Note) Slides and example codes are available:
https://github.com/mint-lab/dl_tutorial

Deep Learning Tutorial with PyTorch

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Image: BBC

Why Deep Learning?

- **AlphaGo** beat Sedol Lee in a five-game Go match. (2016)

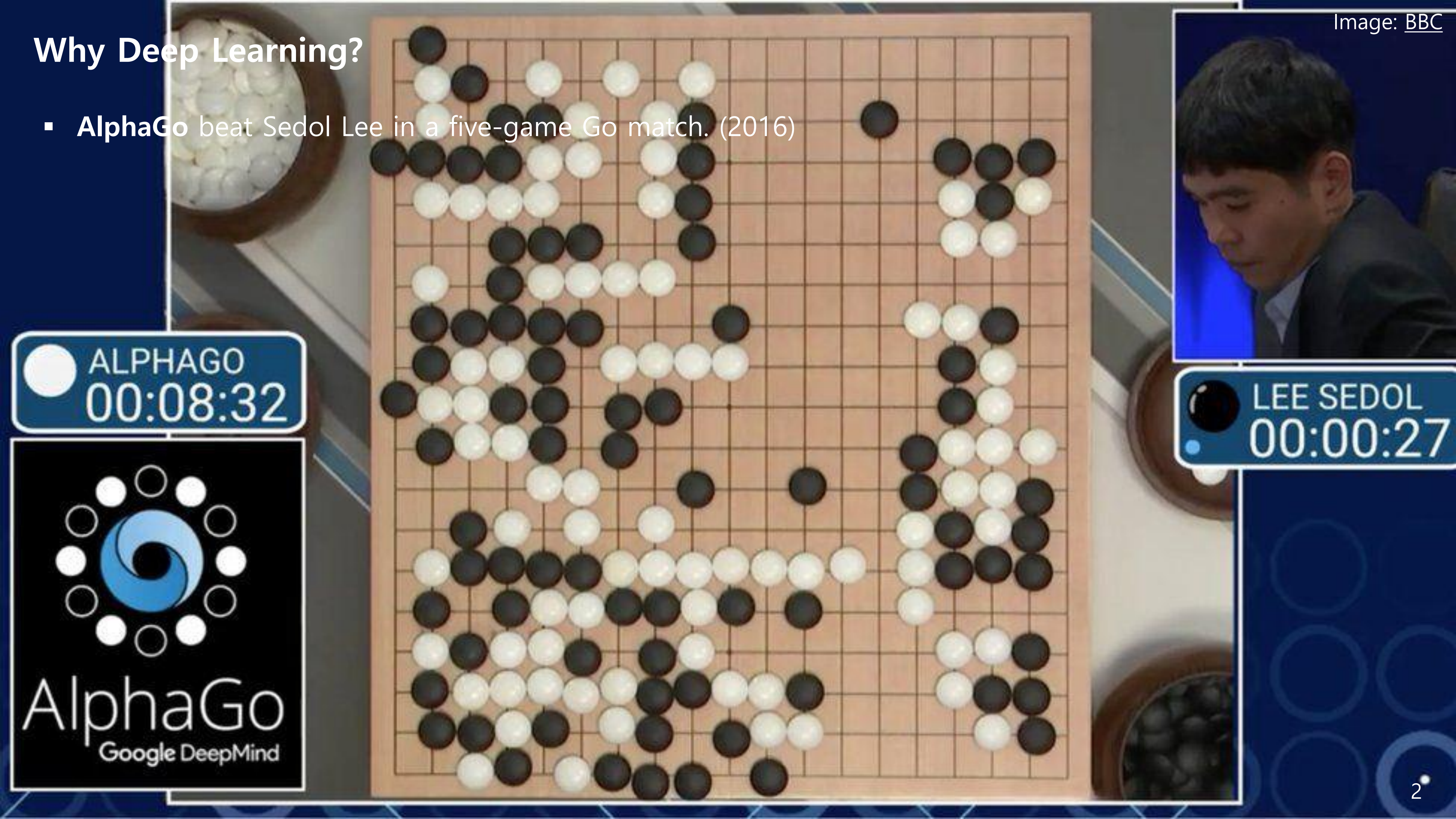
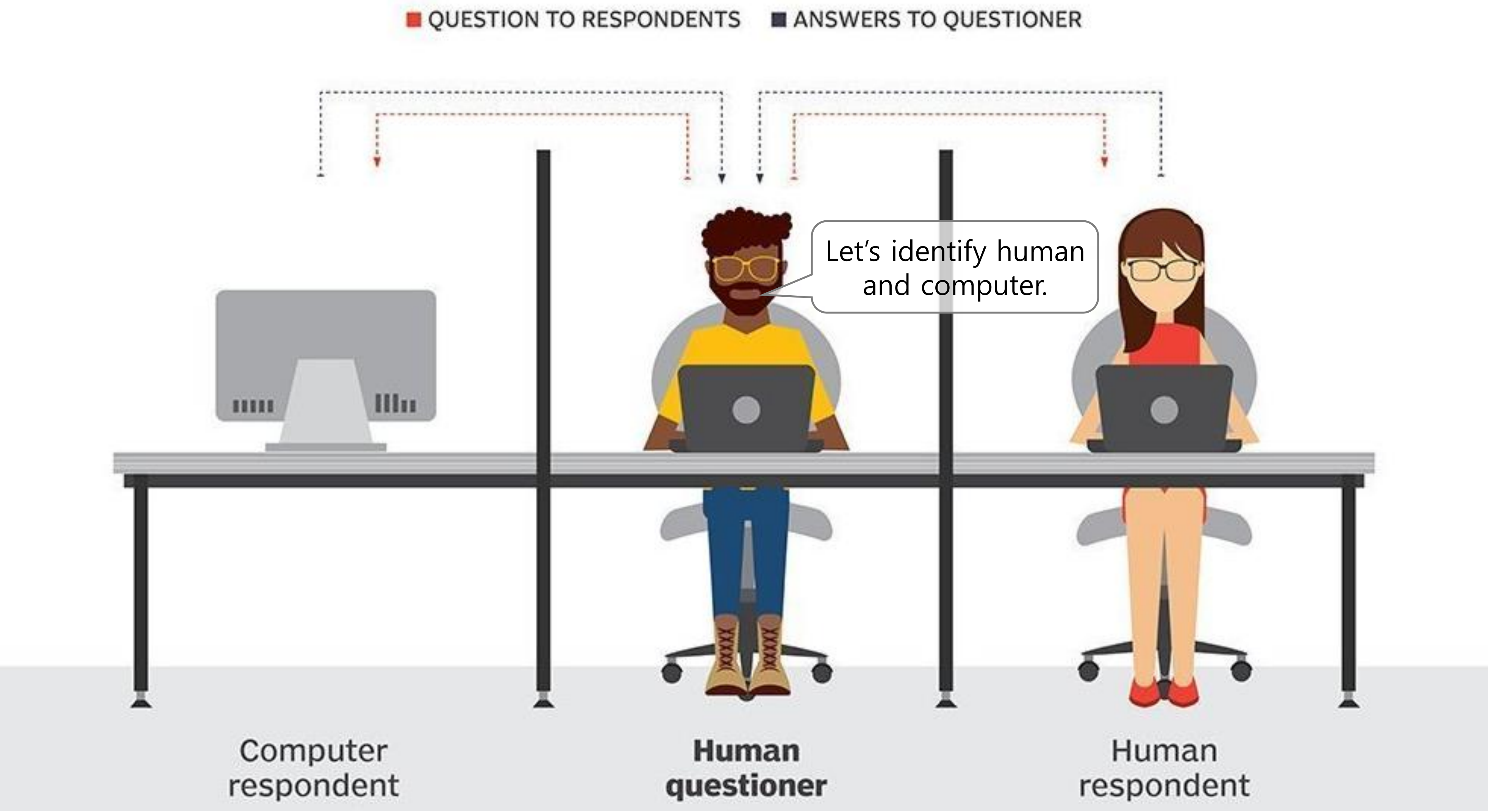


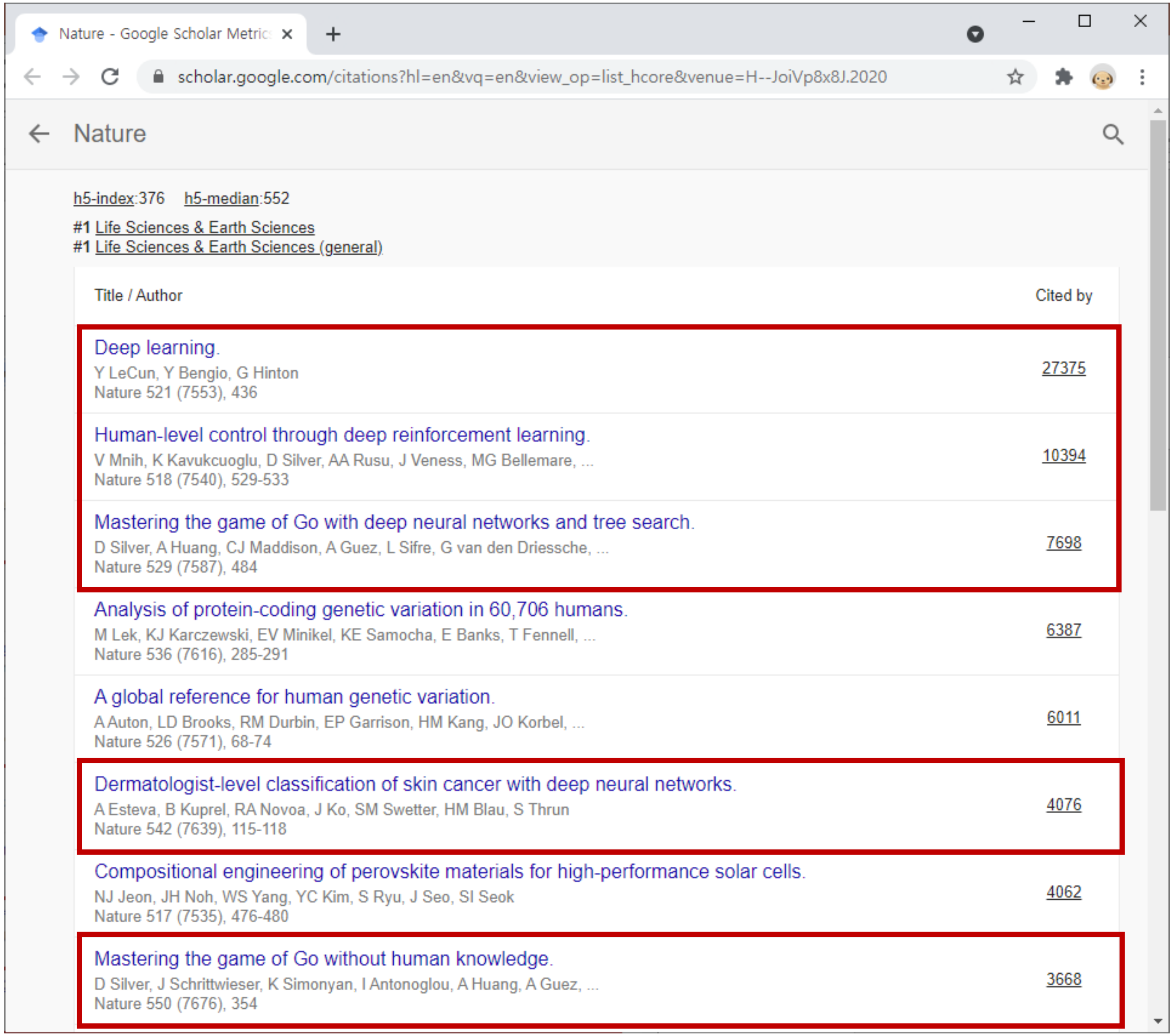
Image: TechTarget

Why Deep Learning?

- **ChatGPT** broke the Turing test. (2022)
  - Reference) Nature, Vol. 619, 2023 DOI



Why Deep Learning?


Nature - Google Scholar Metrics

scholar.google.com/citations?hl=en&vq=en&view_op=list_hcore&venue=H--JoiVp8x8J.2020

Nature

h5-index:376 h5-median:552

#1 Life Sciences & Earth Sciences
#1 Life Sciences & Earth Sciences (general)

Title / Author	Cited by
Deep learning. Y LeCun, Y Bengio, G Hinton Nature 521 (7553), 436	27375
Human-level control through deep reinforcement learning. V Mnih, K Kavukcuoglu, D Silver, AA Rusu, J Veness, MG Bellemare, ... Nature 518 (7540), 529-533	10394
Mastering the game of Go with deep neural networks and tree search. D Silver, A Huang, CJ Maddison, A Guez, L Sifre, G van den Driessche, ... Nature 529 (7587), 484	7698
Analysis of protein-coding genetic variation in 60,706 humans. M Lek, KJ Karczewski, EV Minikel, KE Samocha, E Banks, T Fennell, ... Nature 536 (7616), 285-291	6387
A global reference for human genetic variation. A Auton, LD Brooks, RM Durbin, EP Garrison, HM Kang, JO Korbel, ... Nature 526 (7571), 68-74	6011
Dermatologist-level classification of skin cancer with deep neural networks. A Esteva, B Kuprel, RA Novoa, J Ko, SM Swetter, HM Blau, S Thrun Nature 542 (7639), 115-118	4076
Compositional engineering of perovskite materials for high-performance solar cells. NJ Jeon, JH Noh, WS Yang, YC Kim, S Ryu, J Seo, SI Seok Nature 517 (7535), 476-480	4062
Mastering the game of Go without human knowledge. D Silver, J Schrittwieser, K Simonyan, I Antonoglou, A Huang, A Guez, ... Nature 550 (7676), 354	3668

Image: Google Scholar (retrieved on April 7th, 2021)

Why Deep Learning?

- Yoshua Bengio, Geoffrey Hinton, and Yann LeCun won **Turing Award (2018)**.
  - Note) Chronological listing of A.M. Turing Award Winners

Yoshua Bengio

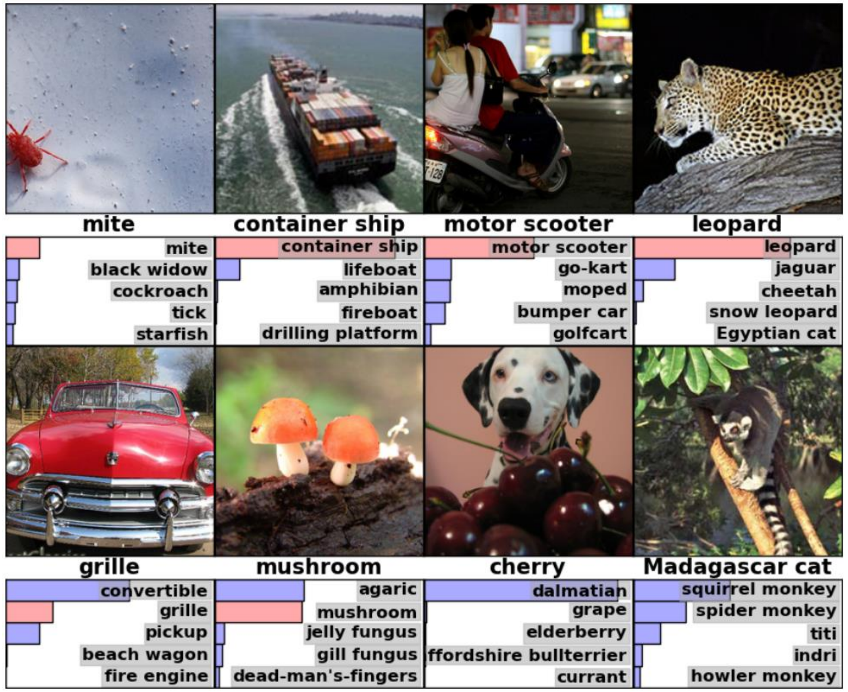
Geoffrey Hinton

Yann LeCun

Image: ACM

Why Deep Learning?

- **AlexNet** won the ILSVRC (ImageNet Large Scale Visual Recognition Competition) 2012 (top-5 error: **16.4%**).
  - A **8-layer** neural network (approx. 61 million parameters) with 2 x GPUs
  - ReLU (rectified linear unit) is used for the vanishing gradient problem and speed-up.
  - Data augmentation (more data) and dropout (regularization) was used to solve the overfitting problem.
  - Local response normalization (~ batch normalization) are used for stable training and generalization.



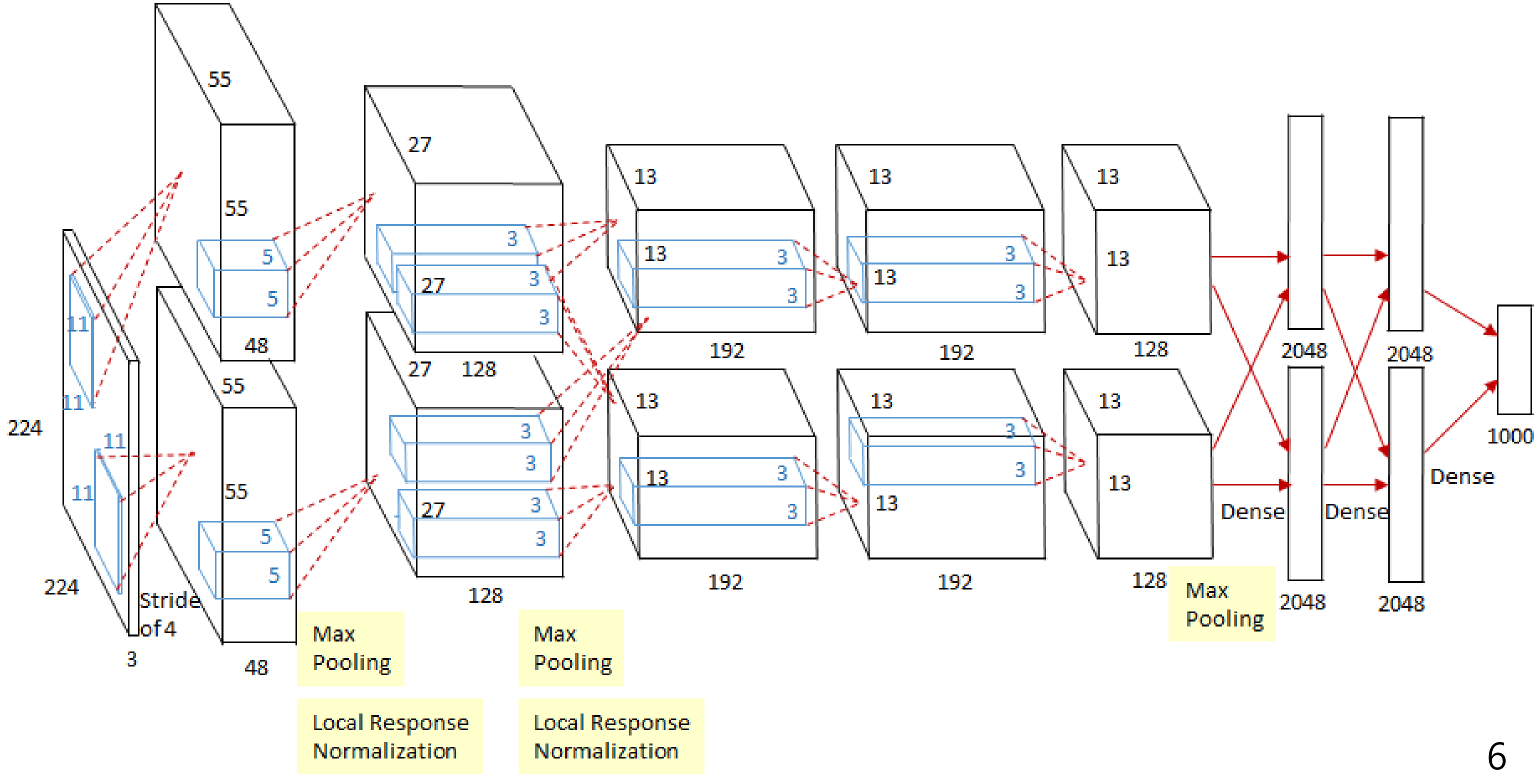
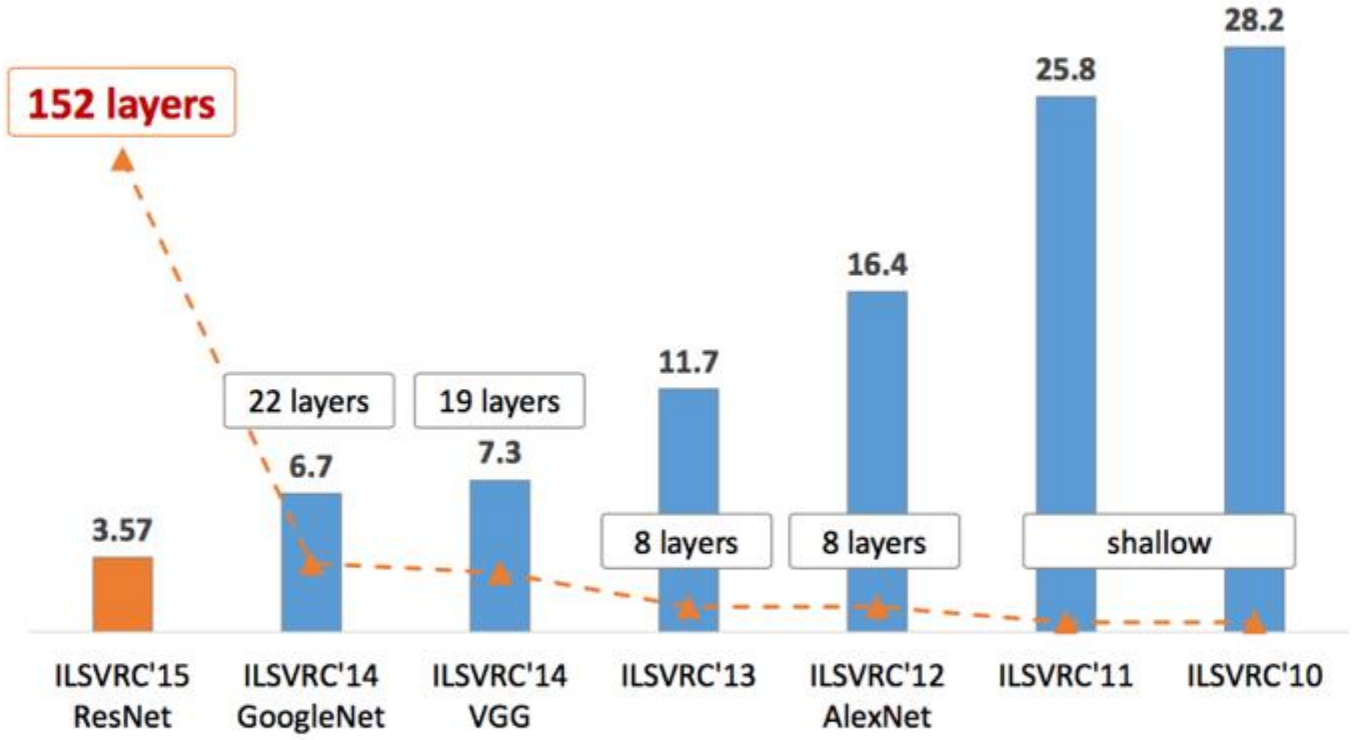


Image: Medium article (by Sik-Ho Tsang)

What is Deep Learning?

