Mathematical Foundations of Deep Neural Networks, M1407.001200 E. Ryu Spring 2024



## Homework 11 Due 5pm, Monday, June 10, 2024

**Problem 1:** VLB for IWAE. The standard variational lower bound (VLB) of VAE is

$$\log(p_{\theta}(x)) \ge \text{VLB}_{\theta,\phi}(x) = \mathbb{E}_{Z \sim q(z|x)} \left[ \log \left( \frac{p_{\theta}(x \mid Z) p_{Z}(Z)}{q_{\phi}(Z \mid x)} \right) \right],$$

where  $p_{\theta}(z \mid x)$  is the true posterior and  $q_{\phi}(z \mid x)$  is the approximate posterior. Define

$$VLB_{\theta,\phi}^{(K)}(x) = \mathbb{E}_{Z_1,\dots,Z_K \sim q_{\phi}(z|x)} \left[ \log \frac{1}{K} \sum_{k=1}^K \frac{p_{\theta}(x \mid Z_k) p_Z(Z_k)}{q_{\phi}(Z_k \mid x)} \right],$$

to be the VLB for importance weighted autoencoders (IWAE) [1]. To clarify,  $Z_1, \ldots, Z_K$  are sampled independently from  $q_{\phi}(z \mid x)$ . Note that IWAE with K = 1 coincides with the standard VAE, and VLB<sup>(1)</sup><sub> $\theta,\phi$ </sub> = VLB<sub> $\theta,\phi$ </sub>. Show:

- (a)  $\log p_{\theta}(x) \geq \text{VLB}_{\theta,\phi}^{(K)}(x)$  for all x and  $K \geq 1$ .
- (b) If  $K \geq M$ , then  $VLB_{\theta,\phi}^{(K)}(x) \geq VLB_{\theta,\phi}^{(M)}(x)$  for all x.
- (c) Let  $X_1, \ldots, X_N$  be data for training the IWAE. Show that if  $q_{\phi}$  is "powerful enough", then

$$\underset{\theta \in \Theta}{\text{maximize}} \quad \sum_{i=1}^{N} \log p_{\theta}(X_i) = \underset{\theta \in \Theta, \phi \in \Phi}{\text{maximize}} \quad \sum_{i=1}^{N} \text{VLB}_{\theta, \phi}^{(K)}(X_i).$$

What should be the precise meaning of "powerful enough"?

*Hint.* For (a), use the Jensen's inequality. For (b), let  $I \subset \{1, \dots, K\}$  with |I| = M be a uniformly distributed subset of distinct indices from  $\{1, \dots, K\}$ . Then,  $\mathbb{E}_{I = \{i_1, \dots, i_M\}} \left[\frac{a_{i_1} + \dots + a_{i_M}}{M}\right] = \frac{a_1 + \dots + a_K}{K}$  for any sequence of numbers  $a_1, \dots, a_K$ .

Remark. This analysis shows that  $VLB_{\theta,\phi}^{(K)}$  provides a tighter approximation of the log likelihood than  $VLB_{\theta,\phi}$ . However, using  $VLB_{\theta,\phi}^{(K)}$  requires more computation than  $VLB_{\theta,\phi}$ .

# References

[1] Y. Burda, R. Grosse, and R. Salakhutdinov, Importance weighted autoencoders, *ICLR*, 2016.

#### Solution.

(a) First, note that

$$p_{\theta}(x) = \int p(x, z) dz = \int p_{\theta}(x \mid z) p_{Z}(z) dz$$

$$= \int \frac{p_{\theta}(x \mid z) p_{Z}(z)}{q_{\theta}(z \mid x)} q_{\theta}(z \mid x) dz = \mathbb{E}_{Z \sim q_{\theta}(\cdot \mid x)} \left[ \frac{p_{\theta}(x \mid Z) p_{Z}(Z)}{q_{\theta}(Z \mid x)} \right]$$

From the concavity of log, we use Jensen's inequality to swap the orders of  $\mathbb{E}$  and log.

