CS 260: Foundations of Data Science

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Fall 2024

HAVERFORD
COLLEGE

Materials by Sara Mathieson

Admin

- **Lab 8** grades & feedback posted on Moodle

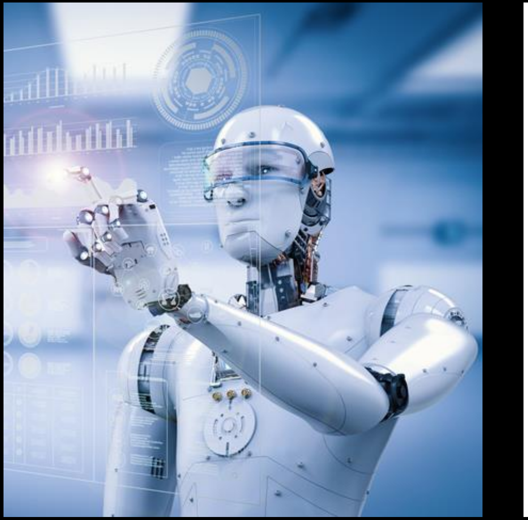
- **End-of-semester survey (link on Piazza)**

Outline for today

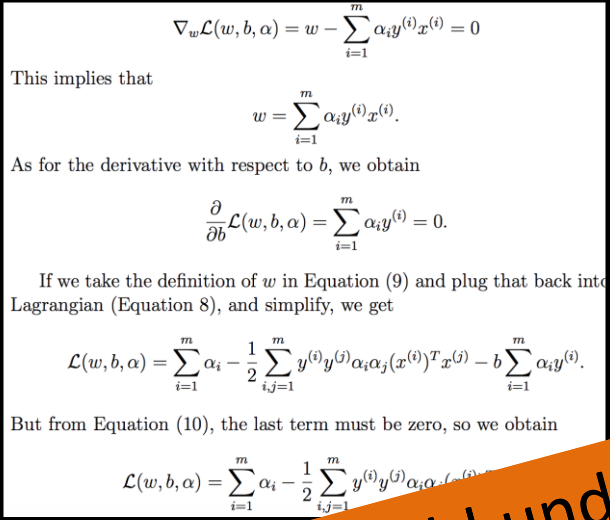
- Neural networks

Adapted from: “Know Your Meme”

MACHINE LEARNING



What society thinks I do



$$\nabla_w \mathcal{L}(w,b,\alpha) = w - \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)} = 0$$

This implies that

$$w = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}.$$

As for the derivative with respect to b, we obtain

$$\frac{\partial}{\partial b}\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i y^{(i)} = 0.$$

If we take the definition of w in Equation (9) and plug that back int Lagrangian (Equation 8), and simplify, we get

$$\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)})^T x^{(j)} - b\sum_{i=1}^{m} \alpha_i y^{(i)}.$$

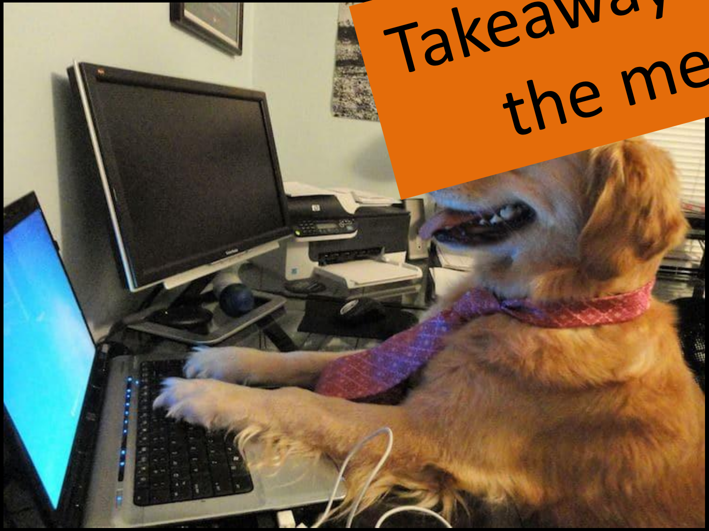
But from Equation (10), the last term must be zero, so we obtain

$$\mathcal{L}(w,b,\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j (x^{(i)}$$

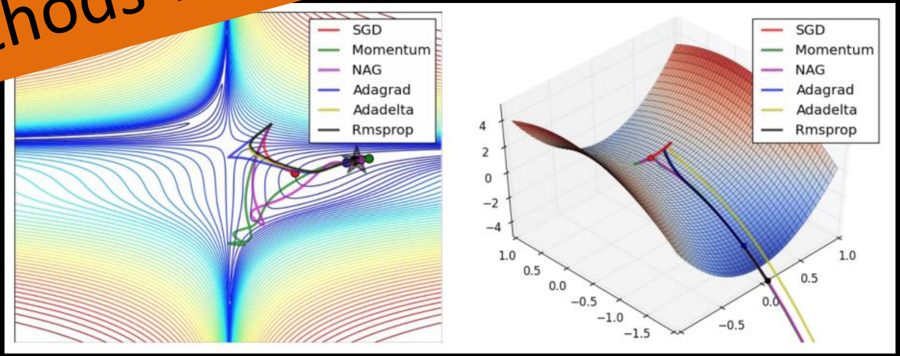
Wh

t other computer scientists think I do

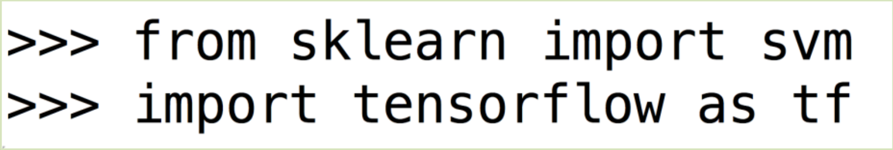
Takeaway: we should understand the methods we are using!



What mathematicians think I do



What I think I do



```
>>> from sklearn import svm
>>> import tensorflow as tf
```

What I really do

Biological Inspiration for Neural Networks

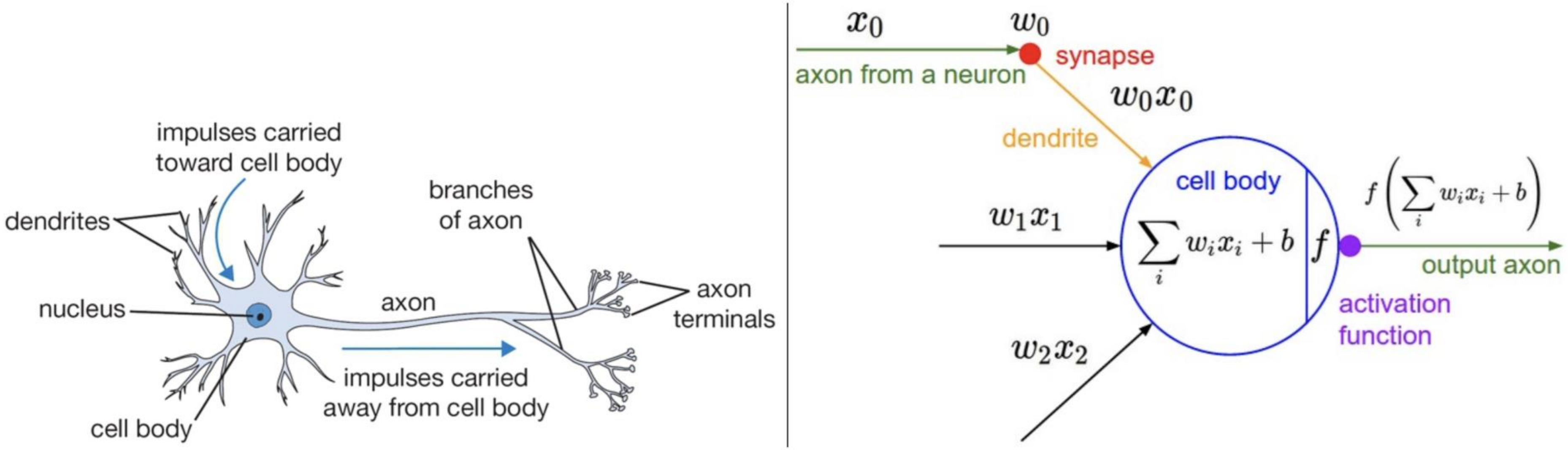
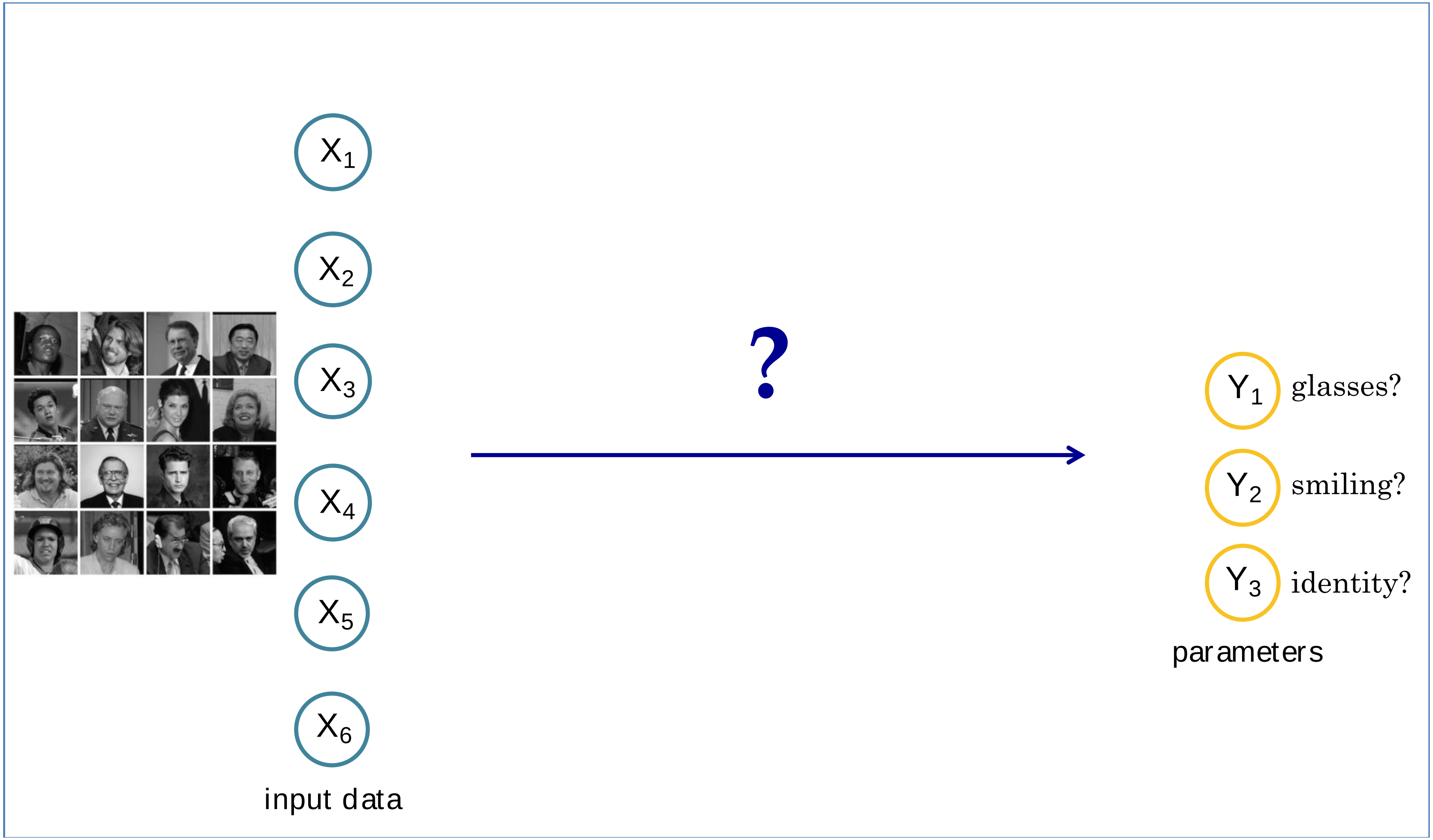


Figure: Stanford CS231n http://cs231n.github.io/neural-networks-1/

Goal: learn from complicated inputs



X_1

X_2

X_3

X_4

X_5

X_6

input data

?

Y_1 glasses?

Y_2 smiling?