- *Deep learning* is machine learning with **deep neural network** (shortly DNN)
  - e.g. **ResNet** (residual neural network)
    - A **152-layer** with skip connection
    - The winner of ImageNet Challenge 2015 (top-5 error: **3.57%**)



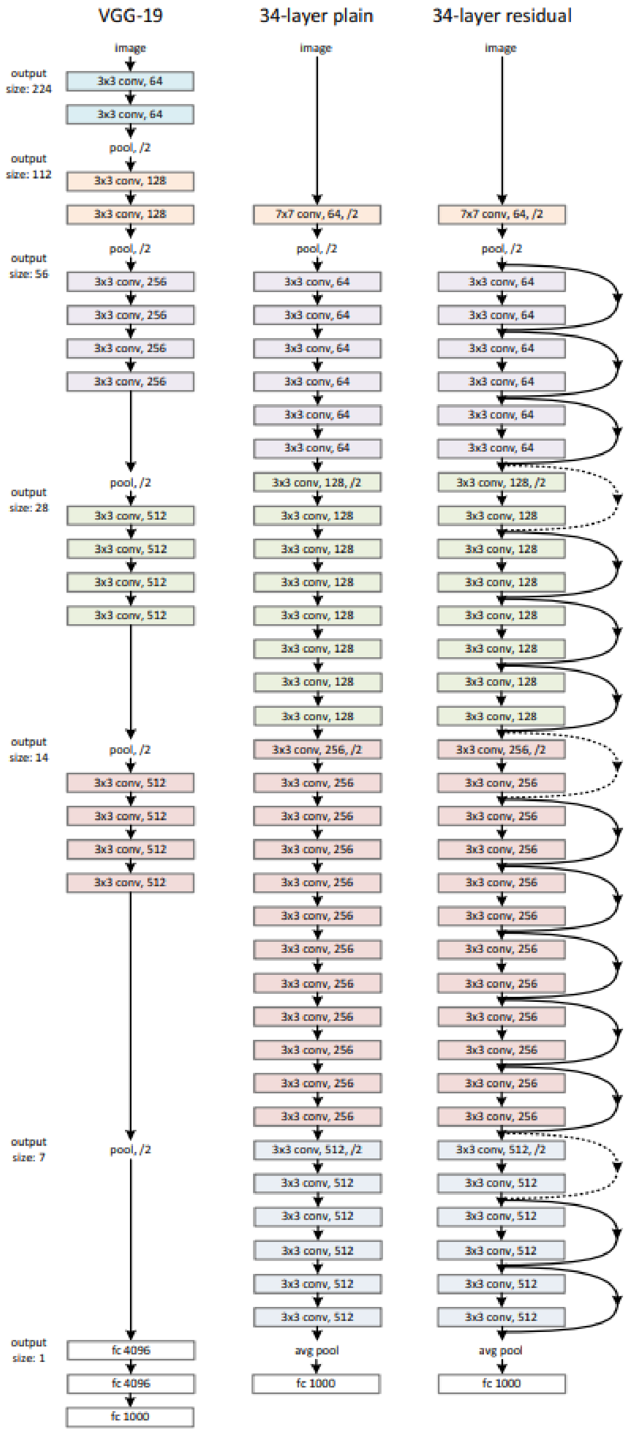
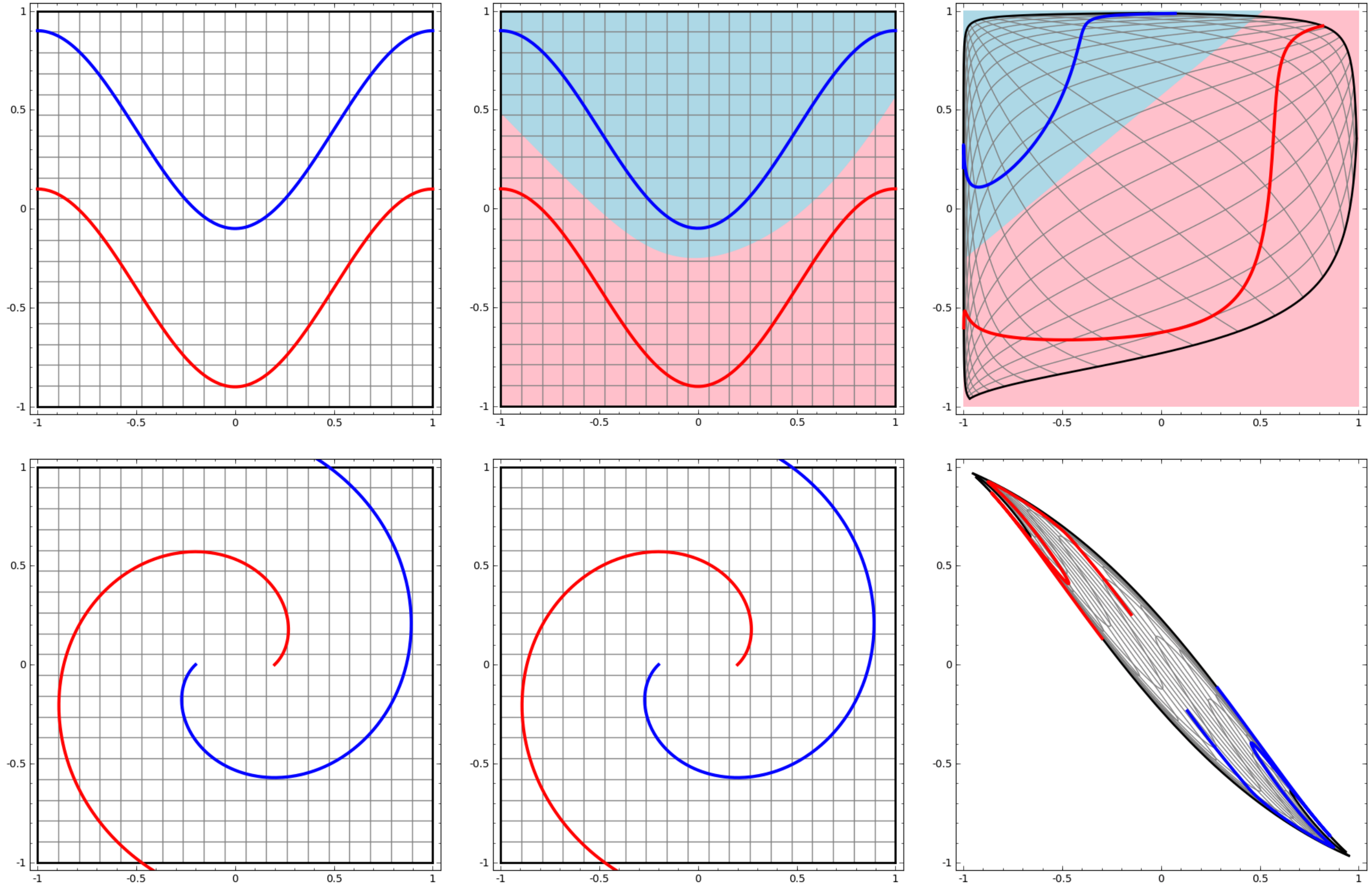


Image: arXiv:1512.03385 and OpenGenus IQ

What is Deep Learning?

- *Deep learning* is **representation learning** (a.k.a. feature learning).
  - e.g. Task: Draw a line to separate the red line and blue line.

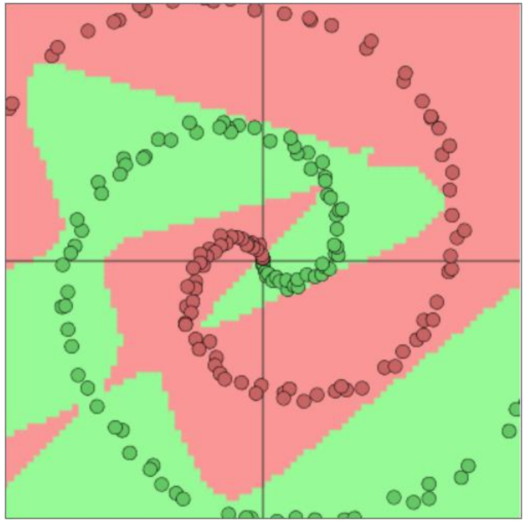


Image/Animation: colah's blog

What is Deep Learning?

- *Deep learning* is **representation learning** (a.k.a. feature learning).
  - e.g. Task: Draw a line to separate the red circle and green circle.
    - Note) Try it at ConvnetJS or TensorFlow Playground.

```
layer_defs = [];
layer_defs.push({type:'input', out_sx:1, out_sy:1, out_depth:2});
layer_defs.push({type:'fc', num_neurons:6, activation: 'tanh'});
layer_defs.push({type:'fc', num_neurons:2, activation: 'tanh'});
layer_defs.push({type:'softmax', num_classes:2});

net = new convnetjs.Net();
net.makeLayers(layer_defs);

trainer = new convnetjs.SGDTrainer(net, {learning_rate:0.01, momentum:0.1, batch_size:10, l2_decay:0.001});
```



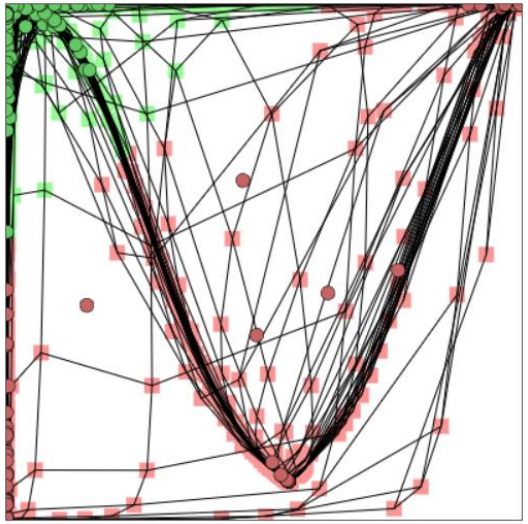


Image: ConvNetJS (retrieved on April 15th, 2021)

What is Deep Learning?

- *Deep learning* is **representation learning** (a.k.a. feature learning).

Machine learning:

Deep learning:

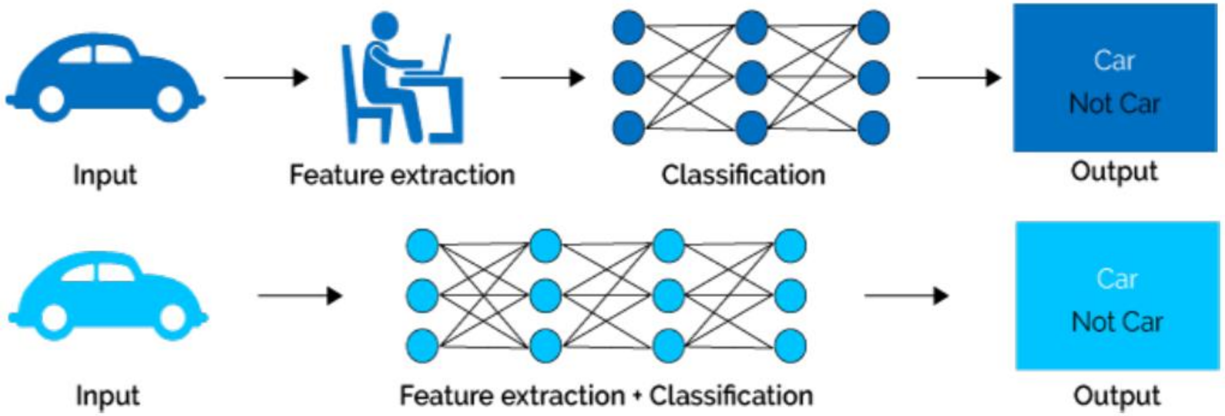


Image: MIT DL Lectures (by Lex Fridman)

What is Deep Learning?

- *Deep learning* is **scalable**.

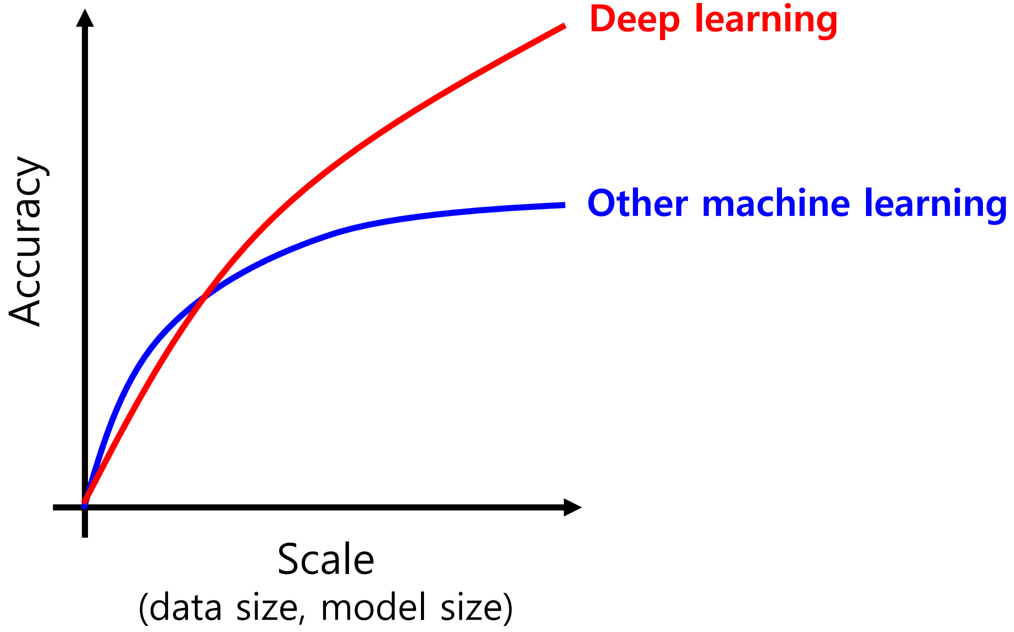


Table of Contents

Why PyTorch?

- **10 reasons why PyTorch is the DL framework of the future**

(by Dhiraj K, September 18th, 2019)

1. PyTorch is Pythonic
2. Easy to learn
3. Higher developer productivity
4. Easy debugging
5. Data parallelism
6. Dynamic computational graph support
7. Hybrid front-end
8. Useful libraries
9. ONNX (Open Neural Network Exchange) support
10. Cloud support

Why PyTorch?

- Popularity (vs. TensorFlow) in academic communities

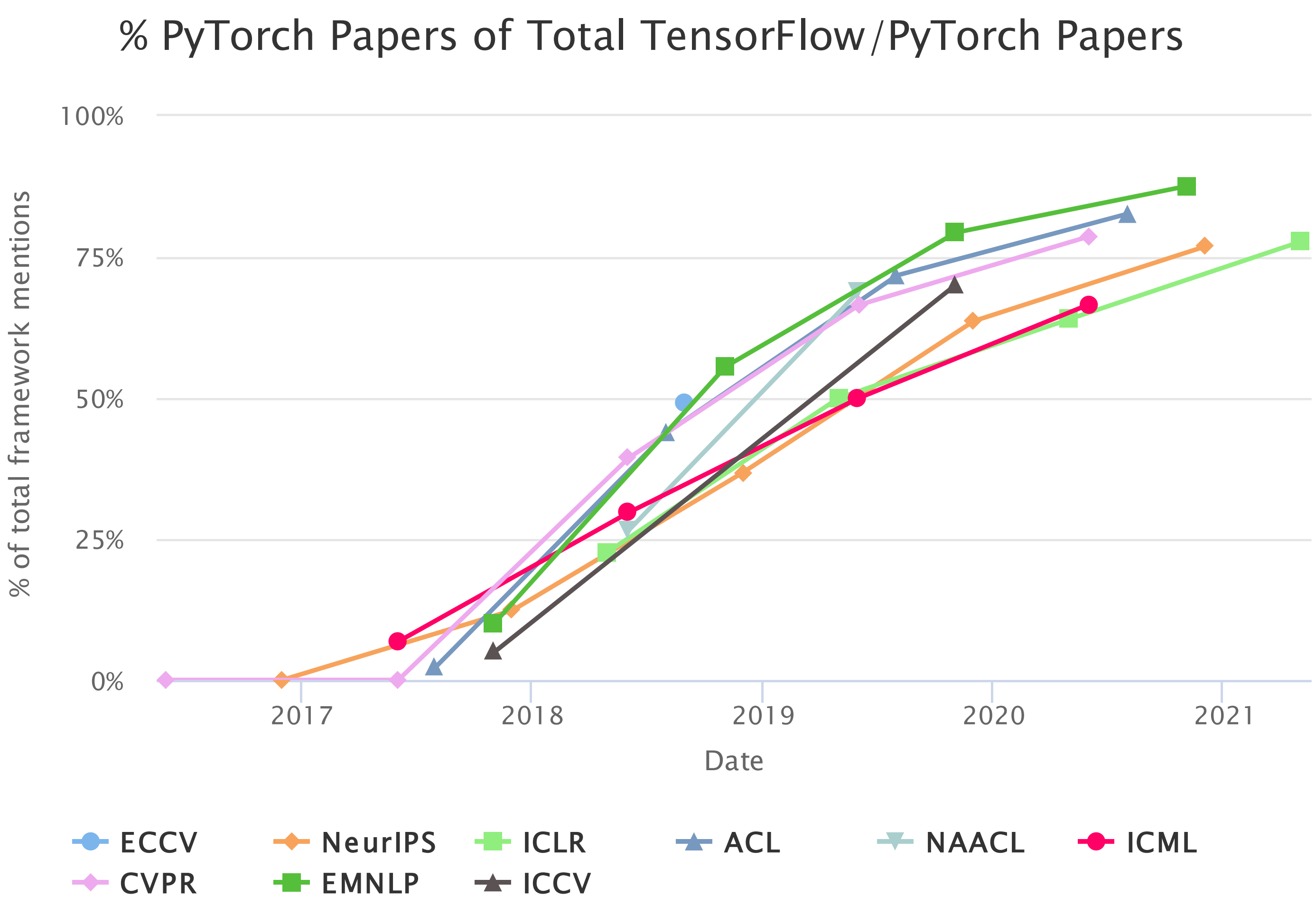


Image: [PyTorch vs TensorFlow (by Horace He)]

What is PyTorch?

- **PyTorch** (2016) is an open source deep learning library based on Python.
  - It originated from *Torch* (2002) based on Lua script language.
  - It is primarily developed by Facebook's AI Research lab (FAIR).

- (From my point of view) PyTorch is a **NumPy extension** with supports of
  - \+ A n-dimensional array with GPU acceleration and automatic differentiation
  - \+ Useful modules for neural networks

- My useful lists on deep learning and PyTorch

Practice) PyTorch Installation

- Please follow PyTorch's instruction of installation for your system.
  - Note) If you want GPU acceleration, please install the matched version of CUDA in advance. Please visit CUDA Toolkit Archive to download a specific version of CUDA.

PyTorch Build	Stable (1.8.1)		Preview (Nightly)	
Your OS	Linux	Mac	Windows	
Package	Conda	Pip	LibTorch	Source
Language	Python		C++ / Java	
Compute Platform	CUDA 10.2	CUDA 11.1	ROCm 4.0 (beta)	CPU
Run this Command:	**NOTE:** 'conda-forge' channel is required for cudatoolkit 11.1 conda install pytorch torchvision torchaudio cudatoolkit=11.1 -c pytorch -c conda-forge			

- Note) You can use Google Colab without local installation of PyTorch.

Image: PyTorch (retrieved on April 7th, 2021)

Note) Python Virtual Environment

- A **Python virtual environment** is an isolated Python runtime environment that contains a particular version of Python and its additional packages.
  - Note) Virtual machine: A computer entirely implemented by software
- Why virtual environments?
  - We can run Python applications with different versions of packages (e.g. PyTorch 0.9 and PyTorch 1.8) together.
- Tool #1) venv in the Python Standard Library
- Tool #2) conda in Anaconda
  - *Conda* is an open source package/dependency/environment management system for programming languages such as Python, R, Java, JavaScript, C/C++, and more.
  - Usage

`conda create --name` *`venv_name`* `python=3.6`	Create a virtual environment
`conda create --name venv_dst --clone venv_src`	Copy a virtual environment
`conda activate` *`venv_name`*	Activate the virtual environment
`conda deactivate`	Deactivate the virtual environment
`conda env remove --name` *`venv_name`*	Remove the virtual environment
`conda env list`	List all virtual environments
`conda list`	List all installed packages

Learning PyTorch with Practice

(From my point of view) PyTorch is a **NumPy extension** with supports of

+ A n-dimensional array with GPU acceleration and automatic differentiation
  so-called a ***tensor*** (Note: A matrix is a second-order tensor.)
+ Useful modules for neural networks

- Practice with tensors
  - Creating a tensor
  - Reshaping a tensor
  - Line fitting from two points
  - CPU vs. GPU-acceleration
  - Automatic differentiation (so called *Autograd*)
- Practice with useful modules for neural networks
  - Gradient descent by hands and `torch.optim`
  - More examples with DNNs, CNNs, and RNNs.

