Supervised Learning: Exercise 2

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November 3, 2023

Exercise 1: Risk Minimizers for 0-1-Loss

Consider the classification learning setting, i.e., $\mathcal{Y} = \{1, \dots, g\}$, and the hypothetis space is $\mathcal{H} = \{h : \mathcal{X} \to \mathcal{Y}\}$. The loss function of interest is the 0-1-loss:

$$L(y, h(\mathbf{x})) = \boldsymbol{I}_{y \neq h(\mathbf{x})} = \begin{cases} 1, & \text{if} y \neq h(\mathbf{x}), \\ 0, & \text{if} y = h(\mathbf{x}). \end{cases} \qquad \triangleleft$$

(a) Consider the hypothesis space of constant models
$\mathcal{H} = \{h : \mathcal{X} \to \mathcal{Y} | h(\mathbf{x}) = \boldsymbol{\theta} \in \mathcal{Y} \; \forall \mathbf{x} \in \mathcal{X}\}$, where $\mathcal{X}$ is the feature space. Show that

$$\hat{h}(\mathbf{x}) = \mathrm{mode}\left\{y^{(i)}\right\}$$

is the empirical risk minimizer for the 0-1-loss in this case.

Solution to Question (a)

The empirical risk is

$$\begin{aligned}\mathcal{R}_{\text{emp}}(h) &= \sum_{i=1}^{n} \boldsymbol{I}_{y^{(i)} \neq h(\mathbf{x}^{(i)})} \\ &= \sum_{i=1}^{n} 1 - \boldsymbol{I}_{y^{(i)} = h(\mathbf{x}^{(i)})} \quad \triangleright\end{aligned}$$

Therefore

$$\arg\min_{h \in \mathcal{H}} \mathcal{R}_{\text{emp}}(h) = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} 1 - \boldsymbol{I}_{y^{(i)} = h(\mathbf{x}^{(i)})}$$

Solution to Question (a)

The empirical risk is

$$\mathcal{R}_{\mathrm{emp}}(h) = \sum_{i=1}^{n} \boldsymbol{I}_{y^{(i)} \neq h(\mathbf{x}^{(i)})}$$
$$= \sum_{i=1}^{n} 1 - \boldsymbol{I}_{y^{(i)} = h(\mathbf{x}^{(i)})} \quad \triangleright$$

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$$= \arg\max_{h \in \mathcal{H}} \sum_{i=1}^{n} \boldsymbol{I}_{y^{(i)} = h(\mathbf{x}^{(i)})}$$

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Therefore

$$\begin{aligned}\arg\min_{h \in \mathcal{H}} \mathcal{R}_{\text{emp}}(h) &= \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} 1 - \boldsymbol{I}_{y^{(i)} = h(\mathbf{x}^{(i)})} \\ &= \arg\max_{h \in \mathcal{H}} \sum_{i=1}^{n} \boldsymbol{I}_{y^{(i)} = h(\mathbf{x}^{(i)})} \\ &= \arg\max_{\boldsymbol{\theta} \in \mathcal{Y}} \sum_{i=1}^{n} \boldsymbol{I}_{y^{(i)} = \boldsymbol{\theta}} = \mathrm{mode}\left\{ y^{(i)} \right\}\end{aligned}$$

Question (b)

(b) What is the optimal constant model interms of the (theoretical) risk for the 0-1-loss and what is its risk?

Constant model:

$$h(\mathbf{x}) = \theta$$

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Solution to Question (b)

$$\mathcal{R}_L(h) = \int_y \int_{\mathbf{x}} \boldsymbol{I}_{y \neq h(\mathbf{x})} p(\mathbf{x}, y) \mathrm{d}\mathbf{x} \mathrm{d}y$$

Therefore, $\arg\min_h \mathcal{R}_L(h) = \arg\max_{\theta \in \mathcal{Y}} \int_y \boldsymbol{I}_{y=\theta} p(y) \mathrm{d}y$. Futhermore, $\mathcal{Y} = \{1, \ldots, g\}$, it follows that $\arg\max_{\theta \in \mathcal{Y}} \int_y \boldsymbol{I}_{y=\theta} p(y) \mathrm{d}y = \arg\max_{\theta \in \mathcal{Y}} \sum_{j=1}^{g} \boldsymbol{I}_{\theta=j} \mathbb{P}(y = j)$. (Show example.)

