Homework 7 - Part B

Note that there are two different notebooks for HW assignment 7. This is part A. There will be two different assignments in gradescope for each part. The deadlines are the same for both parts.

References

• Lectures 27-28 (inclusive).

Instructions

- Type your name and email in the "Student details" section below.
- Develop the code and generate the figures you need to solve the problems using this notebook.
- For the answers that require a mathematical proof or derivation you should type them using latex. If you have never written latex before and you find it exceedingly difficult, we will likely accept handwritten solutions.
- The total homework points are 100. Please note that the problems are not weighed equally.

```
In [ ]: import numpy as np
        import matplotlib.pyplot as plt
        %matplotlib inline
        import matplotlib inline
        matplotlib_inline.backend_inline.set_matplotlib_formats('svg')
        import seaborn as sns
        sns.set_context("paper")
        sns.set_style("ticks")
        import scipy
        import scipy.stats as st
        import urllib.request
        import os
        def download(
            url : str.
            local_filename : str = None
            """Download a file from a url.
                         -- The url we want to download.
            url
            local_filename -- The filemame to write on. If not
                            specified
            if local_filename is None:
               local_filename = os.path.basename(url)
            urllib.request.urlretrieve(url, local filename)
In [ ]: # Run this on Google colab
        #!pip install pyro-ppl
In [ ]: import pyro
```

Student details

import torch

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import pyro.distributions as dist
from pyro.infer import MCMC, NUTS

Problem 1 - Bayesian Linear regression on steroids

The purpose of this problem is to demonstrate that we have learned enough to do very complicated things. In the first part, we will do Bayesian linear regression with radial basis functions (RBFs) in which we characterize the posterior of all parameters, including the length-scales of the RBFs. In the second part, we are going to build a model that has an input-varying noise. Such models are called heteroscedastic models.

We need to write some pytorch code to compute the design matrix. This is absolutely necessary so that pyro can differentiate through all expressions.

Here is how you can use them:

```
In []: # Make the basis
    x_centers = torch.linspace(-1, 1, 10).unsqueeze(-1)
    ell = 0.2
    basis = RadialBasisFunctions(x_centers, ell)

# Some points (need to be N x 1)
    x = torch.linspace(-1, 1, 100).unsqueeze(-1)

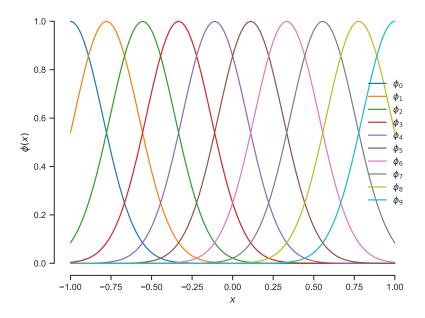
# Evaluate the basis
Phi = basis(x)

# Here is the shape of Phi
    print(Phi.shape)
```

torch.Size([100, 10])

Here is how they look like:

```
In []: fig, ax = plt.subplots()
for i in range(Phi.shape[1]):
          ax.plot(x, Phi[:, i], label=f"$\phi_{i}$")
ax.set(xlabel="$x$", ylabel="$\phi(x)$")
ax.legend(loc="best", frameon=False)
sns.despine(trim=True);
```



Part A - Hierarchical Bayesian linear regression with input-independent noise

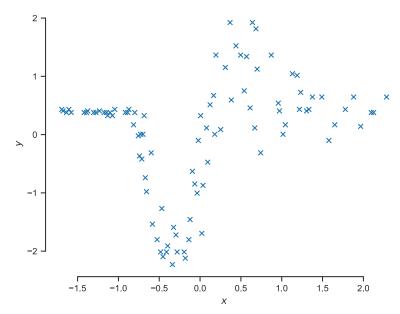
We will analyze the motorcycle dataset. The data is loaded below.

