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Prof. Mu-Yadong's Deep Learning: Algorithms and Applications
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Homework-1

Question 1. Variational Auto-Encoder

VAE is the typical generative model which has a lot of applications. The encoder portion of a VAE yields an approximate posterior distribution $q(z \mid x)$, and is parameterized on a neural network by weights collectively denoted θ. Hence we more properly write the encoder as $q_\theta(z \mid x)$. Similarly, the decoder portion of the VAE yields a likelihood distribution $p(x \mid z)$, and is parameterized on a neural network by weights collectively denoted φ. Hence we more properly denote the decoder portion of the VAE as $p_\varphi(x \mid z)$. The output of the encoder are parameters of the latent distribution, which is sampled to yield the input into the decoder.

a) Draw the model's framework of VAE

b) Derive the objective function e.g. the Evidence Lower Bound (ELBO) using KL divergence.

HINT: 1) Please include the re-parametrisation trick implemented in VAE

HINT: 2) You may need to use Bayes theorem: $p(x \mid y) = \frac{p(y|x)p(x)}{p(y)}$

c) Derive the closed form VAE loss: Gaussian latents, based on question b). e.g. Say we choose:

$$p(z) \rightarrow \frac{1}{\sqrt{2\pi\sigma_p^2}} \exp\left(-\frac{(x-\mu_p)^2}{2\sigma_p^2}\right)$$

and

$$q_\theta\left(z \mid x_i\right) \rightarrow \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp\left(-\frac{(x-\mu_q)^2}{2\sigma_q^2}\right)$$

SOLUTION:

BING AI:

a) The framework of a VAE consists of an encoder and a decoder. The encoder takes in input data x and outputs the parameters of the latent distribution $q_\theta(z \mid x)$. The decoder takes in a sample from the latent distribution z and outputs the reconstructed data $p_\varphi(x \mid z)$.

b) The objective function of a VAE is the Evidence Lower Bound (ELBO), which can be derived using KL divergence. The ELBO can be written as:

$$\mathcal{L}(\theta, \varphi; x) = \mathbb{E}_{q_\theta(z|x)}[\log p_\varphi(x \mid z)] - \mathrm{KL}\left(q_\theta(z \mid x) \| p(z)\right)$$

where KL denotes the Kullback-Leibler divergence. The first term is the expected log-likelihood of the data given the latent variable z, and the second term is the KL divergence between the approximate posterior $q_\theta(z \mid x)$ and the prior $p(z)$.

The re-parametrization trick is used to make the ELBO differentiable with respect to θ. This is done by introducing an auxiliary variable ϵ such that $z = g_\theta(\epsilon, x)$ where g_θ is a differentiable function. This allows us to write the ELBO as:

$$\mathcal{L}(\theta, \varphi; x) = \mathbb{E}_{p(\epsilon)}[\log p_\varphi(x \mid g_\theta(\epsilon, x))] - \mathrm{KL}\left(q_\theta(z \mid x) \| p(z)\right)$$

c) If we choose Gaussian distributions for both the prior and approximate posterior, we can derive a closed-form expression for the VAE loss. Let's say we choose:

$$p(z) = \frac{1}{\sqrt{2\pi\sigma_p^2}} \exp\left(-\frac{(z-\mu_p)^2}{2\sigma_p^2}\right)$$

and

$$q_\theta\left(z \mid x_i\right)=\frac{1}{\sqrt{2 \pi \sigma_q^2}} \exp \left(-\frac{\left(z-\mu_q\right)^2}{2 \sigma_q^2}\right)$$

where μ_p, σ_p, μ_q, and σ_q are learned parameters.

The KL divergence between two Gaussian distributions has a closed-form expression:

$$\mathrm{KL}\left(q_\theta(z \mid x) \| p(z)\right)=\log \frac{\sigma_p}{\sigma_q}+\frac{\sigma_q^2+\left(\mu_q-\mu_p\right)^2}{2 \sigma_p^2}-\frac{1}{2}$$

Substituting this into the ELBO, we get:

$$\mathcal{L}(\theta, \varphi ; x)=\mathbb{E}_{p(\epsilon)}[\log p_\varphi(x \mid g_{<IPAddress>-<IPAddress>})]-\log \frac{\sigma_p}{\sigma_q}-\frac{\sigma_q^2+\left(\mu_q-m u_p\right)^2}{2 \sigma_p^2}+\frac{1}{2}$$

This is the closed-form expression for the VAE loss when using Gaussian latents.