$$VLB_{\theta,\phi}^{(K)}(x) = \mathbb{E}_{Z_1,\dots,Z_K \sim q_{\phi}(z|x)} \left[ \log \frac{1}{K} \sum_{k=1}^K \frac{p_{\theta}(x \mid Z_k) p_Z(Z_k)}{q_{\phi}(Z_k \mid x)} \right]$$

$$\leq \log \mathbb{E}_{Z_1,\dots,Z_K \sim q_{\phi}(z|x)} \left[ \frac{1}{K} \sum_{k=1}^K \frac{p_{\theta}(x \mid Z_k) p_Z(Z_k)}{q_{\phi}(Z_k \mid x)} \right]$$

$$= \log \left( \frac{1}{K} \sum_{k=1}^K \mathbb{E}_{Z_k \sim q_{\phi}(z|x)} \left[ \frac{p_{\theta}(x \mid Z_k) p_Z(Z_k)}{q_{\phi}(Z_k \mid x)} \right] \right) = \log p_{\theta}(x).$$

(b) Using the *Hint*, we get

$$\frac{1}{K} \sum_{k=1}^{K} \frac{p_{\theta}(x \mid Z_{k}) p_{Z}(Z_{k})}{q_{\phi}(Z_{k} \mid x)} = \mathbb{E}_{I = \{i_{1}, \dots, i_{M}\} \subseteq \{1, \dots, K\}} \left[ \frac{1}{M} \sum_{m=1}^{M} \frac{p_{\theta}(x \mid Z_{m}) p_{Z}(Z_{m})}{q_{\phi}(Z_{m} \mid x)} \right].$$

By Jensen's inequality,

$$VLB_{\theta,\phi}^{(K)}(x) = \mathbb{E}_{Z_{1},...,Z_{K} \sim q_{\phi}(z|x)} \left[ \log \frac{1}{K} \sum_{k=1}^{K} \frac{p_{\theta}(x \mid Z_{k})p_{Z}(Z_{k})}{q_{\phi}(Z_{k} \mid x)} \right]$$

$$= \mathbb{E}_{Z_{1},...,Z_{K} \sim q_{\phi}(z|x)} \left[ \log \mathbb{E}_{I=\{i_{1},...,i_{M}\}} \left[ \frac{1}{M} \sum_{m=1}^{M} \frac{p_{\theta}(x \mid Z_{i_{m}})p_{Z}(Z_{i_{m}})}{q_{\phi}(Z_{i_{m}}|x)} \right] \right]$$

$$\geq \mathbb{E}_{Z_{1},...,Z_{K} \sim q_{\phi}(z|x)} \left[ \mathbb{E}_{I=\{i_{1},...,i_{M}\}} \left[ \log \frac{1}{M} \sum_{m=1}^{M} \frac{p_{\theta}(x \mid Z_{i_{m}})p_{Z}(Z_{i_{m}})}{q_{\phi}(Z_{i_{m}}|x)} \right] \right]$$

$$= \mathbb{E}_{Z_{i_{1}},...,Z_{i_{m}} \sim q_{\phi}(z|x)} \left[ \log \frac{1}{M} \sum_{m=1}^{M} \frac{p_{\theta}(x \mid Z_{i_{m}})p_{Z}(Z_{i_{m}})}{q_{\phi}(Z_{i_{M}}|x)} \right] = VLB_{\theta,\phi}^{(M)}(x).$$

