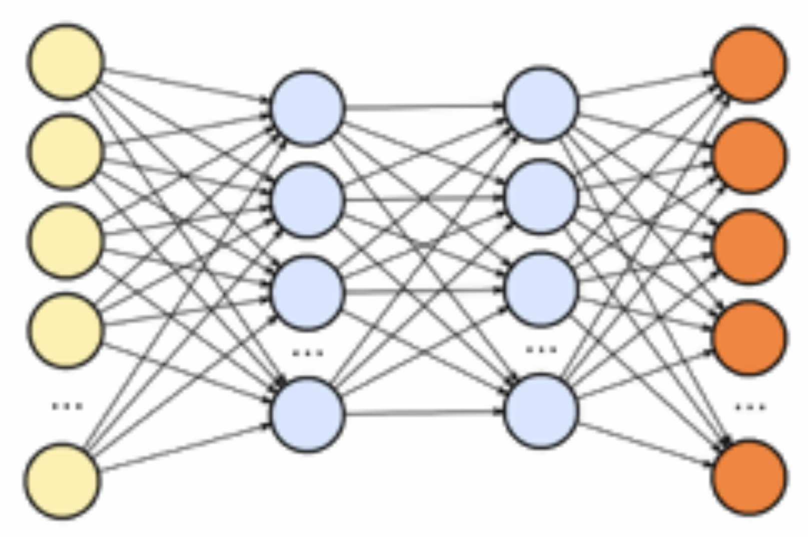
CSE 543

Simon Du



CSE543: Deep Learning

Instructor: Simon Du

Teaching Assistant: Yancheng Liang, Siting Li, Yiping Wang

Course Website (contains all logistic information): https://courses.cs.washington.edu/courses/cse543/24au/

Questions: Ed Discussion

Announcements: Canvas

Homework: Canvas

CSE543: Deep Learning

What this class is:

- **Fundamentals of DL:** Neural network architecture, approximation properties, optimization, generalization, generative models, representation learning
- **Preparation for further learning / research:** the field is fast-moving, you will be able to apply the fundamentals and teach yourself the latest

What this class is not:

- **An easy course:** mathematically easy
- **A survey course:** laundry list of algorithms
- **An application course**: implementation of different architectures on different datasets

Prerequisites

- Working knowledge of:
    - Linear algebra
    - Vector calculus
    - Probability and statistics
    - Algorithms
    - Machine leanring (CSE 446/546)
- Mathematical maturity
- “Can I learn these topics concurrently?”

Lecture

- Time: Tuesday and Thursday 11:30 AM - 12:50PM
- CSE2 G01 or Zoom (see website for the schedule)
- Slides + handwritten notes (e.g., proofs)
- Zoom link on Canvas
- Tentative schedule on course website

Homework (40%)

- 2 homework (20%+20%)
  - Each contains both theoretical questions and programming questions
  - Related to course materials
  - Collaboration okay but must write who you collaborated with. You must write, submit, and understand your answers and code.
  - Submit on Canvas
  - Must be **typed**
  - **Two** late days
  - Tentative timeline:
    - HW 1 due: 10/24
    - HW 2 due: 11/7

Course Project (60%)

- Group of 2 - 4.
- Topic: literature review (state-of-the-art) or original research.
- Post on Ed Discussion to form teams.
- Some potential topics are in listed on Canvas. OK to do a project NOT ~~on~~ listed.
- You can work on a project related to your research.
- Proposal (due: 10/10): **5%**
  - Format: NeurIPS Latex format, ~1 - 1.5 pages
- Presentations on (12/3 and 12/5 on Zoom): **20%**
- Final report (due: 12/13): **35%**
  - Format: NeurIPS Latex format, ~8 pages
- Submit on Canvas

Possible Topics

- Approximation properties
- Advanced optimization methods
- Optimization theory for deep learning
- Generalization theory for deep learning
- Deep reinforcement learning
- Implicit regularization
- Meta-learning
- Robustness
- Neural network compression
- Pre-training, fine-tuning, RLHF
- Deep learning application
- …

Communication Chanels

- **Announcements**
  - Canvas
- **questions about class, homework help**
  - Ed Discussion
  - Office hours:
    - Simon Du: Tu 10:00 - 11:00 AM, CSE2 312
    - Yancheng Liang: W 13:00 - 14:00 PM, on Zoom
    - Siting Li: Tu 16:00 - 17:00, CSE2 151
    - Yiping Wang: W 16:00 - 17:00, CSE2 151
  - **Regrade requests / Personal concerns:**
    - Email to instructor or TAs

Topic 1: Review (Today)

- ML Review: training, generalization
- Neural network basics: fully-connected neural network, gradient descent

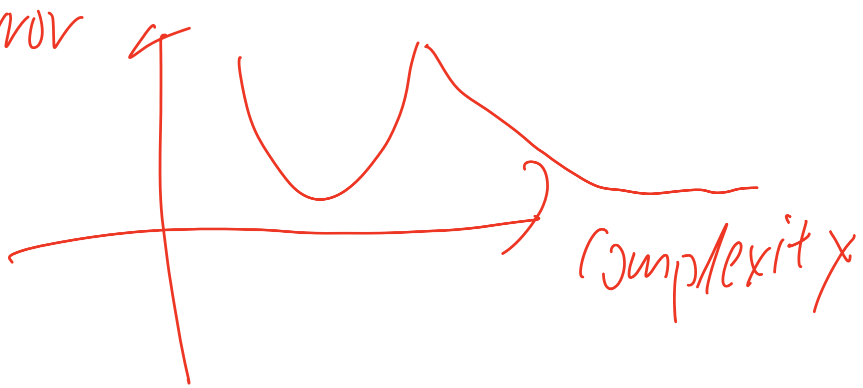
Topic 2: Approximation Theory

- Why neural networks can express the (regression, classification, …) function you want?
- Construction of such desired neural networks
- Universal approximation theorem

