

Solutions to the Exam on Neural Network Theory August 17, 2020

Problem 1

(a) By definition we have

$$g_{B_{n+1}}(\mathbf{x}) = \int_{-\frac{1}{2}}^{\frac{1}{2}} g_{B_n}(\mathbf{x} - t\mathbf{b}_{n+1}) dt.$$

This yields

$$\begin{aligned} \hat{g}_{B_{n+1}}(\xi) &= \int_{\mathbb{R}^n} g_{B_{n+1}}(\mathbf{x}) e^{-i\xi^T \mathbf{x}} d\mathbf{x} \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\int_{\mathbb{R}^n} g_{B_n}(\mathbf{x} - t\mathbf{b}_{n+1}) e^{-i\xi^T \mathbf{x}} d\mathbf{x} \right) dt \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\int_{\mathbb{R}^n} |\det(\mathbf{B}_n)| g_{B_n}(\mathbf{B}_n \mathbf{z}) e^{-i\xi^T (\mathbf{B}_n \mathbf{z} + t\mathbf{b}_{n+1})} d\mathbf{z} \right) dt \end{aligned} \quad (1)$$

$$= \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i\xi^T \mathbf{b}_{n+1} t} dt \prod_{i=1}^n \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i\xi^T \mathbf{b}_i z_i} dz_i, \quad (2)$$

where in (1) we changed variables to $\mathbf{z} = \mathbf{B}_n^{-1}(\mathbf{x} - t\mathbf{b}_{n+1})$ and (2) follows from the fact that

$$|\det(\mathbf{B}_n)| g_{B_n}(\mathbf{B}_n \mathbf{z}) = \begin{cases} 1, & \text{if } \mathbf{z} \in \left[-\frac{1}{2}, \frac{1}{2}\right]^n \\ 0, & \text{else.} \end{cases}$$

As

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-iat} dt = \frac{2}{a} \sin\left(\frac{a}{2}\right), \quad \text{for all } a > 0, \quad (3)$$

we can conclude that

$$\hat{g}_{B_{n+1}}(\xi) = \prod_{i=1}^{n+1} \left(\frac{2}{\xi^T \mathbf{b}_i} \sin\left(\frac{\xi^T \mathbf{b}_i}{2}\right) \right).$$

(b) The result for $q = n + 1$ follows from subproblem (a). For general $q > n$, we proceed by induction as follows. Suppose that the statement holds for $q - 1$, i.e.,

$$\hat{g}_{B_{q-1}}(\xi) = \prod_{i=1}^{q-1} \left(\frac{2}{\xi^T \mathbf{b}_i} \sin\left(\frac{\xi^T \mathbf{b}_i}{2}\right) \right). \quad (4)$$

By definition we have

$$g_{B_q}(\mathbf{x}) = \int_{-\frac{1}{2}}^{\frac{1}{2}} g_{B_{q-1}}(\mathbf{x} - t\mathbf{b}_q) dt.$$

This yields

$$\begin{aligned} \hat{g}_{B_q}(\xi) &= \int_{\mathbb{R}^n} g_{B_q}(\mathbf{x}) e^{-i\xi^T \mathbf{x}} d\mathbf{x} \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\int_{\mathbb{R}^n} g_{B_{q-1}}(\mathbf{x} - t\mathbf{b}_q) e^{-i\xi^T \mathbf{x}} d\mathbf{x} \right) dt \\ &= \int_{-\frac{1}{2}}^{\frac{1}{2}} \left(\int_{\mathbb{R}^n} g_{B_{q-1}}(\mathbf{z}) e^{-i\xi^T (\mathbf{z} + t\mathbf{b}_q)} d\mathbf{z} \right) dt \end{aligned} \quad (5)$$

$$\begin{aligned} &= \hat{g}_{B_{q-1}}(\xi) \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{-i\xi^T \mathbf{b}_q t} dt \\ &= \prod_{i=1}^q \left(\frac{2}{\xi^T \mathbf{b}_i} \sin\left(\frac{\xi^T \mathbf{b}_i}{2}\right) \right), \end{aligned} \quad (6)$$

where in (5) we changed variables to $\mathbf{z} = \mathbf{x} - t\mathbf{b}_q$ and (6) follows from (3) and (4).

