Neural Computation

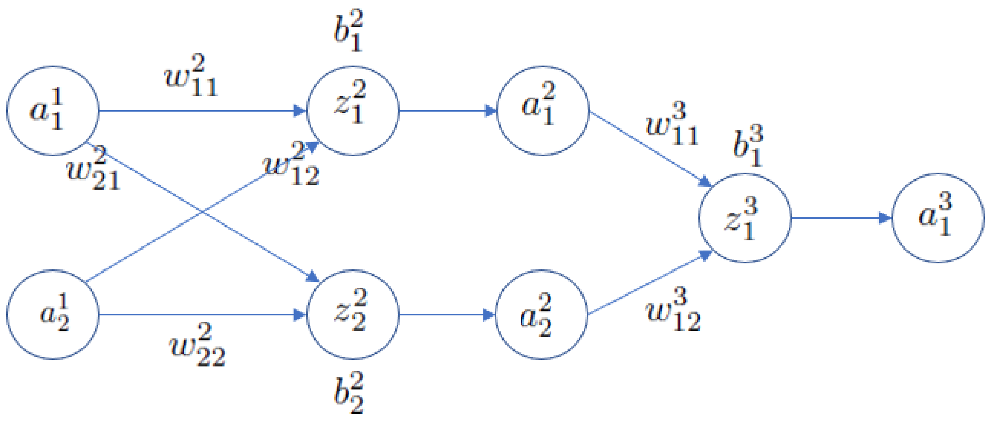
Solutions

Main Summer Examinations 2022

Neural Computation

Question 1

Let us consider solving regression problems with a neural network. In particular, we consider a neural network of the following structure:



As illustrated in the lecture, we have the following relationship between variables in the neural network.

$$\mathbf{z}^2 = \begin{pmatrix} z_1^2 \\ z_2^2 \end{pmatrix} = \begin{pmatrix} \omega_{11}^2 & \omega_{12}^2 \\ \omega_{21}^2 & \omega_{22}^2 \end{pmatrix} \begin{pmatrix} a_1^1 \\ a_2^1 \end{pmatrix} + \begin{pmatrix} b_1^2 \\ b_2^2 \end{pmatrix}, \quad \mathbf{a}^2 = \begin{pmatrix} a_1^2 \\ a_2^2 \end{pmatrix} = \begin{pmatrix} \sigma(z_1^2) \\ \sigma(z_2^2) \end{pmatrix},$$

where σ is the activation function. For simplicity of computation, we always use $\sigma(x) = x^2$ in this neural network. In a similar way, there is also a relationship between z_1^3, a_1^3 and $\mathbf{a}^2$.

(a) Compute the number of trainable parameters required in determining this neural network. Please explain your answer. **[3 marks]**

(b) Suppose

$$\mathbf{W}^2 = \begin{pmatrix} \omega_{11}^2 & \omega_{12}^2 \\ \omega_{21}^2 & \omega_{22}^2 \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad \mathbf{W}^3 = (\omega_{11}^3, \omega_{12}^3) = (1, 1),$$

$$\mathbf{b}^2 = \begin{pmatrix} b_1^2 \\ b_2^2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad b_1^3 = -3.$$

Consider the training example

$$\mathbf{x} = \begin{pmatrix} a_1^1 \\ a_2^1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad y = 1.$$

Let us consider the square loss function $C_{\mathbf{x},y}(\mathbf{W}, \mathbf{b}) = \frac{1}{2}(a_1^3 - y)^2$, where $\mathbf{W} = \{\mathbf{W}^2, \mathbf{W}^3\}, \mathbf{b} = \{\mathbf{b}^2, b_1^3\}$. Use the forward propagation algorithm to compute $\mathbf{a}^2$, a_1^3 and the loss $C_{\mathbf{x},y}(\mathbf{W}, \mathbf{b})$ for using the neural network to do prediction on the above example $(\mathbf{x}, y)$. Please write down your step-by-step calculations. **[7 marks]**

(c) Let us consider the neural network with the above $\mathbf{W}^2, \mathbf{W}^3, \mathbf{b}^2, b_1^3$ and the above training example $\mathbf{x}, y$. Use the back propagation algorithm to compute the gradients. For simplicity, we only require you to compute the explicit number of

$$\frac{\partial C_{\mathbf{x},y}(\mathbf{W},\mathbf{b})}{\partial z_1^3}, \quad \frac{\partial C_{\mathbf{x},y}(\mathbf{W},\mathbf{b})}{\partial z_1^2}, \quad \frac{\partial C_{\mathbf{x},y}(\mathbf{W},\mathbf{b})}{\partial z_2^2}, \quad \frac{\partial C_{\mathbf{x},y}(\mathbf{W},\mathbf{b})}{\partial \omega_{11}^3}, \quad \frac{\partial C_{\mathbf{x},y}(\mathbf{W},\mathbf{b})}{\partial \omega_{12}^3}.$$