We will work with the scaled data:

```
In [ ]: from sklearn.preprocessing import StandardScaler

data = np.loadtxt('motor.dat')
scaler = StandardScaler()
data = scaler.fit_transform(data)
X = torch.tensor(data[:, 0], dtype=torch.float32).unsqueeze(-1)
Y = torch.tensor(data[:, 1], dtype=torch.float32)

fig, ax = plt.subplots()
ax.plot(X, Y, 'x')
ax.set(xlabel="$x$", ylabel="$y$")
sns.despine(trim=True);
```



Part A.I

Your goal is to implement the model described below. We use the radial basis functions (RadialBasisFunction) with centers, x_i at m=50 equidistant points between the minimum and maximum of the observed inputs:

$$\phi_i(x;\ell) = \expigg(-rac{(x-x_i)^2}{2\ell^2}igg),$$

for $i=1,\ldots,m$. We denote the vector of RBFs evaluated at x as $\phi(x;\ell)$.

We are not going to pick the length-scales ℓ by hand. Instead, we will put a prior on it:

 $\ell \sim \text{Exponential}(1)$.

The corresponding weights have priors:

$$w_j | lpha_i \sim N(0,lpha_i^2),$$

and its α_j has a prior:

 $\alpha_i \sim \text{Exponential}(1),$

for $j = 1, \ldots, m$.

Denote our data as:

$$x_{1:n}=(x_1,\ldots,x_n)^T, ext{ (inputs)},$$

and

$$y_{1:n} = (y_1, \dots, y_n)^T$$
, (outputs).

The likelihood of the data is:

$$y_i | \mathbf{w}, \sigma \sim N(\mathbf{w}^T oldsymbol{\phi}(x_i; \ell), \sigma^2),$$

for $i = 1, \ldots, n$.

$$y_n | \ell, \mathbf{w}, \sigma \sim N(\mathbf{w}^T \boldsymbol{\phi}(x_n; \ell), \sigma^2).$$

Complete the pyro implementation of that model:

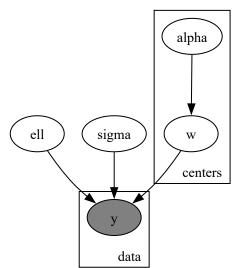
Answer:

```
In [ ]: def model(X, y, num_centers=50):
            with pyro.plate("centers", num centers):
                alpha = pyro.sample("alpha", dist.Exponential(1.0))
                # Notice below that dist.Normal needs the standard deviation - not the variance
                # We follow a different convention in the lecture notes
                w = pyro.sample("w", dist.Normal(0.0, alpha))
            # Complete the code assign to ell the correct prior distribution (an Exponential(1))
            ell = pyro.sample("ell", dist.Exponential(1.0))
            # Hint: Look at alpha.
            # Complete the code assign to sigma the correct prior distribution (an Exponential(1))
            sigma = pyro.sample("sigma", dist.Exponential(1.0))
            x_centers = torch.linspace(X.min(), X.max(), num_centers).unsqueeze(-1)
            Phi = RadialBasisFunctions(x_centers, ell)(X)
            with pyro.plate("data", X.shape[0]):
                pyro.sample("y", dist.Normal(Phi @ w, sigma), obs=y)
            # Notice that I'm making the model return all the variables that I have made.
            # This is not essential for characterizing the posterior, but it does reduce redundant code
            # when we are trying to get the posterior predictive.
            return locals()
```

The graph will help to understand the model:

```
In [ ]: pyro.render_model(model, (X, Y), render_distributions=True)
```

Out[]:



$$\label{eq:alpha} \begin{split} &alpha \sim Exponential \\ &w \sim Normal \\ &ell \sim Exponential \\ &sigma \sim Exponential \\ &y \sim Normal \end{split}$$

Use pyro.infer.autoguide.AutoDiagonalNormal to make the guide:

```
In [ ]: guide = pyro.infer.autoguide.AutoDiagonalNormal(model)
```

We will use variational inference. Here is the training code from the hans-on activity:

```
In [ ]: def train(model, guide, data, num_iter=5_000):
            """Train a model with a guide.
            Arguments
            model -- The model to train.
            guide -- The guide to train.
            data -- The data to train the model with.
            num_iter -- The number of iterations to train.
            Returns
            elbos -- The ELBOs for each iteration.
            param_store -- The parameters of the model.
            pyro.clear_param_store()
            optimizer = pyro.optim.Adam({"lr": 0.001})
            svi = pyro.infer.SVI(
                model,
                guide,
                optimizer,
                loss=pyro.infer.JitTrace_ELBO()
            elbos = []
            for i in range(num_iter):
                loss = svi.step(*data)
                elbos.append(-loss)
                if i % 1_000 == 0:
                    print(f"Iteration: {i} Loss: {loss}")
            return elbos, pyro.get_param_store()
```