Hence, the optimal constant model for the **theorerical** risk is

$$\bar{h}(\mathbf{x}) = \arg\max_{l \in \mathcal{Y}} \mathbb{P}(y = l)$$

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$$\mathcal{R}_L(h) = \int_y \int_{\mathbf{x}} \boldsymbol{I}_{y \neq h(\mathbf{x})} p(\mathbf{x}, y) \mathrm{d}\mathbf{x} \mathrm{d}y$$
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Therefore, $\arg\min_h \mathcal{R}_L(h) = \arg\max_{\theta \in \mathcal{Y}} \int_y \boldsymbol{I}_{y=\theta} p(y) \mathrm{d}y$. Futhermore, $\mathcal{Y} = \{1, \ldots, g\}$, it follows that $\arg\max_{\theta \in \mathcal{Y}} \int_y \boldsymbol{I}_{y=\theta} p(y) \mathrm{d}y = \arg\max_{\theta \in \mathcal{Y}} \sum_{j=1}^{g} \boldsymbol{I}_{\theta=j} \mathbb{P}(y=j)$. (Show example.)

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Therefore, $\arg\min_h \mathcal{R}_L(h) = \arg\max_{\theta\in\mathcal{Y}} \int_y \boldsymbol{I}_{y=\theta} p(y)\mathrm{d}y$. Futhermore, $\mathcal{Y} = \{1, \ldots, g\}$, it follows that $\arg\max_{\theta\in\mathcal{Y}} \int_y \boldsymbol{I}_{y=\theta} p(y)\mathrm{d}y = \arg\max_{\theta\in\mathcal{Y}} \sum_{j=1}^{g} \boldsymbol{I}_{\theta=j}\mathbb{P}(y=j)$. (Show example.)

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&= \int_y \boldsymbol{I}_{y \neq \boldsymbol{\theta}} p(y) \mathrm{d}y \\
&= \int_y \left(1 - \boldsymbol{I}_{y = \boldsymbol{\theta}}\right) p(y) \mathrm{d}y = 1 - \int_y \boldsymbol{I}_{y = \boldsymbol{\theta}} p(y) \mathrm{d}y
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Therefore, $\arg\min_h \mathcal{R}_L(h) = \arg\max_{\boldsymbol{\theta} \in \mathcal{Y}} \int_y \boldsymbol{I}_{y=\boldsymbol{\theta}} p(y) \mathrm{d}y$. Futhermore, $\mathcal{Y} = \{1, \ldots, g\}$, it follows that $\arg\max_{\boldsymbol{\theta} \in \mathcal{Y}} \int_y \boldsymbol{I}_{y=\boldsymbol{\theta}} p(y) \mathrm{d}y = \arg\max_{\boldsymbol{\theta} \in \mathcal{Y}} \sum_{j=1}^{g} \boldsymbol{I}_{\boldsymbol{\theta}=j} \mathbb{P}(y = j)$. (Show example.)