- (c) We first determine the Fourier transform $\widehat{f \star g}(\xi)$ of the convolution $(f \star g)(\mathbf{x})$ for two general functions $f, g: \mathbb{R}^n \rightarrow \mathbb{R}$. Specifically, we have

$$\begin{aligned} \widehat{f \star g}(\xi) &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} f(\mathbf{y}) g(\mathbf{x} - \mathbf{y}) d\mathbf{y} \right) e^{-i\xi^T \mathbf{x}} d\mathbf{x} \\ &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} g(\mathbf{x} - \mathbf{y}) e^{-i\xi^T \mathbf{x}} d\mathbf{x} \right) f(\mathbf{y}) d\mathbf{y} \\ &= \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} g(\mathbf{u}) e^{-i\xi^T \mathbf{u}} d\mathbf{u} \right) f(\mathbf{y}) e^{-i\xi^T \mathbf{y}} d\mathbf{y} \\ &= \hat{f}(\xi) \hat{g}(\xi), \end{aligned} \quad (7)$$

where in (7) we changed variables to $\mathbf{u} = \mathbf{x} - \mathbf{y}$. Particularizing this result to $f = g = g_{B_q}$ yields

$$\begin{aligned} \hat{k}(\xi) &= \widehat{g_{B_q} \star g_{B_q}}(\xi) \\ &= (\hat{g}_{B_q})^2(\xi) \\ &= \prod_{i=1}^q \left(\frac{2}{\xi^T \mathbf{b}_i} \sin\left(\frac{\xi^T \mathbf{b}_i}{2}\right) \right)^2, \end{aligned} \quad (8)$$

where in (8) we used the explicit expression for $\hat{g}_{B_q}(\xi)$ obtained in subproblem (b).

- (d) We have to show that for every $k \in \mathbb{N}$ and all $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{R}^n$, the $k \times k$ Gramian matrix

$$\mathbf{K}(\mathbf{x}_1, \dots, \mathbf{x}_k) = \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \dots & K(\mathbf{x}_1, \mathbf{x}_k) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \dots & K(\mathbf{x}_2, \mathbf{x}_k) \\ \vdots & \vdots & \dots & \vdots \\ K(\mathbf{x}_k, \mathbf{x}_1) & K(\mathbf{x}_k, \mathbf{x}_2) & \dots & K(\mathbf{x}_k, \mathbf{x}_k) \end{pmatrix}$$

is positive semidefinite. This is effected by noting that, for every $k \in \mathbb{N}$, all $\mathbf{x}_1, \dots, \mathbf{x}_k \in \mathbb{R}^n$, and all $\mathbf{c} = (c_1 \dots c_k)^\top \in \mathbb{R}^k$, we have

$$\begin{aligned}
\mathbf{c}^\top \mathbf{K}(\mathbf{x}_1, \dots, \mathbf{x}_k) \mathbf{c} &= \sum_{i,j=1}^k c_i c_j K(\mathbf{x}_i, \mathbf{x}_j) \\
&= \sum_{i,j=1}^k c_i c_j k(\mathbf{x}_i - \mathbf{x}_j) \\
&= \frac{1}{(2\pi)^n} \sum_{i,j=1}^k c_i c_j \int \hat{k}(\xi) e^{i\xi^\top(\mathbf{x}_i - \mathbf{x}_j)} d\xi \\
&= \frac{1}{(2\pi)^n} \int \hat{k}(\xi) \left| \sum_{i=1}^k c_i e^{i\xi^\top \mathbf{x}_i} \right|^2 d\xi \\
&\geq 0,
\end{aligned}$$

which, owing to $\hat{k}(\xi) \geq 0$, for all $\xi \in \mathbb{R}^n$, proves that K is positive semidefinite.

Problem 2

(a) The Lagrange function $L(\mathbf{w}, b, \mathbf{c})$ is given by

$$L(\mathbf{w}, b, \mathbf{c}) = \frac{1}{2} \|\mathbf{w}\|_2^2 + \sum_{i=1}^3 c_i (1 - y_i (\langle \mathbf{w}, \mathbf{x}_i \rangle_2 - b)). \quad (9)$$