Part A.II

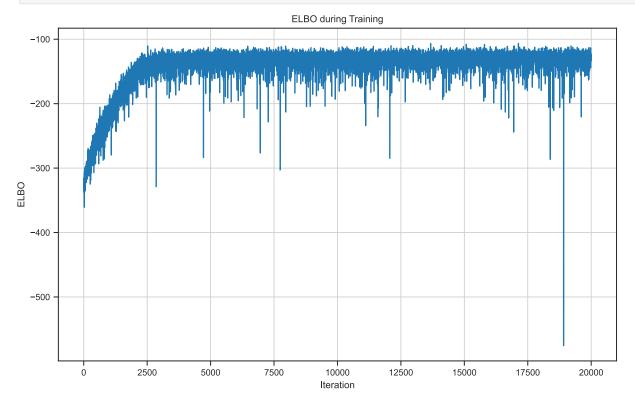
Train the model for 20,000 iterations. Call the train() function we defined above to do it. Make sure you store the returned elbo values because you will need them later.

```
In [ ]: # Your code here
        data = (X, Y)
        elbos, param_store = train(model, guide, data, 20_000)
       Iteration: 0 Loss: 315.35321044921875
       Iteration: 1000 Loss: 214.4072723388672
       Iteration: 2000 Loss: 179.45632934570312
       Iteration: 3000 Loss: 132.06173706054688
       Iteration: 4000 Loss: 132.23574829101562
       Iteration: 5000 Loss: 134.7322998046875
       Iteration: 6000 Loss: 137.6085662841797
       Iteration: 7000 Loss: 139.9112091064453
       Iteration: 8000 Loss: 151.78863525390625
       Iteration: 9000 Loss: 144.66534423828125
       Iteration: 10000 Loss: 139.01451110839844
       Iteration: 11000 Loss: 127.27172088623047
       Iteration: 12000 Loss: 124.31206512451172
       Iteration: 13000 Loss: 124.6731185913086
       Iteration: 14000 Loss: 127.07342529296875
       Iteration: 15000 Loss: 159.40548706054688
       Iteration: 16000 Loss: 125.95035552978516
       Iteration: 17000 Loss: 124.36157989501953
       Iteration: 18000 Loss: 120.1683120727539
       Iteration: 19000 Loss: 135.248779296875
```

Part A.III

Plot the evolution of the ELBO.

```
In []: # Your code here
fig, ax = plt.subplots(figsize=(10, 6))
ax.plot(elbos)
ax.set_xlabel("Iteration")
ax.set_ylabel("ELBO")
ax.set_title("ELBO during Training")
ax.grid(True)
```



Take 1,000 posterior samples.

Answer:

I'm giving you this one because it is a bit tricky. You need to use the pyro.infer.Predictive class to do it. Here is how you can use it:

```
In [ ]: post_samples = pyro.infer.Predictive(model, guide=guide, num_samples=1_000)(X, Y)
# Just modify the call to get the right number of samples
```