Y_3 identity?

parameters

Image: Labeled Faces in the Wild (UMass)

Idea: transform data into lower dimension

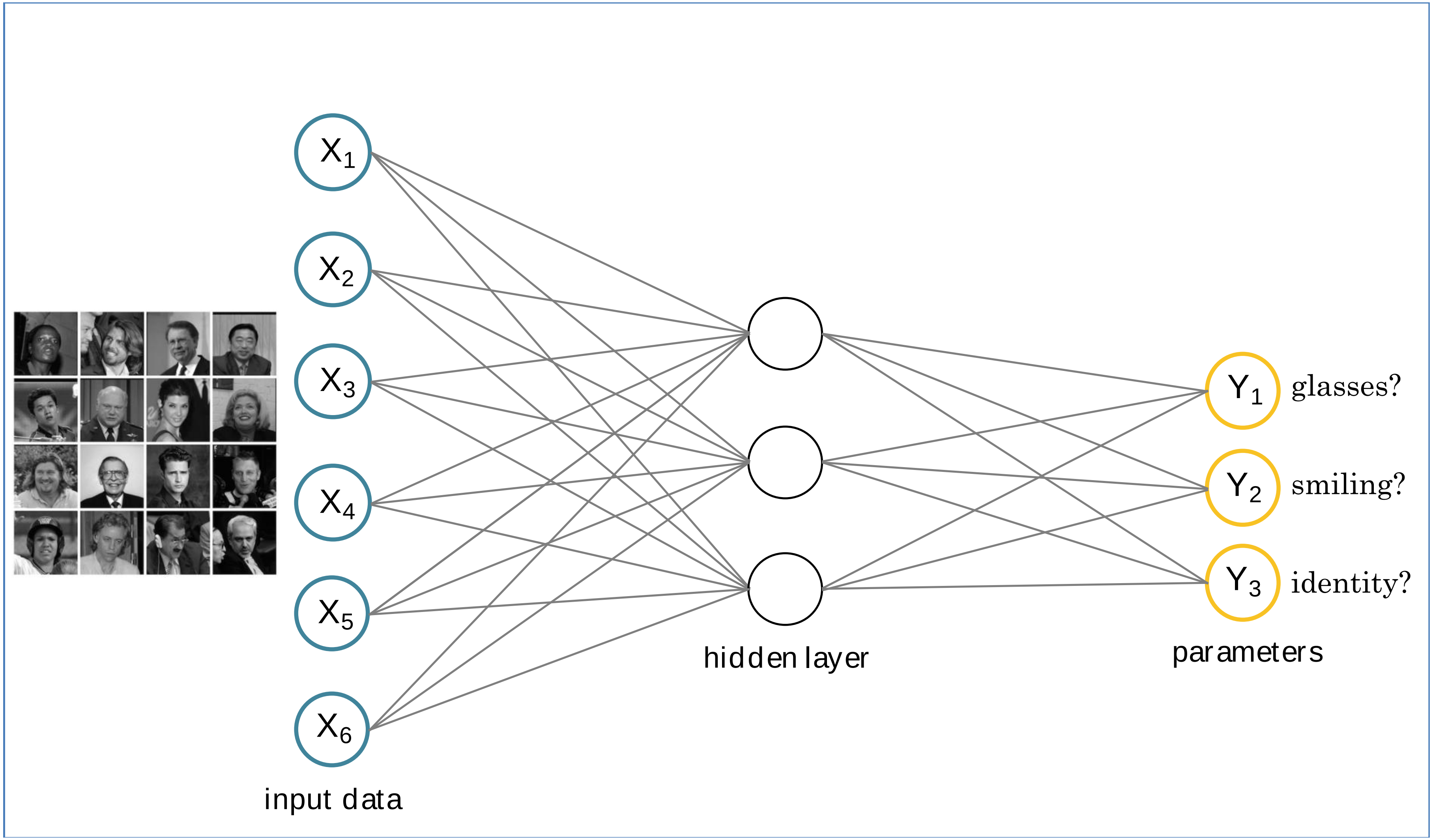
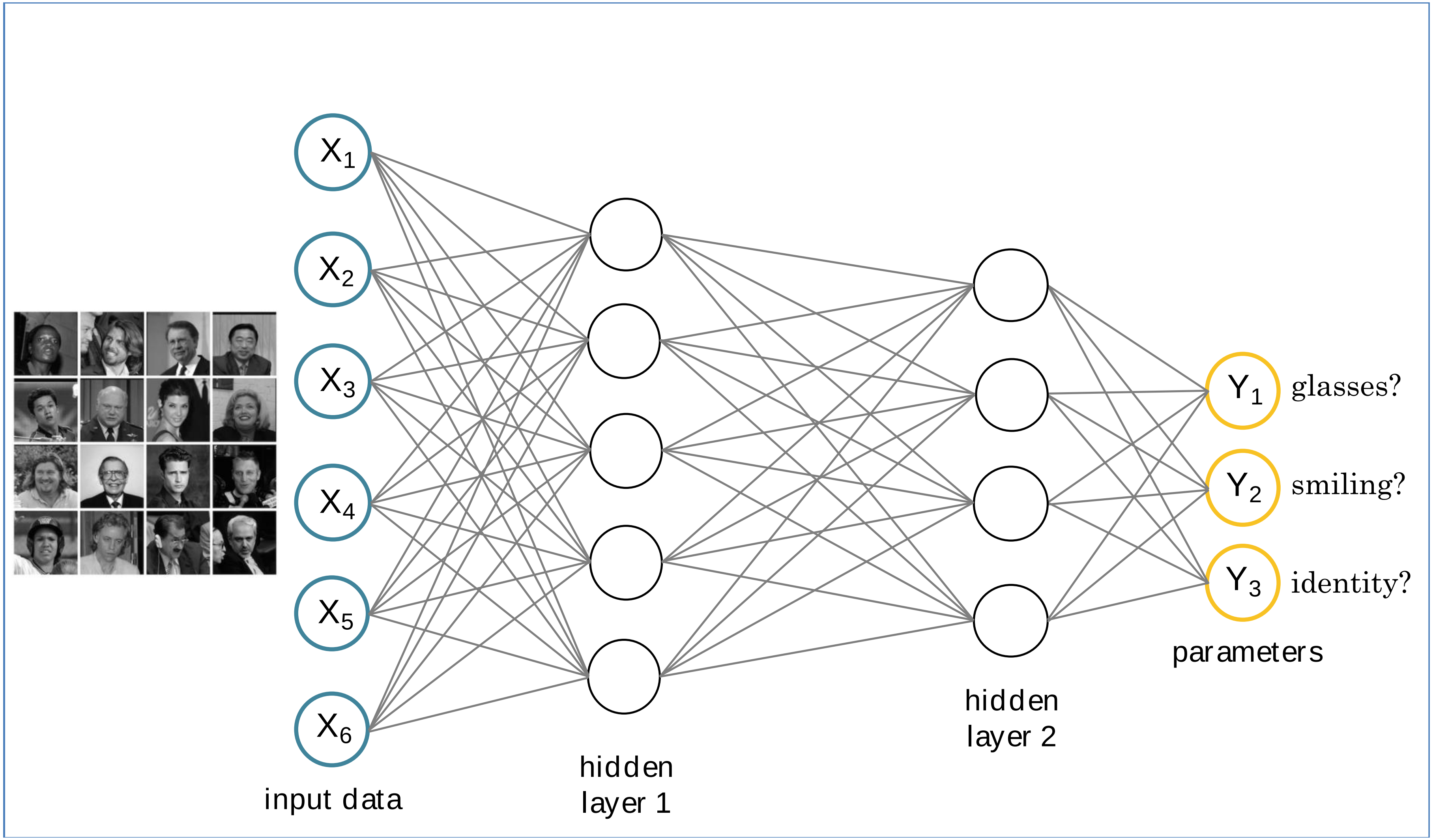


Image: Labeled Faces in the Wild (UMass)

Multi-layer networks = “deep learning”



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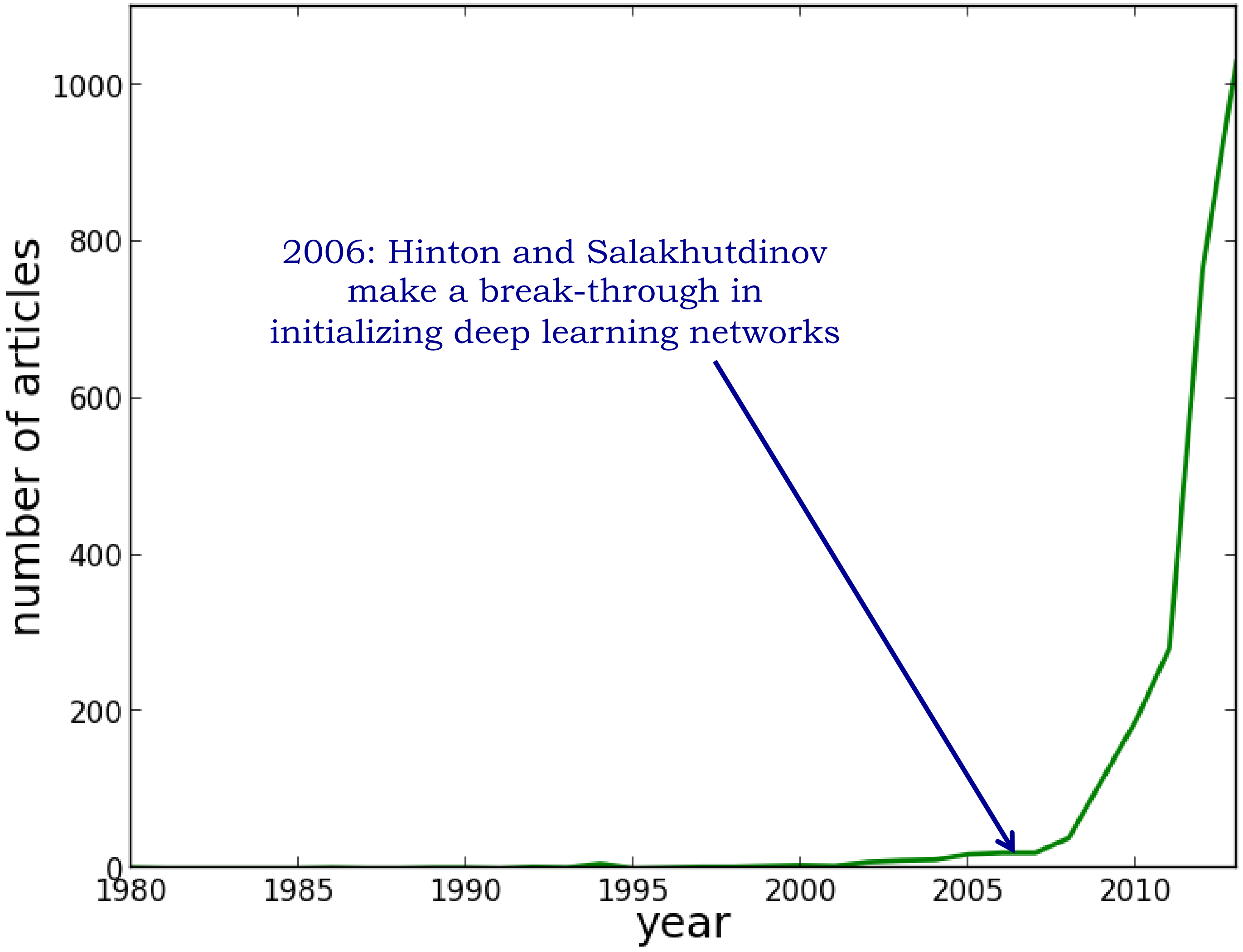
History of Neural Networks

- Perceptron can be interpreted as a simple neural network
- Misconceptions about the weaknesses of perceptrons contributed to declining funding for NN research
- Difficulty of training multi-layer NNs contributed to second setback
- Mid 2000’s: breakthroughs in NN training contribute to rise of “deep learning”

Number of papers that mention "deep learning" over time



2006: Hinton and Salakhutdinov make a break-through in initializing deep learning networks

Big picture for today

- Neural networks can approximate any function!