Please write down your step-by-step calculations. **[10 marks]**

Model answer / LOs / Creativity:

(a) The trainable parameters include the weight matrices and bias vectors, which are as follows

$$\mathbf{W}^2 = \begin{pmatrix} \omega_{11}^2 & \omega_{12}^2 \\ \omega_{21}^2 & \omega_{22}^2 \end{pmatrix}, \quad \mathbf{b}^2 = \begin{pmatrix} b_1^2 \\ b_2^2 \end{pmatrix} \quad \mathbf{W}^3 = (\omega_{11}^3, \omega_{12}^3) \quad b_1^3.$$

In total, we have $4+2+2+1=9$ parameters.

- Type of question: Bookwork
- Learning outcomes: 1 and 4.
- Marking scheme: One mark for correct number, two extra marks for the explanation.

(b) According to the construction of the neural network, we know

$$\mathbf{z}^2 = \mathbf{W}^2\mathbf{a}^1 + \mathbf{b}^2 = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \end{pmatrix} \Longrightarrow \mathbf{a}^2 = \begin{pmatrix} 1 \\ 4 \end{pmatrix}.$$

Furthermore, we have

$$z_1^3 = (\omega_{11}^3, \omega_{12}^3)\begin{pmatrix} a_1^2 \\ a_2^2 \end{pmatrix} + b_1^3 = (1,1)\begin{pmatrix} 1 \\ 4 \end{pmatrix} - 3 = 2 \Longrightarrow a_1^3 = 4$$

The loss function becomes

$$(a_1^3 - y)^2/2 = (4-1)^2/2 = 9/2.$$

- Type of question: Creative
- Learning outcomes: 1 and 4.
- Marking scheme: Three marks for $\mathbf{a}^2$, two marks for a_1^3 and two marks for the loss function.

(c) Note $\sigma'(x) = 2x$. We first compute the backpropagated gradient w.r.t. z_1^3

$$\delta_1^3 = \frac{\partial C}{\partial z_1^3} = \sigma'(z_1^3) * (a_1^3 - y) = 2 * 2 * (4-1) = 12.$$

We then compute the backpropagated gradient w.r.t. $\mathbf{z}^2$. According to the back-propagation algorithm, we have

$$\delta^2 = \begin{pmatrix} \frac{\partial C}{\partial z_1^2} \\ \frac{\partial C}{\partial z_2^2} \end{pmatrix} = \sigma'(\mathbf{z}^2) \odot ((\mathbf{W}^3)^\top \delta_1^3) = \begin{pmatrix} 2z_1^2 \\ 2z_2^2 \end{pmatrix} \odot \left(\begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot 12 \right) = \begin{pmatrix} -2 \\ 4 \end{pmatrix} \odot \begin{pmatrix} 12 \\ 12 \end{pmatrix} = \begin{pmatrix} -24 \\ 48 \end{pmatrix}$$

Furthermore, according to the backpropagation we know

$$\left(\frac{\partial C}{\partial \omega_{11}^3}, \frac{\partial C}{\partial \omega_{12}^3} \right) = \delta^3 (\mathbf{a}^2)^\top = 12 * (1, 4) = (12, 48).$$

- Type of question: Creative
- Learning outcomes: 1 and 4.
- Marking scheme: Two marks of each gradient computation.

Question 2

Given the weights (w_1, w_2, w_3) and the biases (b_2, b_3), we have the following recurrent neural network (RNN) which takes in an input vector x_t and a hidden state vector h_{t-1} and returns an output vector y_t:

$$y_t = \mathbf{g}(w_3 \mathbf{f}(w_1 x_t + w_2 h_{t-1} + b_2) + b_3), \tag{1}$$

where $\mathbf{g}$ and $\mathbf{f}$ are activation functions. The following computational graph depicts such a RNN.

