CS 360: Machine Learning

Prof. Sara Mathieson

Fall 2020

HAVERFORD COLLEGE

Admin

- Office hours **today 11-12pm** (stay on the link)
  - Will talk first to people I didn't get to in lab
- **Lab 8** due Friday Nov 20
  - Let me know if you would like individual deadlines
- After Thanksgiving – **two options for capstone**
  - Midterm 2 (midterm material ends Nov 20)
  - Final project (posted soon)
  - I will update grade percentages soon

Outline for November 13

- Introduction to neural networks
- Fully connected (FC) neural networks
- Convolutional neural networks (CNNs)
- Next week: more details on training NNs

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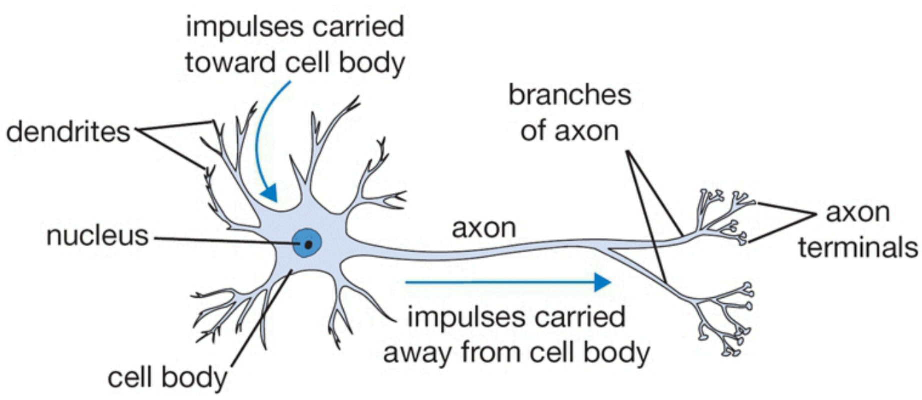
Biological Inspiration



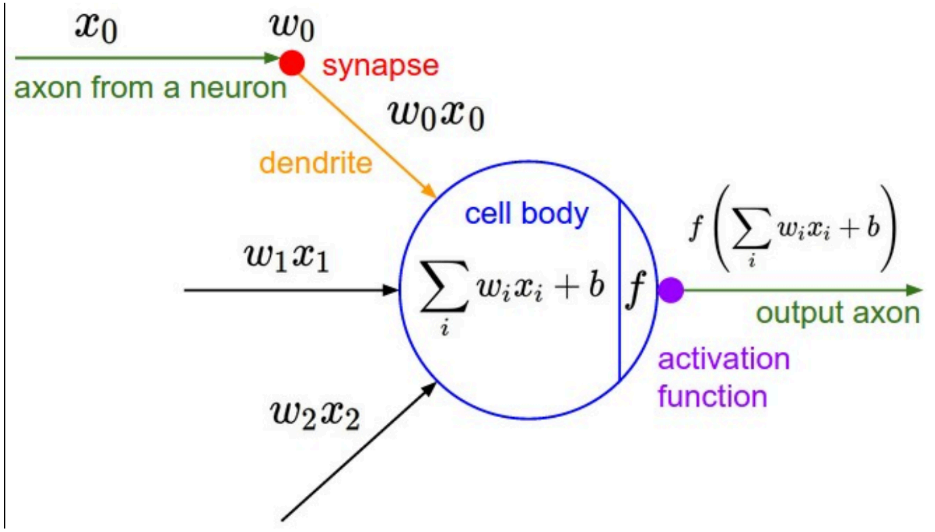


Figure: Stanford CS231n http://cs231n.github.io/neural-networks-1/

Goal: learn from complicated inputs

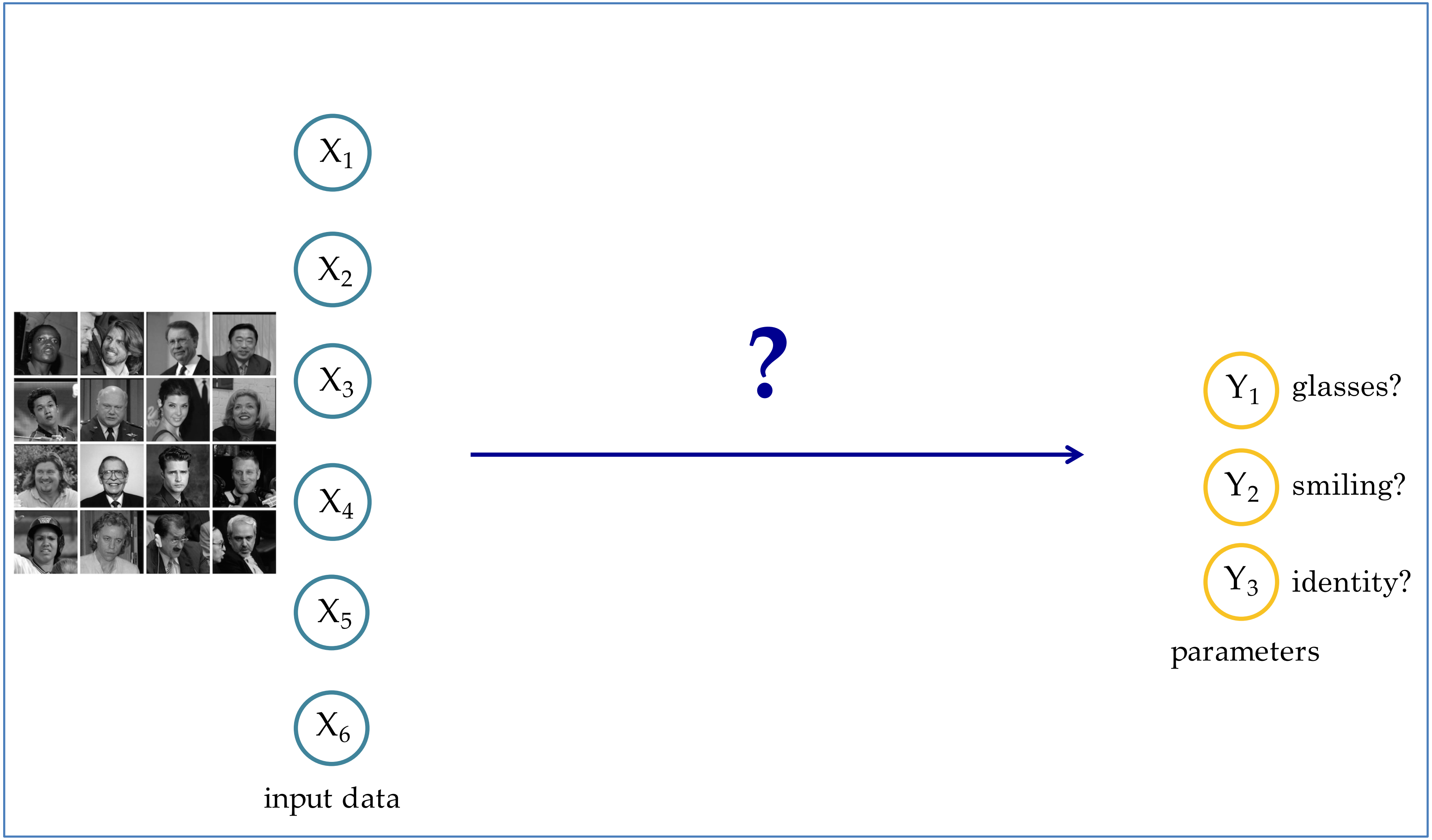
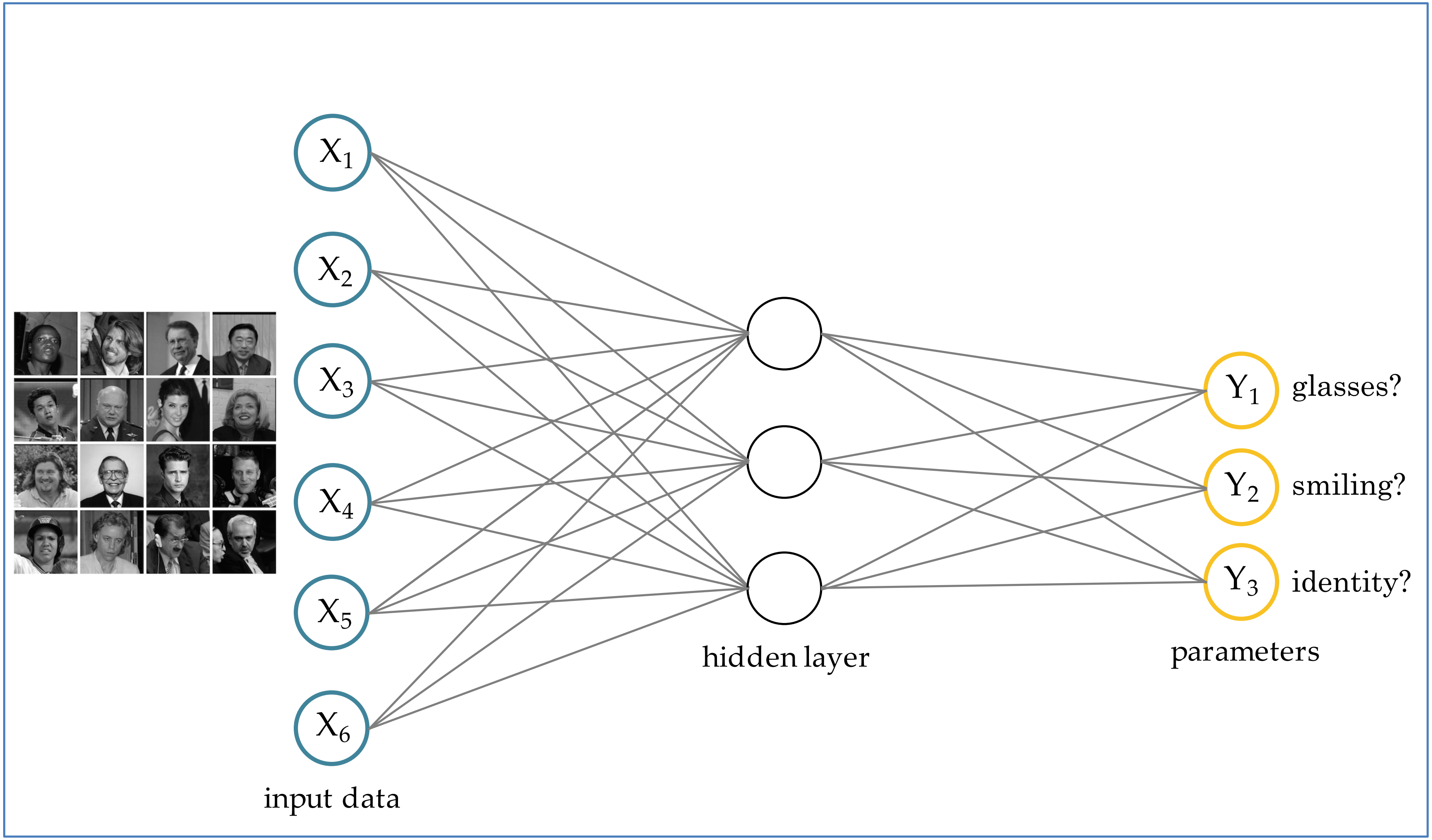


Image: Labeled Faces in the Wild (UMass)

Idea: transform data into lower dimension



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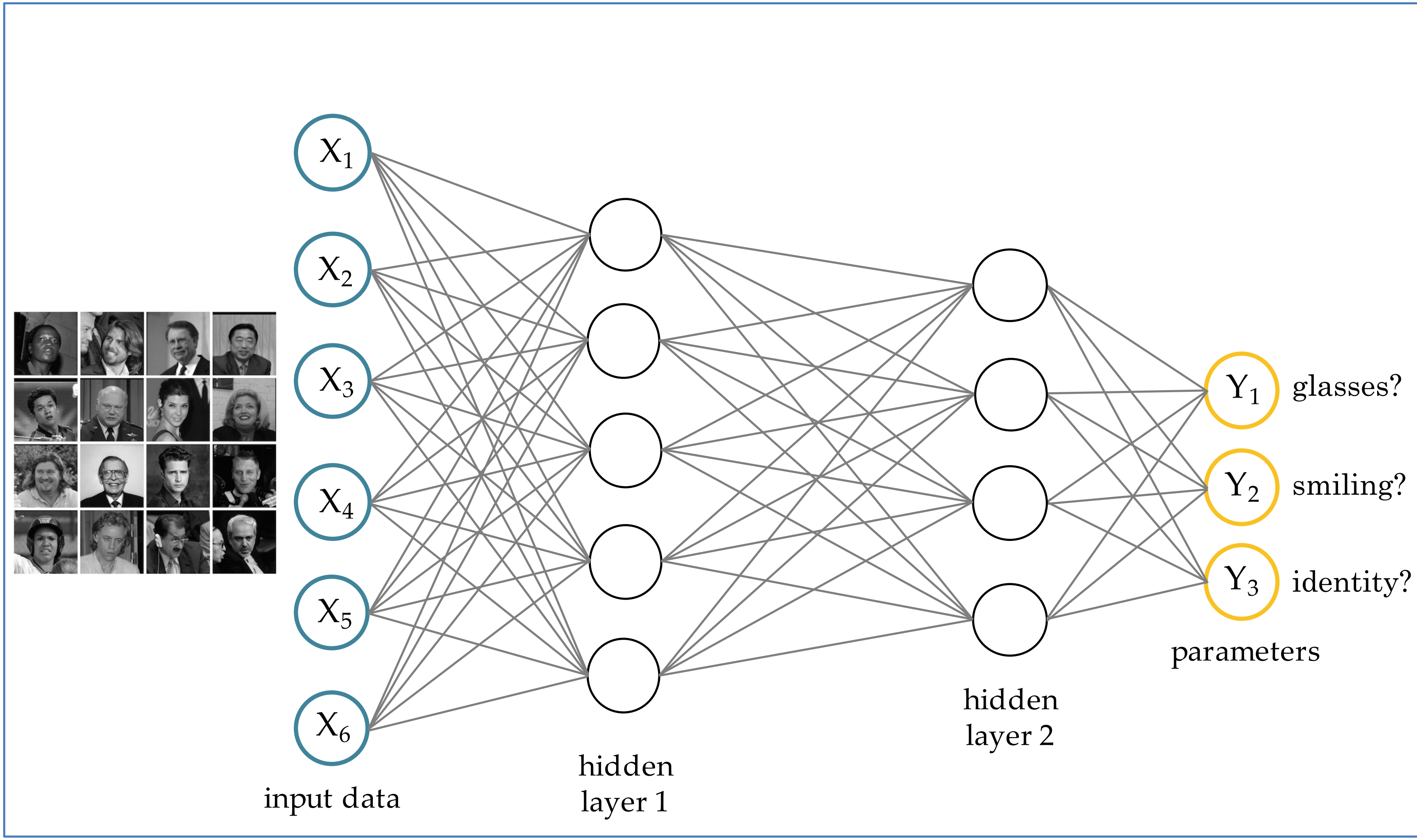
Multi-layer networks = “deep learning”



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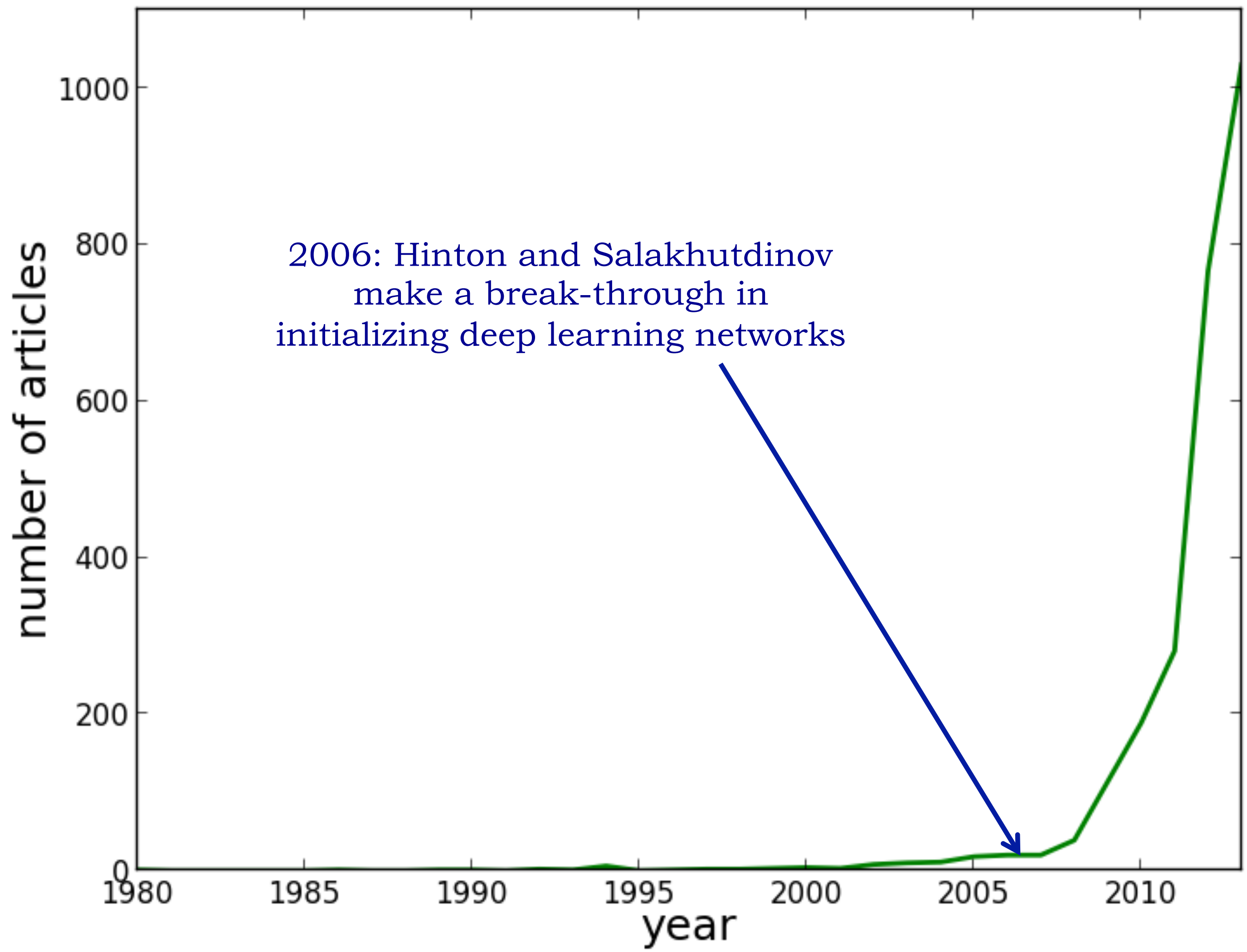
History of Neural Networks

- 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



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

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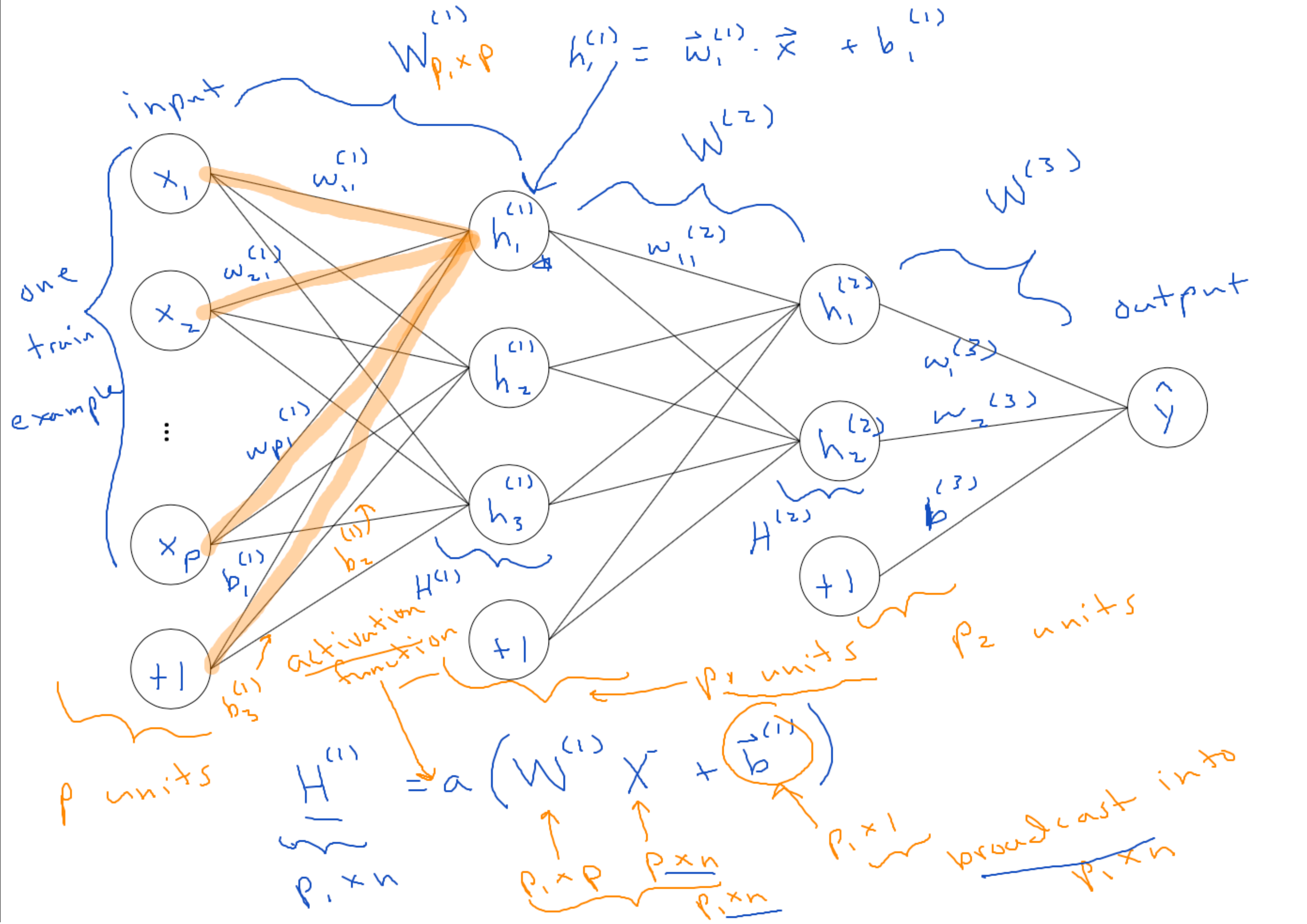
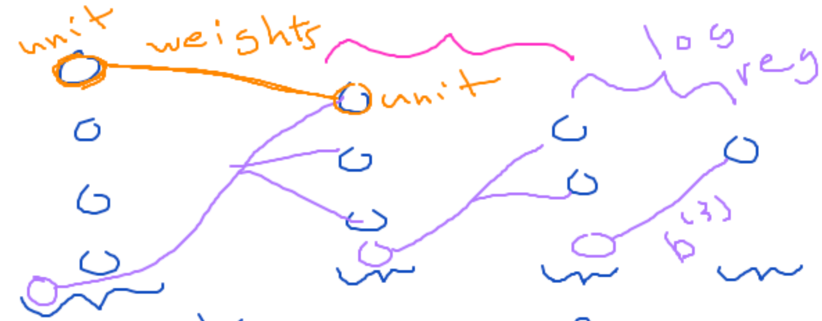
Fully Connected Neural Network Architecture



Fully Connected Neural Network Architecture

input

$$X = \begin{bmatrix} | & | & & | \\ \vec{x}_1 & \vec{x}_2 & \cdots & \vec{x}_n \\ | & | & & | \end{bmatrix}_{p \times n}$$



$$\underset{p_1 \times n}{H^{(1)}} = a\left(\underset{p_1 \times p}{W^{(1)}}\ \underset{p \times n}{X} + \underset{p_1 \times 1}{\vec{b}^{(1)}}\right)$$

$$\underset{p_2 \times n}{H^{(2)}} = a\left(\underset{p_2 \times p_1}{W^{(2)}}\ \underset{p_1 \times n}{H^{(1)}} + \underset{p_2 \times 1}{\vec{b}^{(2)}}\right)$$

$$\underset{1 \times n}{\hat{\vec{y}}} = a\left(\underset{1 \times p_2}{W^{(3)}}\ \underset{p_2 \times n}{H^{(2)}} + \underset{1 \times 1}{b^{(3)}}\right)$$

scalar

prediction

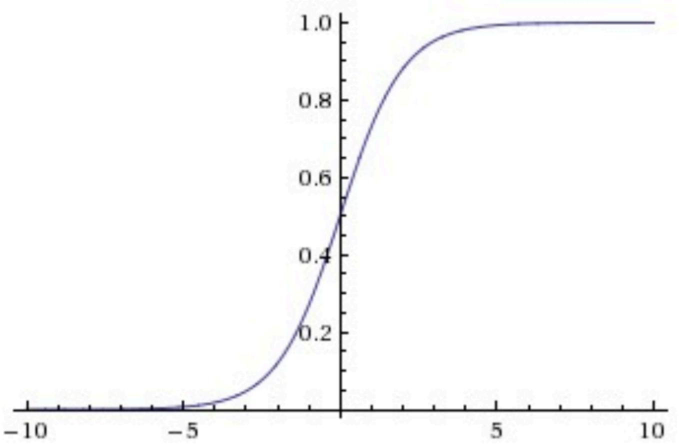
activation function

element-wise

Option 1: sigmoid function

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

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



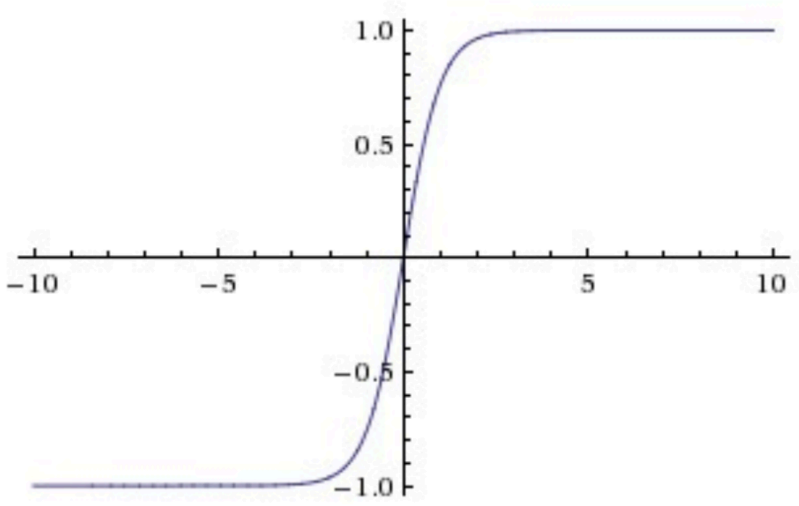
- Derivative is convenient

$$\sigma'(x) = \sigma(x)(1 - \sigma(x))$$

Option 2: hyperbolic tangent

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

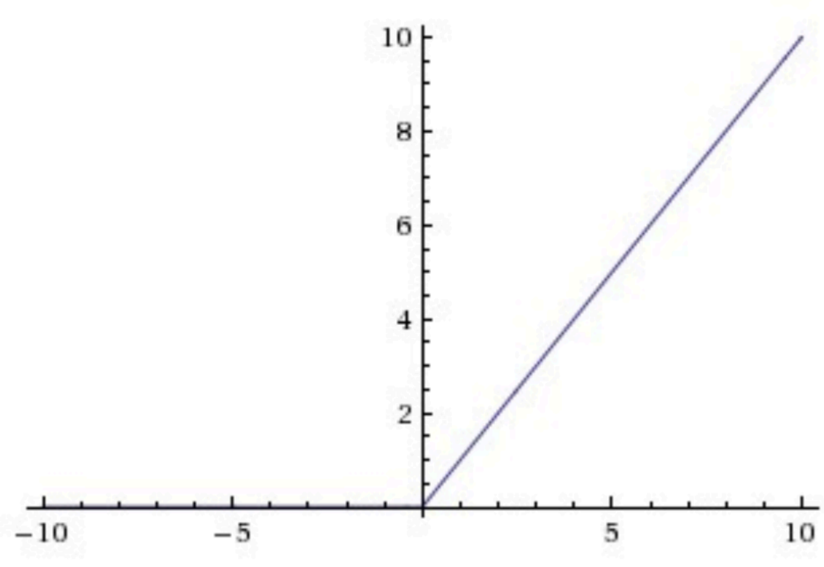
$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$



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 "die" (no signal) if input becomes too negative throughout gradient descent

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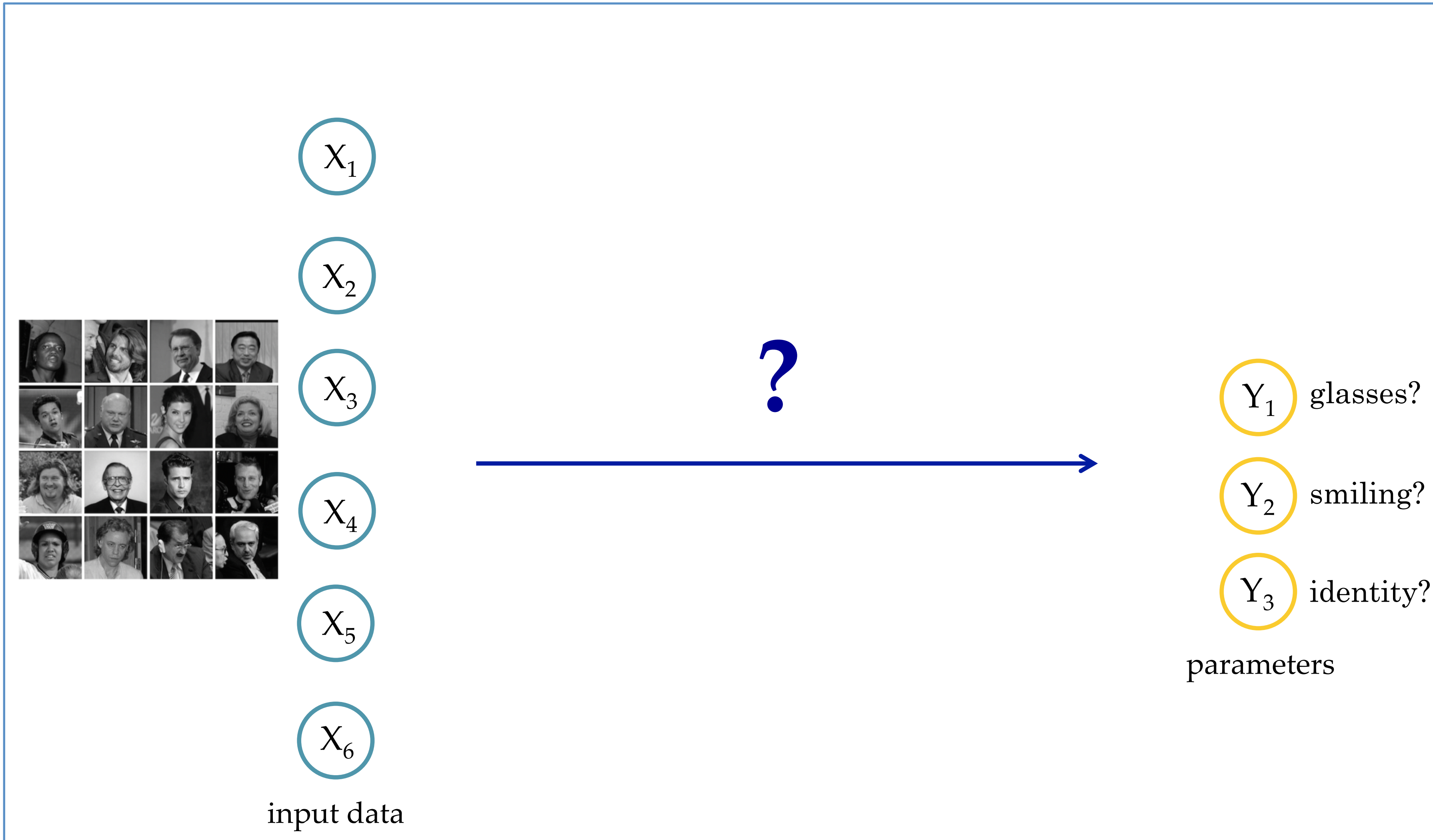
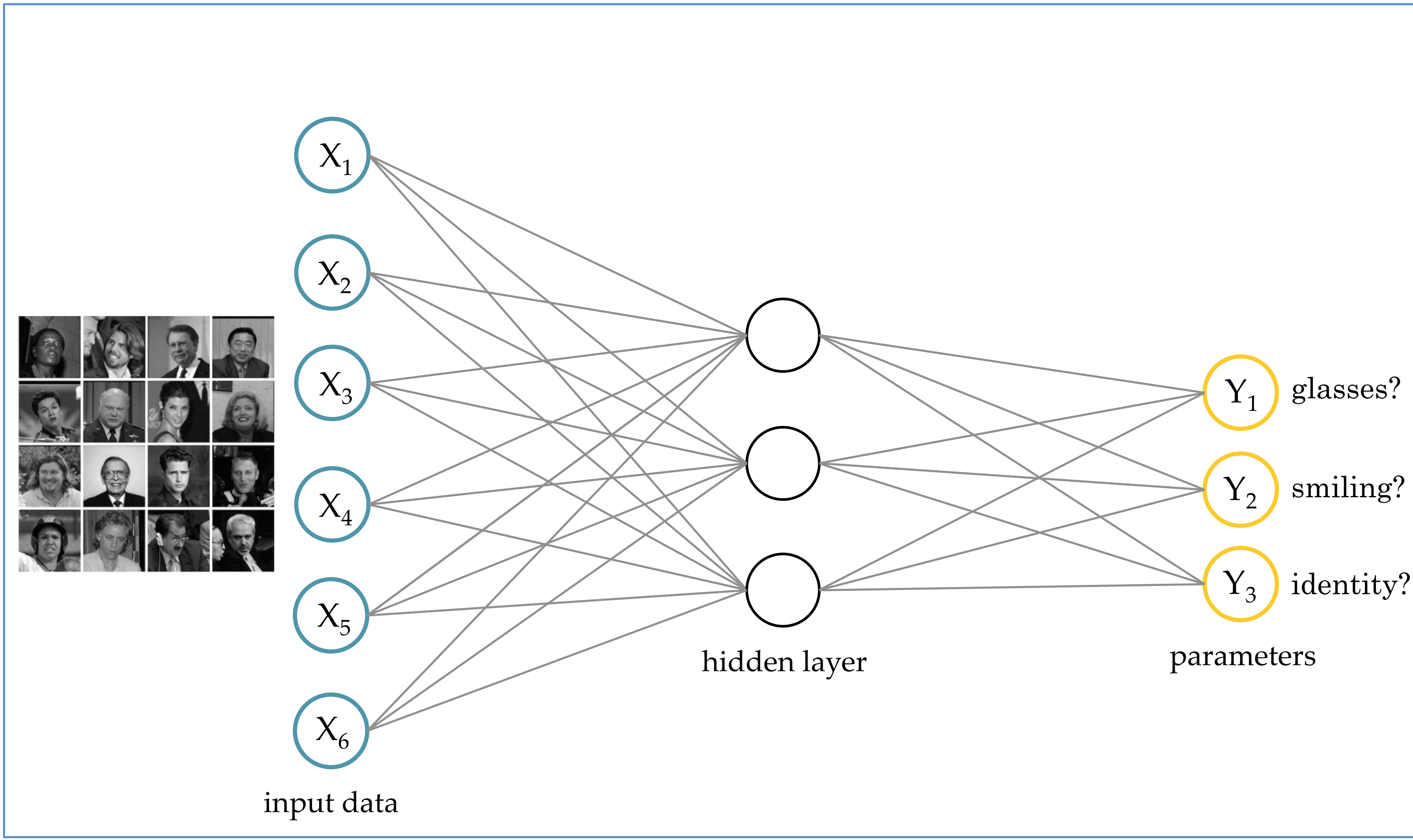
Cross Entropy Loss

NEXT TIME!

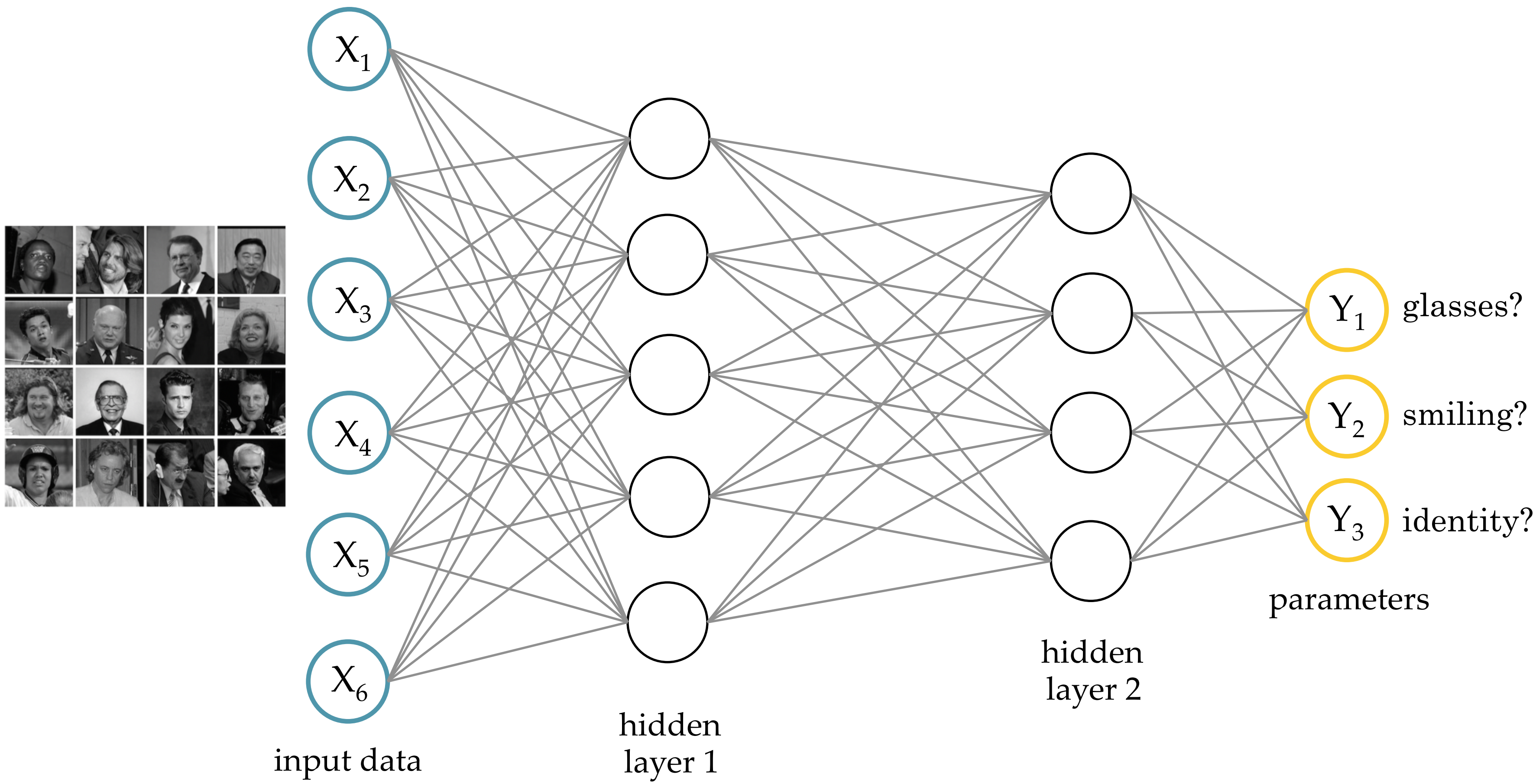
Goal: find a function between input and output



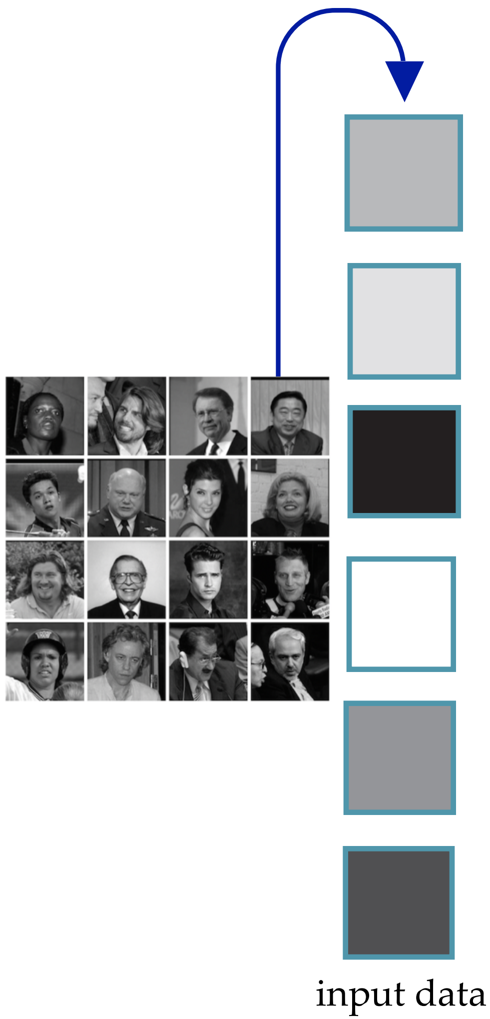
First idea: one hidden layer



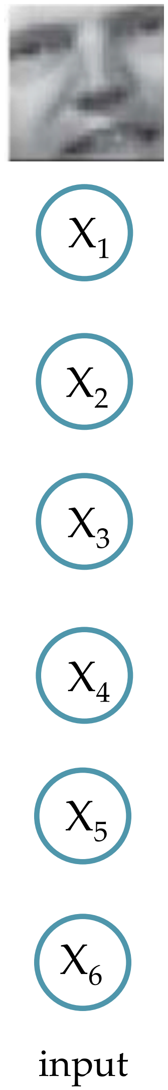
Second idea: more hidden layers (“deep” learning)



Flatten pixels of image into a single vector



Detour to autoencoders



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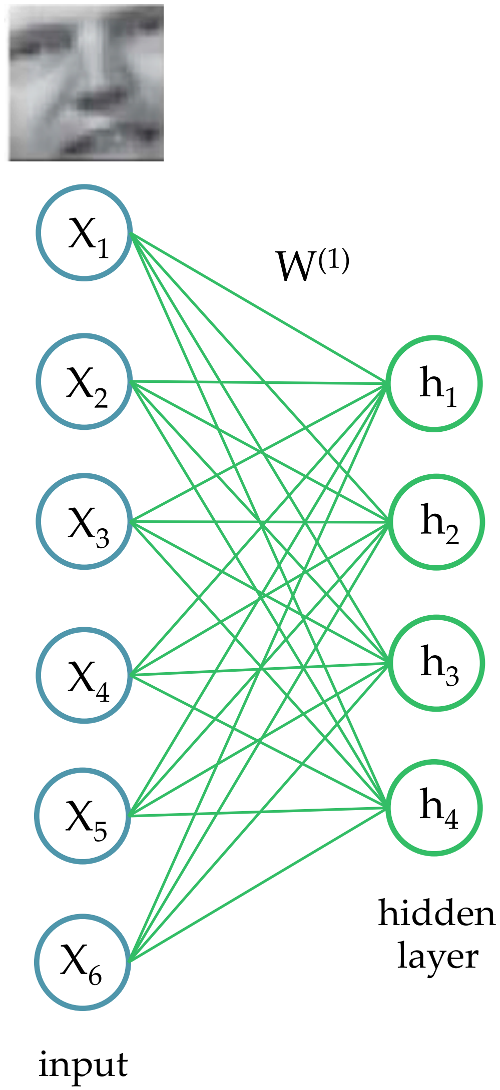

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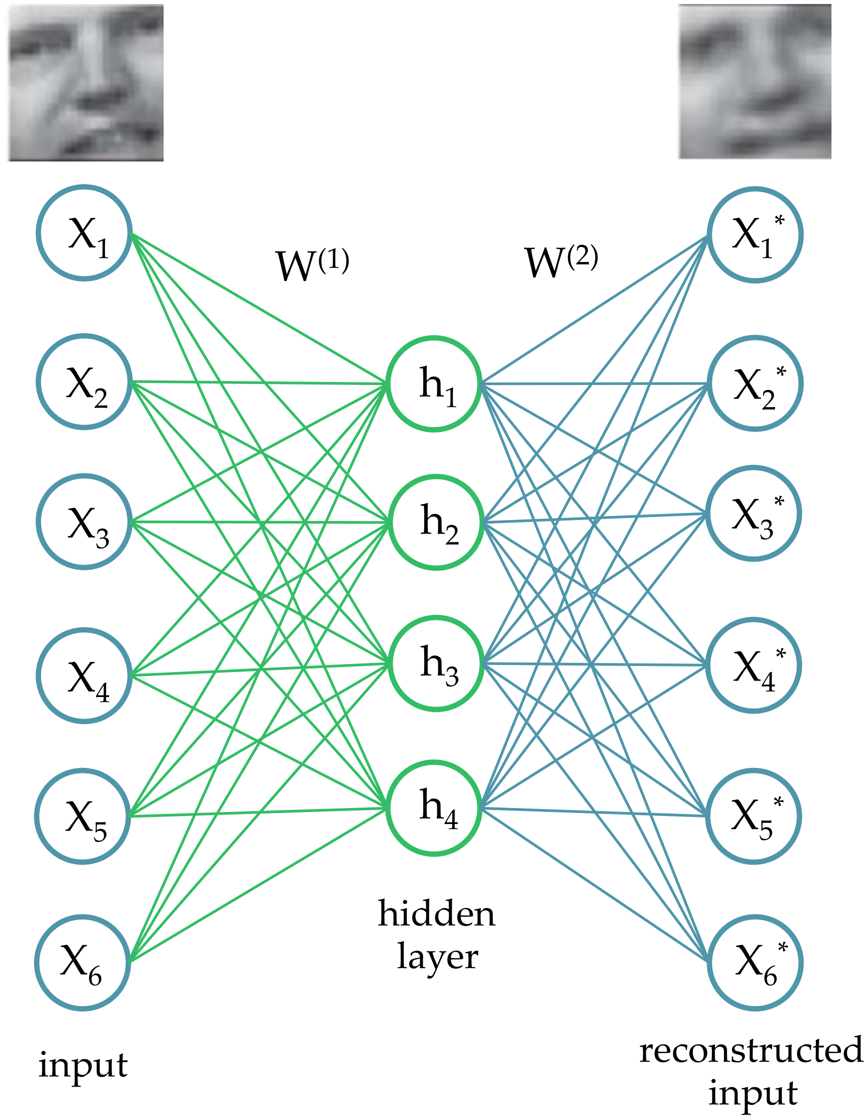

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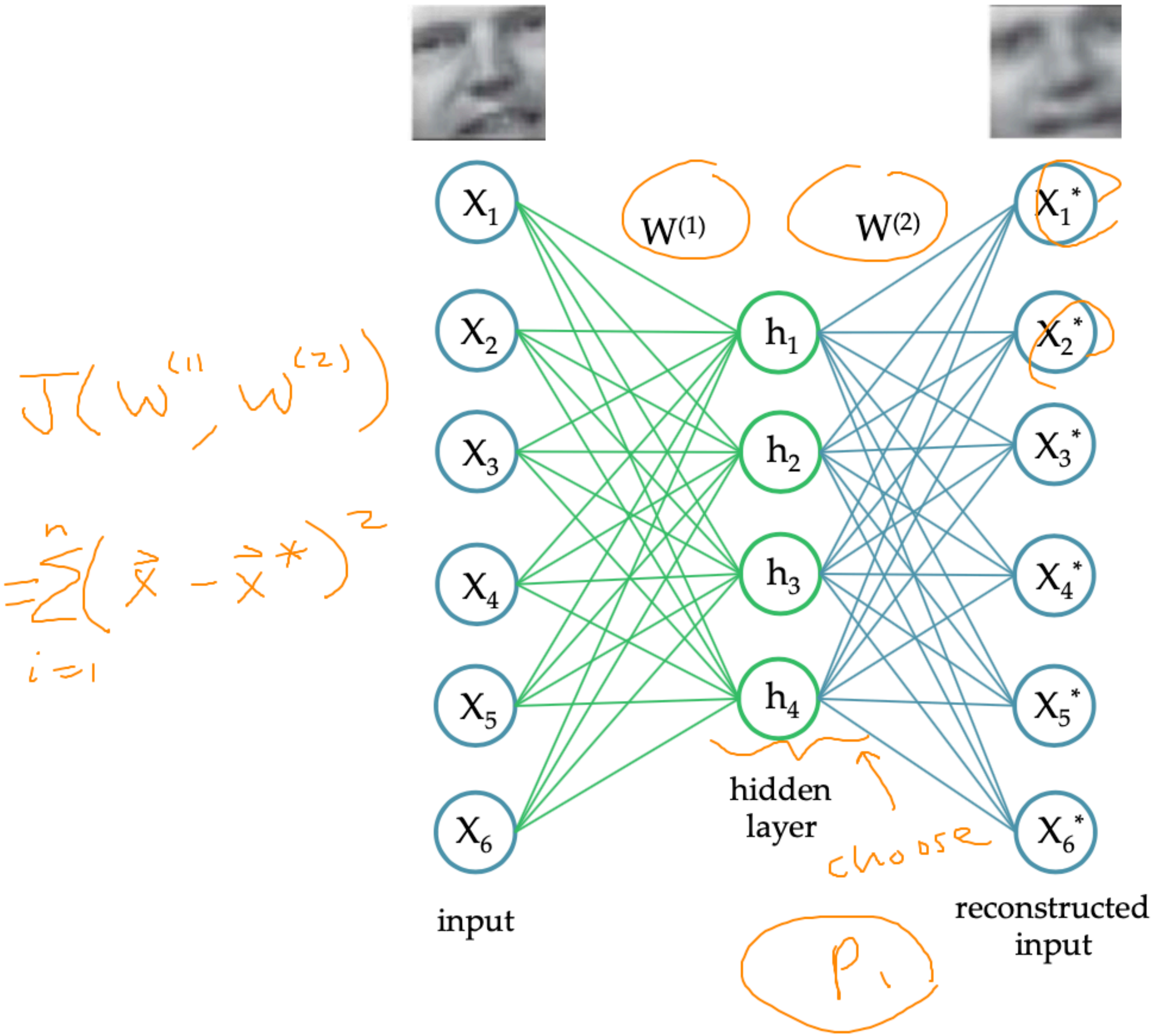
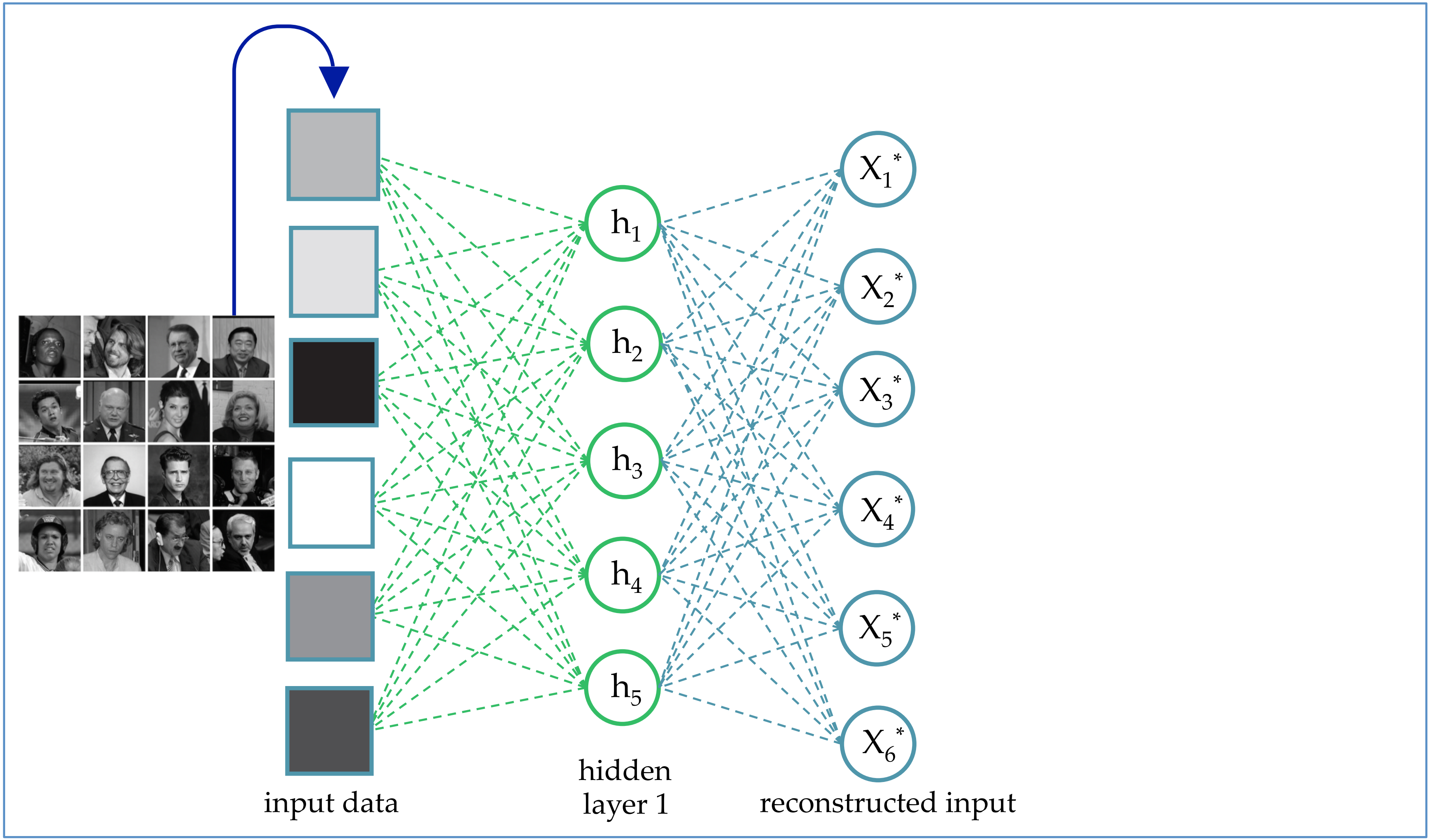
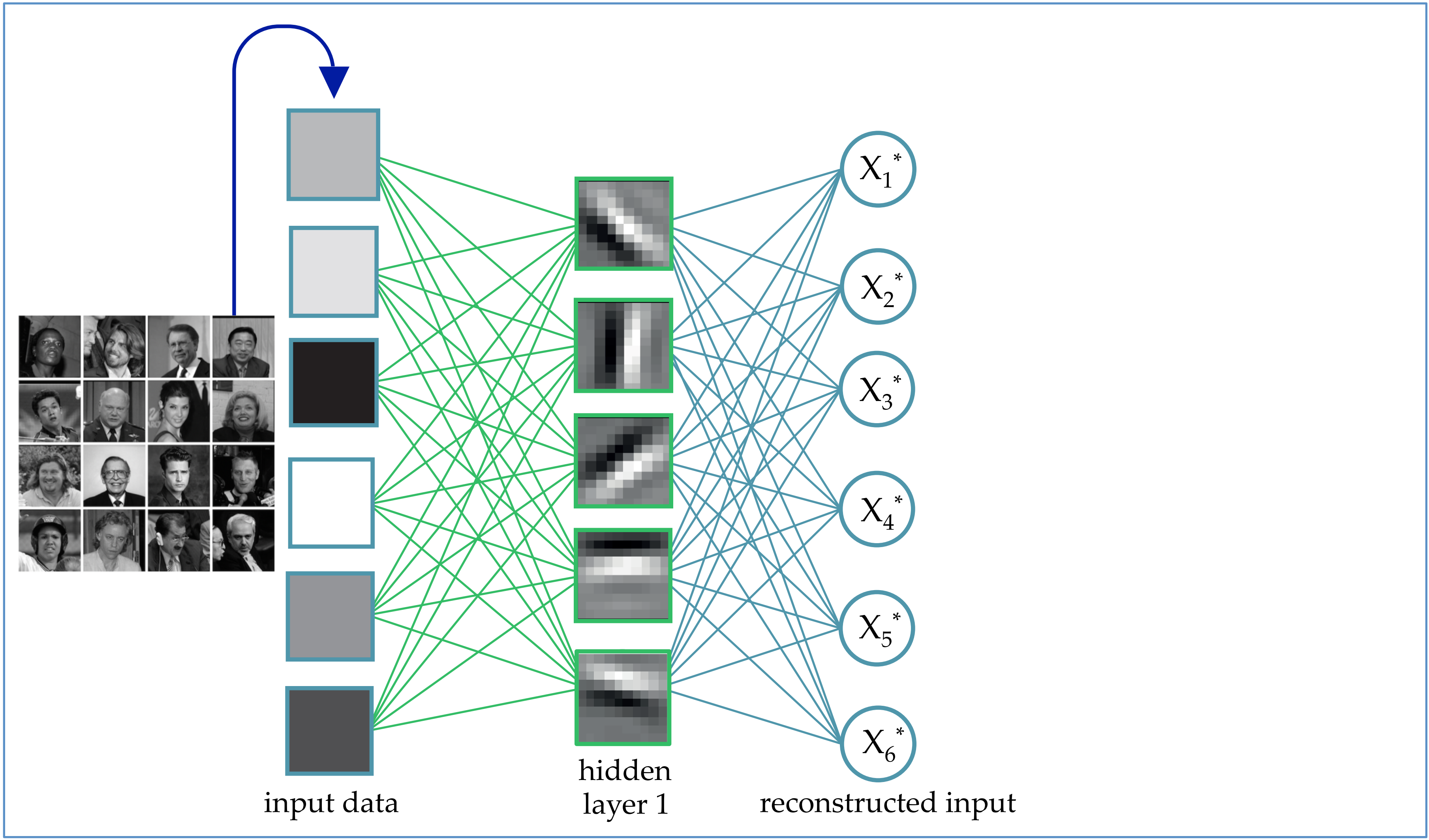


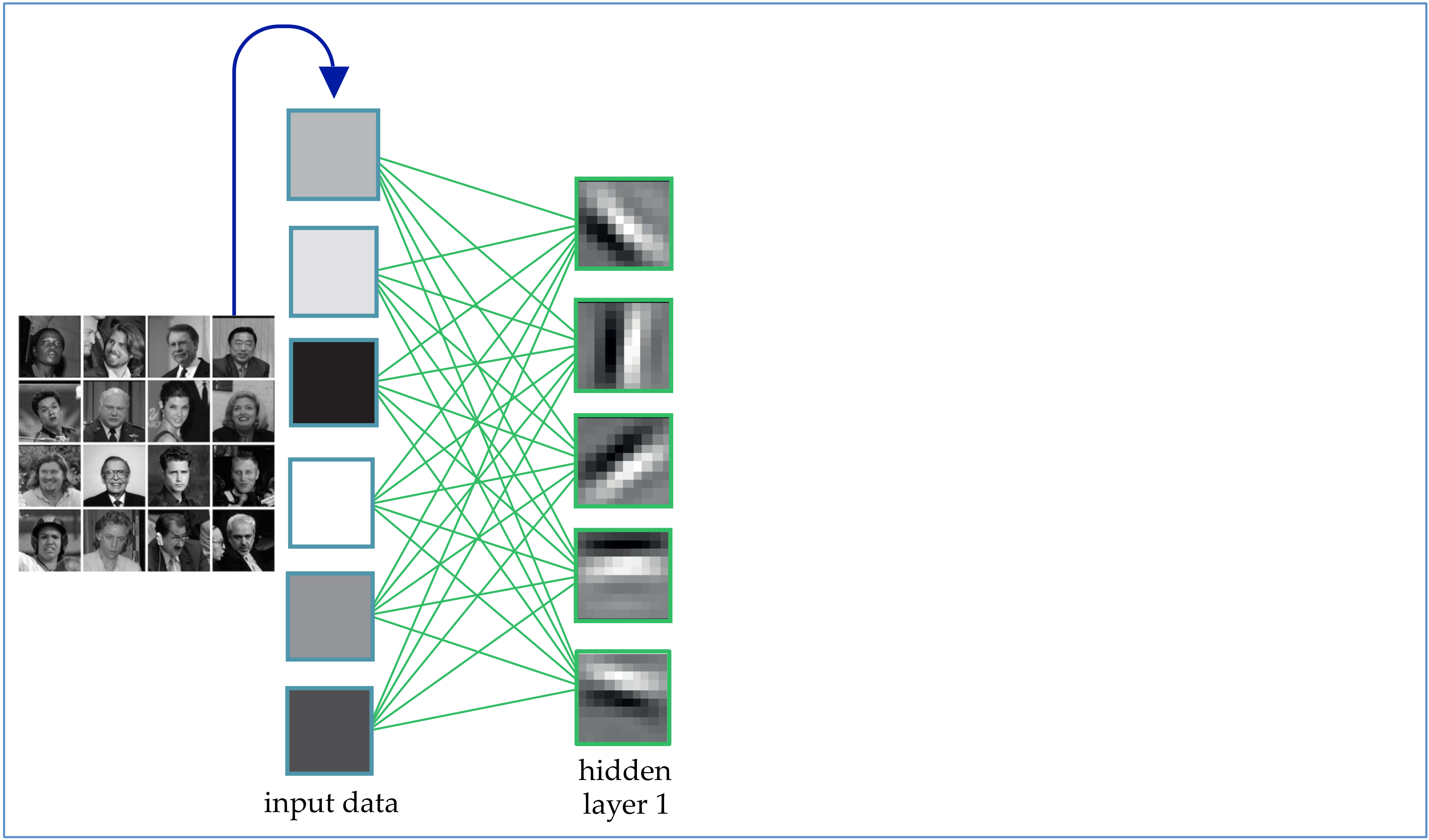
Use unsupervised pre-training to find a function from the input to itself



Hidden units can be interpreted as edges



Now: throw away reconstruction and input



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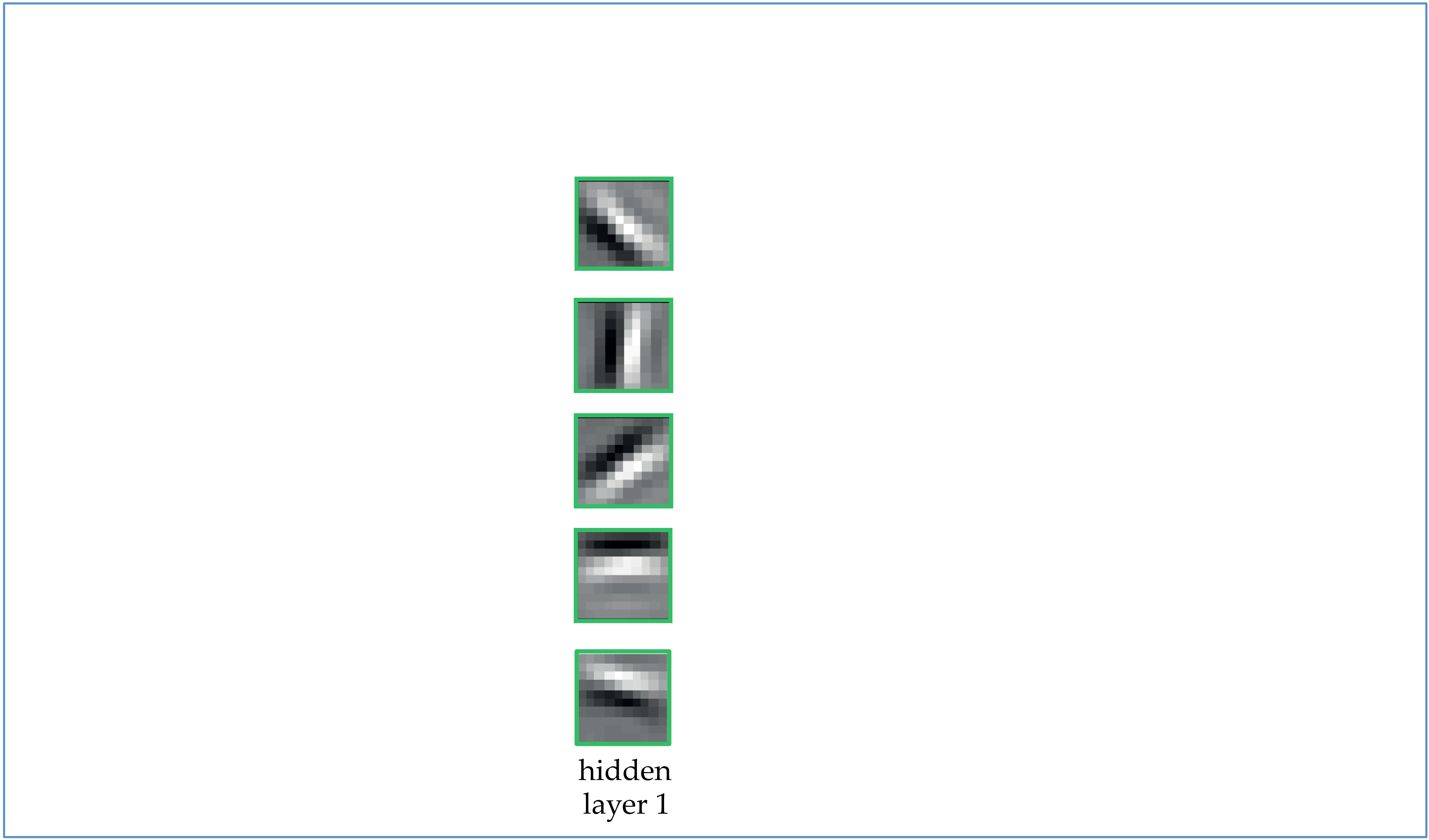
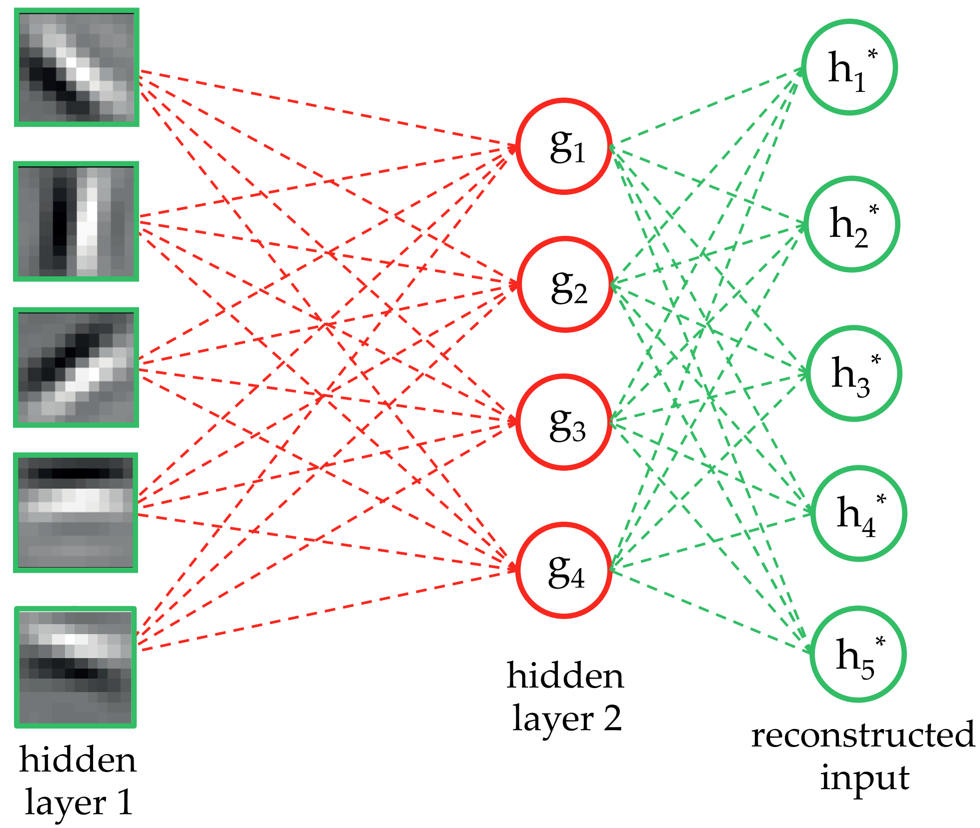


Then repeat the entire process for each layer



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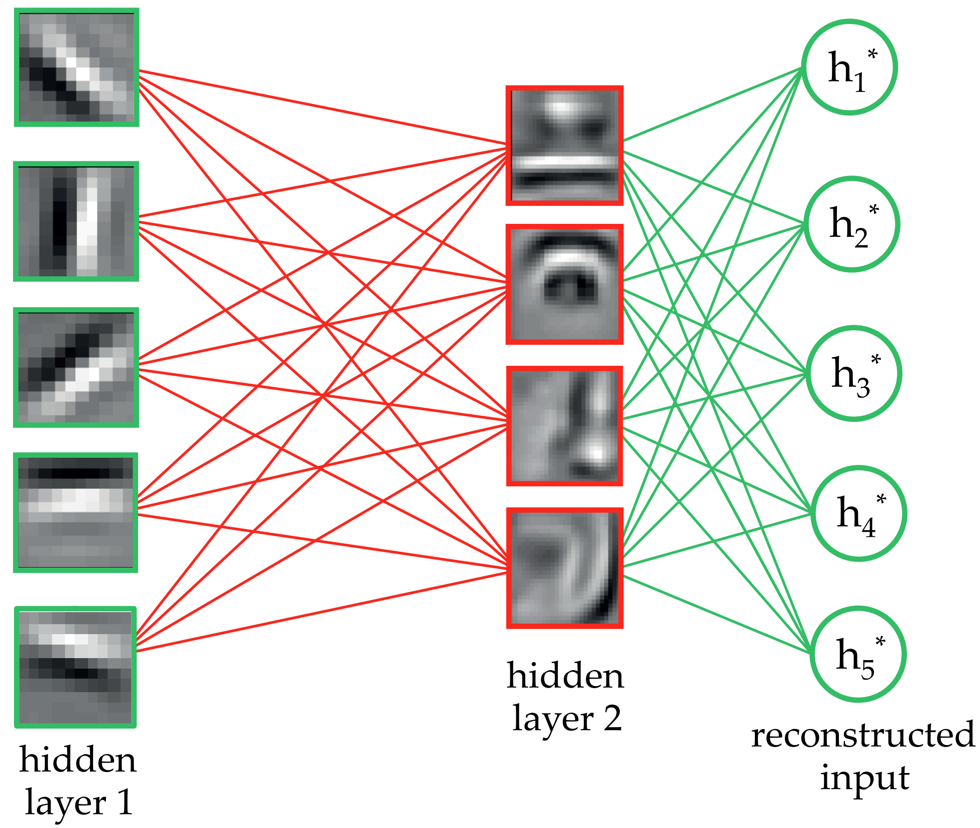

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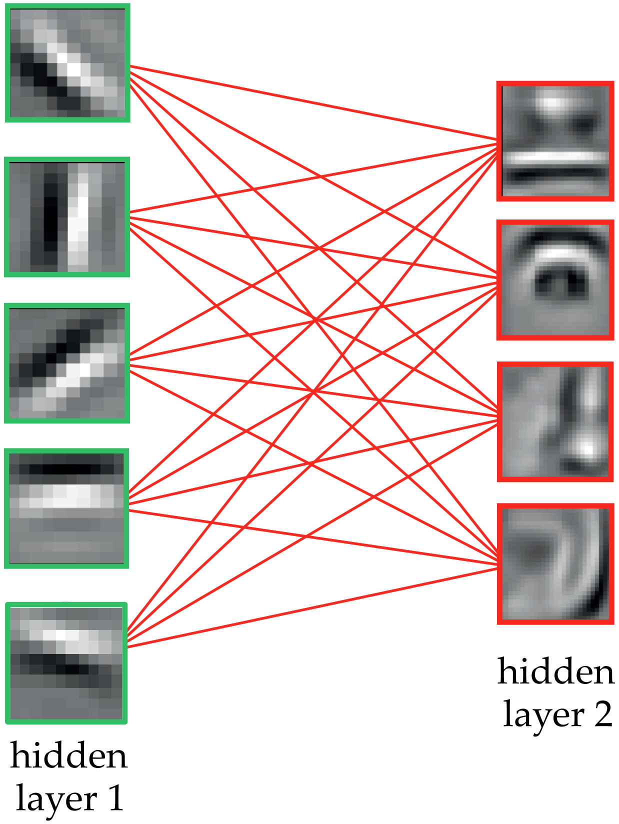

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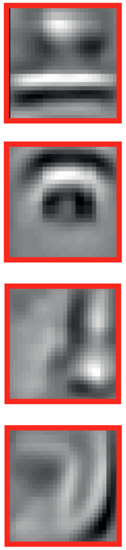
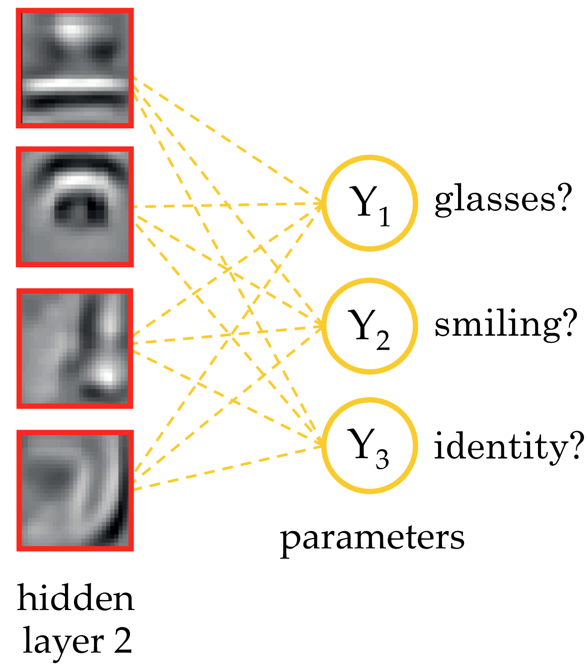


hidden
layer 2

In the last layer, use the outputs (supervised)



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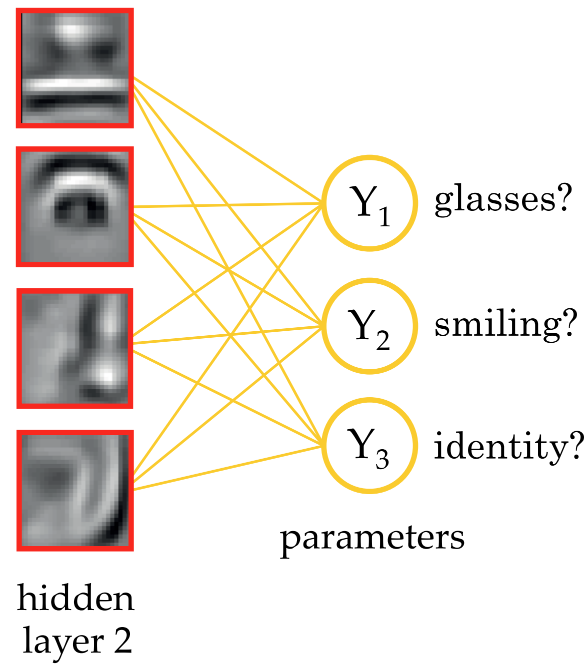
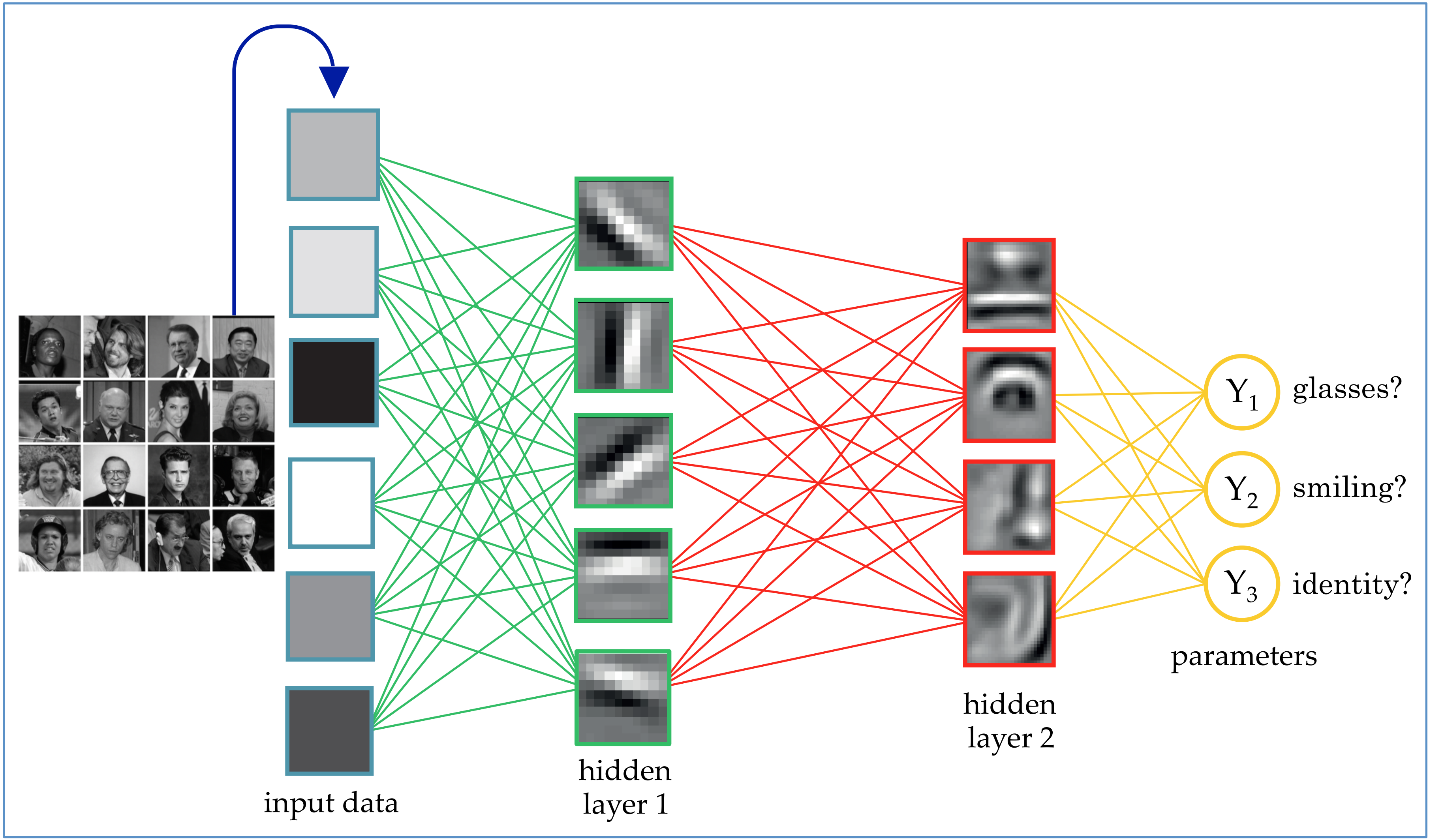
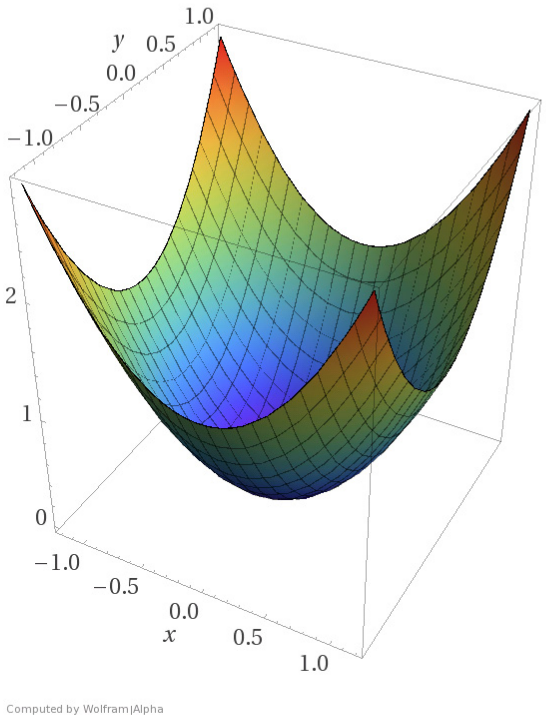


Finally, "fine-tune" the entire network!

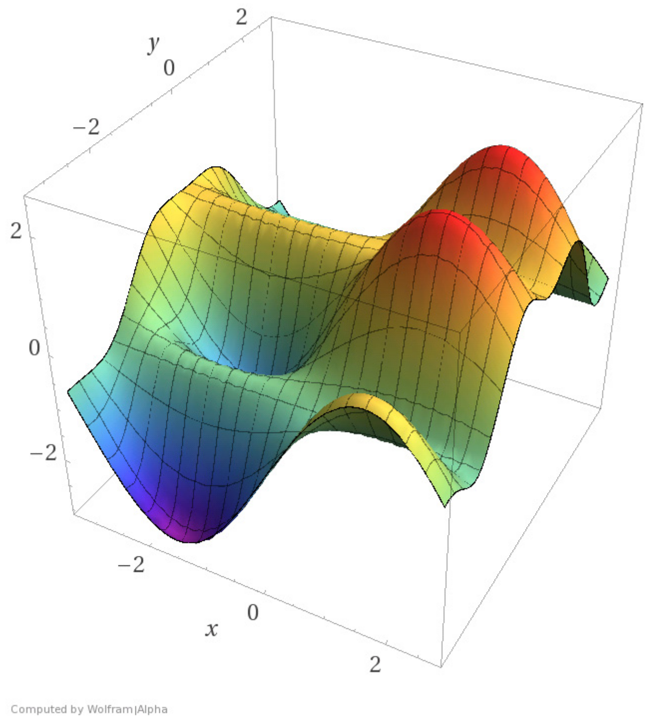


Takeaways

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



Convex



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)

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- Unsupervised pre-training uses latent structure in the data as a starting point for weight initialization
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- In practice this has been found to increase accuracy on specific tasks (which could be specified after feature learning)

Recent Example: OpenAI's GPT-2

- "Language Models are Unsupervised Multitask Learners" https://d4mucfpksywv.cloudfront.net/better-language-models/language-models.pdf

- Decision not to release full model: https://openai.com/blog/better-language-models/

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. This is the approach we will use in Lab 8.

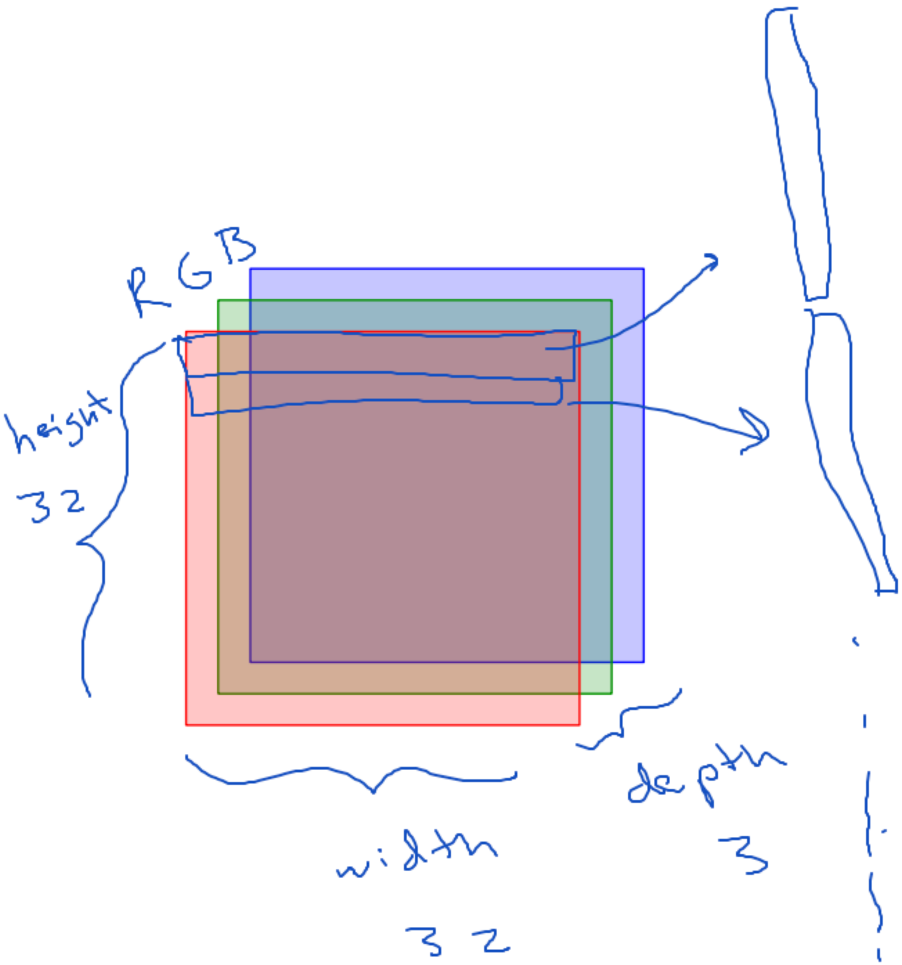
Lab 8 data pre-processing

- It is helpful to have our data be zero-centered, so we will subtract off the mean
- It is also helpful to have the features be on the same scale, so we will divide by the standard deviation
- We will compute the mean and std with respect to the *training data*, then apply the same transformation to all datasets

Lab 8 data pre-processing

- Input is now itself a multi-dimensional array
- For images, often the shape of each image will be (width, height, 3) for RGB channels
- Need to "*flatten*" or "unravel" for fully connected networks

Lab 8 Data



one data point

x.shape = (32, 32, 3)

mini-batch

X.shape = (64, 32, 32, 3)

fully connected

"flatten" unravel

$p = 32 \cdot 32 \cdot 3$

$= 3072$

Notes about scores and softmax

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

- 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

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Think about outside of class:
- Why do we use exp?
- Why don't we just take the max score?

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

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

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

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

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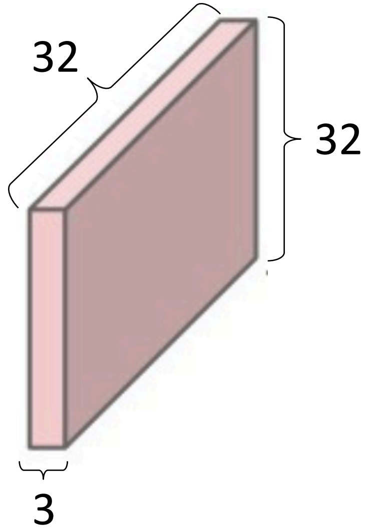

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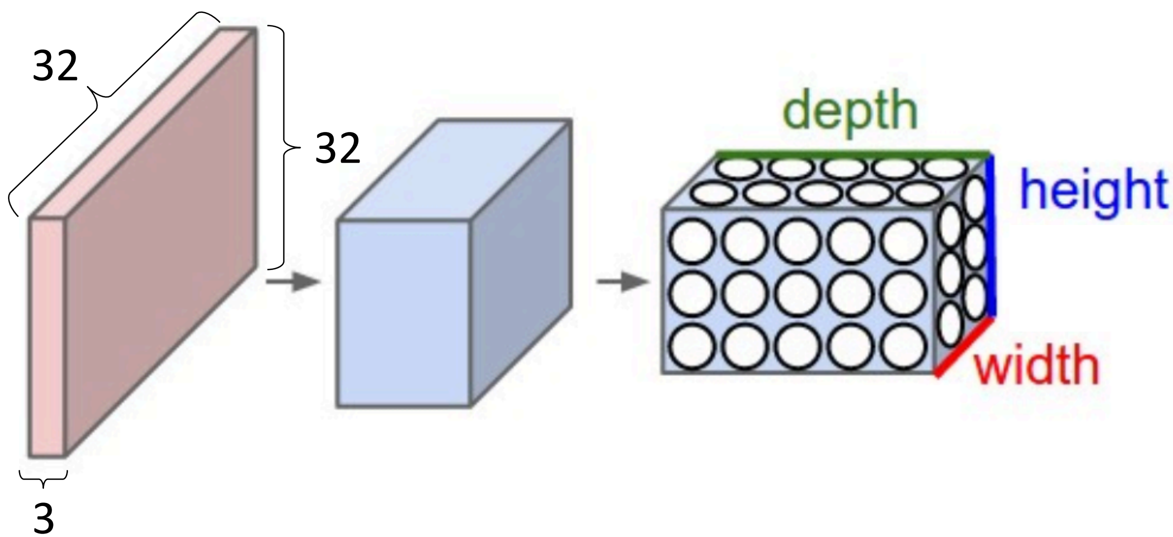

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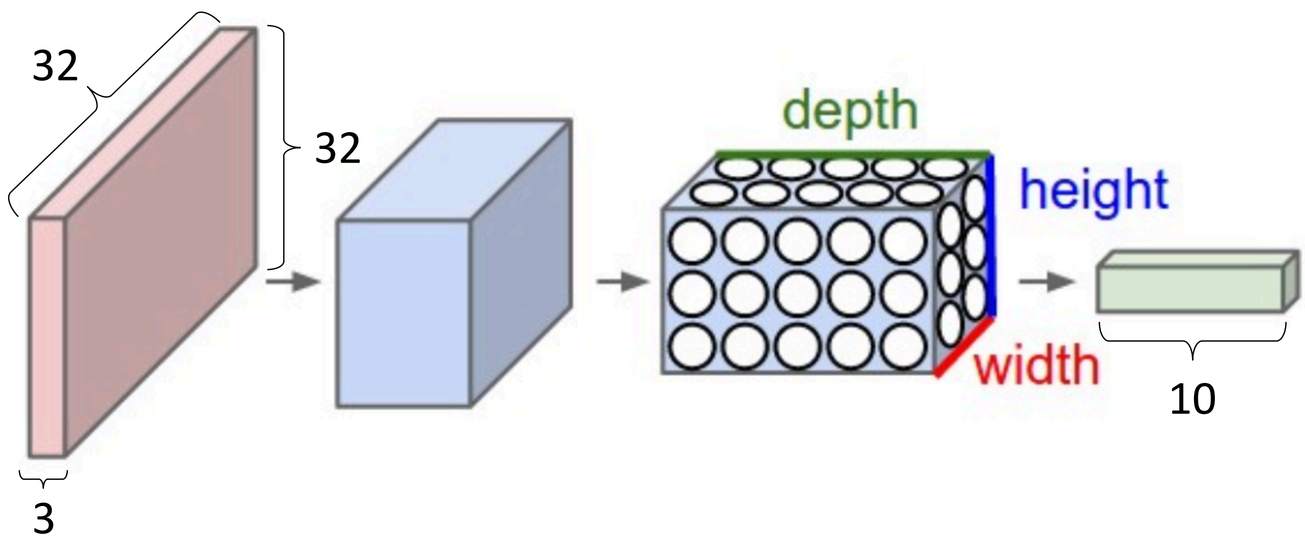
- For **CIFAR-10**, we would have:
  - Width=32, Height=32, Depth=3
- Each layer is also a 3 dimensional volume
- The output layer is 1x1xC, where C is the number of classes (10 for CIFAR-10)



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