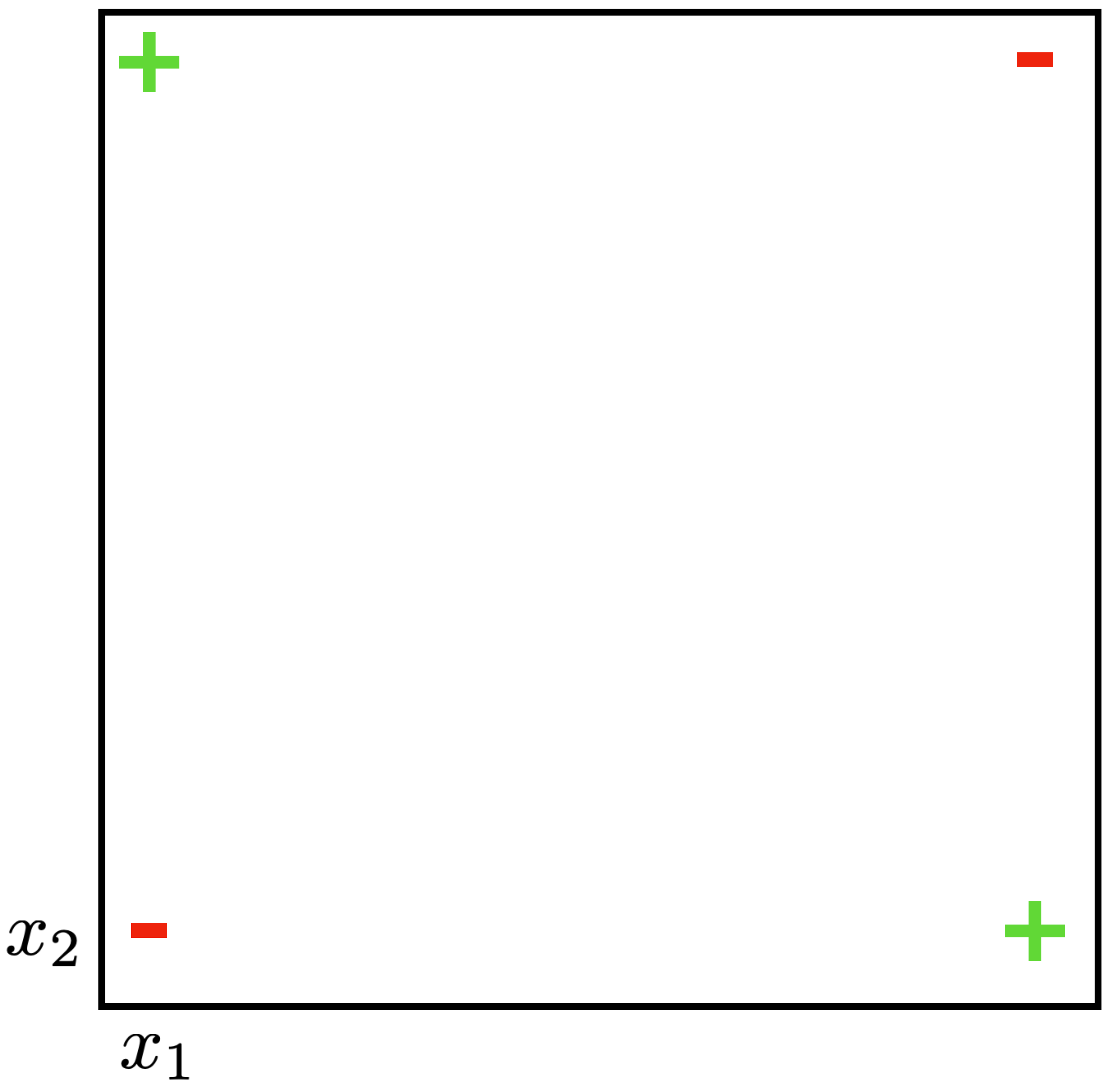
Lecture 7: Neural networks

- Discussion this week: machine learning
- Reading:
  - Szeliski 5.3
  - Goodfellow Deep Feedforward Networks
- Start thinking about project
- PS2 due today – submit to gradescope and canvas

Today

- Brief history of neural networks
- Computation in neural networks
- Multi-layer perceptrons (for PS4)
- Estimating gradients (to be continued next class).

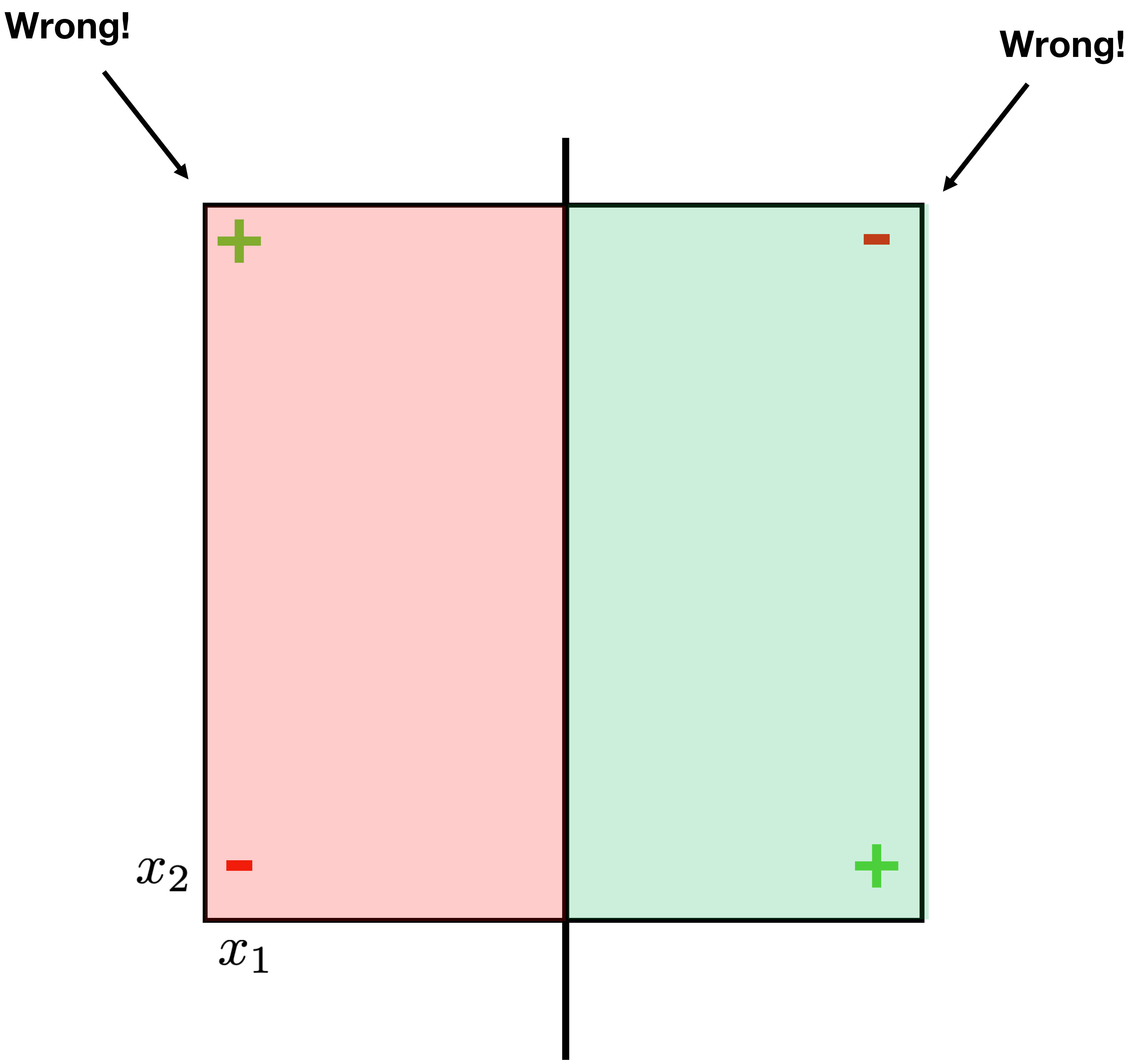
Limitations to linear classifiers



		x_2	
		0	1
x_1	0	0	1
	1	1	0

XOR

Limitations to linear classifiers



		x_2	
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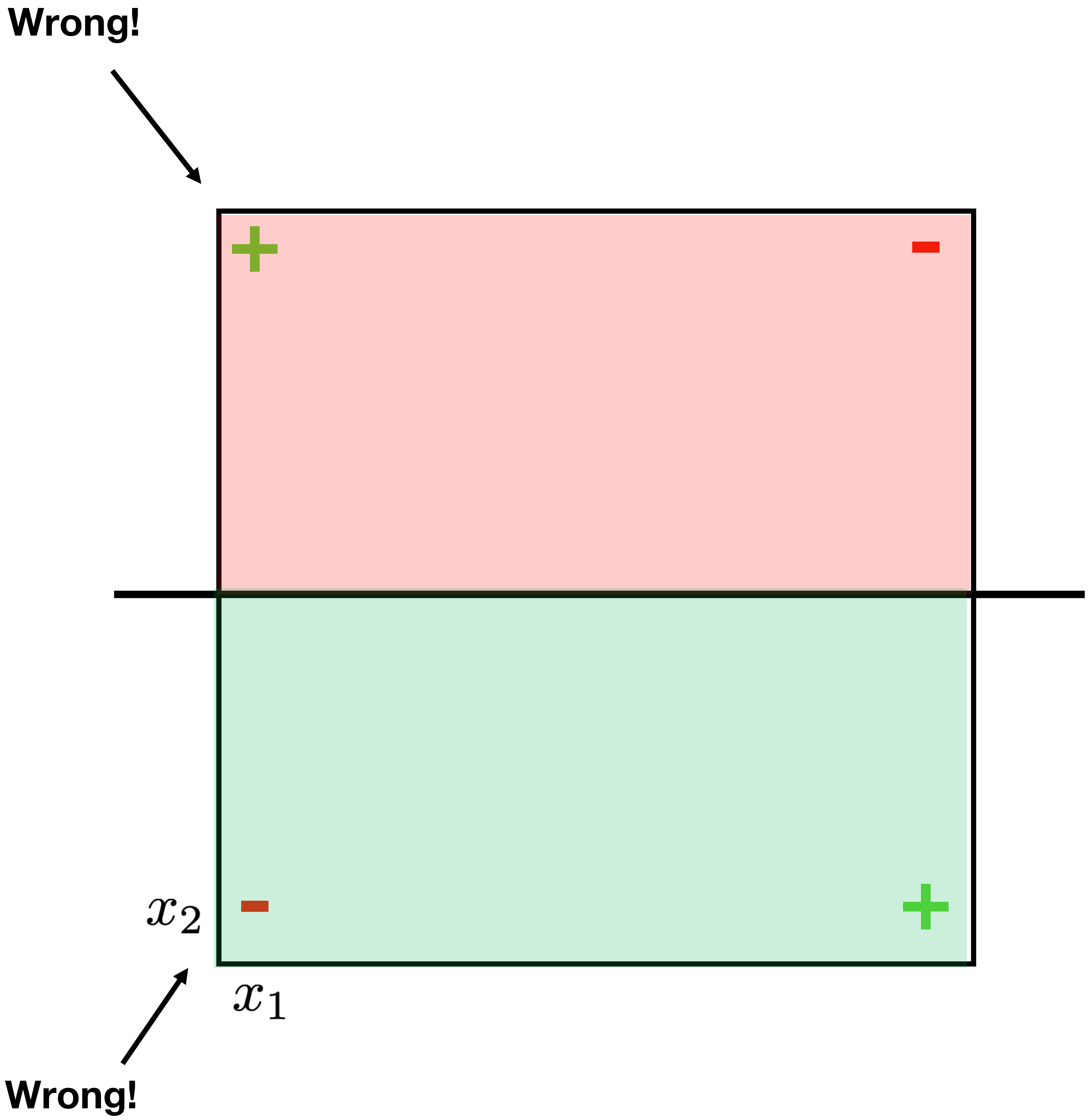
XOR

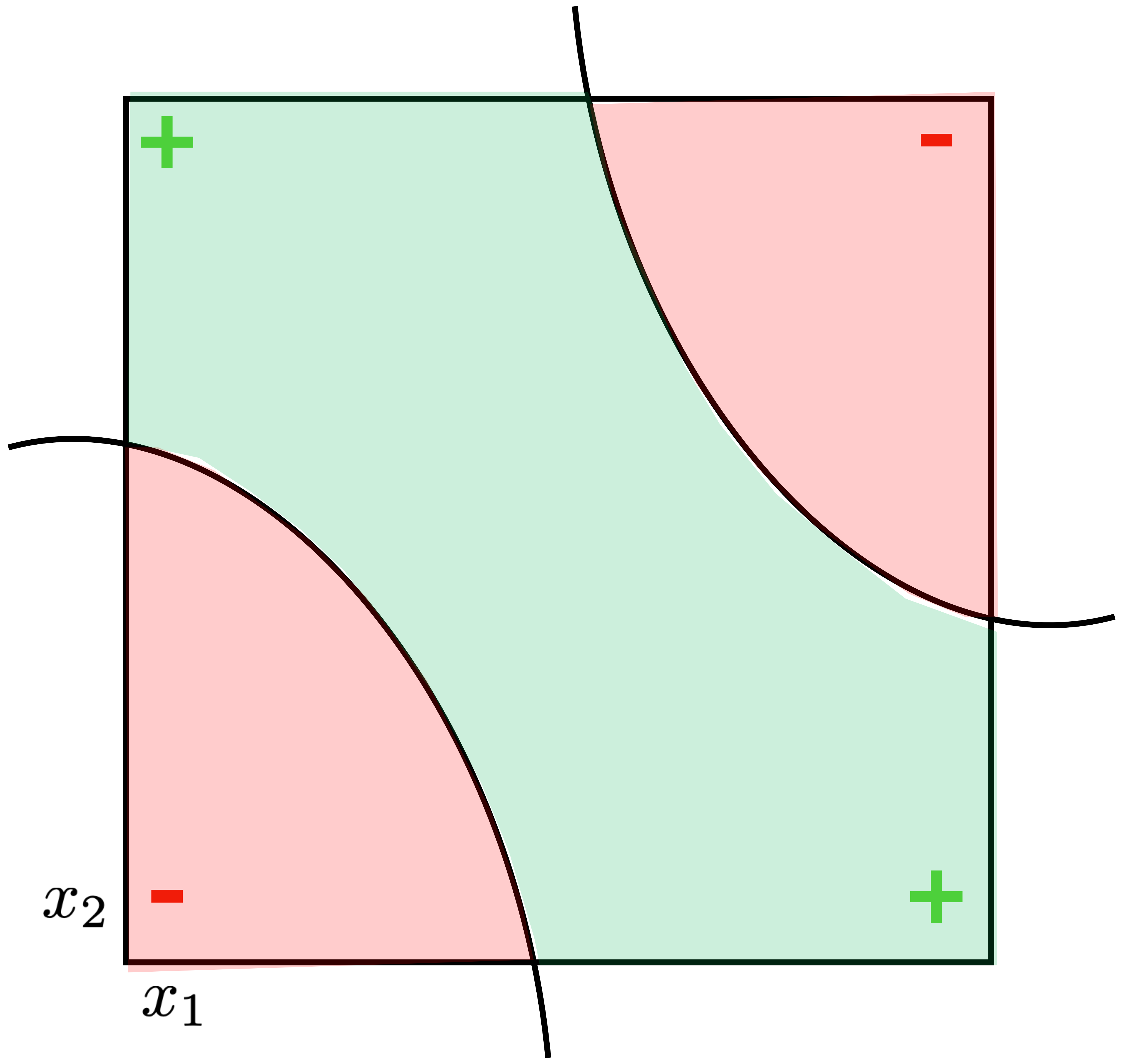
Limitations to linear classifiers



		x_2	
		0	1
x_1	0	0	1
	1	1	0

XOR

Goal: Non-linear decision boundary

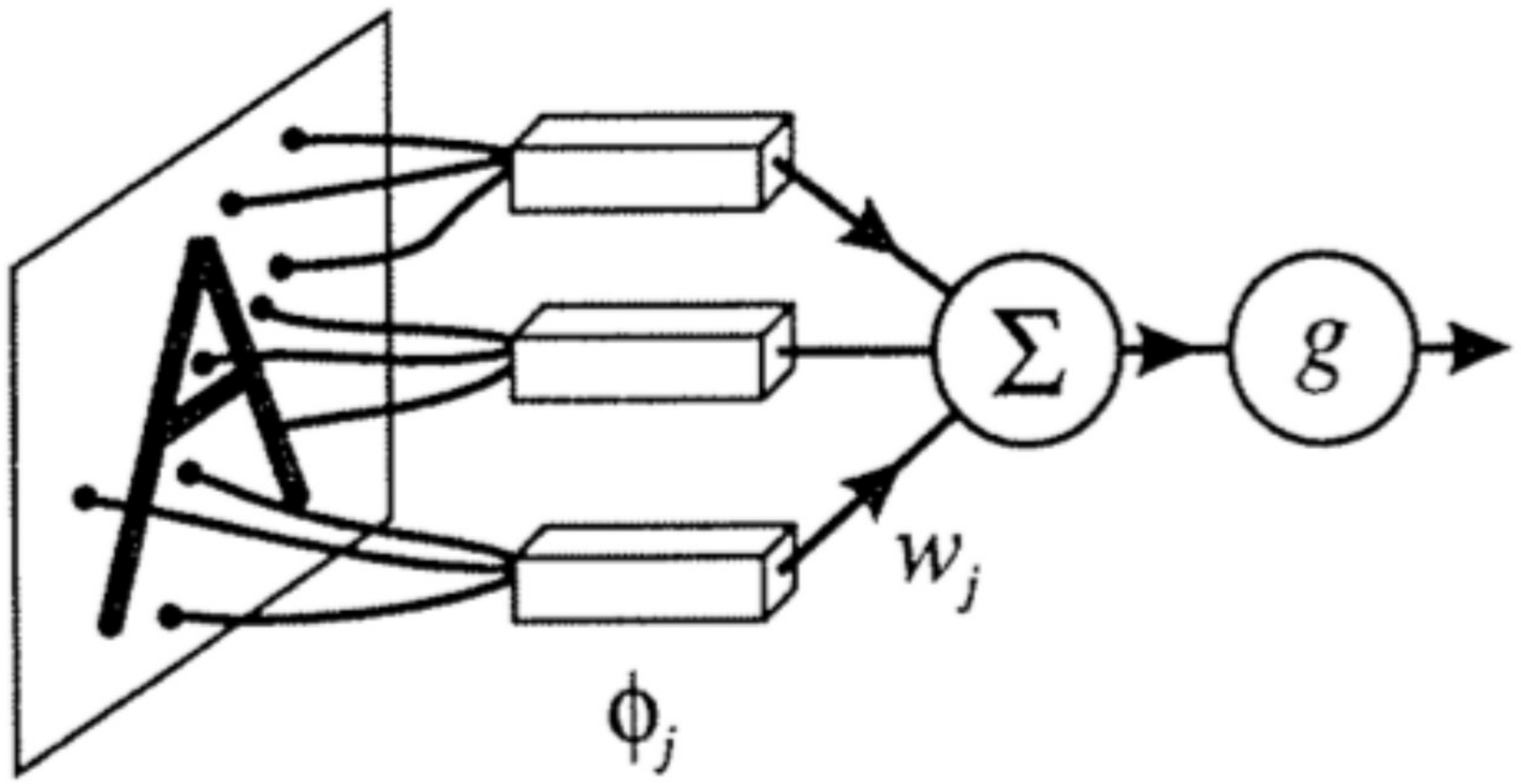


		x_2	
		0	1
x_1	0	0	1
	1	1	0

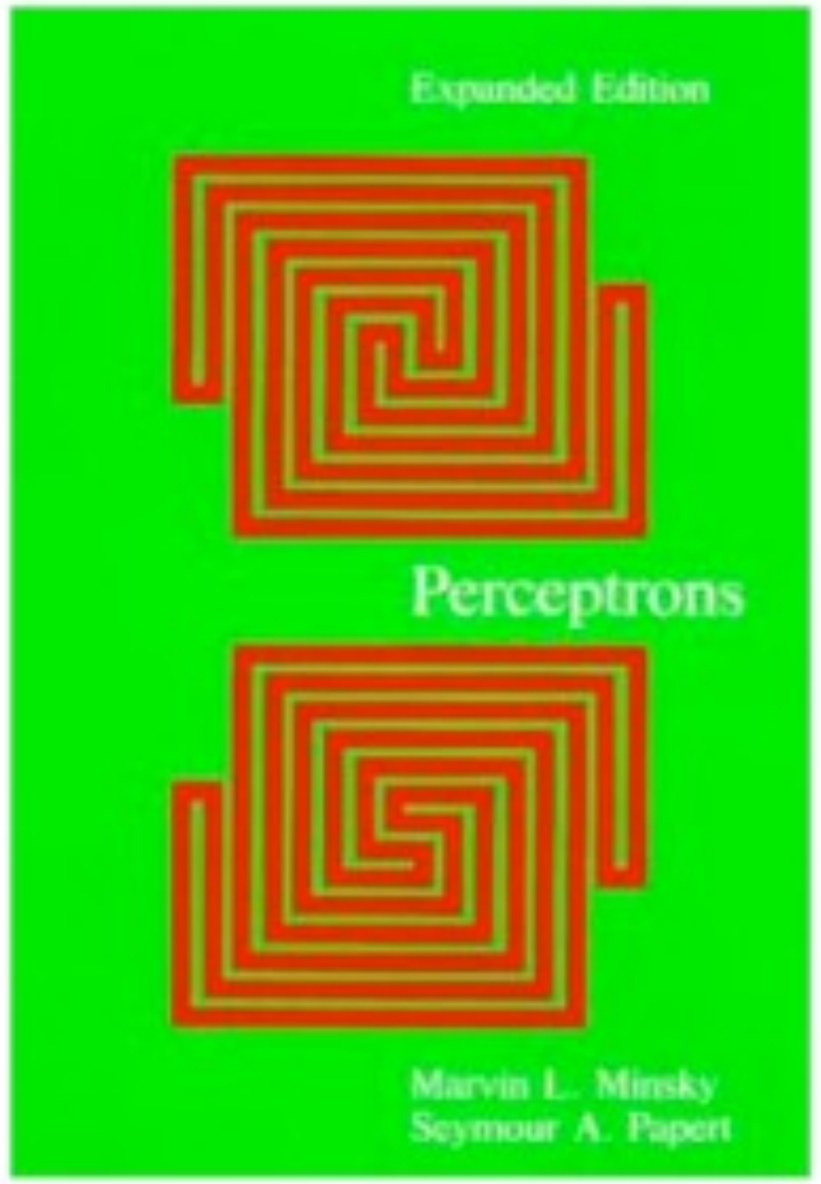
XOR

Perceptron

- In 1957 Frank Rosenblatt invented the perceptron
- Computers at the time were too slow to run the perceptron, so Rosenblatt built a special purpose machine with adjustable resistors
- New York Times Reported: “The Navy revealed the embryo of an electronic computer that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence”



Minsky and Papert, Perceptrons, 1972



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ISBN: 9780262631112 | 308 pp. | 6 x 8.9 in | December 1987

Perceptrons, expanded edition

An Introduction to Computational Geometry

By Marvin Minsky and Seymour A. Papert

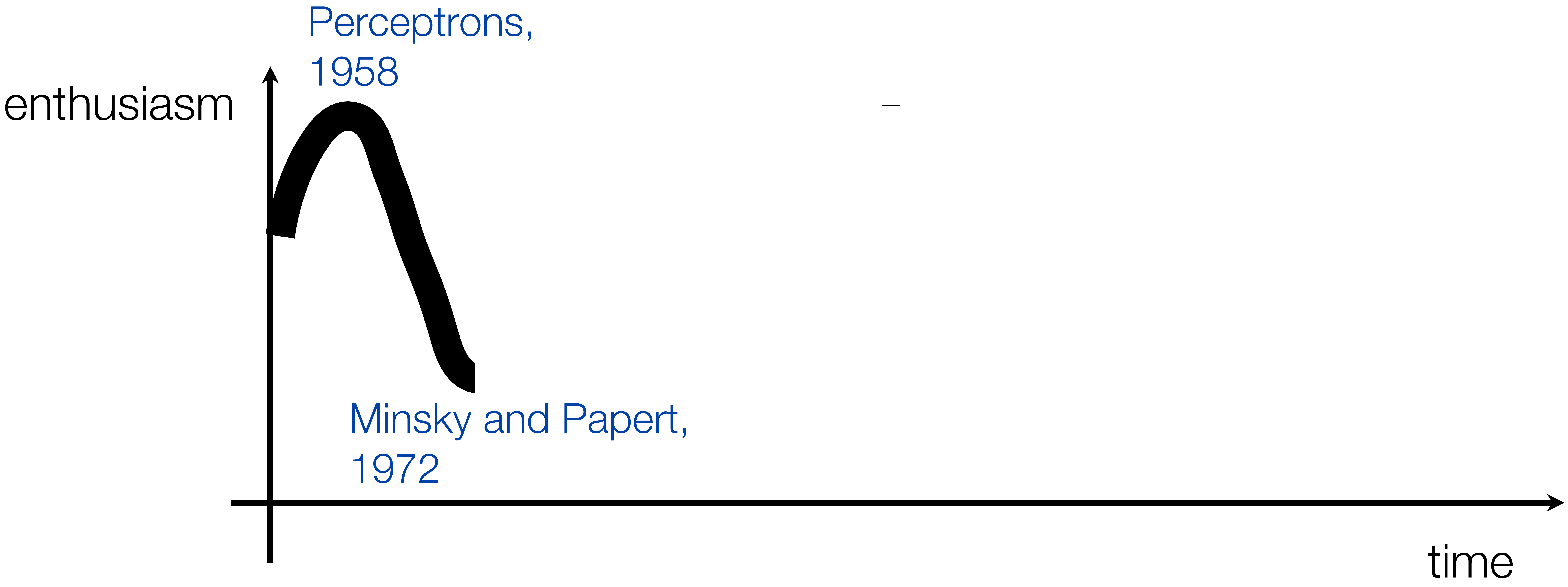
Overview

Perceptrons - the first systematic study of parallelism in computation - has remained a classical work on threshold automata networks for nearly two decades. It marked a historical turn in artificial intelligence, and it is required reading for anyone who wants to understand the connectionist counterrevolution that is going on today.

Artificial-intelligence research, which for a time concentrated on the programming of ton Neumann computers, is swinging back to the idea that intelligence might emerge from the activity of networks of neuronlike entities. Minsky and Papert's book was the first example of a mathematical analysis carried far enough to show the exact limitations of a class of computing machines that could seriously be considered as models of the brain. Now the new developments in mathematical tools, the recent interest of physicists in the theory of disordered matter, the new insights into and psychological models of how the brain works, and the evolution of fast computers that can simulate networks of automata have given *Perceptrons* new importance.

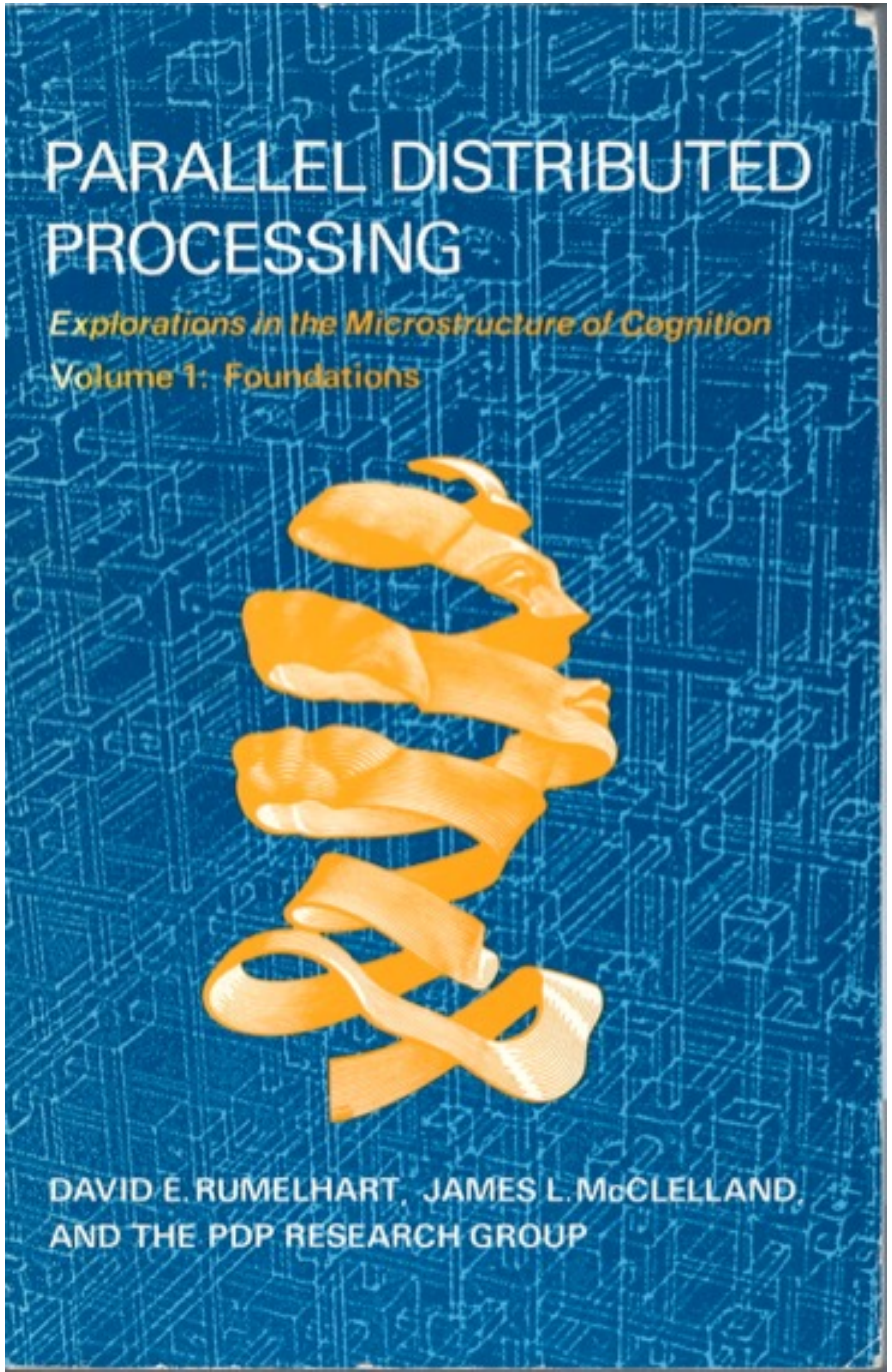
Witnessing the swing of the intellectual pendulum, Minsky and Papert have added a new chapter in which they discuss the current state of parallel computers, review developments since the appearance of the 1972 edition, and identify new research directions related to connectionism. They note a central theoretical challenge facing connectionism: the challenge to reach a deeper understanding of how "objects" or "agents" with individuality can emerge in a network. Progress in this area would link connectionism with what the authors have called "society theories of mind."