Topic 3: Optimization

- Review: Back-propagation
- Auto-differentiation
- Advanced optimizers: momentum (Nesterov acceleration), adaptive method (AdaGrad, Adam)
- Techniques for improving optimization: batch-norm, layer-norm, ..
- Theory: global convergence of gradient of over-parameterized neural networks wide
- Neural Tangent Kernel

Topic 4: Generalization



- Measures of generalization
- Double descent
- Techniques for improving generalization
- Generalization theory beyond VC-dimension
- Implicit regularization
- Why NN outperforms kernel

Topic 5: Architecture

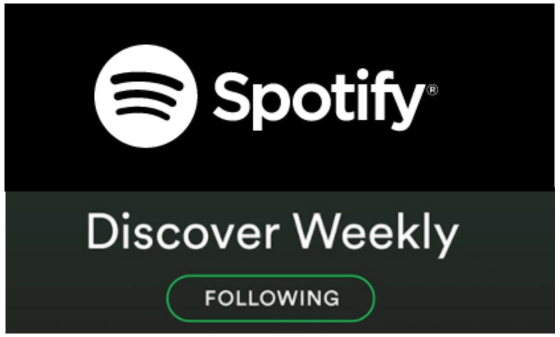
- Convolutional neural network
- Recurrent neural network
    - LSTM
- Attention-based neural network
    - Transformer
- General framework

Topic 6: Representation Learning / Pre-Training

- Multi-task representation learning
- Auto-regressive pre-training
- Multi-modal learning
- Contrastive learning
- Meta-learning
- Data
- Theory

Topic 7: Generative Models

- Generative adversarial network
- Variational Auto-Encoder
- Energy-based models
- Normalizing flows
- Diffusion models



ML uses past data to make predictions

Supervised Learning Process

$\{(x_i, y_i)\}_{i=1}^n \overset{i.i.d.}{\sim} D$

x_i : input $\in \mathbb{R}^d$, image

Collect a **dataset**

y_i $\in \{0, \dots, K\}$ classification, $\mathbb{R}$ regression

Decide on a **model** $f : \mathbb{R}^d \to \mathbb{R}$

$f \in \mathcal{F}$ function class
(1) linear $f(x) = w^T x$, for some w
(2) kernels
(3) trees
(4) neural networks

Find the function which fits the data best

$(f(x) - y)^2$
logistic loss

Choose a loss function $\ell(f(x), y) \to \mathbb{R}$

Pick the function which minimizes loss on data $\hat{f} \leftarrow \underset{f \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i) + \lambda R(f)$

