(x_grid)
  preds = np.stack([posterior_predictive(posterior_samples, i, x, x_grid) for i␣
 ↪in range(n_samples)])
  plt.figure(figsize=np.array([10, 6]))
  plt.contourf(x0, x1, preds.mean(0).reshape(x0.shape), 101,
               cmap=plt.get_cmap('bwr'), vmin=0, vmax=1)
  plt.title(f'Posterior Mean')
  plt.xticks([]); plt.yticks([])
  plt.colorbar()
  scatterplot(x, y)
```

5. Pass the learned posterior samples obtained from `NUTS` inference and the set of training points x to `plot_pyro_predictions` and plot the posterior predictive mean.

[13]:
```
plot_pyro_predictions(samples, x)
```

```
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copy construct from a tensor, it is recommended to use
sourceTensor.clone().detach() or
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