(c) If the approximate posterior  $q_{\phi}$  is 'powerful enough' to exactly represent the true posterior, then there exists a  $\phi^*$  such that  $q_{\phi^*}(Z_k \mid x) = p_{\theta}(Z_k \mid x)$  for  $k = 1, \ldots, K$ . Then

$$VLB_{\theta,\phi^{\star}}^{(K)}(x) = \mathbb{E}_{Z_{1},...,Z_{K} \sim q_{\phi^{\star}}(z|x)} \left[ \log \frac{1}{K} \sum_{k=1}^{K} \frac{p_{\theta}(x \mid Z_{k})p_{Z}(Z_{k})}{q_{\phi^{\star}}(Z_{k} \mid x)} \right]$$

$$= \mathbb{E}_{Z_{1},...,Z_{K} \sim q_{\phi^{\star}}(z|x)} \left[ \log \frac{1}{K} \sum_{k=1}^{K} \frac{p_{\theta}(x \mid Z_{k})p_{Z}(Z_{k})}{p_{\theta}(Z_{k} \mid x)} \right]$$

$$= \mathbb{E}_{Z_{1},...,Z_{K} \sim q_{\phi^{\star}}(z|x)} \left[ \log \frac{1}{K} \sum_{k=1}^{K} p_{\theta}(x) \right] = \log p_{\theta}(x).$$

**Problem 2:** VAE with trainable prior. In this problem, we consider the setup of training a VAE with a trainable prior. Specifically, we assume  $Z \sim r_{\lambda}(z)$ , where  $\lambda$  is a trainable parameter, and  $X \sim p_{\theta}(x \mid Z)$ . Let  $q_{\phi}(z \mid X)$  be the approximate posterior. Let

$$VLB_{\theta,\phi,\lambda}(X_i) = \mathbb{E}_{Z \sim q_{\phi}(z|X_i)} \left[ \log \left( \frac{p_{\theta}(X_i \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_i)} \right) \right].$$

- (a) Show that  $\log p_{\theta}(X_i) \geq \text{VLB}_{\theta,\phi,\lambda}(X_i)$ .
- (b) Describe how to evaluate stochastic gradients of  $VLB_{\theta,\phi,\lambda}(X_i)$  using the log-derivative trick.
- (c) Assume  $r_{\lambda} = \mathcal{N}(\lambda_1, \operatorname{diag}(\lambda_2))$ , where  $\lambda_1, \lambda_2 \in \mathbb{R}^k$ ,  $q_{\phi}(z \mid X_i) = \mathcal{N}(\mu_{\phi}(X_i), \Sigma_{\phi}(X_i))$  with diagonal  $\Sigma_{\phi}$ , and  $p_{\theta}(X_i \mid z) = \mathcal{N}(f_{\theta}(z), \sigma^2 I)$ . Describe how to evaluate stochastic gradients of  $\operatorname{VLB}_{\theta,\phi,\lambda}(X_i)$  using the reparameterization trick.

### Solution.

(a) Using Jensen's inequality,

$$VLB_{\theta,\phi,\lambda}(X_{i}) = \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log \left( \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right]$$

$$\leq \log \left( \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right] \right) = \log p_{\theta}(X_{i}).$$

The last equality follows from the same argument as in problem 1(a).

(b) For the stochastic gradients with respect to  $\theta$  and  $\lambda$ , as we can explicitly evaluate

$$\begin{split} \nabla_{\theta} \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log \left( \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right] &= \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \nabla_{\theta} \left( \log \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right] \\ &= \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \nabla_{\theta} \log p_{\theta}(X_{i} \mid Z) \right] \\ \nabla_{\lambda} \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log \left( \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right] &= \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \nabla_{\lambda} \log r_{\lambda}(Z_{i}) \right], \end{split}$$

the stochastic gradient can be calculated as

$$\frac{1}{K} \sum_{k=1}^{K} \nabla_{\theta} \log p_{\theta}(X_i \mid Z_{i,k}), \qquad \frac{1}{K} \sum_{k=1}^{K} \nabla_{\lambda} \log r_{\lambda}(Z_{i,k})$$

given the sample  $Z_{i,k} \sim q_{\phi}(\cdot \mid X_i)$  for  $k = 1, \dots, K$  where K is the number of elements in a single batch.