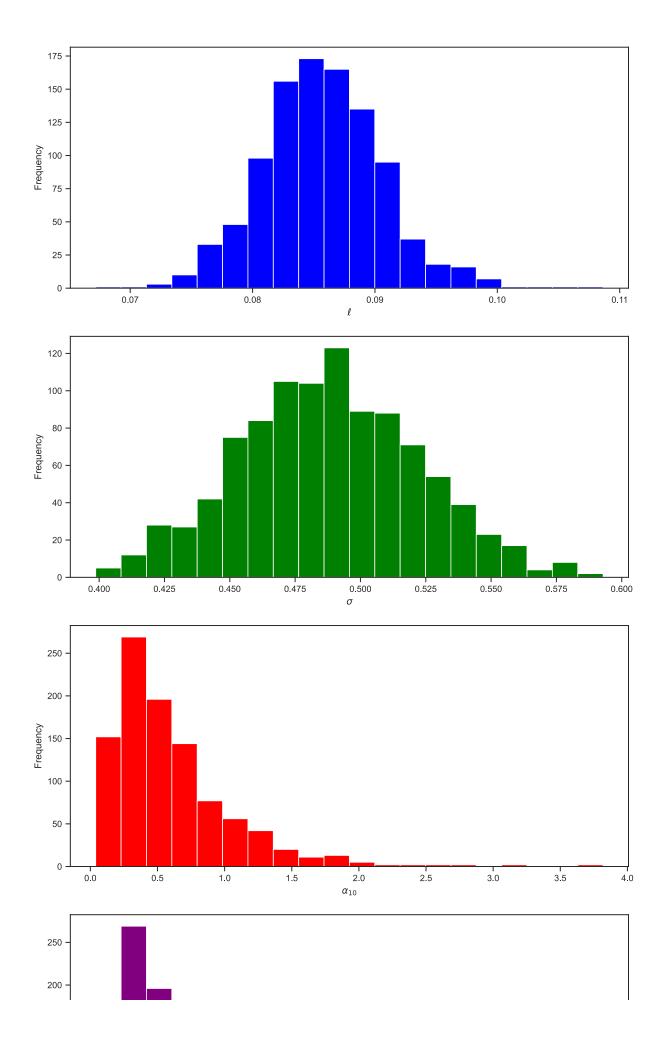
Part A.V

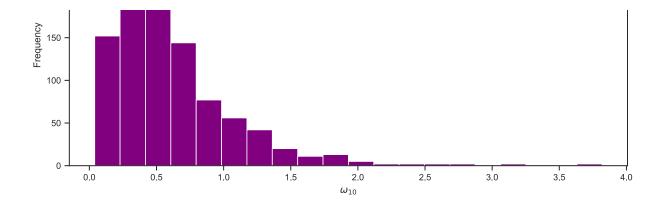
Plot the histograms of the posteriors of ℓ , σ , α_{10} and w_{10} .

Answer:

```
In [ ]: # First, here is how to extract the samples.
        ell = post_samples["ell"]
        # You can do `post_samples.keys()` to see all the keys.
        # But they should correspond to the names of the latent variables in the model.
        sigma = post_samples["sigma"]
        alphas = post_samples["alpha"]
        ws = post_samples["w"]
        alpha_10 = alphas[:,10]
        w_10 = alphas[:,10]
        # Here is the code to make the histogram for the length scale.
        fig, axs = plt.subplots(4,1,figsize=(10, 20))
        # **VERY IMPORTANT** - You need to detach the tensor from the computational graph.
        # Otherwise, you will get very very strange behavior.
        axs[0].hist(ell.detach().numpy(), bins=20, color='blue')
        axs[0].set(xlabel="$\ell$", ylabel="Frequency")
        # Your code for the other histograms here
        # Here is the code to make the histogram for the length scale.
        # **VERY IMPORTANT** - You need to detach the tensor from the computational graph.
        # Otherwise, you will get very very strange behavior.
        axs[1].hist(sigma.detach().numpy(), bins=20, color='green')
        axs[1].set(xlabel="$\sigma$", ylabel="Frequency")
        # **VERY IMPORTANT** - You need to detach the tensor from the computational graph.
        # Otherwise, you will get very very strange behavior.
        axs[2].hist(alpha_10.detach().numpy(), bins=20, color='red')
        axs[2].set(xlabel="$\\alpha_{10}$", ylabel="Frequency")
        \# **VERY IMPORTANT** - You need to detach the tensor from the computational graph.
        # Otherwise, you will get very very strange behavior.
        axs[3].hist(w_10.detach().numpy(), bins=20, color='purple')
        axs[3].set(xlabel="$\omega_{10}$", ylabel="Frequency")
```

Out[]: [Text(0.5, 0, '\$\\omega_{10}\$'), Text(0, 0.5, 'Frequency')]





Part A.VI

Let's extend them model to make predictions.