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Solution to Question (b): Continued

Before we compute $\mathcal{R}_L(\bar{h})$, we write 0-1-loss as follows:

$$L(y, h(\mathbf{x})) = \boldsymbol{I}_{y \neq h(\mathbf{x})} = \sum_{k \in \mathcal{Y}} \boldsymbol{I}_{y=k} \boldsymbol{I}_{k \neq h(\mathbf{x})} = \sum_{k \in \mathcal{Y}} L(k, h(x)).$$

Then, the risk of $\bar{h}$ is

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$$\mathcal{R}_L(\bar{h}) = \mathbb{E}_{xy}[L(y, \bar{h}(\mathbf{x}))]$$

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$$\begin{aligned} \mathcal{R}_L(\bar{h}) &= \mathbb{E}_{xy}[L(y, \bar{h}(\mathbf{x}))] \\ &= \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_{y|\mathbf{x}} \left[L(y, \bar{h}(\mathbf{x})) \mid \mathbf{x} \right] \right] \end{aligned}$$

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\mathcal{R}_L(\bar{h}) &= \mathbb{E}_{xy}[L(y, \bar{h}(\mathbf{x}))] \\
&= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{y|\mathbf{x}}\left[L(y, \bar{h}(\mathbf{x})) \mid \mathbf{x}\right]\right] \\
&= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{y|\mathbf{x}}\left[\sum_{k \in \mathcal{Y}} \boldsymbol{I}_{y=k} L(k, \bar{h}(\mathbf{x})) \mid \mathbf{x}\right]\right]
\end{aligned}$$

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\mathcal{R}_L(\bar{h}) &= \mathbb{E}_{xy}[L(y, \bar{h}(\mathbf{x}))] \\
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&= \mathbb{E}_{\mathbf{x}} \left[\mathbb{E}_{y|\mathbf{x}} \left[\sum_{k \in \mathcal{Y}} \boldsymbol{I}_{y=k} L(k, \bar{h}(\mathbf{x})) \mid \mathbf{x} \right] \right] \\
&= \mathbb{E}_{\mathbf{x}} \left[\sum_{k \in \mathcal{Y}} L(k, \bar{h}(\mathbf{x})) \mathbb{E}_{y|\mathbf{x}} \left[\boldsymbol{I}_{y=k} \mid \mathbf{x} \right] \right] \quad \triangleright
\end{aligned}$$

Solution to Question (b): Continued

$$
\begin{aligned}
\mathcal{R}_L(\bar{h}) &= \mathbb{E}_{\mathbf{x}}\left[\sum_{k\in\mathcal{Y}} L(k,\bar{h}(\mathbf{x}))\mathbb{E}_{y|\mathbf{x}}\left[\boldsymbol{I}_{y=k} \mid \mathbf{x}\right]\right] \\
&= \mathbb{E}_{\mathbf{x}}\left[\sum_{k\in\mathcal{Y}} L(k,\bar{h}(\mathbf{x}))\mathbb{P}(y=k \mid \mathbf{x})\right] \\
&= \sum_{k\in\mathcal{Y}} L(k,\bar{h}(\mathbf{x}))\mathbb{E}_{\mathbf{x}}\left[\mathbb{P}(y=k \mid \mathbf{x})\right] \\
&= \sum_{k\in\mathcal{Y}} L(k,\bar{h}(\mathbf{x}))\mathbb{P}(y=k) \\
&= \sum_{k\in\mathcal{Y}} \boldsymbol{I}_{k\neq\bar{h}(\mathbf{x})}\mathbb{P}(y=k) \\
&= \sum_{k\in\mathcal{Y}} \boldsymbol{I}_{k\neq\arg\max_{l\in\mathcal{Y}}\mathbb{P}(y=l)}\mathbb{P}(y=k) \\
&= 1-\max_{l\in\mathcal{Y}}\mathbb{P}(y=l).
\end{aligned}
$$

Question (c)

(c) Derive the approximation error if the hypothesis space $\mathcal{H}$ consists of the **constant models**.