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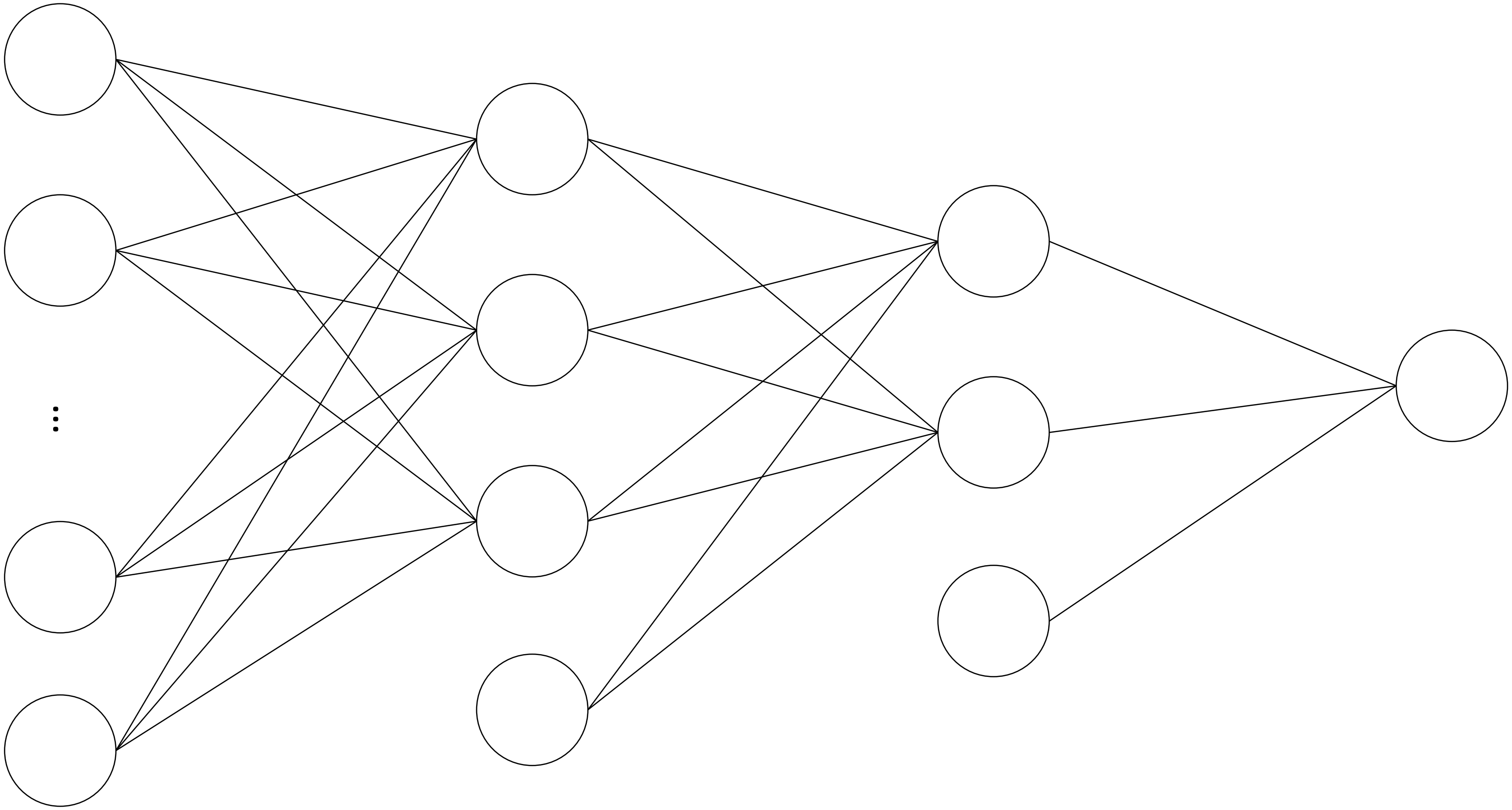
- Neural networks can approximate any function!

- For our purposes in ML, we want to use them to approximate a function from our inputs to our outputs

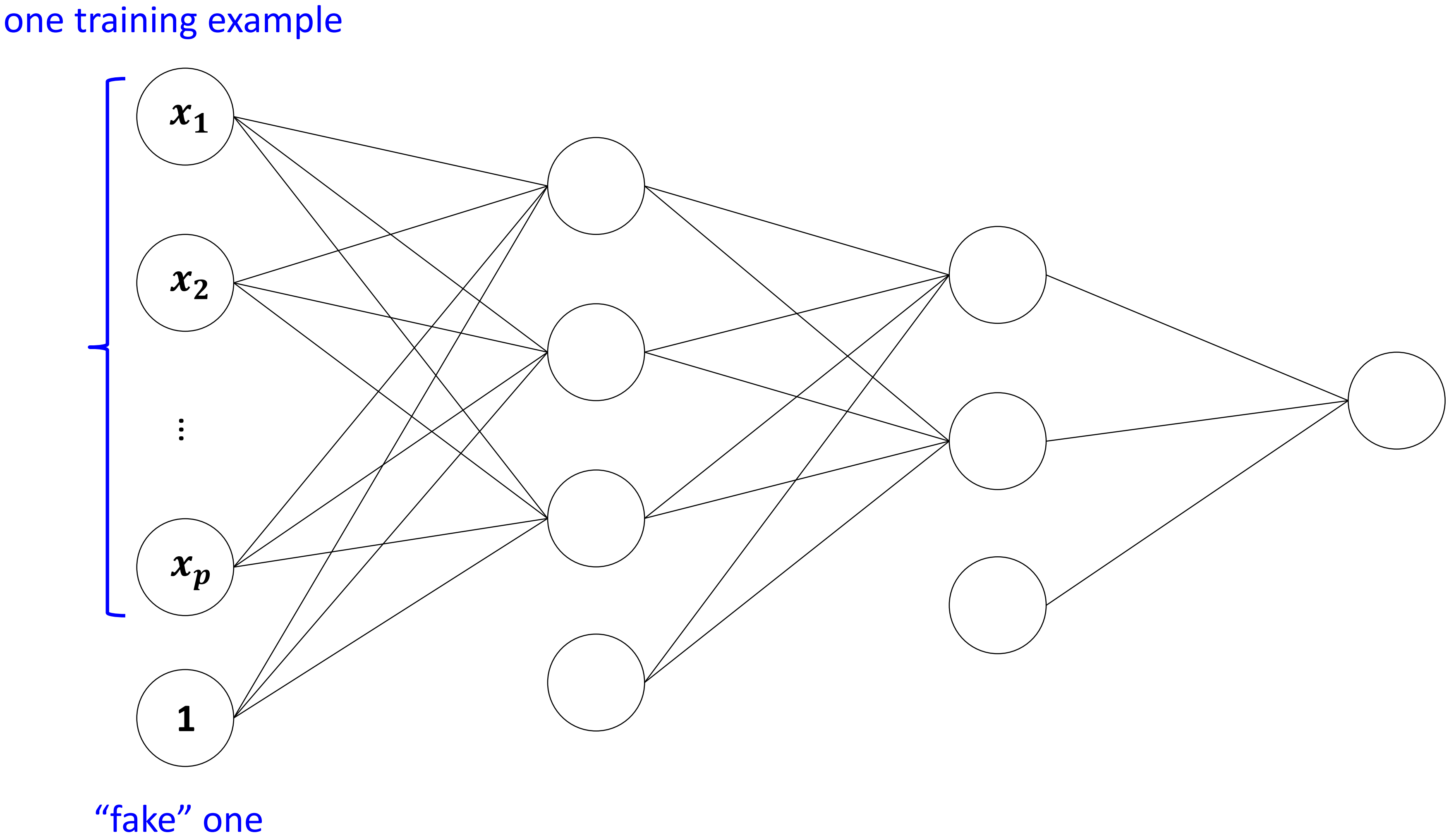
- We will train our network by asking it to minimize the loss between its output and the true output

- We will use SGD-like approaches to minimize loss

Fully Connected Neural Network Architecture

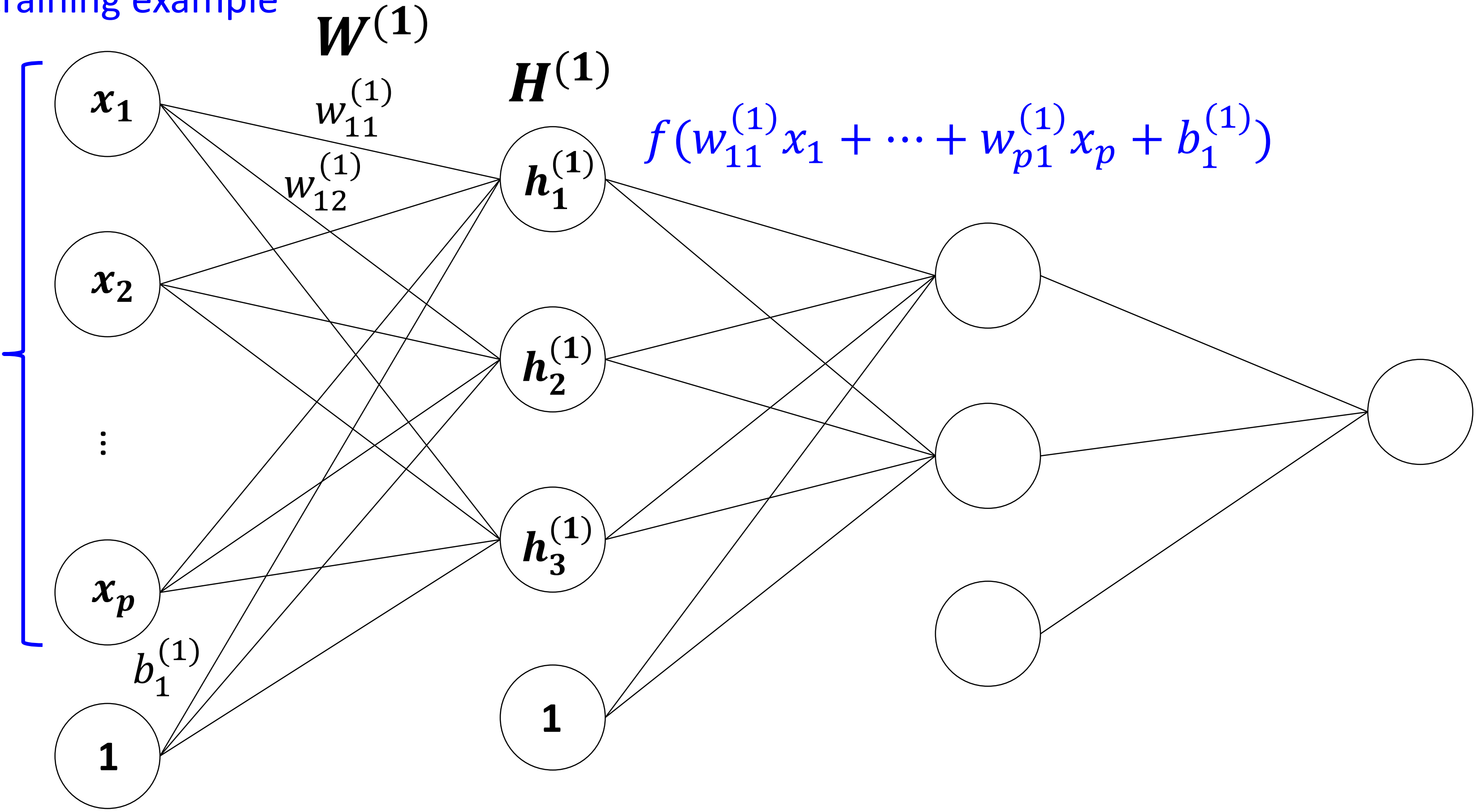


Fully Connected Neural Network Architecture



Fully Connected Neural Network Architecture

one training example



$\boldsymbol{W}^{(\mathbf{1})}$
$\boldsymbol{H}^{(\mathbf{1})}$
$w_{11}^{(1)}$
$w_{12}^{(1)}$
$\boldsymbol{x}_{\mathbf{1}}$
$\boldsymbol{x}_{\mathbf{2}}$
⋮
$\boldsymbol{x}_{\boldsymbol{p}}$
$b_1^{(1)}$
1
$\boldsymbol{h}_{\mathbf{1}}^{(\mathbf{1})}$
$\boldsymbol{h}_{\mathbf{2}}^{(\mathbf{1})}$
$\boldsymbol{h}_{\mathbf{3}}^{(\mathbf{1})}$
1

