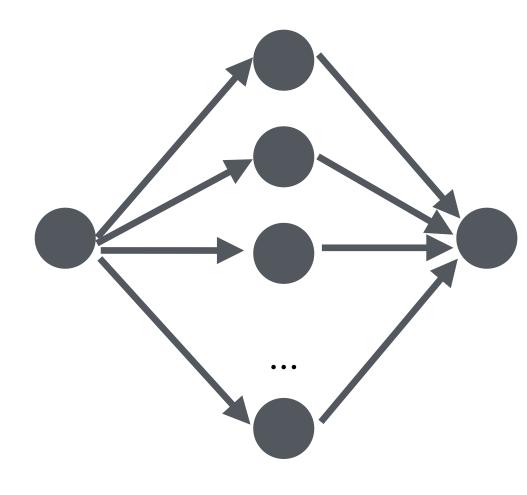
4. Approximation: 3-Layer ReLU net

Recap

- In the last class, we proved our first universal approximation result
 - Simple case, of 1D function with 2-layer threshold nets





Proposition 2.1.

Suppose that $g: \mathbb{R} \to \mathbb{R}$ is ρ -Lipschitz. Then, for any $\varepsilon > 0$, there exists a 2-layer network with $\lceil \rho/\varepsilon \rceil$ threshold nodes, so that

$$\sup_{x \in [0,1]} |f(x) - g(x)| \le \epsilon$$

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Suppose that $g: \mathbb{R} \to \mathbb{R}$ is ρ -Lipschitz. Then, for any $\varepsilon > 0$, there exists a 2-layer network with $\lceil \rho/\varepsilon \rceil$ threshold nodes, so that

$$\sup_{x \in [0,1]} |f(x) - g(x)| \le \epsilon$$

- Recall that the proof consists of two large steps:
 - Approximating $g(\cdot)$ with $h(\cdot)$ a weighted sum of simple bases

$$h(x) = \sum_{i=1}^{k} \alpha_i \cdot b_i(x)$$

• Approximating $h(\cdot)$ with $f(\cdot)$ — a weighted sum of neurons

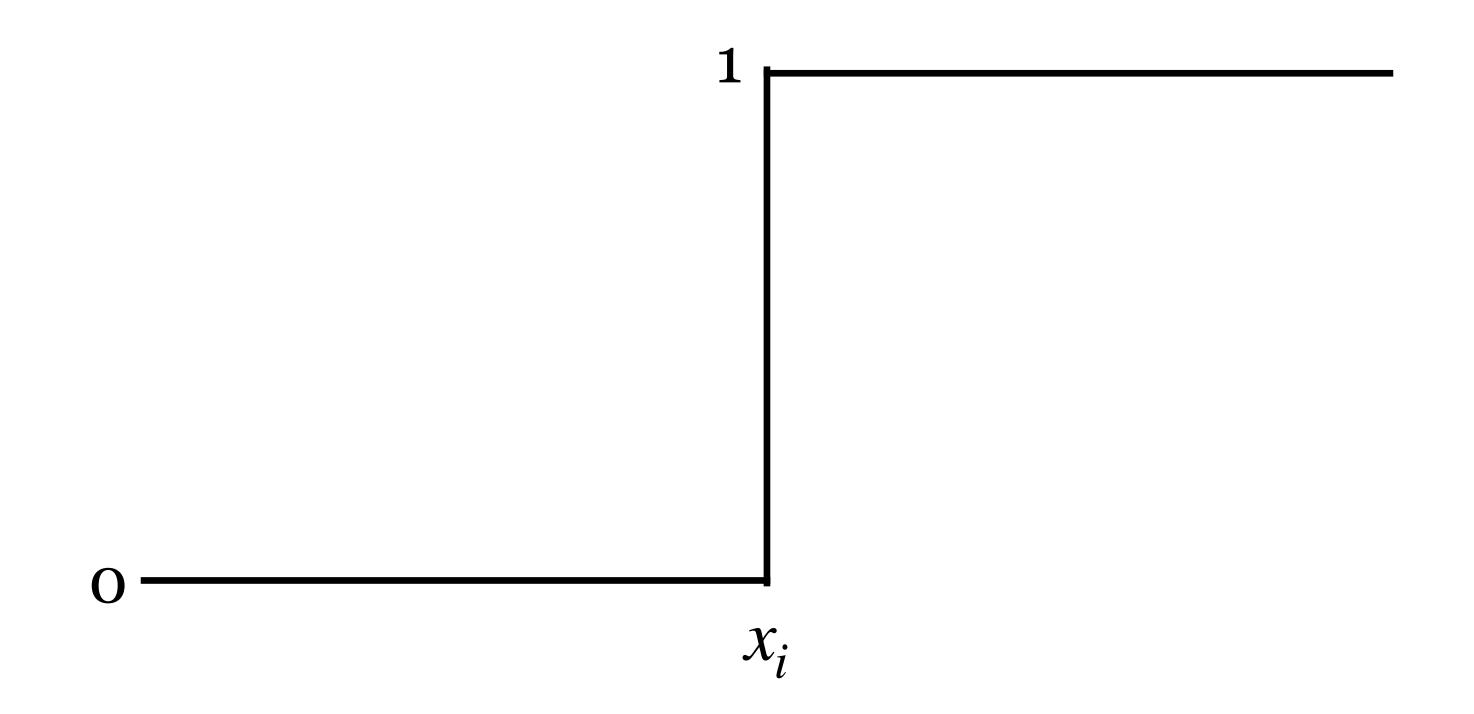
$$f(x) = \sum_{i=1}^{m} a_i \cdot n_i(x)$$

• Establish the relationship $g(\cdot) \approx h(\cdot) \approx f(\cdot)$

Step 1. Approximating $g(\cdot)$ with $h(\cdot)$ — a weighted sum of simple basis

