Neural Networks

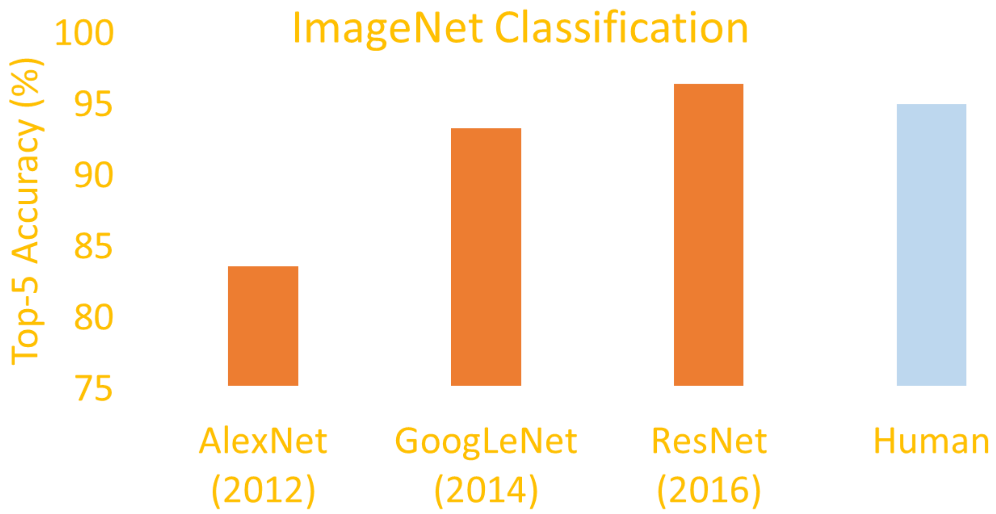
Nov 2022

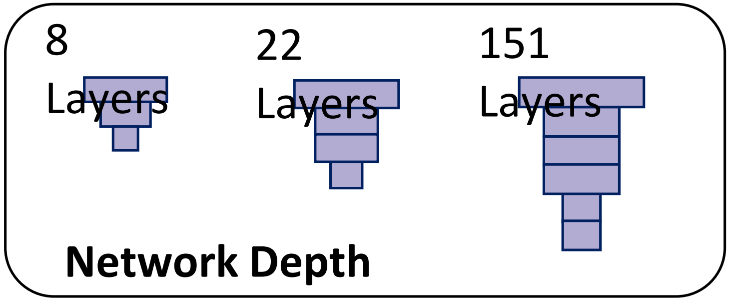
Beibin Li

Summary

- CNN
  - Image Classification
  - Segmentation, Detection, Generation
- RNN
- Transformer
- RL
- PyTorch

Introduction



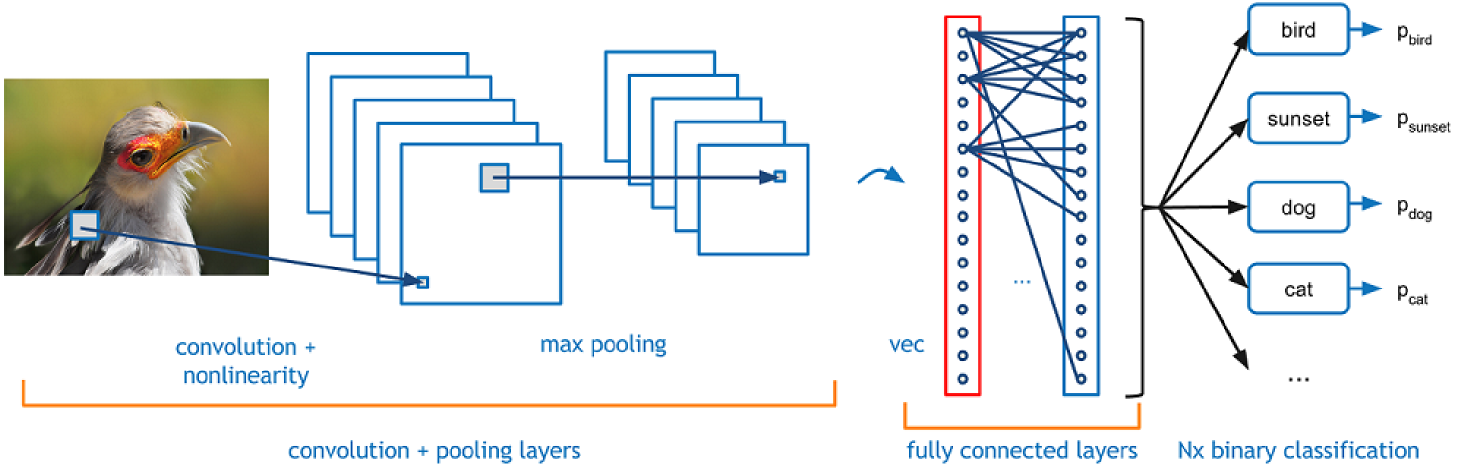



Accuracy **improves**

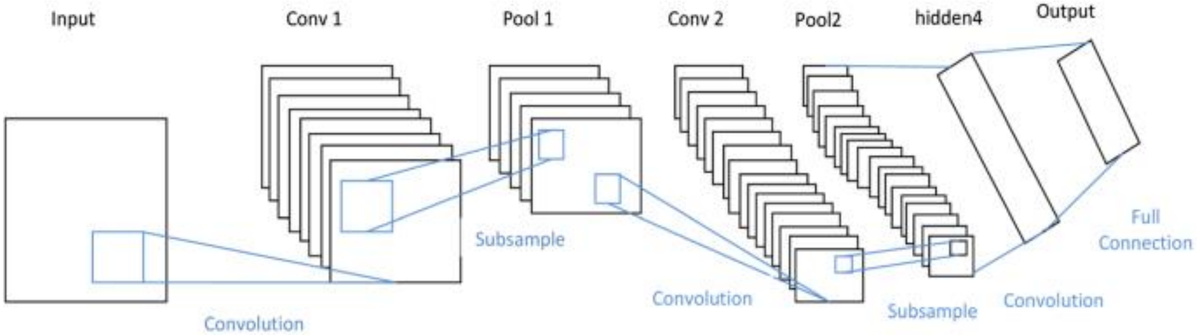

Speed **reduces**

Energy consumption **increases**

CNN



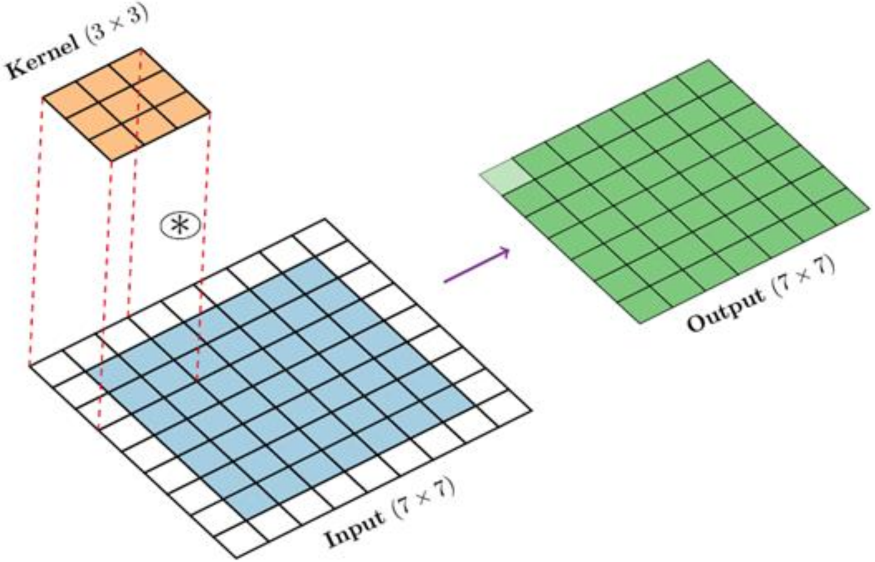
bird
sunset
dog
cat
p_{bird}
p_{sunset}
p_{dog}
p_{cat}
...
convolution +
nonlinearity
max pooling
vec
convolution + pooling layers
fully connected layers
Nx binary classification

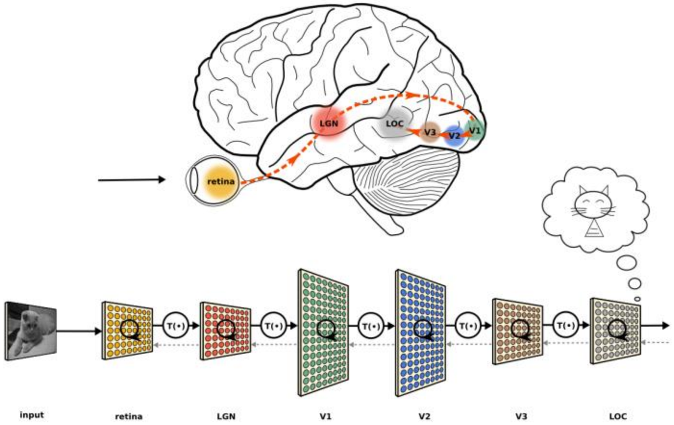


Input
Conv 1
Pool 1
Conv 2
Pool2
hidden4
Output
Convolution
Subsample
Convolution
Subsample
Convolution
Full
Connection

Convolution Operation

Nowadays, we learn kernels from the data.