Practice) Creating a Tensor (1/2)

```
import numpy as np
import torch

# 1. Create a tensor from a composite data
x = np.array([[3, 29, 82], [10, 18, 84]])
y = torch.tensor(x)
print(y.ndim, y.dim())      # 2                       Note) x.ndim
print(y.nelement())         # 6                       Note) x.size
print(y.shape, y.size())    # torch.Size([2, 3])      Note) x.shape
print(y.dtype)              # torch.int32             Note) x.dtype

# 2. Create a tensor using initializers
p = torch.rand(3, 2)        # Try zeros, ones, eyes, empty, arange, linspace,
q = torch.zeros_like(p)     #     and their ..._like
print(p.dtype)              # torch.float32
print(q.shape)              # torch.Size([3, 2])

# 3. Interpret as a tensor (generating only a view)
z = torch.as_tensor(x)      # Or torch.from_numpy(x)  Note) np.asarray()
x[-1,-1] = 86
print(z[-1])                # tensor([10, 18, 86], dtype=torch.int32)
```

Practice) Creating a Tensor (2/2)

```
# 4. Access elements
print(y[:,1])                 # tensor([29, 18])
print(y[0,0])                 # tensor(3)                Note) x[0,0] == 3
print(y[0,0].item())          # 3

# 5. CUDA tensors
if torch.cuda.is_available():
    print(y.device)           # 'cpu'
    y_cuda = y.cuda()         # Or y.to('cuda')
    print(y_cuda.device)      # 'cuda:0'
    y_cpu = y_cuda.cpu()      # Or y.cuda.to('cpu')
    print(y_cpu.device)       # 'cpu'

    x_cpu = y_cpu.numpy()     # Or np.array(y_cpu)
    x_cuda = y_cuda.numpy()   # Error!
```

Practice) Reshaping a Tensor (1/2)

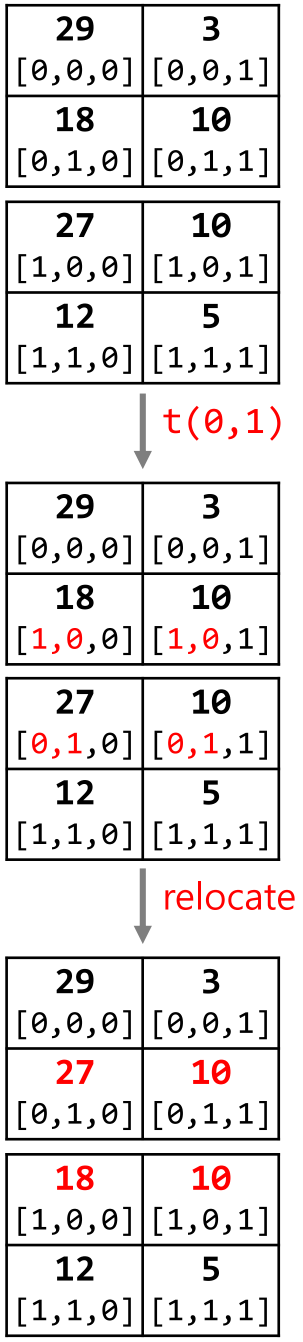
29 [0,0,0]	**3** [0,0,1]
18 [0,1,0]	**10** [0,1,1]

27 [1,0,0]	**10** [1,0,1]
12 [1,1,0]	**5** [1,1,1]

```python
import numpy as np
import torch

x = np.array([[[29, 3], [18, 10]], [[27, 10], [12, 5]]])
y = torch.tensor(x)
print(y.ndim)          # 3
print(y.shape)         # torch.Size([2, 2, 2])

p = y.view(-1)         # tensor([29, 3, 18, 10, 27, 10, 12, 5])
print(p.shape, p)      # torch.Size([8])
q = y.view(1, -1)      # tensor([[29, 3, 18, 10, 27, 10, 12, 5]])
print(q.shape, q)      # torch.Size([1, 8])
r = y.view(2, -1)      # tensor([[29, 3, 18, 10], [27, 10, 12, 5]])
print(r.shape, r)      # torch.Size([2, 4])
# Of course, 'reshape' is also supported and the same with 'view'.
s = y.reshape(2, -1, 1) # tensor([[[29], [3], [18], [10]], [[27], [10], [12], [5]]])
print(s.shape, s)      # torch.Size([2, 4, 1])

ss = s.squeeze(2)      # Note) s.squeeze(0) and s.squeeze(1) have no effect.
print(ss)              # tensor([[29, 3, 18, 10], [27, 10, 12, 5]])
print(ss.shape)        # torch.Size([2, 4])
u0 = ss.unsqueeze(0)   # tensor([[[29, 3, 18, 10], [27, 10, 12,  5]]])
print(u0.shape, u0)    # torch.Size([1, 2, 4])
u1 = ss.unsqueeze(1)   # tensor([[[29, 3, 18, 10]], [[27, 10, 12, 5]]])
print(u1.shape, u1)    # torch.Size([2, 1, 4])
u2 = ss.unsqueeze(2)   # tensor([[[29], [3], [18], [10]], [[27], [10], [12], [5]]])
print(u2.shape, u2)    # torch.Size([2, 4, 1])
```

Practice) Reshaping a Tensor (2/2)

```
# Switch indices each other, (i, j) to (j, i)
t_021 = y.transpose(1, 2)          # tensor([[[29, 18],
print(t_021, t_021.is_contiguous()) #           [ 3, 10]], ... ]) False
c_021 = t_021.contiguous()         # tensor([[[29, 18],
print(c_021, c_021.is_contiguous()) #           [ 3, 10]], ... ]) True
t_102 = y.transpose(0, 1)          # tensor([[[29,  3],
print(t_102, t_102.is_contiguous()) #            27, 10]], ... ]) False

# Assign indices
t_201 = y.permute(2, 0, 1)         # tensor([[[29, 18],
print(t_201, t_201.is_contiguous()) #           [27, 12]], ... ]) False

# Note) Reshaping does not copy contents.
y[0,0,0] = 27
print(p)                           # tensor([27, 3, 18, 10, 27, 10, 12, 5])
print(t_021)                       # tensor([[[27, 18], ...], ...])
print(c_021)                       # tensor([[[29, 18], ...], ...])

# Copy a tensor and detach it from its connected computational graph
z = y.clone().detach()             # Note) x.clone()
y[0,0,0] = 1
print(y)                           # tensor([[[ 1, 3], ...], ...])
print(z)                           # tensor([[[27, 3], ...], ...])
```



Practice) Line Fitting from Two Points

- Find a line which passes two points, $(1, 4)$ and $(4, 2)$
  - The tensor class, `torch.Tensor`, includes member functions of tensor operation and manipulation, and linear algebra (in contrast to `numpy.array`).
  - Note) [PyTorch APIs for `torch.Tensor`]
    - Remind again that a function with `ending_` means an in-place function.

```
import torch

A = torch.tensor([[1., 1.], [4., 1.]])
b = torch.tensor([[4.], [2.]])
A_inv = A.inverse()        # Note) np.linalg.inv(A)
print(A_inv.mm(b))         # Note) np.matmul(A_inv, b)
```

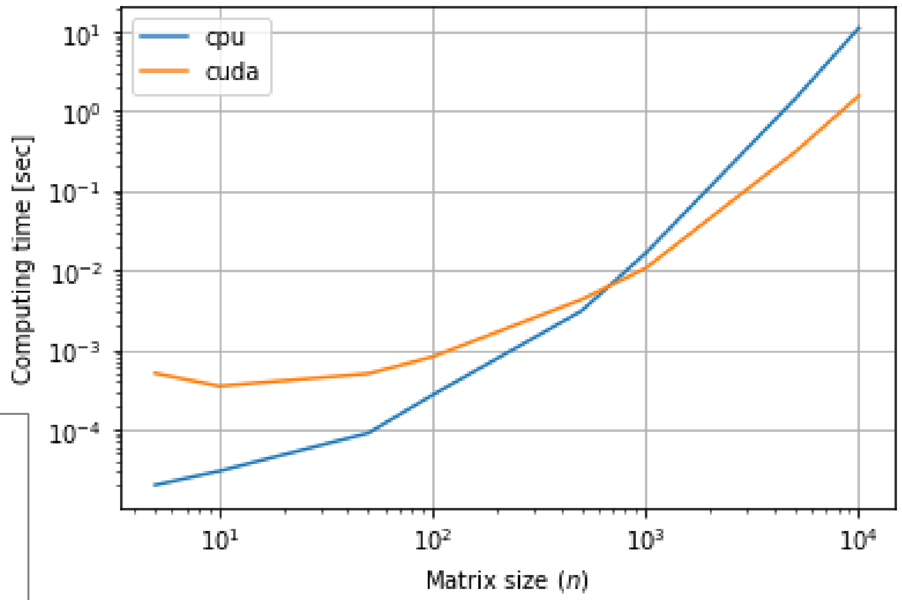
- Note) Line fitting with NumPy

```
import numpy as np

A = np.array([[1., 1.], [4., 1.]])
b = np.array([[4.], [2.]])
A_inv = np.linalg.inv(A)
print(np.matmul(A_inv, b)) # [[-0.66666667], [ 4.66666667]]
```

Practice) CPU vs. GPU-acceleration

- Computing time on my laptop
  - cpu : **1.4** [sec] @ Intel i7-7700HQ 2.8GHz
  - cuda: **0.3** [sec] @ NVIDIA GTX 1060

```
import torch
import time

dev_name = 'cuda' if torch.cuda.is_available() else 'cpu' # Try 'cpu'
n = 5000

A = torch.rand(n, n, device=dev_name)
B = torch.rand(n, n, device=dev_name)
start = time.time()
C = A.inverse() * B
elapse = time.time() - start
print(f'Computing time by {dev_name}: {elapse:.3f} [sec]')
```



Practice) Automatic Differentiation

- A derivative value, `torch.Tensor.grad`, is available after setting `requires_grad=True` and its forward calculation and backward propagation (a.k.a. backpropagation).

```
import torch

x = torch.tensor([2.], requires_grad=True)
y = 0.1*x**3 - 0.8*x**2 - 1.5*x + 5.4
y.backward()
print(x.grad) # Derivative: tensor([-3.5000])
```

- Note) Symbolic differentiation with SymPy

```
import sympy as sp

x, y = sp.symbols('x y')
y = 0.1*x**3 - 0.8*x**2 - 1.5*x + 5.4
yd = sp.diff(y, x)
print(yd)                     # 0.3*x**2 - 1.6*x - 1.5
print(float(yd.subs({x: 2}))) # -3.5
```

Practice) Automatic Differentiation – More Analysis

- Given) $y(x) = x^3$, $z(y) = \log y$
- Q) A derivative value $\frac{\partial z}{\partial x}$ at $x = 5$?

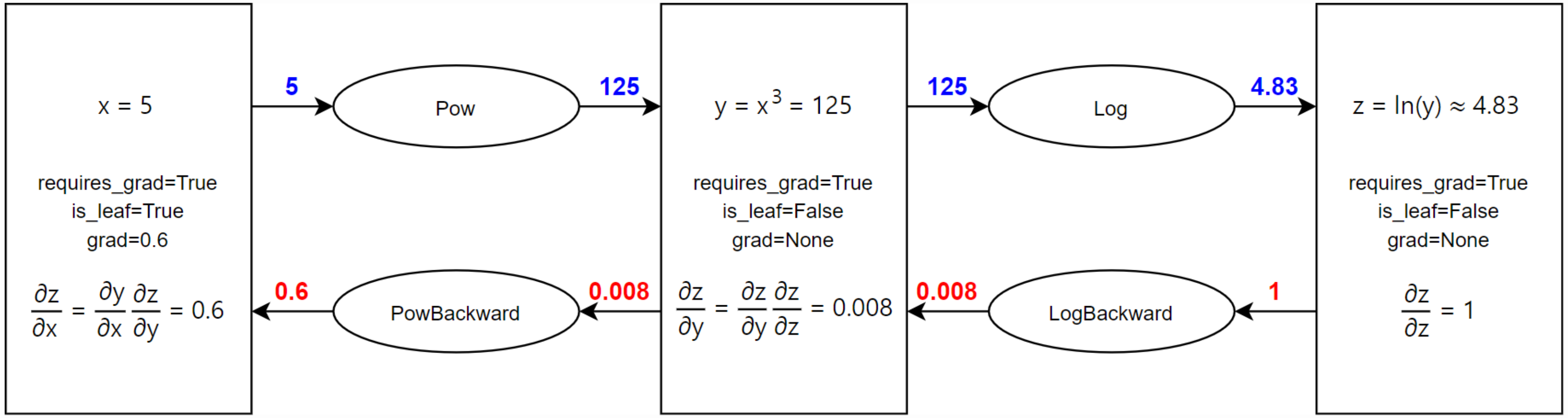
```
import torch

def get_tensor_info(tensor):
  info = []
  for name in ['requires_grad', 'is_leaf', 'retains_grad', 'grad']:
    info.append(f'{name}({getattr(tensor, name, None)})')
  info.append(f'tensor({str(tensor)})')
  return ' '.join(info)

x = torch.tensor(5., requires_grad=True)
y = x ** 3
z = torch.log(y)
print("### Before 'z.backward()'")
print('* x:', get_tensor_info(x))
print('* y:', get_tensor_info(y))
print('* z:', get_tensor_info(z))

y.retain_grad()
z.retain_grad()
z.backward()
print("### After 'z.backward()'")
print('* x:', get_tensor_info(x))
print('* y:', get_tensor_info(y))
print('* z:', get_tensor_info(z))
```

Code/Image: [Dable Tech Blog]()

Practice) Automatic Differentiation – More Analysis

- Given) $y(x) = x^3$, $z(y) = \log y$
- Q) A derivative value $\frac{\partial z}{\partial x}$ at $x = 5$?

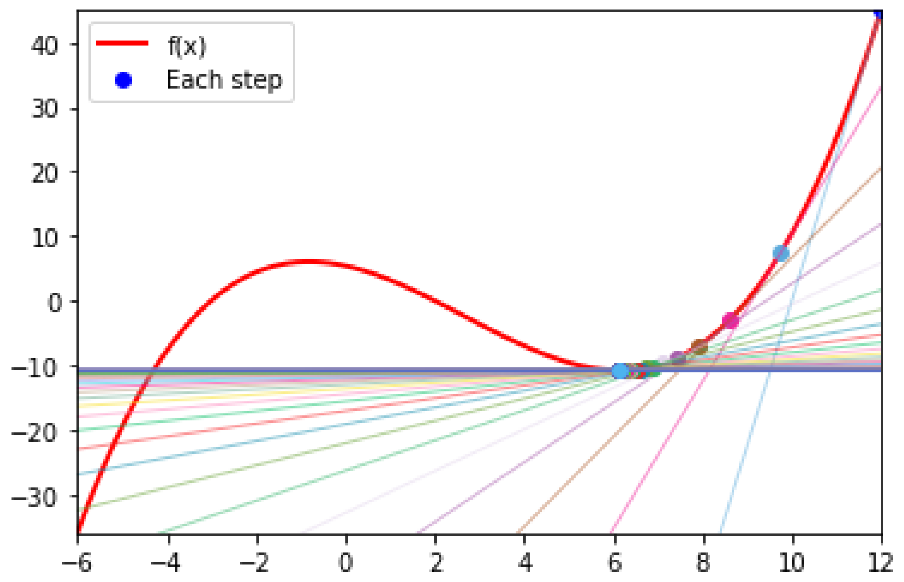
```
### Before 'z.backward()'
* x: requires_grad(True) is_leaf(True)  retains_grad(None) grad(None)  tensor(tensor(5.,   requires_grad=True))
* y: requires_grad(True) is_leaf(False) retains_grad(None) grad(None)  tensor(tensor(125., grad_fn=<PowBackward0>))
* z: requires_grad(True) is_leaf(False) retains_grad(None) grad(None)  tensor(tensor(4.83, grad_fn=<LogBackward>))

### After 'z.backward()'
* x: requires_grad(True) is_leaf(True)  retains_grad(None) grad(0.6)   tensor(tensor(5.,   requires_grad=True))
* y: requires_grad(True) is_leaf(False) retains_grad(True) grad(0.008) tensor(tensor(125., grad_fn=<PowBackward0>))
* z: requires_grad(True) is_leaf(False) retains_grad(True) grad(1.)    tensor(tensor(4.83, grad_fn=<LogBackward>))
```



Code/Image: Dable Tech Blog

Practice) Gradient Descent by Hands

```python
f = lambda x: 0.1*x**3 - 0.8*x**2 - 1.5*x + 5.4
viz_range = torch.FloatTensor([-6, 12])
learn_rate =  0.1
max_iter = 100
min_tol = 1e-6
x_init = 12.

# Prepare visualization
xs = torch.linspace(*viz_range, 100)
plt.plot(xs, f(xs), 'r-', label='f(x)', linewidth=2)
plt.plot(x_init, f(x_init), 'b.', label='Each step', markersize=12)
plt.axis((*viz_range, *f(viz_range)))
plt.legend()

x = torch.tensor(x_init, requires_grad=True)
for i in range(max_iter):
    # Derive gradient with Autograd
    if x.grad != None:
        x.grad.zero_()           # Reset gradient tracking
    y = f(x)                     # Calculate the function (forward)
    y.backward()                 # Calculate the gradient (backward)

    # Run the gradient descent
    xp = x.clone().detach()      # Note) xp = x
    with torch.no_grad():        # Disable gradient tracking
        x -= learn_rate*x.grad   # Note) x = x - learn_rate*fd(x) is an original code.
                                 #       x = x - learn_rate*x.grad() does not work!

    # Update visualization for each iteration
    print(f'Iter: {i}, x = {xp:.3f} to {x:.3f}, f(x) = {f(xp):.3f} to {f(x):.3f} (f\'(x) = {x.grad:.3f})')
    lcolor = torch.rand(3).tolist()
    approx = x.grad*(xs-xp) + f(xp)
    plt.plot(xs, approx, '-', linewidth=1, color=lcolor, alpha=0.5)
    xc = x.clone().detach() # Copy 'x' for plotting
    plt.plot(xc, f(xc), '.', color=lcolor, markersize=12)

    # Check the terminal condition
    if abs(x - xp) < min_tol:
        break;
plt.show()
```



Practice) Gradient Descent by `torch.optim`

```python
f = lambda x: 0.1*x**3 - 0.8*x**2 - 1.5*x + 5.4
viz_range = torch.FloatTensor([-6, 12])
learn_rate =  0.1
max_iter = 100
min_tol = 1e-6
x_init = 12.

# Prepare visualization
xs = torch.linspace(*viz_range, 100)
plt.plot(xs, f(xs), 'r-', label='f(x)', linewidth=2)
plt.plot(x_init, f(x_init), 'b.', label='Each step', markersize=12)
plt.axis((*viz_range, *f(viz_range)))
plt.legend()

x = torch.tensor(x_init, requires_grad=True)
optimizer = torch.optim.SGD([x], lr=learn_rate)
for i in range(max_iter):
    # Run the gradient descent with the optimizer
    optimizer.zero_grad()       # Reset gradient tracking
    y = f(x)                    # Calculate the function (forward)
    y.backward()                # Calculate the gradient (backward)
    xp = x.clone().detach()     # Note) xp = x
    optimizer.step()            # Update 'x'

    # Update visualization for each iteration
    print(f'Iter: {i}, x = {xp:.3f} to {x:.3f}, f(x) = {f(xp):.3f} to {f(x):.3f} (f\'(x) = {x.grad:.3f})')
    lcolor = torch.rand(3).tolist()
    approx = x.grad*(xs-xp) + f(xp)
    plt.plot(xs, approx, '-', linewidth=1, color=lcolor, alpha=0.5)
    xc = x.clone().detach() # Copy 'x' for plotting
    plt.plot(xc, f(xc), '.', color=lcolor, markersize=12)

    # Check the terminal condition
    if abs(x - xp) < min_tol:
        break;
plt.show()
```

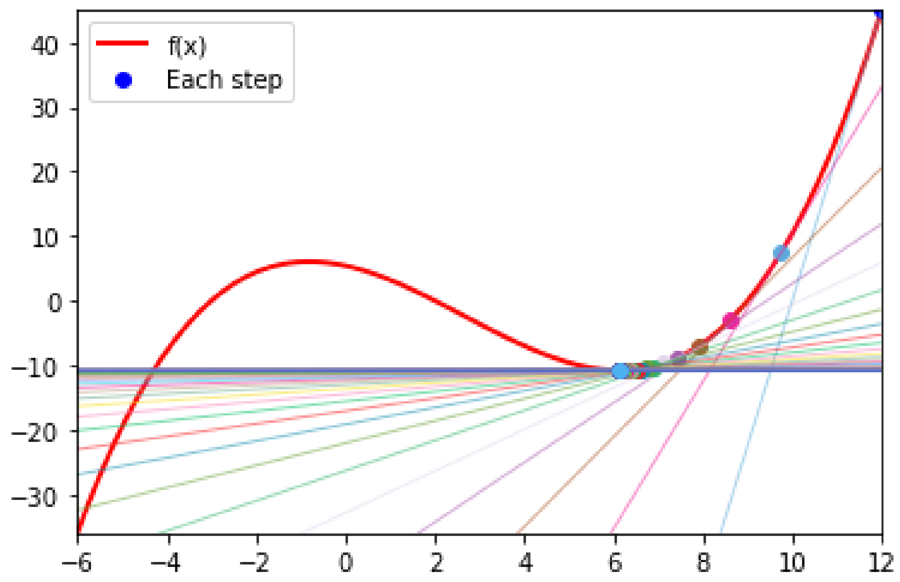
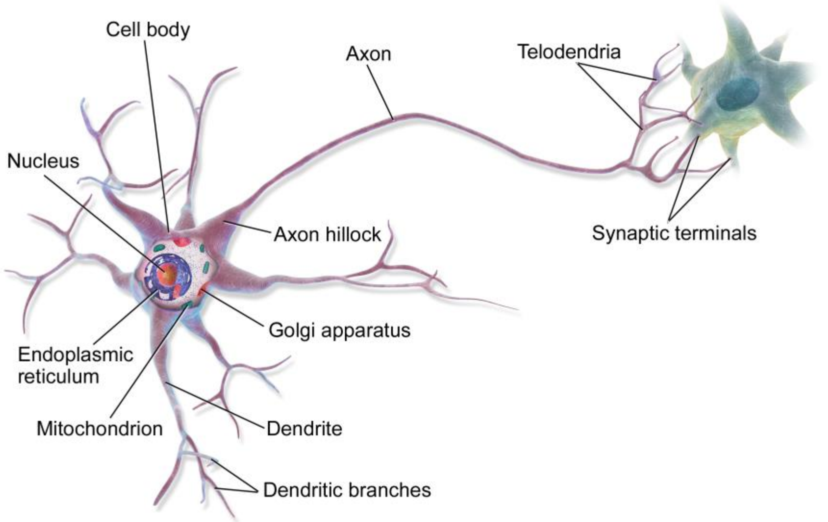
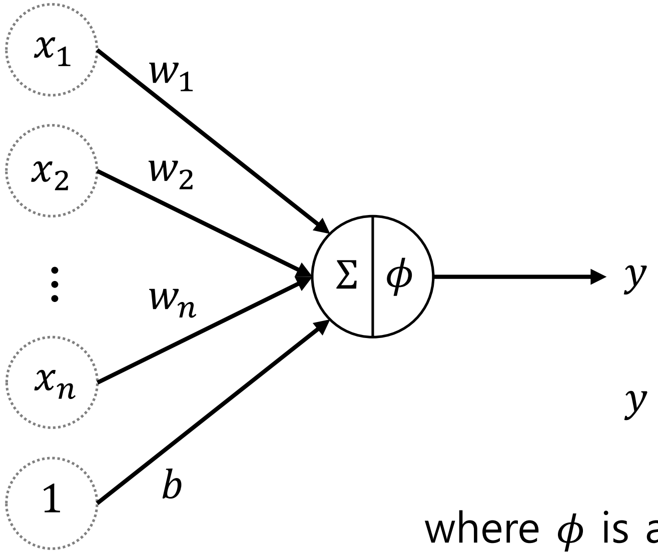


Table of Contents

Neural Network

- A *artificial neural network* (shortly *neural network*, *NN*) is a collection of perceptrons (a.k.a. artificial neurons) and their connection with weights.
  - Inspired by the biological neural networks.
- **Neuron vs. Perceptron**





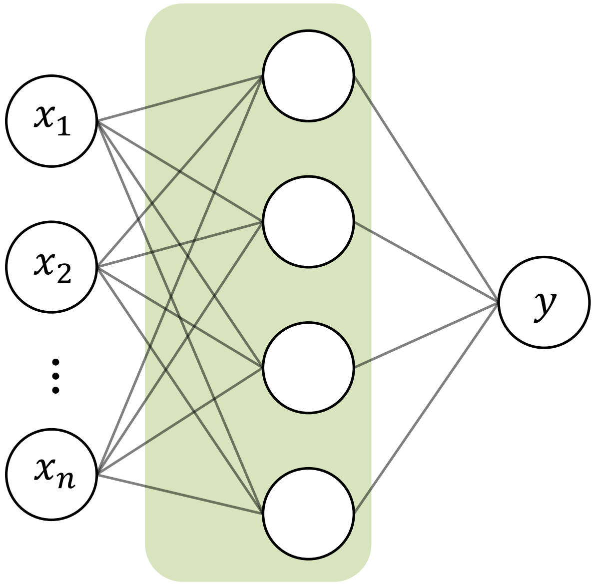
$$y = \phi\left(\sum_{i=1}^{n} w_i x_i + b\right)$$

where ϕ is an activation function (for nonlinearity) and b is bias.

