TTIC 31230 Fundamentals of Deep Learning, winter 2020 ${\it Quiz} \ 4$

Problem 1. The Variational Upper Bound on Mutual Information (25 points)

Consider an arbitrary distribution P(z,y). Show the variational equation

$$I(y,z) = \inf_{O} E_{y \sim P(y)} KL(P(z|y), Q(z))$$

where Q ranges over distributions on z. Hint: It suffices to show

$$I(y,z) \leq E_y KL(P(z|y),Q(z))$$

and that there exists a Q achieving equality.

Problem 2. Rounding RDA (25 points)

We consider the following modification of RDAa

$$\mathrm{RDA}: \; \Phi^* \quad = \quad \underset{\Phi}{\operatorname{argmin}} \; E_{y \sim \mathrm{Pop}, \; z \sim P_{\Phi}(z|y)} \; - \ln \frac{P_{\Phi}(z)}{P_{\Phi}(z|y)} + \lambda \mathrm{Dist}(y, y_{\Phi}(z))$$

Rounding RDA :
$$\Phi^*, \Psi^* = \underset{\Phi}{\operatorname{argmin}} E_{y \sim \operatorname{Pop}, z := \operatorname{round}(z_{\Psi}(y))} - \ln P_{\Phi}(z) + \lambda \operatorname{Dist}(y, y_{\Phi}(z))$$

Here round $(z) \in \mathcal{Z}$ where \mathcal{Z} is a discrete set of vectors defined independent of the choice of y. For example, rounding might map each real number in z to the nearest integer as was done in Balle et al. 2017. Or rounding might map the vector z to the nearest center vector resulting from K-means vector quantization as in VQ-VAE. Other roundings are possible. The Rounding RDA corresponds to practical image compression where $-\log_2 P_{\Phi}(\text{round}(z_{\Phi}(y)))$ is (approximately) the number of bits in the compressed file.

- (a) What is $\nabla_{\Psi} \ln P_{\Phi}(\text{round}(z_{\Psi}(y)))$?
- (b) What is $\nabla_{\Psi} \text{Dist}(y, y_{\Phi}(\text{round}(z_{\Psi}(y))))$?

To optimize Ψ Balle et al. used two tricks. They replaced $P_{\Phi}(\text{round}(z_{\Phi}(y)))$ with $p_{\Phi}(z_{\Phi}(y))$ where $p_{\Phi}(z)$ is a continuous density, and they replace the rounding operation with additive noise. Although rounding will be used for image compression, gradient descent is then done on

$$\Phi^*, \Psi^* = \operatorname*{argmin}_{\Phi, \Psi} E_{y, \epsilon} - \ln p_{\Phi}(z_{\Psi}(y)) + \lambda \mathrm{Dist}(y_{\Phi}(z_{\Psi}(y) + \epsilon))$$

To model rounding to the nearest integer we take each dimension of ϵ to be drawn uniformly over the interval (-1/2, 1/2).

(c) The density $p_{\Phi}(\tilde{z})$ defines a discrete distribution on the discrete values $\tilde{z} \in Z$ defined by

$$P_{\Phi}(\tilde{z}) = P_{z \sim p_{\Phi}}(\text{round}(z) = \tilde{z})$$

Consider the case where \mathcal{Z} is the discrete set of vectors with integer coordinates. Assume that the density $p_{\Phi}(z)$ is locally approximated by its first order Taylor expansion

$$p_{\Phi}(z + \Delta z) = p_{\Phi}(z) + (\nabla_z p_{\Phi}(z))^{\top} \Delta z$$

Assuming the first order Taylor expansion is exact, give a closed-form expression for the discrete distribution $P_{\Phi}(\tilde{z})$ in terms of the continuous density $p_{\Phi}(z)$. Hint: write $P_{\Phi}(\tilde{z})$ as an expectation over ϵ drawn from the uniform distribution on $[-1/2, 1/2]^d$ where d is the dimension of z.

3. VQ-VAEs (50 points)

In a VQ-VAE the rounding operation is parameterized by a tensor C[K, I] giving K center vectors of the form C[k, I]. We now consider rounding-RDAs defined by the following objective.

$$\Phi^*, \Psi^*, C^* = \underset{\Phi, \Psi, C}{\operatorname{argmin}} \ E_{y \sim \operatorname{Pop}, \ \hat{L} := \operatorname{round}_C(L_{\Psi}(y))} \ - \ln P_{\Phi}(\hat{L}) + \lambda \operatorname{Dist}(y, y_{\Phi}(\hat{L}))$$

In the VQ-VAE we are controlling the rate with the parameter K giving the number of clusters. In the optimization problem the prior term $P_{\Phi}(\hat{L})$ is being held as uniform over all \hat{L} and can be ignored. Assuming L_2 distortion we are then left with

$$\Phi^*, \Psi^*, C^* = \underset{\Psi, \Psi, C}{\operatorname{argmin}} E_y \frac{1}{2} ||y - y_{\Phi}(\operatorname{round}_C(L_{\Psi}(y)))||^2$$

This has well defined gradients for Φ and Θ but, because of rounding, not for Ψ . We are now trying to minimize the expected loss of the following forward calculation where L[P,I] is a sequence of vectors.

$$\begin{array}{rcl} y & \sim & \text{Pop} \\ L & = & L_{\Psi}(y) \\ k[p] & = & \underset{k}{\operatorname{argmin}} \; ||C[k,I] - L[p,I]|| \\ \hat{L}[p,I] & = & C[k[p],I] \\ \hat{y} & = & y_{\Phi}(\hat{L}) \\ \text{Loss} & = & \frac{1}{2}||y - \hat{y}||^2 \end{array}$$

The straight through gradient for a rounding operation is given by

$$L.\operatorname{grad} += \hat{L}.\operatorname{grad}$$

- (a) 10 points. Give a for loop for computing C[K, I] grad from \hat{L} grad as defined by backpropagation on the above computation.
- (b) 15 points. The published formulation of VQ-VAE uses the following gradient updates.

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\begin{array}{rcl} L.\mathrm{grad} & += & \hat{L}.\mathrm{grad} \\ & L.\mathrm{grad} & += & \beta(L-\hat{L}) \\ \text{for } p \ C[k(p),I].\mathrm{grad} & += & \tilde{\eta}(C[k(p),I]-L[p,I]) \end{array}
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Actually, this has been modified from the published form to add a learning rate adjustment parameter $\tilde{\eta}$.

Give an additional loss term so that the published version is equivalent to taking the gradient of C[K, I] grad from the new loss term only and L[P, I] grad from both the straight-through gradient and the gradient of the new loss term.

- (c) 15 points. Give a complete set of backpropagation updates defined by backpropagation on both loss terms and using straight-through backpropagation to L[P,I].grad
- (d) 10 points. We now have three versions of training end-to-end with straight through as in part (a), the published version as in part (b), and the backpropagation on the both loss terms with straight-through as defined in part (c). For which of these three training algorithms is it true that at a stationary point C[k, I] is mean of the vectors assigned to class k?