Source: Isola, Torralba, Freeman

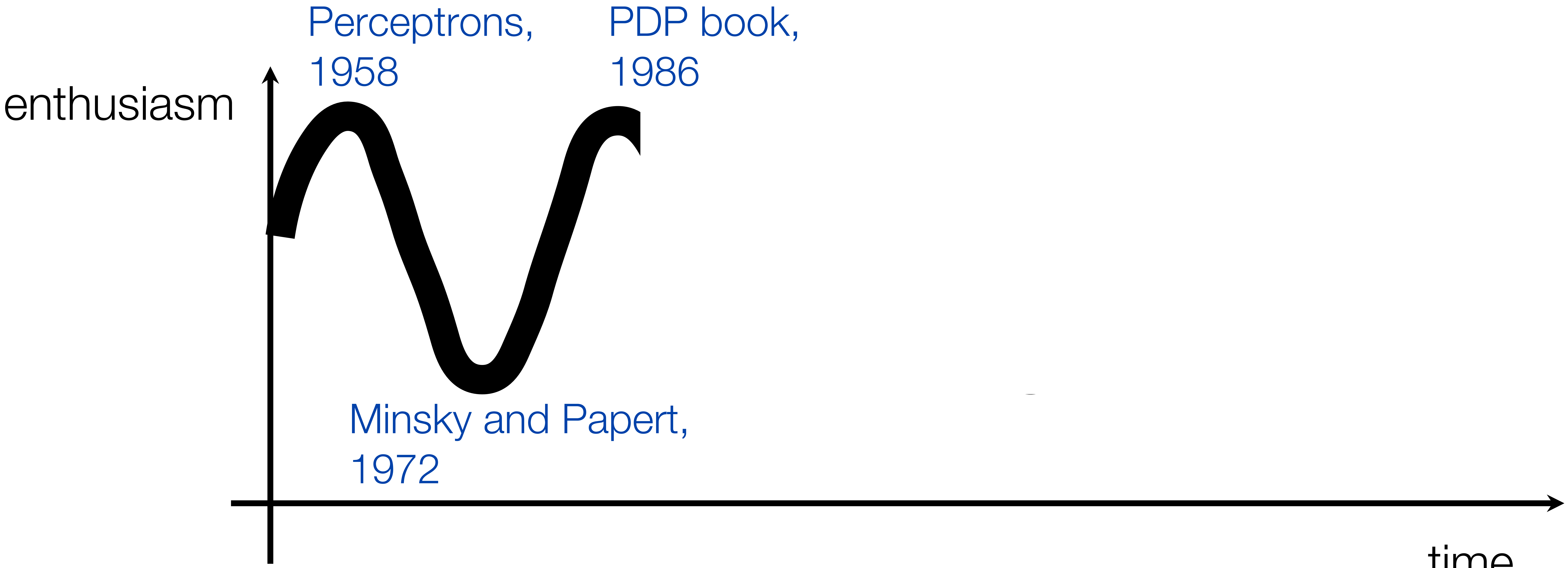


Based on slide by: Isola, Torralba, Freeman

Parallel Distributed Processing (PDP), 1986



Source: Isola, Torralba, Freeman



Source: Isola, Torralba, Freeman

LeCun convolutional neural networks

PROC. OF THE IEEE, NOVEMBER 1998 7

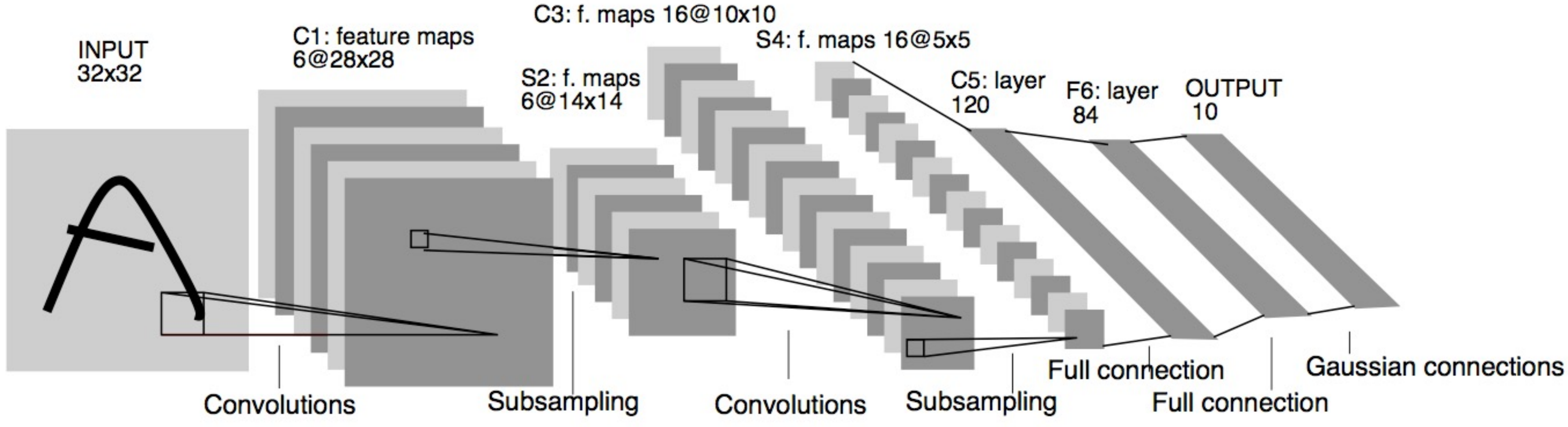


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

Demos:
http://yann.lecun.com/exdb/lenet/index.html

Source: Isola, Torralba, Freeman

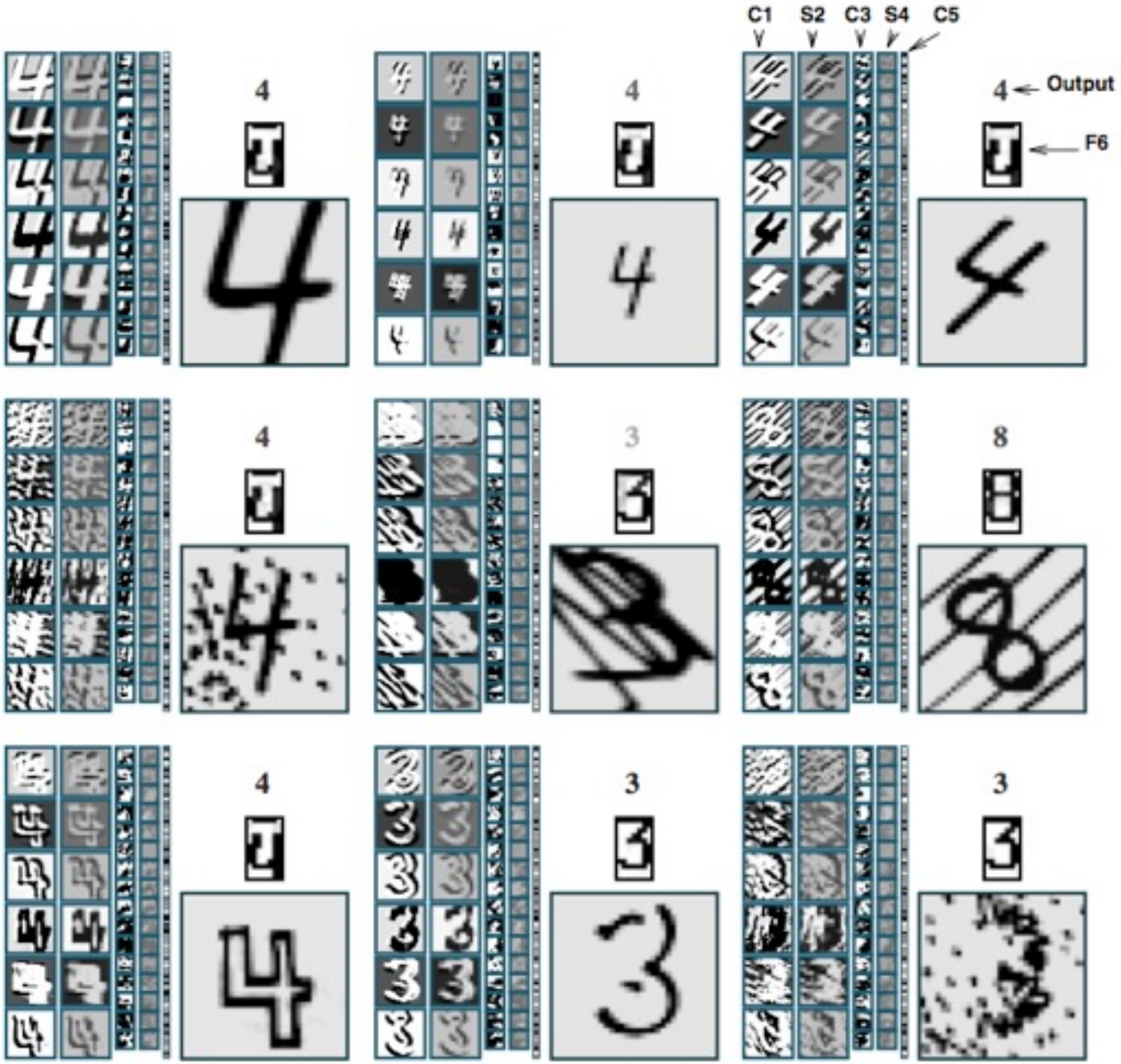
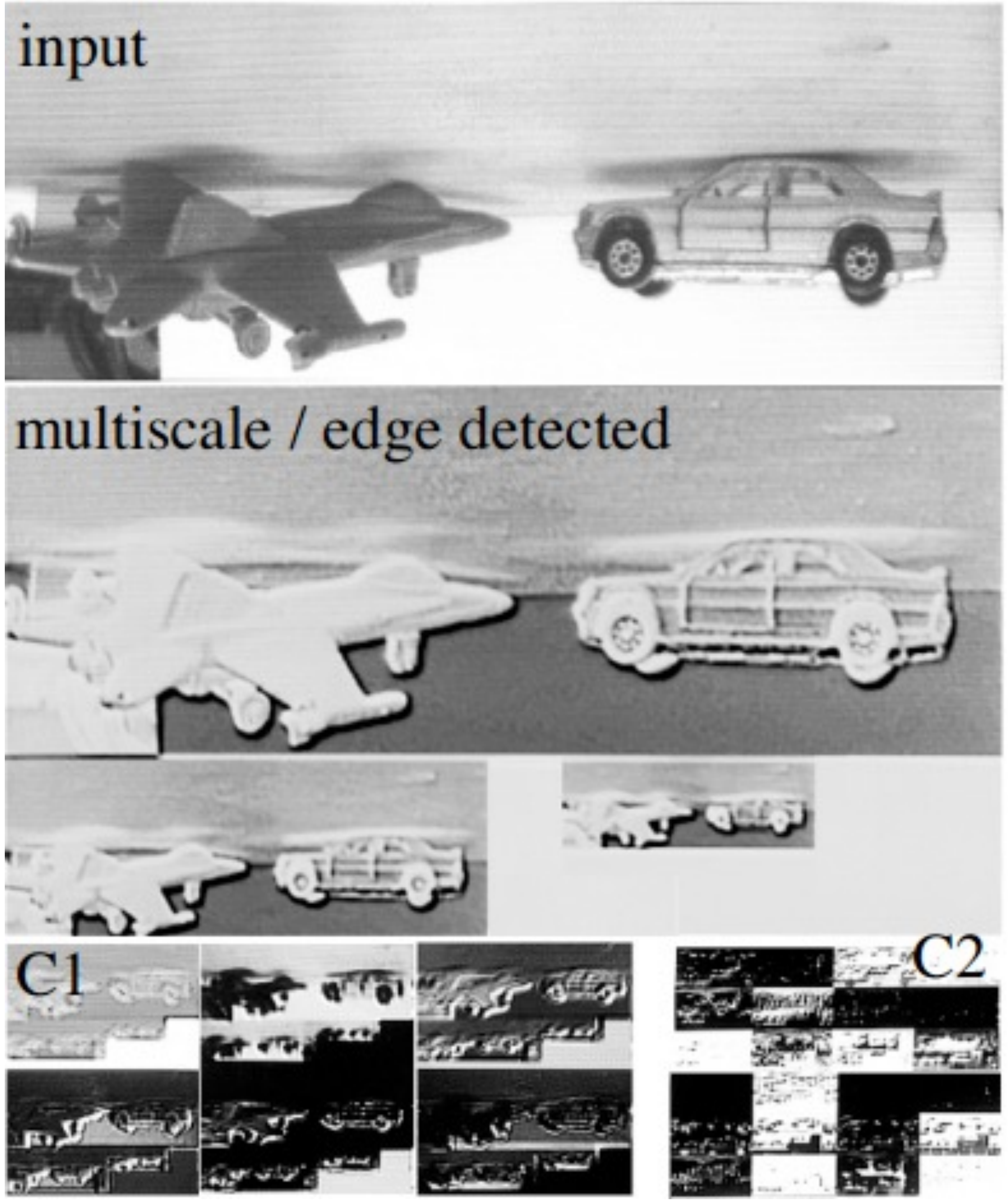


Fig. 13. Examples of unusual, distorted, and noisy characters correctly recognized by LeNet-5. The grey-level of the output label represents the penalty (lighter for higher penalties).

Source: Isola, Torralba, Freeman



http://pub.clement.farabet.net/ecvw09.pdf

Neural networks to recognize handwritten digits and human faces?
yes

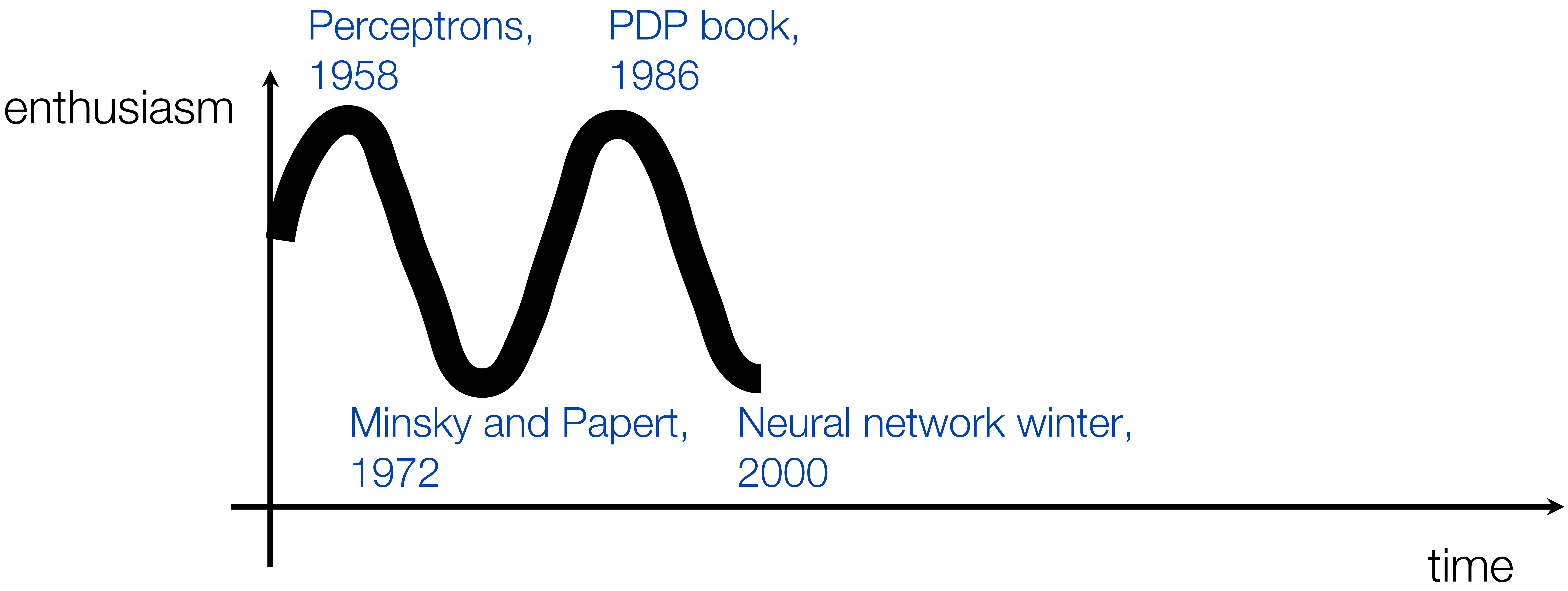
Neural networks for tougher problems?
not really

Source: Isola, Torralba, Freeman

Machine learning circa 2000

- Neural Information Processing Systems (NeurIPS), is a top conference on machine learning.
- For the 2000 conference:
  - title words predictive of paper acceptance: "Belief Propagation" and "Gaussian".
  - title words predictive of paper rejection: "Neural" and "Network".

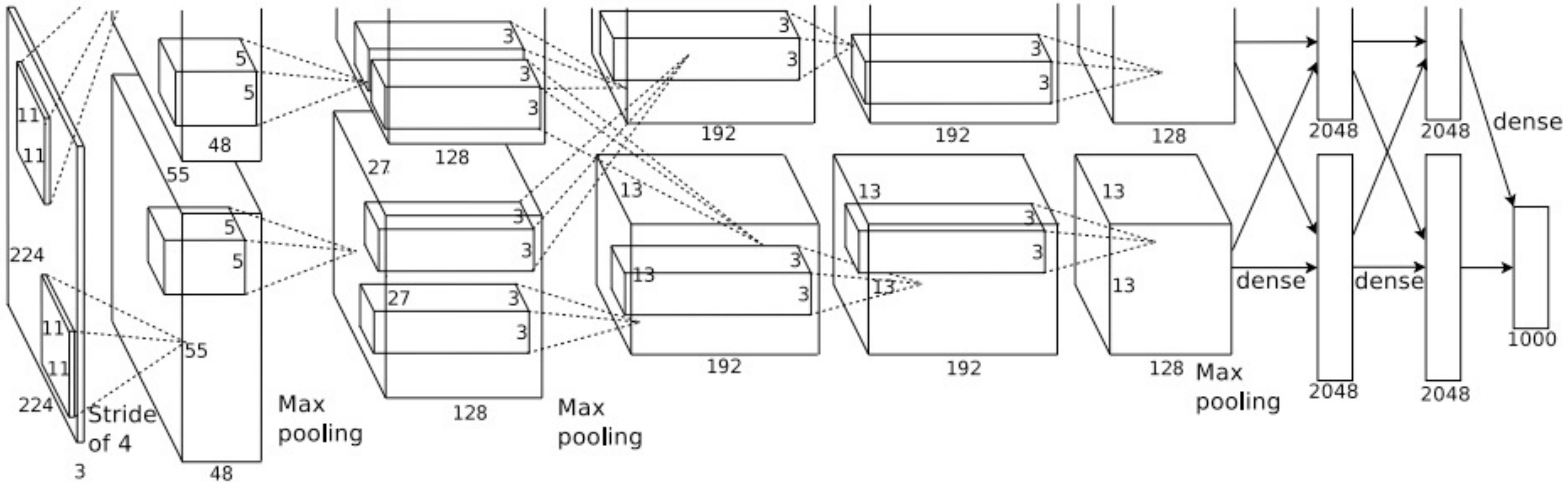
Source: Isola, Torralba, Freeman



Source: Isola, Torralba, Freeman

Krizhevsky, Sutskever, and Hinton, NeurIPS 2012

“AlexNet”



Got all the “pieces” right, e.g.,
- Trained on ImageNet
- 8 layer architecture (for reference: today we have architectures with 100+ layers)
- Allowed for multi-GP training

Source: Isola, Torralba, Freeman

Krizhevsky, Sutskever, and Hinton, NeurIPS 2012

Source: Isola, Torralba, Freeman

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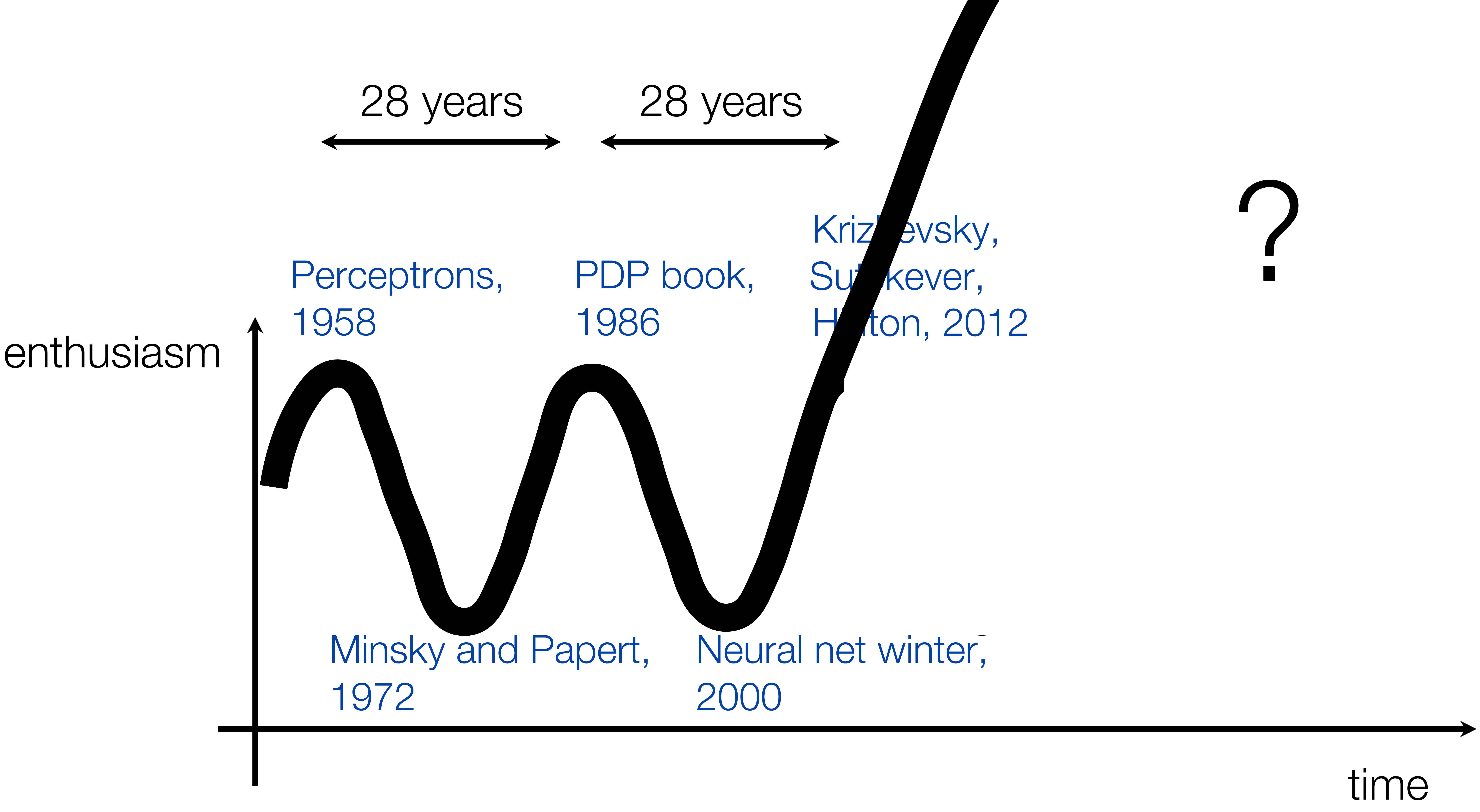
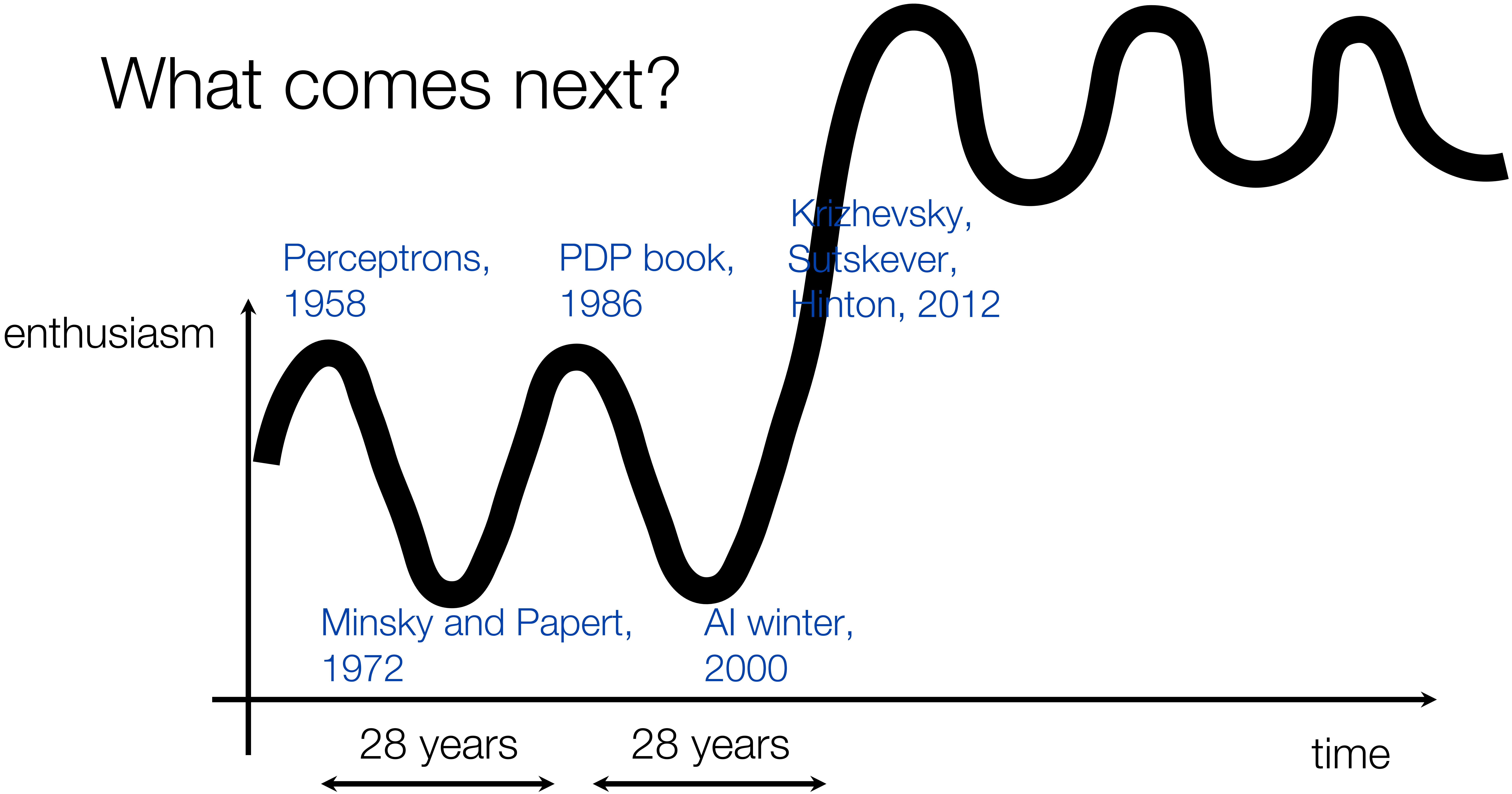


Source: Isola, Torralba, Freeman

What comes next?