For the gradient with respect to  $\phi$ , use the log-derivative trick, following the details in the problem 1 of homework 10:

$$\nabla_{\phi} \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log \left( \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right]$$

$$= \nabla_{\phi} \int \log \left( \frac{p_{\theta}(X_{i} \mid z) r_{\lambda}(z)}{q_{\phi}(z \mid X_{i})} \right) q_{\phi}(z \mid X_{i}) dz$$

$$= \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ (\nabla_{\phi} \log q_{\phi}(Z \mid X_{i})) \log \left( \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right].$$

Here, the stochastic gradient can be calculated as

$$\frac{1}{K} \sum_{k=1}^{K} \left( \nabla_{\phi} \log q_{\phi} \left( Z_{i,k} \mid X_{i} \right) \right) \log \left( \frac{p_{\theta} \left( X_{i} \mid Z_{i,k} \right) r_{\lambda}(Z_{i,k})}{q_{\phi} \left( Z_{i,i} \mid X_{i} \right)} \right)$$

given the sample  $Z_{i,k} \sim q_{\phi}(\cdot \mid X_i)$  for k = 1, ..., K where K is the number of elements in a single batch.

(c) Note that the stochastic gradients with respect to θ and λ can be evaluated as the same way as in (b). Here, we only focus on the stochastic gradient with respect to φ. VLB can be reformulated as:

$$VLB_{\theta,\phi,\lambda}(X_{i}) = \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log \left( \frac{p_{\theta}(X_{i} \mid Z) r_{\lambda}(Z)}{q_{\phi}(Z \mid X_{i})} \right) \right]$$
$$= \mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log p_{\theta}(X_{i} \mid Z) \right] - D_{KL} \left( q_{\phi}(z \mid X_{i}) \parallel r_{\lambda}(z) \right).$$

The first term is as follows:

$$\mathbb{E}_{Z \sim q_{\phi}(z|X_{i})} \left[ \log p_{\theta} \left( X_{i} \mid Z \right) \right] = -\frac{1}{2\sigma^{2}} \mathbb{E}_{Z \sim \mathcal{N} \left( \mu_{\phi}(X_{i}), \Sigma_{\phi}(X_{i}) \right)} \left\| X_{i} - f_{\theta}(Z) \right\|^{2} - \frac{d}{2} \log(2\pi\sigma^{2})$$

But in this equation, the evaluation of the gradient with respect to  $\phi$  is intractable. We use the reparametrization trick to remedy this. The first term becomes

$$-\frac{1}{2\sigma^{2}}\mathbb{E}_{\varepsilon \sim \mathcal{N}(0,I)}\left\|X_{i}-f_{\theta}\left(\mu_{\phi}\left(X_{i}\right)+\Sigma_{\phi}^{1/2}(X_{i})\varepsilon\right)\right\|^{2}-\frac{d}{2}\log(2\pi\sigma^{2})$$

and its gradient with respect to  $\phi$  is

$$-\frac{1}{2\sigma^2} \mathbb{E}_{\varepsilon \sim \mathcal{N}(0,I)} \left[ \nabla_{\phi} \left\| X_i - f_{\theta} \left( \mu_{\phi}(X_i) + \Sigma_{\phi}^{1/2} \varepsilon \right) \right\|^2 \right]$$

In this equation, after sampling, the gradient can be calculated directly. Therefore, back-propagation becomes possible. The second term can be calculated by problem 5 of homework 9 as:

$$-D_{\mathrm{KL}}\left(q_{\phi}\left(z\mid X_{i}\right) \| r_{\lambda}(z)\right)$$

$$= -\frac{1}{2}\left(\mathrm{tr}\left(\left[\mathrm{diag}(\lambda_{2})\right]^{-1} \Sigma_{\phi}(X_{i})\right) + (\lambda_{1} - \mu_{\phi}(X_{i}))^{T}\left[\mathrm{diag}(\lambda_{2})\right]^{-1} (\lambda_{1} - \mu_{\phi}(X_{i})) - k + \log\frac{\det(\mathrm{diag}(\lambda_{2}))}{\det(\Sigma_{\phi}(X_{i}))}\right)$$

and its gradient with respect to  $\phi$  can be calculated accordingly. Therefore, back-propagation is possible for both terms.