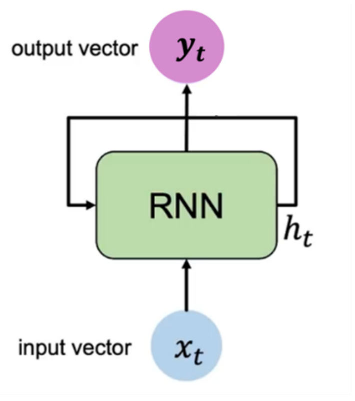


Figure 1: RNN Computational Graph

(a) Write down clearly which part of Equation (1) defines the current (updated) hidden state vector h_t shown in Figure 1. **[3 marks]**

(b) When $t = 3$ (starting from 1), please show how information is propagated through time by drawing an unfolded feedforward neural network that corresponds to the RNN in Figure 1. Please make sure that hidden states, inputs and outputs as well as network weights and biases are annotated on your network. **[4 marks]**

(c) Assume x_t, h_{t-1}, h_t and y_t are all scalars in Equation (1), and the activation functions are a linear unit and a binary threshold unit, respectively defined as:

$$\mathbf{g}(x) = x,$$
$$\mathbf{f}(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}.$$

When $t = 3$ (starting from 1), please calculate the values of the outputs (y_1, y_2, y_3) given $(w_1 = 1, w_2 = -3, w_3 = 5)$, $(b_2 = 1, b_3 = 3)$, $(x_1 = 5, x_2 = 3, x_3 = 1)$ and $h_0 = 0$. Please show your calculations in detail. **[3 marks]**

(d) Again let us assume x_t, h_{t-1}, h_t and y_t are all scalars with $h_0 = 0$ and the activation functions the same as above. Compute (w_1, w_2, w_3) and (b_2, b_3) such that the network outputs 0 initially, but when it receives an input of 1, it outputs 1 for all subsequent time steps. For example, if the input is 00001000100, the output will be 00001111111. Please justify your answer.

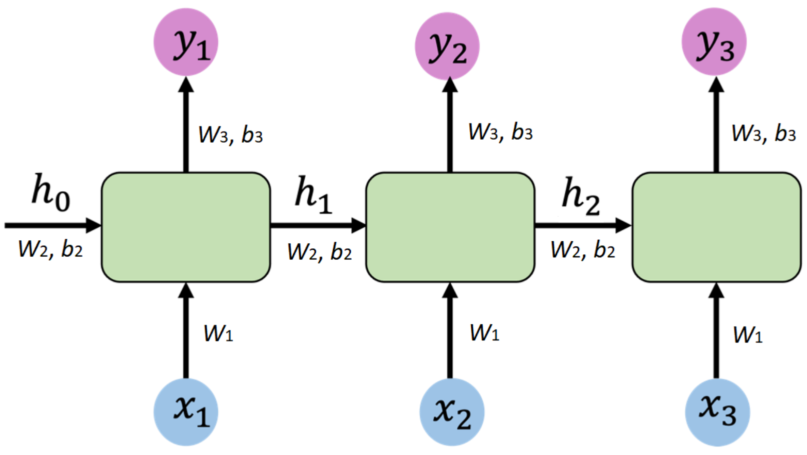
Note: here we want a solution that satisfies (1) the hidden state h_t is zero until the input x_t becomes 1, at which point the hidden state changes to 1 forever, and (2) the output always predicts the same as the hidden state, i.e. $y_t = h_t$. **[10 marks]**

Model answer / LOs / Creativity:

(a) The current hidden state $h_t = \mathbf{f}(w_1 x_t + w_2 h_{t-1} + b_2)$. **[3 marks]**

- Type of question: Bookwork
- Learning outcomes: 1.
- Marking scheme: 3 points for hidden state equation right

(b) Please see the following figure for an unfolded feedforward RNN with $t = 3$. Note: parameters should be shared. **[4 marks]**



- Type of question: Bookwork
- Learning outcomes: 1.
- Marking scheme: 2 point for drawing three cascades correctly and 2 point for making all annotations correctly.

(c)

$$h_1 = \mathbf{f}(w_1 x_1 + w_2 h_0 + b_2) = \mathbf{f}((1x5) + (-3x0) + 1) = 1$$
$$y_1 = \mathbf{g}(w_3 h_1 + b_3) = \mathbf{g}((5x1) + 3) = 8$$

$$h_2 = \mathbf{f}(w_1 x_2 + w_2 h_1 + b_2) = \mathbf{f}((1x3) + (-3x1) + 1) = 1$$
$$y_2 = \mathbf{g}(w_3 h_2 + b_3) = \mathbf{g}((5x1) + 3) = 8$$

$$h_3 = \mathbf{f}(w_1 x_3 + w_2 h_2 + b_2) = \mathbf{f}((1x1) + (-3x1) + 1) = 0$$
$$y_3 = \mathbf{g}(w_3 h_3 + b_3) = \mathbf{g}((5x0) + 3) = 3$$

[3 marks]

- Type of question: Creative
- Learning outcomes: 2 and 4.
- Marking scheme: 2 points for equations correct but answers wrong. 3 points for both equations and answers right.