Image: [Wikipedia]

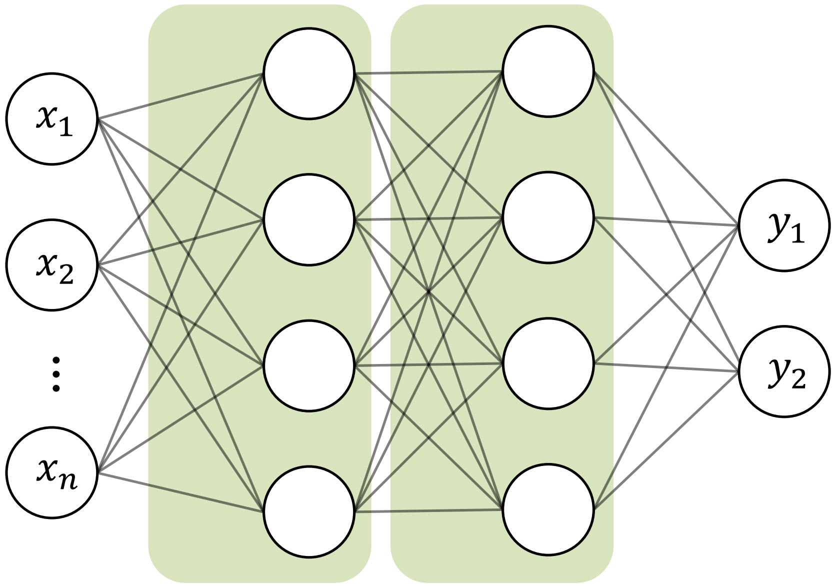
Neural Network

- **Multi-layer perceptrons (MLP)**
  - Note) Fully-connected (shortly FC) layer



2-layer NN

(1 x hidden layer, 1 x output)

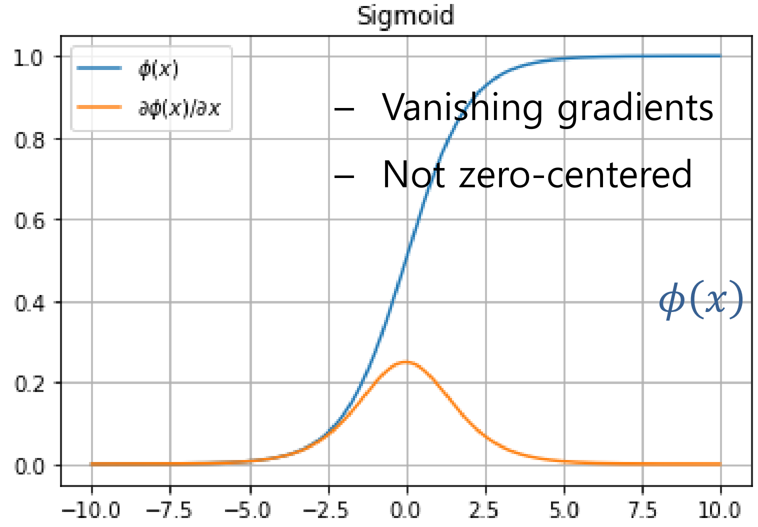


3-layer NN

(2 x hidden layer, 2 x output)

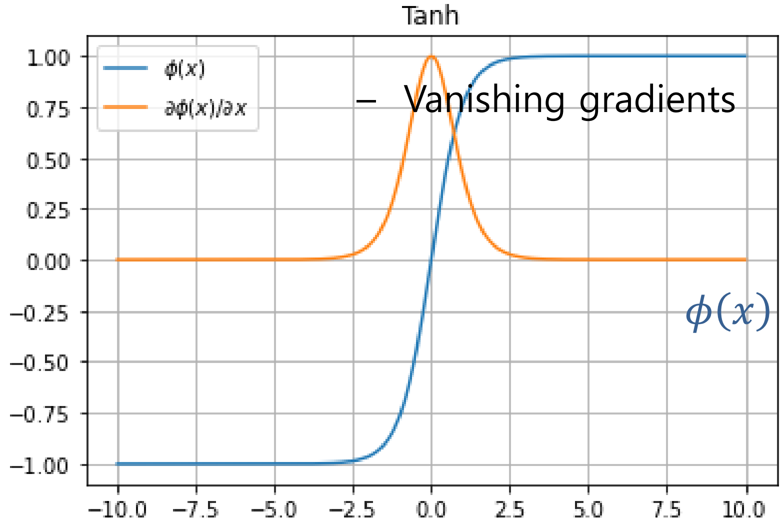
Activation Function

- **Activation function** imposes **nonlinearity** to a neural network.



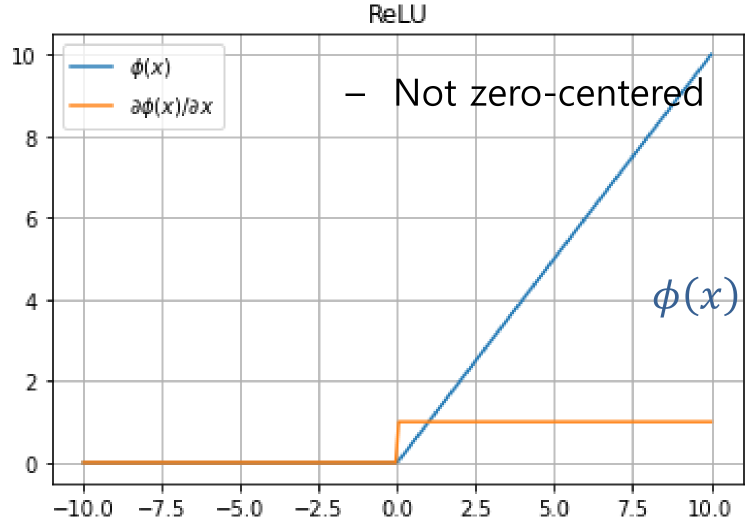
- Vanishing gradients
- Not zero-centered

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



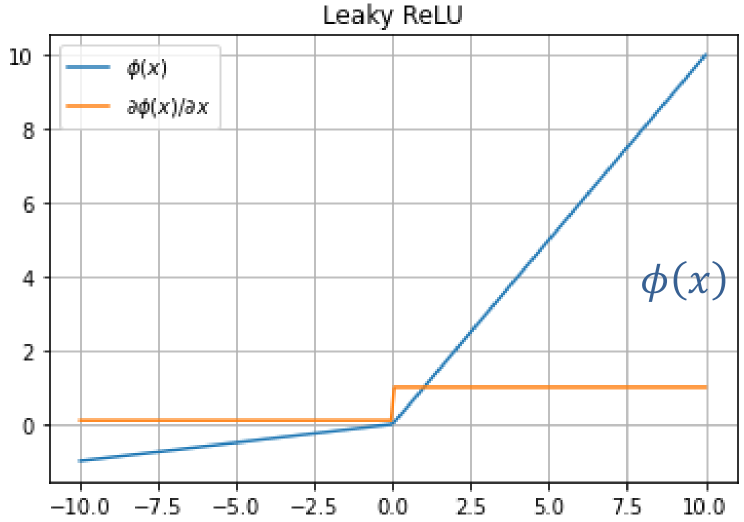
- Vanishing gradients

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



- Not zero-centered

$$\phi(x) = \begin{cases} 0 & \text{if } x \le 0 \\ x & \text{if } x > 0 \end{cases}$$



$$\phi(x) = \begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \ge 0 \end{cases}$$

Practice) Visualizing Activation Functions

- Visualize activation functions and their derivative functions
  - Note) [PyTorch APIs for activation functions]()

```
import torch
import torch.nn as nn
import matplotlib.pyplot as plt

activation_funcs = [
    {'name': 'Sigmoid',    'func': nn.Sigmoid()},
    {'name': 'Tanh',       'func': nn.Tanh()},
    {'name': 'ReLU',       'func': nn.ReLU()},
    {'name': 'Leaky ReLU', 'func': nn.LeakyReLU(0.1)},
    {'name': 'ELU',        'func': nn.ELU()},
    # Try more activation functions
]

for act in activation_funcs:
    x = torch.linspace(-10, 10, 200, requires_grad=True)
    y = act['func'](x)
    y.sum().backward()

    plt.title(act['name'])
    x_np, y_np, grad = x.detach().numpy(), y.detach().numpy(), x.grad.numpy()
    plt.plot(x_np, y_np, label='$\phi(x)$')
    plt.plot(x_np, grad, label='$\partial \phi(x) / \partial x$')
    plt.grid()
    plt.legend()
    plt.show()
```

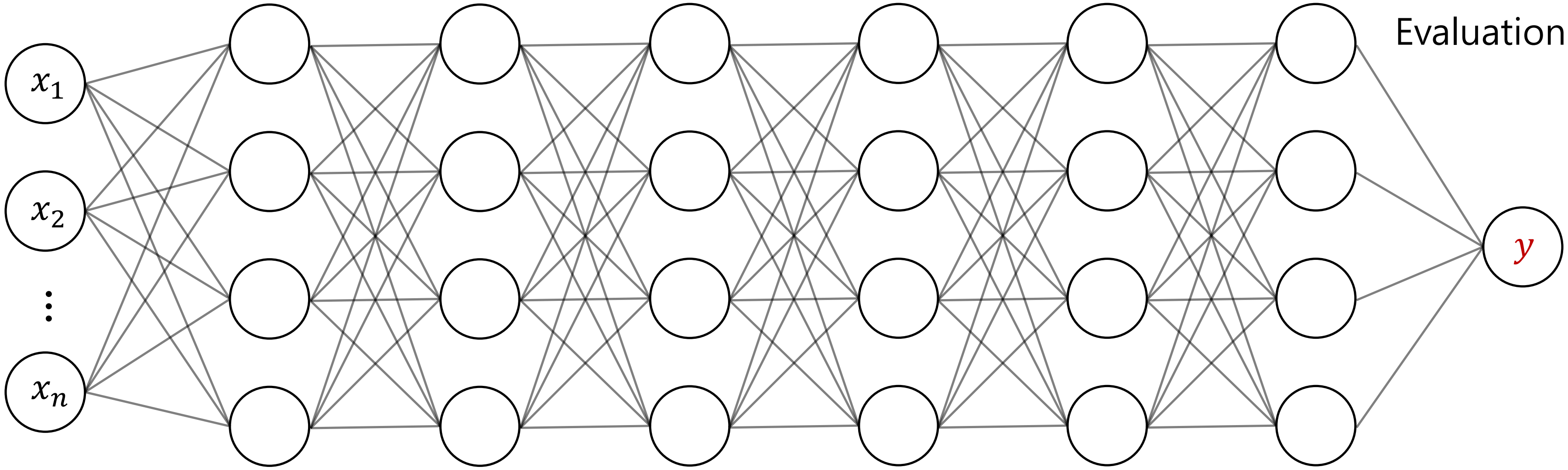
Backpropagation

- **Training a neural network (~ optimization)**

Finding weight variables which minimize a cost function as

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} \frac{1}{N} \sum_{d=1}^{N} l(y^d, \hat{y}^d)$$

where l is a loss function, N is the number of data, and $\hat{y}^d$ is the d-th target value.



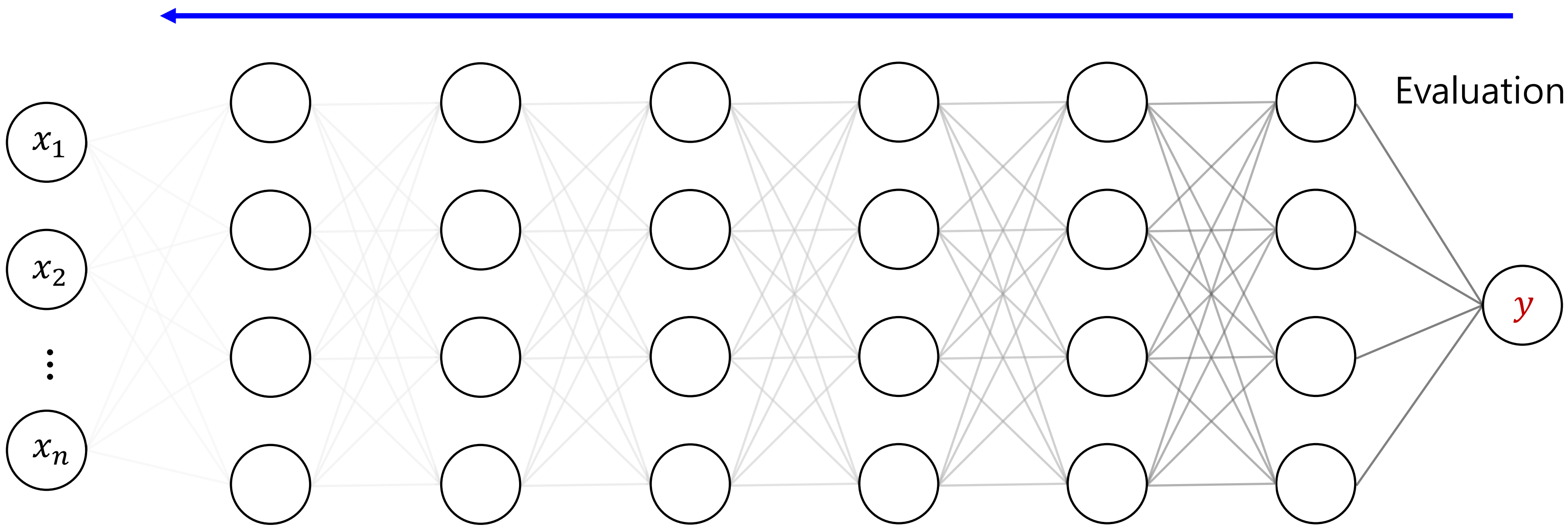
Evaluation with mean squared error

$$MSE = \frac{1}{N} \sum_{d=1}^{N} \left(\hat{y}^d - y^d\right)^2$$

where $l\left(y^d, \hat{y}^d\right) = \left(\hat{y}^d - y^d\right)^2$

Backpropagation

- **Backpropagation** is an algorithm for training a neural network.
  - It tries to find the optimal **weight variables** of a NN by **gradient descent**
- **Vanishing gradient problem**
  - During backpropagation, gradient values of a deep NN become close to 0.

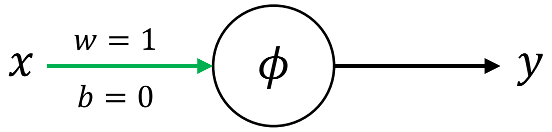


Evaluation with mean squared error

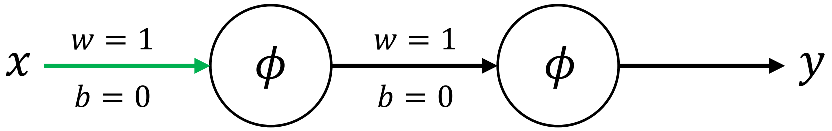
$$MSE = \frac{1}{N}\sum_{d=1}^{N}\left(\hat{y}^d - y^d\right)^2$$

Practice) Observing Vanishing Gradients

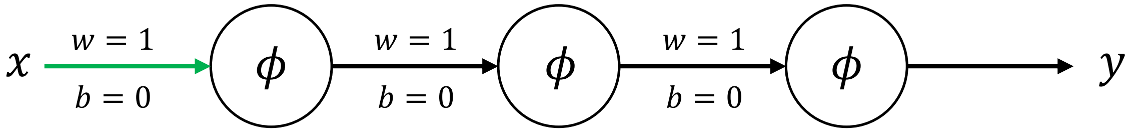
- Gradients of a single-node multi-layer NN
  - 1-layer forward: $y = \phi(wx + b) = \phi(x)$ **if $w = 1$ and $b = 0$**
  - 1-layer backward: $\frac{\partial y}{\partial x} = \phi'(x)$



  - 2-layer forward: $y = \phi(\phi(x))$
  - 2-layer backward: $\frac{\partial y}{\partial x} = \phi'\big(\phi(x)\big)\phi'(x)$ $\because$ **chain rule**



  - 3-layer forward: $y = \phi(\phi(\phi(x)))$
  - 3-layer backward: $\frac{\partial y}{\partial x} = \phi'\Big(\phi\big(\phi(x)\big)\Big)\phi'\big(\phi(x)\big)\phi'(x)$

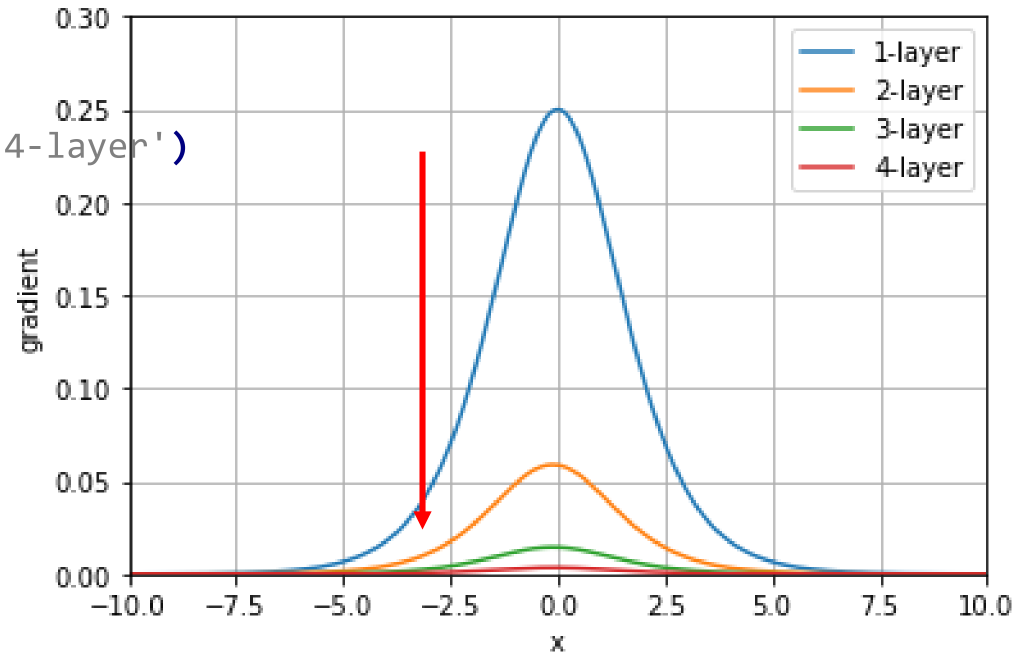


  - …

Practice) Observing Vanishing Gradients

- Gradients of a single-node multi-layer NN with the **sigmoid** function
  - Note) $\phi'(x) = \phi(x)\big(1 - \phi(x)\big)$

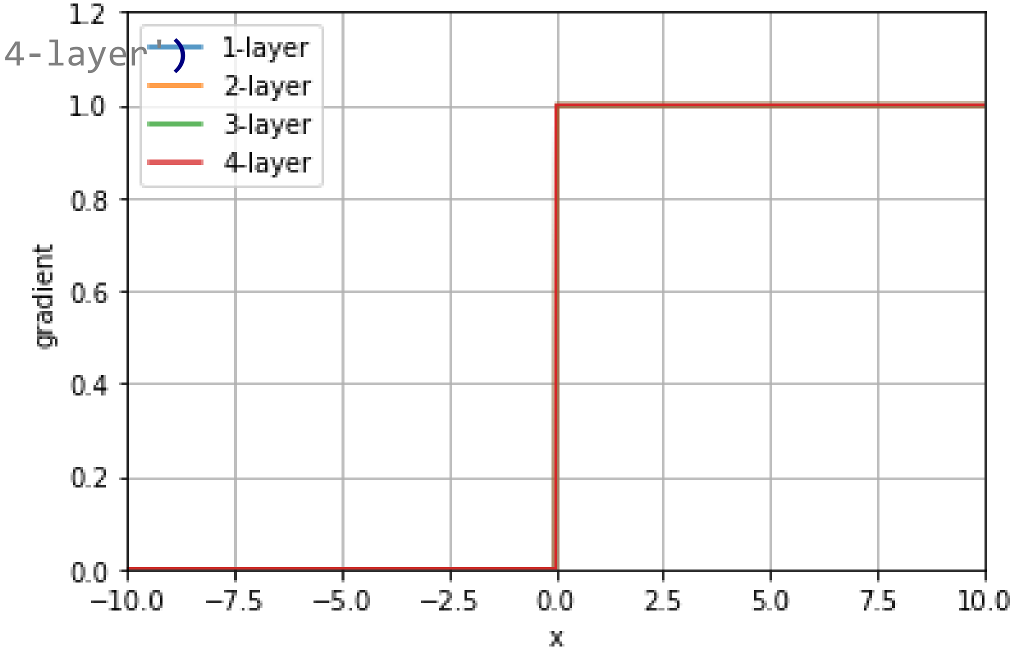
```
import numpy as np
import matplotlib.pyplot as plt

f  = lambda x: 1 / (1 + np.exp(-x))
df = lambda x: f(x) * (1 - f(x))

x = np.linspace(-10, 10, 1000)

plt.plot(x, df(x), label='1-layer')
plt.plot(x, df(f(x))*df(x), label='2-layer')
plt.plot(x, df(f(f(x)))*df(f(x))*df(x), label='3-layer')
plt.plot(x, df(f(f(f(x))))*df(f(f(x)))*df(f(x))*df(x), label='4-layer')
plt.axis((-10, 10, 0, 0.3))
plt.grid()
plt.legend()
plt.show()
```



Practice) Observing Vanishing Gradients

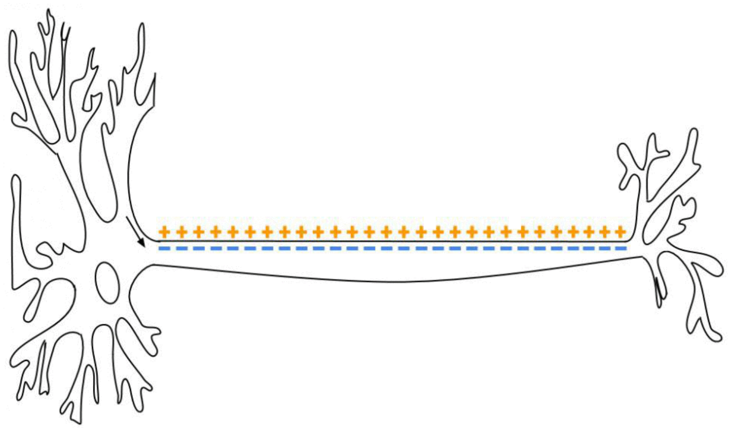
- Gradients of a single-node multi-layer NN with the **ReLU** function

```
import numpy as np
import matplotlib.pyplot as plt

f  = lambda x: x * (x >= 0)
df = lambda x: x >= 0

x = np.linspace(-10, 10, 1000)

plt.plot(x, df(x), label='1-layer')
plt.plot(x, df(f(x))*df(x), label='2-layer')
plt.plot(x, df(f(f(x)))*df(f(x))*df(x), label='3-layer')
plt.plot(x, df(f(f(f(x))))*df(f(f(x)))*df(f(x))*df(x), label='4-layer')
plt.axis((-10, 10, 0, 0.3))
plt.grid()
plt.legend()
plt.show()
```



Activation Function (Revisited)

- **Why ReLU?**
  - It can relax the vanishing gradient problem.
  - In addition, there is a biological analogue such as neural action potential.