(b) Setting $\nabla_{\mathbf{w}} L(\mathbf{w}, b, \mathbf{c}) = 0$ and $\nabla_b L(\mathbf{w}, b, \mathbf{c}) = 0$ yields

$$\mathbf{w} = \sum_{i=1}^3 c_i y_i \mathbf{x}_i \quad (10)$$

and

$$\sum_{i=1}^3 c_i y_i = 0, \quad (11)$$

respectively. Using (10) and (11) in (9) results in

$$\begin{aligned} g(\mathbf{c}) &= \min_{\mathbf{w} \in \mathbb{R}^2, b \in \mathbb{R}} L(\mathbf{w}, b, \mathbf{c}) \\ &= \sum_{i=1}^3 c_i - \frac{1}{2} \sum_{i,j=1}^3 c_i y_i c_j y_j \langle \mathbf{x}_i, \mathbf{x}_j \rangle_2 \\ &= \mathbf{a}^\top \mathbf{c} - \frac{1}{2} \mathbf{c}^\top \mathbf{A} \mathbf{c} \end{aligned}$$

with $\mathbf{a} = (1 \ 1 \ 1)^\top$ and

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -\lambda \\ 0 & -\lambda & 1 + \lambda^2 \end{pmatrix}.$$

(c) It follows from subproblem (b) that the Lagrange dual function $g(\mathbf{c})$ can be written as

$$g(\mathbf{c}) = c_1 + c_2 + c_3 - \frac{1}{2} (c_2^2 + (1 + \lambda^2) c_3^2 - 2\lambda c_2 c_3).$$

Since $-g(\mathbf{c})$ is convex, we can, as mentioned in the hint, consider the Lagrange function

$$\tilde{L}(\mathbf{c}, \boldsymbol{\mu}, \gamma) = -g(\mathbf{c}) - \boldsymbol{\mu}^\top \mathbf{c} + \gamma (c_1 + c_2 - c_3),$$

where $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3)^\top \in \mathbb{R}^3$ and $\gamma \in \mathbb{R}$ are Lagrange multipliers. The KKT conditions now read as follows:

$$c_i \geq 0, \quad \text{for } i = 1, 2, 3 \quad (12)$$

$$c_1 + c_2 - c_3 = 0, \quad (13)$$

$$\mu_i \geq 0, \quad \text{for } i = 1, 2, 3 \quad (14)$$

$$c_i \mu_i = 0, \quad \text{for } i = 1, 2, 3 \quad (15)$$

$$\frac{\partial \tilde{L}(\mathbf{c}, \boldsymbol{\mu}, \gamma)}{\partial c_i} = 0, \quad \text{for } i = 1, 2, 3. \quad (16)$$

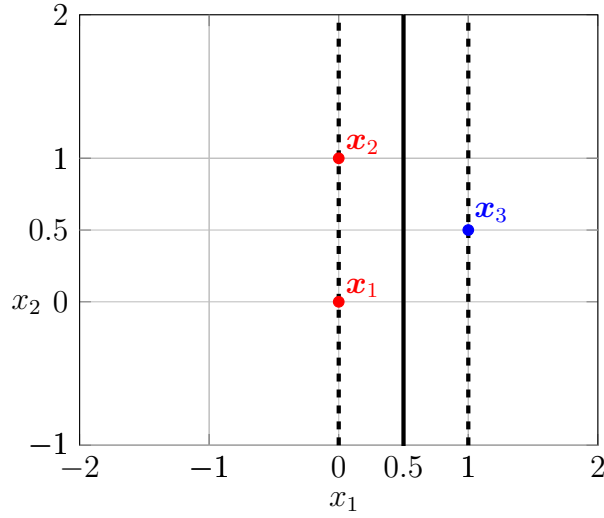
Evaluating the derivatives in (16) yields

$$-1 - \mu_1 + \gamma = 0 \quad (17)$$

$$-1 + c_2 - \lambda c_3 - \mu_2 + \gamma = 0 \quad (18)$$

$$-1 + (1 + \lambda^2)c_3 - \lambda c_2 - \mu_3 - \gamma = 0. \quad (19)$$

Suppose first that $\lambda \in (0, 1)$. The following figure depicts the separating straight line between $\{x_1, x_2\}$ and $\{x_3\}$ of largest possible margins for $\lambda = 1/2$:

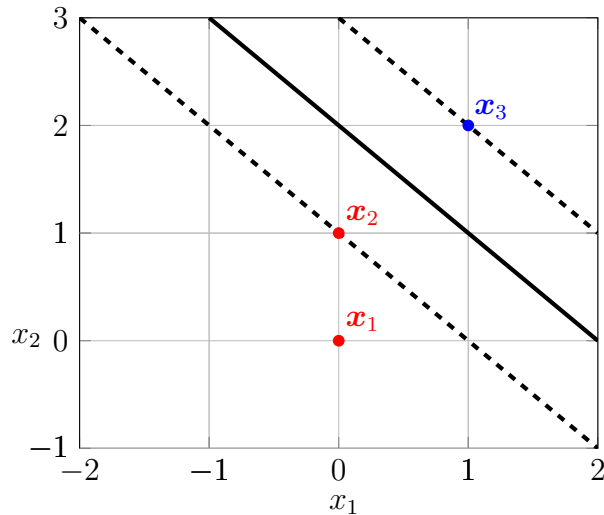


From the figure we can see that x_1, x_2 , and x_3 are all support vectors. We therefore make the ansatz $c_i > 0$ for $i = 1, 2, 3$. Then, (15) implies that $\mu_1 = \mu_2 = \mu_3 = 0$. Using this in (17)–(19) yields $c_2 = 2\lambda$ and $c_3 = 2$. Finally, (13) implies that $c_1 = 2 - 2\lambda$. We can therefore conclude that

$$\mathbf{c}^* = (2 - 2\lambda \quad 2\lambda \quad 2)^\top$$

is a solution of the Lagrange dual problem for $\lambda \in (0, 1)$.

Next, suppose that $\lambda > 1$. The following figure depicts the separating straight line between $\{x_1, x_2\}$ and $\{x_3\}$ of largest possible margins for $\lambda = 2$:



From the figure we can see that now $\mathbf{x}_2$ and $\mathbf{x}_3$ are the support vectors. This leads to the ansatz $c_2 > 0$, $c_3 > 0$, and $c_1 = 0$. Then, (15) implies that $\mu_2 = \mu_3 = 0$ and (13) yields $c_2 = c_3$. Using this in (17)–(19), we obtain

$$\begin{aligned} c_2(\lambda - 1) &= \mu_1 \\ c_2(1 + \lambda^2 - \lambda) &= \mu_1 + 2, \end{aligned}$$

which yields

$$c_2 = \frac{2}{2 - 2\lambda + \lambda^2}.$$

We can therefore conclude that

$$\mathbf{c}^* = \frac{2}{2 - 2\lambda + \lambda^2} (0 \ 1 \ 1)^\top$$

is a solution of the Lagrange dual problem for $\lambda \geq 1$.

- (d) By assumption we have $\lambda \in (0, 1)$. Using (10) and $\mathbf{c}^* = (2 - 2\lambda \ 2\lambda \ 2)^\top$ from subproblem (c), we obtain the following solution $\mathbf{w}^*$ of the optimization problem in subproblem (a):

$$\mathbf{w}^* = 2\lambda\mathbf{x}_2 - 2\mathbf{x}_3 = -\begin{pmatrix} 2 \\ 0 \end{pmatrix}.$$

The solution b^* can be obtained as follows. Since $c_1^* > 0$, i.e., $\mathbf{x}_1$ is a support vector, the corresponding inequality constraint $y_1(\langle \tilde{\mathbf{w}}, \mathbf{x}_1 \rangle_2 - b^*) \geq 1$ must be satisfied with equality. This yields

$$\begin{aligned} b^* &= \langle \tilde{\mathbf{w}}, \mathbf{x}_1 \rangle_2 - y_1 \\ &= -1. \end{aligned}$$

The hard margin binary classifier $g_{\text{hm}}(\mathbf{x})$ is therefore given by

$$\begin{aligned} g_{\text{hm}}(\mathbf{x}) &= (\langle \tilde{\mathbf{w}}, \mathbf{x} \rangle_2 - b^*) \\ &= -2 \begin{pmatrix} 1 & 0 \end{pmatrix} \mathbf{x} + 1. \end{aligned}$$

Problem 3

- (a) Denote the ReLU function as $\rho(x) = \max\{0, x\}$. The function $f(x)$ can be realized according to

$$f(x) = \rho(4x) - \rho(8x - 1.6) + \rho(14x - 5.6) - \rho(20x - 10) + \rho(14x - 8.4) - \rho(8x - 6.4) + \rho(4x - 4).$$

This function can, in turn, be realized through a depth-2 ReLU network according to