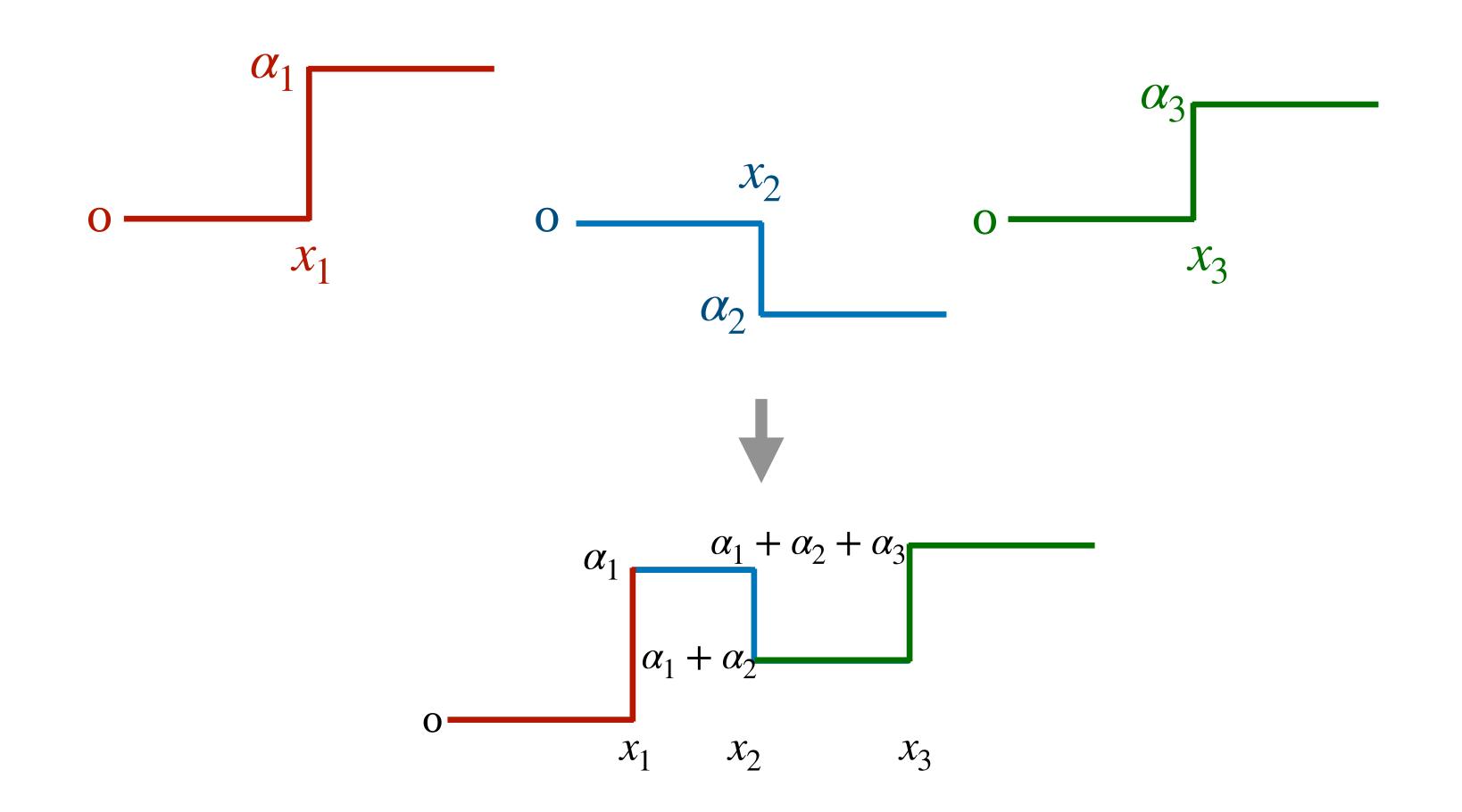
• As the basis, we used shifted step functions

$$b_i(x) = \mathbf{1}\{x - x_i\}$$



• Weighted sum of bases gives histogram-like function

$$h(x) = \sum_{i=1}^{k} \alpha_i \cdot b_i(x)$$



- The histogram $h(\cdot)$ can approximate any Lipschitz function $g(\cdot)$ arbitrarily closely

Step 2. Approximating $h(\cdot)$ with $f(\cdot)$ — a weighted sum of neurons

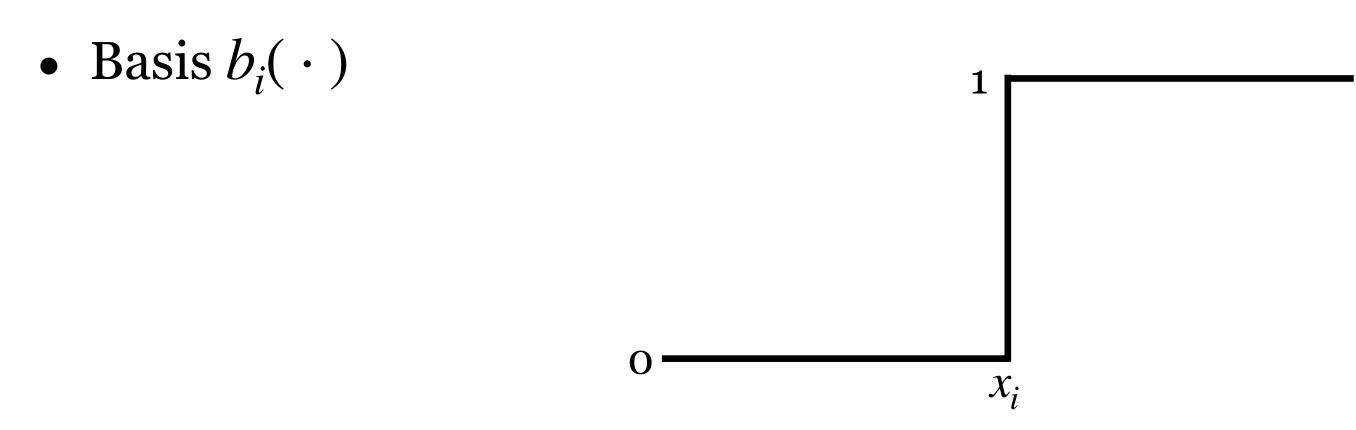
• Two-layer threshold net can be written as a weighted sum of threshold neurons