Source: Isola, Torralba, Freeman

Inspiration: Neurons

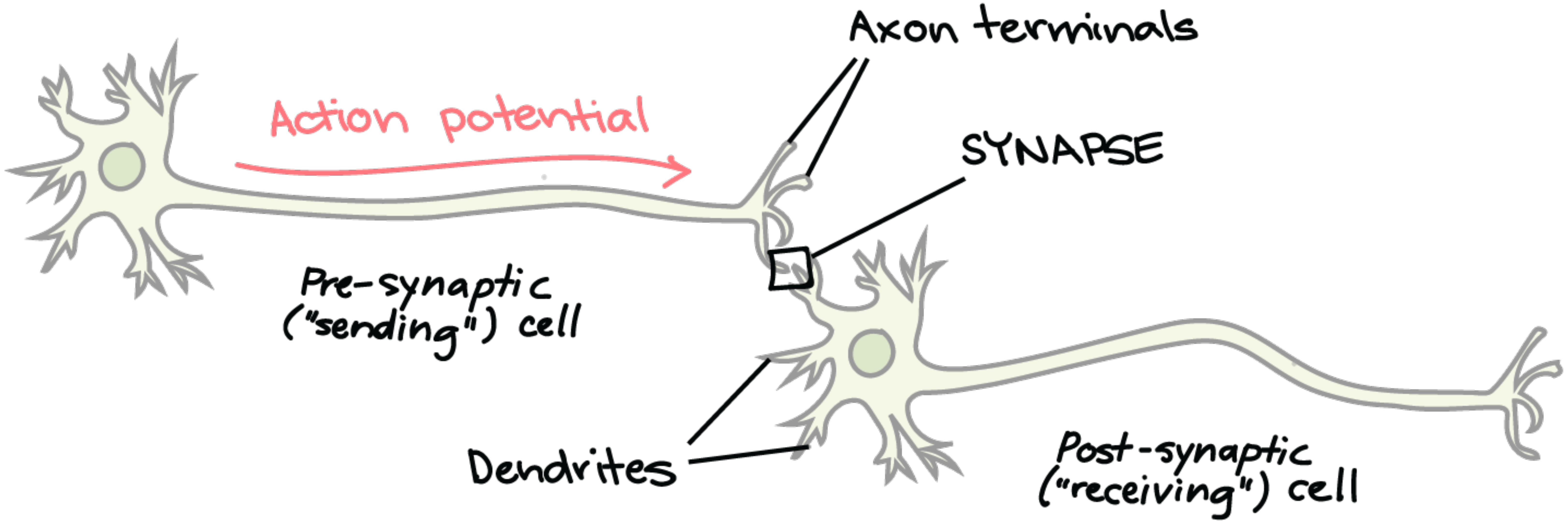
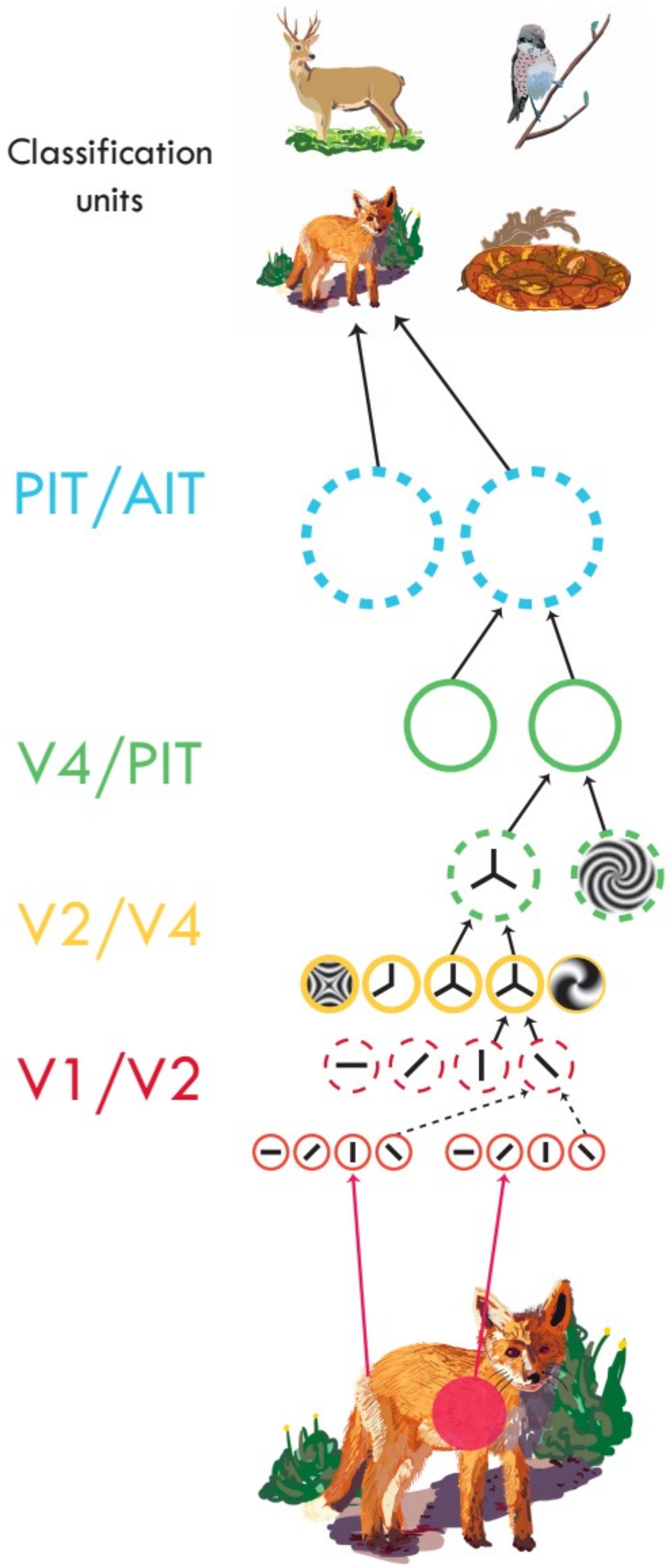


Image source: [Khan academy]

Inspiration: Hierarchical Representations

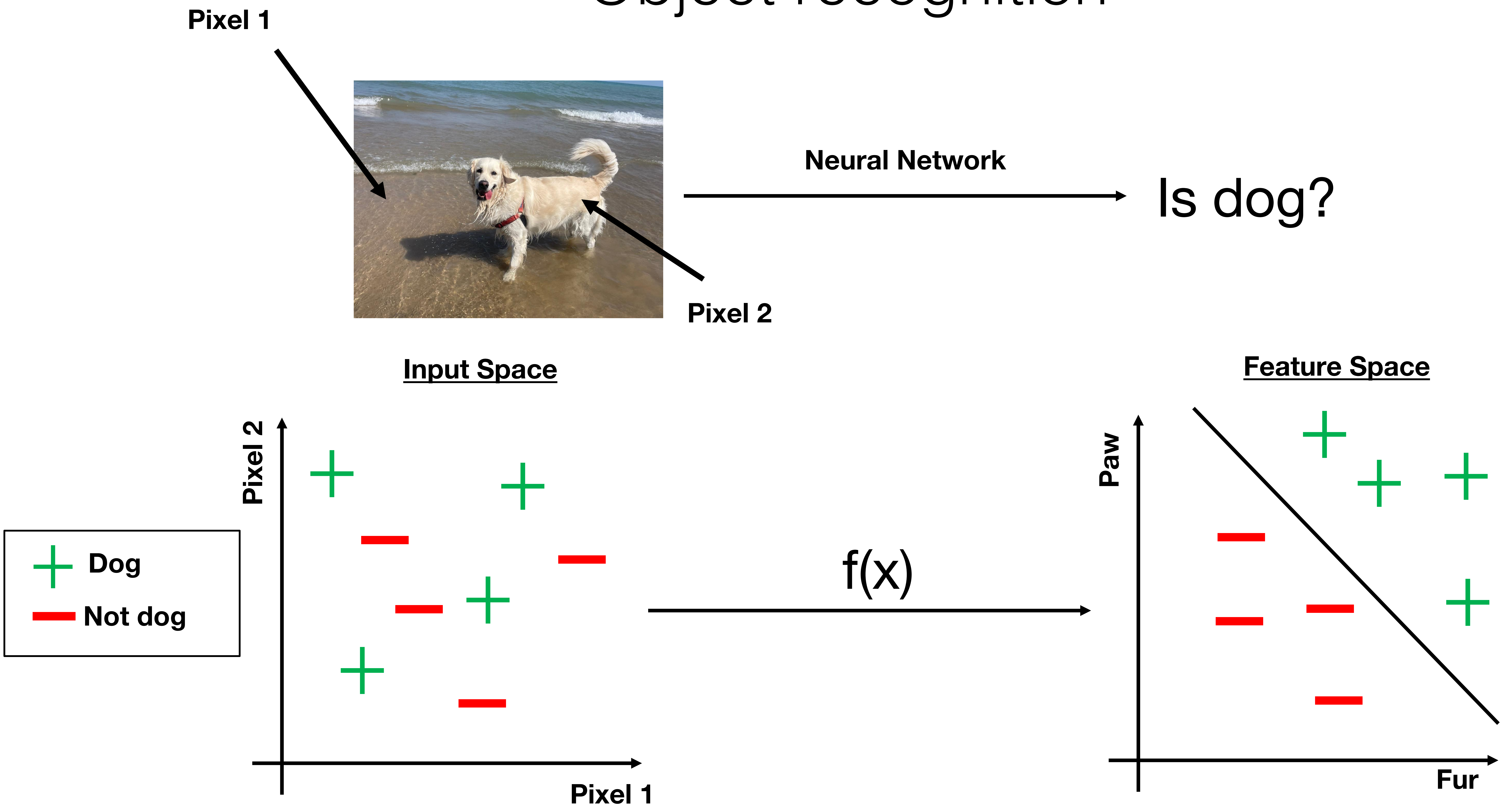


[Serre, 2014]

Best to treat as *inspiration*. The neural nets we'll talk about aren't very biologically plausible.

Source: Isola, Torralba, Freeman

Object recognition

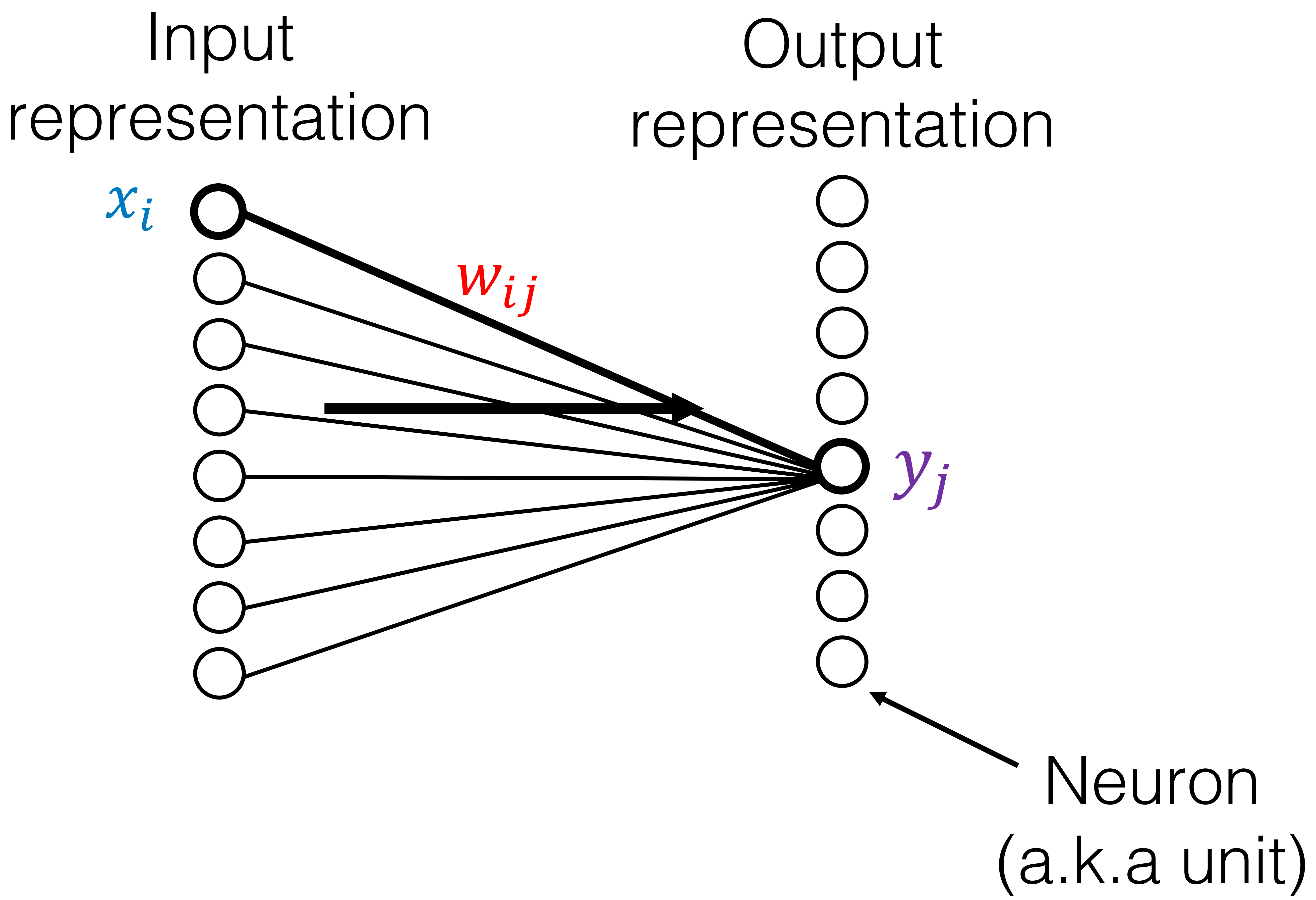


Goal: automatically learn a function that maps data from the input space to a feature space, i.e., "feature learning", rather than use hand-crafted features

Computation in a neural net

Lets say we have some 1D input that we want to convert to some new feature space:

Linear layer



$$y_j = \sum_i w_{ij} x_i$$

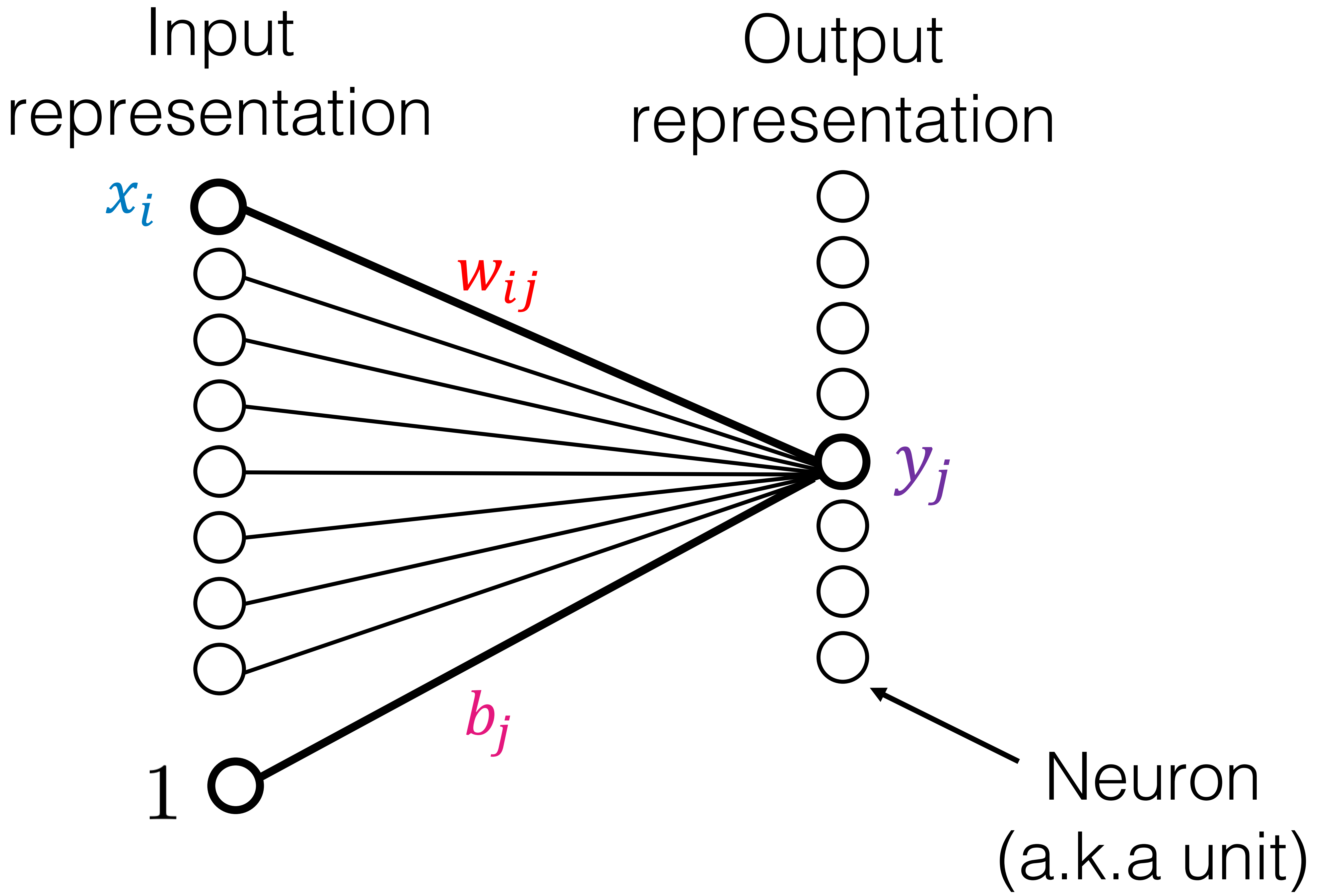
weights

Adapted from: Isola, Torralba, Freeman

Computation in a neural net

Lets say we have some 1D input that we want to convert to some new feature space:

<u>Linear layer</u>



weights

$$y_j = \sum_i w_{ij} x_i + b_j$$

bias

Computation in a neural net – Matrix Multiplication

$$y_j = \sum_i w_{ij} x_i + b_j$$

$$\sum_i \boldsymbol{w_{ij} x_i} = \boldsymbol{x} \cdot \boldsymbol{w_j} = \boldsymbol{x}^T \boldsymbol{w}_j$$

$$y_j = \boldsymbol{x}^T \boldsymbol{w}_j + b_j$$

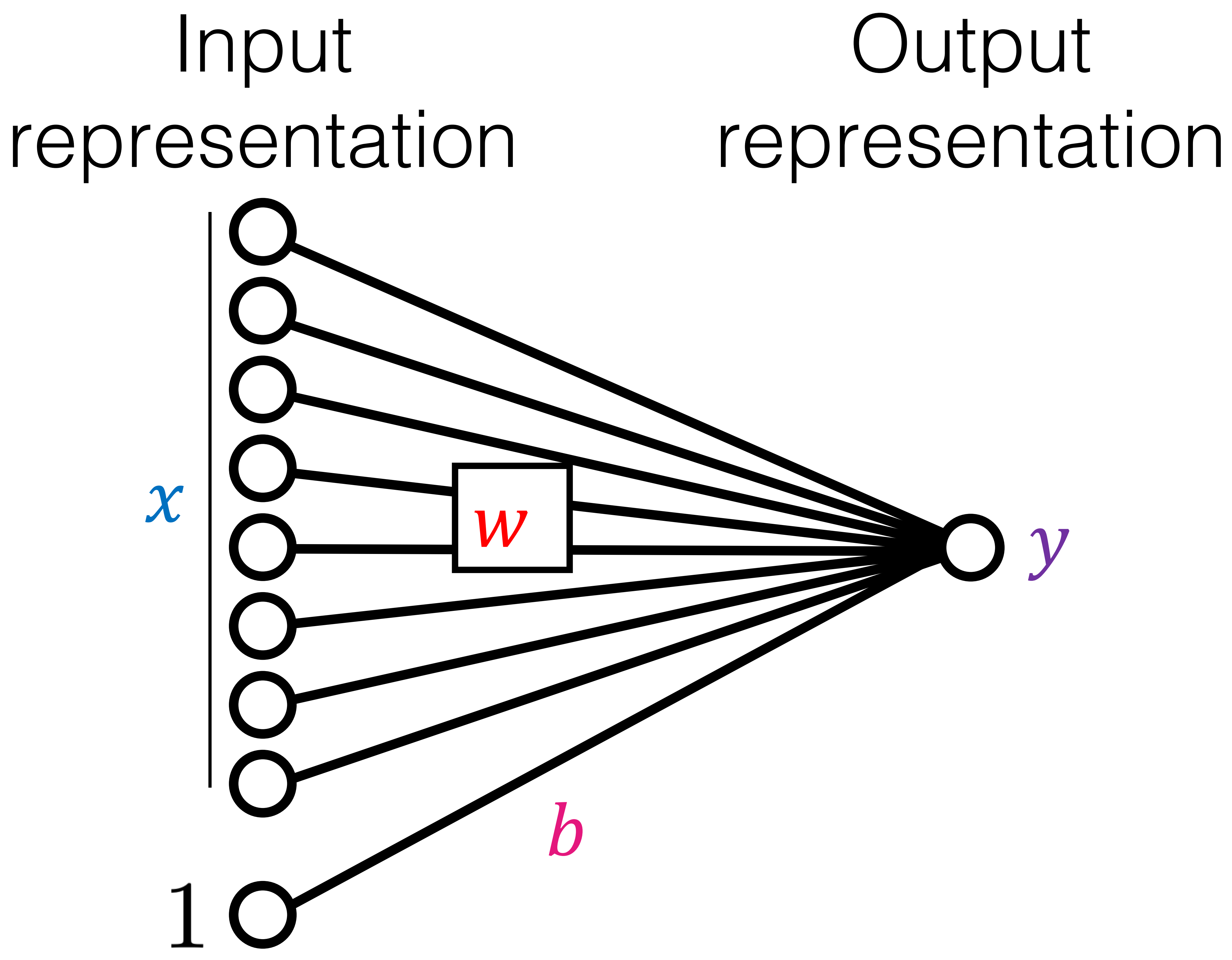
Vector of all input units

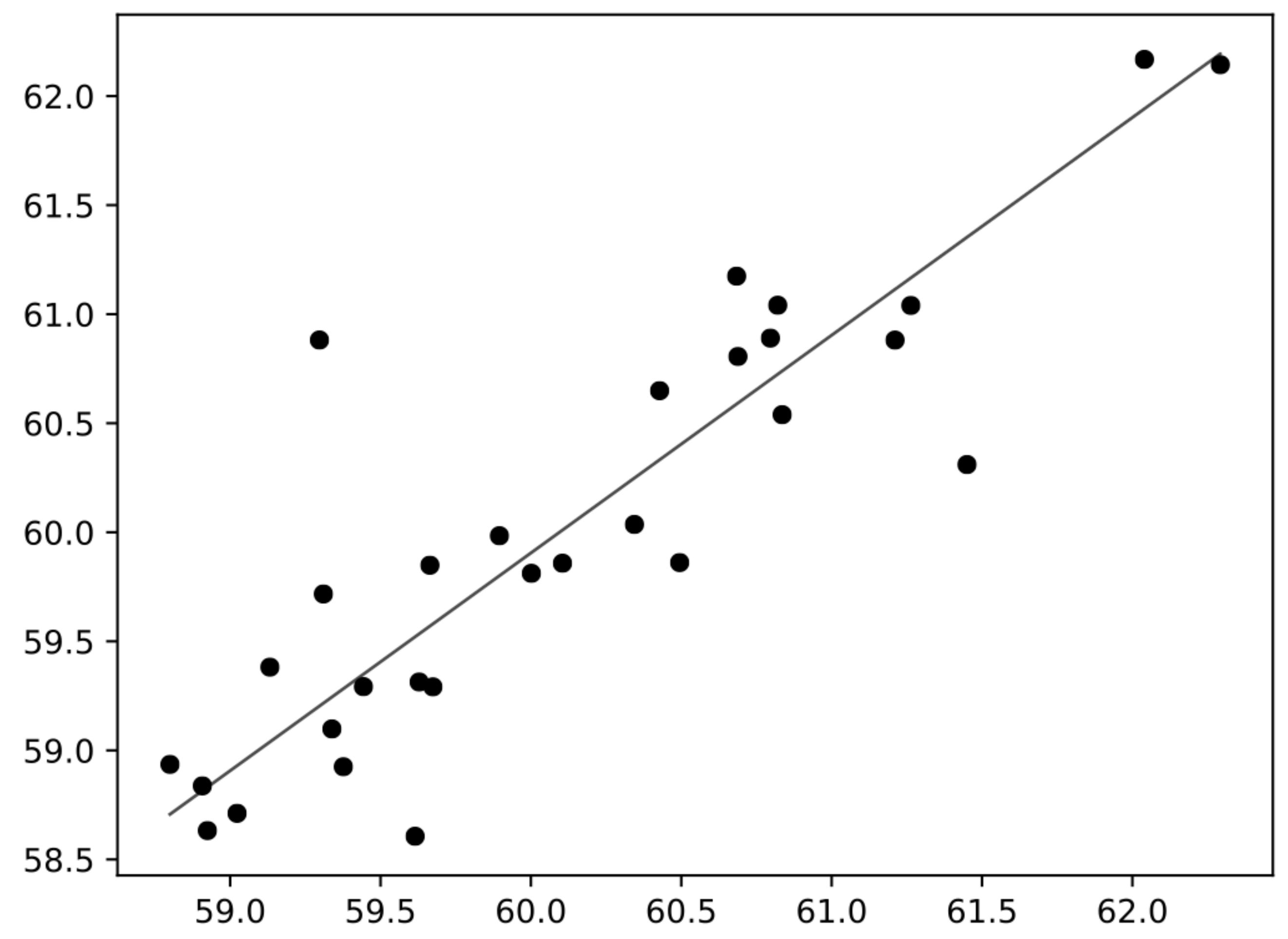
Vector of weights

$$[\boldsymbol{x_1} \;\; \boldsymbol{x_2} \; \ldots \boldsymbol{x_n}] \begin{bmatrix} \boldsymbol{w_1} \\ \boldsymbol{w_2} \\ \ldots \\ \boldsymbol{w_n} \end{bmatrix} + \boldsymbol{b_j} = [\boldsymbol{x_1} \;\; \boldsymbol{x_2} \; \ldots \boldsymbol{x_n} \;\; \boldsymbol{1}] \begin{bmatrix} \boldsymbol{w_1} \\ \boldsymbol{w_2} \\ \ldots \\ \boldsymbol{w_n} \\ \boldsymbol{b_j} \end{bmatrix}$$

Example: Linear Regression

Linear layer



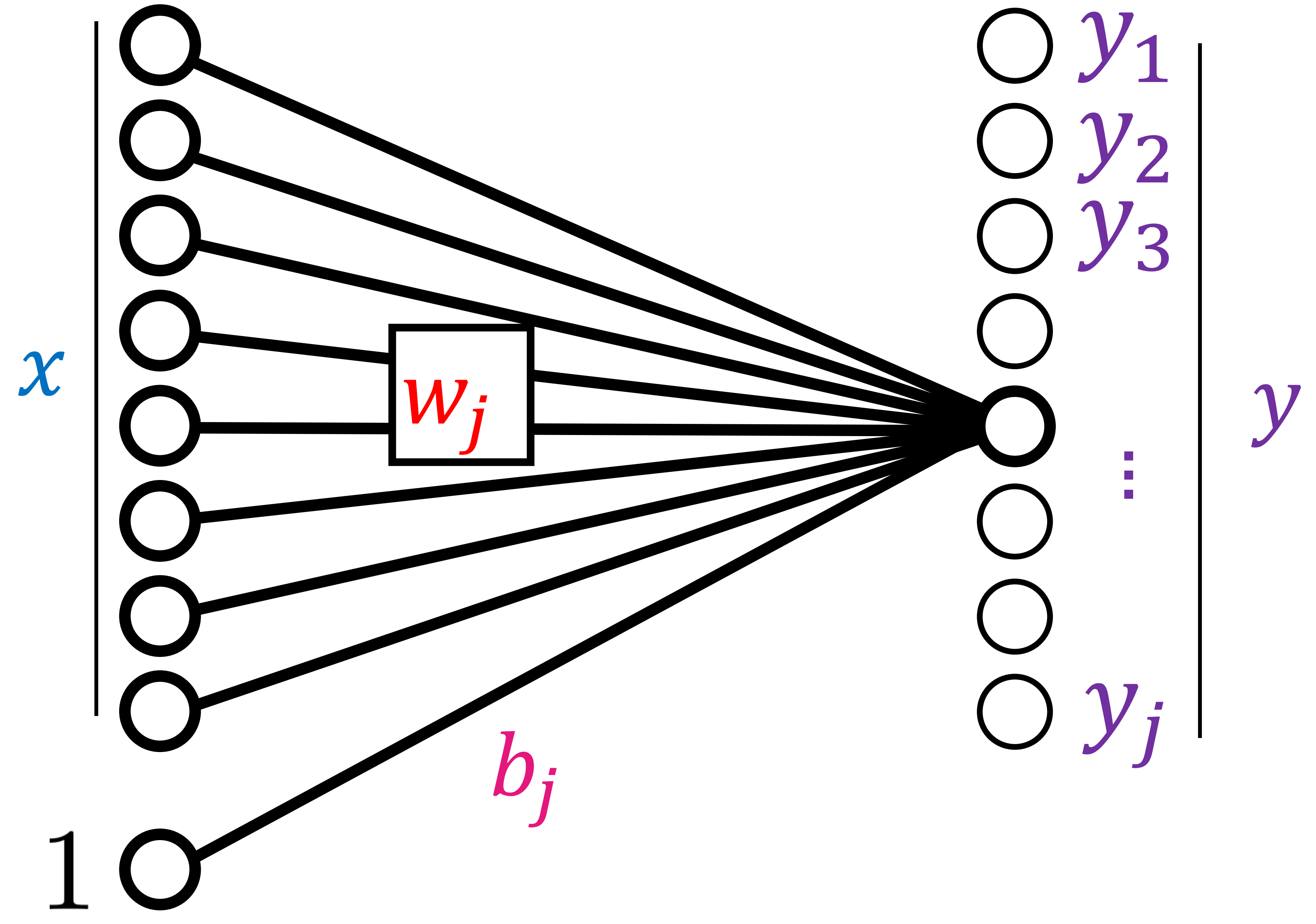


$$f_{\mathbf{w},b}(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b$$

Computation in a neural net – Full Layer

Linear layer

$$y = Wx + b$$



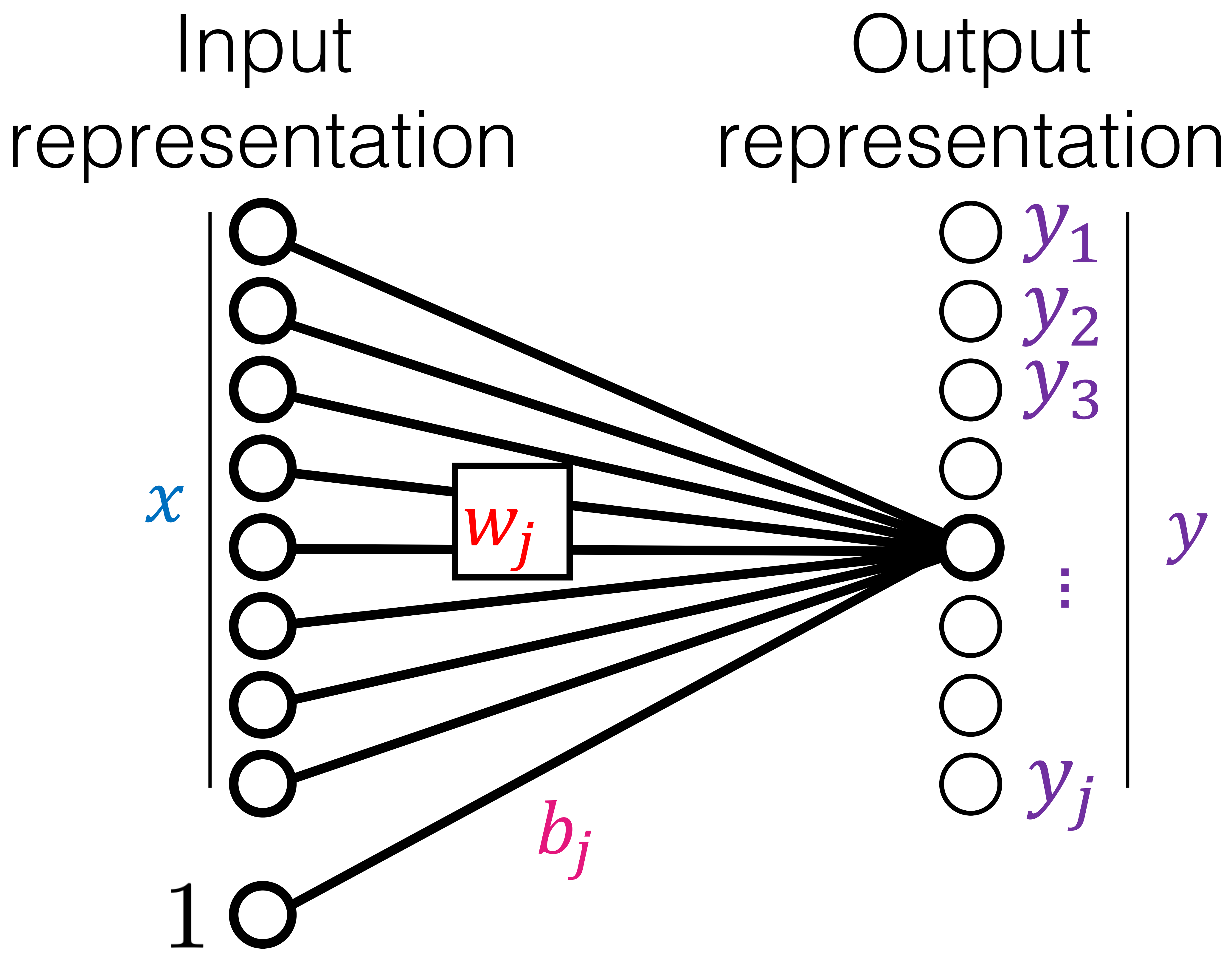
$$\begin{bmatrix} w_{11} & \cdots & w_{1n} \\ \vdots & \ddots & \vdots \\ w_{j1} & \cdots & w_{jn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ \cdots \\ b_j \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_j \end{bmatrix}$$

parameters of the model: $\boldsymbol{\theta} = \{\boldsymbol{W}, \boldsymbol{b}\}$

Adapted from: Isola, Torralba, Freeman

Computation in a neural net – Full Layer

Linear layer



Full layer

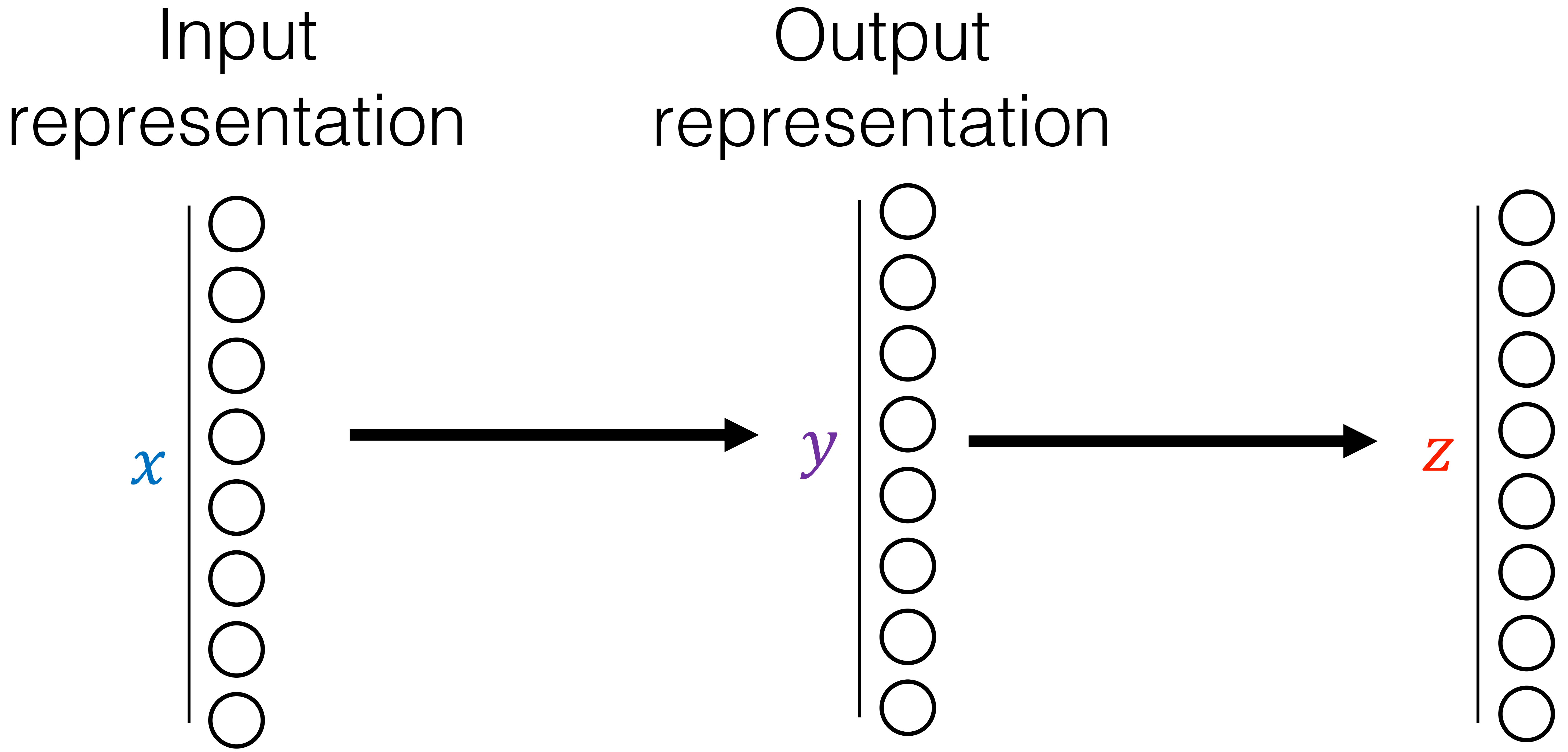
$$y = Wx + b$$

$$\begin{bmatrix} w_{11} & \cdots & w_{jn} & b_1 \\ \vdots & \ddots & \vdots & \vdots \\ w_{j1} & \cdots & w_{jn} & b_j \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdots \\ x_n \\ 1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \cdots \\ y_j \end{bmatrix}$$

Can again simplify notation by appending a 1 to $\mathbf{x}$

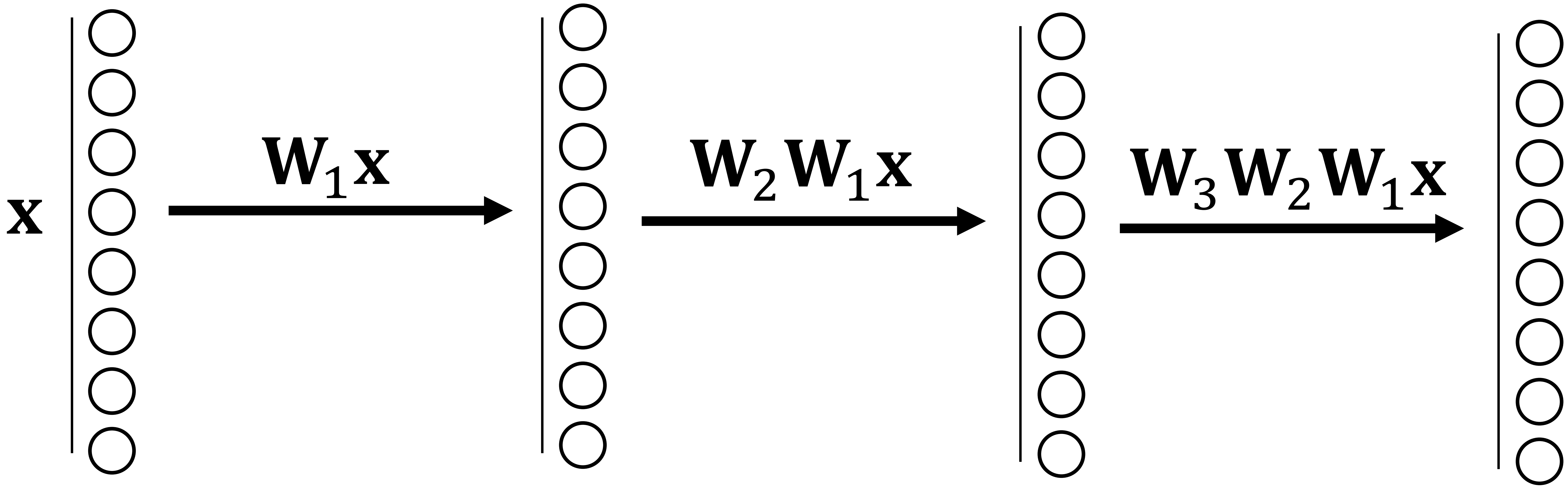
Computation in a neural net – Recap

We can now transform our input representation vector into some output representation vector using a bunch of linear combinations of the input:



We can repeat this as many times as we want!

What is the problem with this idea?



Can be expressed as single linear layer!

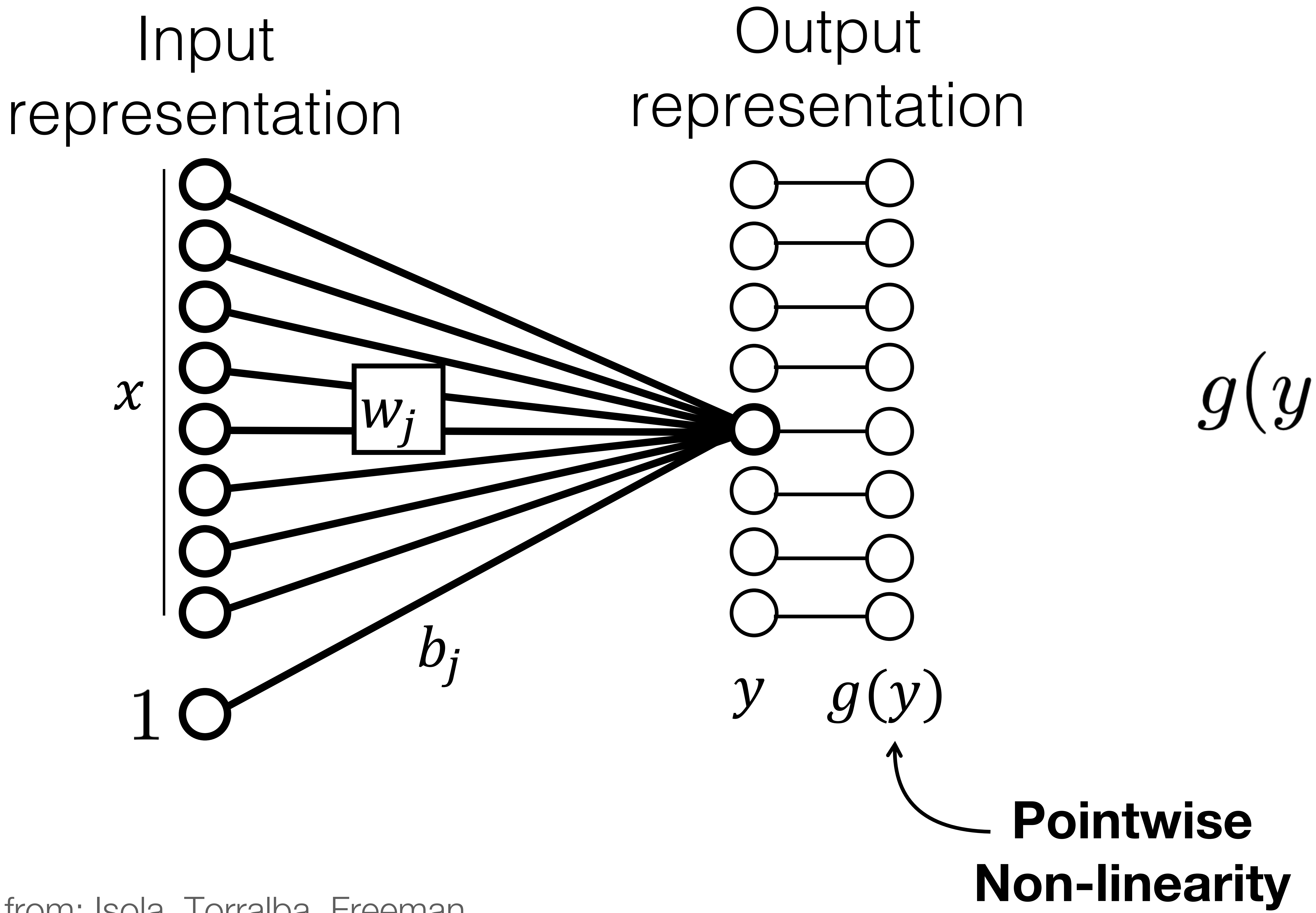
$$\left(\prod_i \mathbf{W}_i\right)\mathbf{x} = \hat{\mathbf{W}}\mathbf{x}$$

Limited power: can't solve XOR :(

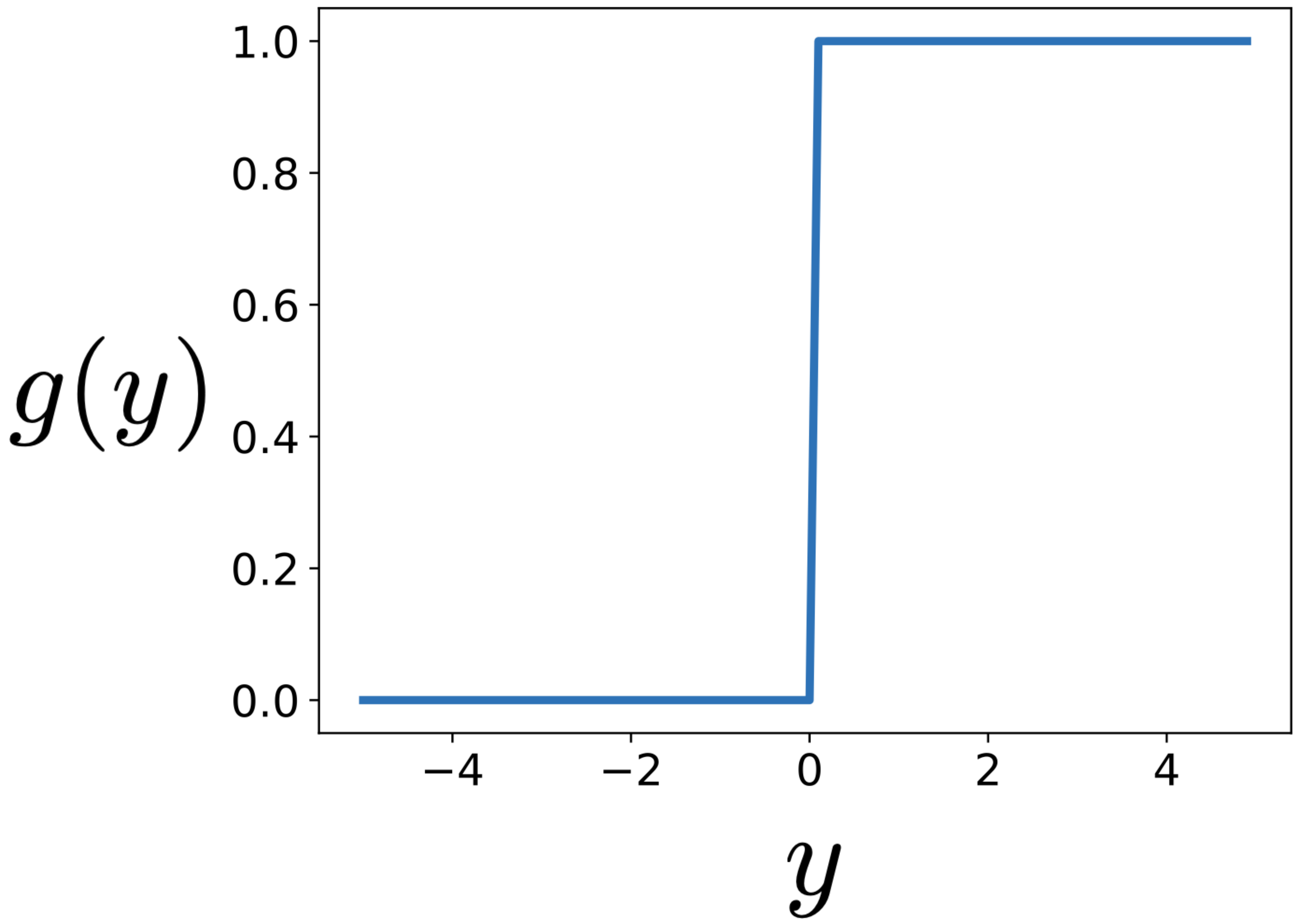
Adapted from: Isola, Torralba, Freeman

Solution: simple nonlinearity

Linear layer

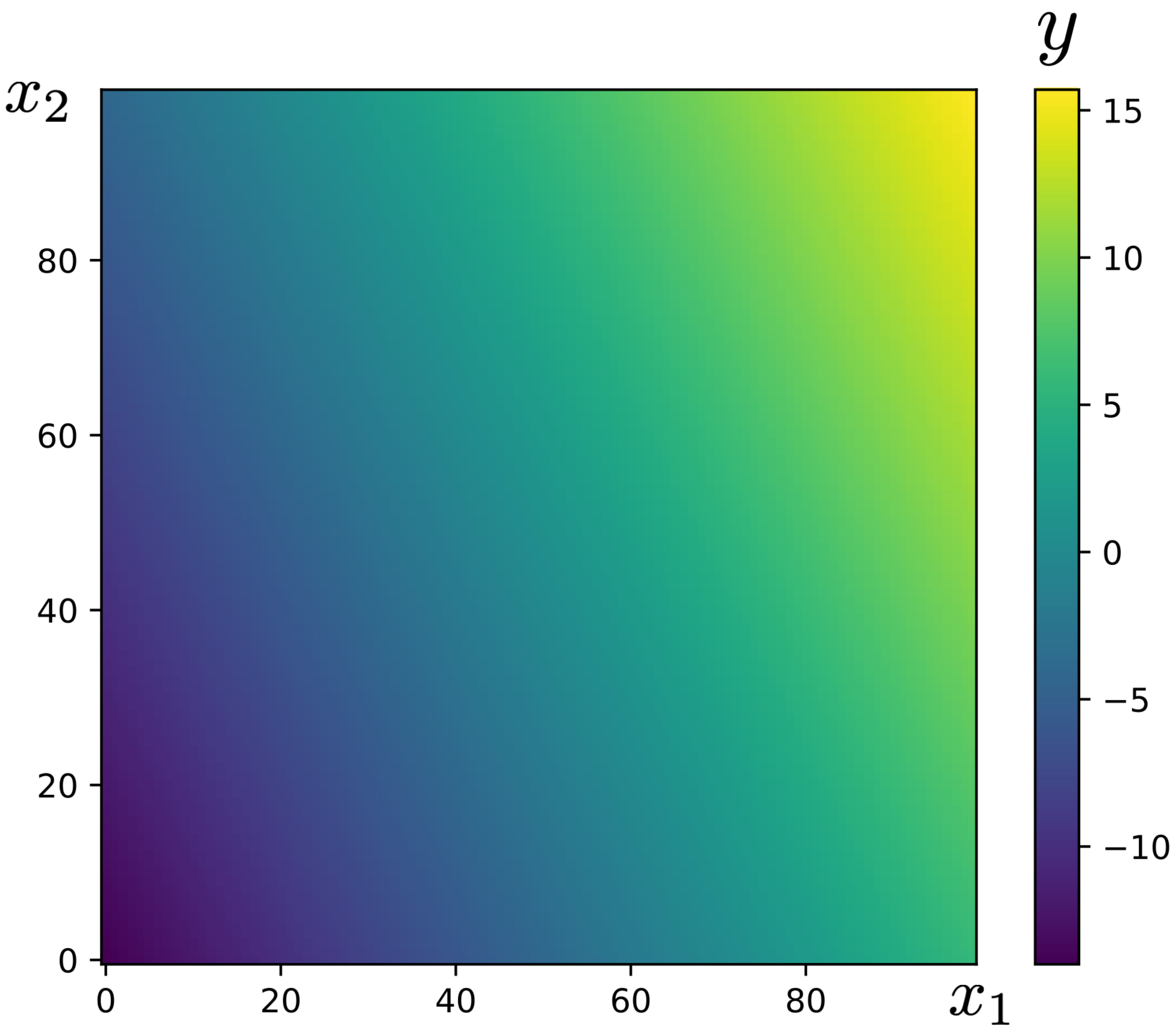


$$g(y) = \begin{cases} 1, & \text{if} \quad y > 0 \\ 0, & \text{otherwise} \end{cases}$$



Adapted from: Isola, Torralba, Freeman

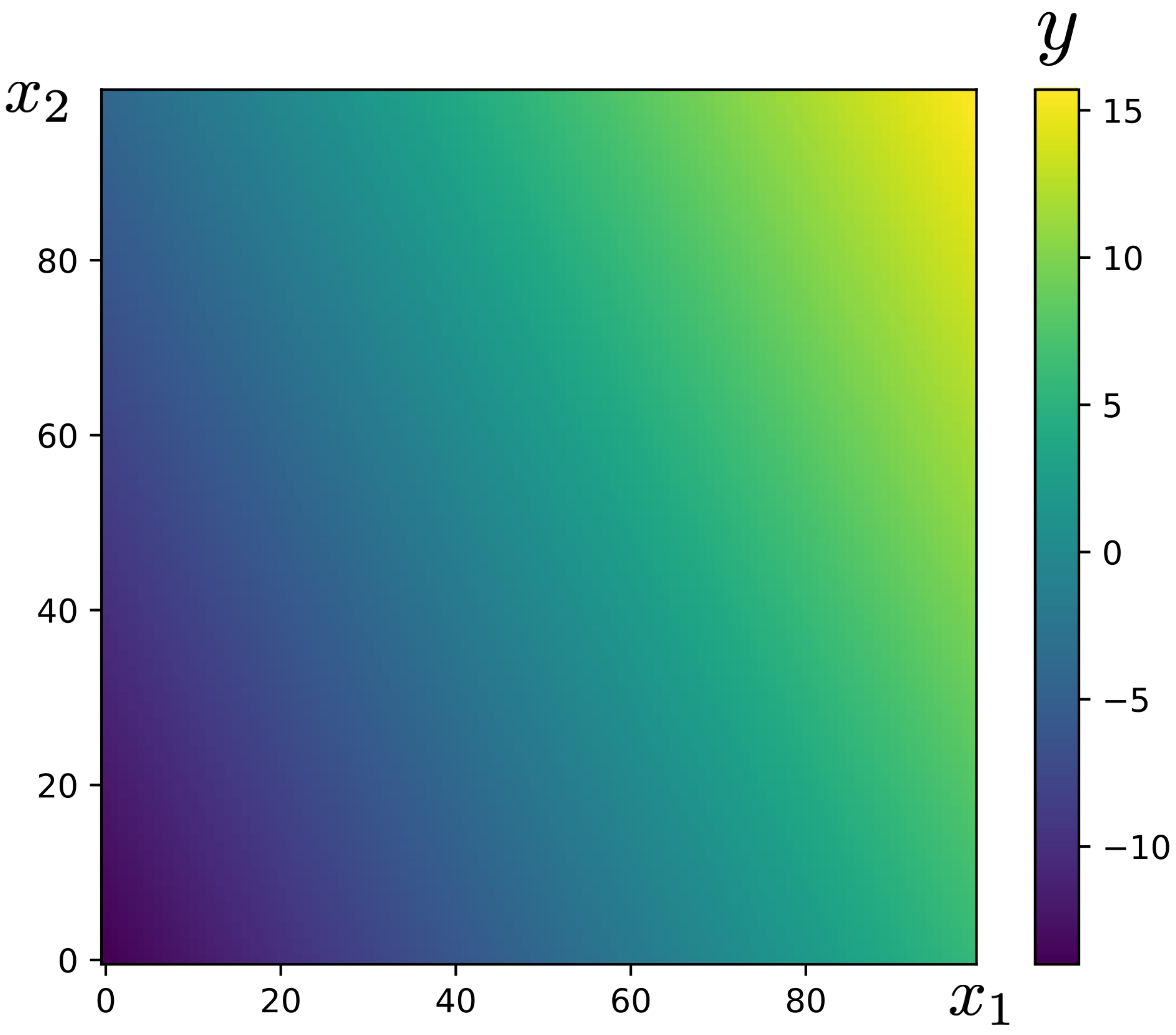
Example: linear classification with a perceptron



$$y = \mathbf{x}^T \mathbf{w} + b$$

Source: Isola, Torralba, Freeman

Example: linear classification with a perceptron



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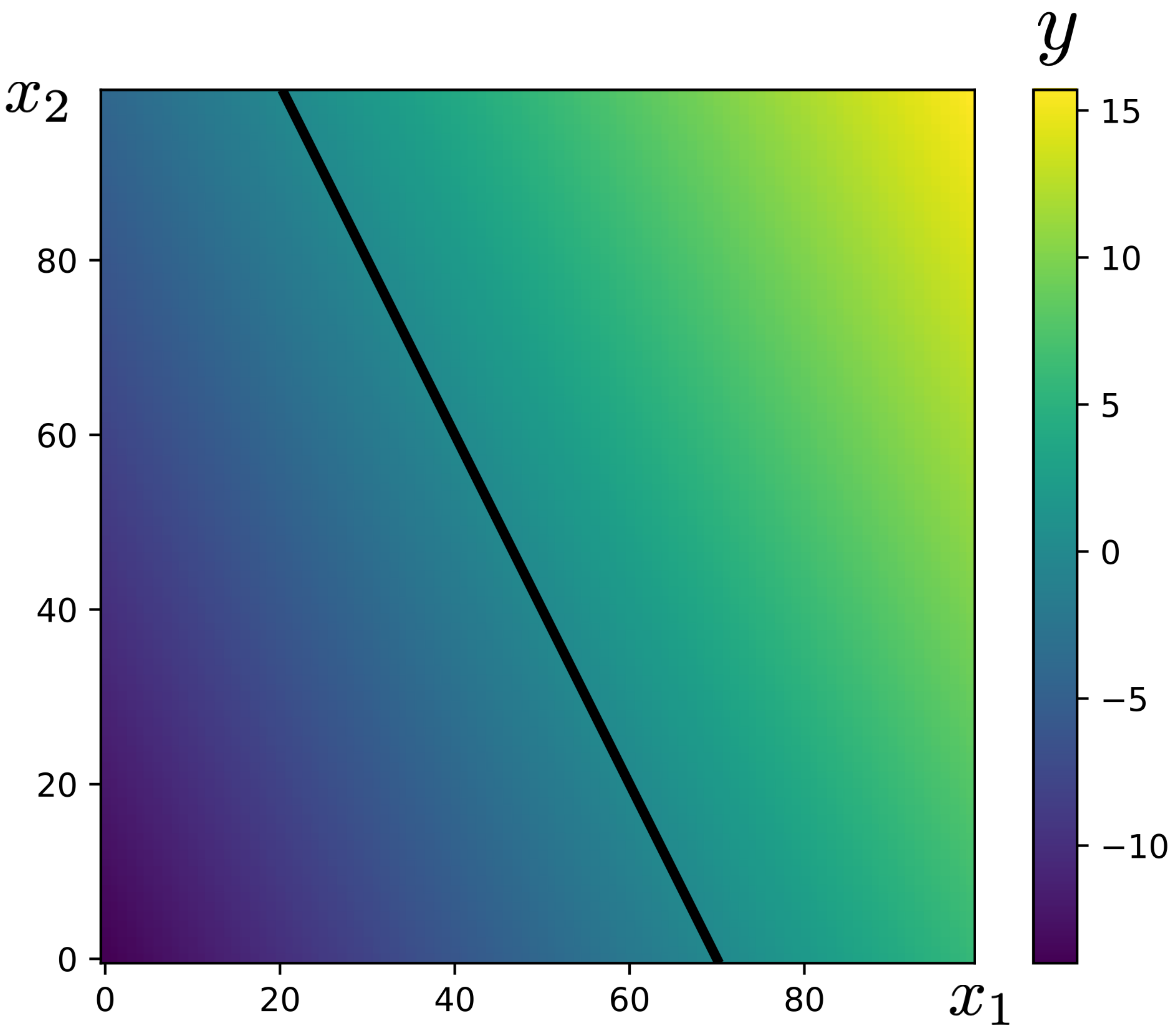
Source: Isola, Torralba, Freeman

Example: linear classification with a perceptron



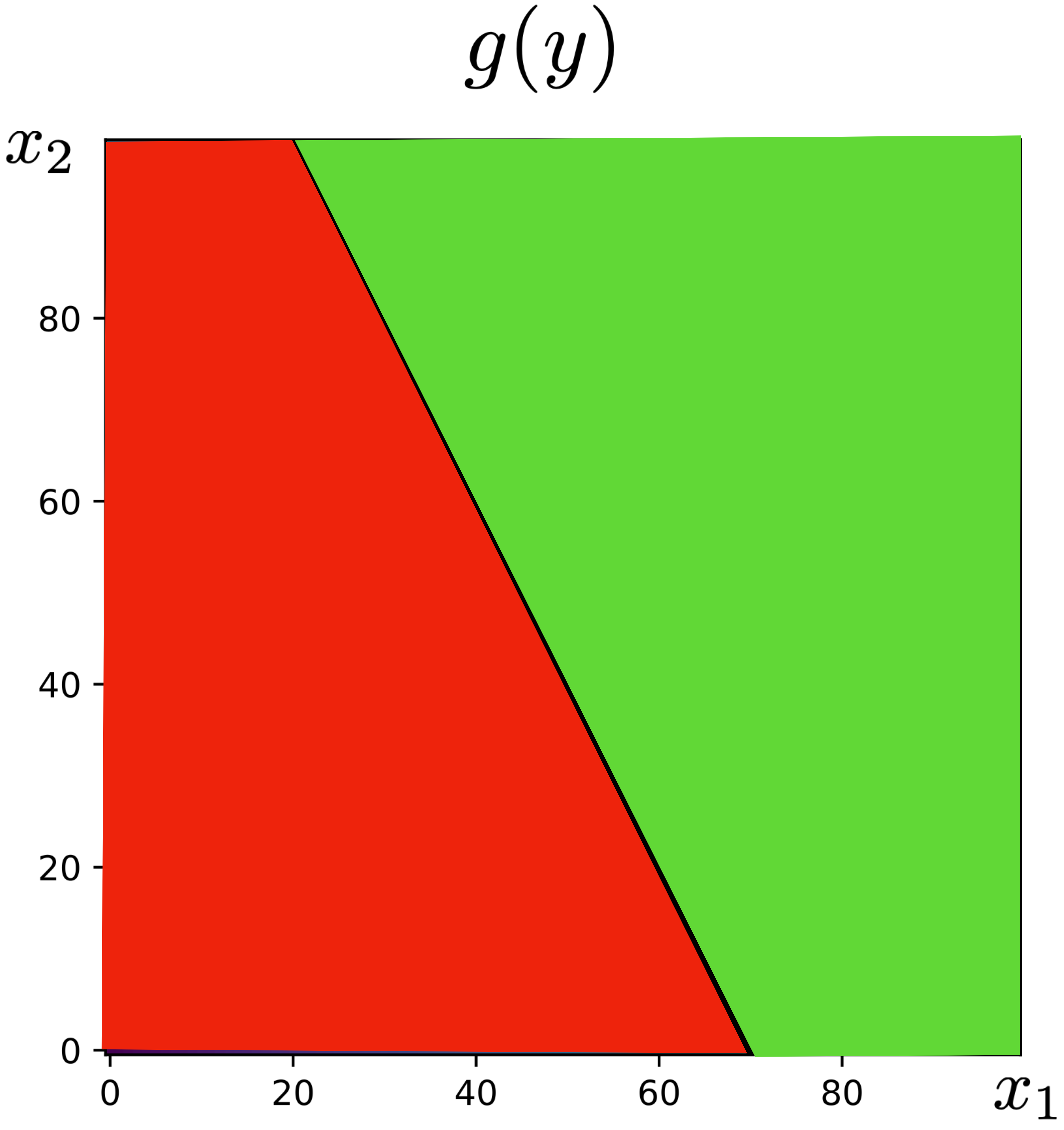
$$y = \mathbf{x}^T \mathbf{w} + b$$

$$g(y) = \begin{cases} 1, & \text{if} \quad y > 0 \\ 0, & \text{otherwise} \end{cases}$$

“when y is greater than 0, set all pixel values to 1 (green), otherwise, set all pixel values to 0 (red)”

Source: Isola, Torralba, Freeman

Example: linear classification with a perceptron



$$y = \mathbf{x}^T \mathbf{w} + b$$

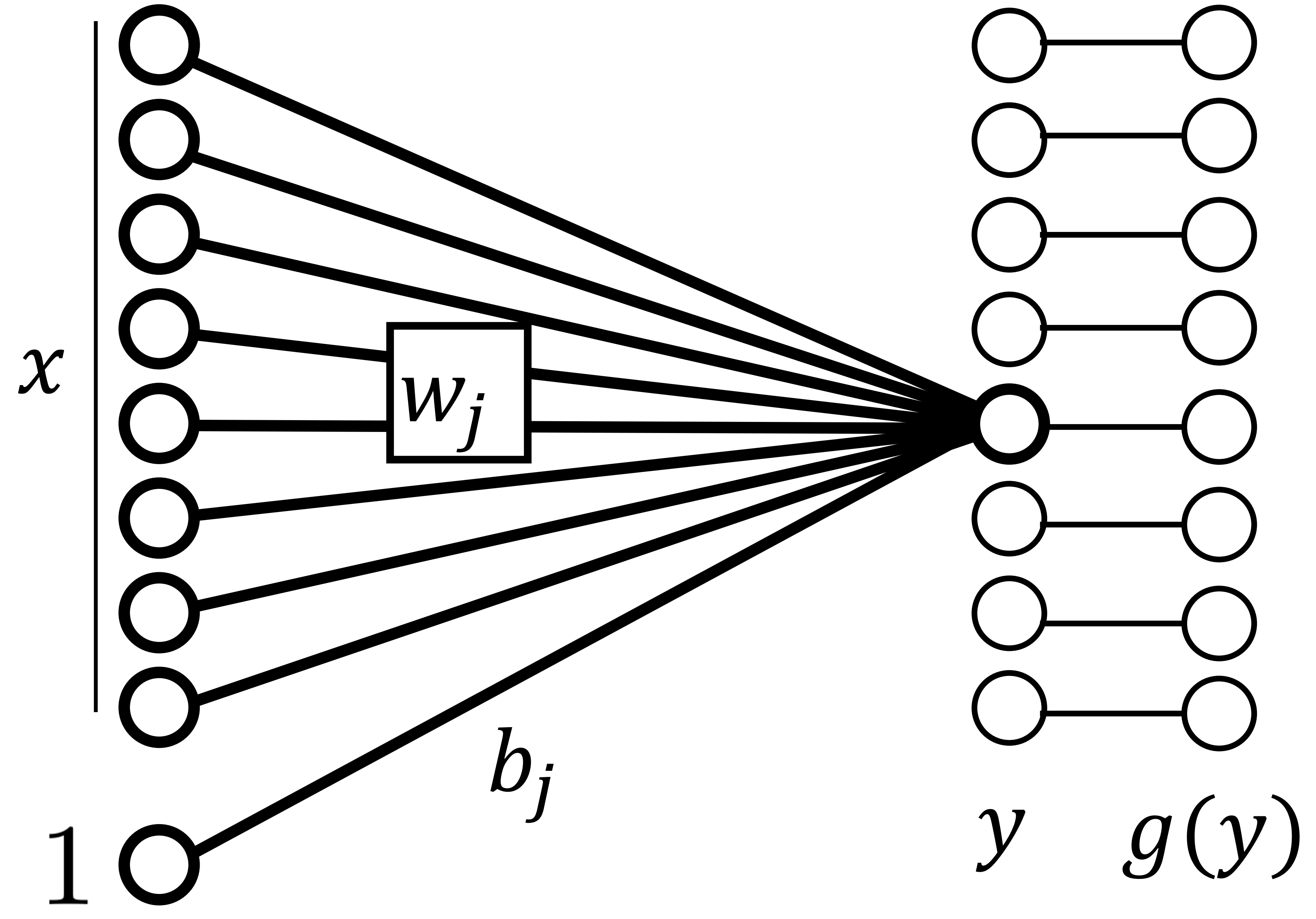
$$g(y) = \begin{cases} 1, & \text{if} \quad y > 0 \\ 0, & \text{otherwise} \end{cases}$$

"when y is greater than 0, set all pixel values to 1 (green), otherwise, set all pixel values to 0 (red)"

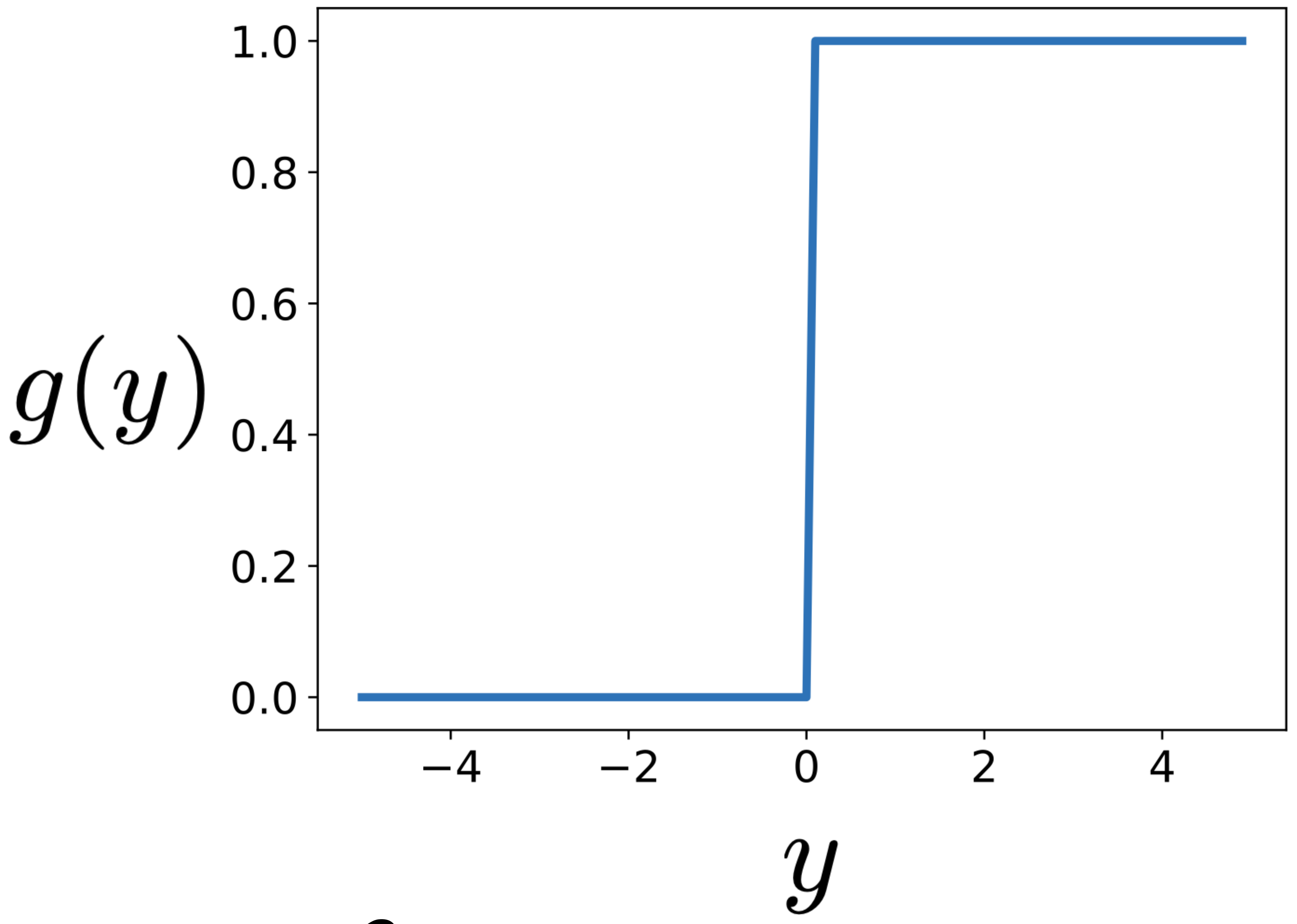
Source: Isola, Torralba, Freeman

Computation in a neural net - nonlinearity

Linear layer



$$g(y) = \begin{cases} 1, & \text{if} \quad y > 0 \\ 0, & \text{otherwise} \end{cases}$$

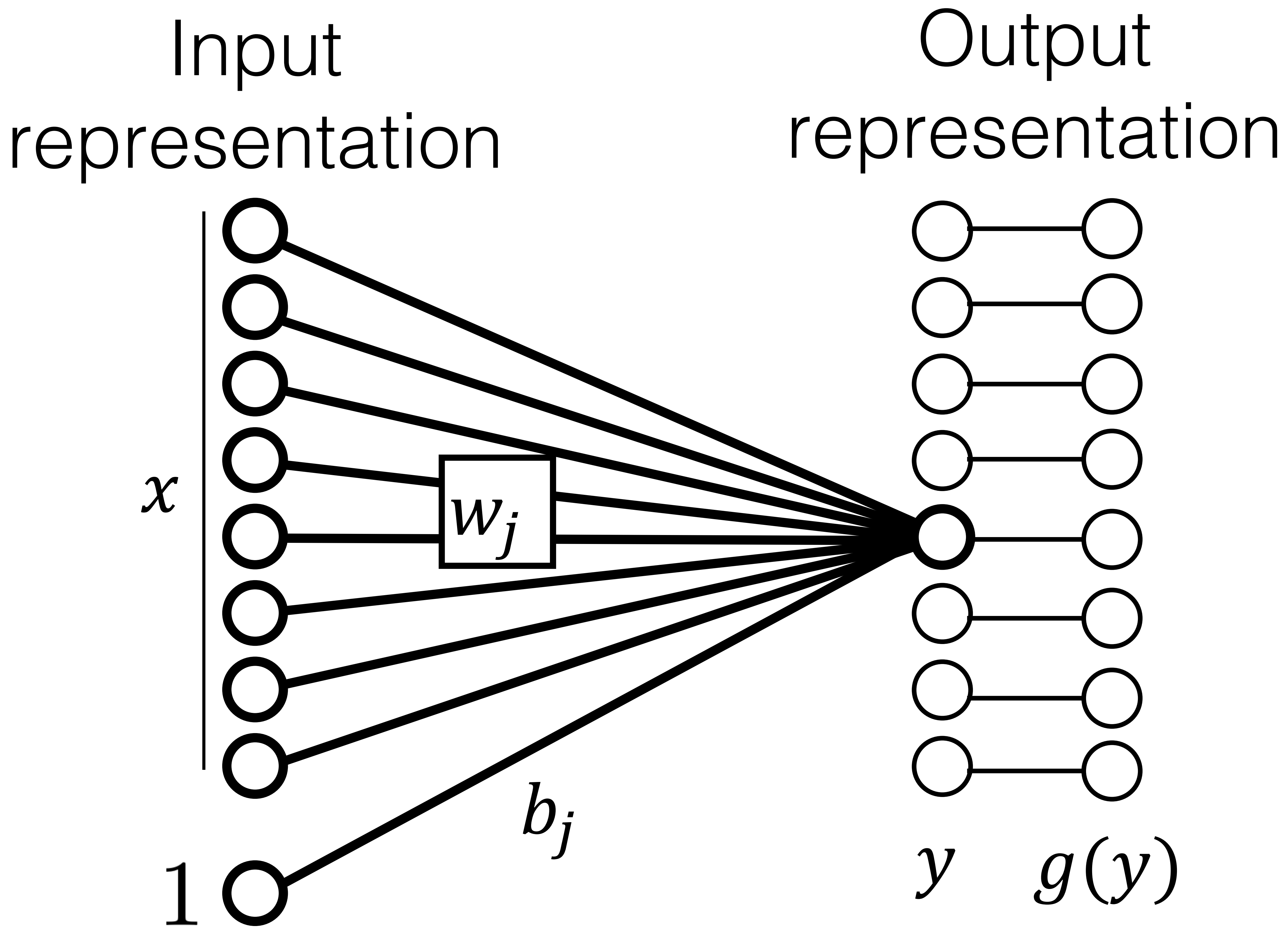


Can't use with gradient descent, $\frac{\partial}{\partial y} g = 0$

Adapted from: Isola, Torralba, Freeman

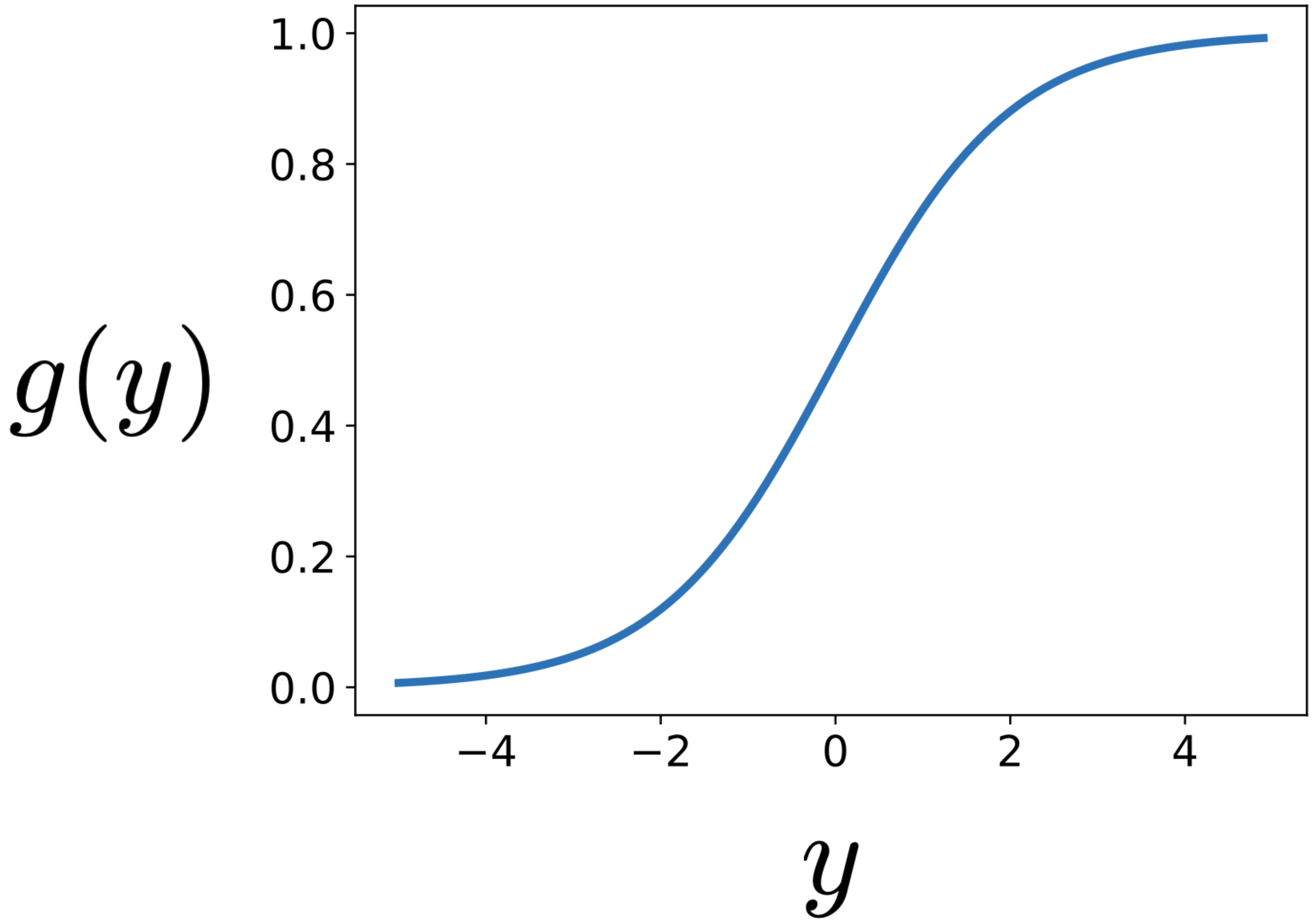
Computation in a neural net - nonlinearity

Linear layer



Sigmoid

$$g(y) = \sigma(y) = \frac{1}{1+e^{-y}}$$



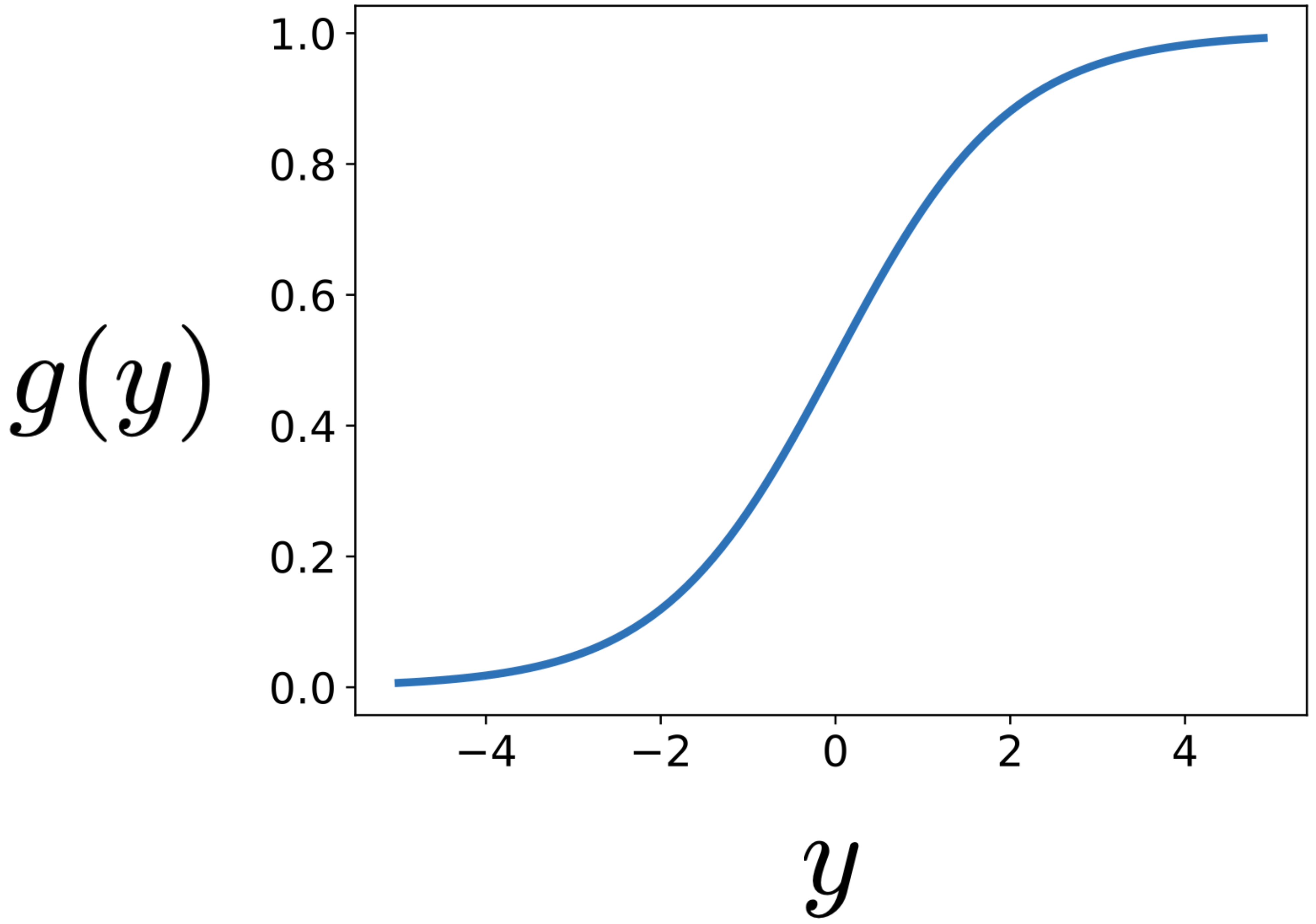
Adapted from: Isola, Torralba, Freeman

Computation in a neural net - nonlinearity

- Bounded between [0,1]
- Saturation for large +/- inputs
- Gradients go to zero
- Better in practice to use: $\tanh(y) = 2g(y) - 1$

Sigmoid

$$g(y) = \sigma(y) = \frac{1}{1+e^{-y}}$$



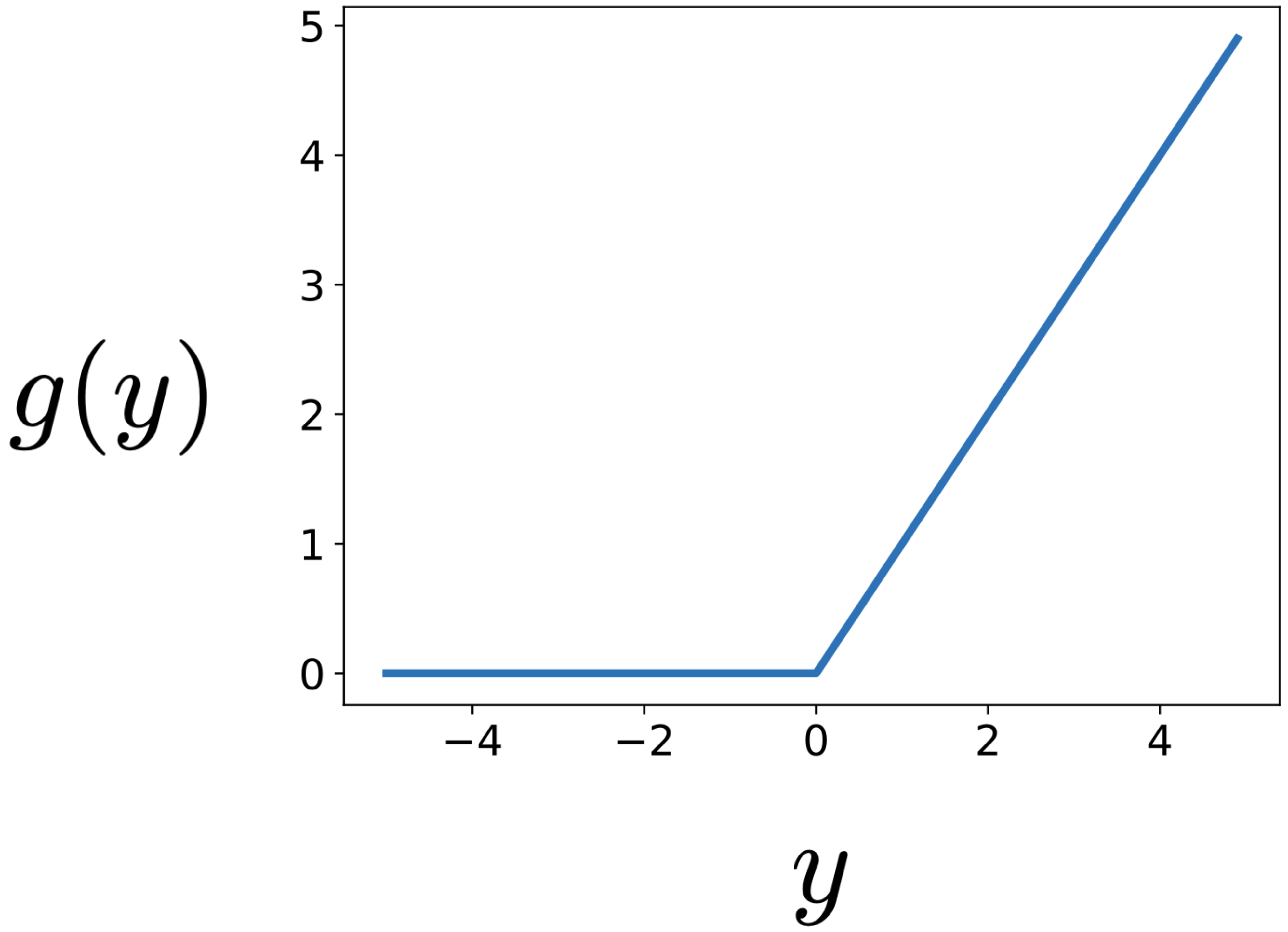
Adapted from: Isola, Torralba, Fre

Computation in a neural net — nonlinearity

- Unbounded output (on positive side)
- Efficient to implement: $\frac{\partial g}{\partial y} = \begin{cases} 0, & \text{if} \quad y < 0 \\ 1, & \text{if} \quad y \geq 0 \end{cases}$
- Also seems to help convergence (6x speedup vs. tanh in [Krizhevsky et al. 2012])
- Drawback: if strongly in negative region, unit is dead forever (no gradient).
- Default choice: widely used in current models!

Rectified linear unit (ReLU)

$$g(y) = \max(0, y)$$

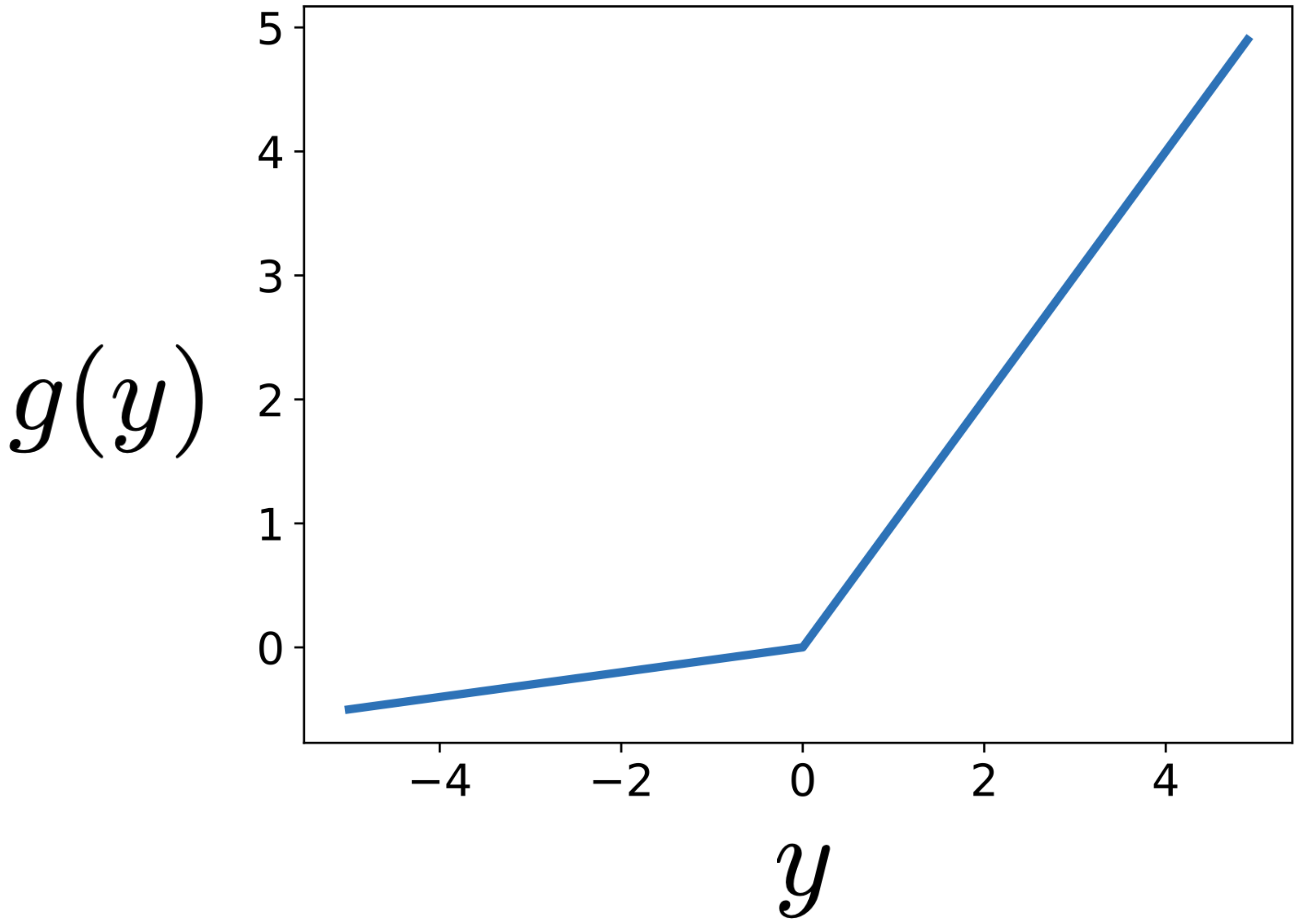


Computation in a neural net — nonlinearity

- where α is small (e.g., 0.02)
- Efficient to implement: $\frac{\partial g}{\partial y} = \begin{cases} -a, & \text{if} \quad y < 0 \\ 1, & \text{if} \quad y \geq 0 \end{cases}$
- Has non-zero gradients everywhere (unlike ReLU)

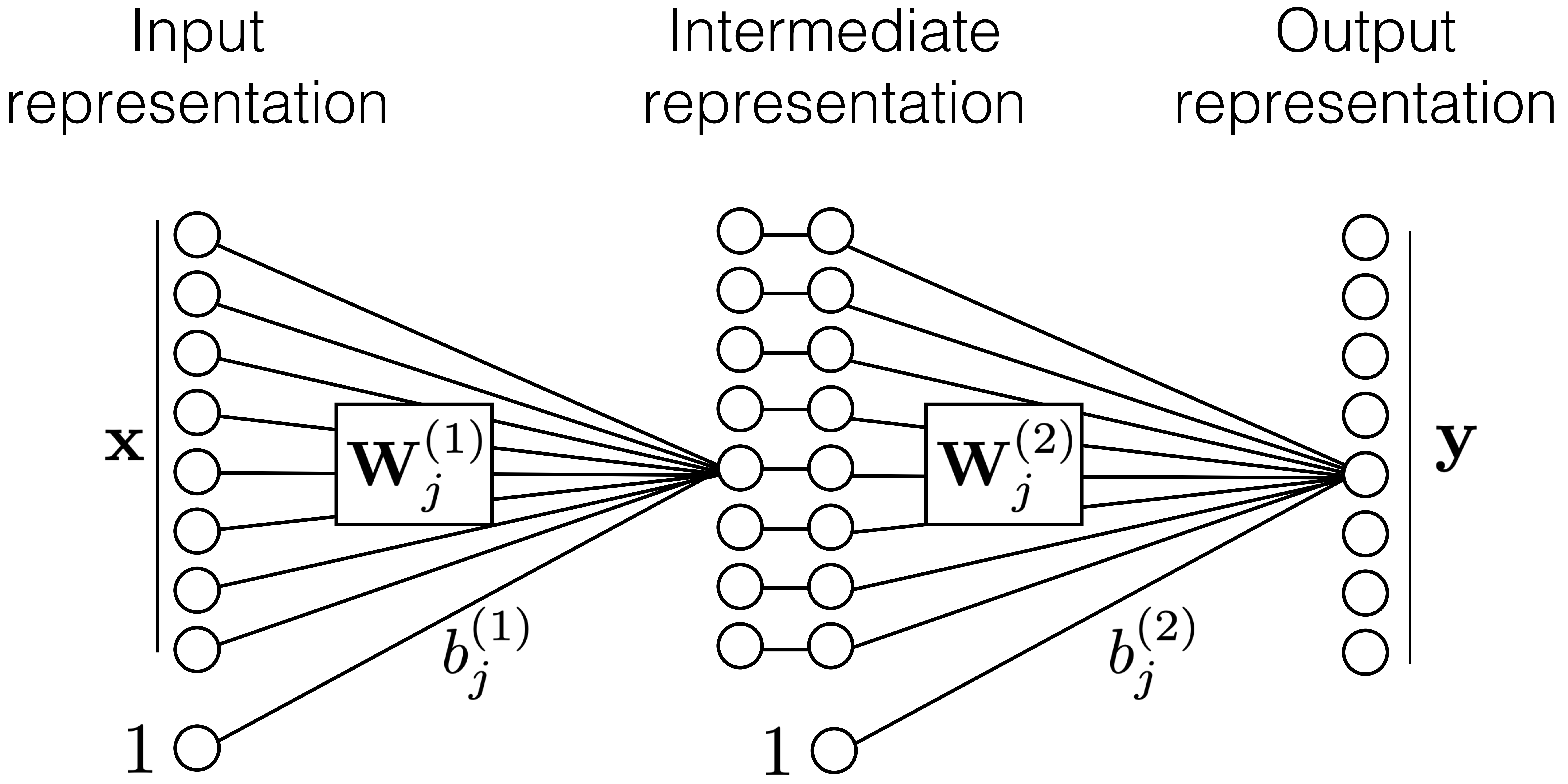
Leaky ReLU

$$g(y) = \begin{cases} \max(0, y), & \text{if} \quad y \geq 0 \\ a \min(0, y), & \text{if} \quad y < 0 \end{cases}$$



Source: Isola, Torralba, Freeman

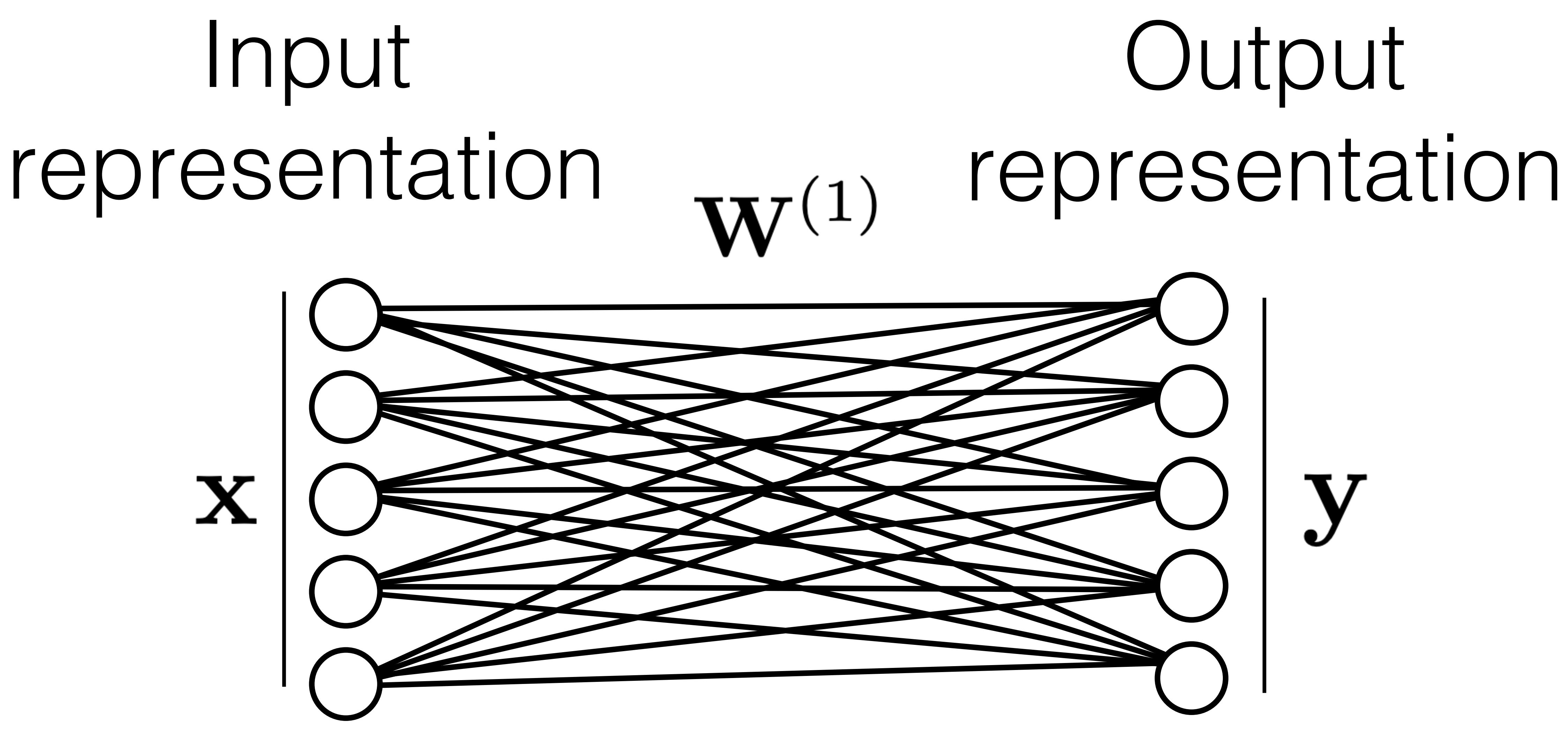
Stacking layers



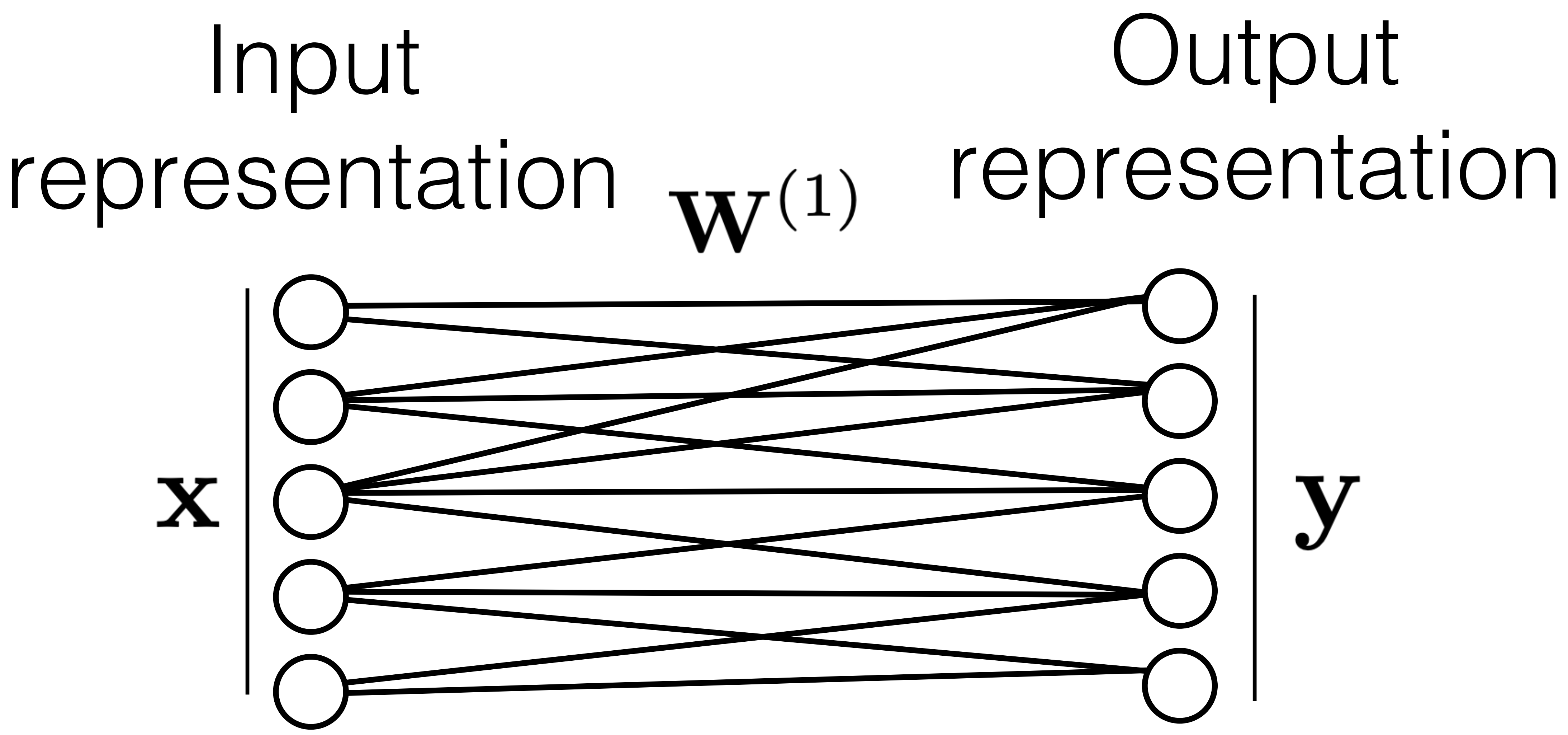
$\mathbf{h}$ = "hidden units"

Adapted from: Isola, Torralba, Freeman

Connectivity patterns



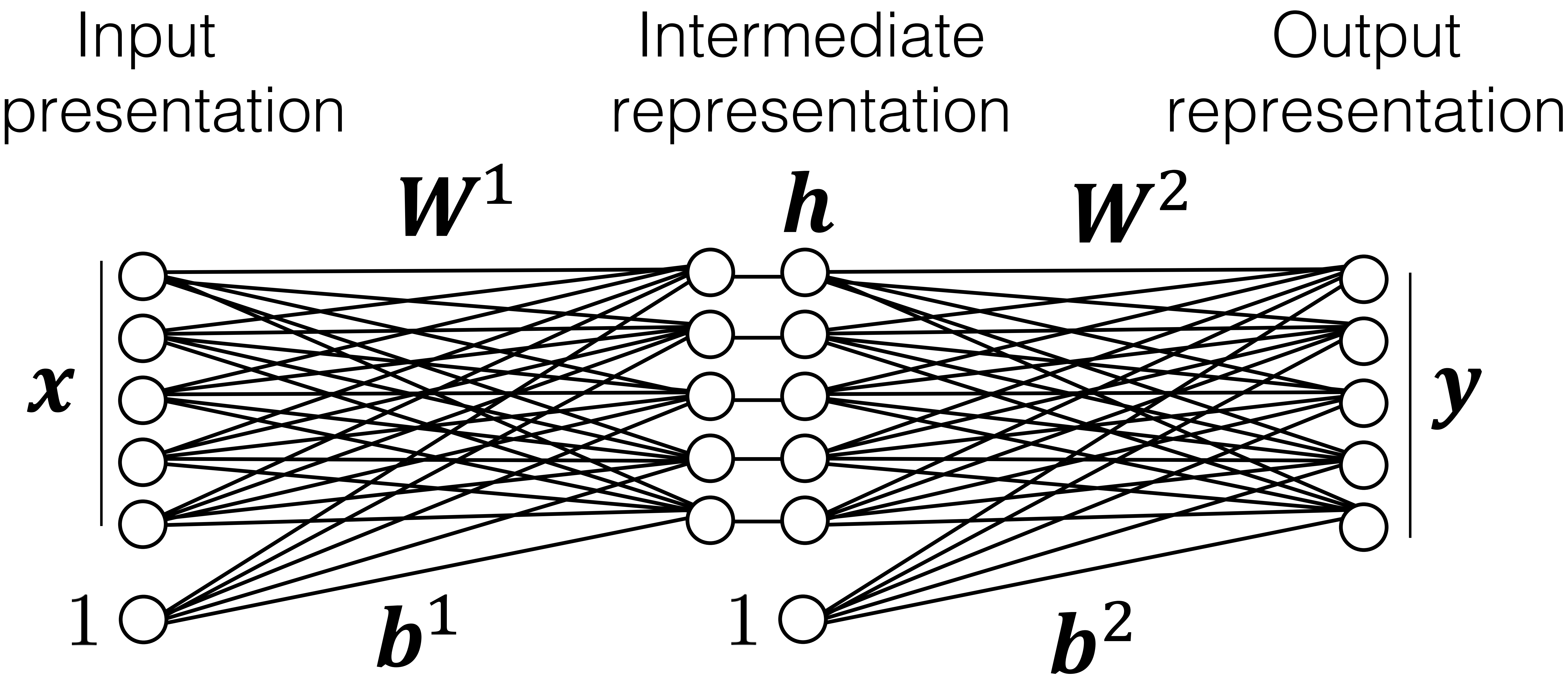
Fully connected layer



Locally connected layer
(Sparse W)

Source: Isola, Torralba, Freeman

Stacking layers



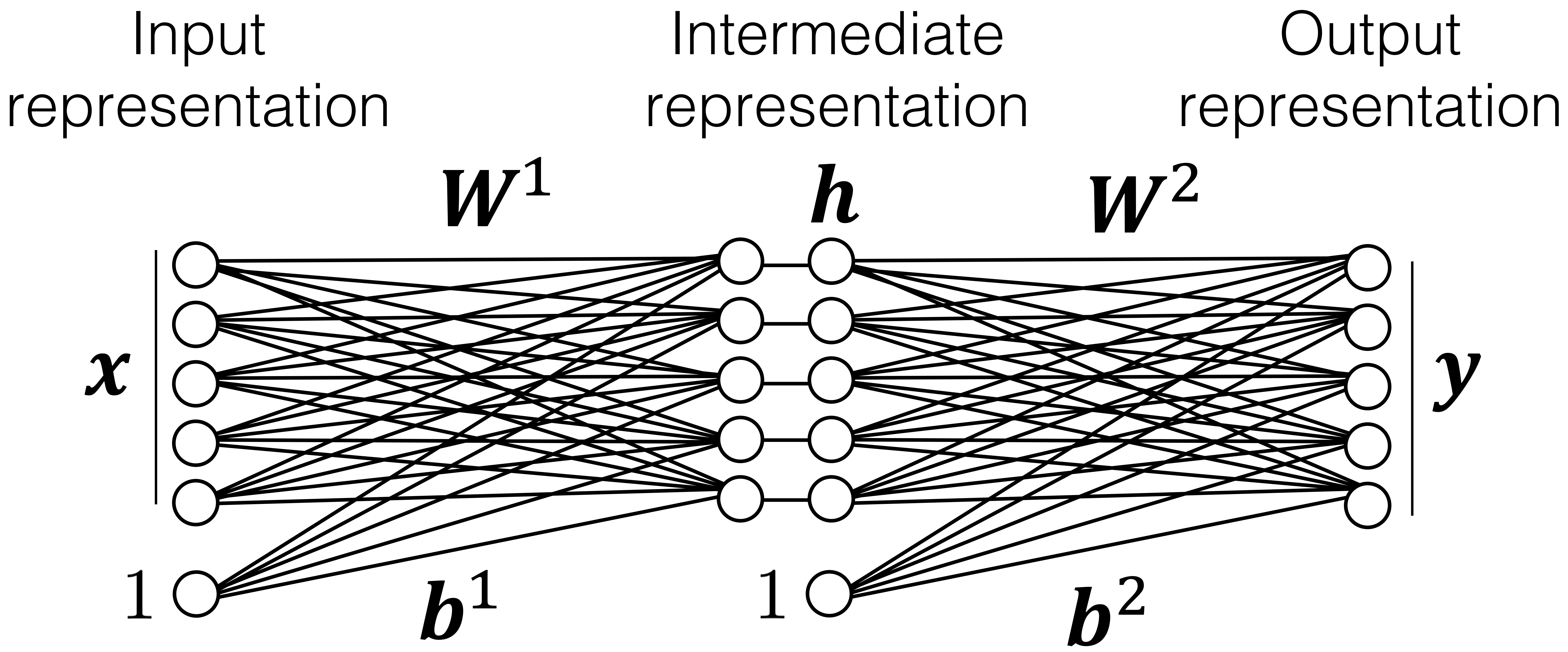
$$\boldsymbol{h} = g(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1) \quad \boldsymbol{y} = g(\boldsymbol{W}^2\boldsymbol{h} + \boldsymbol{b}^2)$$

ReLU

$$\theta = \{\boldsymbol{W}^1, \ldots, \boldsymbol{W}^L, \boldsymbol{b}^1, \ldots, \boldsymbol{b}^L\}$$

Source: Isola, Torralba, Freeman

Stacking layers



positive

negative

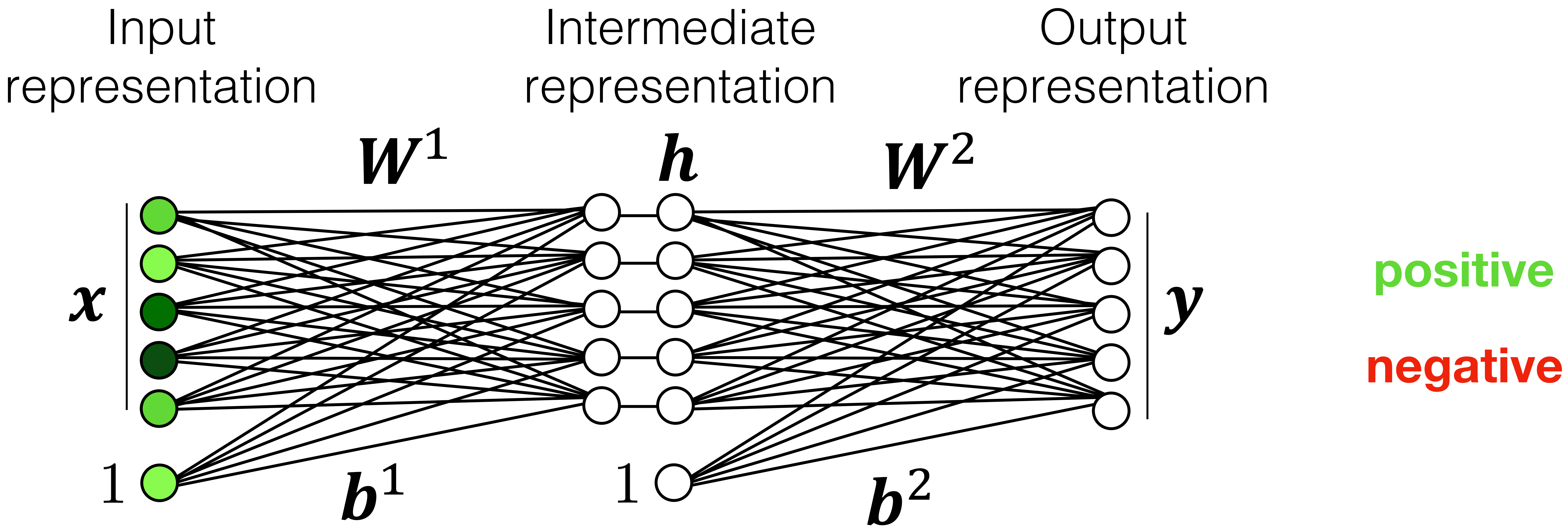
$$\boldsymbol{h} = g(\boldsymbol{W}^1 \boldsymbol{x} + \boldsymbol{b}^1) \qquad \boldsymbol{y} = g(\boldsymbol{W}^2 \boldsymbol{h} + \boldsymbol{b}^2)$$

ReLU

$$\theta = \{\boldsymbol{W}^1, \ldots, \boldsymbol{W}^L, \boldsymbol{b}^1, \ldots, \boldsymbol{b}^L\}$$

Source: Isola, Torralba, Freeman

Stacking layers



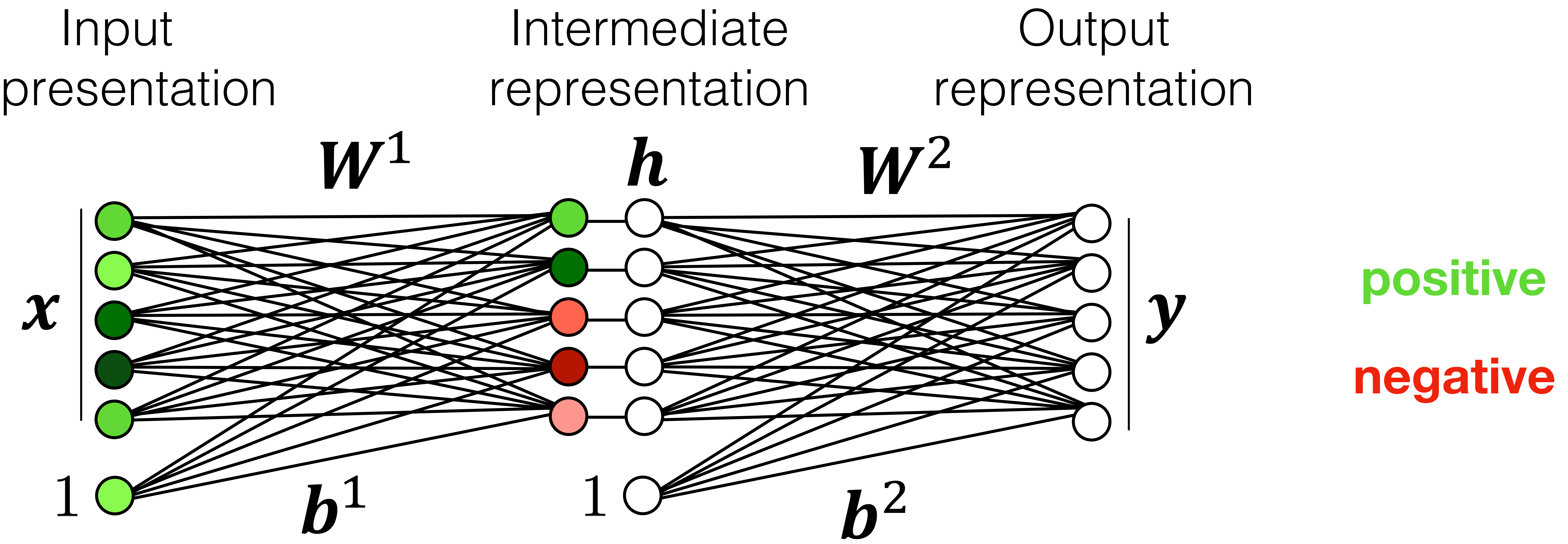
$$h = g(W^1 x + b^1) \quad y = g(W^2 h + b^2)$$

ReLU

$$\theta = \{W^1, \ldots, W^L, b^1, \ldots, b^L\}$$

Source: Isola, Torralba, Freeman

Stacking layers



$$\boldsymbol{h} = g(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1) \quad \boldsymbol{y} = g(\boldsymbol{W}^2\boldsymbol{h} + \boldsymbol{b}^2)$$

ReLU

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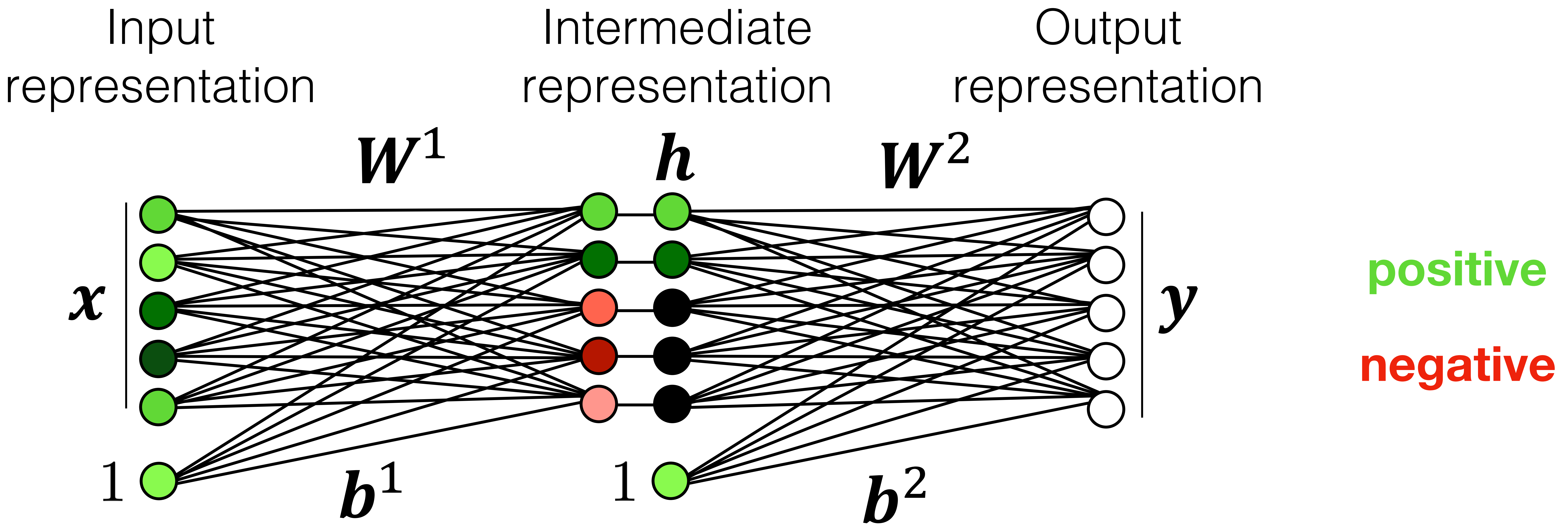
Stacking layers



$$\boldsymbol{h} = g(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1) \quad \boldsymbol{y} = g(\boldsymbol{W}^2\boldsymbol{h} + \boldsymbol{b}^2)$$