**Problem 3:** Anomaly detection via flow models. Assume we have a trained flow model that we use to evaluate the likelihood function  $p_{\theta}$ . In this problem, you will use this trained flow model to perform anomaly detection between the MNIST and KMNIST datasets. In step 1, load the MNIST and KMNIST datasets, and split the MNIST test dataset into "validation" and "test" sets. In step 2, define the flow model. In step 3, load the trained flow model. In step 4, calculate the mean and standard deviation of

$$\{\log p_{\theta}(Y_i)\}_{i=1}^M$$

where  $Y_1, \ldots, Y_M$  are the validation data. Define a threshold to be mean - 3 standard deviations, and define inputs with log likelihood below this threshold to be anomalies. In step 5, check how many of the MNIST images within the test set are classified as anomalies and report the type I error rate. In step 6, check how many of the KMNIST images are classified as non-anomalies and report the type II error rate. Download the starter code flow\_anomaly.py, which provides the implementation of steps 1–3. Complete the implementation of steps 4–6.

Remark. In this problem, we split the test data into validation and test sets because the entire training set was already used to train the flow model. If we were to train the flow model from scratch, it would be better to split the training set into the training and validation sets to set aside the validation data for step 3.

Solution. See flow\_anomaly\_sol.py. ■

**Problem 4:** Rock paper scissors and minimiax optimization. Consider a game of rock paper scissors between players A and B. Players A and B play randomized strategies with

$$p_A = \begin{bmatrix} \mathbb{P}(A \text{ plays rock}) \\ \mathbb{P}(A \text{ plays paper}) \\ \mathbb{P}(A \text{ plays scissors}) \end{bmatrix}, \qquad p_B = \begin{bmatrix} \mathbb{P}(B \text{ plays rock}) \\ \mathbb{P}(B \text{ plays paper}) \\ \mathbb{P}(B \text{ plays scissors}) \end{bmatrix}.$$

Define

$$\Delta^3 = \{ p = (p_1, p_2, p_3) \in \mathbb{R}^3 \mid p_1, p_2, p_3 \ge 0, \ p_1 + p_2 + p_3 = 1 \}$$

so that  $p_A, p_B \in \Delta^3$ . In the game, a player receives 1 point for a win, -1 points for a loss, and 0 points for a draw. Consider the minimax problem

(a) Show that

$$p_A^{\star} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}, \qquad p_B^{\star} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

is the unique solution to the minimax problem.

(b) Note that if  $p_B = (1/3, 1/3, 1/3)$ , then  $\mathbb{E}_{p_A, p_B}[\text{points for } B] = 0$  regardless of how A plays. Does this mean any strategy  $p_A \in \Delta^3$  is optimal for player A? (Here, the word "optimal" is used informally. Think about whether any  $p_A \in \Delta^3$  is a best strategy for A.)

Clarification. We say  $(\theta^*, \phi^*)$  is a solution to the minimax problem

$$\label{eq:loss_eq} \underset{\theta \in \Theta}{\text{minimize}} \quad \underset{\phi \in \Phi}{\text{maximize}} \quad L(\theta, \phi)$$

if  $\theta^* \in \Theta$ ,  $\phi^* \in \Phi$ , and

$$L(\theta^{\star}, \phi) \le L(\theta^{\star}, \phi^{\star}) \le L(\theta, \phi^{\star})$$

for all  $\theta \in \Theta$  and  $\phi \in \Phi$ , i.e., unilaterally deviating from  $\theta^*$  increases the value of L and unilaterally deviating from  $\phi^*$  decreases the value of L.

Remark. In the setup of GANs (which is what this problem is intended to prepare you for), if the generator is perfect, the discriminator cannot do better than a 50-50 guess in detecting fakes. However, the discriminator is still forced to learn to distinguish imperfect fakes, as otherwise, the generator can take advantage of the discriminator.

