Auto-encoding Variational Bayes

Applied Bayesian Methods

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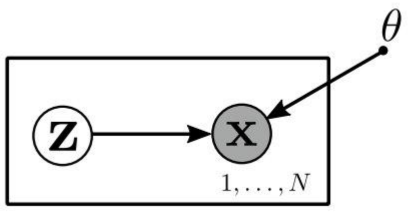
The main objective of this assignment is to develop a variational autoencoder using the working principles of variational inference, and, use this method for doing approximate inference in the MNIST dataset. The probabilistic model considered is a generative model of the form:



Task 1. *Complete the missing parts of the code to allow for training a VAE on the MNIST dataset.*

We are briefly reviewing the implemented steps for each of the four functions designed for this task. Let us begin with `sample_latent_variables_posterior`, the main aim of this function is to generate an unique sample from $Q(z \mid x)$ for each x in the given batch. To this end, the mean and variance of each factor Q is given as input for the function. In order to return the desired samples we are using the decomposition property of the Gaussian distribution, that is

$$\mathcal{N}(\mu, \sigma^2) = \mu + \sigma\mathcal{N}(0, 1).$$

The resulting code is

```
mean, log_std = encoder_output[:, :D], encoder_output[:, D:]
z = npr.randn(*mean.shape)
return mean + z * np.exp(log_std)
```

The `bernoulli_log_prob` function aims to return the log-likelihood of the actual data given the computed logits using the output of the neural network, that is, to compute

$$\begin{aligned}\log P(\boldsymbol{x} \mid \boldsymbol{z}) &= \sum_{x \in \boldsymbol{x}} \log\Big(p(x)^x + (1 - p(x))^{(1-x)}\Big)\\ &= \sum_{x \in \boldsymbol{x}} \log\Big(x\, p(x) + (1 - x)\,(1 - p(x))\Big).\end{aligned}$$

To this end, it is needed to compute the probabilities for the given logits using the sigmoid activation:

```
probs = sigmoid(logits)
log_prob = np.log(targets * probs + (1 - targets) * (1 - probs))
return np.sum(log_prob, axis=-1)
```

On the other hand, function `compute_KL` is used to compute the Kullback-Leibler divergence between the variational distribution $Q(\boldsymbol{z} \mid \boldsymbol{x})$ and the prior distirbution $\mathcal{N}(0, I)$. Given that both distributions are Gaussian, their KL divergence has a closed form which is in turn simplified given that both are diagonal Gaussians. More precisely,

$$\mathcal{KL}\Big(\mathcal{N}\big((\mu_1, \dots, \mu_k)^T, \mathrm{diag}(\sigma_1^2, \dots, \sigma_k^2)\big) \mid \mathcal{N}(\mathbf{0}, \boldsymbol{I})\Big) = \frac{1}{2}\sum_{i=1}^{k}\left(\sigma_i^2 + \mu_i^2 - 1 - \log \sigma_i^2\right).$$

This value can be easily computed given `mean` and `log_stds` from the neural network output as

```
KL = 0.5 * (np.exp(2 * log_std) + mean ** 2 - 1 - 2 * log_std)
return np.sum(KL, axis = -1)
```

Lastly, `vae_lower_bound` is used to compute a noisy estimate of the lower bound by using a single Monte Carlo sample. That is, to approximate the expectation in the objective function with a single observation of the variable. The steps are the following:

1. Compute the encoder output using `neural_net_predict`:

   ```
   output = neural_net_predict(params=rec_params, inputs=data)
   ```

2. Sample the latent variables associated to the batch in data:

   ```
   latents = sample_latent_variables_from_posterior(output)
   ```

3. Reconstruct the image and to compute the log likelihood of the actual data:

   ```
   x_samples = neural_net_predict(gen_params, latents)
   log_prob = bernoulli_log_prob(data, x_samples)
   ```

4. Compute the KL divergence between $Q(\boldsymbol{z} \mid \boldsymbol{x})$ and the prior:

   ```
   KL = compute_KL(output)
   ```

5. Estimate the lower bound by substracting the KL to the data dependent term

   ```
   return np.mean(log_prob - KL, axis=-1)
   ```

Task 2. *Complete the initialization of the ADAM parameters and write the ADAM updates in the main training loop of the code provided in* `vae.py`.