(d) According to the note we provided, y_t should be equal to h_t, hence we have to set $w_3 = 1$ and $b_3 = 0$. Then at the beginning, we have $h_1 = 0$ and $x_1 = 0$ and hence $\mathbf{f}(b_2) = 0$, indicating $b_2 < 0$. Then we have two situations, first $\mathbf{f}(w_1 + b_2) = 1$ for input $x_t = 1$ and $h_t = 0$. In this case, $w_1 + b_2 \geq 0$. Second, for input $x_t = 0$ and $h_t = 1$, the output should be still 1, so in this case, $\mathbf{f}(w_2 + b_2) = 1$, indicating $w_2 + b_2 \geq 0$. Apart from these, we do not have any more scenarios. In conclusion, the following constraints should be satisfied:

$$w_3 = 1$$
$$b_3 = 0$$
$$b_2 < 0$$
$$w_1 + b_2 \geq 0$$
$$w_2 + b_2 \geq 0$$

[10 marks]

- Type of question: Creative
- Learning outcomes: 3.
- Marking scheme: Two points for each of the five constraints correct.

Question 3

Note: Each item below can be answered with approximately 5 lines of text. This is only an informal indication, not a hard constraint. Length of answers will not influence marks.

(a) Consider the Variational Auto-Encoder (VAE), with encoder $f_\phi(x)$ that predicts mean $\mu_\phi(x)$ and standard deviation $\sigma_\phi(x)$ of a multi-dimensional Gaussian that is the conditional $p_\phi(z|x)$, and decoder $g_\theta(z)$. The VAE's loss for each d-dimensional input vector x is:

$$\mathcal{L}_{VAE} = \lambda_{rec}\mathcal{L}_{rec}(x) + \lambda_{reg}\mathcal{L}_{reg}(x), \tag{2}$$

where $\mathcal{L}_{rec}(x) = \frac{1}{d}\sum_{j=1}^{d}(x^{(j)} - g_\theta^{(j)}(\tilde{z}))^2$ for sample $\tilde{z} \sim p_\phi(z|x)$ is reconstruction loss, $\mathcal{L}_{reg}(x) = \frac{1}{2}\sum_{j=1}^{v}\left[(\mu_\phi^{(j)}(x))^2 + (\sigma_\phi^{(j)}(x))^2 - 2\log_e \sigma_\phi^{(j)}(x) - 1\right]$ is the regularizer, z is a v-dimensional vector and $\log_e$ is the natural logarithm. λ_{rec}, λ_{reg} are non-trainable scalars for weighting $\mathcal{L}_{rec}$ and $\mathcal{L}_{reg}$. $h^{(j)}$ denotes the j-th element of vector h.

(i) If you train minimizing only the regularizer $\mathcal{L}_{reg}$ (i.e. $\lambda_{rec} = 0$ and $\lambda_{reg} > 0$), what values do you expect the encoder will tend to predict for means $\mu_\phi(x)$ and standard deviations $\sigma_\phi(x)$? Explain why. **[4 marks]**

(ii) Assume that z is 2 dimensional (i.e. $v = 2$). Assume that for an input data point x_1 the encoder outputs vectors $\mu_\phi(x_1) = (0.5, 0.1)$ and $\sigma_\phi(x_1) = (0.1, 0.3)$. Calculate the value of $\mathcal{L}_{reg}(x_1)$. Show the steps of the calculation. (Note: For simplicity, use $\log_e 0.1 \approx -2.3$ and $\log_e 0.3 \approx -1.2$) **[4 marks]**

(iii) Assume you are given an implementation of the above VAE with a bottleneck (i.e. $v < d$). You are asked to train the VAE so that it will be as good as possible for the task of compressing data (via bottleneck) and uncompressing them with fidelity. Generation of fake data or other applications are not of interest. What values would you choose for λ_{rec} and λ_{reg}? For each, specify either *equal to* 0 or *greater than* 0. Explain why. **[5 marks]**