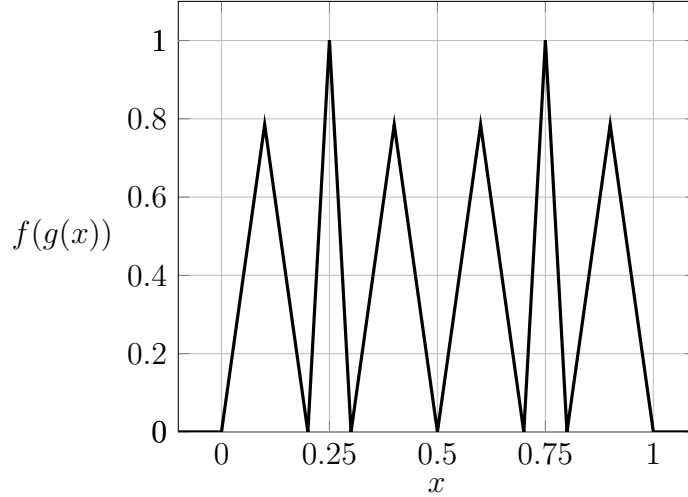
$$\Phi(x) = W_2(\rho(W_1(x)))$$

with

$$W_1(x) = \begin{pmatrix} 4 \\ 8 \\ 14 \\ 20 \\ 14 \\ 8 \\ 4 \end{pmatrix} x + \begin{pmatrix} 0 \\ -1.6 \\ -5.6 \\ -10 \\ -8.4 \\ -6.4 \\ -4 \end{pmatrix}, \quad W_2(x) = \begin{pmatrix} 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix}.$$

The network Φ has depth 2, width 7, and connectivity 20.

- (b) The following figure depicts $f(g(x))$. The axis of symmetry is at $x = 0.5$.



- (c) An alternative way to realize $f(x)$ is obtained by first noting that $f(x)$ is symmetric around $x = 0.5$ and can thus be written as $f(x) = h(g(x))$, where $h(x) = f(0.5x)$, for $x \in [0, 1]$, and $g(x) = \rho(2x) - \rho(4x - 2) + \rho(2x - 2) = W_2^g(\rho(W_1^g(x)))$ is the sawtooth function from subproblem (b). Here,

$$W_1^g(x) = \begin{pmatrix} 2 \\ 4 \\ 2 \end{pmatrix} x + \begin{pmatrix} 0 \\ -2 \\ -2 \end{pmatrix}, \quad W_2^g(x) = \begin{pmatrix} 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}.$$

The function $h(x) = \rho(2x) - \rho(4x - 1.6) + \rho(7x - 5.6) = W_2(\rho(W_1(x)))$ satisfies $h(x) = f(0.5x)$, for $x \in [0, 1]$. Here,

$$W_1(x) = \begin{pmatrix} 2 \\ 4 \\ 7 \end{pmatrix} x + \begin{pmatrix} 0 \\ -1.6 \\ -5.6 \end{pmatrix}, \quad W_2(x) = \begin{pmatrix} 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}.$$

Therefore, $f(x) = h(g(x))$ can be realized through the network

$$\Phi_2(x) = W_2(\rho(W_1(W_2^g(\rho(W_1^g(x))))) = W_3'(\rho(W_2'(\rho(W_1'(x)))))$$

with

$$W_1'(x) = W_1^g(x) = \begin{pmatrix} 2 \\ 4 \\ 2 \end{pmatrix} x + \begin{pmatrix} 0 \\ -2 \\ -2 \end{pmatrix}, \quad W_3'(x) = W_2(x) = \begin{pmatrix} 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix},$$

$$\begin{aligned} W_2'(x) &= W_1(W_2^g(x)) = \begin{pmatrix} 2 \\ 4 \\ 7 \end{pmatrix} \begin{pmatrix} 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} 0 \\ -1.6 \\ -5.6 \end{pmatrix} \\ &= \begin{pmatrix} 2 & -2 & 2 \\ 4 & -4 & 4 \\ 7 & -7 & 7 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} 0 \\ -1.6 \\ -5.6 \end{pmatrix}. \end{aligned}$$

The network Φ_2 has depth 3, width 3, and connectivity 19.