$f(w_{11}^{(1)}x_1 + \cdots + w_{p1}^{(1)}x_p + b_1^{(1)})$

“fake” one

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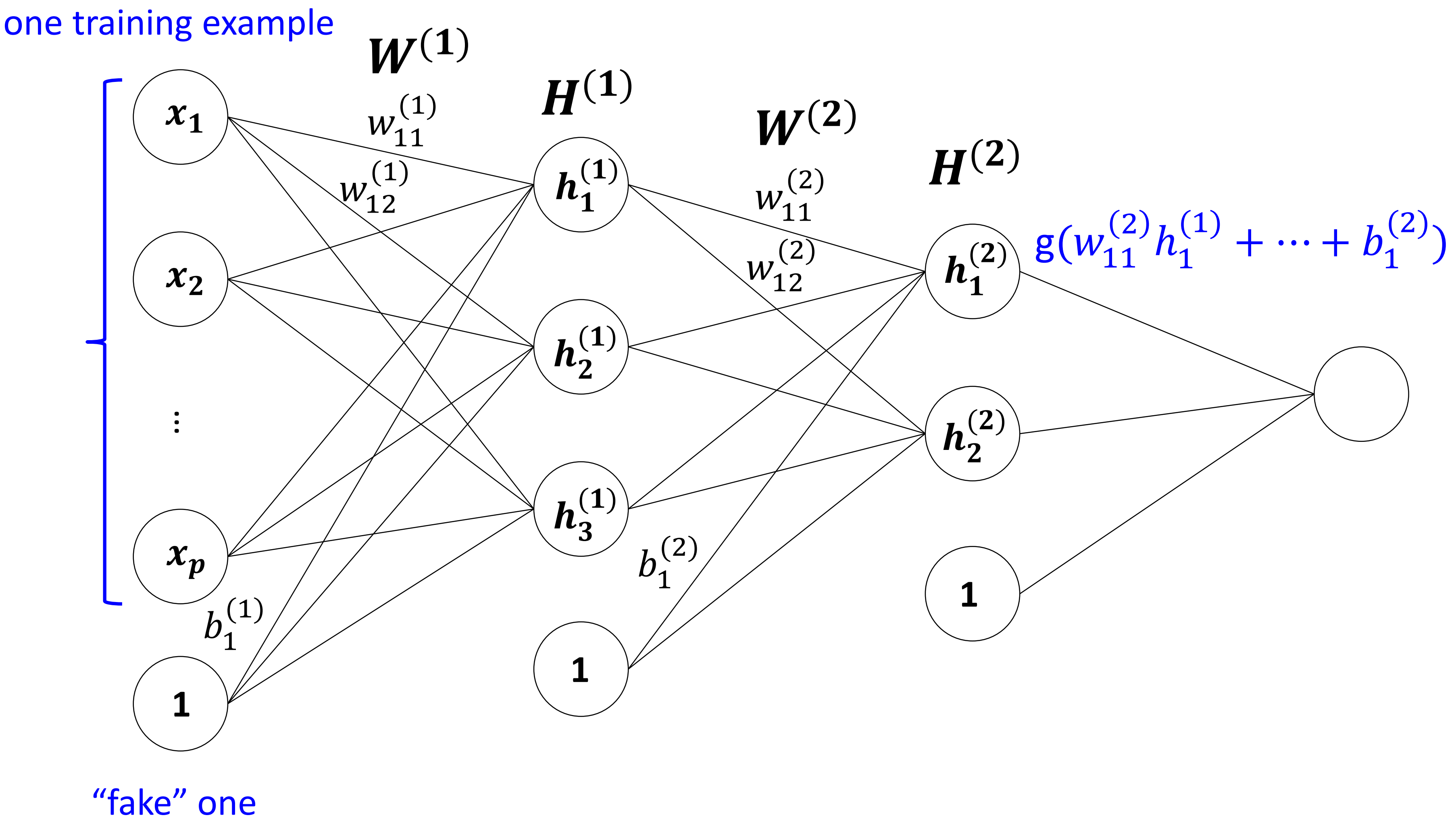

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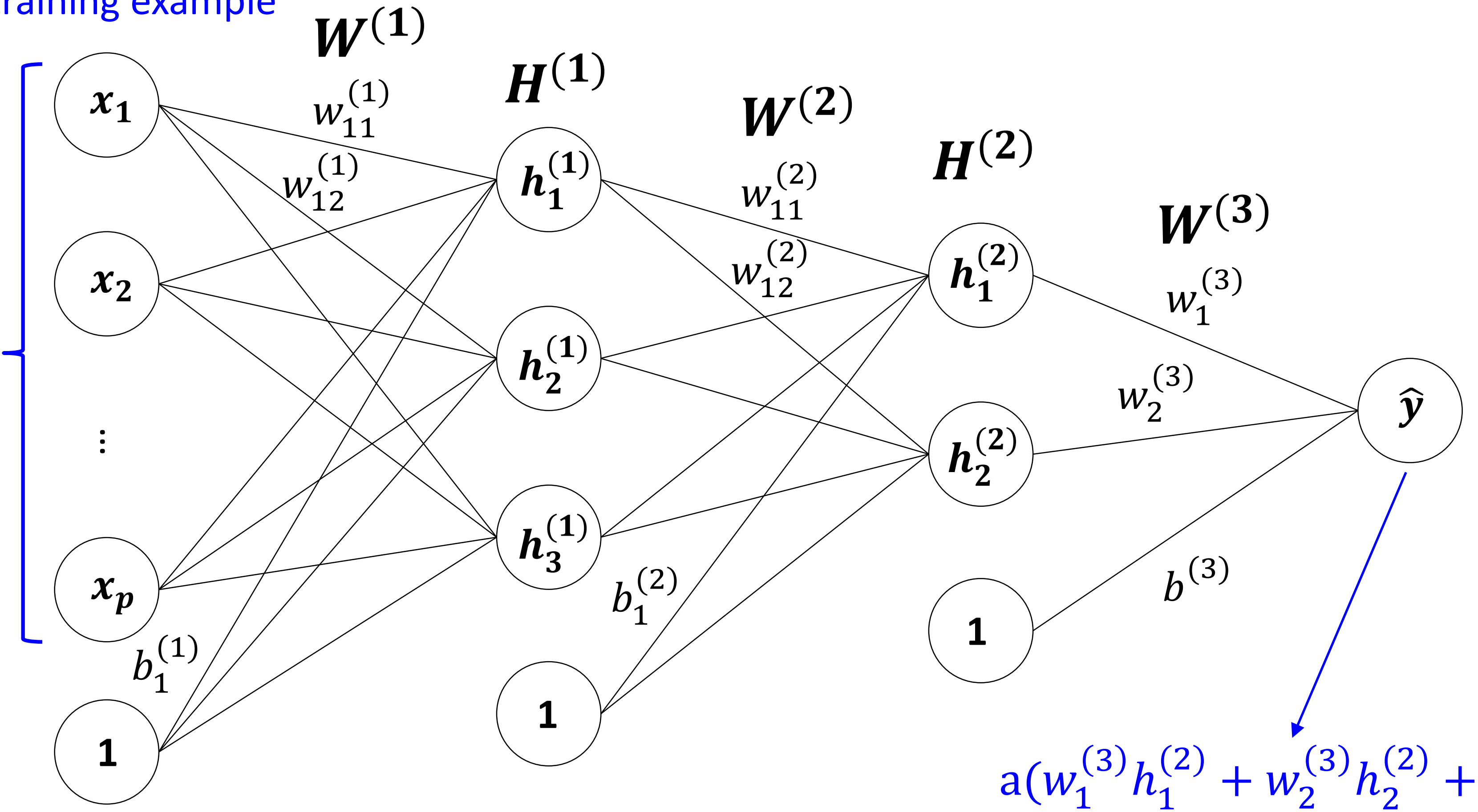


$\mathrm{a}(w_1^{(3)}h_1^{(2)} + w_2^{(3)}h_2^{(2)} + b^{(3)})$

“fake” one

Layer Output

- $$H^{(1)} = \underset{\text{activation function}}{a}\left(\underbrace{\underset{p_1 \times p}{W^{(1)}}\,\underset{p \times n}{X}}_{p_1 \times n} + \underset{p_1 \times 1}{\vec{b}^{(1)}}\right)$$

p_1 = # of nodes in layer 1

- $$H^{(2)} = a\left(W^{(2)}H^{(1)} + \vec{b}^{(2)}\right)$$

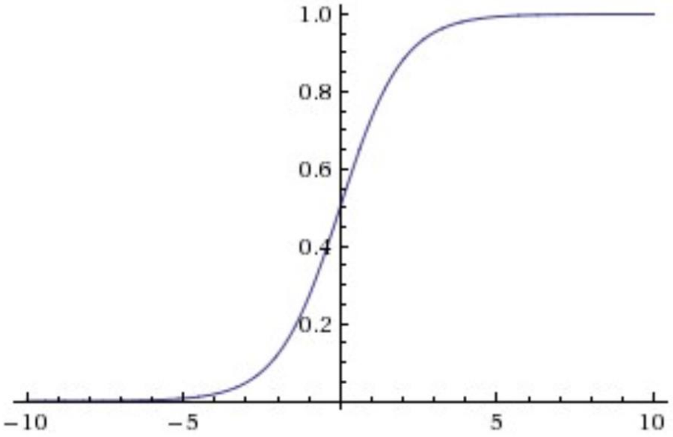
- $$\hat{y} = a\left(W^{(3)}H^{(2)} + b^{(3)}\right)$$

Activation Functions

Option 1: sigmoid function

- Input: all real numbers, output: [0, 1]

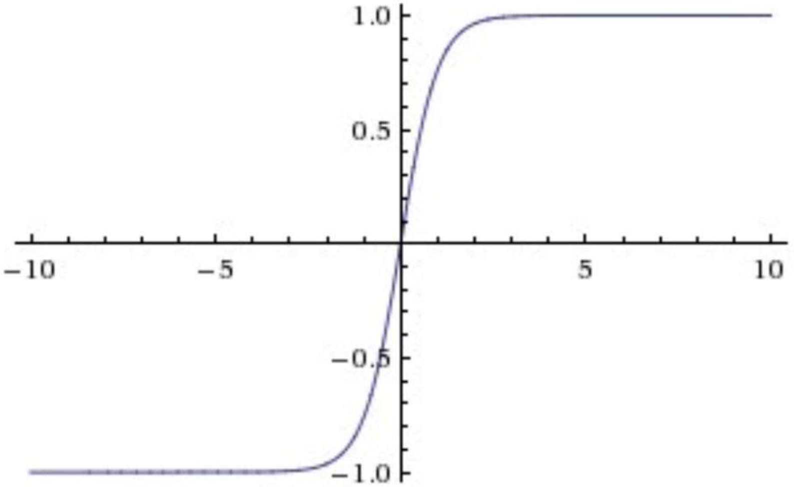
$$\boxed{\sigma(x) = \frac{1}{1 + e^{-x}}}$$



Option 2: hyperbolic tangent

- Input: all real numbers, output: [-1, 1]

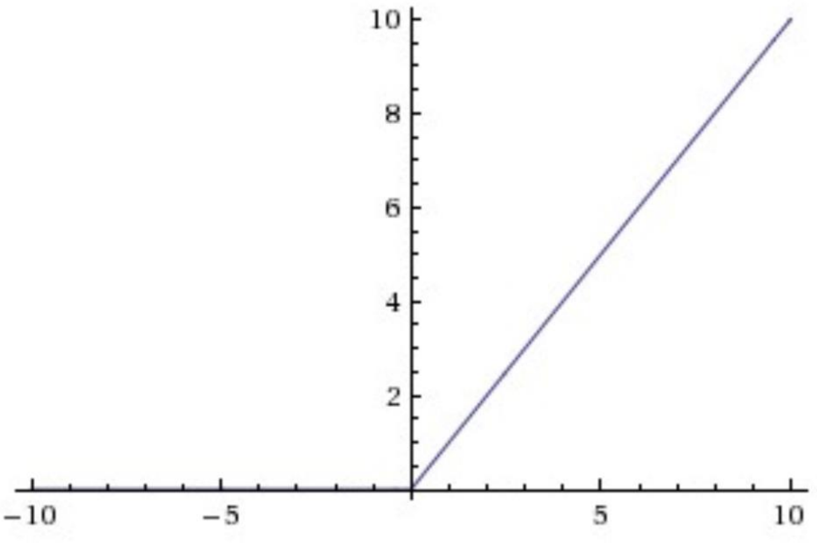
$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$



Option 3: Rectified Linear Unit (ReLU)

- Return *x* if *x* is positive (i.e. threshold at 0)

$$f(x) = \max(0, x)$$



Pros and Cons of Activation Functions

1) Sigmoid

- (-) When input becomes very positive or very negative, gradient approaches 0 (saturates and stops gradient descent)
- (-) Not zero-centered, so gradient on weights can end up all positive or all negative (zig-zag in gradient descent)
- (+) Derivative is easy to compute given function value!