$$f(x) = \sum_{i=1}^{m} a_i \cdot n_i(x)$$

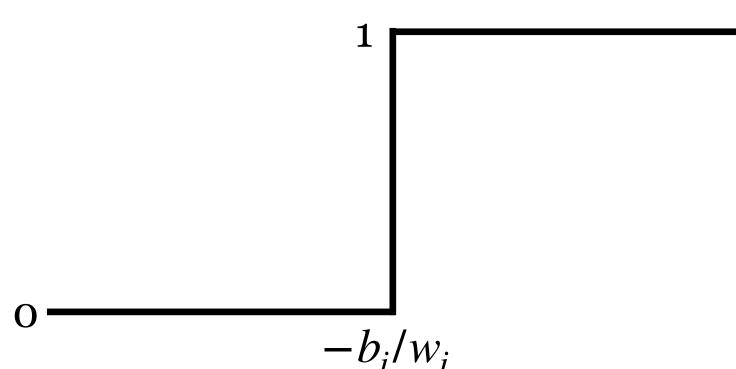
• Each threshold neuron can be written as:

$$n_i(\cdot) = \mathbf{1}\{w_i x + b_i \ge 0\}$$

- Approximate each basis $b_i(\cdot)$ with neuron(s)!
 - Luckily, we can represent each basis using one threshold neuron, without error



• Neuron $n_i(\cdot)$



• Thus, *k*-basis $h(\cdot)$ can be approximated by *k*-neuron network $f(\cdot)$, with $||h(\cdot) - f(\cdot)||_{\infty} = 0$

- Thus we have:
 - $\|g(\cdot) h(\cdot)\|_{\infty} < \varepsilon$, for some good k
 - $\bullet \quad \|h(\,\cdot\,) f(\,\cdot\,)\|_{\infty} = 0$

• By triangle inequality:

$$||g - f||_{\infty} \le ||g - h||_{\infty} + ||h - f||_{\infty}$$

$$< \varepsilon + 0$$

Today

- We depart from non-realistic assumptions
 - Use ReLU, not threshold
 - Use *d*-dimensional input, not 1-dimensional
- This is trickier, so we will first:
 - Use three-layers, not two
 - Upper-bound L_1 norm, not uniform

Main result

• In particular, we prove the following result

Theorem 2.1.

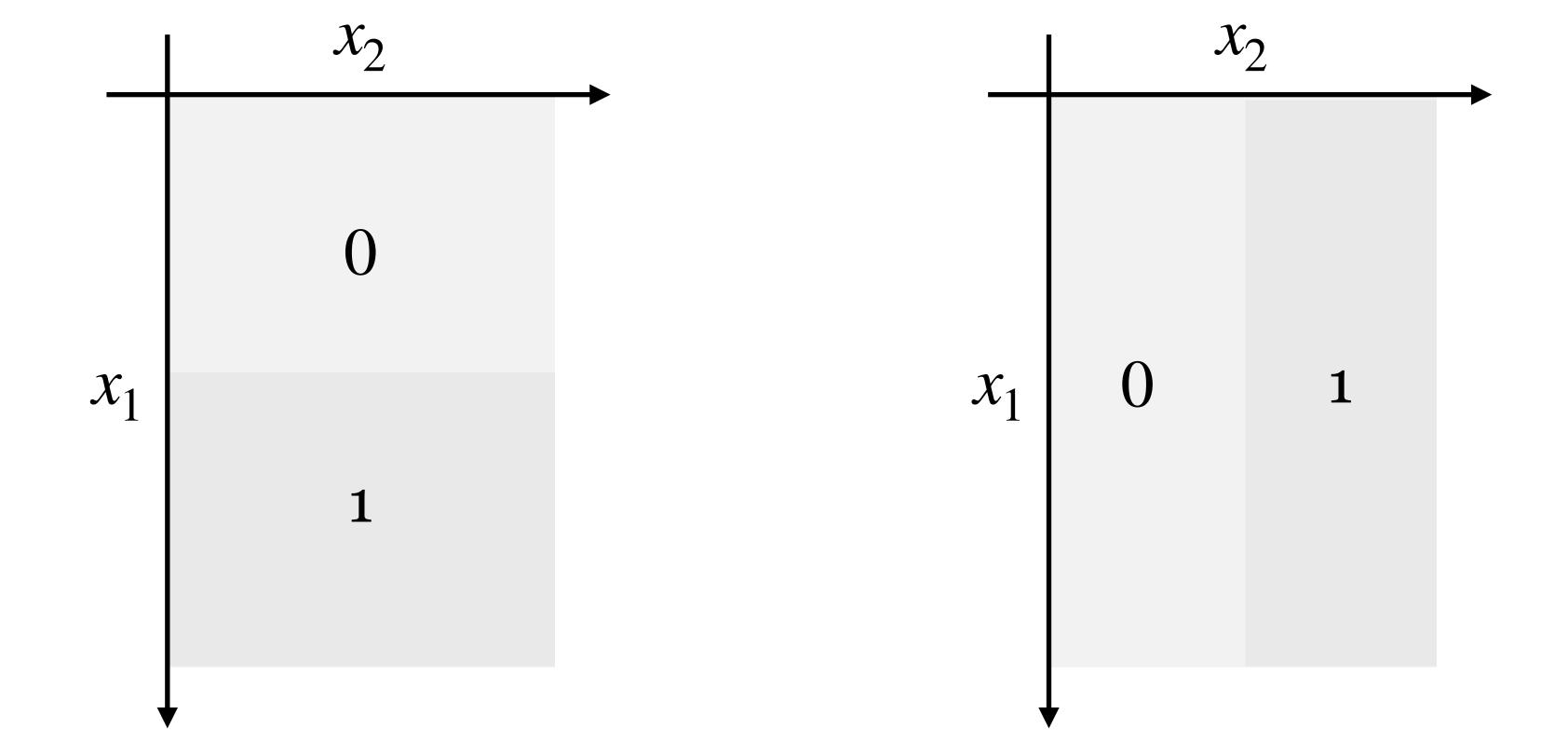
Let $g:[0,1]^d \to \mathbb{R}$ be a ρ -Lipschitz function, and let $\varepsilon > 0$. Then, there exists a three-layer ReLU network with $O(d \cdot \lceil \rho/\varepsilon \rceil^d)$ neurons such that