Recall that the approximation error is defined as

$$\inf_{h \in \mathcal{H}} \mathcal{R}_L(h) - \mathcal{R}_L^*$$

Solution to (c)

$$\begin{aligned}
\inf_{h \in \mathcal{H}} \mathcal{R}_L(h) - \mathcal{R}_L^* &= \mathcal{R}_L(\bar{h}) - \mathcal{R}_L^* \\
&= (1 - \max_{l \in \mathcal{Y}} \mathbb{P}(y = l)) - (1 - \mathbb{E}_{\mathbf{x}}[\max_{l \in \mathcal{Y}} \mathbb{P}(y = l|\mathbf{x})]) \\
&= \mathbb{E}_{\mathbf{x}}[\max_{l \in \mathcal{Y}} \mathbb{P}(y = l|\mathbf{x})] - \max_{l \in \mathcal{Y}} \mathbb{P}(y = l).
\end{aligned}$$

Question (d)

(d) Assume now $g = 2$ (binary classification) and consider now the hypothesis space of probabilistic classifiers $\mathcal{H} = \{\pi : \mathcal{X} \to [0, 1]\}$, that is, $\pi(\mathbf{x})$ (or $1 - \pi(\mathbf{x})$) is an estimate of the posterior distribution $p_{y|\mathbf{x}}(1|\mathbf{x})$ (or $p_{y|\mathbf{x}}(0|\mathbf{x})$). Furthermore, consider the probabilistic 0-1-loss

$$L(y, \pi(\mathbf{x})) = \begin{cases} 1, & \text{if } (\pi(\mathbf{x}) \geq 1/2 \text{ and } y = 0) \text{ or } (\pi(\mathbf{x}) < 1/2 \text{ and } y = 1), \\ 0, & \text{else.} \end{cases}$$

Is the minimum of $\mathbb{E}_{xy}[L(y, \pi(\mathbf{x}))]$ unique over $\pi \in \mathcal{H}$? Is the posterior distribution $p_{y|x}$ a resp. the minimizer of $\mathbb{E}_{xy}[L(y, \pi(\mathbf{x}))]$? Discuss the corresponding (dis-)advantanges of your findings.

Solution to Question (d)

- We can rewrite the 0-1-loss as

$$L(y, \pi(\mathbf{x})) = \boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\boldsymbol{I}_{y=0} + \boldsymbol{I}_{\pi(\mathbf{x})<1/2}\boldsymbol{I}_{y=1}.$$

- Since $\mathcal{H} = \{\pi : \mathcal{X} \to [0, 1]\}$, we can optimize π for each point $\mathbf{x}$.
- In other words, for $\mathbb{E}_{xy}[L(y, \pi(\mathbf{x}))] = \mathbb{E}_{\mathbf{x}}[\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}]]$. we optimize $\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}]$ for each $\mathbf{x}$.

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Solution to Question (d): Continued

$$\mathbb{E}_{y|\mathbf{x}}[L(y,\pi(\mathbf{x})) \mid \mathbf{x}] = \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\boldsymbol{I}_{y=0} + \boldsymbol{I}_{\pi(\mathbf{x})<1/2}\boldsymbol{I}_{y=1} \mid \mathbf{x}]$$

Solution to Question (d): Continued

$$
\begin{aligned}
\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}] &= \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\boldsymbol{I}_{y=0} + \boldsymbol{I}_{\pi(\mathbf{x})<1/2}\boldsymbol{I}_{y=1} \mid \mathbf{x}] \\
&= \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\boldsymbol{I}_{y=0} \mid \mathbf{x}] + \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})<1/2}\boldsymbol{I}_{y=1} \mid \mathbf{x}]
\end{aligned}
$$