Problem 4

- (a) (i) An ϵ -covering of the compact set $\mathcal{C} \subseteq \mathcal{X}$ with respect to the metric ρ is a set $\{x_1, \dots, x_N\} \subset \mathcal{C}$ such that for each $x \in \mathcal{C}$, there exists an $i \in [1, N]$ so that $\rho(x, x_i) \leq \epsilon$. The ϵ -covering number $N(\epsilon; \mathcal{C}, \rho)$ is the cardinality of a smallest ϵ -covering of $\mathcal{C}$.
- (ii) An ϵ -packing of a compact set $\mathcal{C} \subseteq \mathcal{X}$ with respect to the metric ρ is a set $\{x_1, \dots, x_N\} \subset \mathcal{C}$ such that $\rho(x_i, x_j) > \epsilon$, for all distinct i, j . The ϵ -packing number $M(\epsilon; \mathcal{C}, \rho)$ is the cardinality of a largest ϵ -packing of $\mathcal{C}$.
- (iii) $N(2\epsilon; \mathcal{C}, \rho) \leq M(2\epsilon; \mathcal{C}, \rho) \leq N(\epsilon; \mathcal{C}, \rho) \leq M(\epsilon; \mathcal{C}, \rho)$.
- (b) (i) Let $\epsilon < 2^{-n}$ be arbitrary but fixed, take $K = \log_2(1/\epsilon)$, and divide the interval $I_n := [-2^{-n}, 2^{-n}]$ into $L := \lceil 2^{K-n} \rceil \geq 2$ sub-intervals of equal length, centered at the points $\theta_i = -2^{-n} + \frac{(2i-1)2^{-n}}{L}$, for $i \in \{1, 2, \dots, L\}$, and each of length $\frac{2^{1-n}}{L} \leq 2^{1-K} = 2\epsilon$. By construction, for every $\theta \in I_n$, there is hence a $j \in \{1, 2, \dots, L\}$ such that $|\theta - \theta_j| \leq \epsilon$, which proves that $A_n(\epsilon) = \{\theta_i; i \in \{1, 2, \dots, L\}\}$ is an ϵ -covering.
- (ii) For the construction of the 2ϵ -packing, take the points $\theta'_i = -2^{-n} + \frac{2(i-1)2^{-n}}{L-1}$, for $i \in \{1, 2, \dots, L\}$. As for every neighboring pair $\theta'_i, \theta'_j \in I_n$, it holds that $|\theta'_i - \theta'_j| = \frac{2^{1-n}}{L-1} > 2\epsilon$, we have established that $P_n(\epsilon) = \{\theta'_i; i \in \{1, 2, \dots, L\}\}$ constitutes a 2ϵ -packing. We finally note that $|P_n(\epsilon)| = |A_n(\epsilon)| = \lceil 2^{K-n} \rceil$.
- (iii) By (b.i) we have

$$N(\epsilon; I_n, \rho_1) \leq |A_n(\epsilon)| = \lceil 2^{K-n} \rceil$$

and by (b.ii),

$$M(2\epsilon; I_n, \rho_1) \geq |P_n(\epsilon)| = \lceil 2^{K-n} \rceil.$$

Combining this with $M(2\epsilon; \mathcal{C}, \rho) \leq N(\epsilon; \mathcal{C}, \rho)$ for every compact set $\mathcal{C}$ in the metric space $(\mathcal{X}, \rho)$, yields $N(\epsilon; I_n, \rho_1) = \lceil 2^{K-n} \rceil$.

- (c) (i) An ϵ -covering of $\mathcal{C}$ can be obtained by forming the Cartesian product, across $n \in \mathbb{N}$, of the ϵ -coverings of $[-2^{-n}, 2^{-n}]$ according to $A(\epsilon) = \{f : \mathbb{N} \rightarrow \mathbb{R}; f(n) \in A_n(\epsilon), \forall n \in \mathbb{N}\}$, where, for $\epsilon < 2^{-n}$, $A_n(\epsilon)$ is the ϵ -covering of $[-2^{-n}, 2^{-n}]$ constructed in subproblem (b.i) and $A_n(\epsilon) = \{0\}$, for $\epsilon \geq 2^{-n}$.
- (ii) Fix $\epsilon \leq 1/2$ and take $K = \log_2(1/\epsilon)$. By subproblems (b.iii) and (c.i), we have

$$\begin{aligned} N(\epsilon; \mathcal{C}, \rho_2) &\leq |A(\epsilon)| = \prod_{n=1}^{\infty} |A_n(\epsilon)| \leq \prod_{n=1}^{\lceil K \rceil - 1} 2^{\lceil K \rceil - n} = 2^{(\lceil K \rceil - 1)\lceil K \rceil / 2} \\ &\leq \left(\frac{1}{\epsilon}\right)^{\lceil K \rceil / 2} \leq \left(\frac{1}{\epsilon}\right)^{\frac{1}{2} \log_2(1/\epsilon) + C}, \end{aligned}$$

for some $C > 0$ that is independent of ϵ .