Learning

$$\begin{bmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{bmatrix} = \textbf{Convolution}\left(\begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \\ X_{31} & X_{32} & X_{33} \end{bmatrix}, \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \right)$$

$$O_{11} = F_{11}X_{11} + F_{12}X_{12} + F_{21}X_{21} + F_{22}X_{22}$$

$$O_{12} = F_{11}X_{12} + F_{12}X_{13} + F_{21}X_{22} + F_{22}X_{23}$$

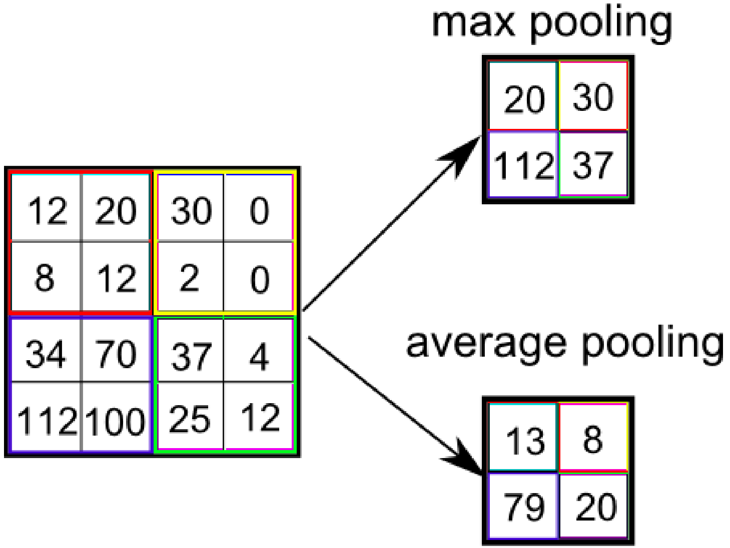
$$O_{21} = F_{11}X_{21} + F_{12}X_{22} + F_{21}X_{31} + F_{22}X_{32}$$

$$O_{22} = F_{11}X_{22} + F_{12}X_{23} + F_{21}X_{32} + F_{22}X_{33}$$

- Details:
- https://www.slideshare.net/EdwinEfranJimnezLepe/example-feedforward-backpropagation
- https://medium.com/@2017csm1006/forward-and-backpropagation-in-convolutional-neural-network-4dfa96d7b37e

Pooling

e.g. kernel size = 2, stride = 2 for both width and height.



CNN Structures
Image Classification

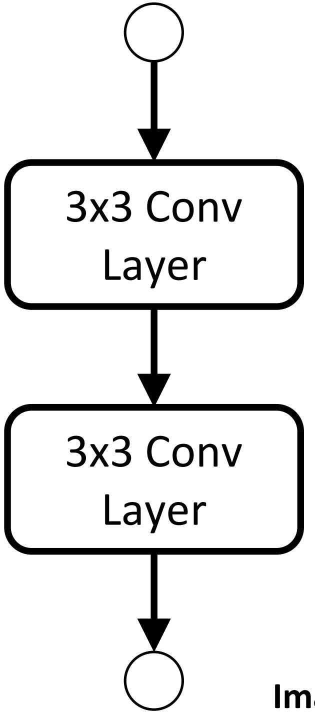
Image Classification

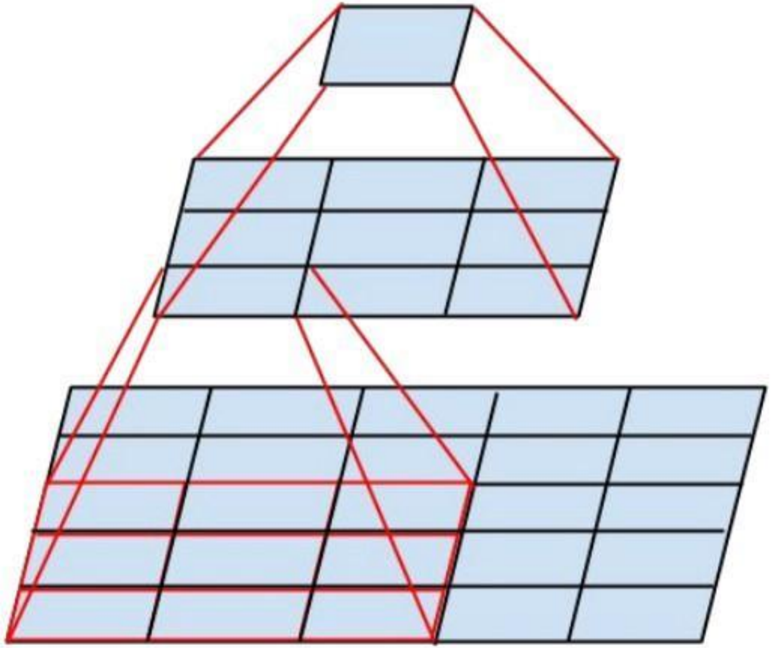
CU	Convolutional Unit
DU	Down-sampling Unit
FC	Fully-connected Or Linear Layer
GAP	Global Avg. Pooling

28 x 28
= $[28]^2$

→ CU $[28]^2$ → DU $[14]^2$ → CU $[14]^2$ → DU $[7]^2$ → CU $[7]^2$ → GAP $[1]^2$ → FC → Cat

Convolutional Unit (CU) - VGG





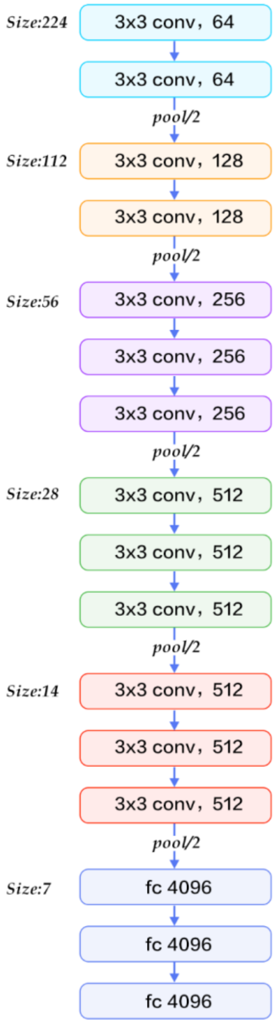
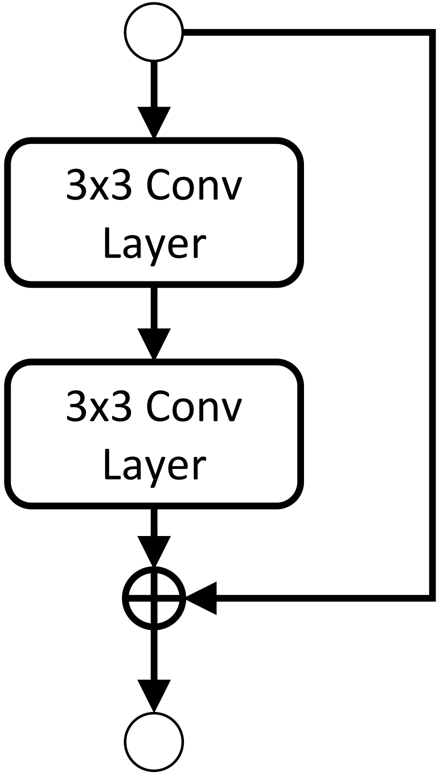