ReLU

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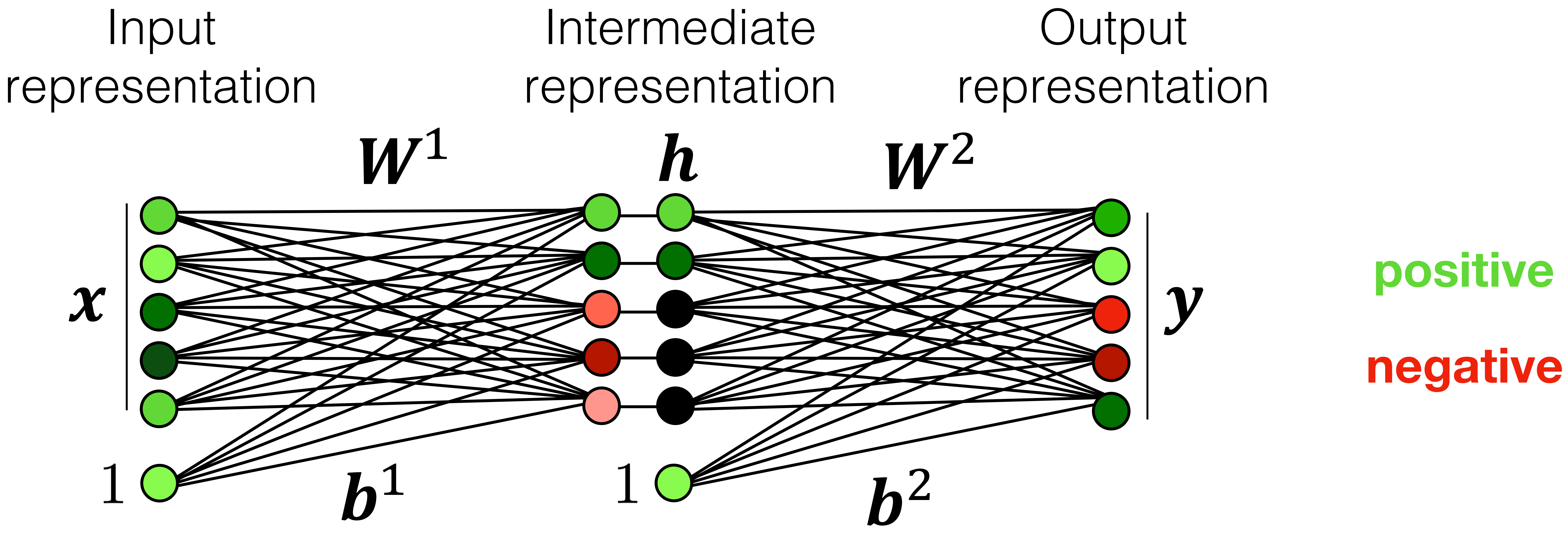
Source: Isola, Torralba, Freeman

Stacking layers



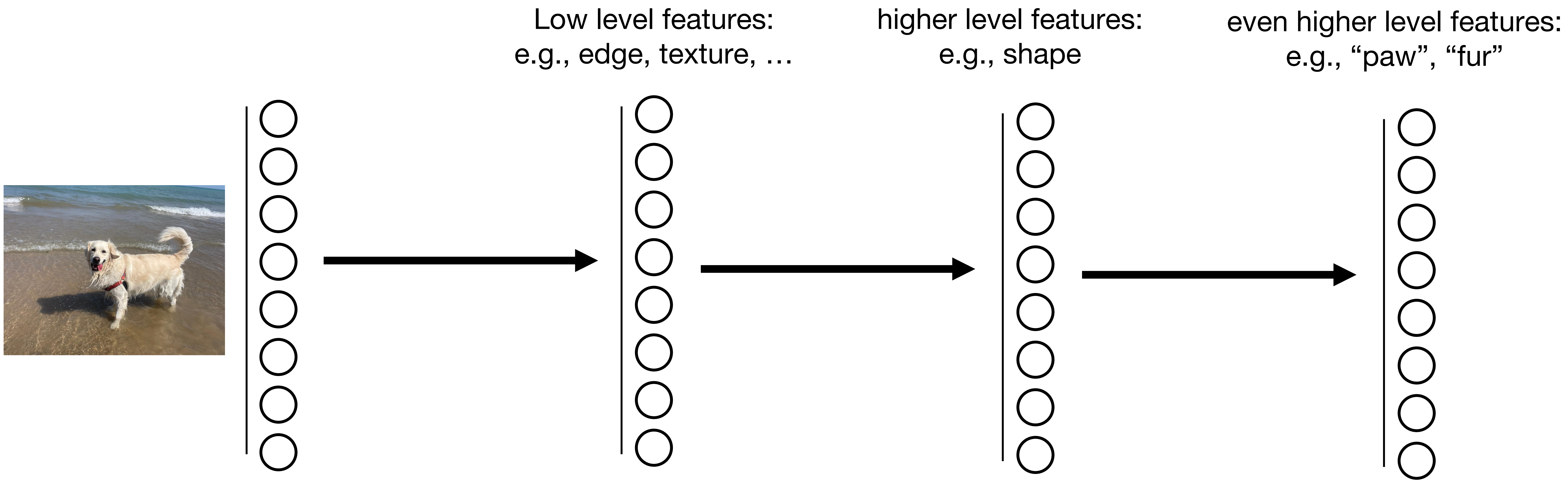
$$\boldsymbol{h} = g(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1) \quad \boldsymbol{y} = g(\boldsymbol{W}^2\boldsymbol{h} + \boldsymbol{b}^2)$$

ReLU

$$\theta = \{\boldsymbol{W}^1, \ldots, \boldsymbol{W}^L, \boldsymbol{b}^1, \ldots, \boldsymbol{b}^L\}$$

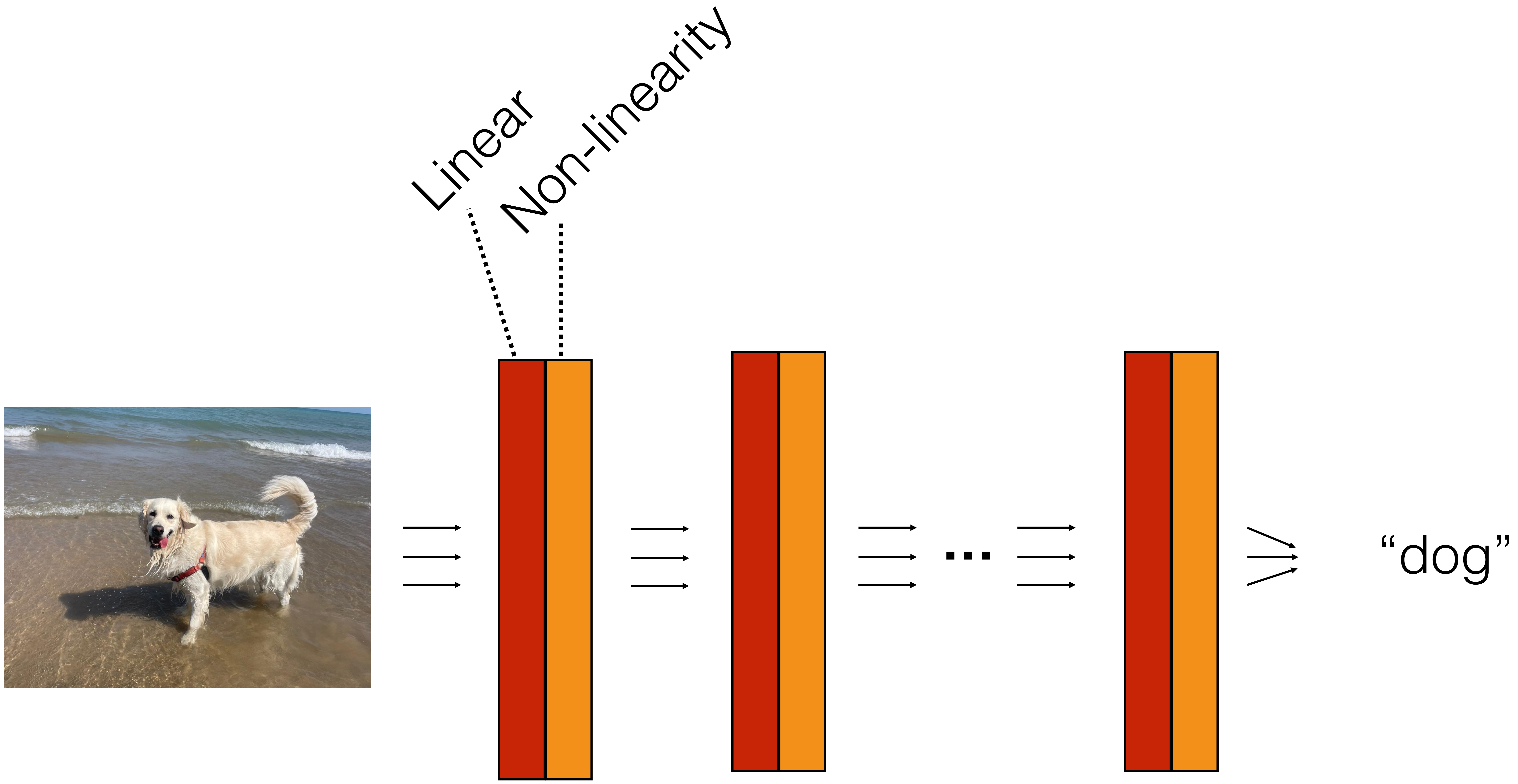
Source: Isola, Torralba, Freeman

Stacking layers - What's actually happening?



Source: Isola, Torralba, Freeman

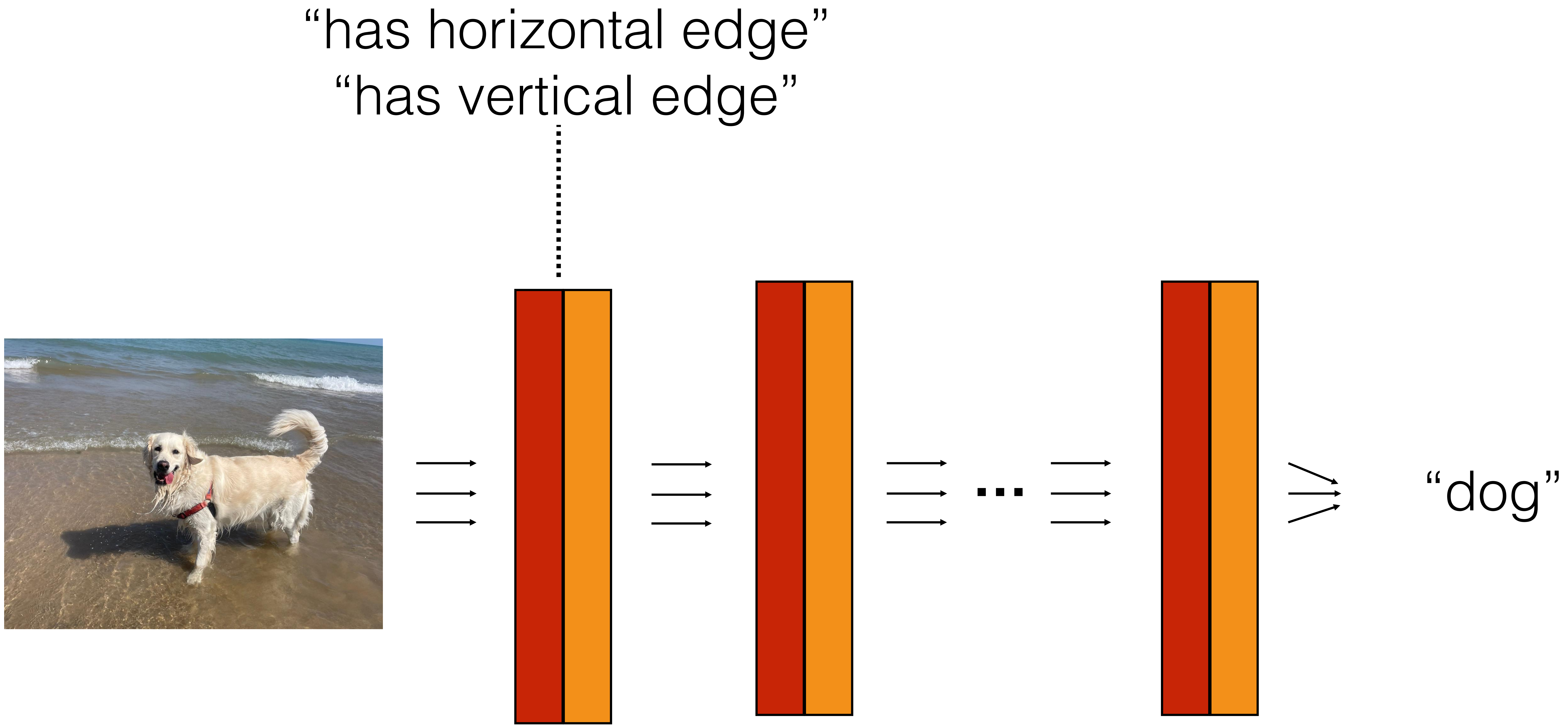
Deep nets



$$f(x) = f_L(\ldots f_3(f_2(f_1(x))))$$

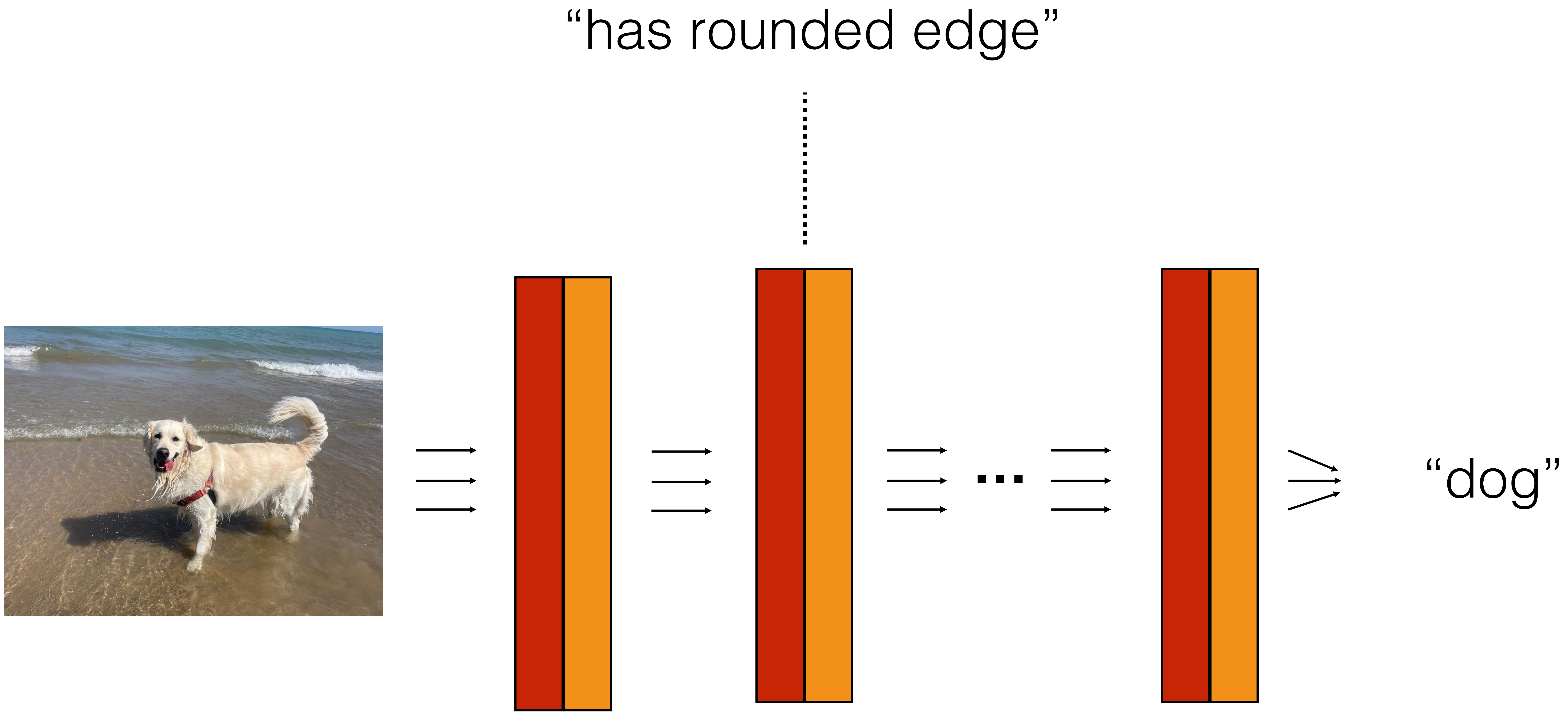
Source: Isola, Torralba, Freeman

Deep nets - Intuition



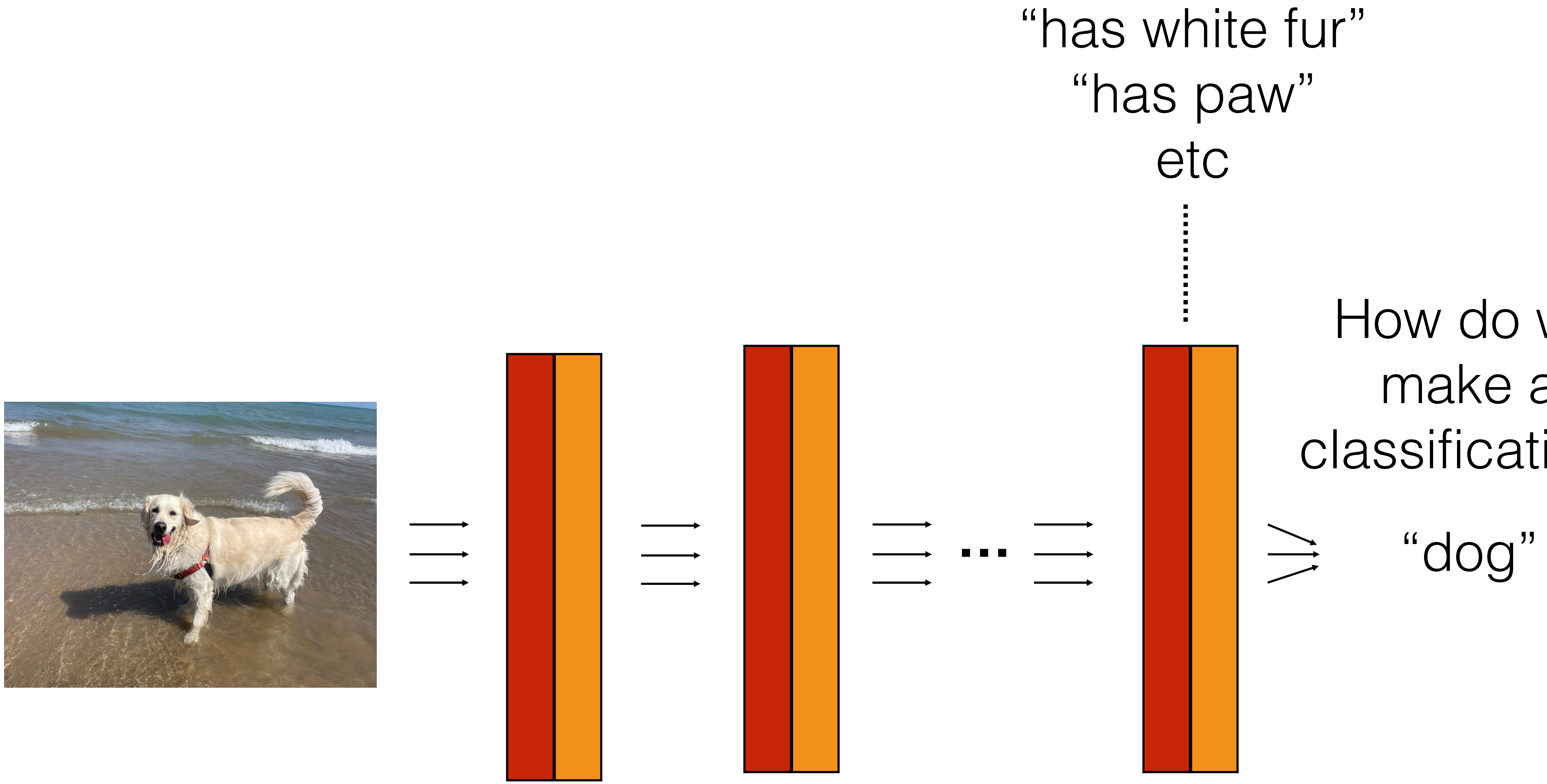
Source: Isola, Torralba, Freeman

Deep nets - Intuition



Source: Isola, Torralba, Freeman

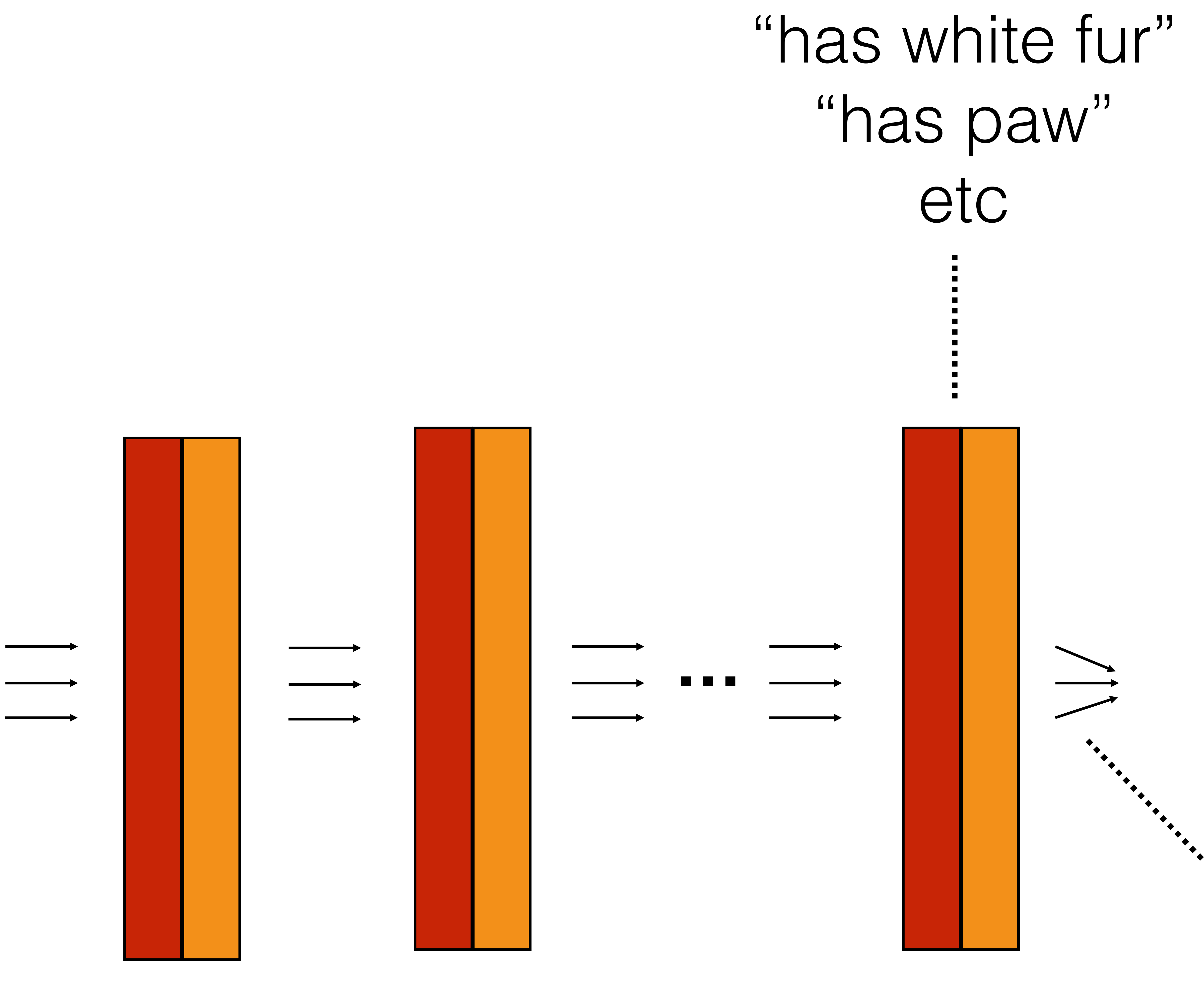
Deep nets - Intuition

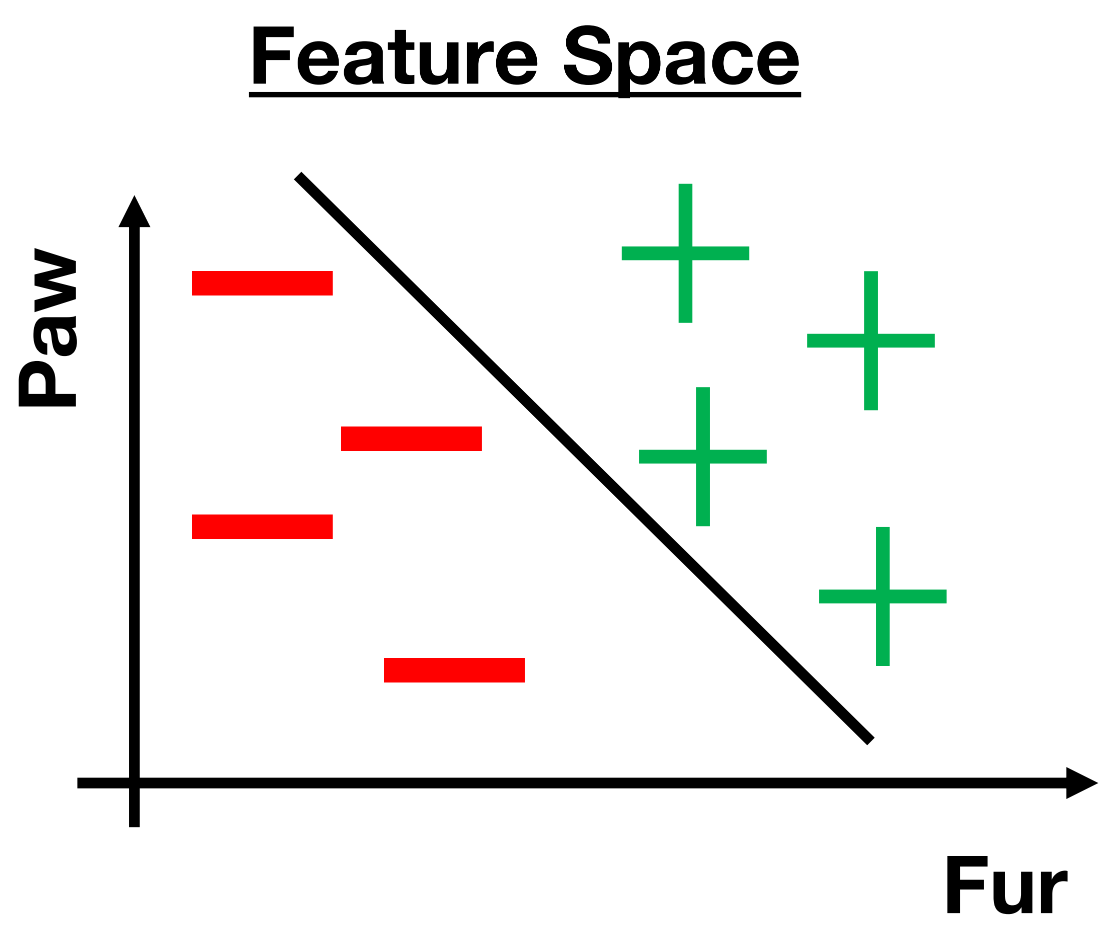


How do we make a classification?

Deep nets - Intuition

Recall:





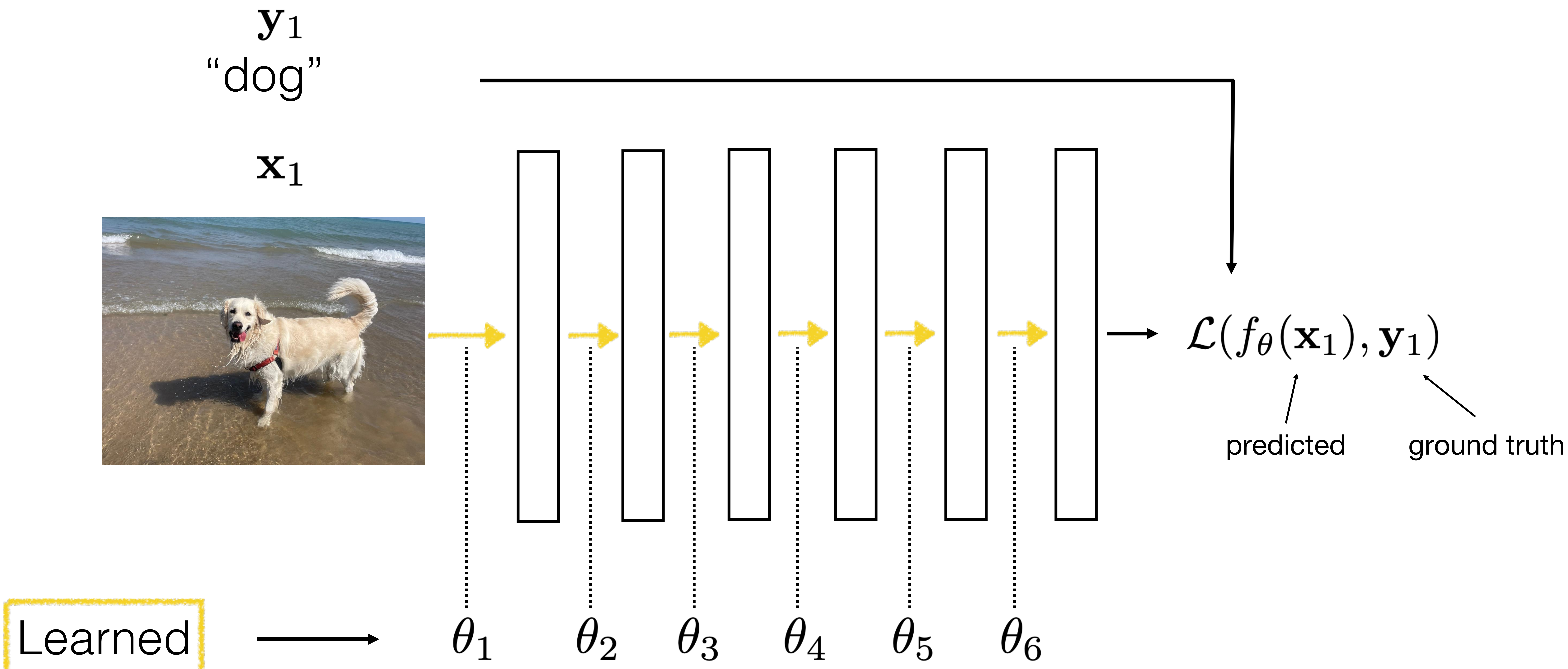
Source: Isola, Torralba, Freeman

Computation has a simple form

- Composition of linear functions with nonlinearities in between
- E.g. matrix multiplications with ReLU, $max(0, \mathbf{x})$ afterwards
- Do a matrix multiplication, set all negative values to 0, repeat

But where do we get the weights from?