$$\int_{[0,1]^d} |f(\mathbf{x}) - g(\mathbf{x})| \, \mathrm{d}x \le 2\varepsilon$$

- Here, the Lipschitz constant is w.r.t. $\|\cdot\|_{\infty}$ at the input and $\|\cdot\|$ at the output
- Our strategy is basically the same:
 - Build a nice $h(\cdot)$, but with d-dimensional bases
 - Approximate each basis with neurons, but with ReLU neurons
- Let's think about these questions first, then move onto the final proof

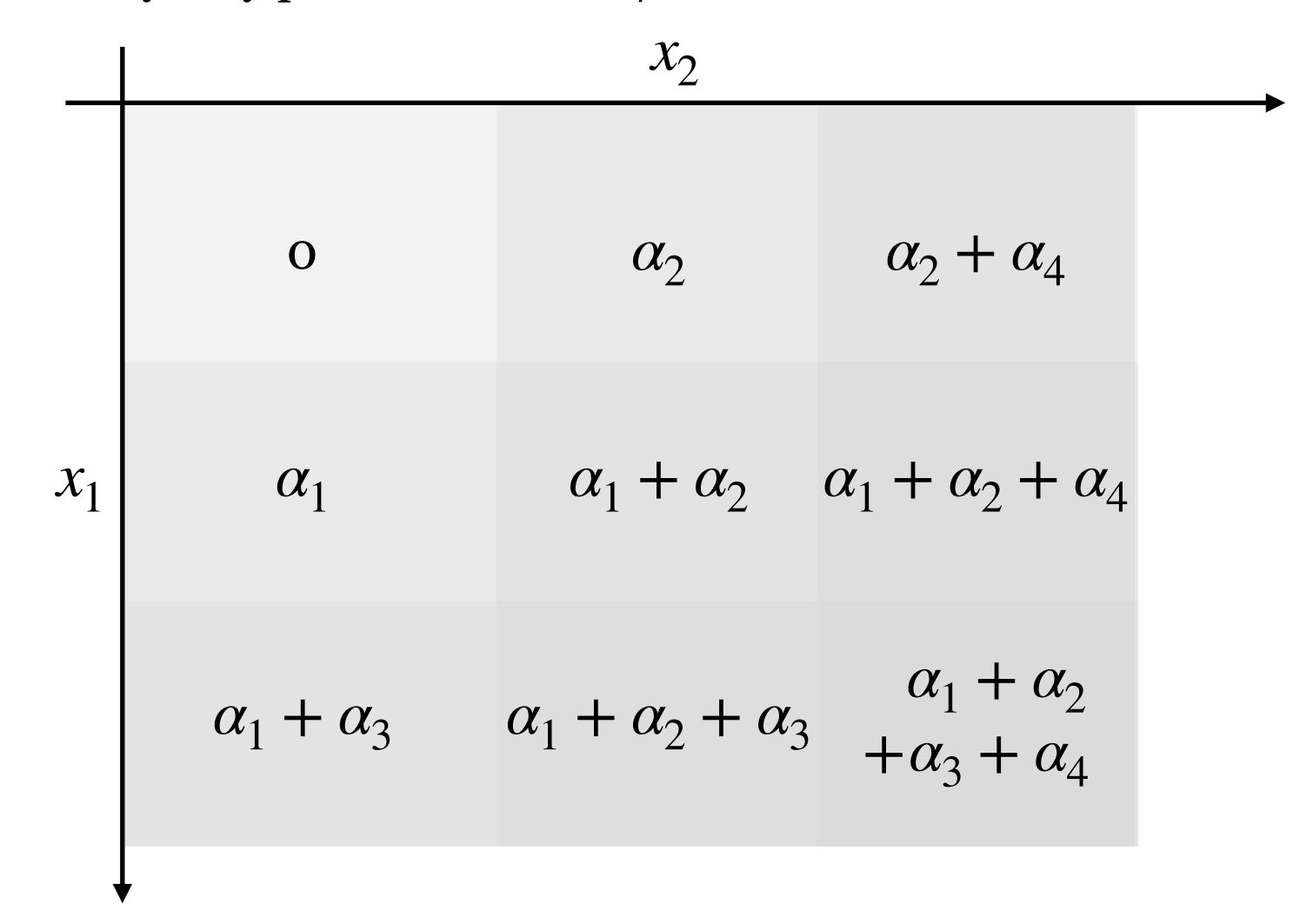
Basis

- In 1D, we used step functions...
 - Can we also use axis-parallel 1D step functions?



Basis

- Problem. Not exactly sure whether we can decouple everything...
 - Brainteaser: Can anybody prove that we can/cannot do this?