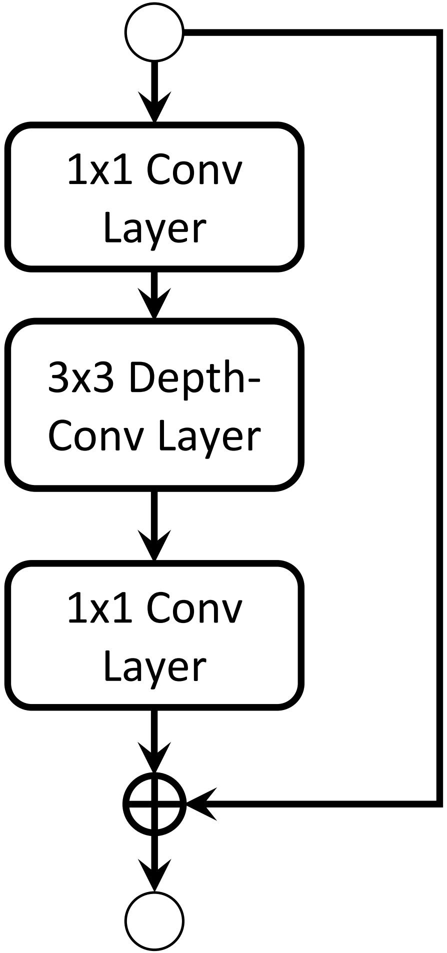
Image Source (Inception): Szegedy, Christian, et al. "Rethinking the inception architecture for computer vision." *CVPR*. 2016.

Basic Block in ResNet



ResNet: He, Kaiming, et al. "Deep residual learning for image recognition." CVPR. 2016.

- Residual Connection
- Element-wise addition of input and output
- Improves gradient flow and accuracy
- In ResNet-18 and ResNet-34
- Still computationally expensive
  - Hard to train very deep networks (> 100 layers)



Bottleneck in ResNet

- Used in ResNet-50, ResNet-101, ResNet-152, etc...
- Computationally Efficient

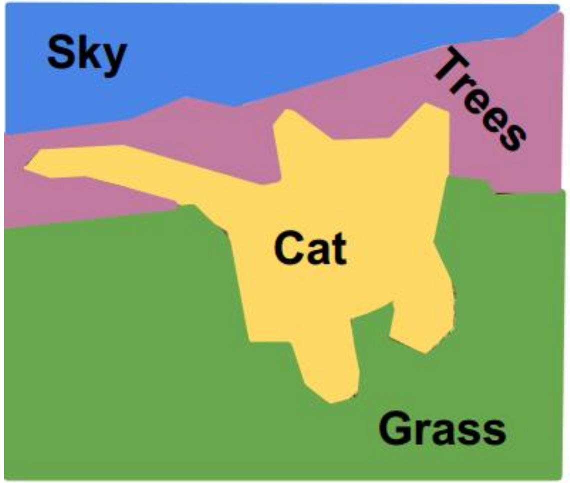
Influence:

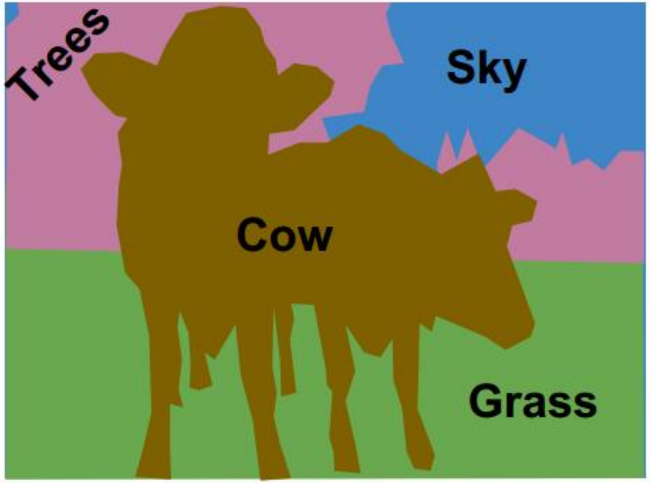
- Bottleneck unit with Depth-wise convs
  - MobileNetv2
  - ShuffleNetv2

- **MobileNetv2:** Sandler, Mark, et al. "Mobilenetv2: Inverted residuals and linear bottlenecks." CVPR, 2018.
- **ShuffleNetv2:** Ma, Ningning, et al. "Shufflenet v2: Practical guidelines for efficient cnn architecture design." ECCV, 2018.