ChatGPT:

a) The framework of the VAE is as follows:

$$\begin{aligned} z & \sim q_\theta(z \mid x) \\ x & \sim p_\varphi(x \mid z)\end{aligned}$$

b) The Evidence Lower Bound (ELBO) objective function of VAE is derived as follows:

$$\begin{aligned}
\log p_\varphi(x) & \geq \mathbb{E}_{q_\theta(z \mid x)}\left[\log p_\varphi(x \mid z)\right]-D_{\mathrm{KL}}\left[q_\theta(z \mid x) \| p(z)\right] \\
& =\mathbb{E}_{q_\theta(z \mid x)}\left[\log p_\varphi(x \mid z)-\log \frac{q_\theta(z \mid x)}{p(z)}\right] \\
& =\mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)}\left[\log p_\varphi\left(x \mid z=\mu_\theta(x)+\sigma_\theta(x) \odot \epsilon\right)-\log \frac{q_\theta\left(z=\mu_\theta(x)+\sigma_\theta(x) \odot \epsilon \mid x\right)}{p(z=\epsilon)}\right] \\
& =\mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)}\left[\log p_\varphi\left(x \mid z=\mu_\theta(x)+\sigma_\theta(x) \odot \epsilon\right)-\log \frac{1}{\sqrt{2 \pi} \sigma_p} \exp \left(-\frac{(\epsilon-0)^2}{2 \sigma_p^2}\right)-\log \frac{1}{\sqrt{2 \pi} \sigma_\theta(x)} \exp \left(-\frac{(\epsilon -\right.\right. \\
& =\mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)}\left[\log p_\varphi\left(x \mid z=\mu_\theta(x)+\sigma_\theta(x) \odot \epsilon\right)-\frac{1}{2} \log (2 \pi \sigma_p^2)-\frac{(\epsilon^2)}{2 \sigma_p^2}+\frac{1}{2} \log \left(2 \pi\left(\sigma_\theta^2(x)\right)\right)+\frac{\left(\epsilon-\frac{\mu_\theta(x)}{\sigma_\theta(x)}\right)^2}{2 \sigma_\theta^2(x)}\right] \\
& =\mathbb{E}_{\epsilon \sim \mathcal{N}(0, I)}\left[\log p_\varphi\left(x \mid z=\mu_\theta(x)+\sigma_\theta(x) \odot \epsilon\right)-\frac{1}{2}\left(1+\log (\sigma_\theta^2(x))-\mu_\theta^2(x)-\sigma_\theta^2(x)\right)-\frac{1}{2} \log \left(\frac{\sigma_p^2}{\sigma_\theta^2(x)}\right)\right]
\end{aligned}$$

c) The closed-form VAE loss with Gaussian latent variables is as follows:

$$\mathcal{L}(x, \theta, \varphi)=\frac{1}{2} \sum_{j=1}^J\left(1+\log (\sigma_j^2)-\mu_j^2-\sigma_j^2\right)-\frac{1}{N} \sum_{i=1}^N \sum_{j=1}^J\left[\log p_\varphi\left(x_i \mid z_j\right)-\frac{1}{2}\left(1+\log (\sigma_{q_j}^2(x_i))-\mu_{q_j}(x_i)^2-\sigma_{q_j}^2(x_i)\right)\right]$$

where N is the number of data points, J is the dimension of the latent space, $\mu_{q_j}(x_i), \sigma_{q_j}^2(x_i)$ are the parameters of the Gaussian $q_\theta(z_j \mid x_i)$ for the j^{th} dimension, and μ_j, σ_j^2 are the parameters of the prior Gaussian $p(z_j)$.