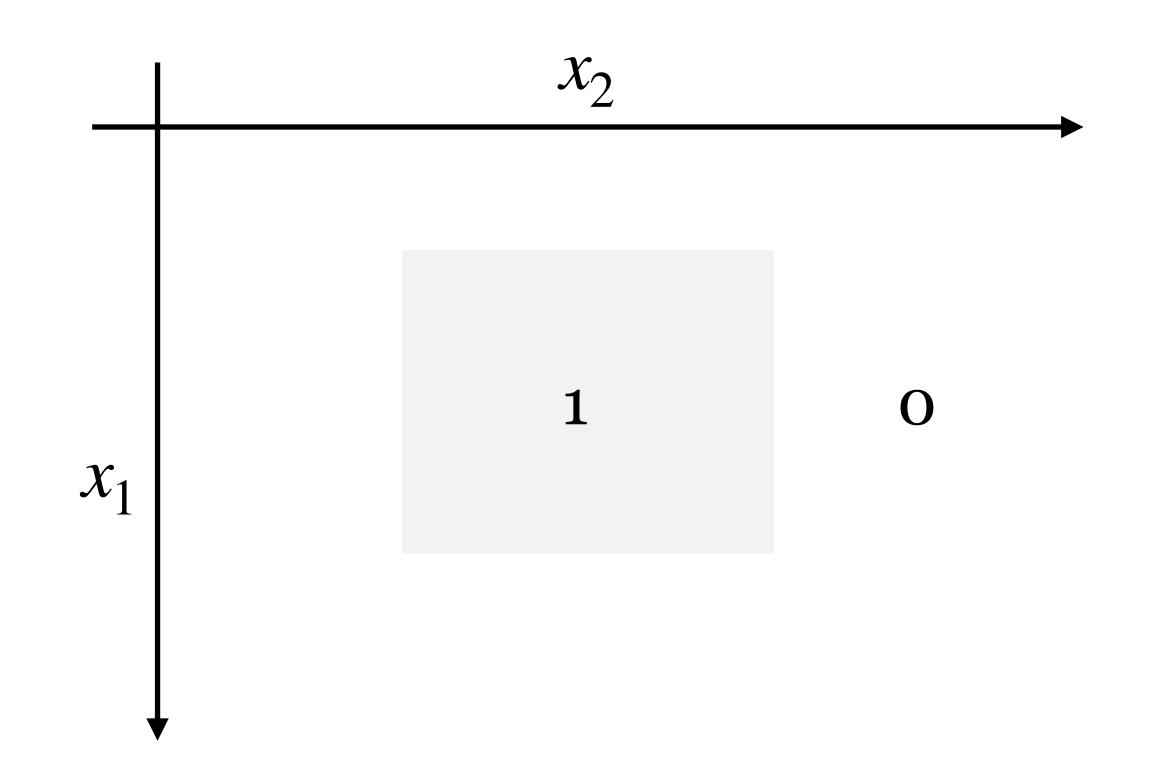


Basis

• Choice. For now, we will use "high-D pulse" as our basis

$$b_i(\mathbf{x}) = \mathbf{1}\{\mathbf{x} \in R_i\}$$
 (R_i is some hypercube)

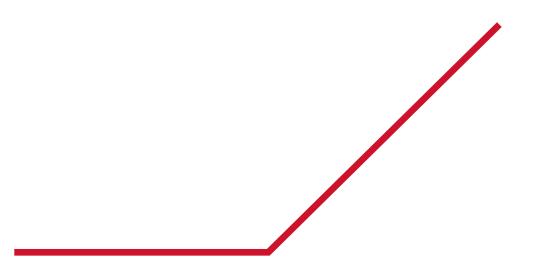
- Much easier to approximate $g(\cdot)$
- Somewhat involved, to be approximated by ReLU neurons



• Now let's think about what a ReLU neuron can approximate:

$$\sigma(\mathbf{w}_i^{\mathsf{T}}\mathbf{x} + b_i)$$

• For 1D input, a single ReLU neuron looks like this:



• Question. Can this approximate 1D pulse, i.e., $1\{x \in [a,b]\}$?

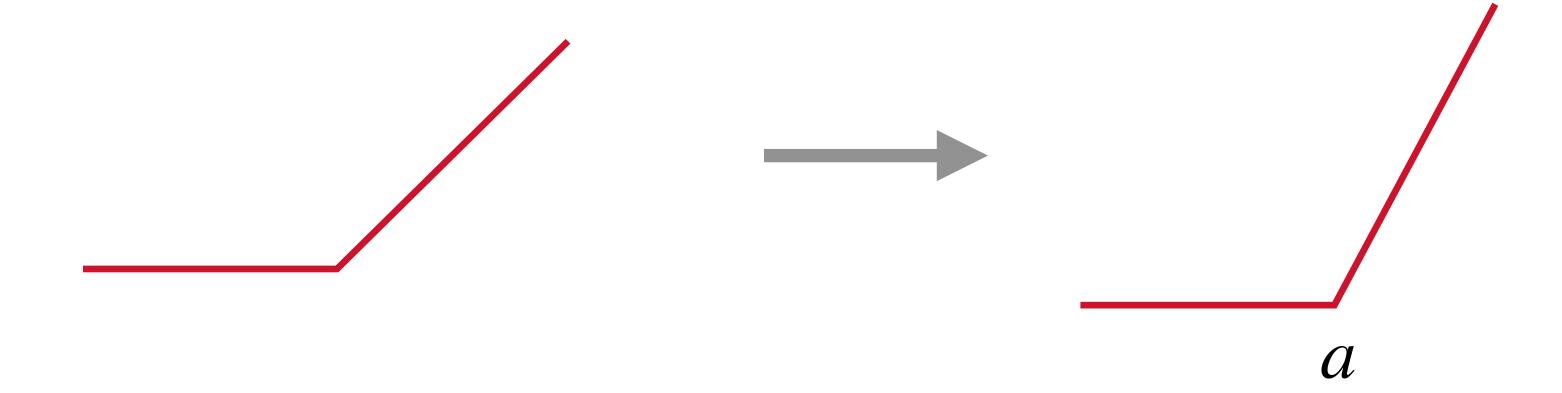
• We do it in three steps:

Step 1. Sharpen up ReLU

• Build ReLU like:

$$\sigma\left(\frac{x-a}{\gamma}\right)$$

using very small γ $(w = 1/\gamma, b = -a/\gamma)$



• We do it in three steps:

Step 2. Combine two ReLU to build a hard sigmoid

• Group two ReLU neurons

$$s_{a,\gamma}(x) = \sigma\left(\frac{x - (a - \gamma)}{\gamma}\right) - \sigma\left(\frac{x - a}{\gamma}\right)$$

• Brainteaser: What if we used sigmoid activations from the first place?

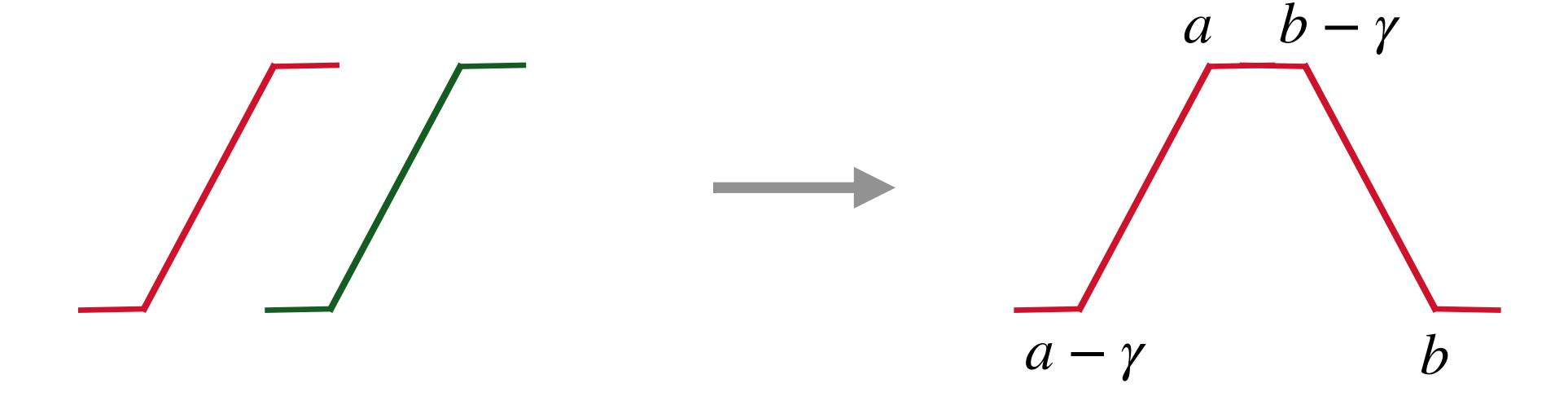


• We do it in three steps:

Step 3. Combine two hard sigmoids to build a pulse

• Group two hard sigmoids as:

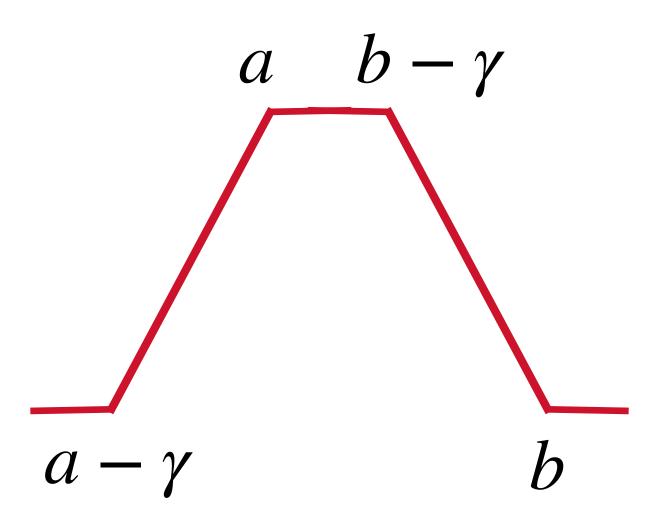
$$u_{a,b,\gamma}(x) = s_{a,\gamma}(x) - s_{b,\gamma}(x)$$



• Summing up, a pulse $\mathbf{1}\{x \in [a,b]\}$ can be approximated by:

$$u_{a,b,\gamma}(x) = \sigma\left(\frac{x - (a - \gamma)}{\gamma}\right) - \sigma\left(\frac{x - a}{\gamma}\right) - \sigma\left(\frac{x - (b - \gamma)}{\gamma}\right) + \sigma\left(\frac{x - b}{\gamma}\right)$$

- Question. How good is this approximation?
 - Of course, the goodness depends on the sharpening factor γ
 - In fact, the L_1 error is exactly γ



• Question. How do we extend it to multivariate pulse?