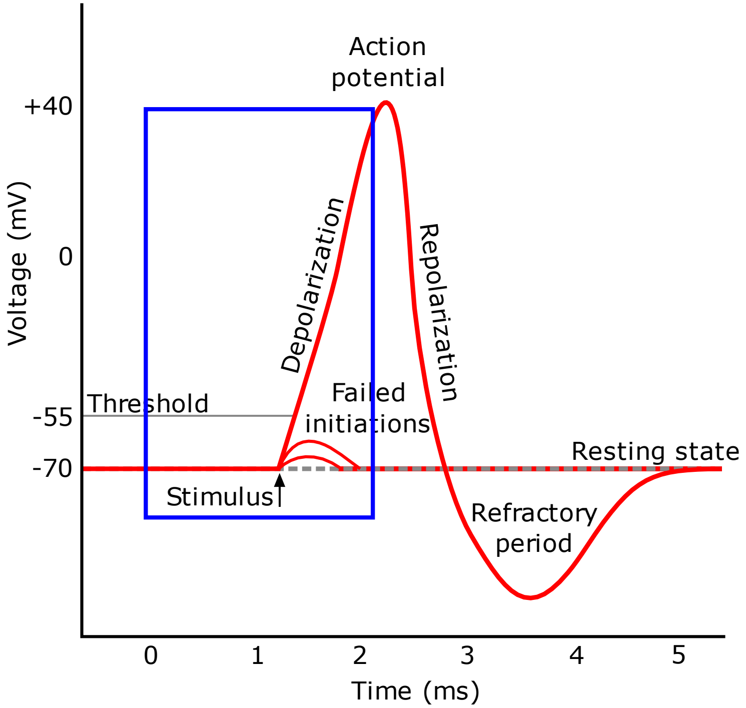


Image: Wikipedia

Loss Function

- **Training a neural network (~ optimization)**

  Finding weight variables which minimize a cost function as

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} \frac{1}{N} \sum_{d=1}^{N} l(y^d, \hat{y}^d)$$

  where l is a loss function, N is the number of data, and $\hat{y}^d$ is the d-th target value.

- **Loss function**
  - A *loss function* quantifies gap between the ground truth and prediction.
  - e.g. **Mean squared error** (usually for *regression*)

$$l(y, \hat{y}) = (\hat{y} - y)^2$$

    where $\hat{y}$ is the ground truth, y is prediction, and N is the number of data.

  - e.g. **Binary cross entropy error** (usually for *binary classification*)

$$l(y, \hat{y}) = -\hat{y} \log y - (1 - \hat{y}) \log(1 - y)$$

    In general, $-\sum \hat{y}_i \log y_i$ for *multi-class classification*

Loss Function

- **Loss function**
  - e.g. **Cross entropy error** (usually for *multi-class classification*)

$$l(\mathbf{y}, \hat{\mathbf{y}}) = -\sum_{i=1}^{C} \hat{y}_i \log y_i$$

where $\hat{y}_i$ is the one-hot-encoded truth, y_i is the predicted (softmax) confidence

	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_3$
$\hat{\mathbf{y}}$:	0	1	0

	y_1	y_2	y_3
$\mathbf{y}$:	0.012	0.929	0.058

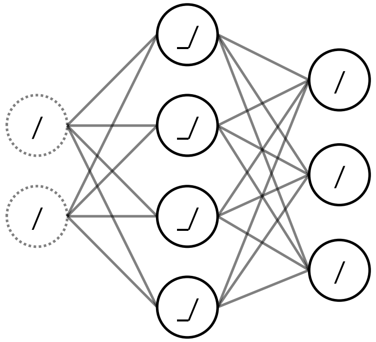
Softmax: $y_i = \exp z_i \,/\, \sum_{j=1}^{C} \exp z_j$

NN output $\mathbf{z}$	-1.03	3.29	0.52

  - Note) PyTorch APIs for loss functions

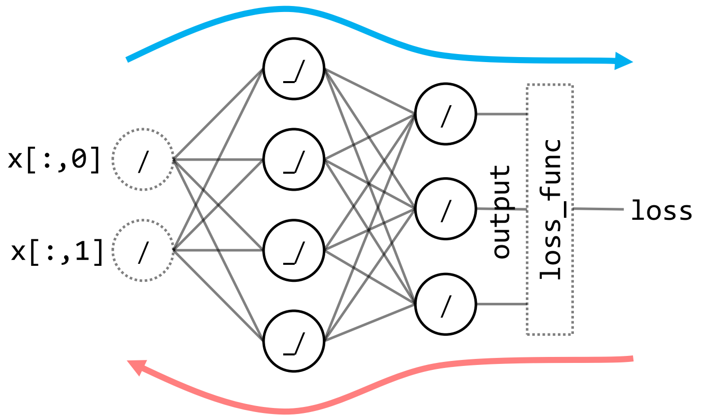
Practice) Iris Flower Classification (1/3)

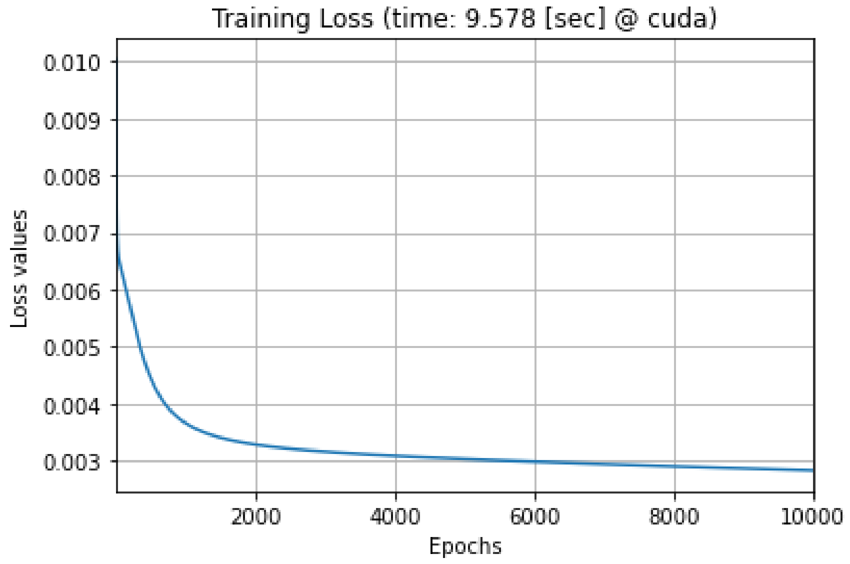
```
import torch
import torch.nn as nn
import numpy as np
import matplotlib.pyplot as plt
from sklearn import (datasets, metrics)
from matplotlib.colors import ListedColormap
import time

# 1.1. Load a dataset partially
iris = datasets.load_iris()
iris.data = iris.data[:,0:2]
iris.feature_names = iris.feature_names[0:2]
iris.color = np.array([(1, 0, 0), (0, 1, 0), (0, 0, 1)])

# 1.2. Load the dataset as tensors
dev_name = 'cuda' if torch.cuda.is_available() else 'cpu' # Try 'cpu'
x = torch.tensor(iris.data,   device=dev_name).float()
y = torch.tensor(iris.target, device=dev_name).long()

# 2. Define a model
# - Try the different number of hidden layers
# - Try less or more layers with different transfer functions
input_size, output_size = len(iris.feature_names), len(iris.target_names)
model = nn.Sequential(
    nn.Linear(input_size, 4),
    nn.ReLU(),
    nn.Linear(4, output_size),
).to(dev_name)
```



Practice) Iris Flower Classification (2/3)

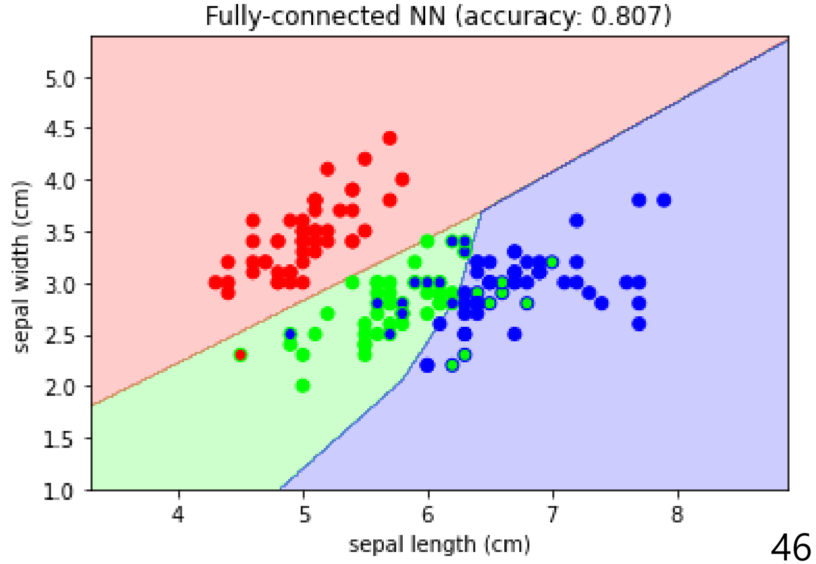
```
# 3. Train the model
loss_func = nn.CrossEntropyLoss()
optimizer = torch.optim.SGD(model.parameters(), lr=0.01) # Try other optimizers
epoch_max = 10000
loss_list = []
start = time.time()
for i in range(epoch_max):
    # Train one iteration
    optimizer.zero_grad()
    output = model(x)
    loss = loss_func(output, y)
    loss.backward()
    optimizer.step()

    # Record the loss
    loss_list.append(loss / len(x))
elapse = time.time() - start

# 4.1. Visualize the training loss curve
plt.title(f'Training Loss (time: {elapse/60:.2f} [min] @ {dev_name})')
plt.plot(range(1, epochs + 1), loss_list)
plt.xlabel('Epochs')
plt.ylabel('Loss values')
plt.xlim((1, epochs))
plt.grid()
plt.show()
```





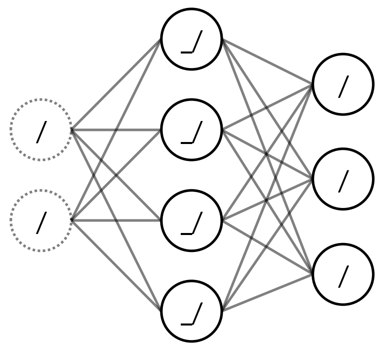
Practice) Iris Flower Classification (3/3)

```
# 4.2. Visualize training results (decision boundaries)
x_min, x_max = iris.data[:, 0].min() - 1, iris.data[:, 0].max() + 1
y_min, y_max = iris.data[:, 1].min() - 1, iris.data[:, 1].max() + 1
xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.01), np.arange(y_min, y_max, 0.01))
xy = np.vstack((xx.flatten(), yy.flatten())).T
xy_tensor = torch.from_numpy(xy).float().to(dev_name)
zz = torch.argmax(model(xy_tensor), dim=1).cpu().detach().numpy()
plt.contourf(xx, yy, zz.reshape(xx.shape), cmap=ListedColormap(iris.color), alpha=0.2)

# 4.3. Visualize data with their classification
predict = torch.argmax(model(x), dim=1).cpu().detach().numpy()
accuracy = metrics.balanced_accuracy_score(iris.target, predict)
plt.title(f'Fully-connected NN (accuracy: {accuracy:.3f})')
plt.scatter(iris.data[:,0], iris.data[:,1], c=iris.color[iris.target], edgecolors=iris.color[predict])
plt.xlabel(iris.feature_names[0])
plt.ylabel(iris.feature_names[1])
plt.show()
```



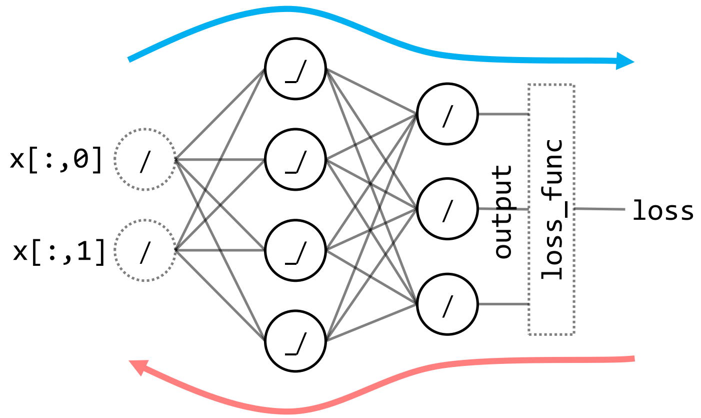
Practice) Iris Flower Classification – My Style (1/5)

```python
import torch
import torch.nn as nn
import torch.nn.functional as F
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets
from matplotlib.colors import ListedColormap
import time

# Define hyperparameters
EPOCH_MAX = 10000
EPOCH_LOG = 1000
OPTIMIZER_PARAM = {'lr': 0.01}
DATA_LOADER_PARAM = { 'batch_size': 50, 'shuffle': True }
USE_CUDA = torch.cuda.is_available()
RANDOM_SEED = 777

# A two-layer NN model
class MyDNN(nn.Module):
    def __init__(self, input_size=2, output_size=3):
        super(MyDNN, self).__init__()
        self.fc1 = nn.Linear(input_size, 4)
        self.fc2 = nn.Linear(4, output_size)

        nn.init.xavier_uniform_(self.fc1.weight)
        nn.init.xavier_uniform_(self.fc2.weight)

    def forward(self, x):
        x = F.relu(self.fc1(x))
        x = self.fc2(x)
        return x
```



Practice) Iris Flower Classification – My Style (2/5)

```python
# Train a model with the given batches
def train(model, batch_data, loss_func, optimizer):
    model.train() # Notify layers (e.g. DropOut, BatchNorm) that it’s now training
    train_loss, n_data = 0, 0
    dev = next(model.parameters()).device
    for batch_idx, (x, y) in enumerate(batch_data):
        x, y = x.to(dev), y.to(dev)
        optimizer.zero_grad()
        output = model(x)
        loss = loss_func(output, y)
        loss.backward()
        optimizer.step()

        train_loss += loss.item()
        n_data += len(y)
    return train_loss / n_data

# Evaluate a model with the given batches
def evaluate(model, batch_data, loss_func):
    model.eval() # Notify layers (e.g. DropOut, BatchNorm) that it’s now testing
    test_loss, n_correct, n_data = 0, 0, 0
    with torch.no_grad():
        dev = next(model.parameters()).device
        for x, y in batch_data:
            x, y = x.to(dev), y.to(dev)
            output = model(x)
            loss = loss_func(output, y)
            y_pred = torch.argmax(output, dim=1)

            test_loss += loss.item()
            n_correct += (y == y_pred).sum().item()
            n_data += len(y)
    return test_loss / n_data, n_correct / n_data
```



Practice) Iris Flower Classification – My Style (3/5)

```
if __name__ == '__main__':
    # 0. Preparation
    torch.manual_seed(RANDOM_SEED)
    if USE_CUDA:
        torch.cuda.manual_seed_all(RANDOM_SEED)
    dev = torch.device('cuda' if USE_CUDA else 'cpu')

    # 1.1. Load the Iris dataset partially
    iris = datasets.load_iris()
    iris.data = iris.data[:,0:2]
    iris.feature_names = iris.feature_names[0:2]
    iris.color = np.array([(1, 0, 0), (0, 1, 0), (0, 0, 1)])

    # 1.2. Wrap the dataset with torch.utils.data.DataLoader
    x = torch.tensor(iris.data, dtype=torch.float32, device=dev)
    y = torch.tensor(iris.target, dtype=torch.long, device=dev)
    data_train = torch.utils.data.TensorDataset(x, y)
    loader_train = torch.utils.data.DataLoader(data_train, **DATA_LOADER_PARAM)
```

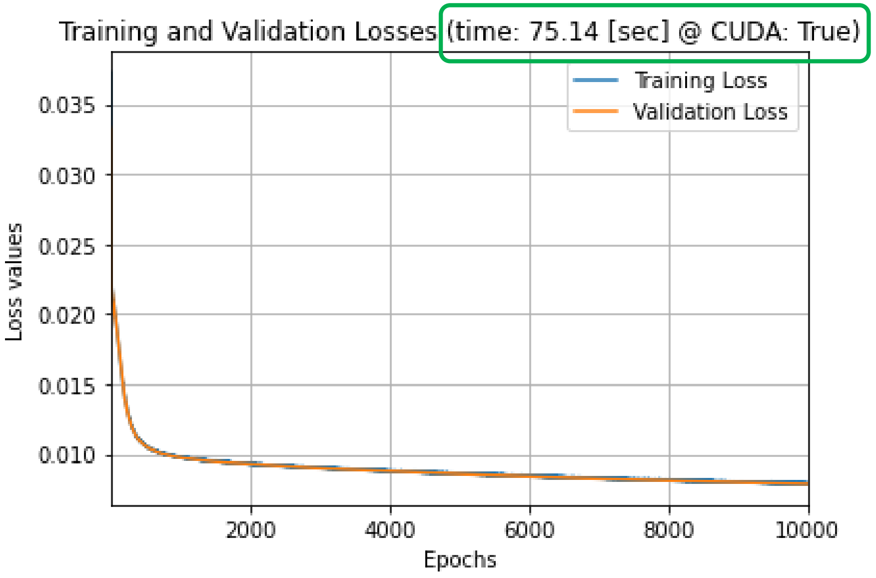
Practice) Iris Flower Classification – My Style (4/5)

```
# 2. Instantiate a model, loss function, and optimizer
model = MyDNN().to(dev)
loss_func = F.cross_entropy
optimizer = torch.optim.SGD(model.parameters(), **OPTIMIZER_PARAM)

# 3. Train the model
loss_list = []
start = time.time()
for epoch in range(1, EPOCH_MAX + 1):
    train_loss = train(model, loader_train, loss_func, optimizer)
    valid_loss, valid_accuracy = evaluate(model, loader_train, loss_func)

    loss_list.append([epoch, train_loss, valid_loss, valid_accuracy])
    if epoch % EPOCH_LOG == 0:
        elapse = time.time() - start
        print(f'{epoch:>6} ({elapse:>6.2f} sec), TrLoss={train_loss:.6f}, VaLoss={valid_loss:.6f}, VaAcc={valid_accuracy:.3f}')
elapse = time.time() - start

# 4.1. Visualize the loss curves
# 4.2. Visualize training results (decision boundaries)
# 4.3. Visualize data with their classification
```

Practice) Iris Flower Classification – My Style (5/5)

```
 1000 (  7.71 sec), TrLoss=0.009773, VaLoss=0.009769, VaAcc=0.707
 2000 ( 15.17 sec), TrLoss=0.009300, VaLoss=0.009281, VaAcc=0.747
 3000 ( 22.85 sec), TrLoss=0.009022, VaLoss=0.009007, VaAcc=0.780
 4000 ( 30.41 sec), TrLoss=0.008800, VaLoss=0.008786, VaAcc=0.800
 5000 ( 37.85 sec), TrLoss=0.008606, VaLoss=0.008594, VaAcc=0.813
 6000 ( 45.49 sec), TrLoss=0.008433, VaLoss=0.008420, VaAcc=0.813
 7000 ( 53.06 sec), TrLoss=0.008274, VaLoss=0.008262, VaAcc=0.813
 8000 ( 60.31 sec), TrLoss=0.008138, VaLoss=0.008118, VaAcc=0.807
 9000 ( 67.91 sec), TrLoss=0.008008, VaLoss=0.007990, VaAcc=0.800
10000 ( 75.14 sec), TrLoss=0.007928, VaLoss=0.007880, VaAcc=0.800
```

Discussion) CPU vs. GPU
Data as raw tensors vs. Data as `DataLoader`



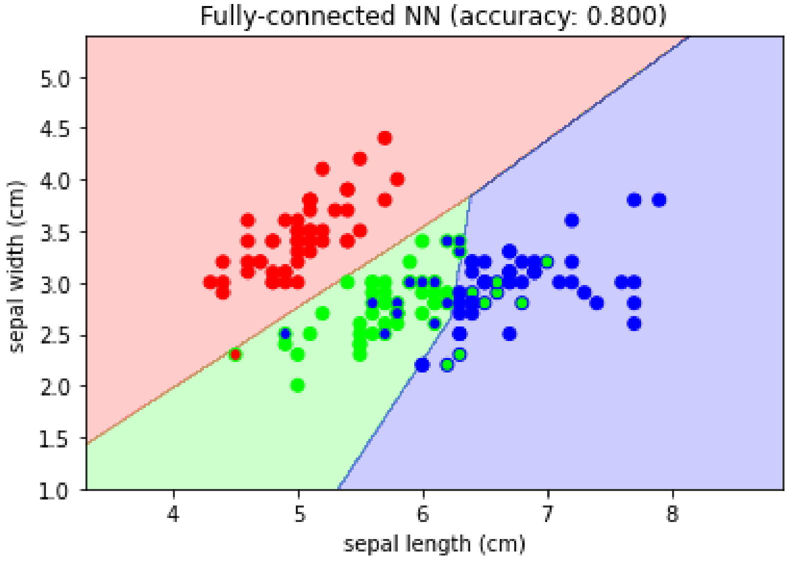


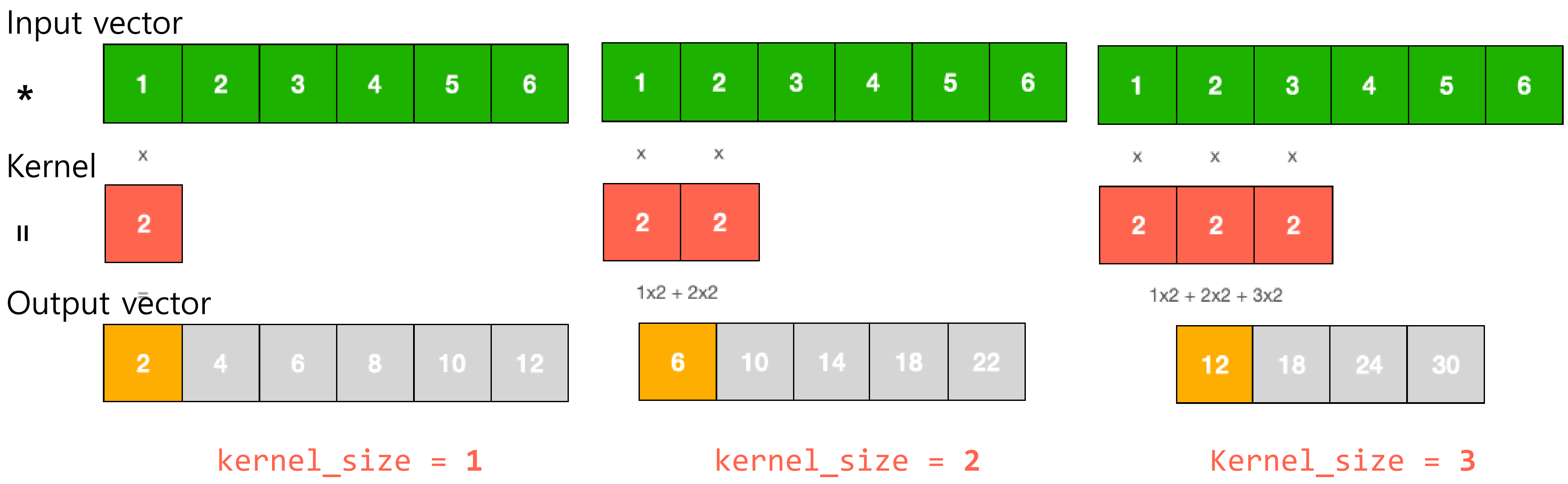
Table of Contents

Convolution

- **Discrete convolution**

$$(f * g)(k) = \sum_{i=-\infty}^{\infty} f(i)g(k-i)$$

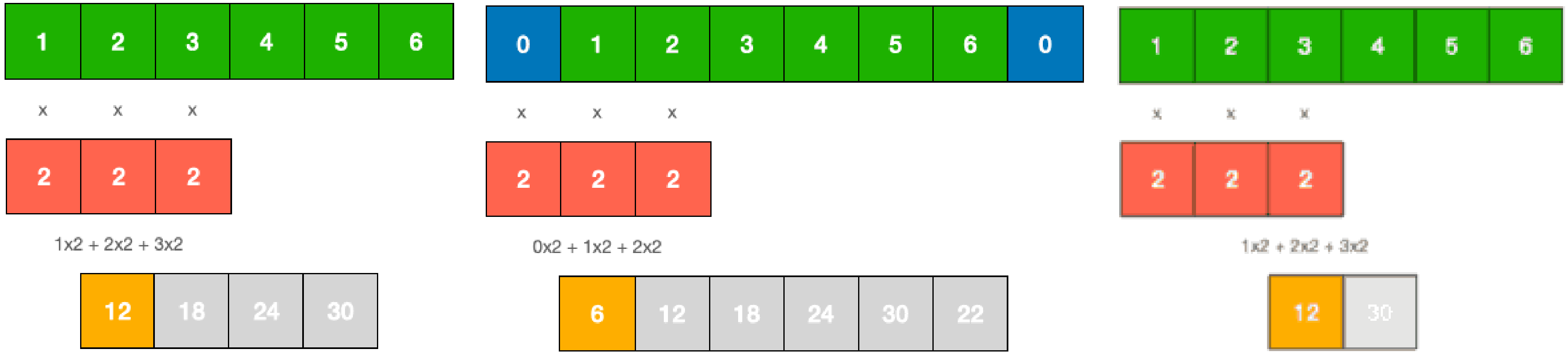
- 1D discrete convolution (e.g. voice)