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3) ReLU

- (+) Works well in practice (accelerates convergence)
- (+) Function value very easy to compute! (no exponentials)
- (-) Units can have no signal if input becomes too negative throughout gradient descent

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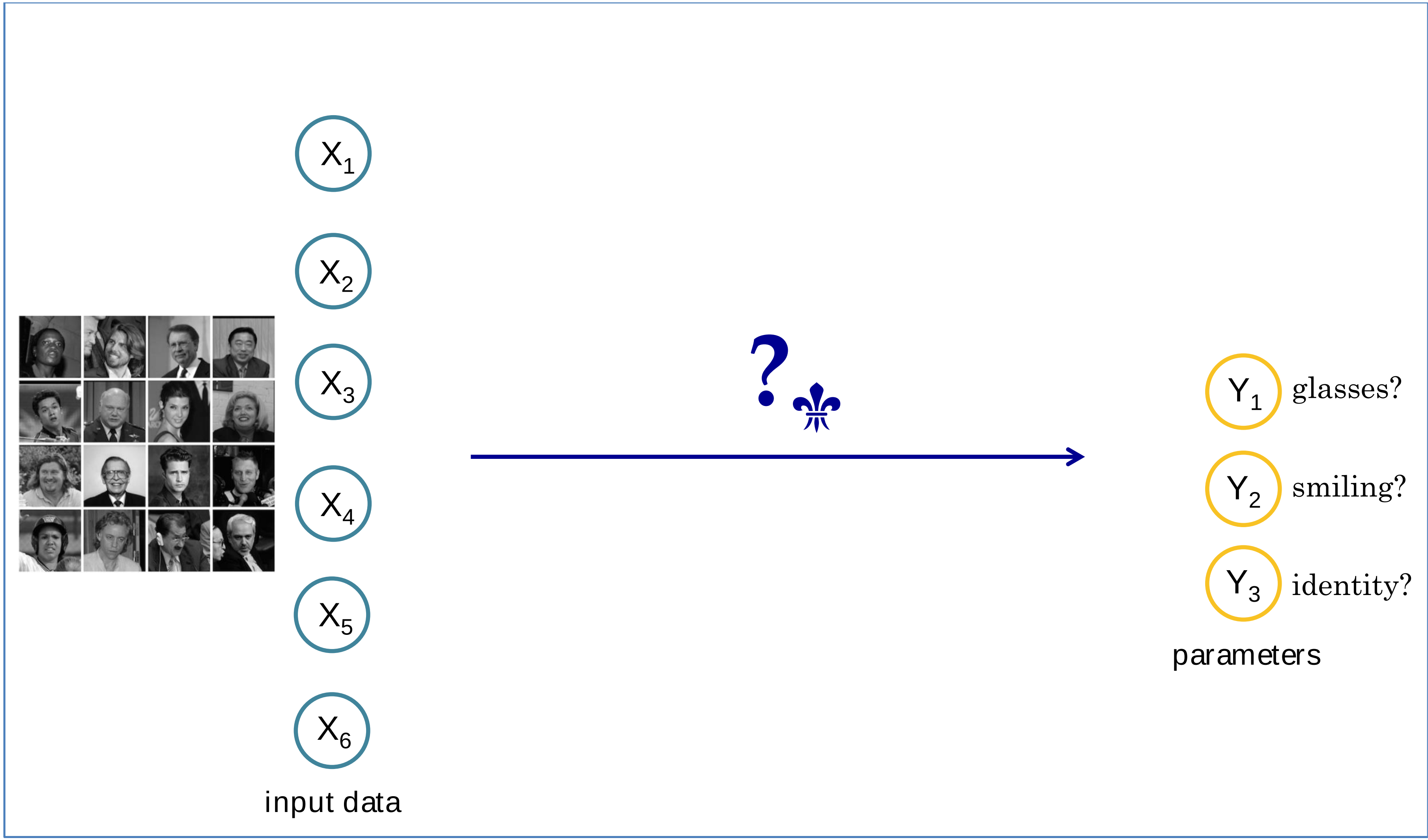
Goal: find a function between input and output



X_1

X_2

X_3

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X_6

input data

? ⚜

Y_1 glasses?

Y_2 smiling?

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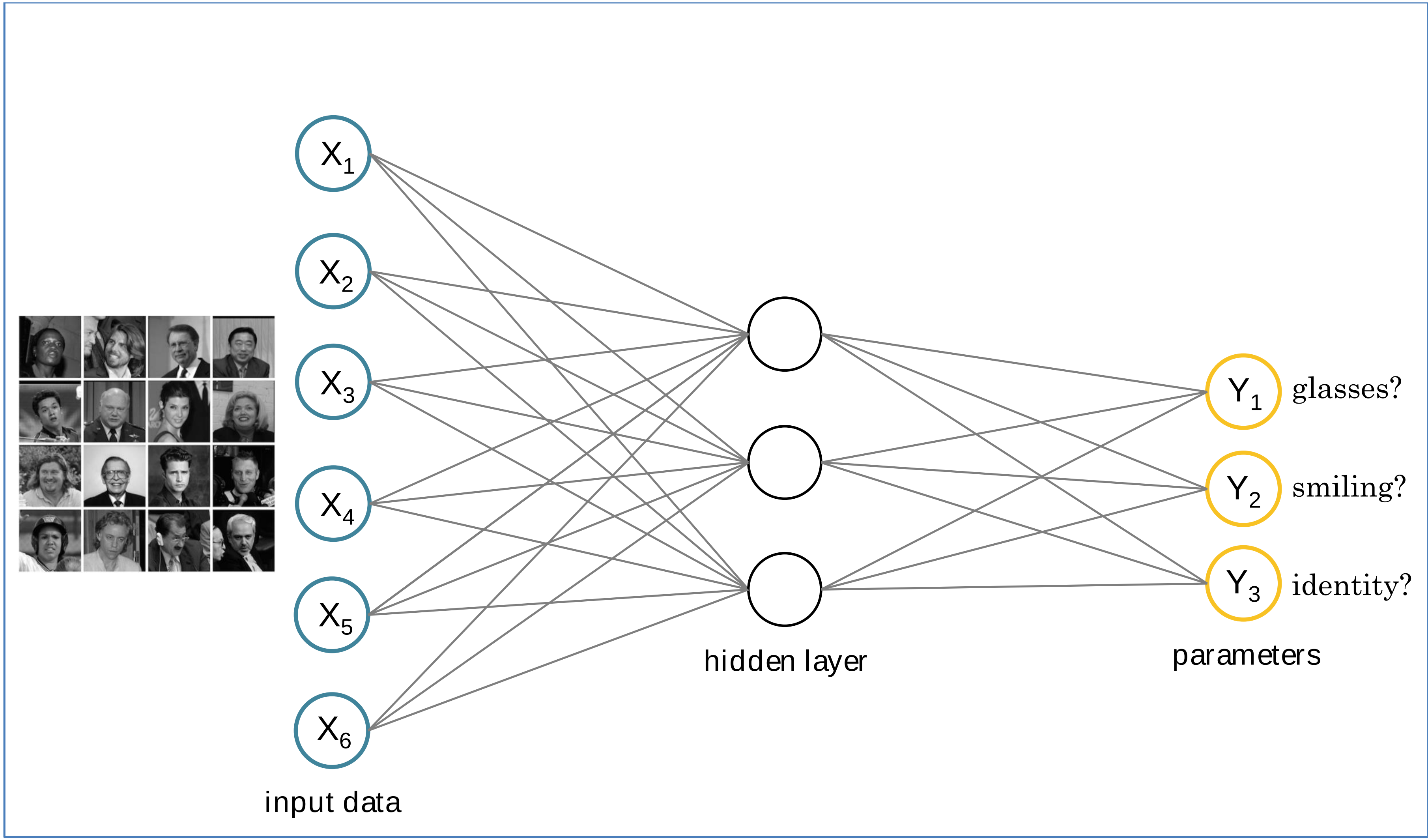
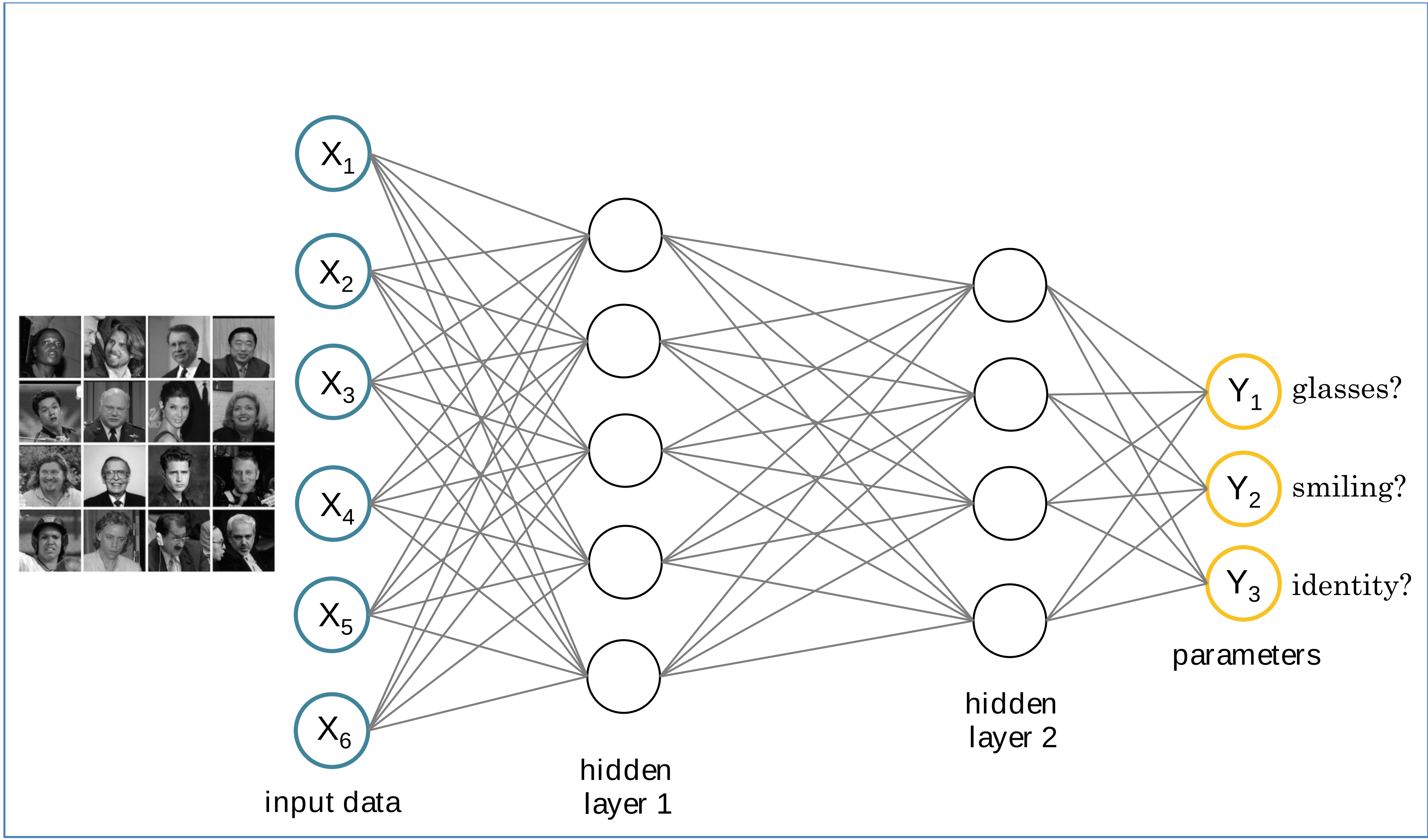
parameters

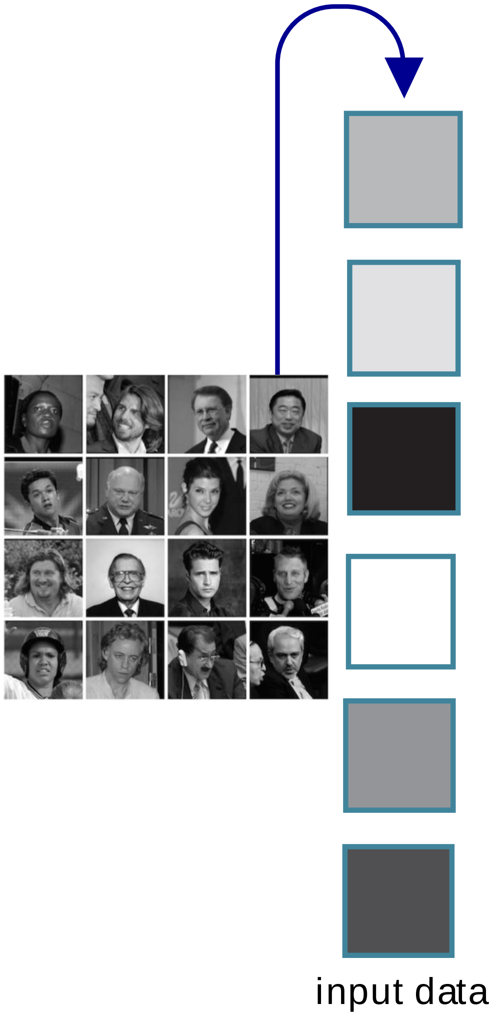
First idea: one hidden layer



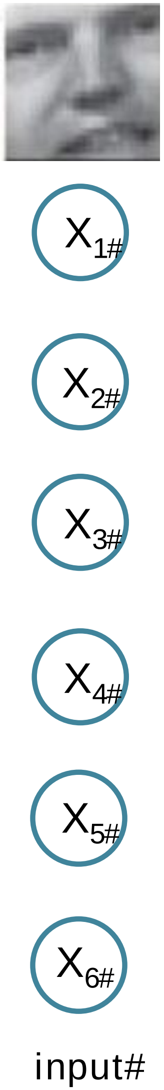
Second idea: more hidden layers (“deep” learning)