How do we learn the parameters?



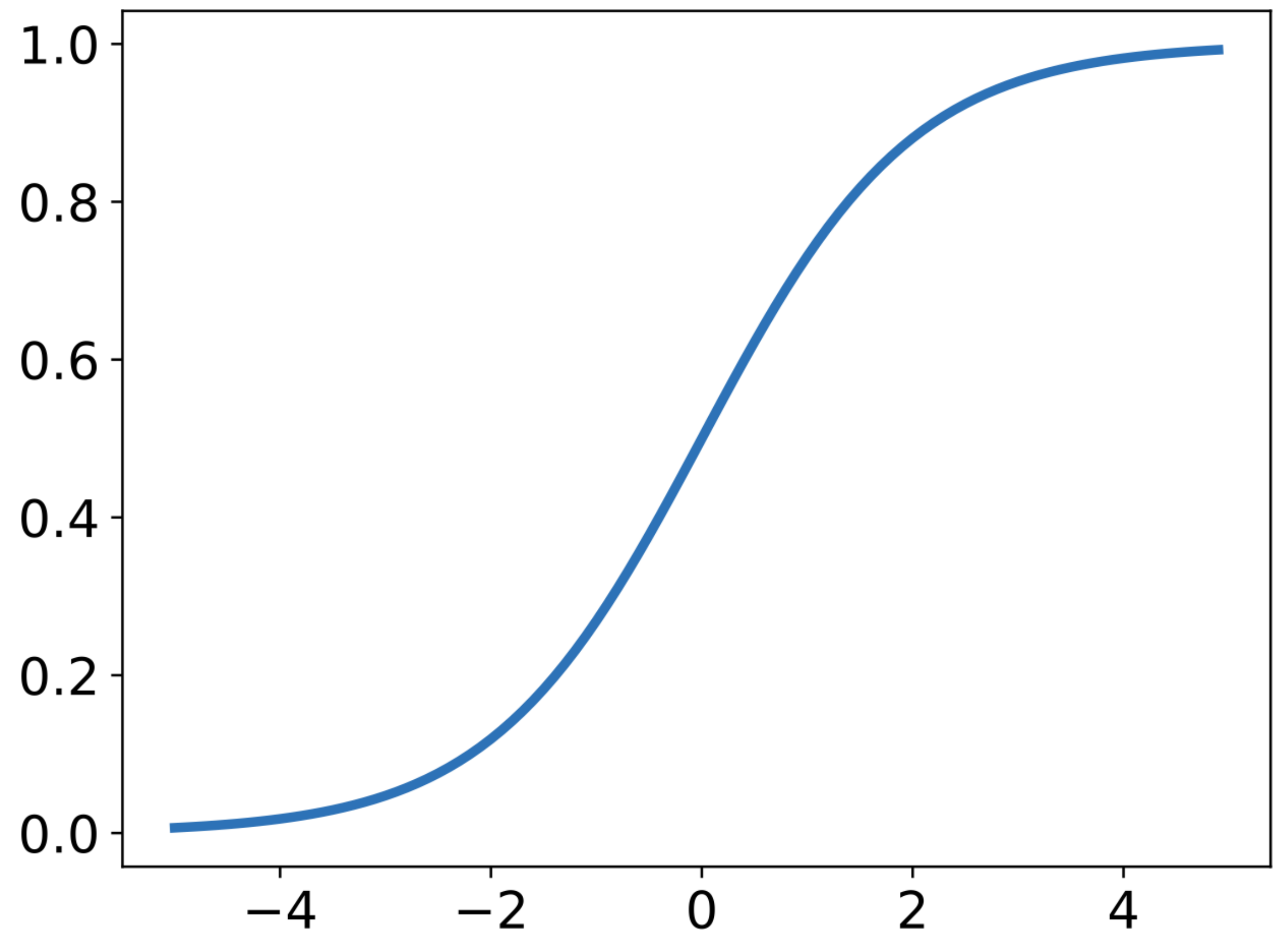
$$\boxed{\theta^* = \arg\min_\theta \sum_{i=1}^{N} \mathcal{L}(f_\theta(\mathbf{x}_i), \mathbf{y}_i)}$$

Source: Isola, Torralba, Freeman

Learning parameters

Squared loss with single-variable network:

$$\sigma(y) = \frac{1}{1+e^{-y}}$$



$$L = \frac{1}{2}(y - f(x))^2$$

$$L = \frac{1}{2}(y - \sigma(wx + b))^2$$

Want: derivatives $\frac{\partial L}{\partial w}, \frac{\partial L}{\partial b}$

X

Example source: Roger Grosse

Computing derivatives with the chain rule

Given: $L = \frac{1}{2}(y - \sigma(wx + b))^2$

Writing out the layers explicitly:

$$z = wx + b$$

$$t = \sigma(\mathrm{z})$$

$$L = \frac{1}{2}(y - t)^2$$

$$\rightarrow \frac{\partial L}{\partial w} = \frac{\partial L}{\partial t}\frac{\partial t}{\partial z}\frac{\partial z}{\partial w}$$

Example source: Roger Grosse

Computing derivatives with the chain rule

$$\frac{\partial L}{\partial w} = \frac{\partial}{\partial w}\left[\frac{1}{2}(y - \sigma(wx + b))^2\right]$$

$$= (y - \sigma(wx + b))\frac{\partial}{\partial w}(y - \sigma(wx + b))$$

$$= (y - \sigma(wx + b))\sigma'(wx + b)\frac{\partial}{\partial w}(wx + b)$$

$$= (y - \sigma(wx + b))\sigma'(wx + b)x$$

$$\frac{\partial L}{\partial b} = \frac{\partial}{\partial b}\left[\frac{1}{2}(y - \sigma(wx + b))^2\right]$$

$$= (y - \sigma(wx + b))\frac{\partial}{\partial b}(y - \sigma(wx + b))$$

$$= (y - \sigma(wx + b))\sigma'(wx + b)\frac{\partial}{\partial b}(wx + b)$$

$$= (y - \sigma(wx + b))\sigma'(wx + b)$$

Note: For each of these derivatives, you’ll have to compute many things multiple times!

Example source: Roger Grosse

Limitations to this approach

- Inefficient! Lots of redundant computation
- We'll also need to extend this to multivariable functions
- **Next lecture:** backpropagation

Representational power

- 1 layer? Linear decision surface.
- 2+ layers? In theory, can represent any function! (if it was infinitely wide with infinite data)
  - Simple proof by M. Nielsen http://neuralnetworksanddeeplearning.com/chap4.html
- But issue is efficiency: very wide two layers vs narrow deep model? In practice, more layers helps.

Source: Isola, Torralba, Freeman

Backup Slides

Sigmoid vs. Softmax

Softmax outputs a probability distribution over all predicted classes:

$$\underset{\text{Input vector}}{\overset{\mathrm{X}}{\begin{bmatrix} 3 \\ 1.75 \\ -2 \\ 0.5 \end{bmatrix}}} \xrightarrow[\frac{e^{x_i}}{\sum_{j=1}^{K} e^{x_j}}]{\text{SoftMax}} \underset{\text{Output vector}}{\overset{\mathrm{Out}}{\begin{bmatrix} 0.725 \\ 0.21 \\ 0.005 \\ 0.06 \end{bmatrix}}}$$

Probability distribution

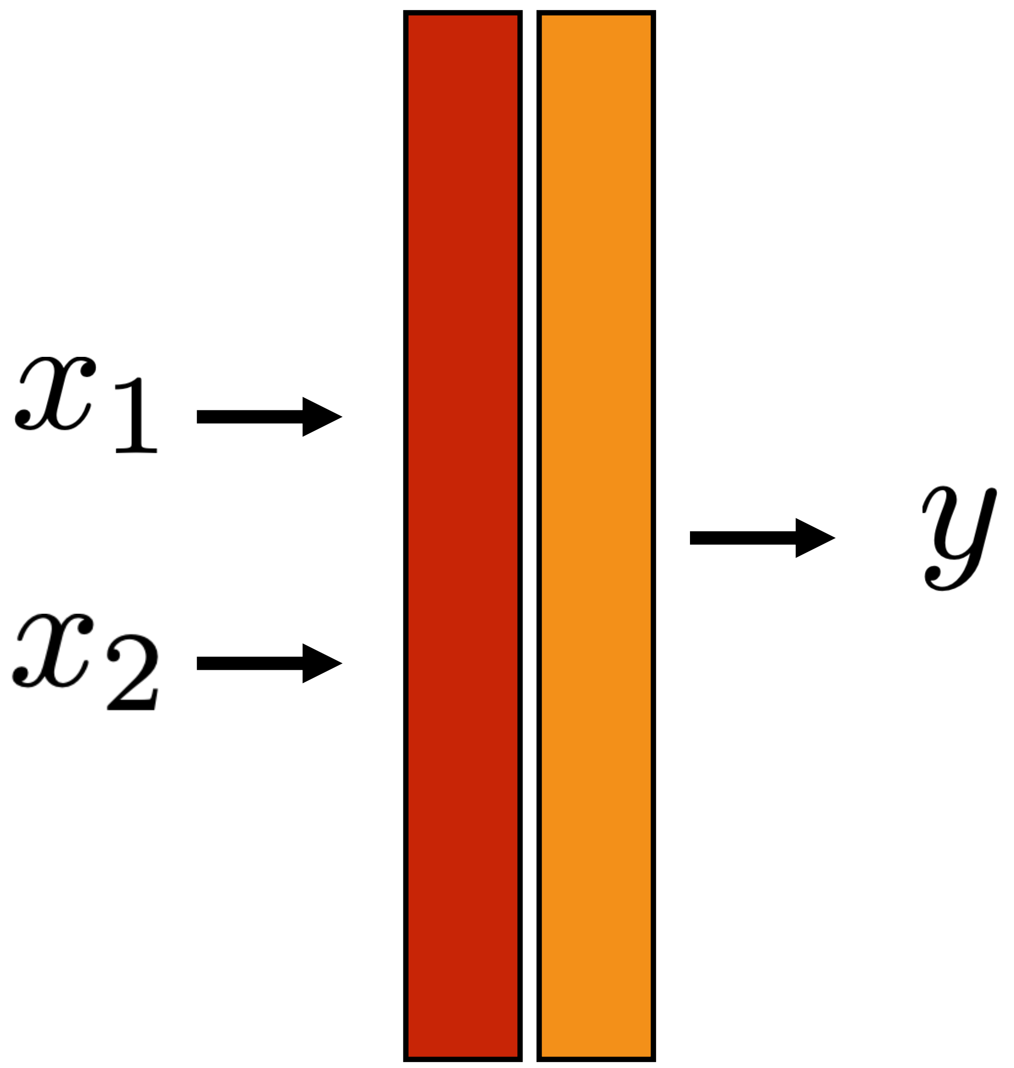
Sigmoid – not a probability distribution:

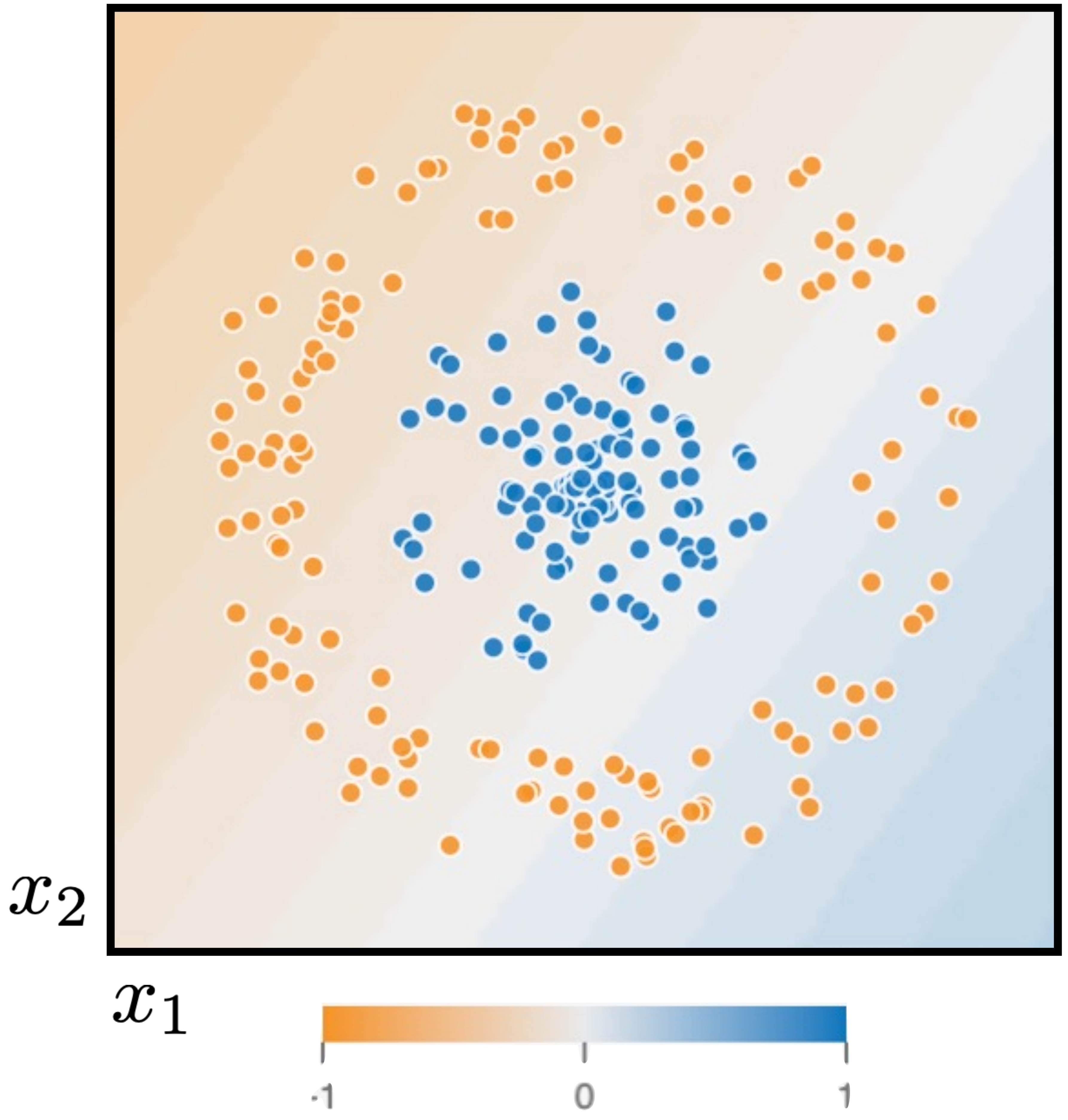
$$\underset{\text{Input vector}}{\overset{\mathrm{X}}{\begin{bmatrix} 3 \\ 1.75 \\ -2 \\ 0.5 \end{bmatrix}}} \xrightarrow[\frac{1}{1+e^{-X}}]{\text{Sigmoid}} \underset{\text{Output vector}}{\overset{\mathrm{Out}}{\begin{bmatrix} 0.95 \\ 0.85 \\ 0.12 \\ 0.62 \end{bmatrix}}}$$

Not a probability distribution

Example: perceptron

$$\mathbf{y} = \sigma(\mathbf{W}^{(1)}\mathbf{x})$$

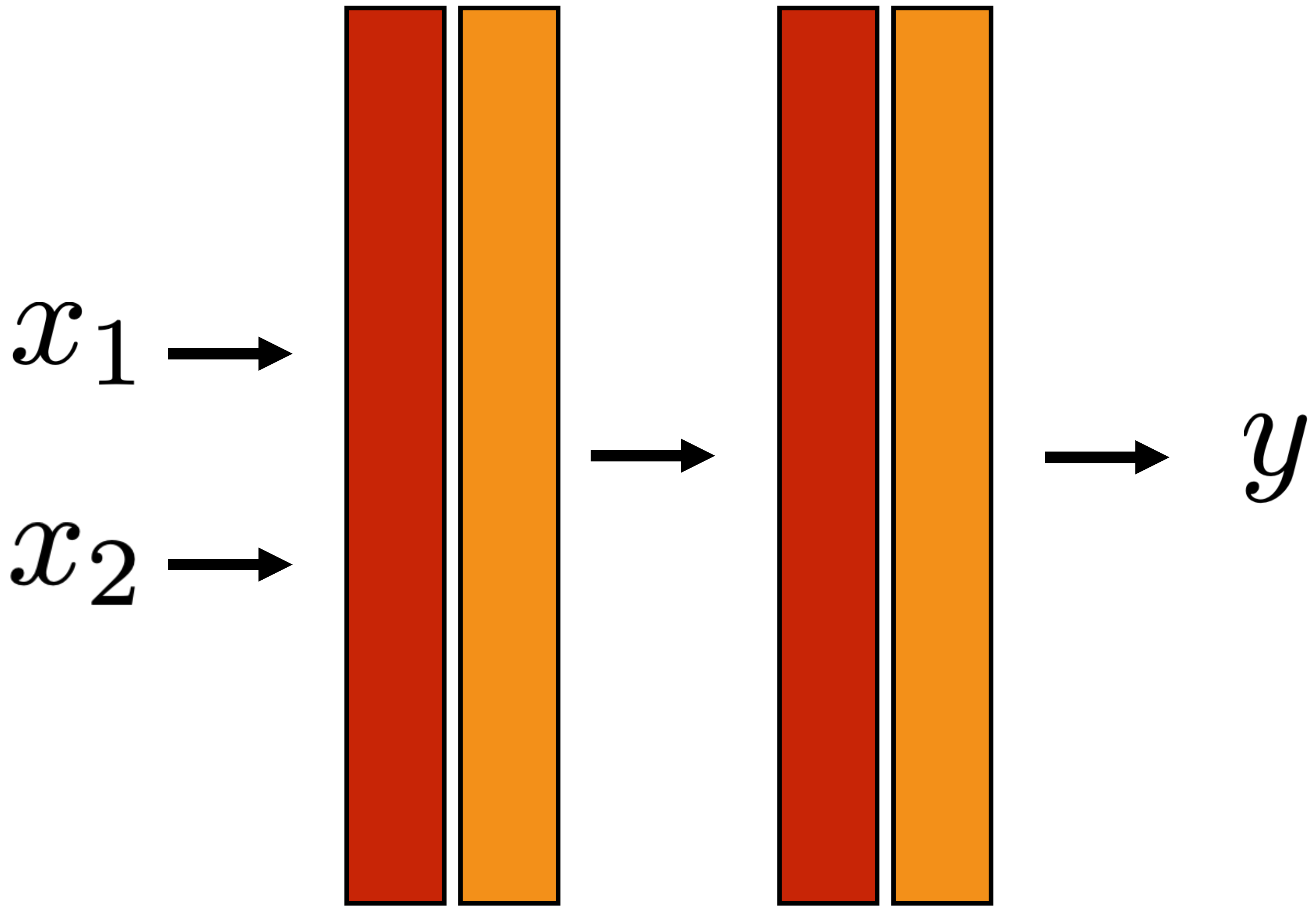


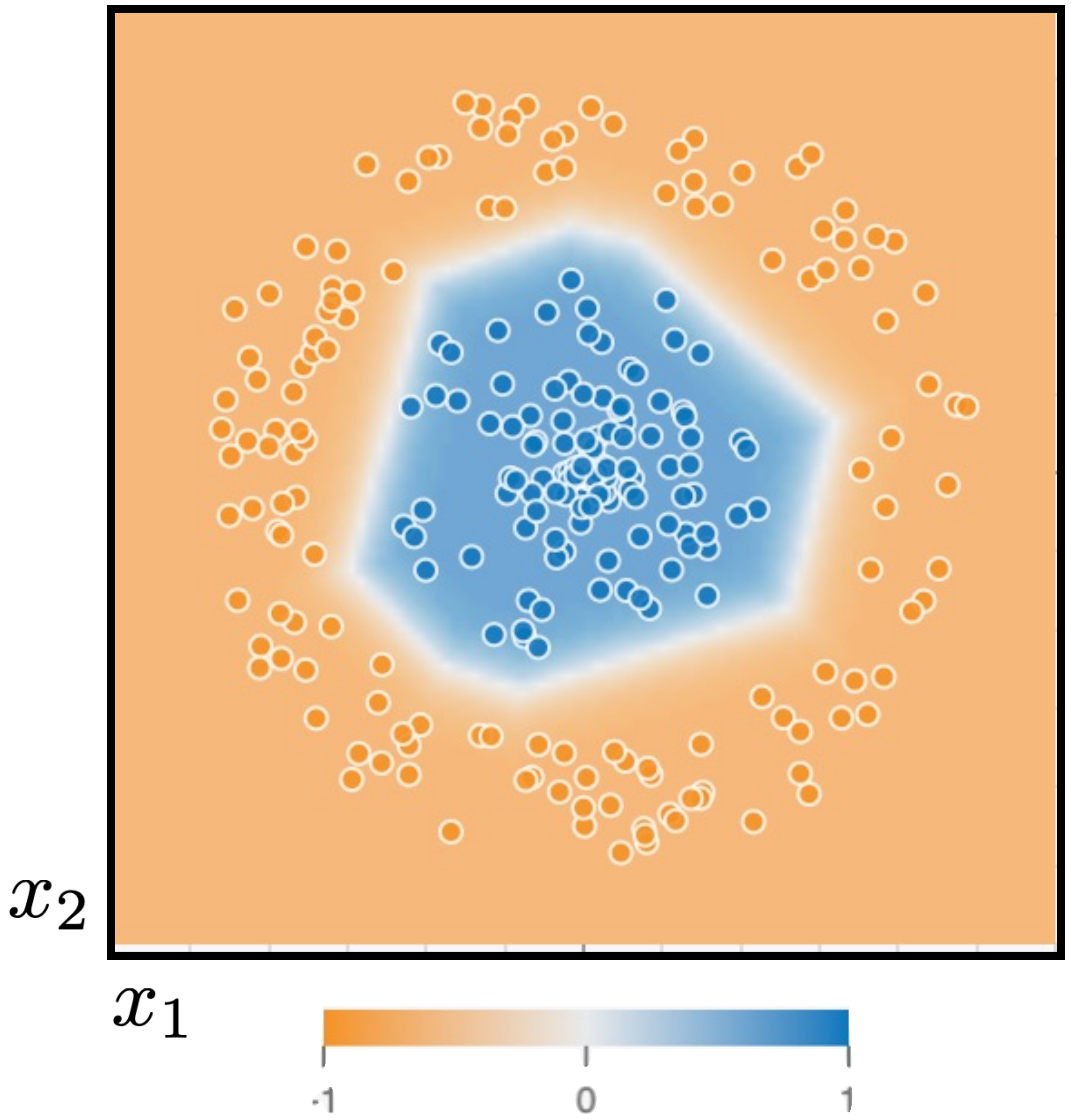


Example source: http://playground.tensorflow.org

Example: multilayer perceptron (MLP)

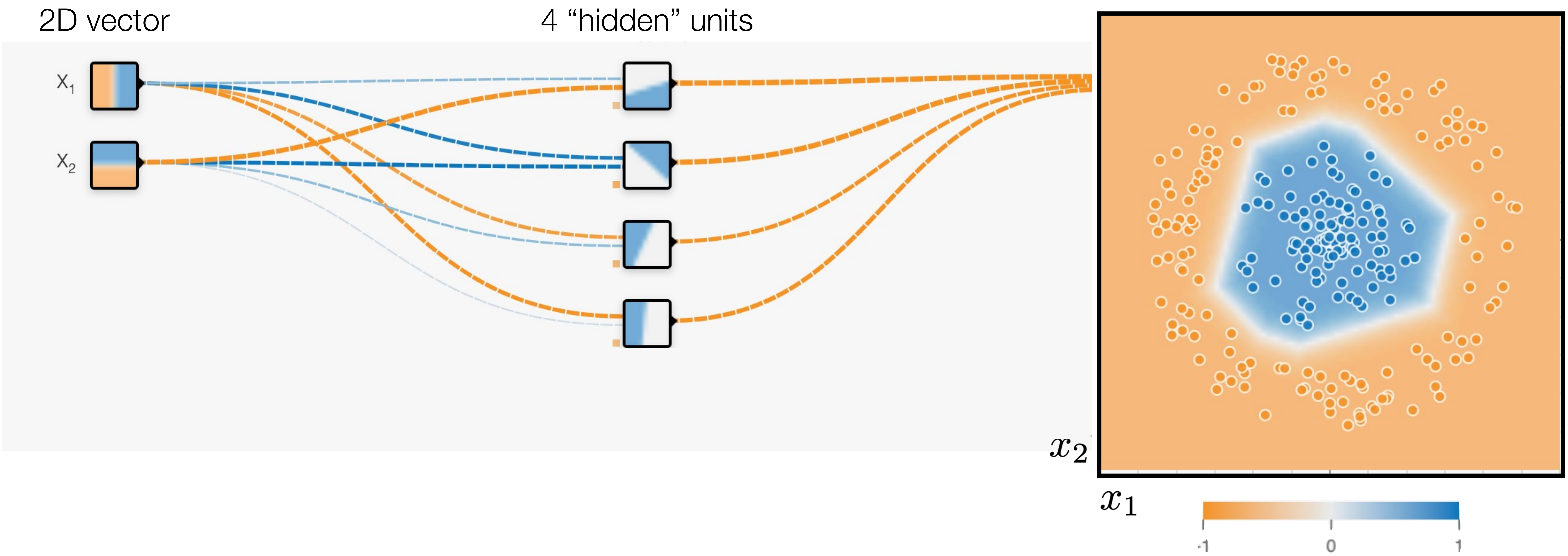
$$\mathbf{y} = \sigma(\mathbf{W}^{(2)} max(0, \mathbf{W}^{(1)}\mathbf{x}))$$





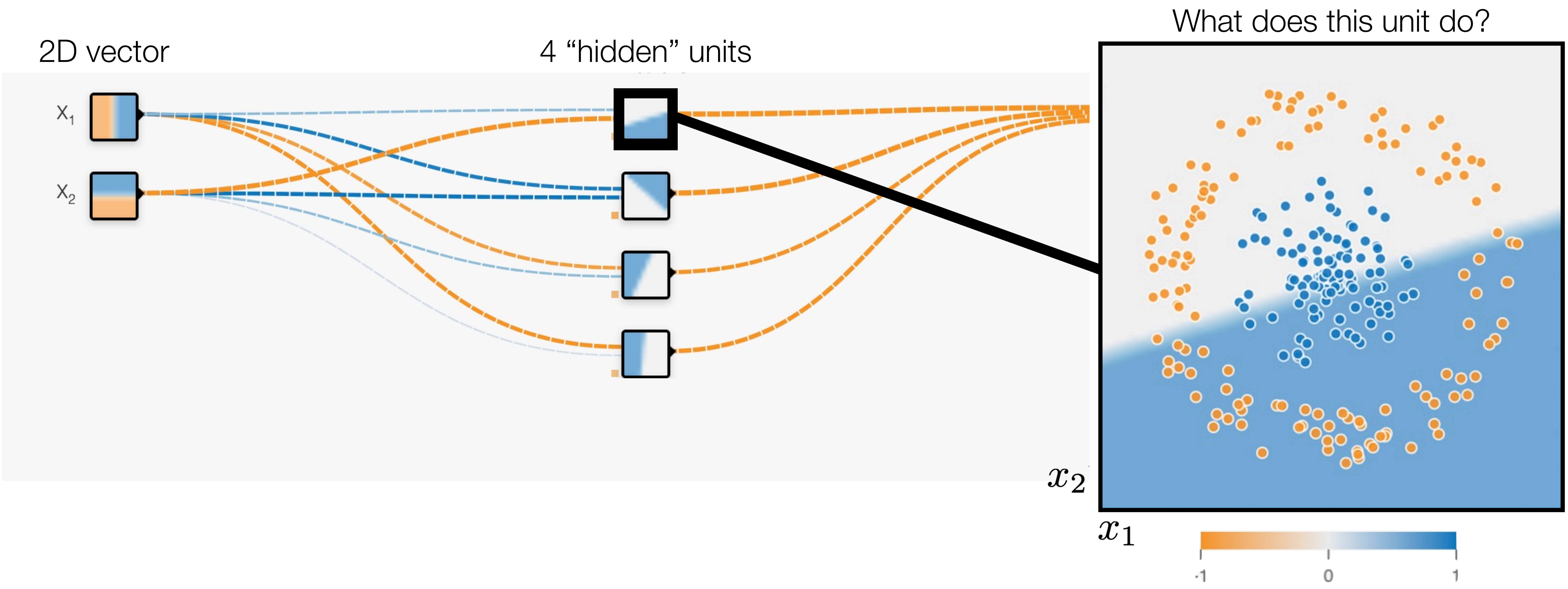
Example source: http://playground.tensorflow.org

Example: multilayer perceptron (MLP)



Example source: http://playground.tensorflow.org

Example: multilayer perceptron (MLP)



Example source: http://playground.tensorflow.org