$\lambda \in \mathbb{R}_+$

if f is linear $f(x) = w^T x$
$\Rightarrow R(f) = \|w\|_2^2$

Use function to make prediction on new examples x_{new}

prediction : $\hat{f}(x_{new}) \approx y_{new}$

Framework

Fix $f \in \mathcal{F}$

Goal : test error

$$L_{te}(f) = \mathbb{E}_{(x,y)\sim D}\left[\ell(f(x), y)\right]$$

$$L_{tr}(f) = \frac{1}{n}\sum_{i=1}^{n} \ell(f(x_i), y_i)$$

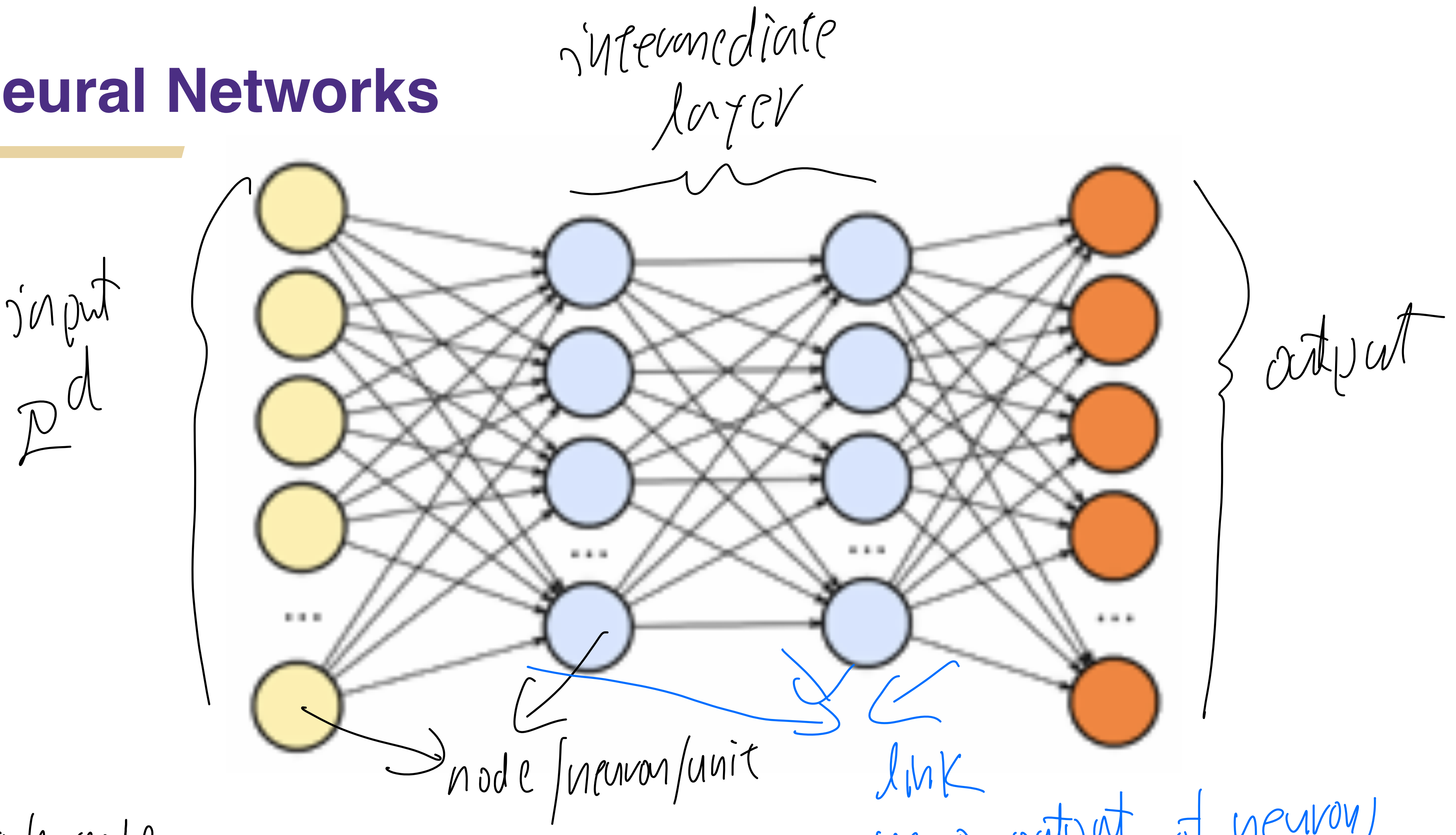
$$L_{te}(f) = L_{tr}(f) + L_{te}(f) - L_{tr}(f)$$

$$= \underbrace{\min_{\tilde{f}\in\mathcal{F}} L_{tr}(\tilde{f})}_{\text{approximation error}}$$

$$+ \underbrace{L_{tr}(f) - \min_{\tilde{f}\in\mathcal{F}} L_{tr}(\tilde{f})}_{\text{optimization error}}$$

$$+ \underbrace{L_{te}(f) - L_{tr}(f)}_{\text{generalization error}}$$

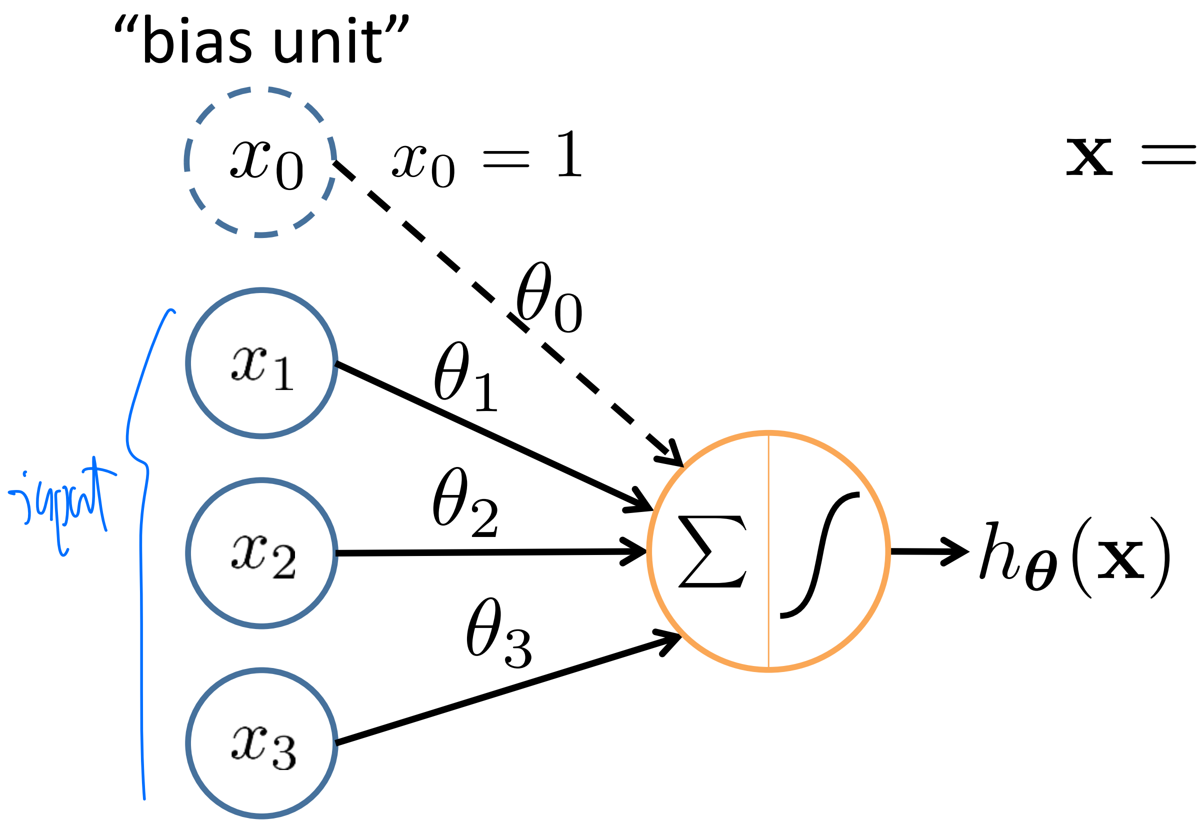
Neural Networks



each node
1) input
2) activation
3) output

- map output of neuron to the input of neuron
- each link has a weight $\in \mathbb{R}$

Single Node



$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix}$$

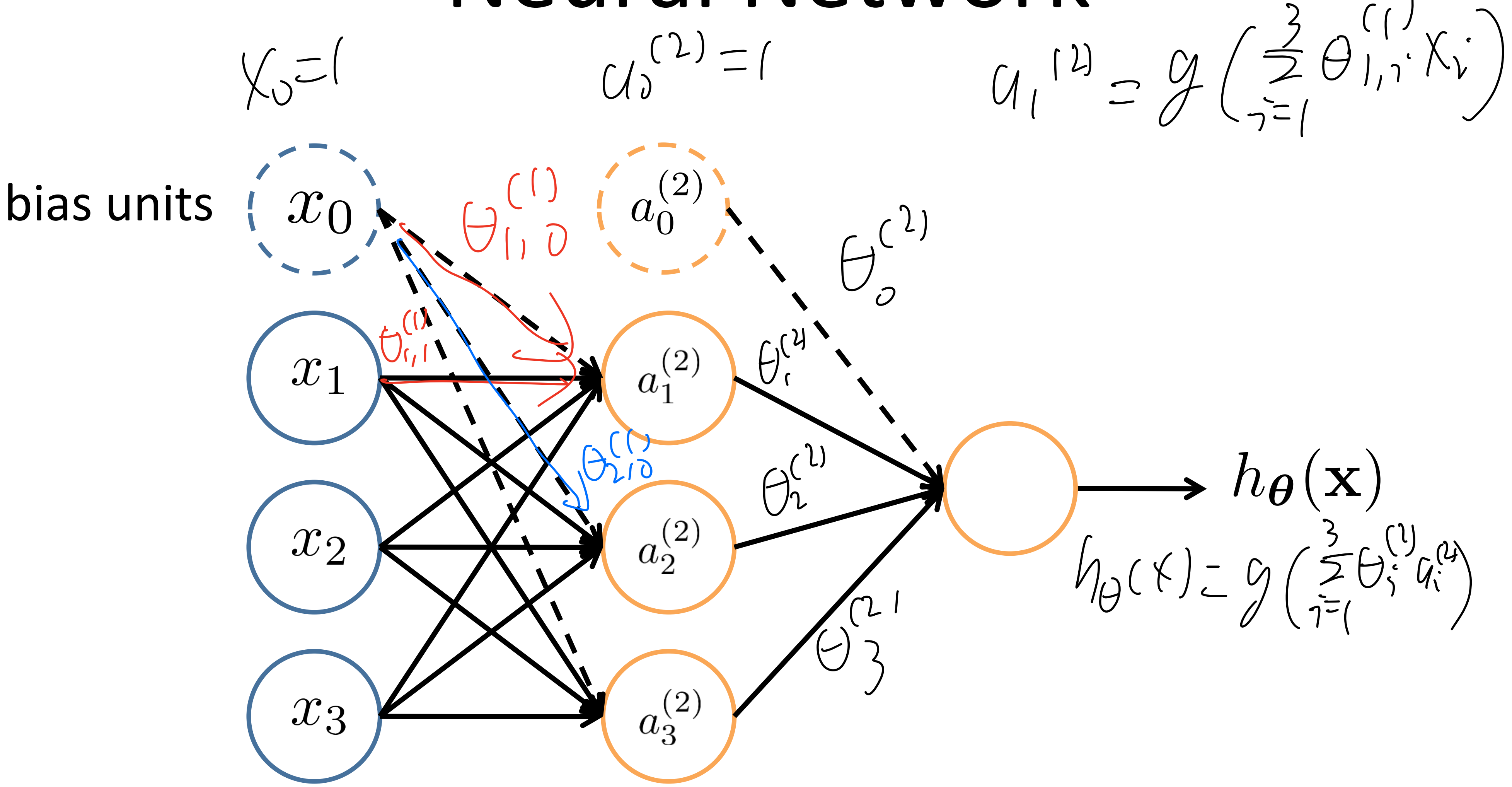
$$h_{\boldsymbol{\theta}}(\mathbf{x}) = g\left(\boldsymbol{\theta}^\top \mathbf{x}\right) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \mathbf{x}}}$$

Binary
Logistic
Regression

Sigmoid (logistic) activation function: $g(z) = \dfrac{1}{1 + e^{-z}}$

Neural Network

$a_1^{(2)} = g\left(\sum_{i=1}^{3} \theta_{1,i}^{(1)} x_i\right)$



Layer 1

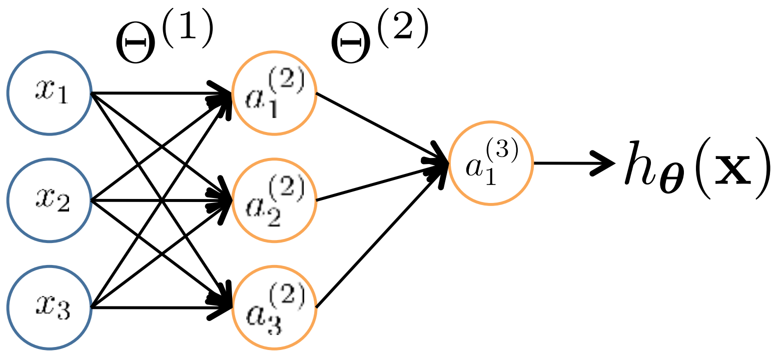
(Input Layer)

Layer 2

(Hidden Layer)

Layer 3

(Output Layer)



$a_i^{(j)}$ = "activation" of unit *i* in layer *j*

$\Theta^{(j)}$ = weight matrix stores parameters from layer *j* to layer *j* + 1

$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

If network has s_j units in layer *j and* s_{j+1} units in layer *j*+1, then $\Theta^{(j)}$ has dimension $s_{j+1} \times (s_j+1)$.

$$\Theta^{(1)} \in \mathbb{R}^{3\times 4} \qquad \Theta^{(2)} \in \mathbb{R}^{1\times 4}$$

Multi-layer Neural Network - Binary Classification

pointwise

$$a^{(1)} = x$$

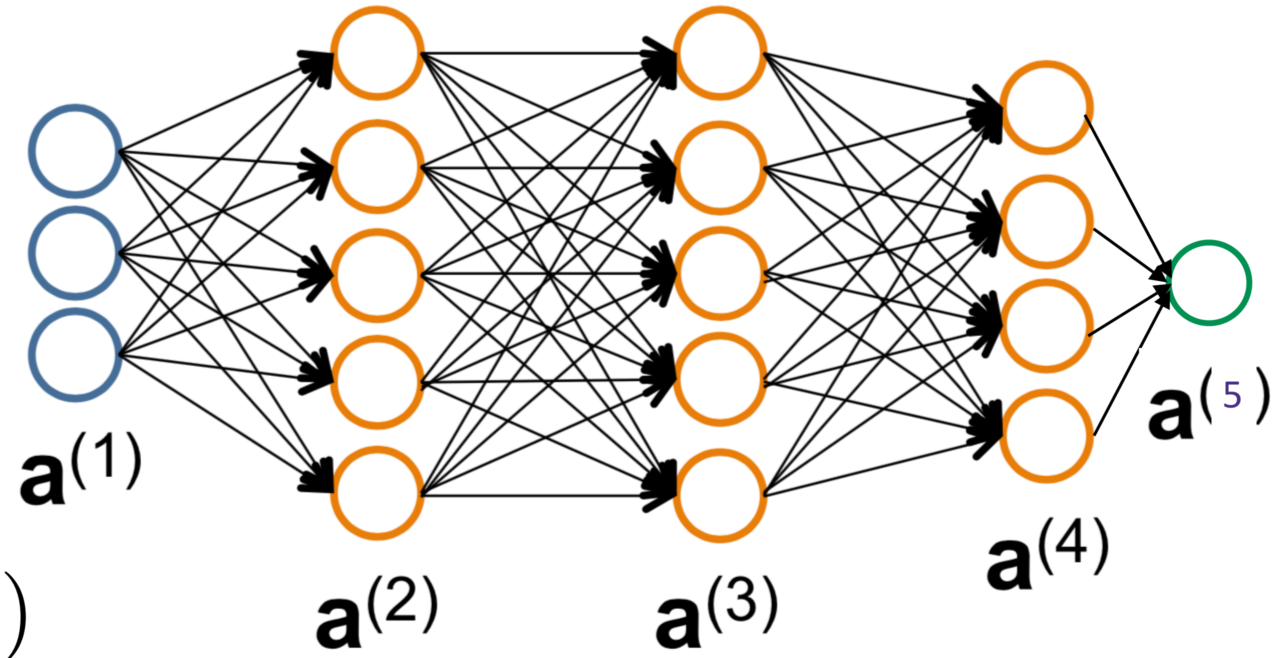
$$a^{(2)} = g(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

$$a^{(l+1)} = g(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

$$\widehat{y} = g(\Theta^{(L)} a^{(L)})$$



$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1 - y)\log(1 - \widehat{y})$$

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

Binary
Logistic
Regression

Multi-layer Neural Network - Binary Classification

$$a^{(1)} = x$$

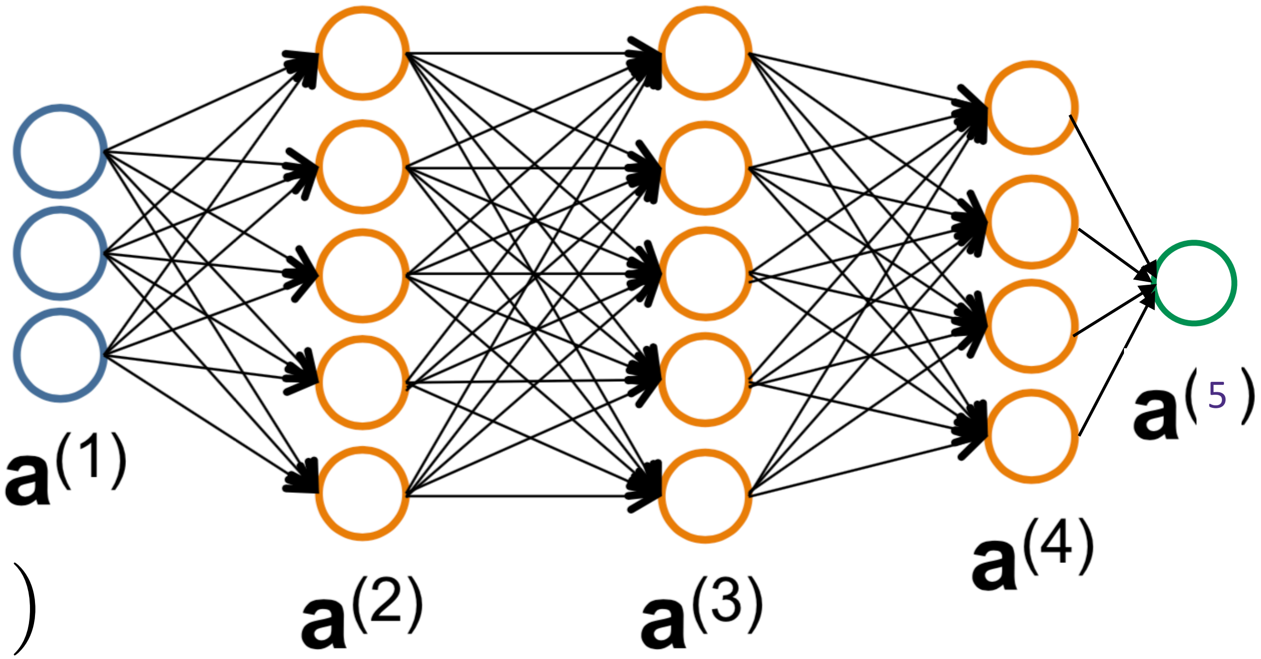
$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

$$\widehat{y} = g(\Theta^{(L)} a^{(L)})$$



$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1 - y)\log(1 - \widehat{y})$$

$$\sigma(z) = \max\{0, z\} \quad g(z) = \frac{1}{1 + e^{-z}}$$

Binary
Logistic
Regression

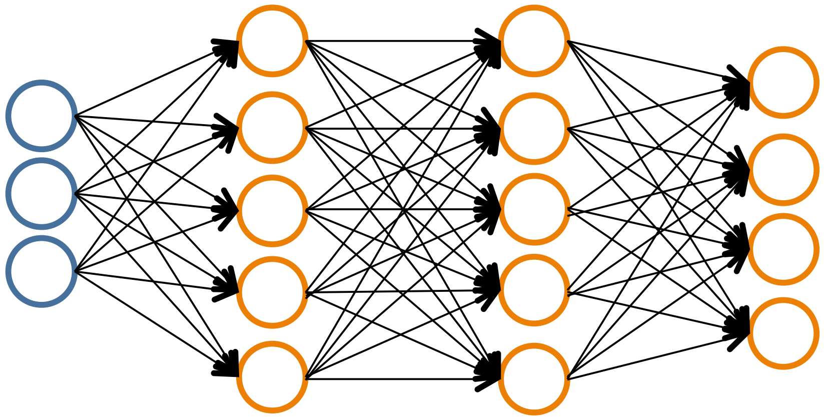
Multiple Output Units: One-vs-Rest

Pedestrian

Car

Motorcycle

Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

Multi-class
Logistic
Regression

We want:

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$
when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$
when motorcycle

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
when truck

Multi-layer Neural Network - Regression

$$a^{(1)} = x$$

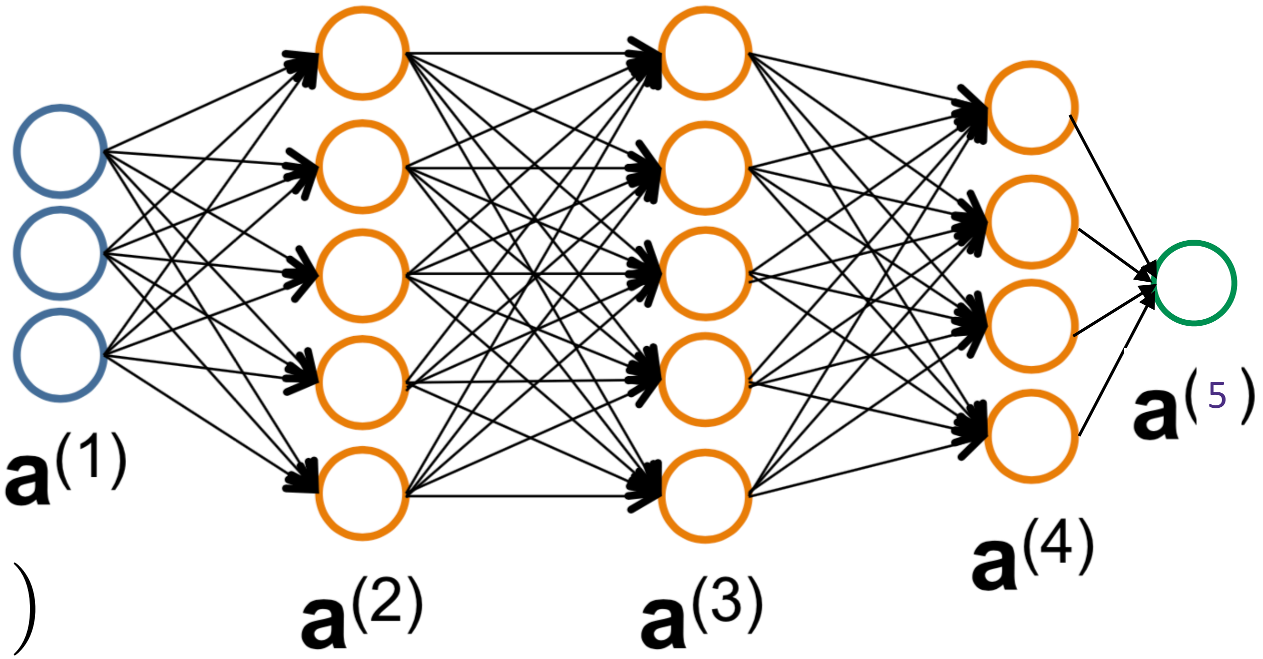
$$a^{(2)} = \sigma(\Theta^{(1)} a^{(1)})$$

$$\vdots$$

$$a^{(l+1)} = \sigma(\Theta^{(l)} a^{(l)})$$

$$\vdots$$

$$\widehat{y} = \Theta^{(L)} a^{(L)}$$



$$L(y, \widehat{y}) = (y - \widehat{y})^2$$

$$\sigma(z) = \max\{0, z\}$$

Regression

$$a^{(1)} = x$$

$$z^{(2)} = \Theta^{(1)} a^{(1)}$$

$$a^{(2)} = g\left(z^{(2)}\right)$$

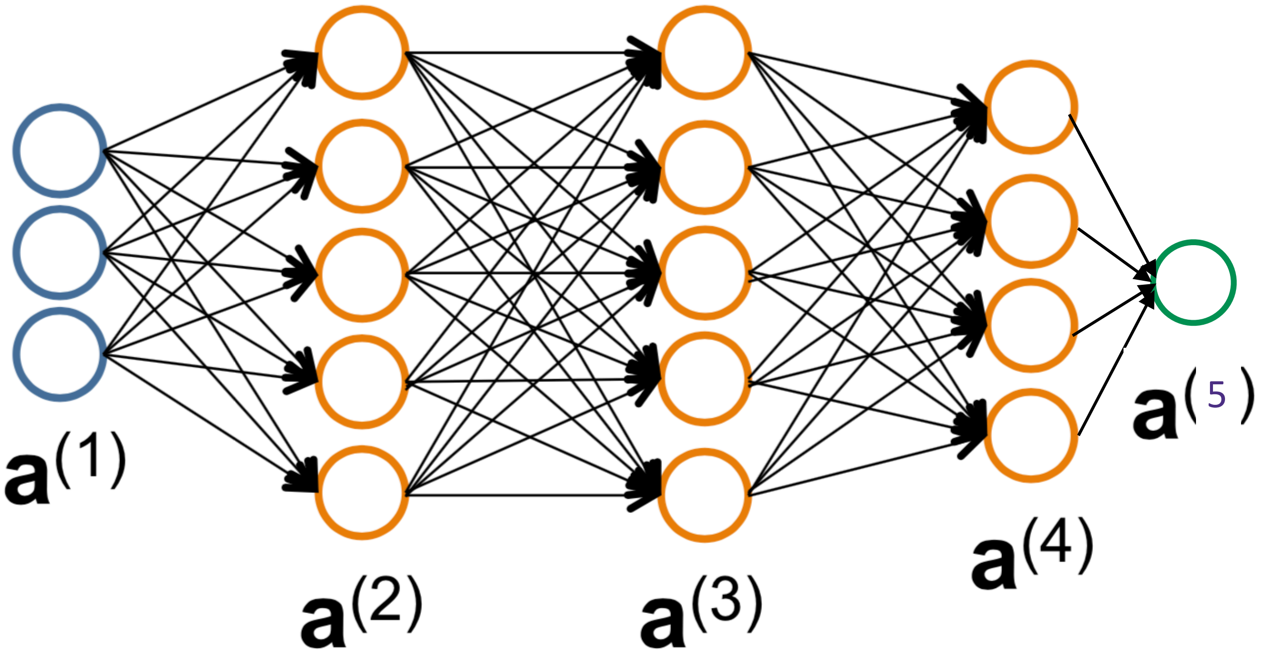
$$\vdots$$

$$z^{(l+1)} = \Theta^{(l)} a^{(l)}$$

$$a^{(l+1)} = g\left(z^{(l+1)}\right)$$

$$\vdots$$

$$\widehat{y} = g(\Theta^{(L)} a^{(L)})$$



$$L(y, \widehat{y}) = y \log(\widehat{y}) + (1 - y)\log(1 - \widehat{y})$$

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

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \widehat{y}) \qquad \forall l$

Gradient Descent: $\Theta^{(l)} \leftarrow \Theta^{(l)} - \eta \nabla_{\Theta^{(l)}} L(y, \widehat{y}) \qquad \forall l$

Seems simple enough, why are packages like PyTorch, Tensorflow, Theano, Cafe, MxNet synonymous with deep learning?

1. Automatic differentiation

2. Convenient libraries

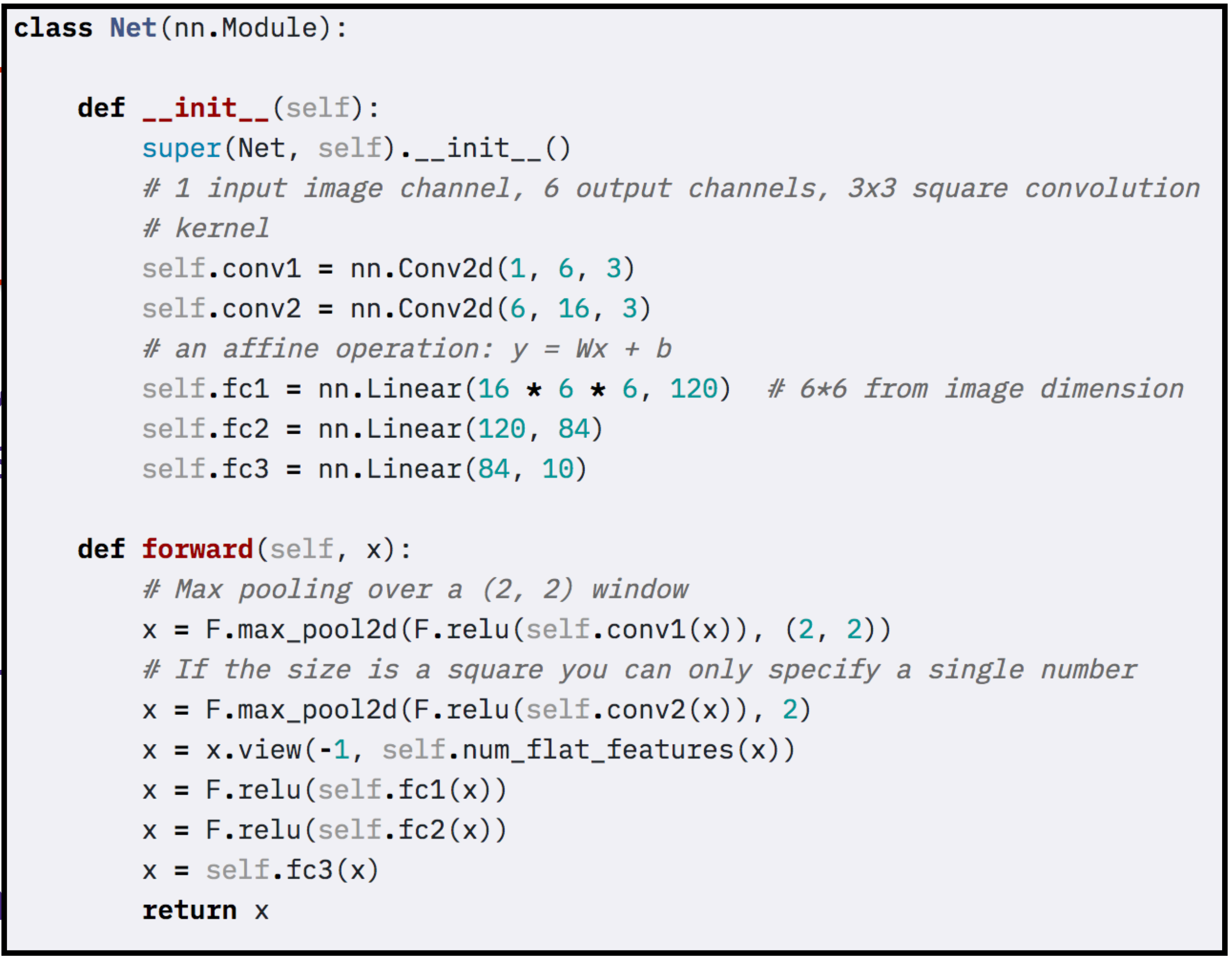
3. GPU support

Gradient Descent:

Seems simple enough,
Theano, Cafe, MxNet s

1. Automatic differ

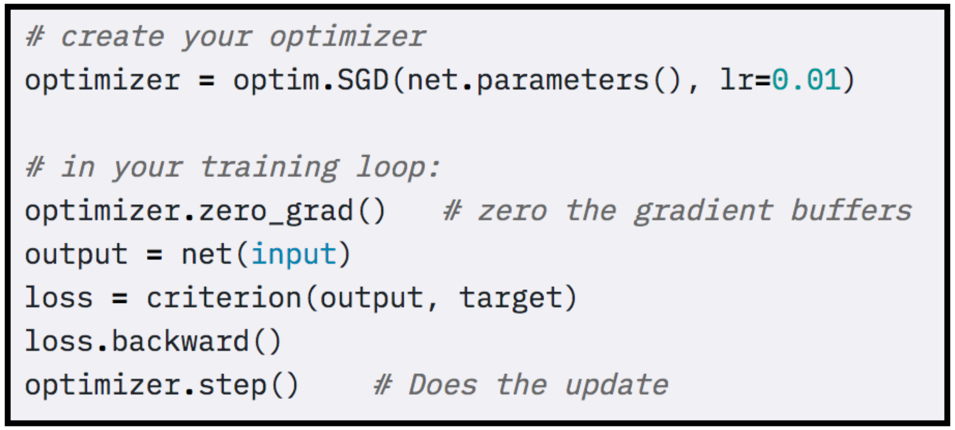
2. Convenient libra



```
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        # 1 input image channel, 6 output channels, 3x3 square convolution
        # kernel
        self.conv1 = nn.Conv2d(1, 6, 3)
        self.conv2 = nn.Conv2d(6, 16, 3)
        # an affine operation: y = Wx + b
        self.fc1 = nn.Linear(16 * 6 * 6, 120)  # 6*6 from image dimension
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)

    def forward(self, x):
        # Max pooling over a (2, 2) window
        x = F.max_pool2d(F.relu(self.conv1(x)), (2, 2))
        # If the size is a square you can only specify a single number
        x = F.max_pool2d(F.relu(self.conv2(x)), 2)
        x = x.view(-1, self.num_flat_features(x))
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x
```



```
# create your optimizer
optimizer = optim.SGD(net.parameters(), lr=0.01)

# in your training loop:
optimizer.zero_grad()   # zero the gradient buffers
output = net(input)
loss = criterion(output, target)
loss.backward()
optimizer.step()    # Does the update
```