Another idea: Flatten pixels of image into a single vector



Detour to autoencoders



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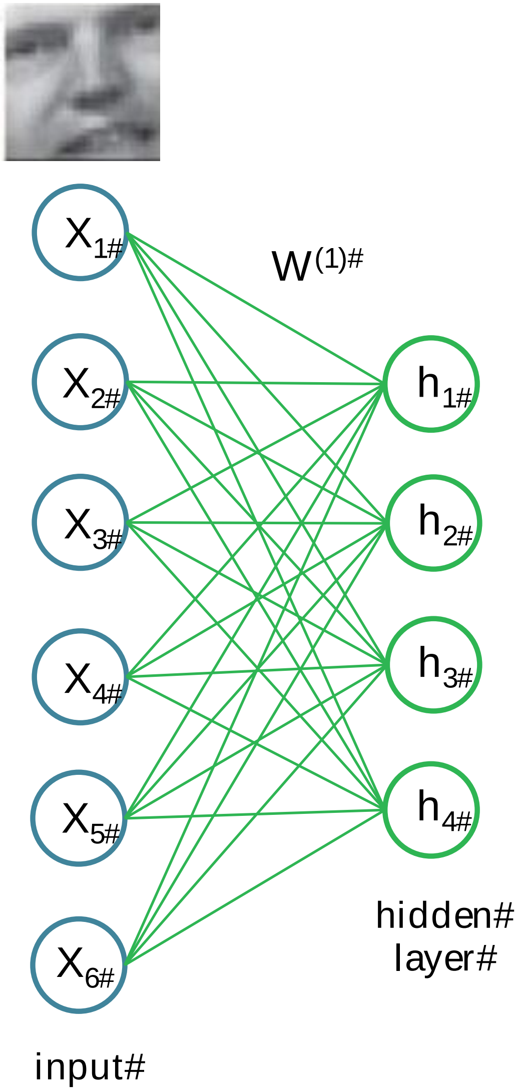

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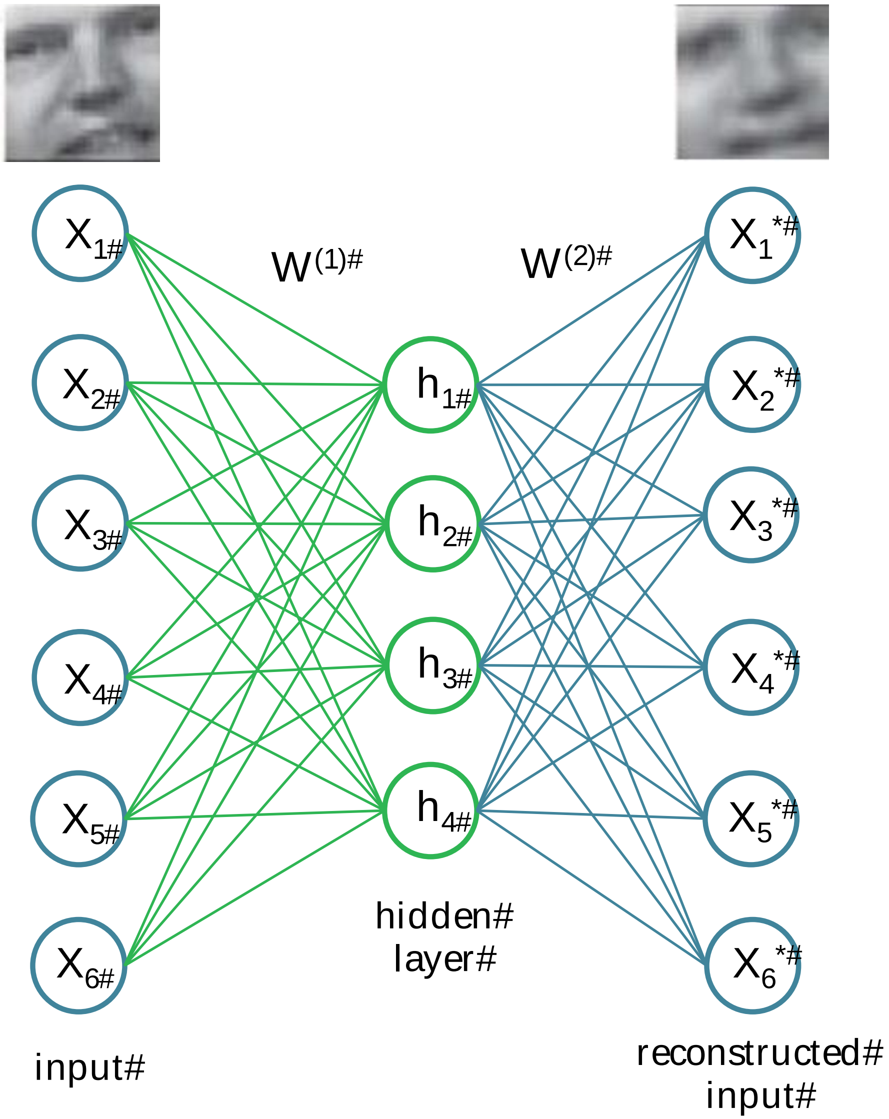
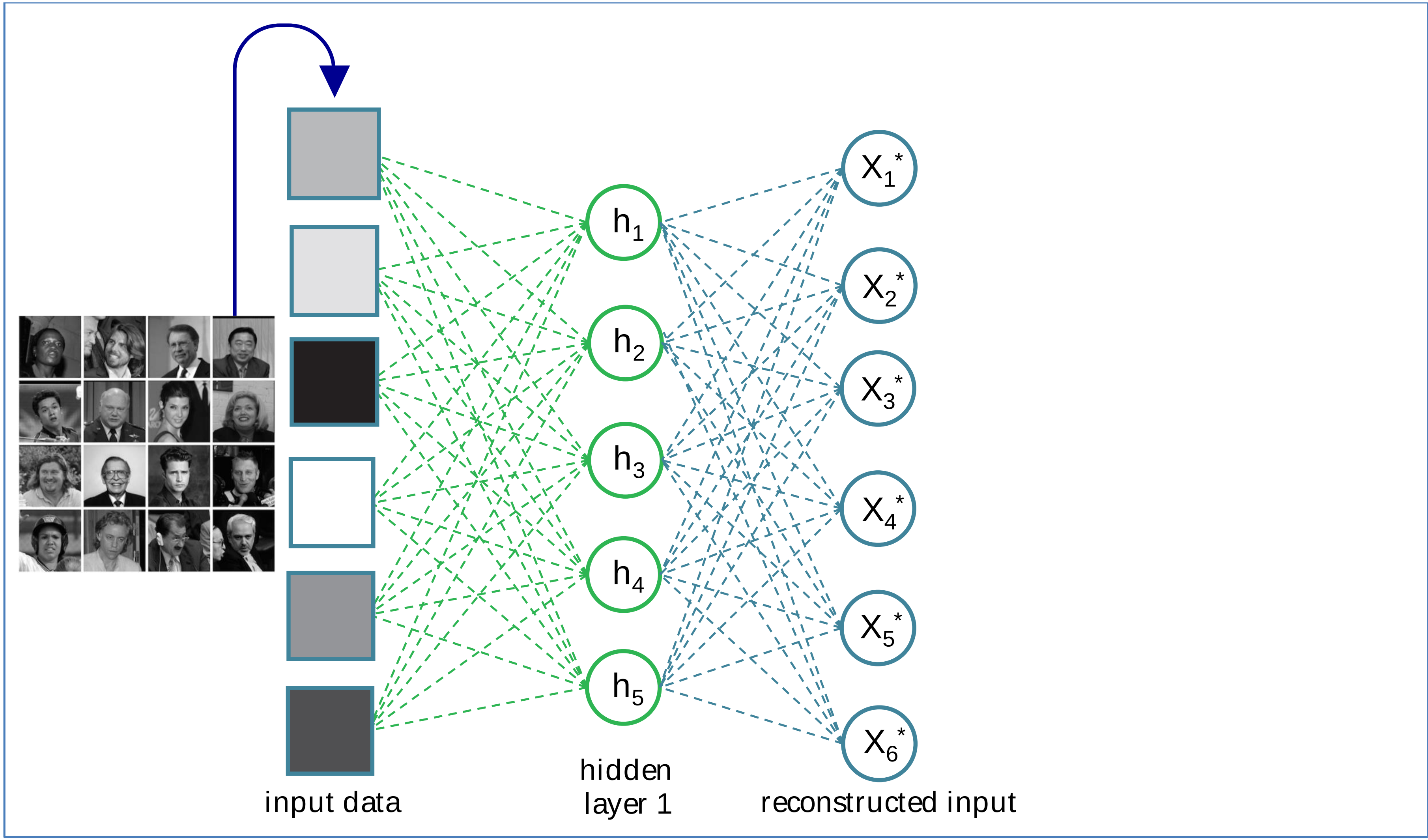
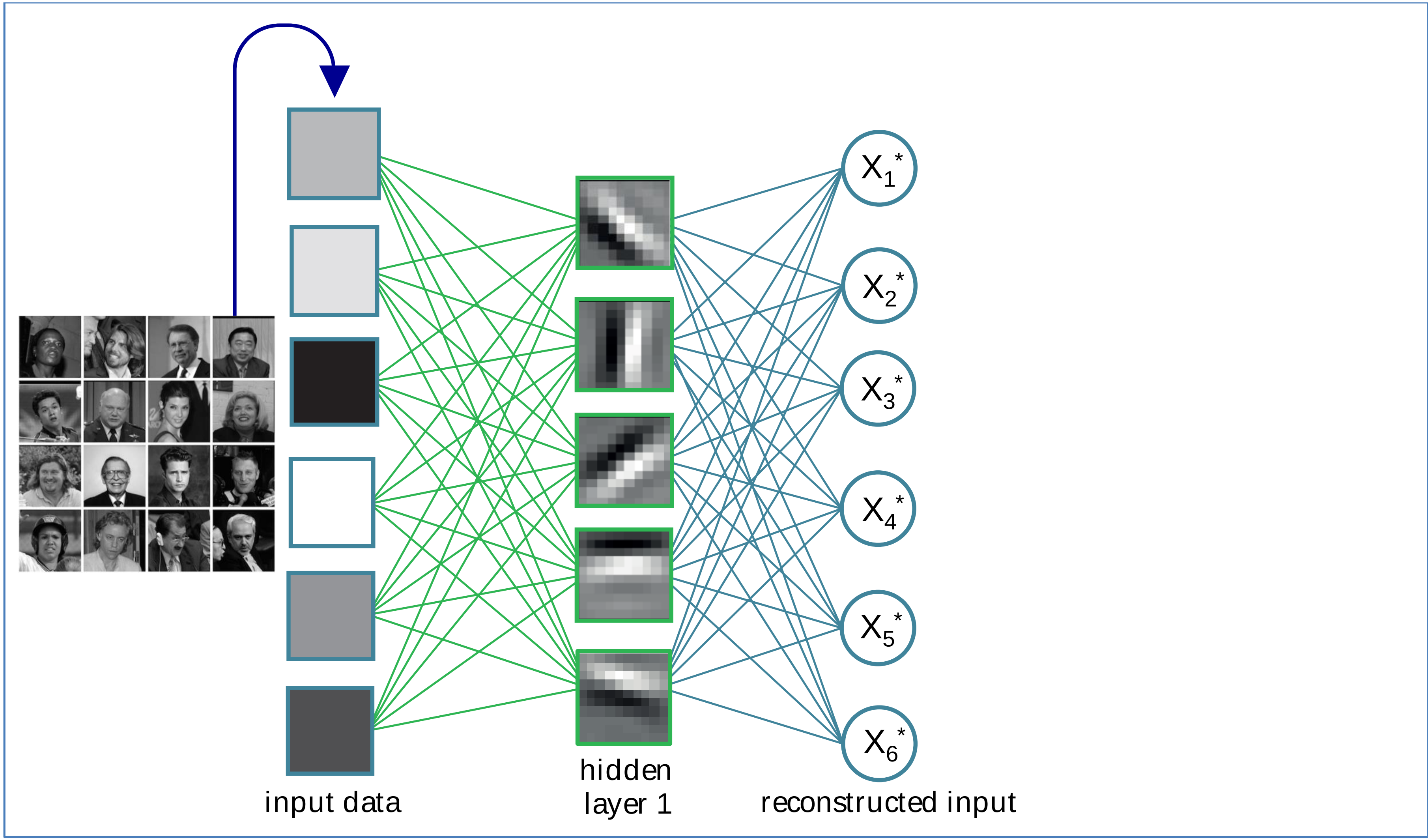