Using the provided description of the algorithm, the parameter updates can be computed as the following:

```
m = beta1 * m + (1 - beta1) * grad
v = beta2 * v + (1 - beta2) * grad ** 2
m_unbiased = m / (1 - beta1 ** t)
v_unbiased = v / (1 - beta2 ** t)

flattened_current_params += (
      alpha * m_unbiased / (np.sqrt(v_unbiased) + epsilon)
)
```

With initial values given by

```
alpha = 0.001
beta1 = 0.9
beta2 = 0.999
```

```
epsilon = 1e-8
m = np.zeros_like(flattened_current_params)
v = np.zeros_like(flattened_current_params)
```

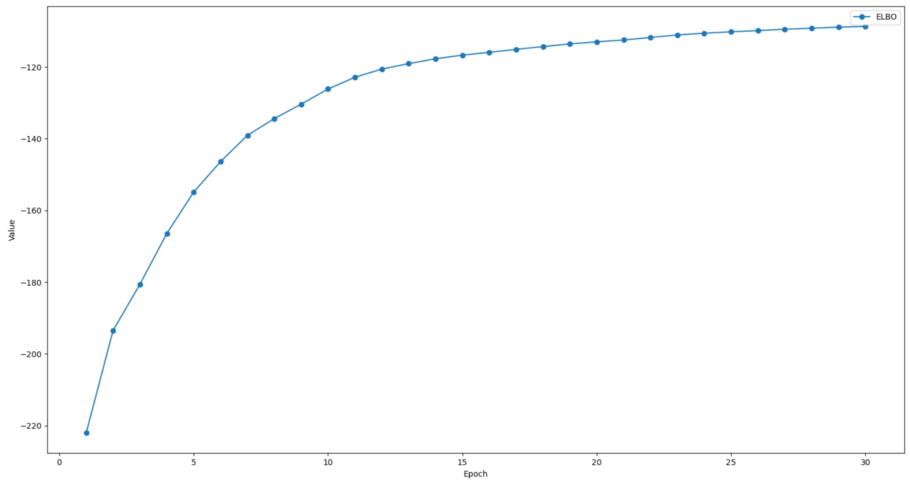


Figure 1: Evolution of the ELBO during 30 training epochs.

Task 3.1. *Generate* 25 *images from the generative model. This should be done by drawing* $\boldsymbol{z}$ *from the prior, to then generate* $\boldsymbol{x}$ *using the conditional distribution* $P_\theta(\boldsymbol{x} \mid \boldsymbol{z})$*. Set the pixel intensity of the image equal to the activation probability. Do not binarizethe images.*

The needed block of code for this subtask generates 25 samples from the prior distribution $\mathcal{N}(0, 1)$, computes the higher dimensional representation using the output of the neural network and saves the given images.

```
z_samples_prior = npr.randn(25, latent_dim)
x_samples = neural_net_predict(gen_params, z_samples_prior)
save_images(sigmoid(x_samples), "images_from_prior")
```

The generated images can be seen at Figure 2.

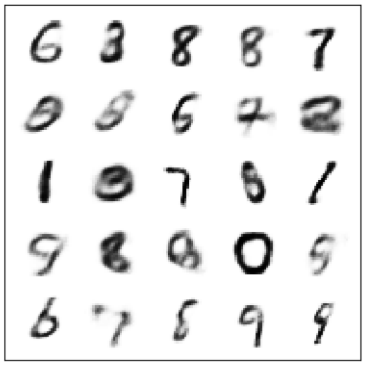


Figure 2: Generated images from the prior distibution $\mathcal{N}(0, I)$.