Animation: [Towards Data Science article (by Jingles)]

Convolution

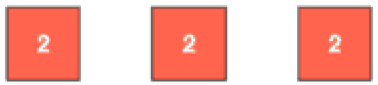
- 1D discrete convolution (continued)




```
kernel_size = 3
padding = 0
stride = 1
dilation = 1
```

```
kernel_size = 3
padding = 1
stride = 1
dilation = 1
```

```
kernel_size = 3
padding = 0
stride = 3
dilation = 1
```




```
dilation = 2
```

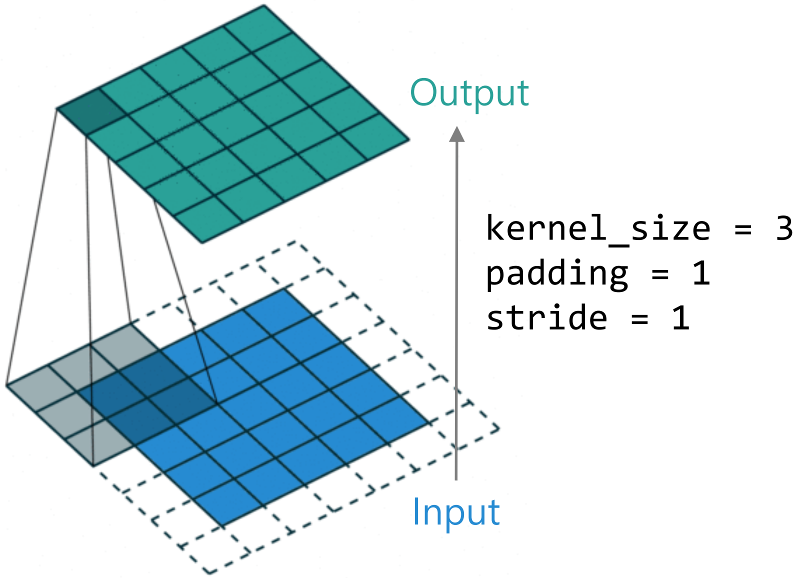
- The size of output vectors

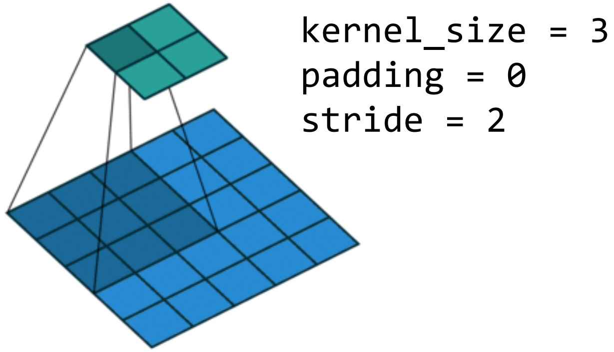
$$\text{output\_size} = \left\lfloor \frac{\text{input\_size} + 2 \times \text{padding} - (\text{dilation} \times (\text{kernel}_{\text{size}} - 1) + 1)}{\text{stride}} + 1 \right\rfloor$$

Animation: [Towards Data Science article (by Jingles)]

Convolution

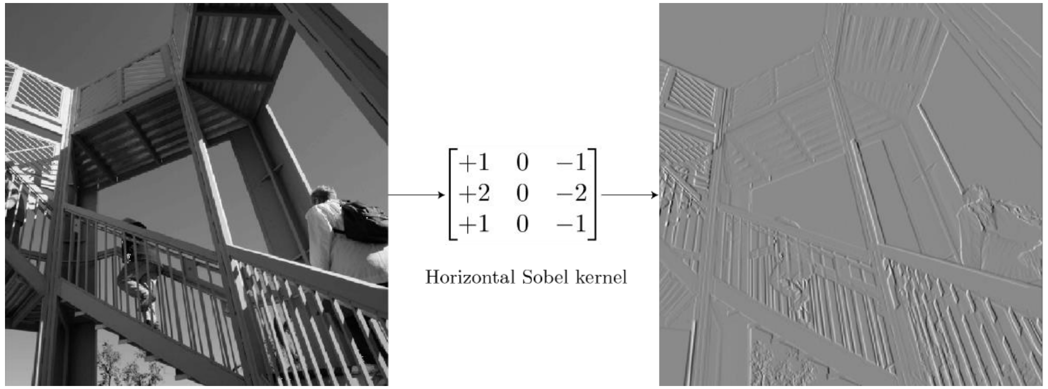
- 2D discrete convolution (e.g. image)





– A kernel and its output are also called as a *filter* and *feature map* (or *activation map*), respectively.

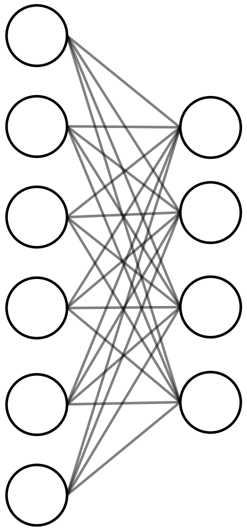
  - CNN visualization examples: ConvNetJS, ~~CNN Explainer~~
  - e.g. When a kernel is a horizontal Sobel filter,

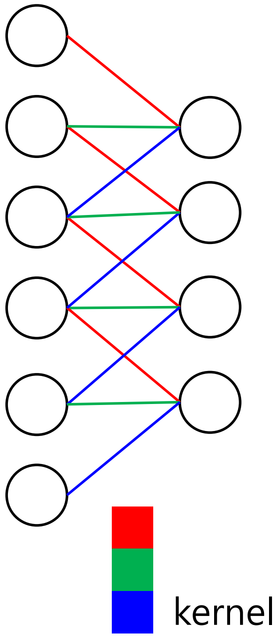


Convolutional Layer

- A **convolutional layer** (shortly *conv layer*) is a NN layer which uses *convolution* as its <u>feedforward propagation</u> and *kernel* as <u>weight variables</u>.
- (In contrast to a FC layer) A convolutional layer has two important points, **weight sharing** and **local connectivity**.
  - e.g. `input_size = 6`, `output_size = 4`, `kernel_size = 3`

    <u>FC layer</u> has 24 weight variables, but <u>conv layer</u> has only 3 weight variables.

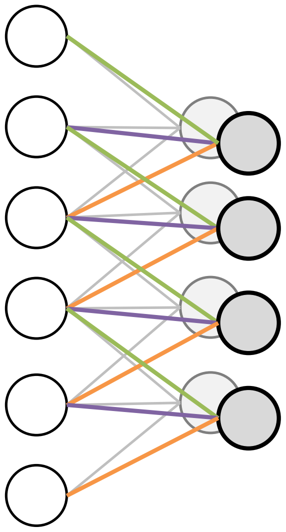




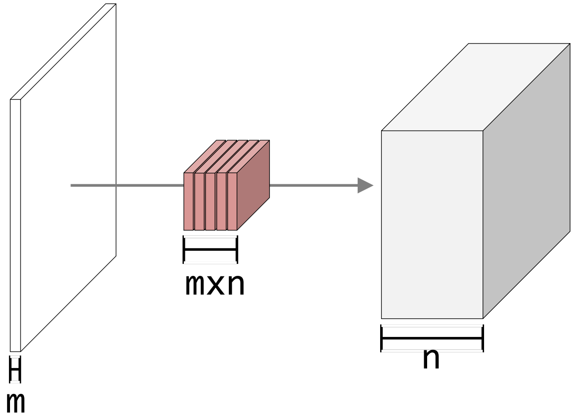
Why it works?

Convolutional Layer

- A convolutional layer can have multiple kernels so that its output will be multiple *channels*.
  - e.g. `in_channel_size = 1`, `out_channel_size = 2`, `kernel_size = 3`
  - e.g. `in_channel_size = m`, `out_channel_size = n`, `kernel_size = 3`



# of weights (w/o bias): 3 x 2



# of weights (w/o bias): 3 x 3 x m x n

  - Note) The number of weights is independent from input and output size in a convolutional layer.
    - Note) The number of weight (w/o bias) in a FC layer = input size x output size
      - e.g. The left example: 6 x 8 = 48

Pooling Layer

- A **pooling layer** is a non-linear down-sampling.
- Especially max pooling is common.
  - Note) [PyTorch APIs for pooling layers]
- Its parameters and working is similar to a convolutional layer.
  - In PyTorch, `stride` is assigned as `kernel_size` if it is not given.

3	16	10	18
12	29	84	20
82	5	3	10
1	27	21	14

```
kernel_size = 2
stride = 2
padding = 0
```

Max pooling

29	84
82	21

Average pooling

15	33
29	12

```
kernel_size = 3
stride = 1
padding = 0
```

Max pooling

84	84
84	84

Average pooling

27	22
29	24

Pooling Layer

- Why is pooling important?
  - It reduces the network size. → Less time/space complexity
  - It provide larger receptive fields with a limited size of kernels.

bag

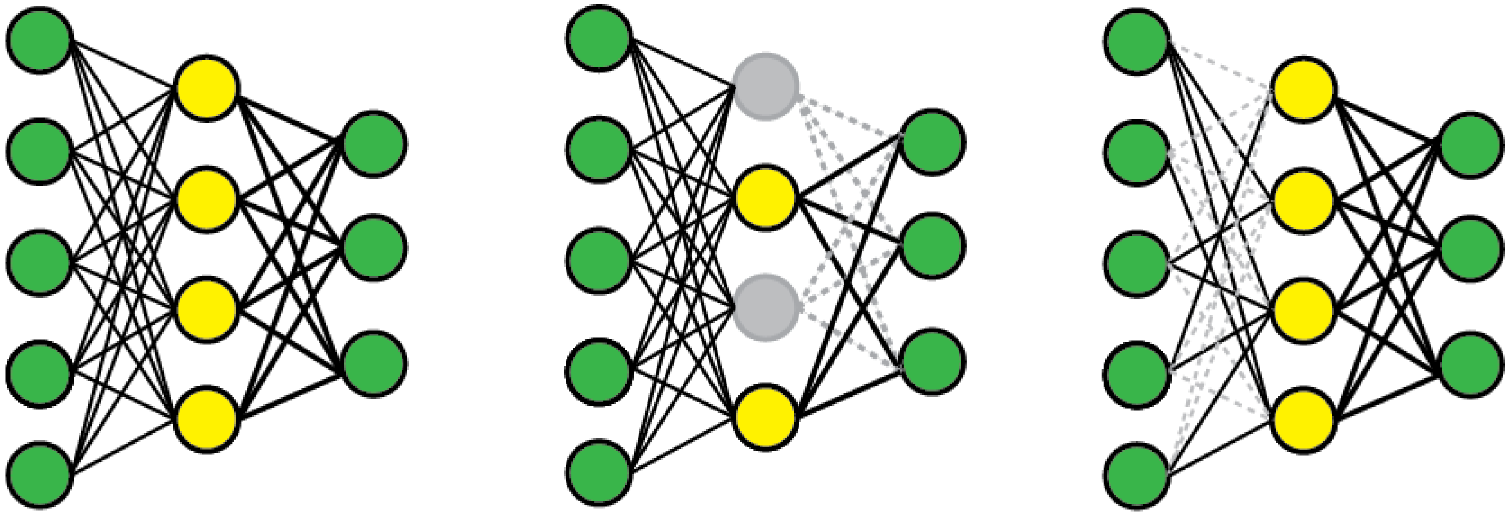
human upper body

human full body

bridge

Dropout

- A **dropout** is one of regularization methods against overfitting.
- It randomly drops a ratio of hidden units during training.
  - It prevents hidden units from co-adaptation.
  - e.g. When some hidden units has high weights, the others in the same layers have little contribution (low weight values, rarely training) to their output.

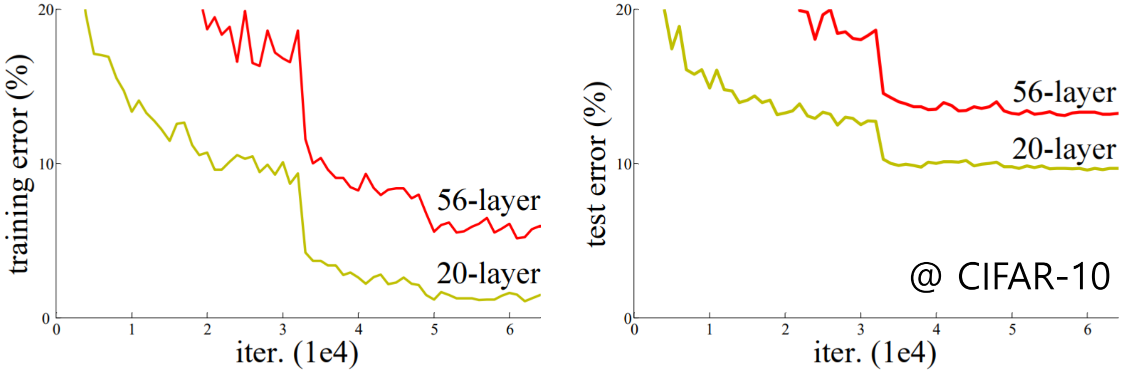


Standard Dropout DropConnect

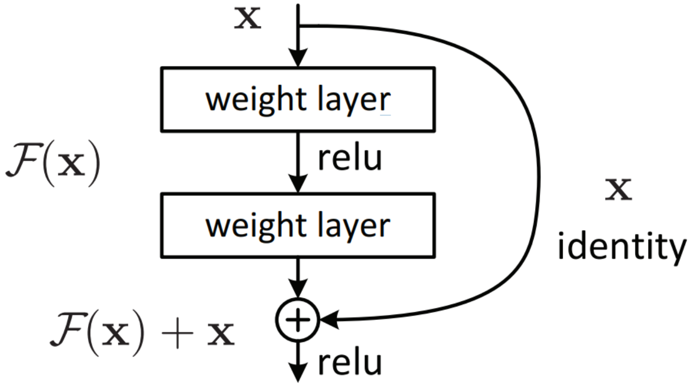
Image: Stack Exchange comment (by Matt Krause)

Skip Connection

- Motivation) Why is a deeper network worse?



- A **skip connection** is a shortcut connection between several layers which contain nonlinearities (e.g. ReLU) and [batch normalization](#).
  - Alias: *Residual connection* (used in *residual neural network, ResNet*)
  - It resolves the vanishing gradient problem.



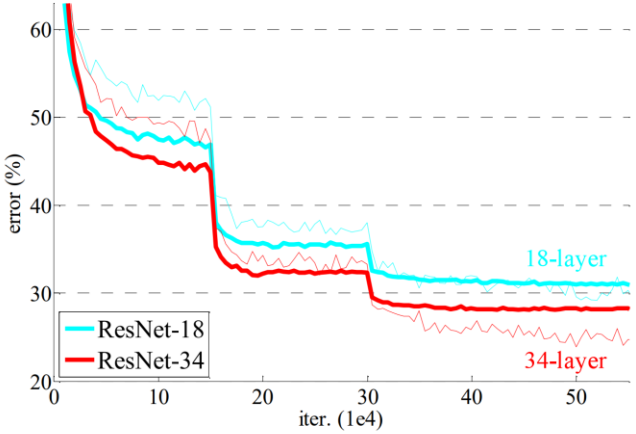


Image: [arXiv:1512.03385](#)

Skip Connection

- Biological analogue [Wikipedia]
  - Cortical layer VI neurons @ the cerebral cortex

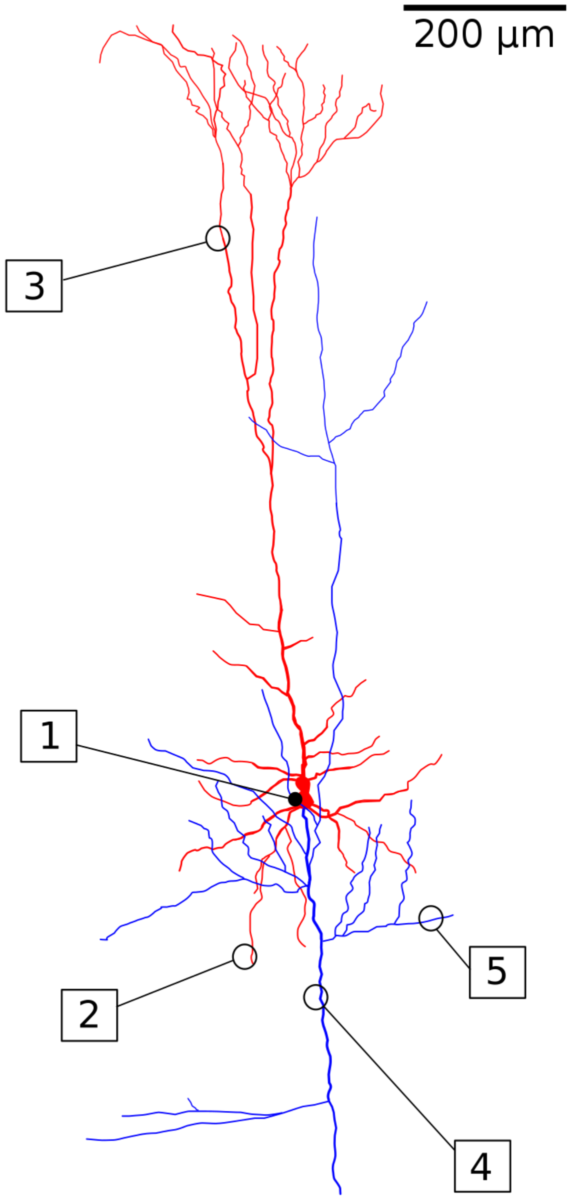


Image: Wikipedia

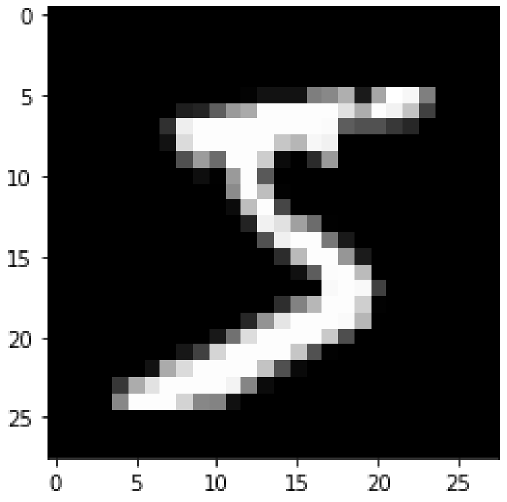
MNIST Dataset

- The MNIST dataset is a large database of handwritten digits. [Wikipedia]
- It was constructed by “re-mixing” the NIST’s original datasets.
  - Full name: *Modified* National Institute of Standards and Technology Database
- Specification
  - Classes: 10 (0, 1, 2, …, 9)
  - Images: 28 x 28 (8-bit gray scale)
  - The number of data: 60,000 for training and 10,000 for test

Image: Wikipedia

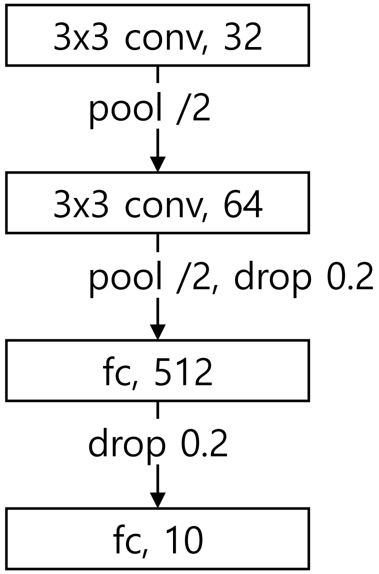
Practice) Loading the MNIST Dataset

```
import torchvision
import matplotlib.pyplot as plt

# Note) You can download the MNIST dataset through its mirror.
# - Reference: https://stackoverflow.com/questions/66577151/http-error-when-trying-to-download-mnist-data
torchvision.datasets.MNIST.resources = [
    ('https://ossci-datasets.s3.amazonaws.com/mnist/train-images-idx3-ubyte.gz', 'f68b3c2dcbeaaa9fbdd348bbdeb94873'),
    ('https://ossci-datasets.s3.amazonaws.com/mnist/train-labels-idx1-ubyte.gz', 'd53e105ee54ea40749a09fcbcd1e9432'),
    ('https://ossci-datasets.s3.amazonaws.com/mnist/t10k-images-idx3-ubyte.gz',  '9fb629c4189551a2d022fa330f9573f3'),
    ('https://ossci-datasets.s3.amazonaws.com/mnist/t10k-labels-idx1-ubyte.gz',  'ec29112dd5afa0611ce80d1b7f02629c')
]

# Load the MNIST dataset
DATA_PATH = './data'
data_train = torchvision.datasets.MNIST(DATA_PATH, train=True, download=True)
data_valid = torchvision.datasets.MNIST(DATA_PATH, train=False)

# Look inside of the dataset
print(data_train)                       # ... 60000 ...
print(data_valid)                       # ... 10000 ...
print(data_train.data.shape)            # torch.Size([60000, 28, 28])
print(data_train.data.dtype)            # torch.uint8
print(data_train.data[0,:,:])           # tensor([[0, 0, ...], ..., [..., 166, 255, 247, ...], ...])
plt.imshow(data_train.data[0,:,:], cmap='gray')
plt.show()
print(data_train.targets[0])            # Guess and check it!
```



Practice) Digit Classification with the MNIST Dataset (1/4)

```
# A four-layer CNN model
# - Try more or less layers, channels, and kernel size
# - Try to apply batch normalization (e.g. 'nn.BatchNorm' and 'nn.BatchNorm2d')
# - Try to apply skip connection (used in ResNet)
class MyCNN(nn.Module):
    def __init__(self):
        super(MyCNN, self).__init__()
        # Notation:    (batch_size, channel, height, width)
        # Input :      (batch_size,  1, 28, 28)
        # Layer1: conv (batch_size, 32, 28, 28)
        #         pool (batch_size, 32, 14, 14)
        self.conv1 = nn.Conv2d(1, 32, kernel_size=3, stride=1, padding=1)
        self.pool1 = nn.MaxPool2d(kernel_size=2)

        # Layer2: conv (batch_size, 64, 14, 14)
        #         pool (batch_size, 64,  7,  7)
        self.conv2 = nn.Conv2d(32, 64, kernel_size=3, stride=1, padding=1)
        self.pool2 = nn.MaxPool2d(kernel_size=2)
        self.drop2 = nn.Dropout(0.2)

        # Input :      (batch_size, 64*7*7)
        # Layer3: fc   (batch_size, 512)
        self.fc3   = nn.Linear(64*7*7, 512)
        self.drop3 = nn.Dropout(0.2)

        # Layer4: fc   (batch_size, 10)
        self.fc4   = nn.Linear(512, 10)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        x = self.pool1(x)

        x = F.relu(self.conv2(x))
        x = self.pool2(x)
        x = self.drop2(x)
        x = torch.flatten(x, 1)

        x = F.relu(self.fc3(x))
        x = self.drop3(x)

        x = F.log_softmax(self.fc4(x), dim=1)
        return x
```



Practice) Digit Classification with the MNIST Dataset (2/4)

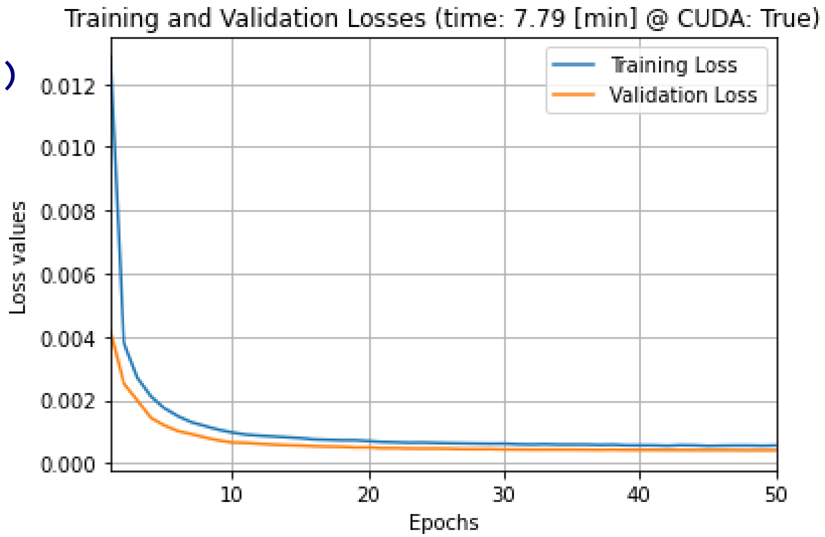
```
if __name__ == '__main__':
    # 0. Preparation
    torch.manual_seed(RANDOM_SEED)
    if USE_CUDA:
        torch.cuda.manual_seed_all(RANDOM_SEED)
    dev = torch.device('cuda' if USE_CUDA else 'cpu')

    # 1. Load the MNIST dataset
    preproc = torchvision.transforms.ToTensor()
    data_train = torchvision.datasets.MNIST(DATA_PATH, train=True,  download=True, transform=preproc)
    data_valid = torchvision.datasets.MNIST(DATA_PATH, train=False, transform=preproc)
    loader_train = torch.utils.data.DataLoader(data_train, **DATA_LOADER_PARAM)
    loader_valid = torch.utils.data.DataLoader(data_valid, **DATA_LOADER_PARAM)

    # 2. Instantiate a model, loss function, and optimizer
    model = MyCNN().to(dev)
    loss_func = F.cross_entropy
    optimizer = torch.optim.SGD(model.parameters(), **OPTIMIZER_PARAM)
    scheduler = torch.optim.lr_scheduler.StepLR(optimizer, **SCHEDULER_PARAM)
```

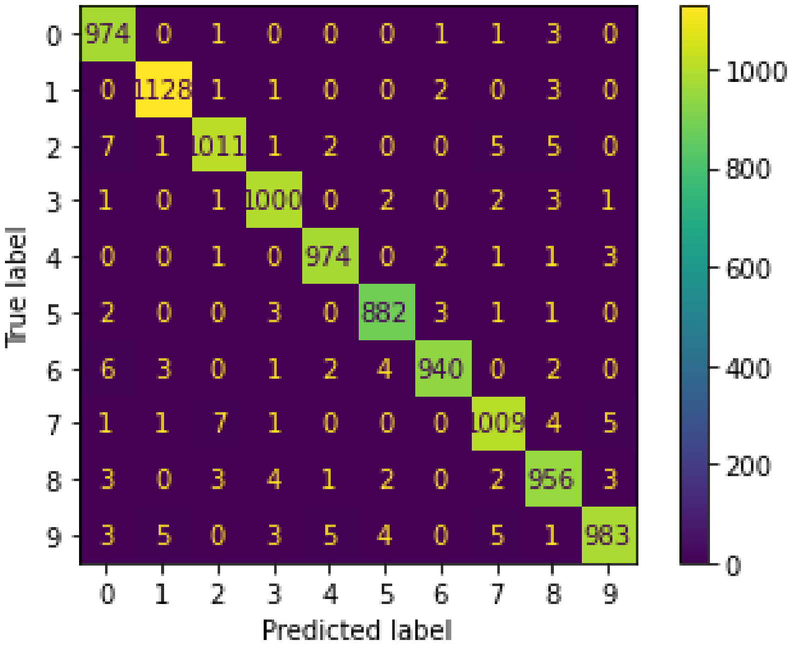
Note) `SCHEDULER_PARAM = { 'step_size': 10, 'gamma': 0.5 }`

```
    # 3.1. Train the model
    loss_list = []
    start = time.time()
    for epoch in range(1, EPOCH_MAX + 1):
        train_loss = train(model, loader_train, loss_func, optimizer)
        valid_loss, valid_accuracy = evaluate(model, loader_valid, loss_func)
        scheduler.step()

        loss_list.append([epoch, train_loss, valid_loss, valid_accuracy])
        if epoch % EPOCH_LOG == 0:
            elapse = (time.time() - start) / 60
            print(f'{epoch:>6} ({elapse:>6.2f} min), TrLoss={train_loss:.6f}, VaLoss={valid_loss:.6f}, VaAcc={valid_accuracy:.3f}, lr={scheduler.get_last_lr()}')
    elapse = (time.time() - start) / 60

    # 3.2. Save the trained model if necessary
    if SAVE_MODEL:
        torch.save(model.state_dict(), SAVE_MODEL)
```

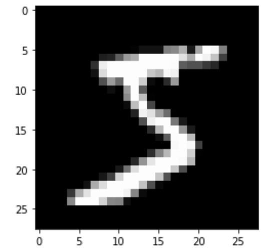
Practice) Digit Classification with the MNIST Dataset (3/4)

```python
# 4.1. Visualize the loss curves
plt.title(f'Training and Validation Losses (time: {elapse:.2f} [min] @ CUDA: {USE_CUDA})')
loss_array = np.array(loss_list)
plt.plot(loss_array[:,0], loss_array[:,1], label='Training Loss')
plt.plot(loss_array[:,0], loss_array[:,2], label='Validation Loss')
plt.xlabel('Epochs')
plt.ylabel('Loss values')
plt.xlim(loss_array[0,0], loss_array[-1,0])
plt.grid()
plt.legend()
plt.show()

# 4.2. Visualize the confusion matrix
predicts = [predict(datum, model) for datum in data_valid.data]
conf_mat = metrics.confusion_matrix(data_valid.targets, predicts)
conf_fig = metrics.ConfusionMatrixDisplay(conf_mat)
conf_fig.plot()

# 5. Test your image
print(predict(data_train.data[0], model)) # 5
with PIL.Image.open('data/cnn_mnist_test.png').convert('L') as image:
    print(predict(image, model))          # 3
```

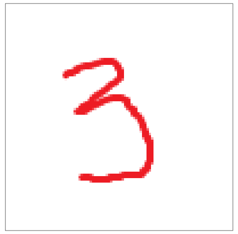




data_train.data[0]



'data/cnn_mnist_test.png'



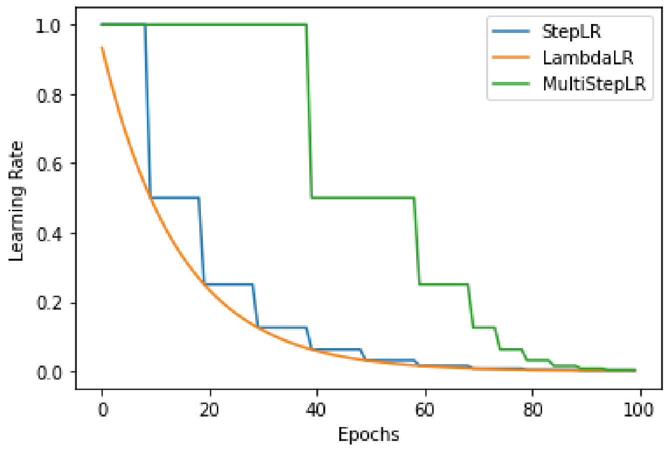
Practice) Digit Classification with the MNIST Dataset (4/4)

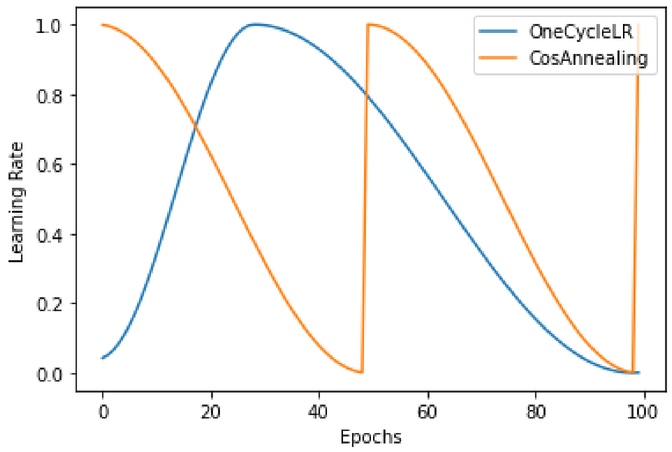
```
# Predict a digit using the given model
def predict(image, model):
    model.eval()
    with torch.no_grad():
        # Convert the given image to its 1 x 1 x 28 x 28 tensor
        if type(image) is torch.Tensor:
            tensor = image.type(torch.float) / 255  # Normalize to [0, 1]
        else:
            tensor = 1 - TF.to_tensor(image)        # Invert (white to black)
        if tensor.ndim < 3:
            tensor = tensor.unsqueeze(0)
        if tensor.shape[0] == 3:
            tensor = TF.rgb_to_grayscale(tensor)    # Make grayscale
        tensor = TF.resize(tensor, 28)              # Resize to 28 x 28
        dev = next(model.parameters()).device
        tensor = tensor.unsqueeze(0).to(dev)        # Add onw more dims

        output = model(tensor)
        digit = torch.argmax(output, dim=1)
        return digit.item()
```

Practice) Loading My Network and Testing My Image

```
import torch, PIL
from cnn_mnist import MyCNN, predict

# Load a model
model = MyCNN()
model.load_state_dict(torch.load('cnn_mnist.pt'))

# Test the model
with PIL.Image.open('data/cnn_mnist_test.png').convert('L') as image:
    print(predict(image, model))
```

Practice) Visualizing Learning Rate Schedulers (1/2)






```python
import torch
import torch.optim.lr_scheduler as lr_scheduler
import matplotlib.pyplot as plt

base_lr = 1.
epoch_max = 100
schedulers = [
    {'name': 'StepLR',        'class': lr_scheduler.StepLR,
                              'param': {'step_size': 10, 'gamma': 0.5}},
    {'name': 'LambdaLR',      'class': lr_scheduler.LambdaLR,
                              'param': {'lr_lambda': lambda epoch: 0.5**(epoch / 10)}},
    {'name': 'MultiStepLR',   'class': lr_scheduler.MultiStepLR,
                              'param': {'milestones': [40, 60, 70, 75, 80, 85, 90, 95], 'gamma': 0.5}},
    {'name': 'OneCycleLR',    'class': lr_scheduler.OneCycleLR,
                              'param': {'max_lr': base_lr, 'total_steps': epoch_max}},
    {'name': 'CosAnnealing', 'class': lr_scheduler.CosineAnnealingWarmRestarts,
                              'param': {'T_0': 50}},
    # Try more learning rate schedulers
]
```

Practice) Visualizing Learning Rate Schedulers (2/2)

```python
for sch in schedulers:
    x = torch.tensor(1., requires_grad=True)             # A dummy parameter
    optimizer = torch.optim.SGD([x], lr=base_lr)         # Instantiate an optimizer
    scheduler = sch['class'](optimizer, **sch['param']) # Instantiate a LR scheduler
    lr_values = []
    for i in range(epoch_max):
        optimizer.step()
        scheduler.step()
        lr_values.append(optimizer.param_groups[0]['lr'])
    plt.plot(range(epoch_max), lr_values, label=sch['name'])

plt.xlabel('Epochs')
plt.ylabel('Learning Rate')
plt.legend()
plt.show()
```

Practice) Different Styles for NN Classes (1/2)

My style

```python
class MyCNN(nn.Module):
    def __init__(self):
        super(MyCNN, self).__init__()
        self.conv1 = nn.Conv2d(1, 32, 3, 1, 1)
        self.pool1 = nn.MaxPool2d(2)

        self.conv2 = nn.Conv2d(32, 64, 3, 1, 1)
        self.pool2 = nn.MaxPool2d(2)
        self.drop2 = nn.Dropout(0.2)

        self.fc3   = nn.Linear(64*7*7, 512)
        self.drop3 = nn.Dropout(0.2)

        self.fc4   = nn.Linear(512, 10)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        x = self.pool1(x)

        x = F.relu(self.conv2(x))
        x = self.pool2(x)
        x = self.drop2(x)
        x = torch.flatten(x, 1)

        x = F.relu(self.fc3(x))
        x = self.drop3(x)

        x = F.log_softmax(self.fc4(x), dim=1)
        return x
```

Functional-oriented style

```python
class MyCNN_Functional(nn.Module):
    def __init__(self):
        super(MyCNN_FStyle, self).__init__()
        self.conv1 = nn.Conv2d( 1, 32, 3, 1, 1)
        self.conv2 = nn.Conv2d(32, 64, 3, 1, 1)
        self.fc1 = nn.Linear(64*7*7, 512)
        self.fc2 = nn.Linear(512, 10)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        x = F.max_pool2d(x, 2)

        x = F.relu(self.conv2(x))
        x = F.max_pool2d(x, 2)
        x = F.dropout(x, 0.2, self.training)
        x = torch.flatten(x, 1)

        x = F.relu(self.fc1(x))
        x = F.dropout(x, 0.2, self.training)

        x = F.log_softmax(self.fc2(x), dim=1)
        return x
```

Practice) Different Styles for NN Classes (2/2)

Object-oriented style

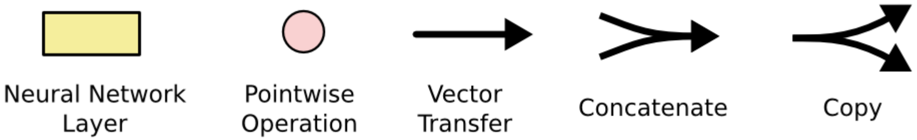
```
class MyCNN_Object(nn.Module):
    def __init__(self):
        super(MyCNN_ObjStyle, self).__init__()
        self.conv1 = nn.Conv2d(1, 32, 3, 1, 1)
        self.relu1 = nn.ReLU()
        self.pool1 = nn.MaxPool2d(2)

        self.conv2 = nn.Conv2d(32, 64, 3, 1, 1)
        self.relu2 = nn.ReLU()
        self.pool2 = nn.MaxPool2d(2)
        self.drop2 = nn.Dropout(0.2)

        self.fc3   = nn.Linear(64*7*7, 512)
        self.relu3 = nn.ReLU()
        self.drop3 = nn.Dropout(0.2)

        self.fc4   = nn.Linear(512, 10)
        self.smax4 = nn.LogSoftmax(dim=1)

    def forward(self, x):
        x = self.conv1(x)
        x = self.relu1(x)
        x = self.pool1(x)

        x = self.conv2(x)
        x = self.relu2(x)
        x = self.pool2(x)
        x = self.drop2(x)
        x = torch.flatten(x, 1)

        x = self.fc3(x)
```

Layer-oriented style

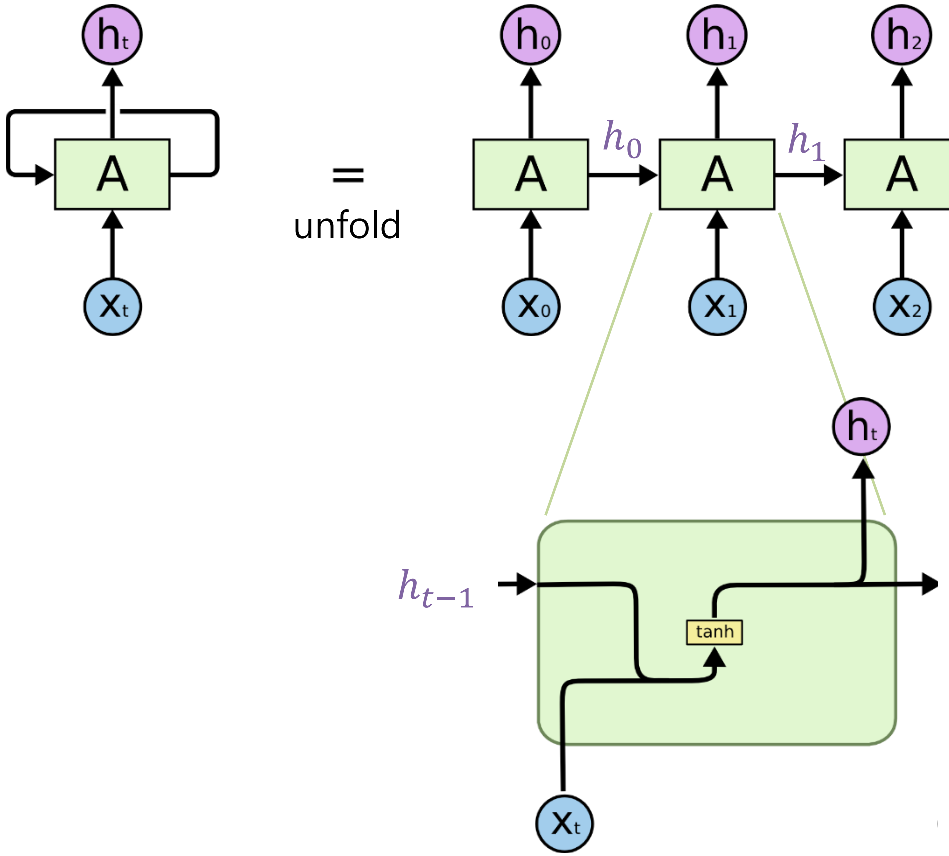
```
class MyCNN_Layer(nn.Module):
    def __init__(self):
        super(MyCNN_SeqStyle, self).__init__()
        self.layer1 = nn.Sequential(
            nn.Conv2d(1, 32, 3, 1, 1),
            nn.ReLU(),
            nn.MaxPool2d(2))

        self.layer2 = nn.Sequential(
            nn.Conv2d(32, 64, 3, 1, 1),
            nn.ReLU(),
            nn.MaxPool2d(2),
            nn.Dropout(0.2))

        self.layer3 = nn.Sequential(
            nn.Linear(64*7*7, 512),
            nn.ReLU(),
            nn.Dropout(0.2))

        self.layer4 = nn.Sequential(
            nn.Linear(512, 10),
            nn.LogSoftmax(dim=1))

    def forward(self, x):
        x = self.layer1(x)
        x = self.layer2(x)
        x = torch.flatten(x, 1)
        x = self.layer3(x)
        x = self.layer4(x)
        return x
```

Table of Contents

Recurrent Neural Network (RNN)



- A **recurrent neural network** (shortly *RNN*) is a NN with a **loop**.
- A RNN can preserve a *memory* or *(hidden) state* or *information* inside.
  - Note) ~ sequential logic circuits (vs. combinatorial logic circuits) in digital circuits



Note) All $\boxed{\textbf{A}}$s have same weight.

$$h_t = \phi(W_h x_t + U_h h_{t-1} + b_h)$$

Image: colah's blog

Recurrent Neural Network (RNN)

- **Multi-layer RNNs**

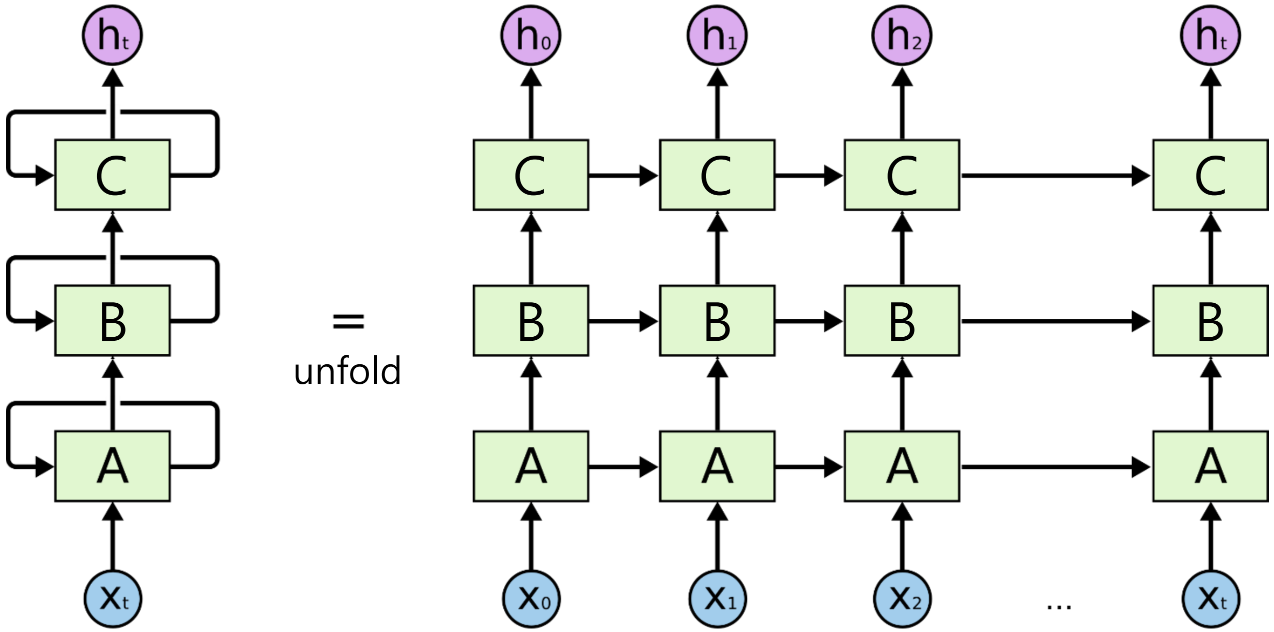
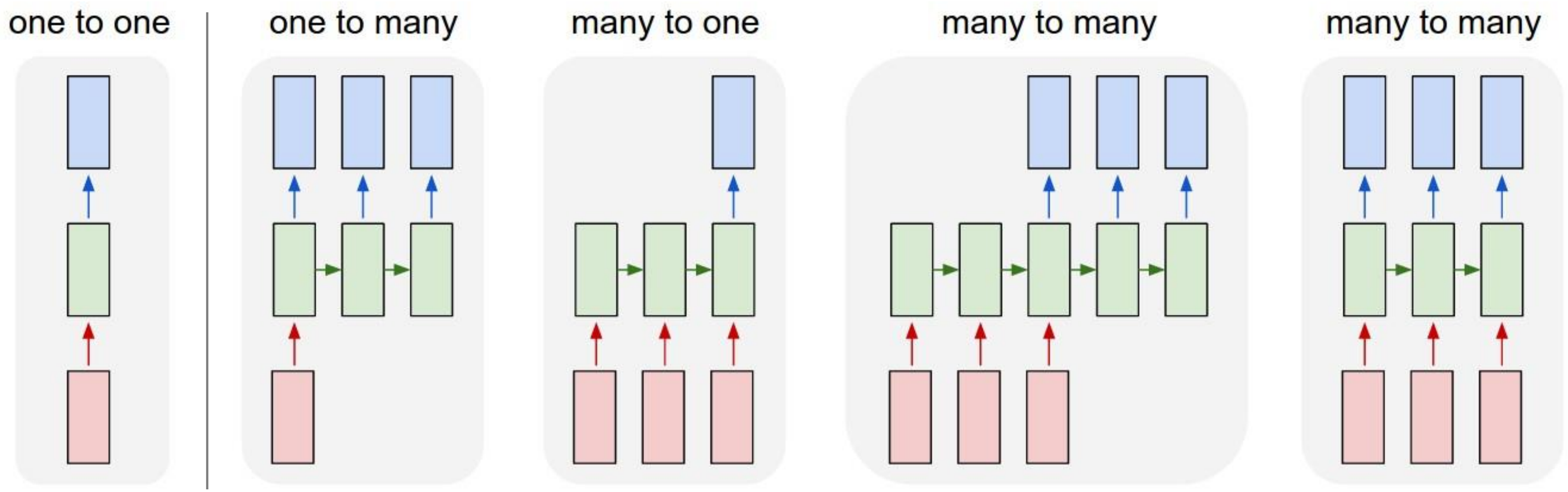


Image: [colah's blog]

Recurrent Neural Network (RNN)

- Memory in a RNN allows it can deal with *sequential* or *temporal* data.
- A RNN can deal with **various lengths of input vectors** and **output vectors** by attaching more hidden/output layers and at the its end.



not RNN
image captioning
sentiment analysis (classification)
machine translation
video classification

Image: [Andrej Karpathy blog]

Recurrent Neural Network (RNN)

- The **vanishing gradient problem** in training a long sequence data
  - A vanilla RNN cannot deal with long-term dependency.
  - e.g. Guessing the last word, “I grew up in France … I speak fluent French.”