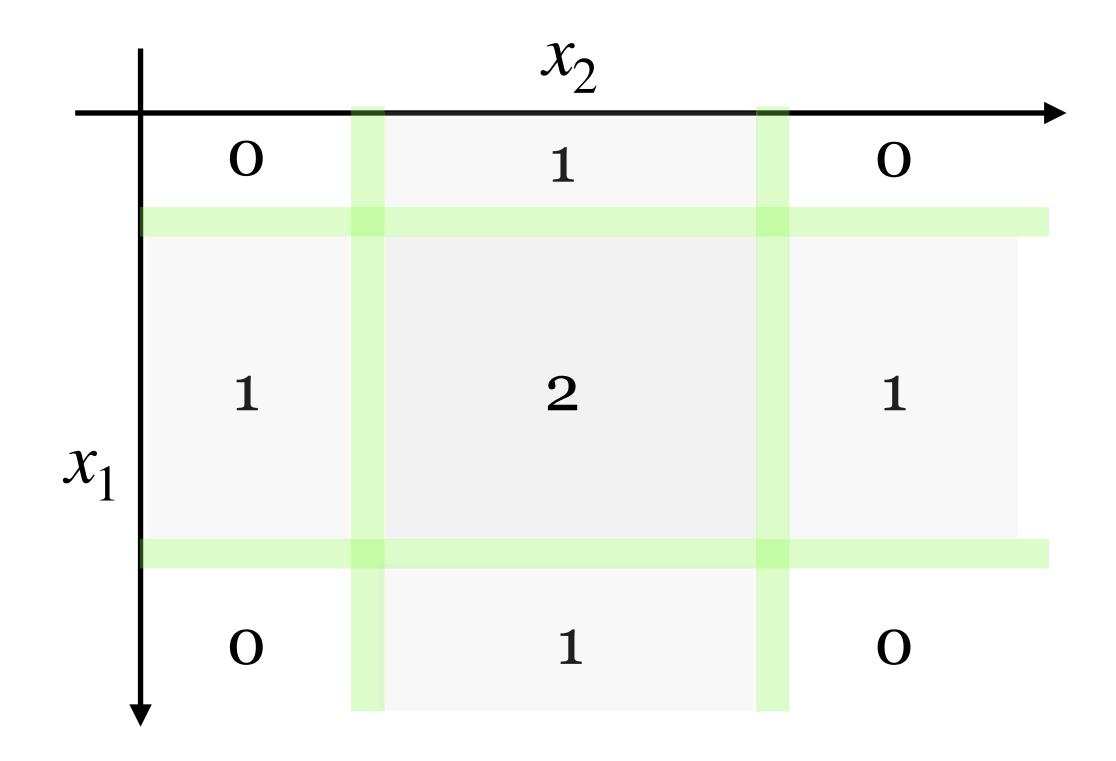
$$\prod_{i} \mathbf{1}\{x_i \in [a_j, b_j]\}$$

- Answer.
 - Very difficult if we use two layers (try it!)
 - Much easier if we use three layers

• Again, we proceed in three steps:

Step 1. Sum univariate pulses in d axes

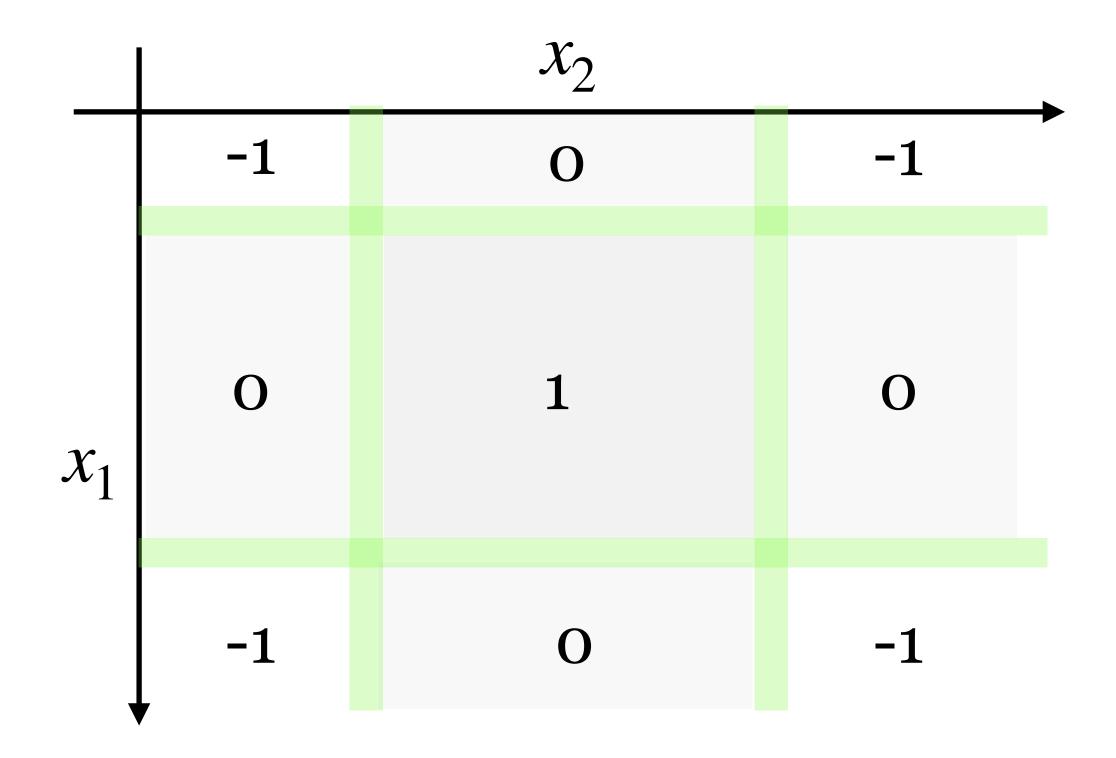
- We'll get something very ugly
- Total 4d ReLU neurons added, so far



• Again, we proceed in three steps:

Step 2. Subtract d-1

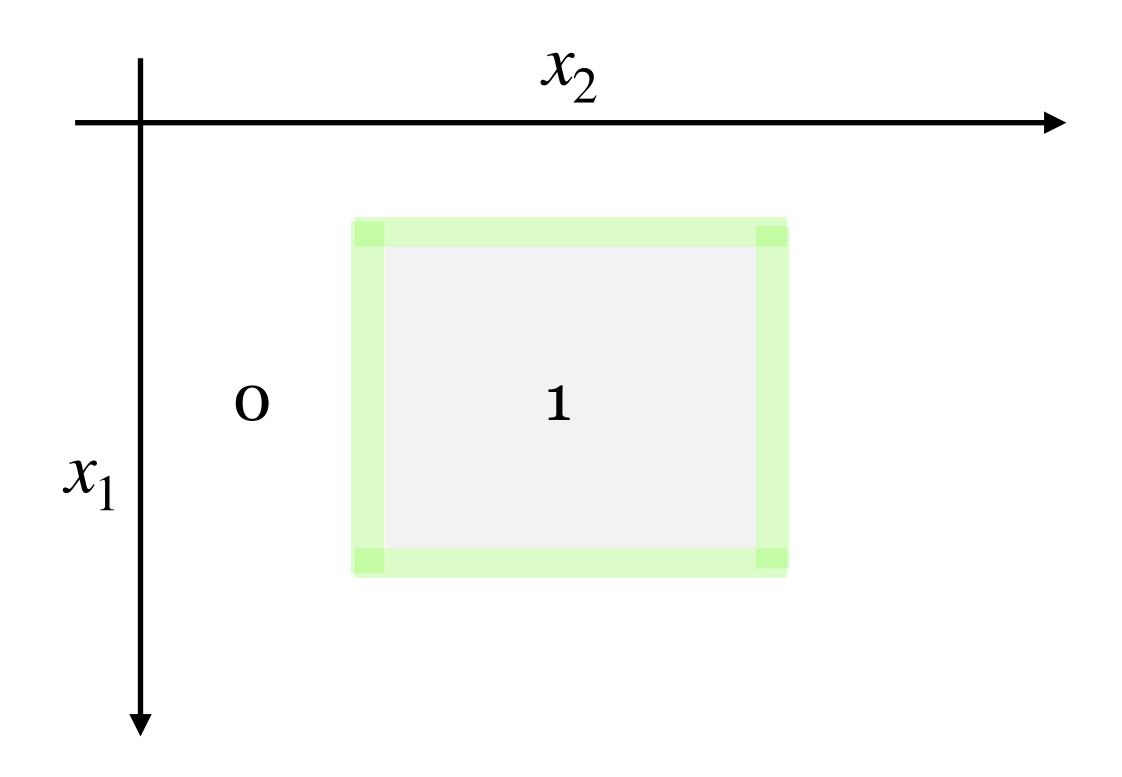
• Think of this as adding a bias, while adding the second hidden layer



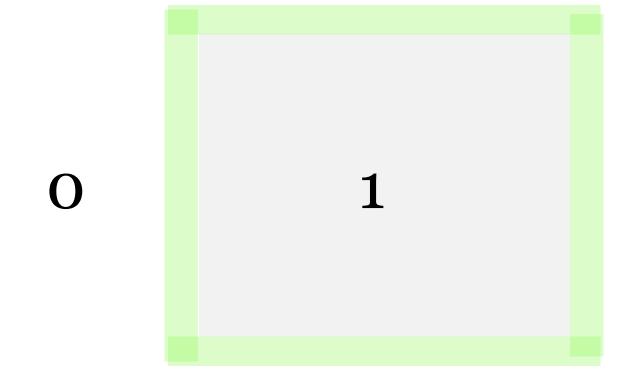
• Again, we proceed in three steps:

Step 3. Remove negative parts, with ReLU

- We have fully added the second hidden layer
 - Total number of neurons used: 4d in the 1st layer, 1 in the second layer



- If we analyze the L1 error, it will be of order at most γ
 - Now we are ready for a formal proof!



- We will prove three claims:
 - Claim 1. Existence of some $h(\cdot)$ with $||g h||_{\infty} \le \varepsilon$
 - Claim 2. Approximating bases with neurons
 - Claim 3. Connecting two claims

Claim 1. There exists an $h(\cdot)$ such that

$$\|g(\mathbf{x}) - h(\mathbf{x})\|_{\infty} \le \varepsilon$$
, where $h(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i \cdot \mathbf{1}\{\mathbf{x} \in R_i\}$ for $N = \lceil \rho/\varepsilon \rceil^d$.

<u>Idea</u>.

- Divide the domain $[0,1]^d$ into many sub-hypercubes, with sidelengths ε/ρ
- Select $\alpha_i = g(\mathbf{x}_{(i)})$, for some $\mathbf{x}_{(i)} \in R_i$

Claim 2. For each R_i , there exists a three-layer neural net $f_i(\cdot)$ such that

$$||f_i(\mathbf{x}) - \mathbf{1}\{\mathbf{x} \in R_i\}||_1 \le \frac{\varepsilon}{\sum_{i=1}^N |\alpha_i|}, \quad \forall i \in [N]$$

<u>Idea</u>.

• Already have the construction — all that remains is to choose the right γ

Claim 3. We have $||f - g||_1 \le 2\varepsilon$, for the three-layer neural network

$$f(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i \cdot f_i(\mathbf{x})$$

<u>Idea</u>.

• Use the triangle inequality

• Congratulations — you have the claim!

Discussion

Theorem 2.1.

Let $g:[0,1]^d \to \mathbb{R}$ be a ρ -Lipschitz function, and let $\varepsilon > 0$. Then, there exists a three-layer ReLU network with $O(d \cdot \lceil \rho/\varepsilon \rceil^d)$ neurons such that

$$\int_{[0,1]^d} |f(\mathbf{x}) - g(\mathbf{x})| \, \mathrm{d}x \le 2\varepsilon$$

- We have used a lot of neurons exponential dependence on *d*
 - Generally unavoidable, but gets better as we increase depth
- We can also use two layers
 - Requires sophisticated tools (next lecture)