#### Solution.

(a) Let

$$p_A = \begin{bmatrix} P_{Ar} \\ P_{Ap} \\ P_{As} \end{bmatrix}, \qquad p_B = \begin{bmatrix} P_{Br} \\ P_{Bp} \\ P_{Bs} \end{bmatrix}, \qquad \mathbf{M} = \begin{bmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{bmatrix}$$

where  $p_{A_r}$ ,  $p_{A_p}$ , and  $p_{A_s}$  are the probability of A playing rock, paper, and scissors, respectively, and  $p_{B_r}$ ,  $p_{B_p}$ , and  $p_{B_s}$  are the same thing for B.

Then, minimax problem becomes

$$\underset{p_A \in \Delta^3}{\text{minimize}} \quad \underset{p_B \in \Delta^3}{\text{maximize}} \quad \mathbb{E}_{p_A, p_B}[\text{points for } B] = p_A^{\mathsf{T}} \mathbf{M} p_B.$$

We start by proving

First of all,

$$\begin{array}{lll} p_A {}^\intercal \mathbf{M} p_B & \geq & \underset{p_A \in \Delta^3}{\operatorname{minimize}} & p_A {}^\intercal \mathbf{M} p_B, \\ \\ \Longrightarrow & \underset{p_B \in \Delta^3}{\operatorname{maximize}} & p_A {}^\intercal \mathbf{M} p_B & \geq & \underset{p_B \in \Delta^3}{\operatorname{maximize}} & \underset{p_A \in \Delta^3}{\operatorname{minimize}} & p_A {}^\intercal \mathbf{M} p_B. \\ \\ \Longrightarrow & \underset{p_A \in \Delta^3}{\operatorname{minimize}} & \underset{p_B \in \Delta^3}{\operatorname{maximize}} & p_A {}^\intercal \mathbf{M} p_B & \geq & \underset{p_B \in \Delta^3}{\operatorname{maximize}} & \underset{p_A \in \Delta^3}{\operatorname{minimize}} & p_A {}^\intercal \mathbf{M} p_B. \end{array}$$

Also,

$$\underset{p_A \in \Delta^3}{\text{minimize}} \quad \underset{p_B \in \Delta^3}{\text{maximize}} \quad p_A^{\mathsf{T}} \mathbf{M} p_B \ \leq \ \underset{p_B \in \Delta^3}{\text{maximize}} \quad p_A^{\mathsf{T}} \mathbf{M} p_B = 0$$

Since  $\mathbf{M} = -\mathbf{M}^{\mathsf{T}}$ ,

$$0 \geq \underset{p_{A} \in \Delta^{3}}{\operatorname{minimize}} \quad \underset{p_{B} \in \Delta^{3}}{\operatorname{maximize}} \quad p_{A}^{\mathsf{T}} \mathbf{M} p_{B}$$

$$= \underset{p_{A} \in \Delta^{3}}{\operatorname{minimize}} \quad \underset{p_{B} \in \Delta^{3}}{\operatorname{maximize}} \quad (p_{A}^{\mathsf{T}} \mathbf{M} p_{B})^{\mathsf{T}} \qquad (\because p_{A}^{\mathsf{T}} \mathbf{M} p_{B} \text{ is a scalar})$$

$$= \underset{p_{A} \in \Delta^{3}}{\operatorname{minimize}} \quad \underset{p_{B} \in \Delta^{3}}{\operatorname{maximize}} \quad -p_{B}^{\mathsf{T}} \mathbf{M} p_{A} \qquad (\because \mathbf{M}^{\mathsf{T}} = -\mathbf{M})$$

$$= \underset{p_{A} \in \Delta^{3}}{\operatorname{minimize}} \quad \left[ -\underset{p_{B} \in \Delta^{3}}{\operatorname{minimize}} \quad p_{B}^{\mathsf{T}} \mathbf{M} p_{A} \right]$$