Answer:

```
In [ ]: # Again, I'm giving you most of the code here.
        def predictive_model(X, y, num_centers=50):
            # First we run the original model get all the variables
            params = model(X, y, num_centers)
            # Here is how you can access the variables
            w = params["w"]
            ell = params["ell"]
            sigma = params["sigma"]
            x_centers = params["x_centers"]
            # Here are the points where we want to make predictions
            xs = torch.linspace(X.min(), X.max(), 100).unsqueeze(-1)
            # Evaluate the basis on the prediction points
            Phi = RadialBasisFunctions(x_centers, ell)(xs)
            # Make the predictions - we use a deterministic node here because we want to
            # save the results of the predictions.
            predictions = pyro.deterministic("predictions", Phi @ w)
            # Finally, we add the measurement noise
            predictions_with_noise = pyro.sample("predictions_with_noise", dist.Normal(predictions, sigma))
            return locals()
```

Part A.VII

Extract the posterior predictive distribution using 10,000 samples. Separate aleatory and epistemic uncertainty.

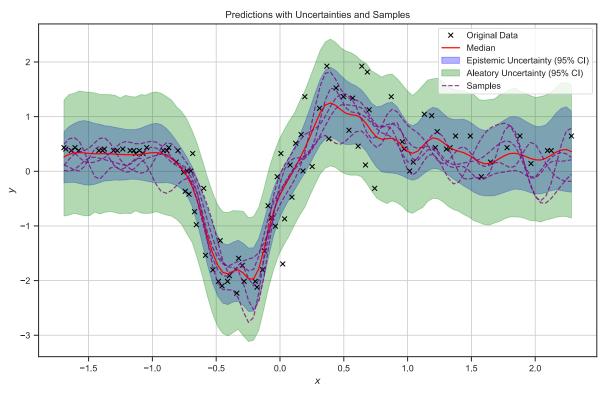
Answer:

```
In []: # Here is how to make the predictions. Just change the number of samples to the right number.
    post_pred = pyro.infer.Predictive(predictive_model, guide=guide, num_samples=10_000)(X, Y)
    # We will predict here:
    xs = torch.linspace(X.min(), X.max(), 100).unsqueeze(-1)
    # You can extract the predictions from post_pred like this:
    predictions = post_pred["predictions"]
    # Note that we extracted the deterministic node called "predictions" from the model.
    # Get the epistemic uncertainty in the usual way:
    p_500, p_025, p_975 = np.percentile(predictions, [50, 2.5, 97.5], axis=0)
    # Extract predictions with noise
    predictions_with_noise = post_pred["predictions_with_noise"]
    # Get the aleatory uncertainty
    ap_025, ap_975 = np.percentile(predictions_with_noise, [2.5, 97.5], axis=0)
```

Part A.VIII

Plot the data, the median, the 95% credible interval of epistemic uncertainty and the 95% credible interval of aleatory uncertainty, along with five samples from the posterior.

```
In [ ]: # Your code here. You have everything you need to make the plot.
        xs = xs.squeeze().numpy()
        p_500 = p_500.squeeze()
        p_{025} = p_{025.squeeze()}
        p_975 = p_975.squeeze()
        ap_025 = ap_025.squeeze()
        ap_975 = ap_975.squeeze()
        # data and median
        fig, ax = plt.subplots(figsize=(10, 6))
        ax.plot(X.numpy(), Y.numpy(), 'x', label='Original Data', color='black')
        ax.plot(xs, p_500, label='Median', color='red')
        # epistemic uncertainty
        ax.fill_between(xs, p_025, p_975, color='blue', alpha=0.3, label='Epistemic Uncertainty (95% CI)')
        # aleatory uncertainty
        ax.fill_between(xs, ap_025, ap_975, color='green', alpha=0.3, label='Aleatory Uncertainty (95% CI)')
        # five samples
        for i in range(5):
            sample_idx = np.random.choice(predictions.shape[0])
            if i == 0:
                ax.plot(xs, predictions[sample_idx].squeeze(), color='purple', alpha=0.75, linestyle='--', label='Samples')
            else:
                ax.plot(xs, predictions[sample_idx].squeeze(), color='purple', alpha=0.75, linestyle='--')
        ax.set_xlabel("$x$")
        ax.set_ylabel("$y$")
        ax.set_title("Predictions with Uncertainties and Samples")
        ax.legend(loc='best')
        ax.grid(True)
```



Part B - Heteroscedastic regression

We are going to build a model that has an input-varying noise. Such models are called heteroscedastic models. Here I will let you do more of the work.

Everything is as before for ℓ , the α_j 's, and the w_j 's. We now introduce a model for the noise that is input dependent. It will use the same RBFs as the mean function. But let's use a different length-scale, ℓ_{σ} . So, we add:

$$\ell_{\sigma} \sim \operatorname{Exponential}(1),$$
 $\alpha_{\sigma,j} \sim \operatorname{Exponential}(1),$

and

$$w_{\sigma,j} | lpha_{\sigma,j} \sim N(0,lpha_{\sigma,j}^2),$$

for $j=1,\ldots,m$.

Our model for the input-dependent noise variance is:

$$\sigma(x; \mathbf{w}_{\sigma}, \ell) = \exp(\mathbf{w}_{\sigma}^T \boldsymbol{\phi}(x; \ell_{\sigma})).$$

So, the likelihood of the data is:

$$y_i | \mathbf{w}, \mathbf{w}_{\sigma} \sim N\left(\mathbf{w}^T \boldsymbol{\phi}(x_i; \ell), \sigma^2(x_i; \mathbf{w}_{\sigma}, \ell)\right),$$

You will implement this model.

Part B.I

Complete the code below:

```
In [ ]: def model1(X, y, num_centers=50):
            with pyro.plate("centers", num_centers):
                alpha = pyro.sample("alpha", dist.Exponential(1.0))
                w = pyro.sample("w", dist.Normal(0.0, alpha))
                # Let's add the generalized linear model for the log noise.
                alpha_noise = pyro.sample("alpha_noise", dist.Exponential(1.0))
                w_noise = pyro.sample("w_noise", dist.Normal(0.0, alpha_noise))
            ell = pyro.sample("ell", dist.Exponential(1.))
            ell_noise = pyro.sample("ell_noise", dist.Exponential(1.))
            x_centers = torch.linspace(X.min(), X.max(), num_centers).unsqueeze(-1)
            Phi = RadialBasisFunctions(x_centers, ell)(X)
            Phi_noise = RadialBasisFunctions(x_centers, ell_noise)(X)
            # This is the new part 2/2
            model_mean = Phi @ w
            model_mean_noise = Phi_noise @ w_noise
            sigma = torch.exp(model_mean_noise)
            with pyro.plate("data", X.shape[0]):
                pyro.sample("y", dist.Normal(model_mean, sigma), obs=y)
            return locals()
```

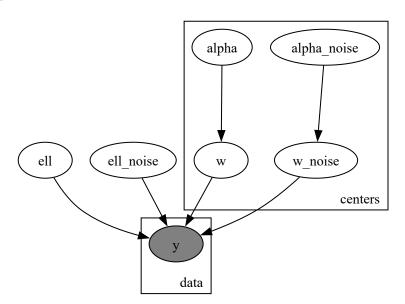
Make a pyro.infer.autoguide.AutoDiagonalNormal guide:

```
In [ ]: # Your code here
    from pyro.infer.autoguide import AutoDiagonalNormal
guide = AutoDiagonalNormal(model1)
```

Make the graph of the model using pyro functionality:

```
In [ ]: # Your code here
pyro.render_model(model1, (X, Y), render_distributions=True)
```

Out[]:

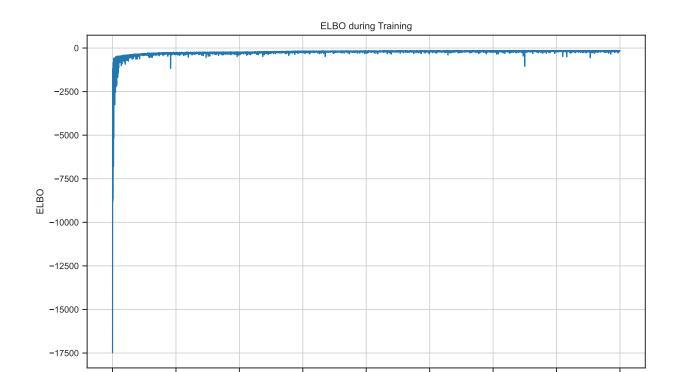


alpha ~ Exponential w ~ Normal alpha_noise ~ Exponential w_noise ~ Normal ell ~ Exponential ell_noise ~ Exponential y ~ Normal

Part B.II

Train the model using 20,000 iterations. Then plot the evolution of the ELBO.

```
In [ ]: # Your code here
        elbos, param_store = train(model1, guide, data, 20_000)
       Iteration: 0 Loss: 17485.99609375
       Iteration: 1000 Loss: 442.5928039550781
       Iteration: 2000 Loss: 294.19573974609375
       Iteration: 3000 Loss: 250.58798217773438
       Iteration: 4000 Loss: 250.0611114501953
       Iteration: 5000 Loss: 256.95355224609375
       Iteration: 6000 Loss: 227.28453063964844
       Iteration: 7000 Loss: 228.33297729492188
       Iteration: 8000 Loss: 216.1748809814453
       Iteration: 9000 Loss: 184.82057189941406
       Iteration: 10000 Loss: 197.52110290527344
       Iteration: 11000 Loss: 178.23306274414062
       Iteration: 12000 Loss: 181.9312286376953
       Iteration: 13000 Loss: 169.94644165039062
       Iteration: 14000 Loss: 188.04452514648438
       Iteration: 15000 Loss: 174.4930877685547
       Iteration: 16000 Loss: 171.0874481201172
       Iteration: 17000 Loss: 188.9711456298828
       Iteration: 18000 Loss: 161.92019653320312
       Iteration: 19000 Loss: 179.12355041503906
In [ ]: fig, ax = plt.subplots(figsize=(10, 6))
        ax.plot(elbos)
        ax.set_xlabel("Iteration")
        ax.set_ylabel("ELBO")
        ax.set_title("ELBO during Training")
        ax.grid(True)
```



Part B.III

Extend the model to make predictions.

2500

5000

7500

10000

Iteration

12500

15000

17500

20000

Answer:

```
In [ ]: def predictive_model(X, y, num_centers=50):
            params = model1(X, y, num_centers)
            w = params["w"]
            w_noise = params["w_noise"]
            ell = params["ell"]
            ell_noise = params["ell_noise"]
            sigma = params["sigma"]
            x_centers = params["x_centers"]
            xs = torch.linspace(X.min(), X.max(), 100).unsqueeze(-1)
            Phi = RadialBasisFunctions(x_centers, ell)(xs)
            Phi_noise = RadialBasisFunctions(x_centers, ell_noise)(xs)
            #Phi = params["Phi"]
            #Phi_noise = params["Phi_noise"]
            predictions = pyro.deterministic("predictions", Phi @ w)
            sigma = pyro.deterministic("sigma", torch.exp(Phi_noise @ w_noise))
            predictions_with_noise = pyro.sample("predictions_with_noise", dist.Normal(predictions, sigma))
            return locals()
```

Part B.IV

Now, make predictions and calculate the epistemic and aleatory uncertainties as in part A.VII.

```
# Your code here
# Here is how to make the predictions. Just change the number of samples to the right number.
post_pred = pyro.infer.Predictive(predictive_model, guide=guide, num_samples=10_000)(X, Y)
# We will predict here:
xs = torch.linspace(X.min(), X.max(), 100).unsqueeze(-1)
# You can extract the predictions from post_pred like this:
predictions = post_pred["predictions"]
# Note that we extracted the deterministic node called "predictions" from the model.
# Get the epistemic uncertainty in the usual way:
p_500, p_025, p_975 = np.percentile(predictions, [50, 2.5, 97.5], axis=0)
```

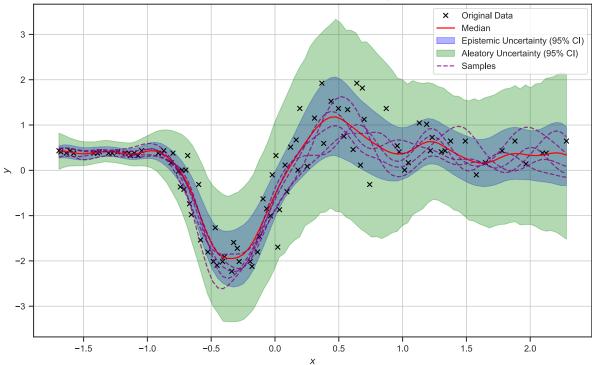
```
# Extract predictions with noise
predictions_with_noise = post_pred["predictions_with_noise"]
# Get the aleatory uncertainty
ap_025, ap_975 = np.percentile(predictions_with_noise, [2.5, 97.5], axis=0)
```