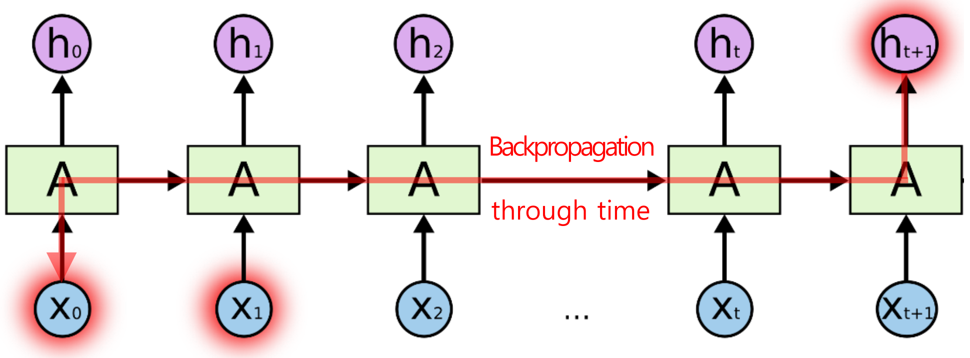
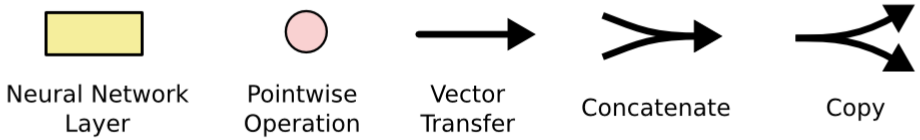


Image: colah's blog

Long Short-Term Memory (LSTM)



- A **long short-term memory** (shortly *LSTM*) is a recurrent neural network unit to deal with the vanishing gradient problem of a vanilla RNN. [Wikipedia]
- It is composed of a **forget gate**, an **input gate**, a **cell**, and an **output gate**.

forget gate	How much forget c_{t-1} to the cell state	$f_t = \sigma\left(W_f x_t + U_f h_{t-1} + b_f\right)$
input gate	How much write $\tilde{c}_t$ to the cell state	$i_t = \sigma(W_i x_t + U_i h_{t-1} + b_i)$
cell	The intermediate cell state	$\tilde{c}_t = \tanh(W_o x_t + U_o h_{t-1} + b_o)$
output gate	How much reveal c_t to the hidden state	$o_t = \sigma(W_o x_t + U_o h_{t-1} + b_o)$

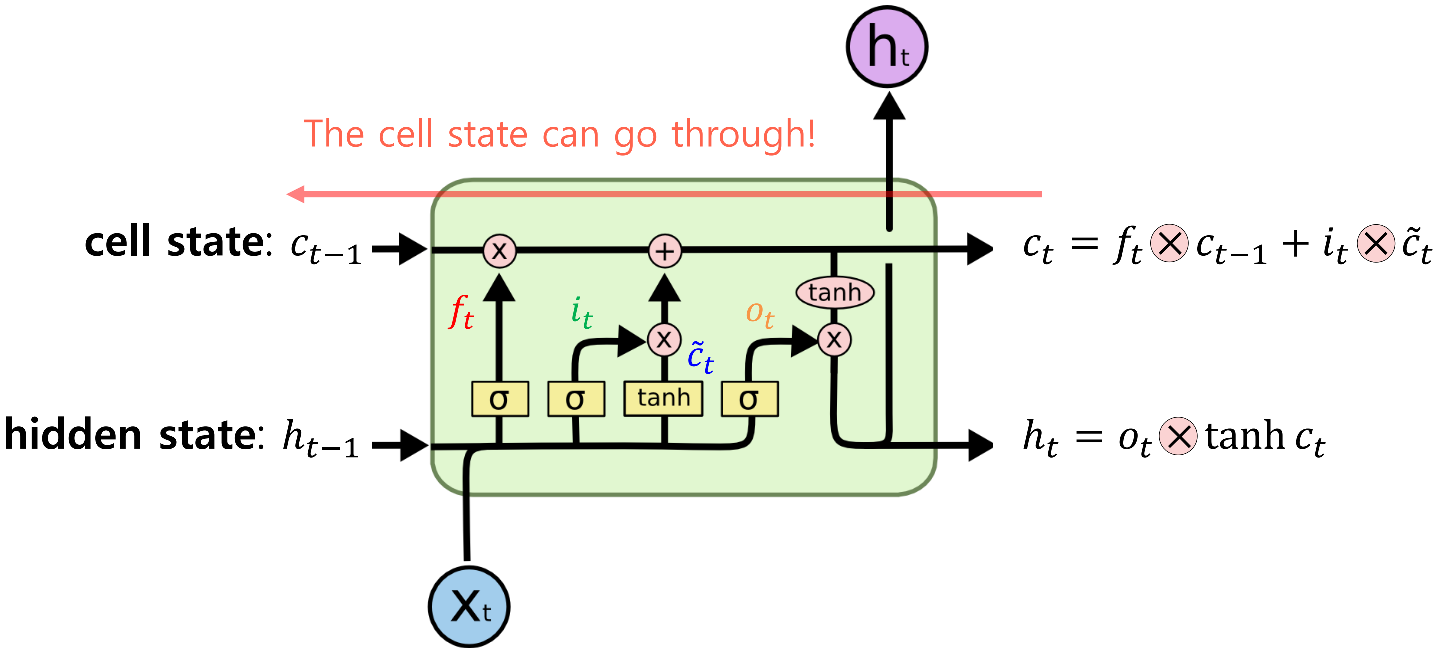
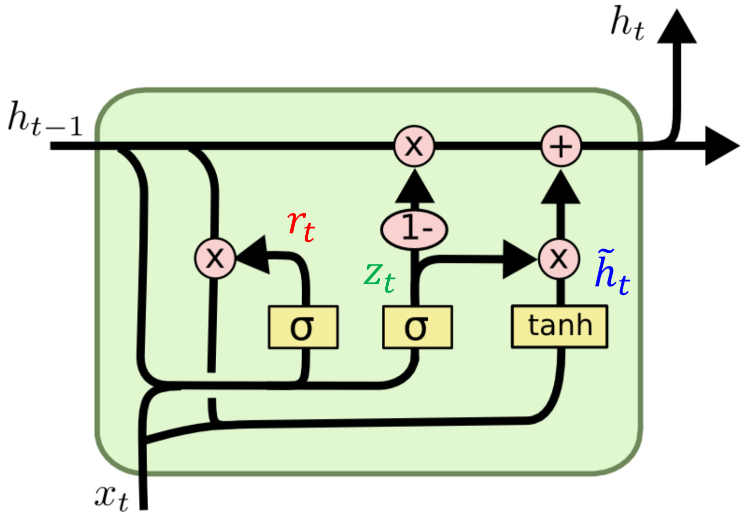


Image: colah's blog

Gated Recurrent Unit (GRU)

- A **gated recurrent unit** (shortly *GRU*) is a LSTM variant with a simplified structure, but still has similar performance. [Wikipedia]

reset gate	How much forget h_{t-1} to the hidden state	$r_t = \sigma(W_r x_t + U_r h_{t-1} + b_r)$
update gate	How much write $\tilde{h}_t$ to the hidden state	$z_t = \sigma(W_z x_t + U_z h_{t-1} + b_z)$
	The intermediate hidden state	$\tilde{h}_t = \tanh(W_h x_t + U_h(r_t \otimes h_{t-1}) + b_h)$



$$h_t = (1 - z_t) \otimes h_{t-1} + z_t \otimes \tilde{h}_t$$

Image: colah's blog

Practice) Name2Lang Classification with a Character-level RNN (1/7)

- Motivation: A registration form on Internet

  First Name | Last Name

  E-mail address

  Country

- Input: **Name** (string; a sequence of characters)
  - e.g. 'Choi', 'Jane', 'Daniel', 'Chow', 'Tanaka', ...
- Classes: **18 languages** (integer; 0-17)
  - e.g. Arabic, Chinese, Czech, Dutch, English, French, German, Greek, Iris, Italian, Japanese, Korean, Polish, Portuguese, Russian, Scottish, Spanish, Vietnamese
- The dataset and bottom-up implementation is available on the PyTorch official tutorial.

Practice) Name2Lang Classification with a Character-level RNN (2/7)

- Input: **Name** (string; a sequence of characters)
  - e.g. 'Choi', 'Jane', 'Daniel', 'Chow', 'Tanaka', …
- How to represent the **name**?
  - The name is represented using 57 characters (52 alphabets and 5 special letters).
    - e.g. `'a'` (0x61), `'b'` (0x62), `'c' (0x63)`, …, `'-'` (0x45) in ASCII code
  - Each character is encoded as a 57-bit one-hot vector.
    - e.g.

a:	**1**	0	0	0	…
b:	0	**1**	0	0	…
c:	0	0	**1**	0	…

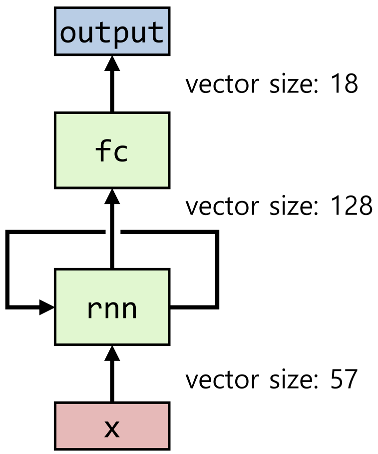
Why one-hot encoding?

    - e.g. `'Choi'`: 4 x 57 크기의 배열로 표현

C:	0	…	0	0	0	…	0	0	…	**1**	0	…
h:	0	…	**1**	0	0	…	0	0	…	0	0	…
o:	0	…	0	0	0	…	**1**	0	…	0	0	…
i:	0	…	0	**1**	0	…	0	0	…	0	0	…
Index)			7	8			14			28		

Practice) Name2Lang Classification with a Character-level RNN (3/7)

```
# A simple RNN model
# - Try a different RNN unit such LSTM and GRU
# - Try less or more hidden units
# - Try more layers (e.g. 'num_layers=2') and dropout (e.g. 'dropout=0.4')
class MyRNN(nn.Module):
    def init(self, input_size, output_size):
        super(MyRNN, self).init()
        self.rnn = torch.nn.RNN(input_size, 128)
        self.fc = torch.nn.Linear(128, output_size)

    def forward(self, x):
        output, hidden = self.rnn(x)
        x = self.fc(output[-1])  # Use output of the last sequence
        return x
```



Practice) Name2Lang Classification with a Character-level RNN (4/7)

```
# Convert Unicode to ASCII
# e.g. Ślusàrski to Slusarski
def unicode2ascii(s):
    return ''.join(
        c for c in unicodedata.normalize('NFD', s)
        if unicodedata.category(c) != 'Mn' and c in LETTER_DICT)

# Read raw files which contain names belong to each language
# Note) Each filename is used as its target's name.
def load_name_dataset(files):
    data = []
    targets = []
    target_names = []
    for idx, filename in enumerate(files):
        lang = os.path.splitext(os.path.basename(filename))[0]
        names = open(filename, encoding='utf-8').read().strip().split('\n')

        data += [unicode2ascii(name) for name in names]
        targets += [idx] * len(names)
        target_names.append(lang)
    return data, targets, target_names

# Transform the given text to its one-hot encoded tensor
# Note) Tensor size: len(text) x 1 x len(LETTER_DICT)
#                    sequence_length x batch_size x input_size
def text2onehot(text, device='cpu'):
    tensor = torch.zeros(len(text), 1, len(LETTER_DICT), device=device)
    for idx, letter in enumerate(text):
        tensor[idx][0][LETTER_DICT.find(letter)] = 1
    return tensor
```

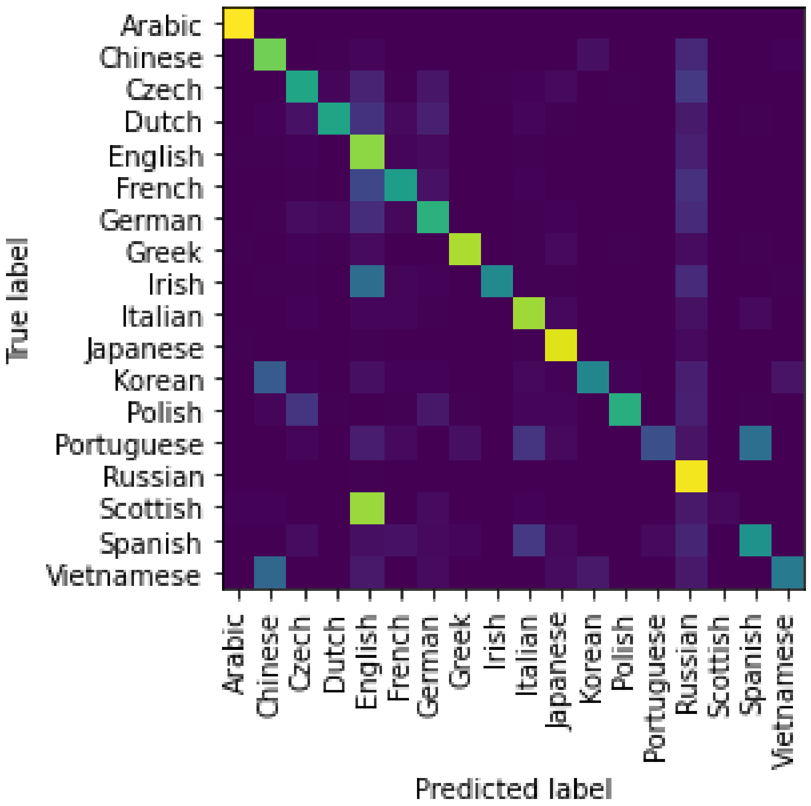
Arabic.txt	13KB
Chinese.txt	2KB
Czech.txt	4KB
Dutch.txt	3KB
English.txt	27KB
French.txt	3KB
German.txt	6KB
Greek.txt	2KB
Irish.txt	2KB
Italian.txt	6KB
Japanese.txt	8KB
Korean.txt	1KB
Polish.txt	2KB
Portuguese.txt	1KB
Russian.txt	84KB
Scottish.txt	1KB
Spanish.txt	3KB
Vietnamese.txt	1KB

Practice) Name2Lang Classification with a Character-level RNN (5/7)

```
if __name__ == '__main__':
    # 0. Preparation
    # 1. Load the name2lang dataset
    data, targets, target_names = load_name_dataset(glob.glob(DATA_PATH))
    data_train = [(text2onehot(data[i], device=dev), torch.LongTensor(
        [targets[i]]).to(dev)) for i in range(len(data))]
    random.shuffle(data_train)

    # 2. Instantiate a model, loss function, and optimizer
    # 3.1. Train the model
    # 3.2. Save the trained model if necessary

    # 4.1. Visualize the loss curves
    # 4.2. Visualize the confusion matrix
    predicts = [predict(datum, model) for datum in data]
    conf_mat = sklearn.metrics.confusion_matrix(targets, predicts, normalize='true')
    plt.imshow(conf_mat)
    plt.xlabel('Predicted label')
    plt.ylabel('True label')
    plt.gca().set_xticklabels([''] + target_names, rotation=90)
    plt.gca().set_yticklabels([''] + target_names)
    plt.gca().xaxis.set_major_locator(ticker.MultipleLocator(1))
    plt.gca().yaxis.set_major_locator(ticker.MultipleLocator(1))
    plt.show()

    # 5. Test your texts
    report_predict('Choi', model, target_names)
    report_predict('Jane', model, target_names)
    report_predict('Daniel', model, target_names)
    report_predict('Chow', model, target_names)
    report_predict('Tanaka', model, target_names)
```

Practice) Name2Lang Classification with a Character-level RNN (6/7)

```
* Name: Choi
  1. Korean    : 50.5 %
  2. Chinese   : 36.1 %
  3. Vietnamese: 11.8 %
  4. Russian   :  0.9 %
  5. Arabic    :  0.5 %
* Name: Jane
  1. English   : 62.4 %
  2. German    : 10.5 %
  3. Korean    :  9.0 %
  4. Chinese   :  7.0 %
  5. Dutch     :  6.2 %
* Name: Daniel
  1. English   : 48.4 %
  2. French    : 20.6 %
  3. Czech     : 13.1 %
  4. Russian   :  6.6 %
  5. Portuguese:  3.1 %
* Name: Chow
  1. Korean    : 69.8 %
  2. Chinese   : 16.0 %
  3. English   :  4.7 %
  4. Vietnamese:  4.3 %
  5. Russian   :  3.1 %
* Name: Tanaka
  1. Japanese  : 84.4 %
  2. Russian   : 14.0 %
  3. Czech     :  1.3 %
  4. English   :  0.1 %
  5. Irish     :  0.1 %
```



Practice) Name2Lang Classification with a Character-level RNN (7/7)

```
# Predict the best result of the given text
def predict(text, model):
    model.eval()
    with torch.no_grad():
        dev = next(model.parameters()).device
        text_tensor = text2onehot(text, dev) # Convert text to one-hot vectors
        output = model(text_tensor)[0]       # Get the last output
        lang = torch.argmax(output)          # Get the best among 18 classes
        return lang.item()

# Predict and report top-k results of the given text
def report_predict(text, model, target_names, n_predict=5):
    print(f'* Name: {text}')
    model.eval()
    with torch.no_grad():
        dev = next(model.parameters()).device
        text_tensor = text2onehot(text, dev)
        output = model(text_tensor)[0]
        prob = nn.functional.softmax(output, dim=0) # Make output as probability
        top_val, top_idx = prob.topk(n_predict)     # Get top-k among 18 classes
        for i in range(len(top_val)):
            print(f'  {i+1}. {target_names[top_idx[i].item()]:<10}: 
{top_val[i]*100:4.1f} %')
```

y_i:	0.012	0.929	0.058

Softmax: $y_i = \exp z_i \,/\, \sum_{j=1}^{C} \exp z_j$

NN output z_i:	-1.03	3.29	0.52

Summary

- **DNN**: Deep neural network
- **CNN**: Feedforward with convolution (and pooling)
- **RNN**: NN with a loop → state/memory → sequential/temporal data

- **Issue #1) Vanishing gradient problem**
  - Activation functions such as ReLU
  - Skip connection ~ LSTM and GRU
- **Issue #2) Overfitting problem**
  - More data by data collection or data augmentation or data synthesis
  - Data separation (train/validation/test data), cross-validation, and early stopping
  - More simplified models (e.g. CNN ← weight sharing and local connectivity; a.k.a. inductive bias)
  - Loss functions with regularization terms
- Other improvement
  - Dropout
  - Batch normalization
  - …

Further Information

- Natural Language Processing (NLP)
  - **Seq2seq** (2014), **attention mechanism** (2015)
  - **Transformer** (2017), **BERT** (Bidirectional Encoder Representations from Transformers), **GPT** (Generative Pretrained Transformer), …
- Computer Vision
  - CNN backbone networks: **AlexNet** (2012), **VGGNet** (2014), **Inception Net** (2014), **ResNet** (2015), …
  - CNN object detection networks
    - Two-stage detectors: **R-CNN** (2014), **Fast R-CNN** (2015), **Faster R-CNN** (2015), **Mask R-CNN** (2017), …
    - One-stage detectors: **YOLO** (You Only Look Once; 2015), **SSD** (Single Shot MultiBox Detector; 2015), …
  - Vision Transformers (ViT) and Vision Foundation Models (VFM)
    - **ViT** (Vision Transformer; 2020), **Swin Transformer** (2021), …, **SAM** (Segment Anything; 2023), …
  - Generative models
    - **Autoencoder** (2006), …, **GAN** (Generative Adversarial Networks; 2014), **CycleGAN** (2017), …
    - **Diffusion model** (2020), **Stable Diffusion** (2022), …
  - Others
    - **NeRF** (Neural Radiance Field; 2020), **CLIP** (Contrastive Language-Image Pre-Training; 2021), …
- Others
  - Incremental/continual learning, …, transfer learning/domain adaptation, …, contrastive learning, …
  - Network compression/pruning, knowledge distillation (2015), …, ML model deployment, …

How To Understand New Methods (or Read Papers)

- **Model**
  - Network design
  - Input and output
    - e.g. Normalization, positional encoding
- **Training**
  - Dataset
    - e.g. Data augmentation, data synthesis
    - e.g. Data labeling, unsupervised or weakly-supervised approaches
  - Objective functions
    - e.g. Regularization terms, Huber loss (for robust regression), focal loss
  - Optimization
    - e.g. Optimization algorithms, hyperparameters