Additionally, we can simplify the ELBO objective to the following expression:

$$\mathcal{L}(x, \theta, \varphi)=-\mathrm{KL}\left(q_\theta(z \mid x) \| p(z)\right)+\frac{1}{N} \sum_{i=1}^N \mathbb{E}_{q_\theta(z \mid x_i)}\left[\log p_\varphi(x_i \mid z)\right]$$

This is equivalent to the previous expression, but highlights the two components of the objective: the KL divergence term, which encourages the approximate posterior $q_\theta(z \mid x)$ to be close to the prior $p(z)$, and the reconstruction term, which encourages the decoder $p_\varphi(x \mid z)$ to generate data that is similar to the input x given the latent variable z.

Bard:

Sure, here are the answers to your questions:

a) Draw the model's framework of VAE

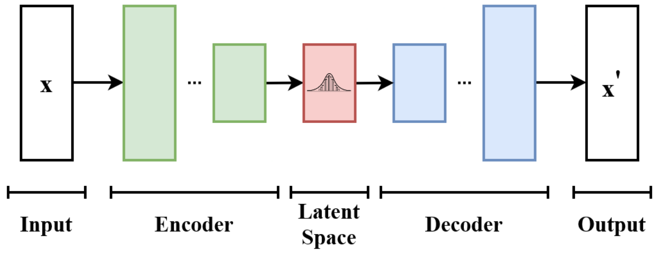

FIGURE 1. VAE model framework

b) Derive the objective function e.g. the Evidence Lower Bound (ELBO) using KL divergence.

The objective function of a VAE is to maximize the Evidence Lower Bound (ELBO), which is given by:

$$ELBO = \mathbb{E}_{q(z|x)}[\log p(x|z)] - D_{KL}(q(z|x)||p(z))$$

where:

* $q(z|x)$ is the approximate posterior distribution over the latent variables, * $p(x|z)$ is the likelihood function, * $p(z)$ is the prior distribution over the latent variables, and * D_{KL} is the Kullback-Leibler divergence.

The first term in the ELBO, $\mathbb{E}_{q(z|x)}[\log p(x|z)]$, is the expected log-likelihood of the data under the approximate posterior distribution. This term encourages the model to generate realistic data. The second term in the ELBO, $D_{KL}(q(z|x)||p(z))$, is the Kullback-Leibler divergence between the approximate posterior distribution and the prior distribution. This term encourages the model to choose latent variables that are likely under the prior distribution.

c) Derive the closed form VAE loss: Gaussian latents, based on question b). e.g. Say we choose:

$$p(z) \to \frac{1}{\sqrt{2\pi\sigma_p^2}} \exp\left(-\frac{(x-\mu_p)^2}{2\sigma_p^2}\right)$$

and

$$q_\theta\left(z \mid x_i\right) \to \frac{1}{\sqrt{2\pi\sigma_q^2}} \exp\left(-\frac{(x-\mu_q)^2}{2\sigma_q^2}\right)$$

The closed form VAE loss for Gaussian latents is given by:

$$L = -\frac{1}{2}\sum_{i=1}^{N}\left(\frac{(x_i-\mu_p)^2}{\sigma_p^2} + \frac{(x_i-\mu_q)^2}{\sigma_q^2} - \log\sigma_p^2 - \log\sigma_q^2 + \log 2\pi\right)$$

where:

* N is the number of data points, * x_i is the ith data point, * μ_p is the mean of the prior distribution, * σ_p is the standard deviation of the prior distribution, * μ_q is the mean of the approximate posterior distribution, and * σ_q is the standard deviation of the approximate posterior distribution.

This loss can be minimized using any standard optimization algorithm, such as stochastic gradient descent.

FREE AI:

a) The framework of VAE consists of an encoder neural network $q_\theta(z \mid x)$ that maps an input data point x to the parameters (μ_z, σ_z^2) of a Gaussian distribution in the latent space z, and a decoder neural network $p_\varphi(x \mid z)$ that maps a sample z from the latent space to a reconstructed data point $\hat{x}$. The overall model can be represented graphically:

$$x \overset{q_\theta(z|x)}{\longrightarrow} z \overset{p_\varphi(x|z)}{\longrightarrow} \hat{x}$$

b) The objective function of VAE is derived by maximizing the evidence lower bound (ELBO), which can be expressed as:

$$\mathcal{L}_{\text{VAE}} = E_{q_\theta(z|x)}[\log p_\varphi(x|z)] - D_{KL}(q_\theta(z|x)||p(z))$$

where the first term measures the reconstruction loss and the second term is the Kullback-Leibler (KL) divergence between the approximated posterior distribution $q_\theta(z|x)$ and the prior distribution $p(z)$. To obtain a differentiable and noise-aware estimator for z, we apply the reparametrization trick:

$$z = \mu_z + \sigma_z \odot \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1)$$

where μ_z and σ_z are the mean and standard deviation outputs of the encoder for z, respectively, and $\odot$ denotes element-wise multiplication.

c) When the prior and approximate posterior distributions are both Gaussian with diagonal covariance matrices, we can rewrite the KL divergence term in the ELBO as:

$$D_{KL}(q_\theta(z|x)||p(z)) = -\frac{1}{2}\sum_{j=1}^{J}\left(1 + \log(\sigma_{z_j}^2) - \mu_{z_j}^2 - \sigma_{z_j}^2\right)$$

where J is the dimensionality of z. Thus, the closed-form VAE loss for a dataset of N samples becomes:

$$\mathcal{L}_{\text{VAE}} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{1}{2}\sum_{j=1}^{J}\left(1 + \log(\sigma_{z_{ij}}^2) - \mu_{z_{ij}}^2 - \sigma_{z_{ij}}^2\right) - \frac{1}{2}\sum_{j=1}^{J}\frac{(x_{ij} - \hat{x}_{ij})^2}{\sigma_{x_{ij}}^2}\right)$$

where $\hat{x}_{ij}$ and $\sigma_{x_{ij}}^2$ are the mean and variance outputs of the decoder for the j-th feature of the i-th input data point, respectively.

To further explain the closed-form VAE loss for a dataset of N samples, the first term in the objective function is the reconstruction loss, which measures the similarity between the input data point and its reconstruction. Since the decoder outputs a Gaussian distribution, the reconstruction loss is computed as the negative log-likelihood of the input data point under the Gaussian distribution. Specifically, we assume that the reconstruction error is normally distributed with zero mean and variance $\sigma_{x_{ij}}^2$, and therefore the negative log-likelihood is given by:

$$-\log p_\varphi(x_i|z_i) = \frac{1}{2}\sum_{j=1}^{J}\left[\log(2\pi\sigma_{x_{ij}}^2) + \frac{(x_{ij} - \hat{x}_{ij})^2}{\sigma_{x_{ij}}^2}\right]$$

where x_{ij} and $\hat{x}_{ij}$ are the j-th feature of the input data point and its reconstruction, respectively.

The second term in the objective function is the KL divergence between the approximated posterior distribution $q_\theta(z|x)$ and the prior distribution $p(z)$. It encourages the posterior distribution to be close to the prior distribution, which helps in avoiding overfitting and enforcing the regularization. The KL divergence term in the closed-form VAE loss can be interpreted as a regularization term that encourages the encoder to distribute the latent variable representation of each input across its dimensions and to avoid overfitting by producing latent variables with high variance.

Question 2. Policy based Reinforcement Learning

Please write down the detailed derivation of the policy gradient method in the episodic case, e.g. Show that $\nabla J(\boldsymbol{\theta}) \propto \mathbb{E}_\pi\left[\sum_a q_\pi(s, a) \nabla \pi(a \mid s)\right]$

Some definitions you may need:

$$J(\boldsymbol{\theta}) = v_{\pi_\theta}\left(s_0\right)$$

where v_{π_θ} is the true state value function for π_θ, the policy determined by θ state value function:

$$v_\pi = \mathbb{E}_\pi\left[G_t \mid S_t = s\right] = \sum_a \pi(a \mid s) q_\pi(s, a)$$

state-action value function:

$$q_\pi(s, a) = \mathbb{E}_\pi\left[G_t \mid S_t = s, A_t = a\right] = \sum_{s', r} p\left(s', r \mid s, a\right)\left(r + v_\pi\left(s'\right)\right)$$

where we have the return defined as:

$$G_t = R_{t+1} + R_{t+2} + \ldots$$

SOLUTION: