XOR-problem for One Hidden Layer

(A problem posted by 戴晨洋)

Sign function

For a vector $u = (u_1, u_2, \ldots, u_d) \in \mathbb{R}^d$, define the vector $\mathrm{sgn}(u) \in \mathbb{R}^d$ whose i-th position is

$$\mathrm{sgn}(u)_i = \begin{cases} 1, & \text{if } u_i > 0; \\ 0, & \text{if } u_i \leq 0, \end{cases}$$

and define $u' = (1, u_1, \ldots, u_d) \in \mathbb{R}^{d+1}$.

Example

$$\mathrm{sgn}(2, -3, 0, 1, 2)' = (1, 1, 0, 0, 1, 1).$$

Hidden layer is necessary in solving XOR-problem

Proposition

There is **no** *column vector* $\Theta = (\theta_0, \theta_1, \theta_2)^T$ *that satisfies*

$$\operatorname{sgn}(x'\Theta) = \operatorname{sgn}(\theta_0 + x_1\theta_1 + x_2\theta_2) = \begin{cases} 0, & \text{if } x_1 = x_2; \\ 1, & \text{if } x_1 \neq x_2, \end{cases}$$

where $x' = (1, x_1, x_2)$ *is binary vector.*

Proof.

If such triple $(\theta_0, \theta_1, \theta_2)$ exists, then applying the four cases $(x_1, x_2) = (0,0), (1,1), (1,0), (0,1)$ into the above equation, we have

$$-\theta_0 \geq 0, \quad -\theta_0 - \theta_1 - \theta_2 \geq 0, \quad \theta_0 + \theta_1 > 0, \quad \theta_0 + \theta_2 > 0,$$

but summing these four inequalities will yield the contradiction $0 > 0$. $\square$

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Proposition

For any positive integer d there exists a positive integer n, a $(d+1) \times n$ matrix Θ and $(n+1) \times 1$ matrix Λ such that

$$\mathrm{sgn}(\mathrm{sgn}(x'\Theta)'\Lambda) = \begin{cases} 1, & \text{if } x_1 + \cdots + x_d \text{ is odd;} \\ 0, & \text{if } x_1 + \cdots + x_d \text{ is even,} \end{cases}$$

where $x = (x_1, \ldots, x_d)$ is a binary vector.

Proof. Let

$$n = d, \; \Theta = \begin{pmatrix} \frac{-1}{2} & \frac{-3}{2} & \cdots & -\frac{(2d+1)}{2} \\ 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \; \Lambda = \begin{pmatrix} -\frac{1}{2} \\ 1 \\ -1 \\ \vdots \\ (-1)^{d+1} \end{pmatrix}.$$

Continue the proof

Then the i-th position of $\operatorname{sgn}(x'\Theta)$ is

$$\begin{aligned}(\operatorname{sgn}(x'\Theta))_i =& \operatorname{sgn}(x_1 + x_2 + \cdots + x_d - i + \frac{1}{2}) \\ =& \begin{cases} 1, & \text{if } i \le x_1 + x_2 + \cdots + x_d; \\ 0, & \text{if } i > x_1 + x_2 + \cdots + x_d, \end{cases}\end{aligned}$$

and

$$\operatorname{sgn}(x'\Theta)'\Lambda = -\frac{1}{2} + \begin{cases} 1, & \text{if } x_1 + x_2 + \cdots + x_d \text{ is odd,} \\ 0, & \text{if } x_1 + x_2 + \cdots + x_d \text{ is even.} \end{cases}$$

Hence

$$\operatorname{sgn}(\operatorname{sgn}(x'\Theta)'\Lambda) = \begin{cases} 1, & \text{if } x_1 + \cdots + x_d \text{ is odd;} \\ 0, & \text{if } x_1 + \cdots + x_d \text{ is even.} \end{cases}$$

□

Remark

Let $n(d)$ denote the minimum n such that the $(d+1) \times n$ matrix Θ in the above proposition exists. The proof of the above proposition implies that $n(d) \leq d$.

Problem. Determine $n(d)$.

$n(d) \neq 1$

Lemma

There is no $(d+1) \times 1$ *matrix* $\Theta = (\theta_0, \theta_1, \ldots, \theta_d)^T$ *and* 2×1 *matrix* $\Lambda = (\lambda_0, \lambda_1)^T$ *such that for any binary vector* $x = (x_1, \ldots, x_d)$*,*

$$\mathrm{sgn}(\mathrm{sgn}(x'\Theta)'\Lambda) = \begin{cases} 1, & \text{if } x_1 + \cdots + x_d \text{ is odd;} \\ 0, & \text{if } x_1 + \cdots + x_d \text{ is even.} \end{cases}$$

Proof. If such Θ, Λ exist, then by assigning $x_3 = x_4 = \cdots = x_d = 0$ and $(x_1, x_2) = (0,0)$, $(1,0)$, $(0,1)$ or $(1,1)$, we have

$$\begin{aligned} -\lambda_0 - \lambda_1 \mathrm{sgn}(\theta_0) &\geq 0, \\ \lambda_0 + \lambda_1 \mathrm{sgn}(\theta_0 + \theta_1) &> 0, \\ \lambda_0 + \lambda_1 \mathrm{sgn}(\theta_0 + \theta_2) &> 0, \\ -\lambda_0 - \lambda_1 \mathrm{sgn}(\theta_0 + \theta_1 + \theta_2) &\geq 0. \end{aligned}$$

Continue the proof

Summing the above first two terms and the remaining two terms respectively, we have

$$\lambda_1(\mathrm{sgn}(\theta_0+\theta_1)-\mathrm{sgn}(\theta_0)) > 0,$$
$$\lambda_1(\mathrm{sgn}(\theta_0+\theta_2)-\mathrm{sgn}(\theta_0+\theta_1+\theta_2)) > 0.$$

Hence $\lambda \neq 0$. We might assume $\lambda_1 > 0$ and the case $\lambda_1 < 0$ is similar. Hence

$$\begin{aligned} \theta_0+\theta_1 &> 0, \\ -\theta_0 &\geq 0, \\ \theta_0+\theta_2 &> 0, \\ -\theta_0-\theta_1-\theta_2 &\geq 0. \end{aligned}$$

Summing the above four inequalities yields $0 > 0$, a contradiction. $\square$