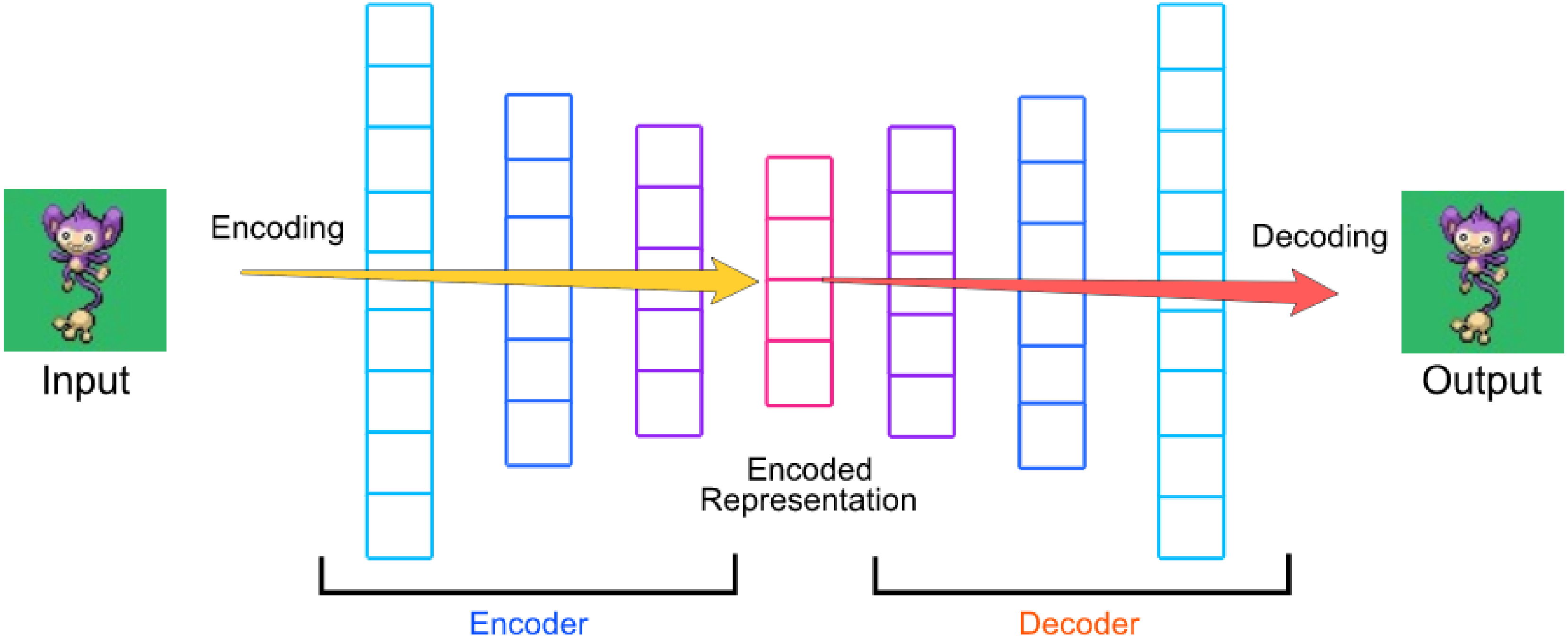
CNN Structures

Segmentation, Detection, Generation

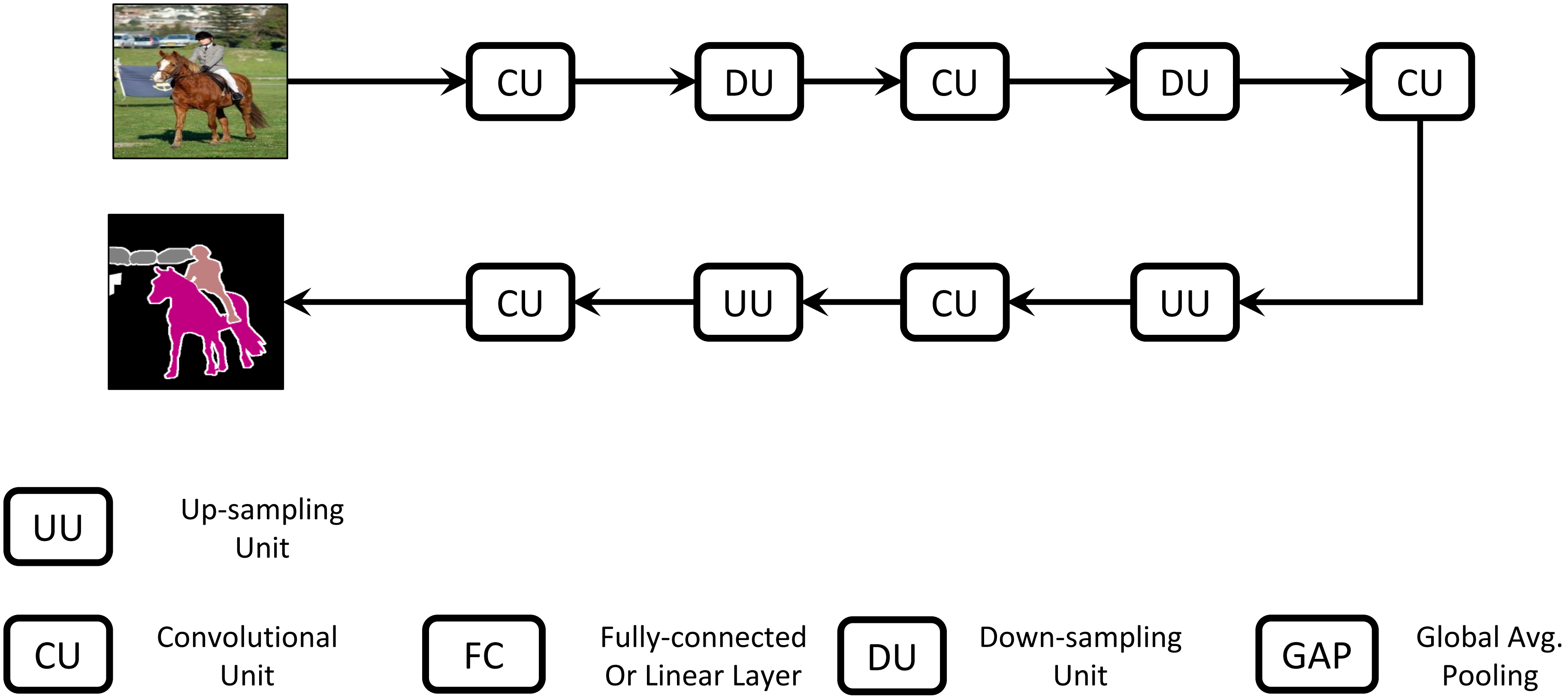

Sky
Trees
Cat
Grass


Trees
Sky
Cow
Grass

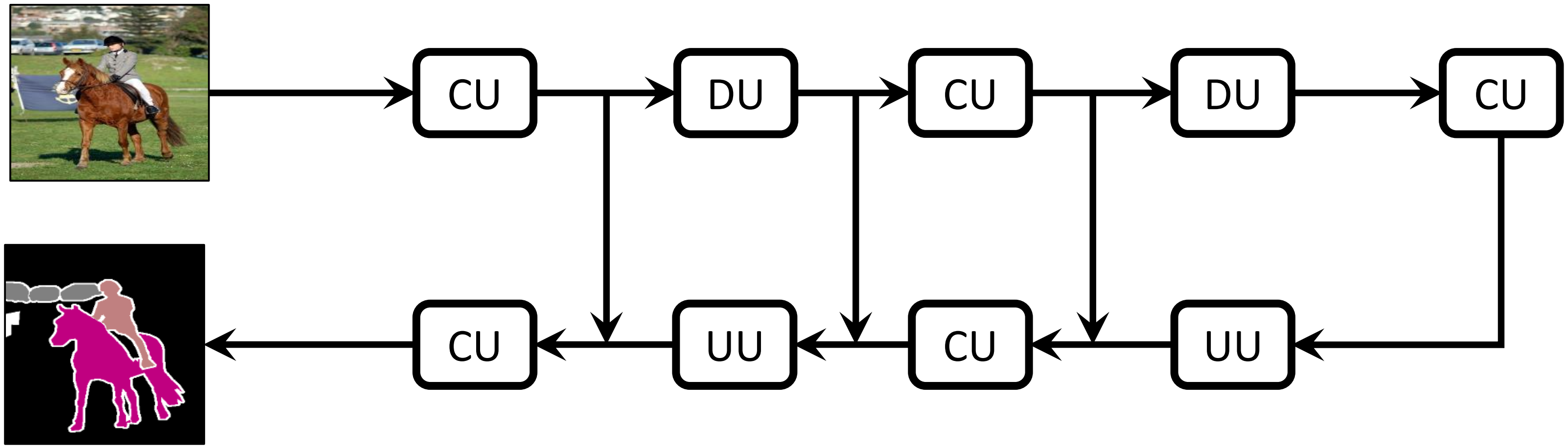
Encoder-Decoder



Encoder-Decoder in Semantic Segmentation

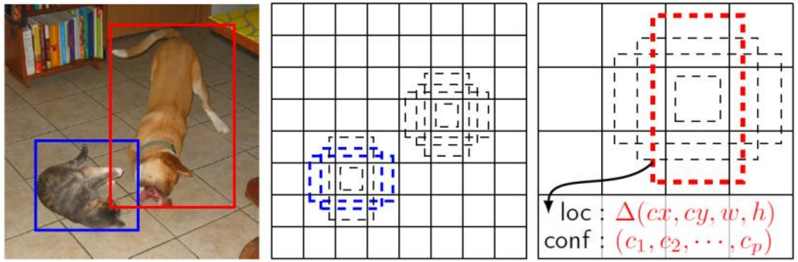


U-Net

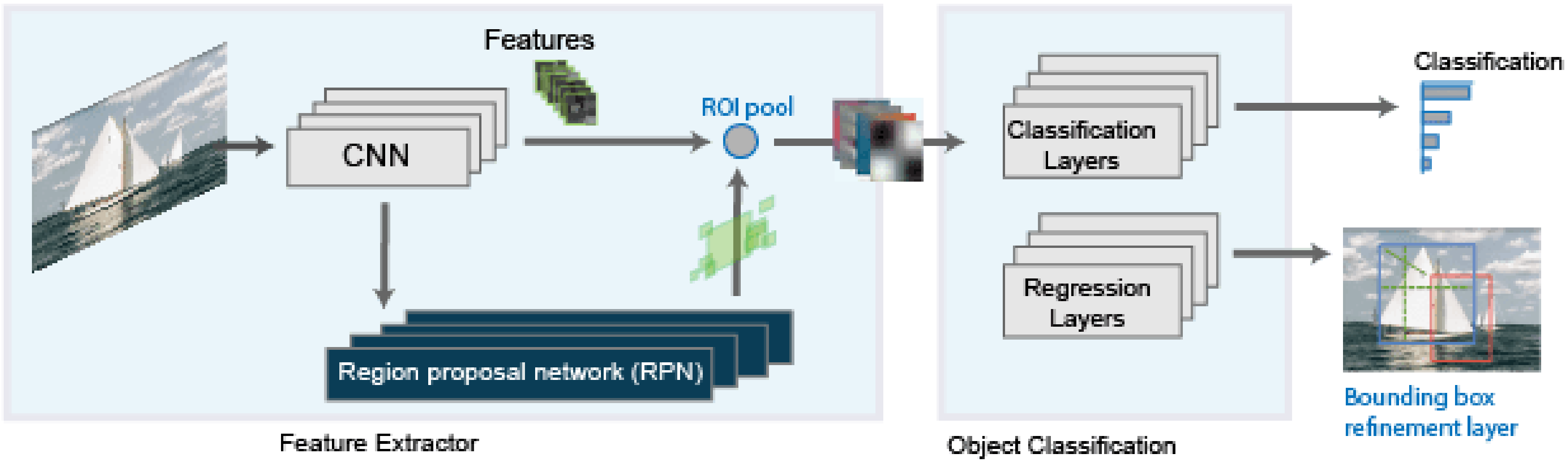


UU	Up-sampling Unit
CU	Convolutional Unit
FC	Fully-connected Or Linear Layer
DU	Down-sampling Unit
GAP	Global Avg. Pooling

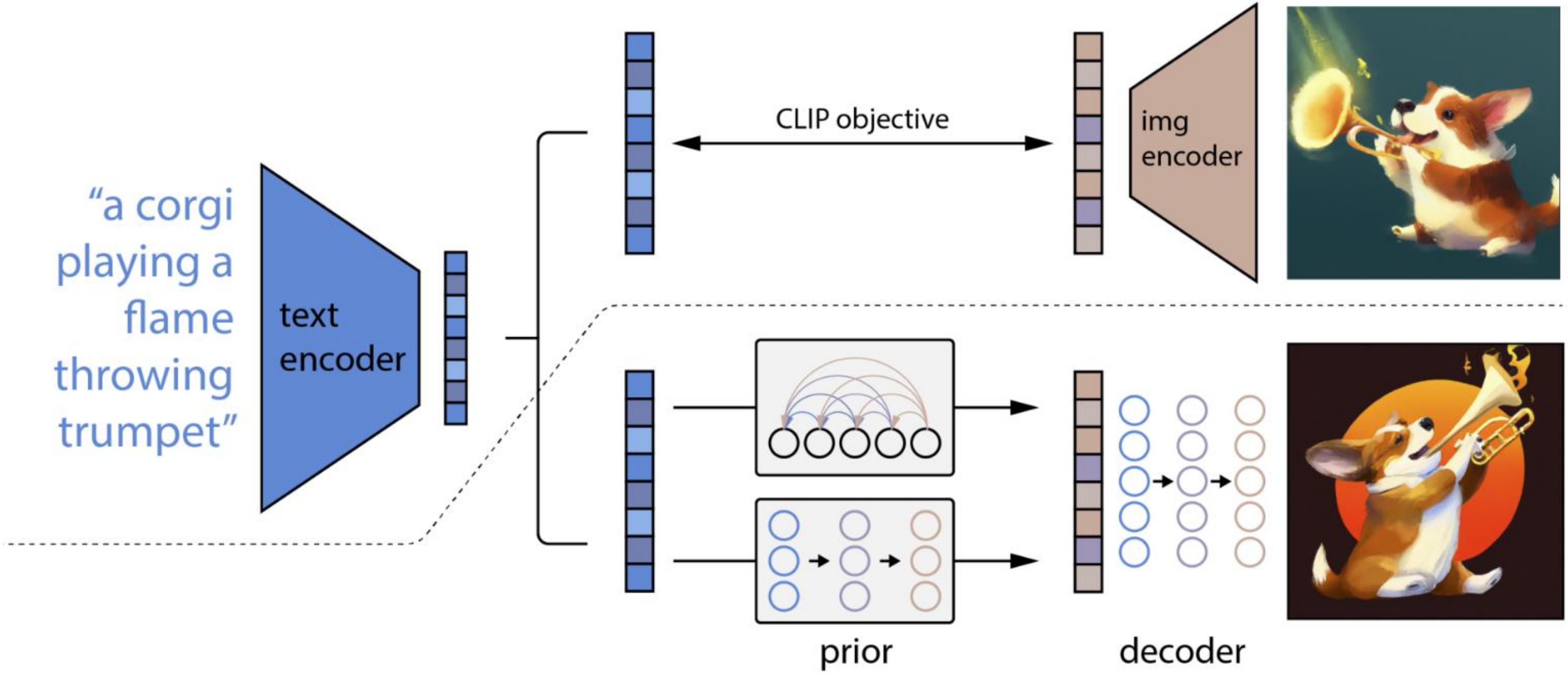
Faster R-CNN



(a) Image with GT boxes (b) 8 × 8 feature map (c) 4 × 4 feature map



Diffusion (DALL·E 2)

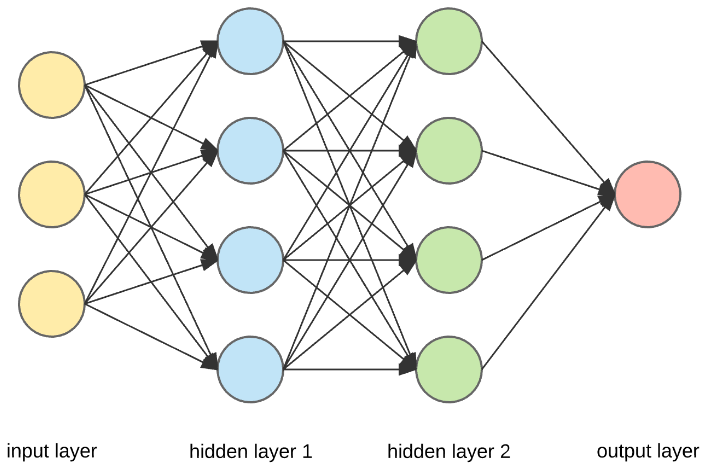


RNN Structures

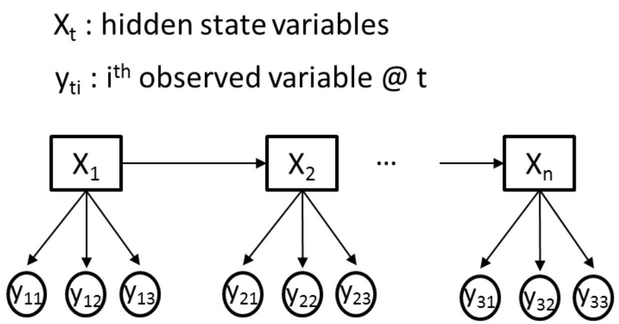
Challenges for time-series signals

- Different signal length
- Online inference for new timepoint

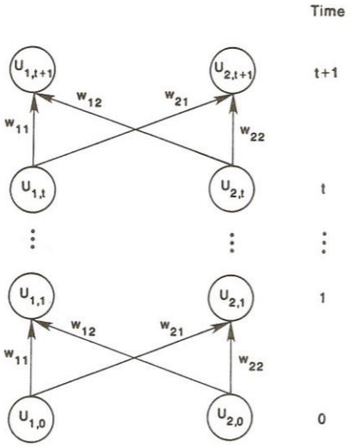
(Vanilla) Neural Network
1940s - 1980s



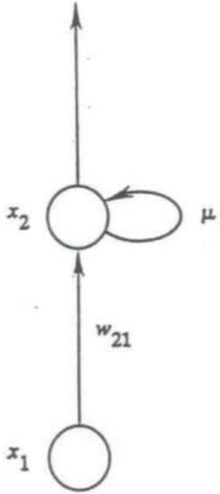
Hidden Markov Model
Andrew Viterbi, 1967
Lawrence Rabiner, 1989



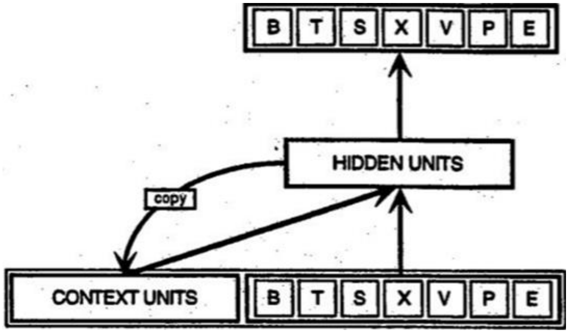
Learning internal representations by error propagation
Rumelhart, Hinton, and Williams (1985)



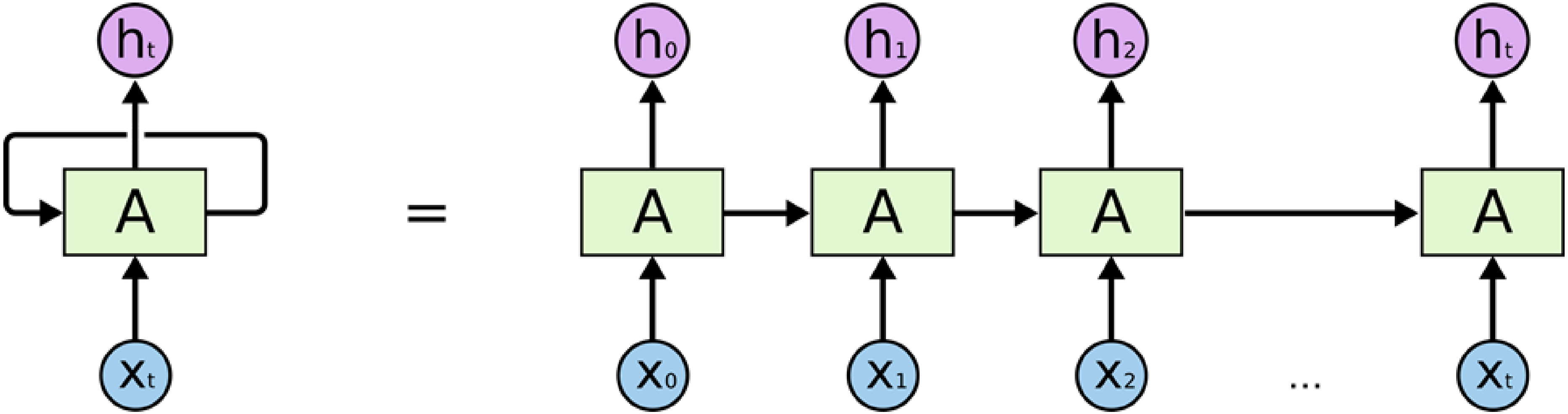
A parallel distributed processing approach
Jordan (1986)



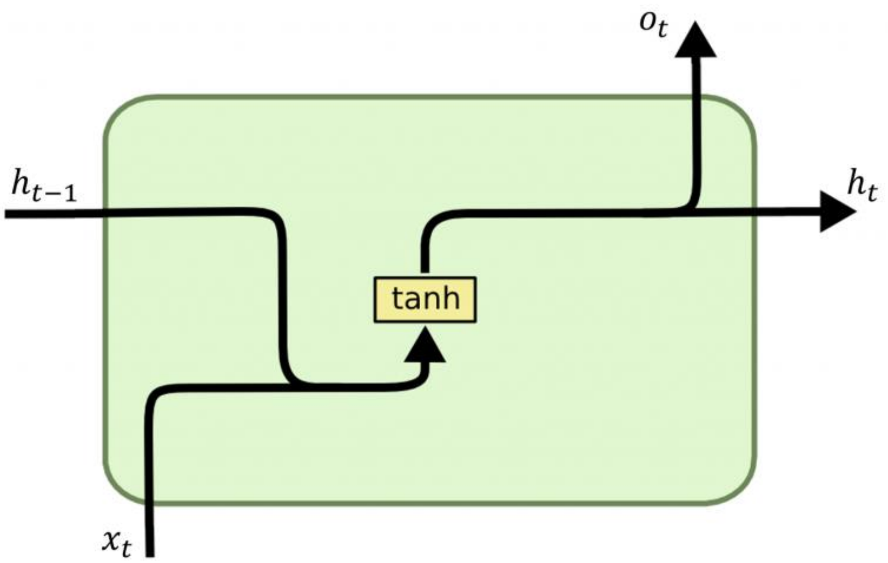
Graded state machines
Servan-Schreiber, Cleeremans, and McClelland (1991)



Recurrent Neural Network



Parameters in Recurrent Neural Network



x_t : input vector $(m \times 1)$.

h_t : hidden layer vector $(n \times 1)$.

o_t : output vector $(n \times 1)$.

b_h : bias vector $(n \times 1)$.

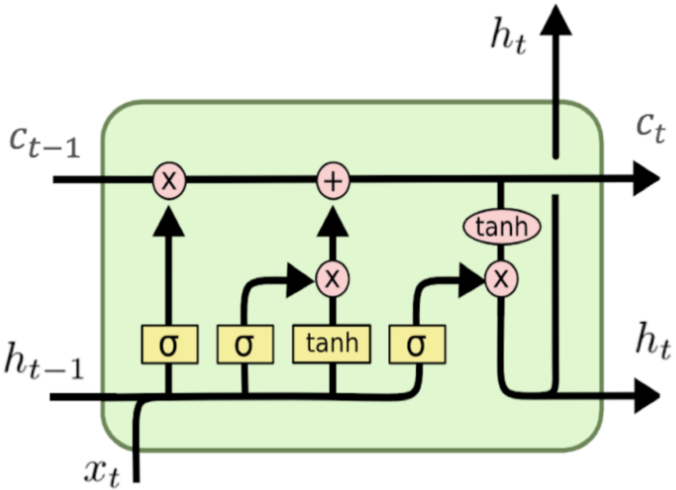
U, W : parameter matrices $(n \times m)$.

V : parameter matrix $(n \times n)$.

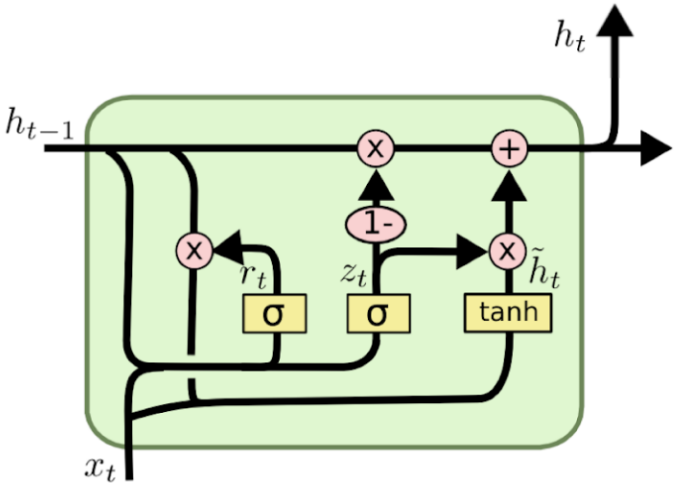
σ_h, σ_y : activation functions.

$$h_t = \sigma_h(i_t) = \sigma_h(U_h x_t + V_h h_{t-1} + b_h)$$
$$y_t = \sigma_y(a_t) = \sigma_y(W_y h_t + b_h)$$

LSTM and GRU: Memory for RNNs



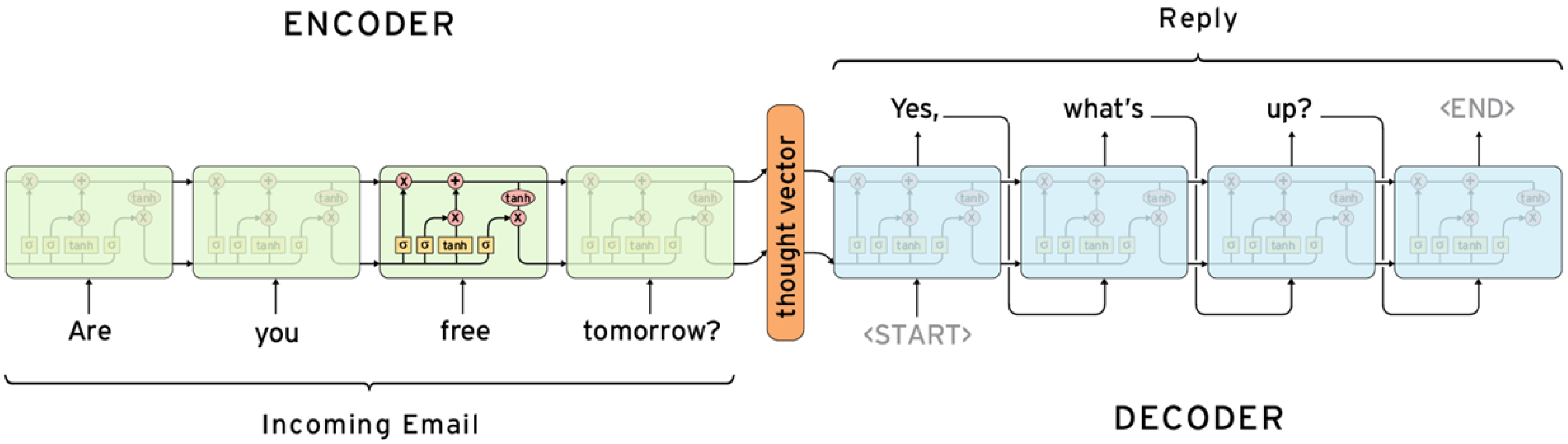
LSTM
(Long-Short Term Memory)



GRU
(Gated Recurrent Unit)

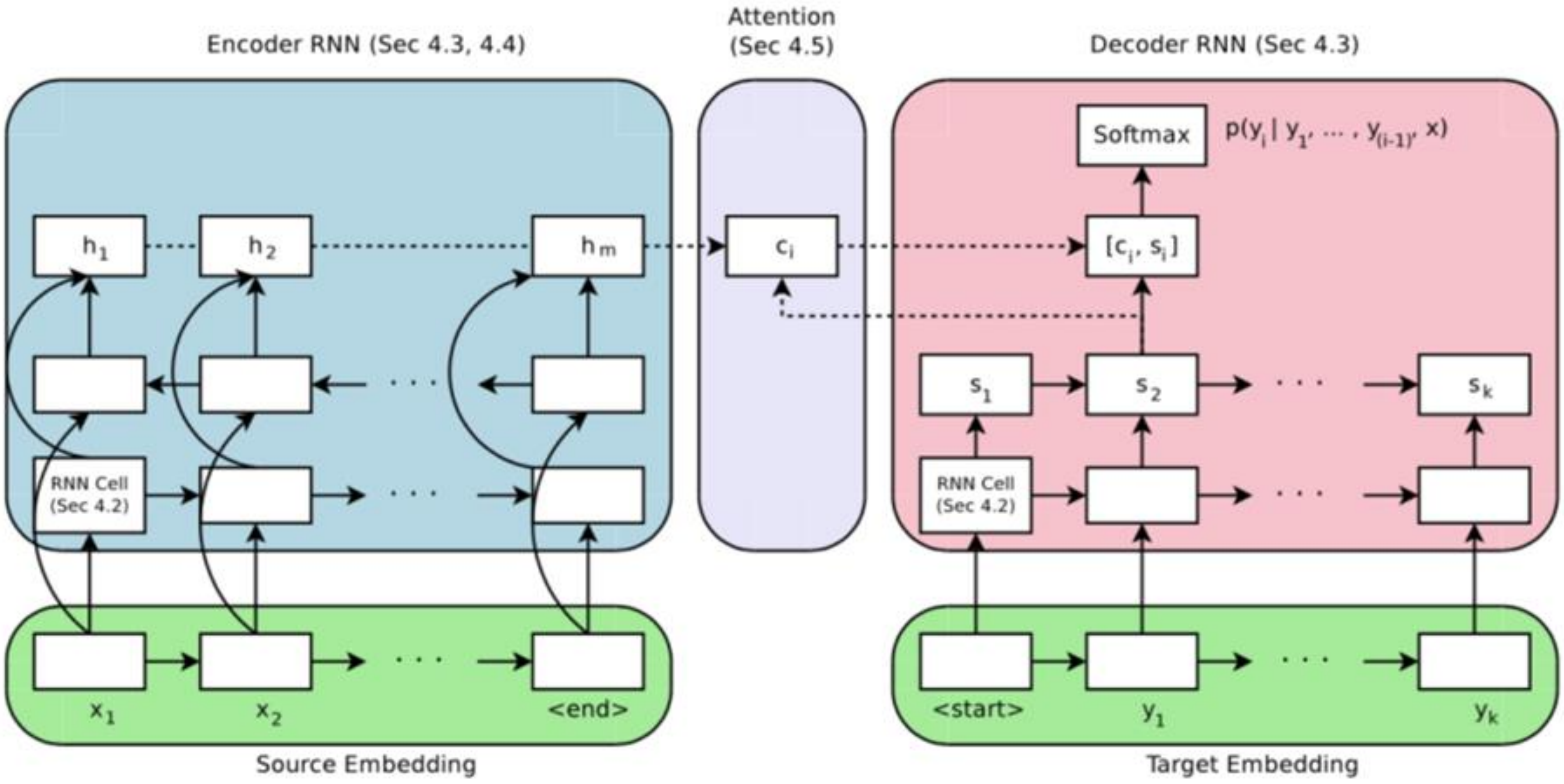
http://dprogrammer.org/rnn-lstm-gru
https://towardsdatascience.com/grus-and-lstm-s-741709a9b9b1

Seq-2-Seq



- Encoder maps a variable-length source sequence (input) to a fixed-length vector
- Decoder maps the vector representation back to a variable-length target sequence (output)
- Two RNNs are trained jointly to maximize the conditional probability of the target sequence given a source sequence

Seq-2-Seq with Attention



Transformer

Limitations of CNN and RNN

1. “Locality” of the convolution operation
    a. Reduce dimension (compared to fully-connected layers) while maintaining useful local information
    b. It could NOT see two pixels that are far away

1. “Recurrentness” of recurrent neural network
    a. It can take an input with arbitrary size (length)
    b. “Vanishing of gradient” problem when sequence length is too long (during backpropagation)

Well, forget about convolution and recurrent

IS ALL YOU NEED

Attention Is All You Need

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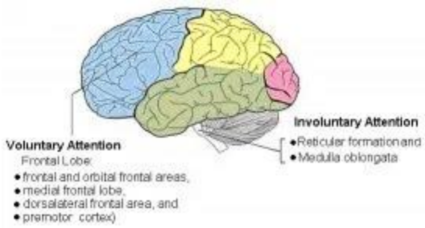
Xiv:1706.03762v5 [cs.CL] 6 Dec 2017

Abstract

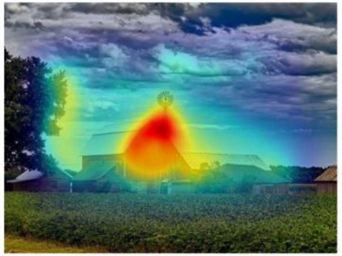
The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.8 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature. We show that the Transformer generalizes well to other tasks by applying it successfully to English constituency parsing both with large and limited training data.

What is attention?



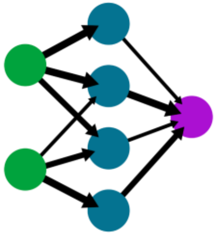
Psychology

Eye-tracking

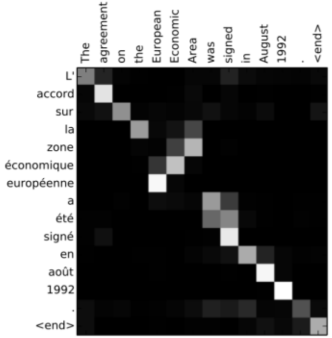


Computer Vision
(Saliency Map)

Computer Vision
(Backpropagation)

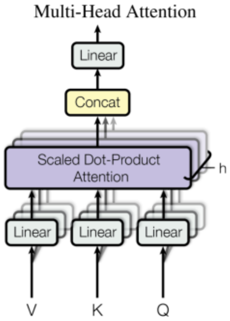


Neural Network
(weights)