Task 3.2. *Generate 10 image reconstructions using the recognition model and then the generative model. Choose the first 10 images from the test set. The reconstructions are obtained by generating $\boldsymbol{z}$ using $Q_\phi(\boldsymbol{z} \mid \boldsymbol{x})$ and then generating $\boldsymbol{x}$ again using $P_\theta(\boldsymbol{x} \mid \boldsymbol{z})$. Set the pixel intensity of the image equal to the activation probability.*

The needed steps to complete this task correspondto the first three steps done in `vae_lower_bound`:

```
output = neural_net_predict(params=rec_params, inputs=test_images[:10])
latents = sample_latent_variables_from_posterior(output)
decoding = neural_net_predict(gen_params, latents)
save_images(np.append(test_images[:10], sigmoid(decoding), axis = 0),
            "reconstructions")
```

The obtained reconstructions are shown in Figure 3.

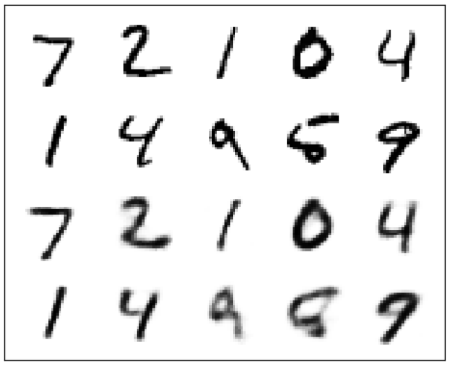


Figure 3: Original data samples (first two rows) and their reconstruction through the autoencoder (last two rows)

Task 3.3. *Generate 5 interpolations in the latent space from one image to another. Consider the first and second image in the test set, the third and fourth image in the test set and so on. The interpolations should be obtained by finding the latent representation of each image. Consider only the mean of the predictive model $Q(\boldsymbol{z} \mid \boldsymbol{x})$ as the latent representation. Ignore the variance.*

Given a pair of images `image1` and `image2`, the needed steps (with simplified code) to compute the interpolation are:

1. Compute the output of the neural network for each image.

   ```
   first_image = neural_net_predict(rec_params, image1)
   second_image = neural_net_predict(rec_params, image2)
   ```

2. Get hidden representation from the mean values:

   ```
   latents1 = first_image[:, :D]
   latents2 = second_image[:, :D]
   ```

3. Compute interpolation scalars.

   ```
   S = np.linspace(0, 1, interpolation_steps)[::-1]
   ```

4. Compute interpolation

   ```
   interp = np.array([s * latents1 + (1 - s) * latents2 for s in S])
   ```

5. Reconstruct interpolated image.

```
    image = neural_net_predict(gen_params, interp)
```

The obtained reconstructions can be seen in Figure 4.

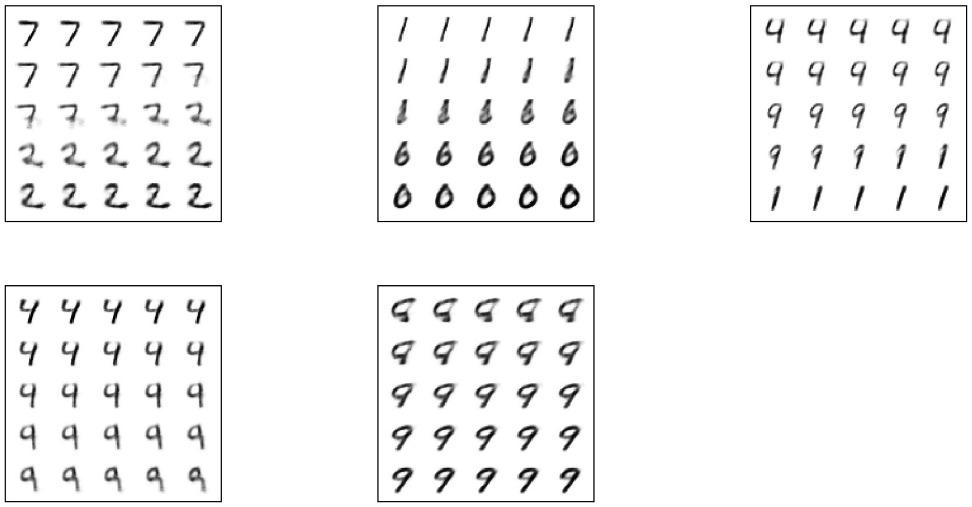


Figure 4: Reconstruction of latent interpolation of data samples.