Autoencoders, Multivariate Normal KL

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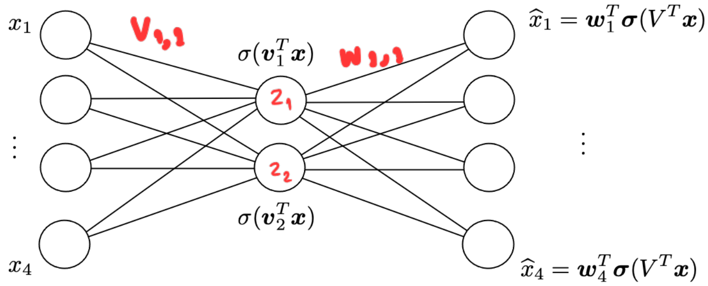
1. Consider the undercomplete autoencoder shown in the figure below. In this problem, there is no activation function on the output layer (the first output is given as $\widehat{x}_1 = \boldsymbol{w}_1^T \boldsymbol{\sigma}(V^T \boldsymbol{x})$).



→ V and W V → 2×4, W → 4×2 → 16 parameters in total

a) How many parameters do you need to learn to train your autoencoder?

b) Let $w_{1,1}$ denote the weight associated with the connection between the first (top) hidden node and the first output node, and $w_{2,1}$ denote the weight associated with the bottom hidden node and the first output. Compute the partial derivative of the output $\widehat{x}_1$ with respect to weight $w_{1,1}$ when $\sigma(\cdot)$ is the logistic activation function. $\sigma(v_1^T x)$

c) Let $v_{1,1}$ denote the weight associated with the connection between the first (top) input note and the first hidden note. Compute the partial derivative of the output $\widehat{x}_1$ with respect to weight $v_{1,1}$ when $\sigma(\cdot)$ is the logistic activation function.

$\frac{d}{dv_{1,1}} \hat{x}_1 = \frac{d}{dz_1} \hat{x} \frac{d}{dv_{1,1}} z_1 = w_{1,1} (\sigma(z_1)(1-\sigma(z_1)) x_1$

d) You decide to use the squared error loss function, i.e, $\ell(\widehat{\boldsymbol{x}}, \boldsymbol{x}) = ||\widehat{\boldsymbol{x}} - \boldsymbol{x}||^2$. Compute the partial derivative of $\ell(\widehat{\boldsymbol{x}}, \boldsymbol{x})$ first with respect to $w_{1,1}$, and then with respect to $v_{1,1}$.

$\frac{\partial}{\partial v_{1,1}} \ell(\hat{x}, x) = \sum_{i=1}^{4} \left(\frac{\partial}{\partial v_{1,1}} \hat{x}_i \right) 2(x_i - \hat{x}_i) = 2 \sum_{i=1}^{4} (x_i - \hat{x}_i) w_{1,i} (\sigma(z_1)(1-\sigma(z_1)) x_i$

2. In this problem we will compute the Kullback–Leibler divergence between two multivariate normal distributions (a quantity we will use in a later lecture). For reference, recall the general form of a multivariate normal distribution:

$$p(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right)$$

and the definition of KL divergence:

$$D(p(\boldsymbol{x}) || q(\boldsymbol{x})) = \int p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} d\boldsymbol{x}.$$

Let $p(\boldsymbol{x}) \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$ and $q(\boldsymbol{x}) \sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$. Describe and justify each step in the derivation of the KL divergence between the two multivariate normal distributions:

$$D(p(\boldsymbol{x})||q(\boldsymbol{x}))$$

$$\overset{(1)}{=} \int p(\boldsymbol{x}) \left(\frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}_2^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_2) - \frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_1^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_1) \right) d\boldsymbol{x}$$

$$\overset{(2)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} E_p \left[(\boldsymbol{x} - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}_2^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_2) \right] - \frac{1}{2} E_p \left[(\boldsymbol{x} - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_1^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_1) \right]$$

de fn. of expectation
$E[g(x)] = \int g(x) p(x) dx$

$$\overset{(3)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} E_p \left[\mathrm{tr} \left((\boldsymbol{x} - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}_2^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_2) \right) \right] - \frac{1}{2} E_p \left[\mathrm{tr} \left((\boldsymbol{x} - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}_1^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_1) \right) \right]$$

$\to$ is a scalar,
trace is the identity
transformation!

$$\overset{(4)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_2^{-1} E_p \left[(\boldsymbol{x} - \boldsymbol{\mu}_2)(\boldsymbol{x} - \boldsymbol{\mu}_2)^T \right] \right) - \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_1^{-1} E_p \left[(\boldsymbol{x} - \boldsymbol{\mu}_1)(\boldsymbol{x} - \boldsymbol{\mu}_1)^T \right] \right)$$

$\to$ $tr(AB) = tr(BA)$
we may remove Σ_1^{-1} out of expectation
bc. $A = (X-\mu)^T$, $B = \Sigma^{-1}(X-\mu)$

$$\overset{(5)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_2^{-1} E_p \left[(\boldsymbol{x} - \boldsymbol{\mu}_2)(\boldsymbol{x} - \boldsymbol{\mu}_2)^T \right] \right) - \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_1^{-1} \boldsymbol{\Sigma}_1 \right)$$

definition of covariance
$\Sigma_1 = E_p[(X_1 - \mu_1)^T (X_1 - \mu_1)]$

$$\overset{(6)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_2^{-1} E_p \left[\boldsymbol{x}\boldsymbol{x}^T - 2\boldsymbol{x}\boldsymbol{\mu}_2^T + \boldsymbol{\mu}_2\boldsymbol{\mu}_2^T \right] \right) - \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_1^{-1} \boldsymbol{\Sigma}_1 \right)$$

expansion

$$\overset{(7)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_2^{-1} \left(\boldsymbol{\Sigma}_1 + \boldsymbol{\mu}_1\boldsymbol{\mu}_1^T - 2\boldsymbol{\mu}_1\boldsymbol{\mu}_2^T + \boldsymbol{\mu}_2\boldsymbol{\mu}_2^T \right) \right) - \frac{1}{2} n$$

$E_p[X] = \mu_1$, $E_p[X^T X] = \Sigma_1$

$$\overset{(8)}{=} \frac{1}{2} \log \frac{|\boldsymbol{\Sigma}_2|}{|\boldsymbol{\Sigma}_1|} + \frac{1}{2} \mathrm{tr} \left(\boldsymbol{\Sigma}_2^{-1} \boldsymbol{\Sigma}_1 \right) + \frac{1}{2} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}_2^{-1} (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) - \frac{1}{2} n$$

arrangement of terms