$$= -\underset{p_{A} \in \Delta^{3}}{\operatorname{maximize}} \quad \underset{p_{B} \in \Delta^{3}}{\operatorname{minimize}} \quad p_{A}^{\mathsf{T}} \mathbf{M} p_{B}$$

$$= -\underset{p_{B} \in \Delta^{3}}{\operatorname{minimize}} \quad \underset{p_{A} \in \Delta^{3}}{\operatorname{maximize}} \quad p_{A}^{\mathsf{T}} \mathbf{M} p_{B}$$

$$\geq -\underset{p_{A} \in \Delta^{3}}{\operatorname{minimize}} \quad \underset{p_{B} \in \Delta^{3}}{\operatorname{maximize}} \quad p_{A}^{\mathsf{T}} \mathbf{M} p_{B} \geq 0$$
(Swapped  $p_{A}$  and  $p_{B}$ )

Therefore,

$$\underset{p_A \in \Delta^3}{\text{minimize}} \quad \underset{p_B \in \Delta^3}{\text{maximize}} \quad \underset{p_B \in \Delta^3}{\text{maximize}} \quad \underset{p_A \in \Delta^3}{\text{minimize}} \quad p_A^{\mathsf{T}} \mathbf{M} p_B \ = 0.$$

Now, we prove that  $p_A^{\star}$  and  $p_B^{\star}$  are the unique solution to the given minimax problem by showing that

$$p_A^{\star \mathsf{T}} \mathbf{M} p_B \leq p_A^{\star \mathsf{T}} \mathbf{M} p_B^{\star} = 0 \leq p_A^{\mathsf{T}} \mathbf{M} p_B^{\star}, \qquad \forall p_A, p_B \in \Delta^3$$

holds only for  $p_A^{\star} = p_B^{\star} = \begin{bmatrix} 1/3 & 1/3 & 1/3 \end{bmatrix}^{\mathsf{T}}$ .

Suppose  $\mathbf{M}p_B^{\star} \neq \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^{\mathsf{T}}$ . From  $p_A^{\mathsf{T}}\mathbf{M}p_B^{\star} \geq 0, \forall p_A \in \Delta^3$  and  $p_A$  having nonnegative entries, at least one entry of  $\mathbf{M}p_B^{\star} = \begin{bmatrix} P_{Bs} - P_{Bp} \\ P_{Br} - P_{Bs} \\ P_{Bp} - P_{Br} \end{bmatrix}$  should be negative. Then, we may

choose  $p_A$  so that  $p_A^{\mathsf{T}} \mathbf{M} p_B^{\star} < 0$ , which contradicts the fact that  $0 \leq p_A^{\mathsf{T}} \mathbf{M} p_B^{\star}$  for all  $p_A \in \Delta^3$ . Therefore,  $\mathbf{M} p_B^{\star} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^{\mathsf{T}}$ , and the only possible solution is  $p_B^{\star} = \begin{bmatrix} 1/3 & 1/3 & 1/3 \end{bmatrix}^{\mathsf{T}}$ 

From the left inequality  $p_A^{\star \intercal} \mathbf{M} p_B \leq 0, \forall p_B \in \Delta^3$ , with the similar reasoning (flipping negative to positive and vice versa),  $p_A^{\star \intercal} \mathbf{M} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}$ . Therefore,  $p_A^{\star} = \begin{bmatrix} 1/3 & 1/3 & 1/3 \end{bmatrix}^{\intercal}$ .

(b) The answer is **negative**. If B fixes its strategy to equalize each probability, A can choose any strategy because  $\mathbb{E}_{p_A,p_B}[\text{points for }B]$  is always 0. However, when A chooses

 $p_A \neq \begin{bmatrix} \frac{1}{3} \\ \frac{1}{3} \end{bmatrix}$ , then B can choose one of the strategy  $P_B = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ to make

 $\mathbb{E}_{p_A,p_B}$ [points for B] > 0. Therefore, in minimax problem, considering only one variable while the other one fixed is not a good approach to find the optimal solution.