Quiz 3	**Name:**	______________________
Week 13, Dec/20/2023	**On your left:**	______________________
CS 280: Fall 2023	**On your right:**	______________________
Instructor: Lan Xu		

Problem 1. (5 points) **Learning of VAE.** Given observation X, and assume a latent variable model according to

$$P(X) = \int_z P(X|z;\theta)P(z)dz$$

with latent variables z lying in high-dimensional space, VAE deals with both the inference problem of the posterior $P(z|X)$ and the learning of the LVM.
Denote the approximating family Q, VAE finds a variational distribution $q \in Q$ most similar to $P(z|X)$, and learns $P(X|z;\theta)$ that explains the data.

1. (3) Derive the objective function of VAE. Use the notation provided above, and suppose you are optimizing w.r.t. q and θ. (Hint: Considering the second question, you'd better choose one specific derivation that involves no inequality)

2. (2) Explain why optimizing the objective deals with the inference problem of $P(z|X)$ and the learning problem of $P(X|z;\theta)$.

Solution:

1. We begin with the KL divergence:

$$\begin{aligned}
&KL(q(z|X)||P(z|X)) \\
&= \mathbb{E}_{z\sim q}[\log q - \log P(z|X)] \\
&= \mathbb{E}_{z\sim q}[\log q - \log \frac{P(X|z)P(z)}{P(X)}] \\
&= \mathbb{E}_{z\sim q}[\log q - \log P(X|z)P(z)] + \log P(X).
\end{aligned}$$

   Rearrange the above to separate the constants and the parameterized distribution:

$$\log P(X) - KL(q(z|X)||P(z|X)) = \mathbb{E}_{z\sim q}[P(X|z;\theta)] - KL(q||P(z)),$$

   and the RHS is the objective function.

2. When q is fixed, maximizing the RHS is equivalent to maximizing the evidence $\log P(X)$ on the LHS since the KL term is constant. When θ is fixed, maximizing the RHS is equivalent to minimizing the KL term since the predicted likelihood of the observation is fixed.

Problem 2. (5 points) **Evaluation of GAN.**

1. (1) What's the discriminator and generator loss curve like for a DCGAN if it is well trained?
2. (2) If the loss for the discriminator has gone to zero or close to zero while the loss of the generator also rises and continues to rise over the same period, what's the possible reason?
3. (2) If the DCGAN converges, does it means that it must be a well trained GAN? If not, what will the generator output in such a state?

Solution:

1. The generator and discriminator are competing against each other, hence improvement on the one means the higher loss on the other, if a GAN converges, both discriminator and generator losses are converging to some permanent numbers.
2. Sometimes the loss for the discriminator has gone to zero or close to zero while the loss of the generator also rise and continue to rise over the same period. This type of loss is most commonly caused by the generator outputting garbage images that the discriminator can easily identify.
3. Even though the model may converges well, it still may suffer mode collapse problem, while a generator is only capable of generating one or a small subset of different outcomes, or modes.

Problem 3. (10 points) **Diffusion Models** and **Score-based Models**

1. (4) Please select all the correct statement(s) in the following:
   - ○ Diffusion Model is a special case of Markovian Hierarchical VAE.
   - ○ In diffusion models, the latent dimension is exactly equal to the data dimension.
   - ○ In diffusion models, the structure of the latent encoder at each timestep is not learned, but a Gaussian distribution centered around the output of the previous timestep.
   - ○ Optimizing a diffusion model boils down to learning a neural network to predict the original ground truth data from an arbitrarily noised version.

2. (6) According to the forward diffusion process and reparameterization trick, we have:

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I}),$$
$$\boldsymbol{x}_0 = \frac{\boldsymbol{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar{\alpha}_t}}.$$

And Tweedie's Formula states that: for a Gaussian variable $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}_{\boldsymbol{z}}, \boldsymbol{\Sigma}_{\boldsymbol{z}})$, it has

$$\mathbb{E}[\boldsymbol{\mu}_{\boldsymbol{z}} \mid \boldsymbol{z}] = \boldsymbol{z} + \boldsymbol{\Sigma}_{\boldsymbol{z}} \nabla_{\boldsymbol{z}} \log p(\boldsymbol{z}).$$

Please make use of the two prerequisites above to derive the score function $\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)$. ***(Hint: the result should be expressed using $\bar{\alpha}_t$ and ϵ_0)***

Solution:

1. All the statements are correct.

2. According to the given Tweedie's formula, we have:

$$\mathbb{E}[\boldsymbol{\mu}_{\boldsymbol{x}_t} \mid \boldsymbol{x}_t] = \boldsymbol{x}_t + \boldsymbol{\Sigma}_{\boldsymbol{x}_t} \nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t).$$

And the forward diffusion process tells that:

$$\boldsymbol{\mu}_{\boldsymbol{x}_t} = \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0,$$
$$\boldsymbol{\Sigma}_{\boldsymbol{x}_t} = (1-\bar{\alpha}_t)\mathbf{I}.$$

So we can get:

$$\sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 = \boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t),$$
$$\boldsymbol{x}_0 = \frac{\boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)}{\sqrt{\bar{\alpha}_t}}.$$

Then we can construct the euqation:

$$\boldsymbol{x}_0 = \frac{\boldsymbol{x}_t + (1-\bar{\alpha}_t)\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)}{\sqrt{\bar{\alpha}_t}} = \frac{\boldsymbol{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar{\alpha}_t}},$$

which means $(1-\bar{\alpha}_t)\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t) = -\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0$. Therefore, we have:

$$\nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_0.$$