(b) Consider a Generative Adversarial Network (GAN) that consists of a Generator G that takes input noise vector z and outputs $G(z)$, and Discriminator D that given input x it outputs $D(x)$. We assume that $D(x) = 1$ means that D predicts with certainty that input x is a real data point, and $D(x) = 0$ means D predicts with certainty that x is a fake, generated sample. Figure 2 shows two loss functions that could be used for training G. Which of the two loss functions in Figure 2 is more appropriate for training G in practice? Explain why, based on the gradients for lowest and highest values of $D(G(z))$ and how they would influence training. **[7 marks]**

Model answer / LOs / Creativity:

(a) (i) Regardless the input the encoder will tend to predict mean equal (or close to) zero, and standard deviation equal (or close to) one. The regularizer minimizes

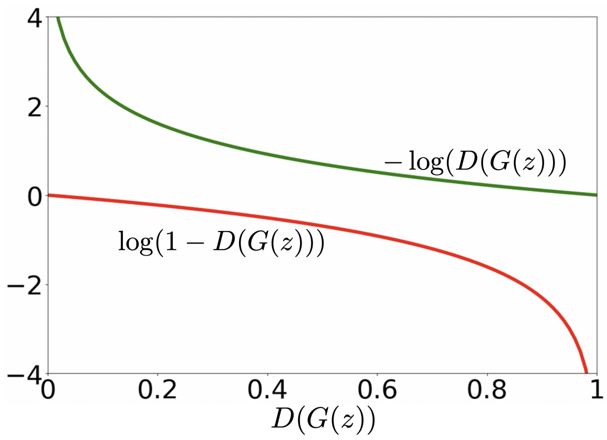


Figure 2: Two loss functions that could be used (minimized) for training Generator G of a GAN. Shown as a function of Discriminator's D predicted probability that a generated sample $G(z)$ is real. On the x-axis, $D(G(z)) = 1$ means D predicts with certainty that $G(z)$ is real, whereas $D(G(z)) = 0$ means D predicts with certainty that $G(z)$ is fake.

the KL divergence between predicted conditional $p(z|x)$ and the prior, $N(0, I)$, i.e. make all means 0 and standard deviations 1. **[4 marks]**

- Type of question: Bookwork
- Learning outcomes: 1 and 2.
- Marking scheme: 1 mark for correct answer about means, 1 for standard deviations. 2 marks for correct explanation.

(ii) Below are the calculations:

$$\begin{aligned}
\mathcal{L}_{reg}(x_1) &= \frac{1}{2}(0.5^2 + 0.1^2 - 2\log_e 0.1 - 1 + 0.1^2 + 0.3^2 - 2\log_e 0.3 - 1) && (3)\\
&= \frac{1}{2}(0.25 + 0.01 - 2(-2.3) - 1 + 0.01 + 0.09 - 2(-1.2) - 1) && (4)\\
&= \frac{1}{2}(0.26 + 3.6 + 0.1 + 1.4) && (5)\\
&= \frac{1}{2}(3.86 + 1.5) && (6)\\
&= \frac{1}{2}5.36 && (7)\\
&= 2.68 && (8)
\end{aligned}$$

[4 marks]

- Type of question: Creative
- Learning outcomes: 1.
- Marking scheme: 1 mark for correctly substituting means and standard deviations in equation. 3 marks for correct solution.

(iii) The correct answer is $\lambda_{rec} > 0$ and $\lambda_{reg} = 0$. This is because for the application of compression only care about being able to reconstruct, not about covering the prior $N(0, I)$. The regularizer opposes the reconstruction loss by enforcing codes to cover the prior. The reconstruction loss alone is the optimal objective for compression and reconstruction. **[5 marks]**

- Type of question: Creative
- Learning outcomes: 1 and 4.
- Marking scheme: 1 mark for correct answer. 2 marks for explaining we only care about reconstruction, not covering the prior. 2 marks for explaining the regularizer opposes reconstruction.

(b) Answer is $-\log(D(G(z)))$. Early in training, G will generate bad output, which D will easily separate from real examples, therefore $D(G(z))$ will be close to 0. Then gradients of $\log(1 - D(G(z)))$ are small, impeding training. In contrast, gradients of $-\log(D(G(z)))$ are large, training G. If $G(z)$ generates some realistic samples, $D(G(z))$ approaches 1 for them. For realistic samples, we would like the loss to saturate, giving gradients close to 0, so that parameters only change by gradients from bad samples, to improve those. $-\log(D(G(z)))$ has this property, whereas $\log(1 - D(G(z)))$ does not. **[7 marks]**

- Type of question: Creative
- Learning outcomes: 1 and 2.
- Marking scheme: 1 mark for answer correct loss. 3 marks for correct explanation for early training. 3 marks for correct explanation regarding very good samples.