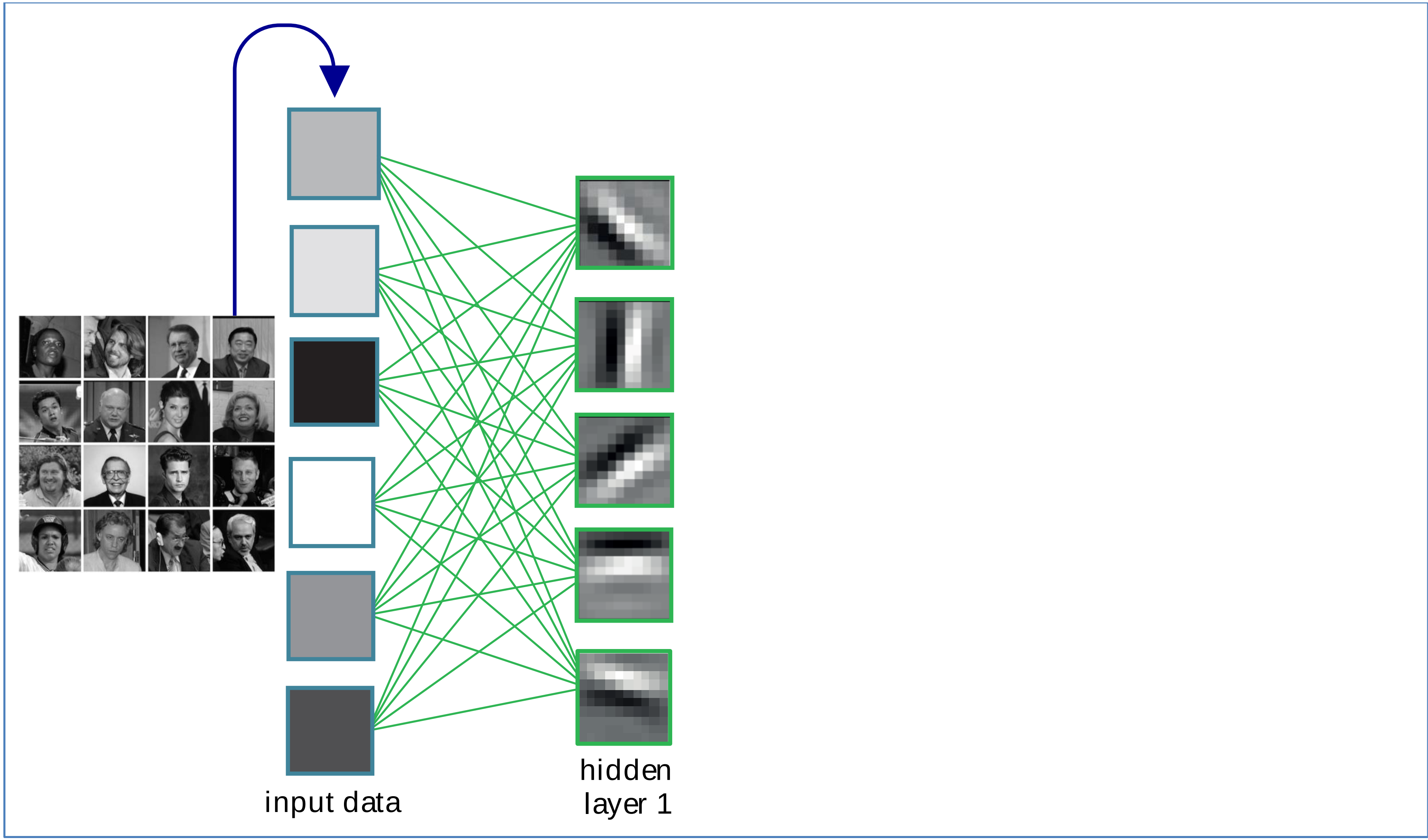
Use unsupervised pre-training to find a function from the input to itself



Hidden units can be interpreted as edges



Now: throw away reconstruction and input



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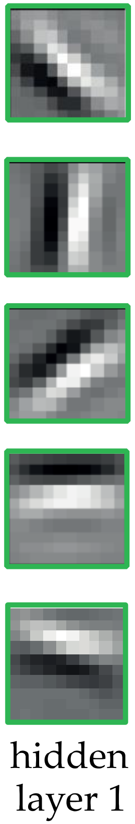
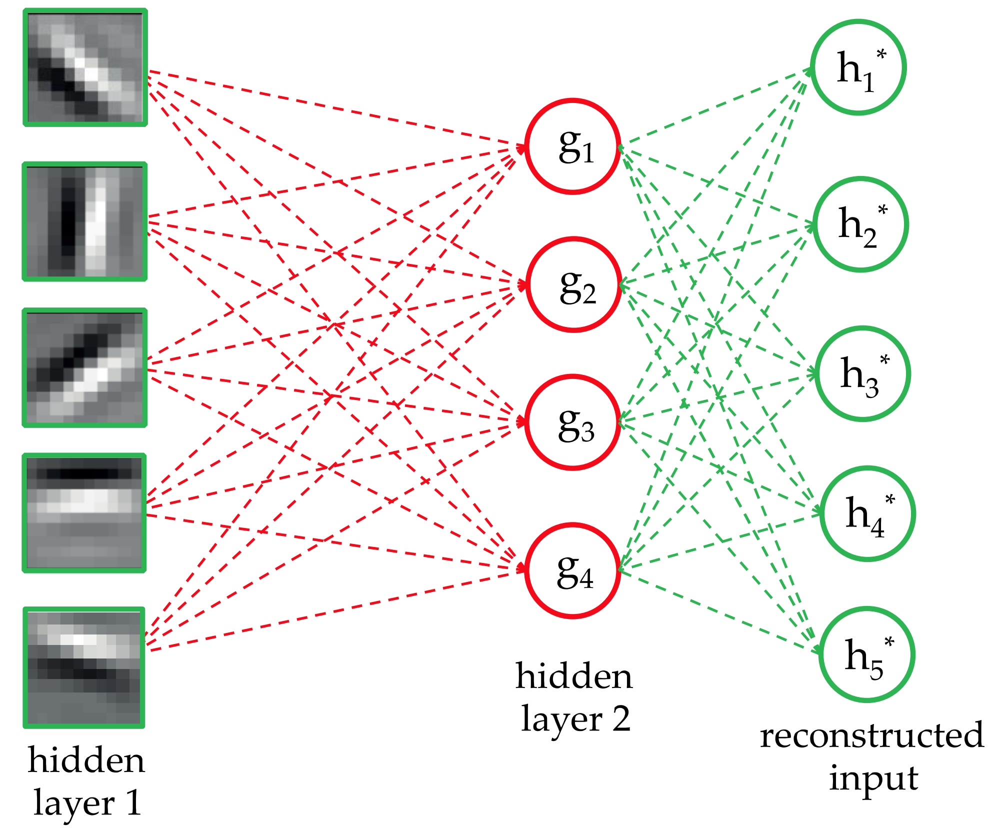


Then repeat the entire process for each layer



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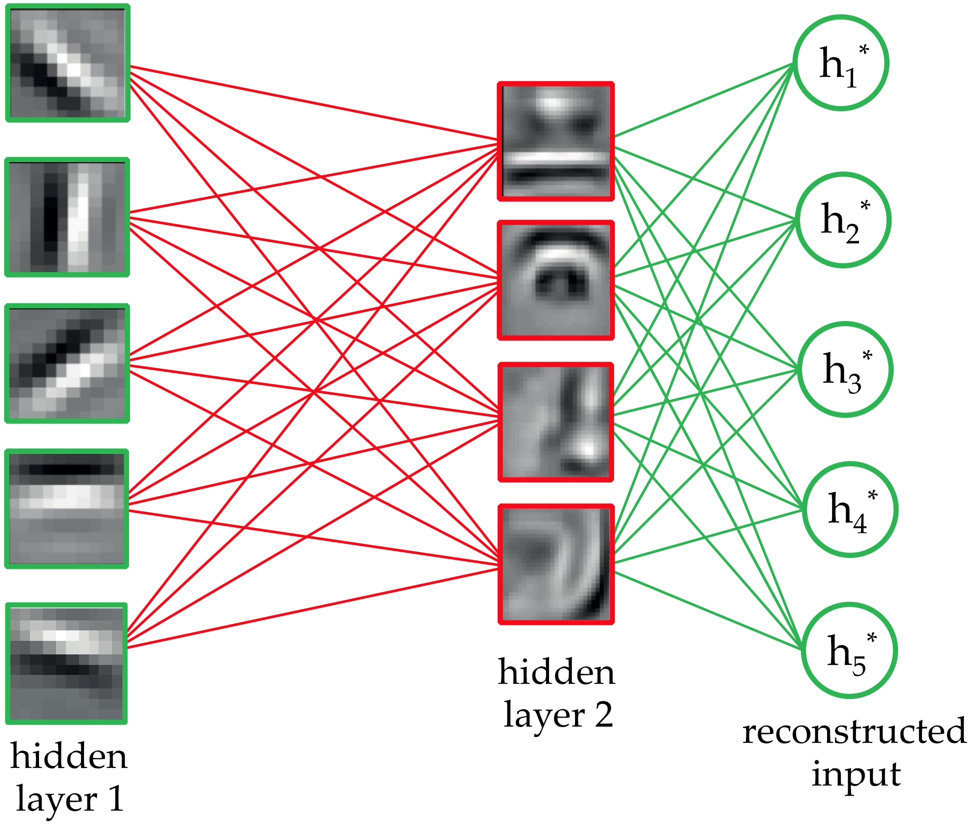

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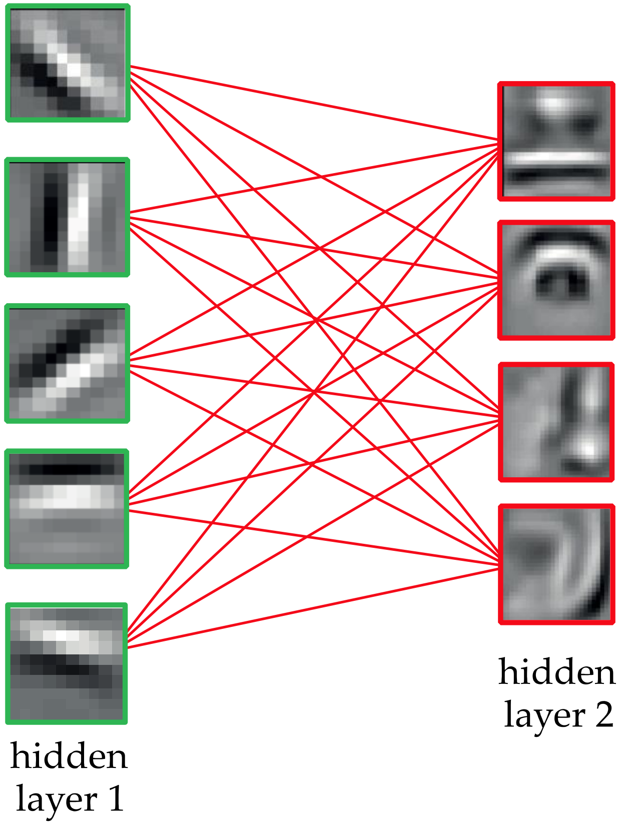

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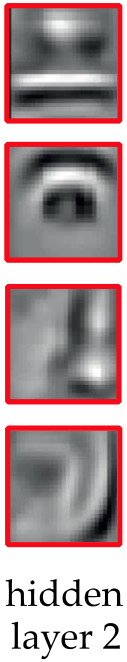
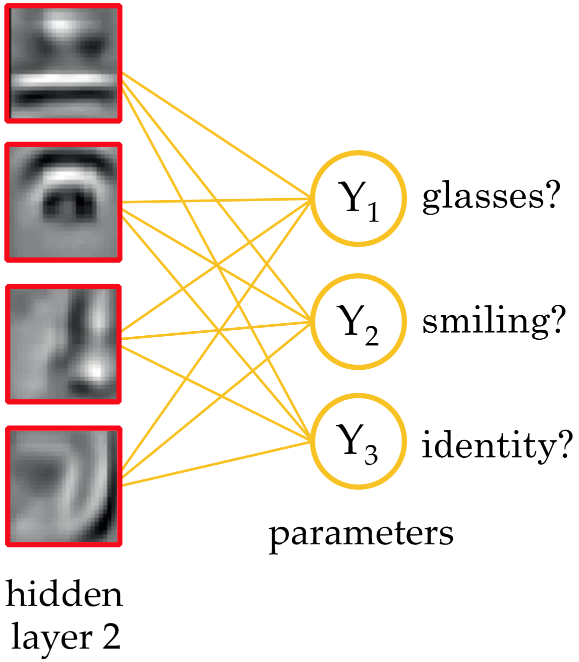
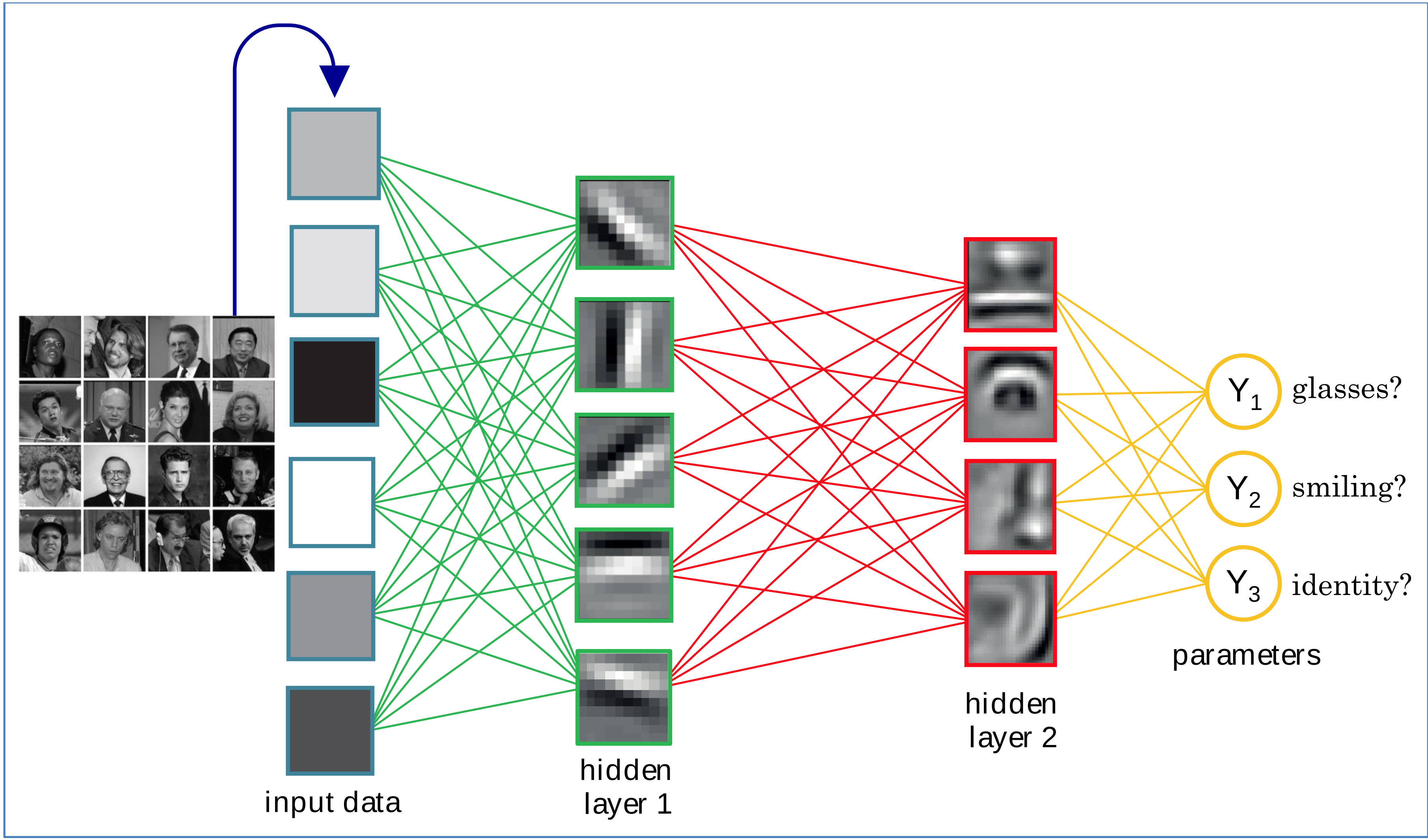


In the last layer, use the outputs (supervised)

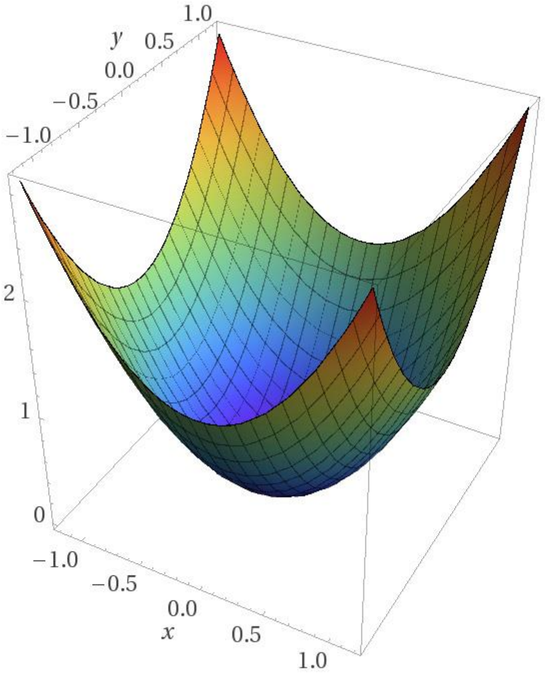


Finally, "fine-tune" the entire network!



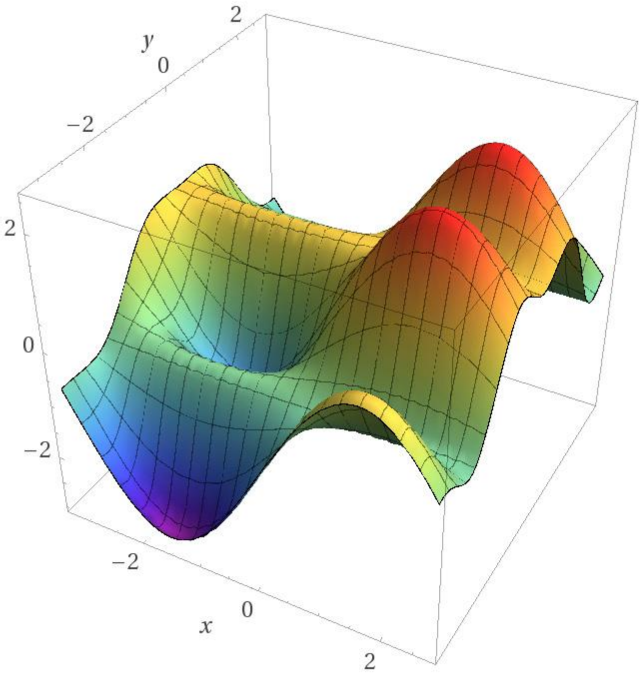
Takeaways

- As the number of parameters grows, a non-convex function often has more and more local minima
- Starting at a “good” point is crucial!



Computed by Wolfram|Alpha

Convex



Computed by Wolfram|Alpha

Non-convex

Image: O’Reilly Media

Takeaways

- Unsupervised pre-training uses latent structure in the data as a starting point for weight initialization

- After this process, the network is “fine-tuned”

- In practice this has been found to increase accuracy on specific tasks (which could be specified after feature learning)

Weight initialization

- We still have to initialize the pre-training

- All 0's initialization is bad! Causes nodes to compute the same outputs, so then the weights go through the same updates during gradient descent

- Need asymmetry! => usually use small random values

Mini-batches

- So far in this class, we have considered *stochastic gradient descent*, where one data point is used to compute the gradient and update the weights

- On the flipside is *batch gradient descent*, where we compute the gradient with respect to all the data, and then update the weights

- A middle ground uses *mini-batches* of examples before updating the weights

Notes about scores and softmax

- The output of the final fully connected layer is a vector of length *K* (number of classes)

Notes about scores and softmax

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- The raw scores are transformed into probabilities using the *softmax function*: (let s_k be the score for class *k*)

$$\hat{y}_k = \frac{e^{s_k}}{\sum_{j=1}^{K} e^{s_j}}$$

- Then we apply *cross-entropy loss* to these probabilities

Motivation for moving away from FC architectures

- For a 32x32x3 image (very small!) we have *p*=3072 features in the input layer

- For a 200x200x3 image, we would have *p*=120,000! *doesn’t scale*

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- Fully connected networks do not explicitly account for the structure of an image and the correlations/ relationships between nearby pixels

Idea: 3D volumes of neurons

- Do not “flatten” image, keep it as a volume with *width*, *height*, and *depth*

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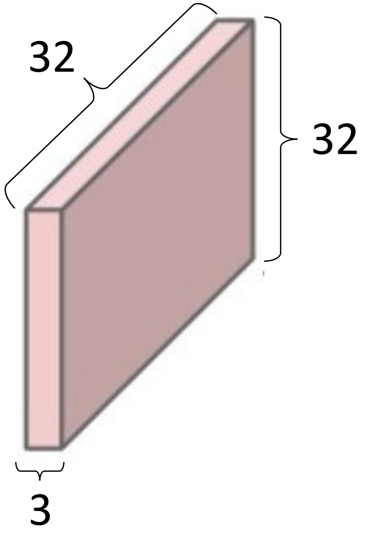

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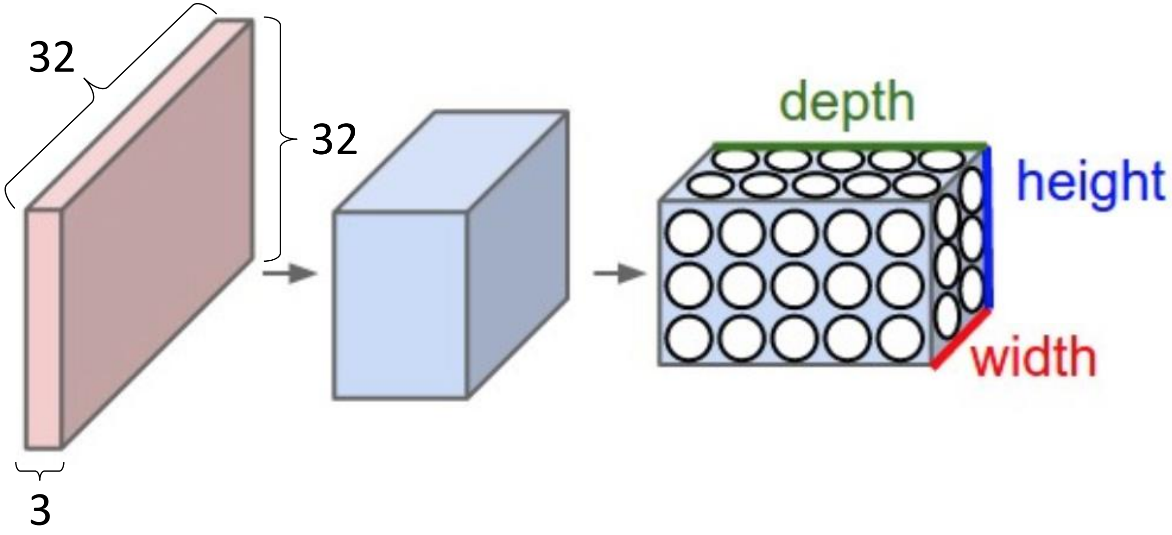

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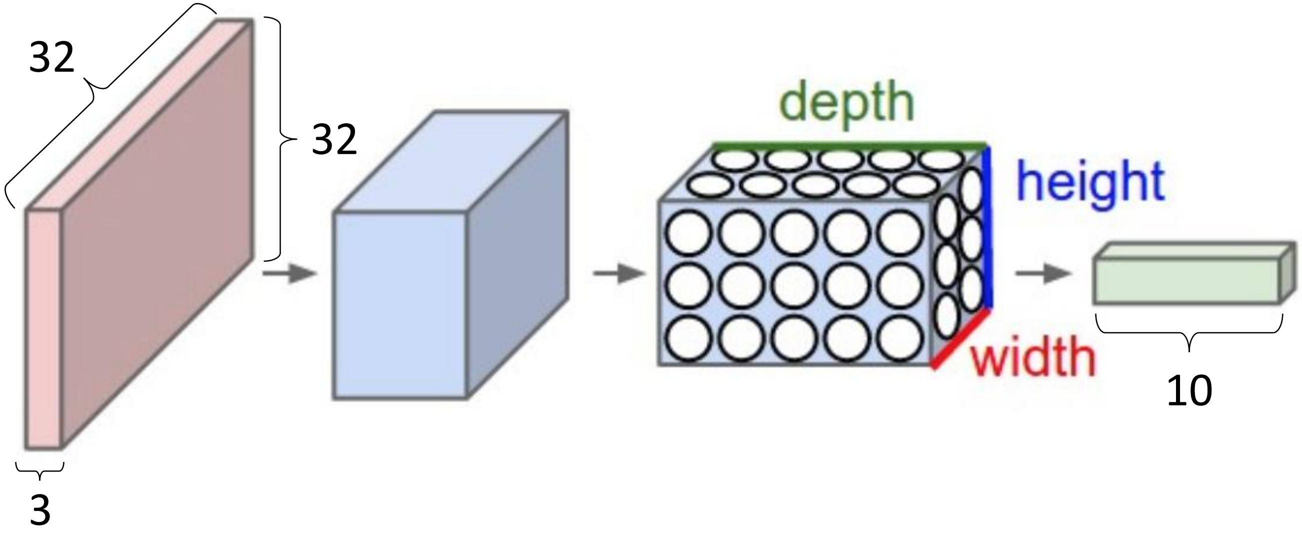
- Each layer is also a 3 dimensional volume
- The output layer is 1x1xC, where C is the number of classes (10 for CIFAR-10)



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