Solution to Question (d): Continued

$$\begin{aligned}
\mathbb{E}_{y|\mathbf{x}}[L(y,\pi(\mathbf{x})) \mid \mathbf{x}] &= \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\boldsymbol{I}_{y=0} + \boldsymbol{I}_{\pi(\mathbf{x})<1/2}\boldsymbol{I}_{y=1} \mid \mathbf{x}] \\
&= \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\boldsymbol{I}_{y=0} \mid \mathbf{x}] + \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x})<1/2}\boldsymbol{I}_{y=1} \mid \mathbf{x}] \\
&= \boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2} \cdot \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{y=0} \mid \mathbf{x}] + \boldsymbol{I}_{\pi(\mathbf{x})<1/2} \cdot \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{y=1} \mid \mathbf{x}] \quad \triangleright
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\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}] &= \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{\pi(\mathbf{x}) \geq 1/2} \boldsymbol{I}_{y=0} + \boldsymbol{I}_{\pi(\mathbf{x}) < 1/2} \boldsymbol{I}_{y=1} \mid \mathbf{x}] \\
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&= \boldsymbol{I}_{\pi(\mathbf{x}) \geq 1/2} \cdot \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{y=0} \mid \mathbf{x}] + \boldsymbol{I}_{\pi(\mathbf{x}) < 1/2} \cdot \mathbb{E}_{y|\mathbf{x}}[\boldsymbol{I}_{y=1} \mid \mathbf{x}] \quad \triangleright \\
&= \boldsymbol{I}_{\pi(\mathbf{x}) \geq 1/2} \mathbb{P}(y = 0 \mid \mathbf{x}) + \boldsymbol{I}_{\pi(\mathbf{x}) < 1/2} \mathbb{P}(y = 1 | \mathbf{x}).
\end{aligned}
$$

Solution to Question (d): Continued

$$\mathbb{E}_{y|\mathbf{x}}[L(y,\pi(\mathbf{x})) \mid \mathbf{x}] = \boldsymbol{I}_{\pi(\mathbf{x})\geq 1/2}\mathbb{P}(y=0 \mid \mathbf{x}) + \boldsymbol{I}_{\pi(\mathbf{x})<1/2}\mathbb{P}(y=1|\mathbf{x}).$$

We can distinguish between two cases:

- If $\mathbb{P}(y=0 \mid \mathbf{x}) \geq 1/2$, then any $\pi(\mathbf{x}) < 1/2$ minimizes $\mathbb{E}_{y|\mathbf{x}}[L(y,\pi(\mathbf{x})) \mid \mathbf{x}]$.
- If $\mathbb{P}(y=0 \mid \mathbf{x}) \leq 1/2$, then any $\pi(\mathbf{x}) \geq 1/2$ minimizes $\mathbb{E}_{y|\mathbf{x}}[L(y,\pi(\mathbf{x})) \mid \mathbf{x}]$.

In other words:

$$\pi(\mathbf{x}) = \begin{cases} < 1/2, & \text{if } \mathbb{P}(y=0 \mid \mathbf{x}) \geq 1/2, \\ \geq 1/2, & \text{if } \mathbb{P}(y=1 \mid \mathbf{x}) < 1/2. \end{cases}$$

The posterior distribution $p_{y|\mathbf{x}}(1 \mid \mathbf{x})$ is quite naturally of this form, but it is not the only π of this kind. As a consequence, the minimize is not unique.

Solution to Question (d): Continued

$$\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}] = \boldsymbol{I}_{\pi(\mathbf{x}) \geq 1/2} \mathbb{P}(y = 0 \mid \mathbf{x}) + \boldsymbol{I}_{\pi(\mathbf{x}) < 1/2} \mathbb{P}(y = 1 | \mathbf{x}).$$

We can distinguish between two cases:

- If $\mathbb{P}(y = 0 \mid \mathbf{x}) \geq 1/2$, then any $\pi(\mathbf{x}) < 1/2$ minimizes $\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}]$.
- If $\mathbb{P}(y = 0 \mid \mathbf{x}) \leq 1/2$, then any $\pi(\mathbf{x}) \geq 1/2$ minimizes $\mathbb{E}_{y|\mathbf{x}}[L(y, \pi(\mathbf{x})) \mid \mathbf{x}]$.

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Solution to Question (d): Continued

Disadvantages of using $p_{y|\mathbf{x}}$:

- TODO (The solution is not very clear. Ask people around.)