Part B.V

Make the same plot as in part A.VIII.

```
In [ ]: # Your code here
        xs = xs.squeeze().numpy()
        p_{500} = p_{500.squeeze()}
        p_{025} = p_{025.squeeze()}
        p_{975} = p_{975.squeeze()}
        ap_025 = ap_025.squeeze()
        ap_975 = ap_975.squeeze()
        fig, ax = plt.subplots(figsize=(10, 6))
        # data, median
        ax.plot(X.numpy(), Y.numpy(), 'x', label='Original Data', color='black')
        ax.plot(xs, p_500, label='Median', color='red')
        # epistemic uncertainty
        ax.fill_between(xs, p_025, p_975, color='blue', alpha=0.3, label='Epistemic Uncertainty (95% CI)')
        # aleatory uncertainty
        ax.fill_between(xs, ap_025, ap_975, color='green', alpha=0.3, label='Aleatory Uncertainty (95% CI)')
        # five samples
        for i in range(5):
            sample\_idx = np.random.choice(predictions.shape[0])
            if i == 0:
                ax.plot(xs, predictions[sample_idx].squeeze(), color='purple', alpha=0.75, linestyle='--', label='Samples')
            else:
                ax.plot(xs, predictions[sample_idx].squeeze(), color='purple', alpha=0.75, linestyle='--')
        ax.set_xlabel("$x$")
        ax.set_ylabel("$y$")
        ax.set_title("Predictions with Uncertainties and Samples")
        ax.legend(loc='best')
        ax.grid(True)
```





Part B.VI

Plot the estimated noise standard deviation as a function of of the input along with a 95% credible interval.

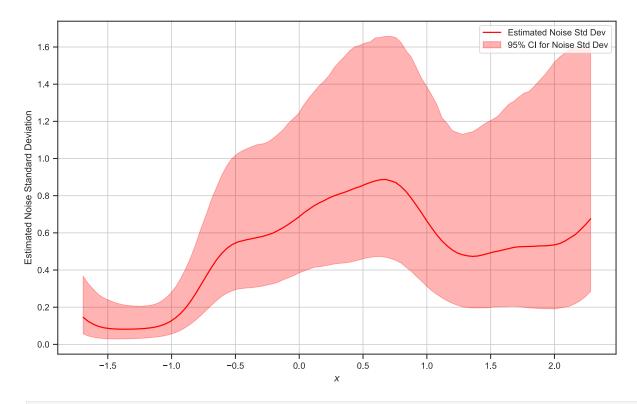
```
In []: # Your code here

# standard deviation
sigma = post_pred["sigma"]

sigma_500, sigma_025, sigma_975 = np.percentile(sigma, [50, 2.5, 97.5], axis=0)

sigma_500 = sigma_500.squeeze()
sigma_025 = sigma_025.squeeze()
sigma_975 = sigma_975.squeeze()

fig, ax = plt.subplots(figsize=(10, 6))
ax.plot(xs, sigma_500, label='Estimated Noise Std Dev', color='red')
ax.fill_between(xs, sigma_025, sigma_975, color='red', alpha=0.3, label='95% CI for Noise Std Dev')
ax.set_xlabel("$x$")
ax.set_ylabel("Estimated Noise Standard Deviation")
ax.legend()
ax.grid(True)
```



In []:

Part B.VII

Which model do you prefer? Why?

Answer:

I prefer the heteroscedastic model (part B). The beginning of input in part b.V has all posterior samples within a small uncertainty, and all the samples stay within a small uncertainty until 0.5. The median also follows the original data closer, getting most of the original data points to fall on the line. Overall, the graph shows that the data points are closer to the samples and median of the heteroscedastic model, so I prefer that model.

Part B.IX

Can you think of any way to improve the model? Go crazy! This is the last homework assignment! There is no right or wrong answer here. But if you have a good idea, we will give you extra credit.

In []: ## Your code and answers here