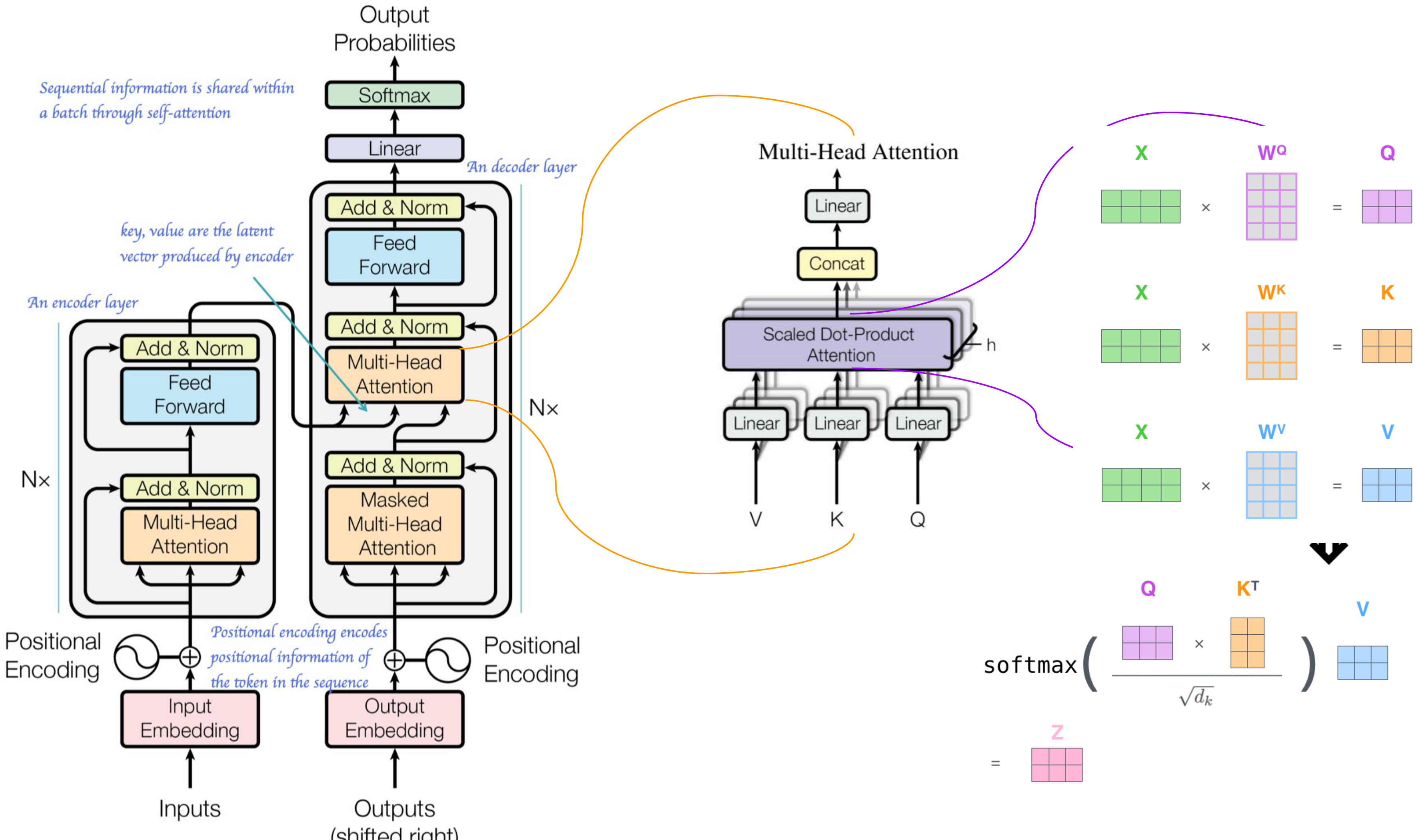


NLP (align)
Bahdanau, Cho, Bengio, 2015, ICLR

Value, Key, Query

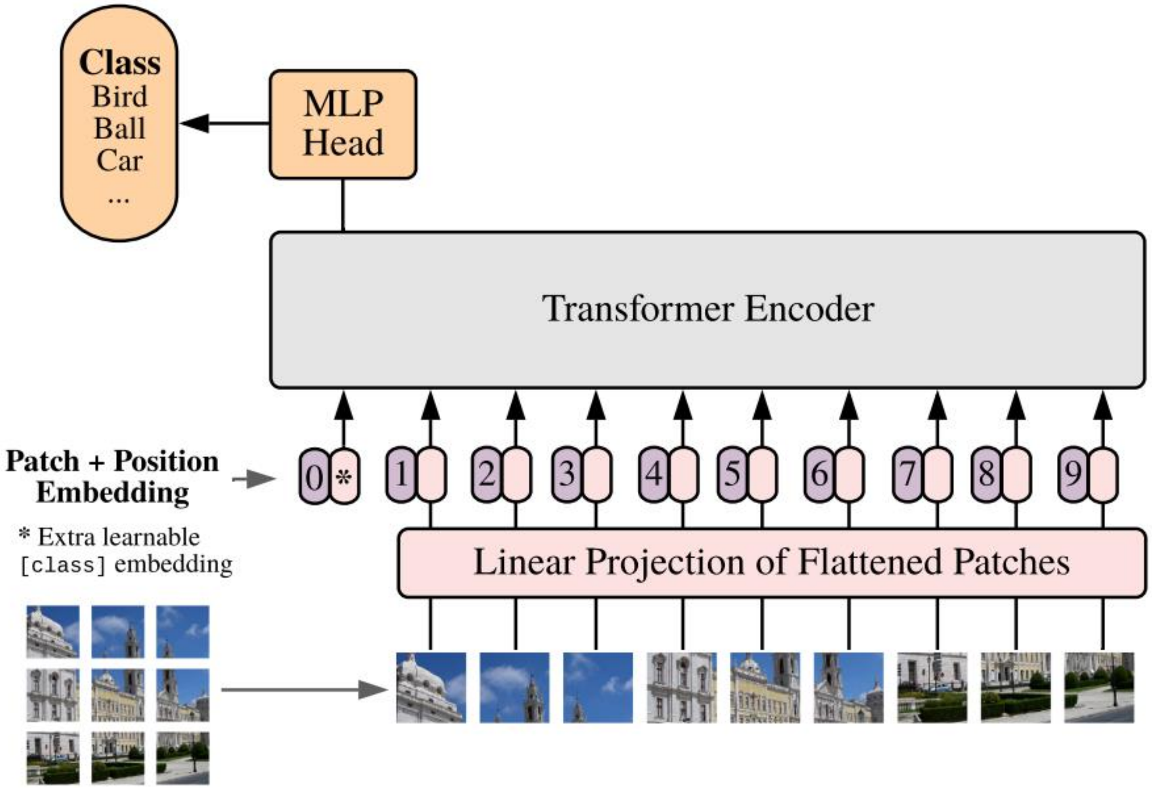


Transformer



http://jalammar.github.io/illustrated-transformer/

Vision Transformer



Limitations of Transformer

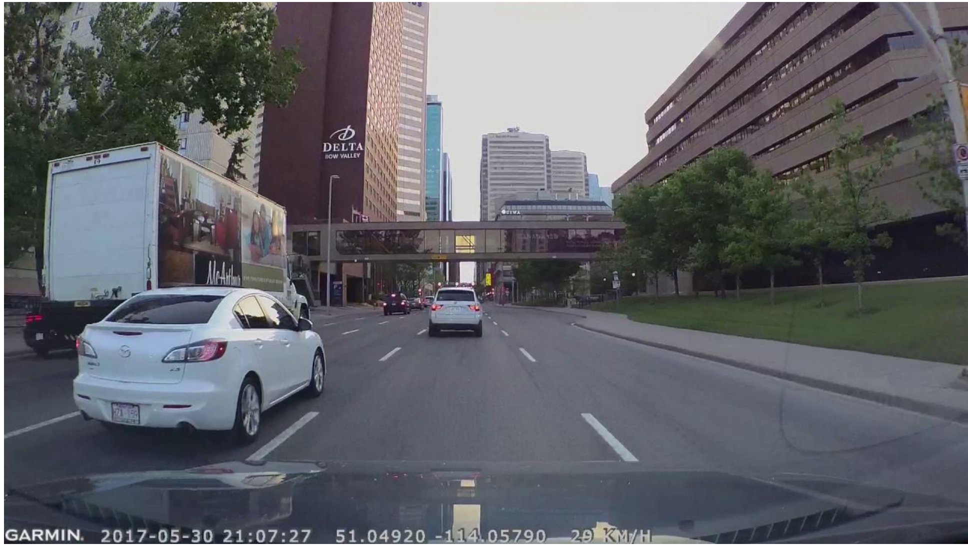
1. It cannot learn hierarchical features efficiently (while CNN can)
2. It cannot model periodic finite-state language (while RNN can)
3. It requires lots for computer memory
   a. Solution: efficient transformers, e.g., BigBird, Longformer, etc.
4. It requires more training data than CNN/RNN
   a. Not a big problem for natural images
   b. Solution: smarter architecture design and learning paradigms for low-resource datasets
   c. Solution: self-supervised learning, transfer learning, etc.

NN for RL

Which Direction

Regression:

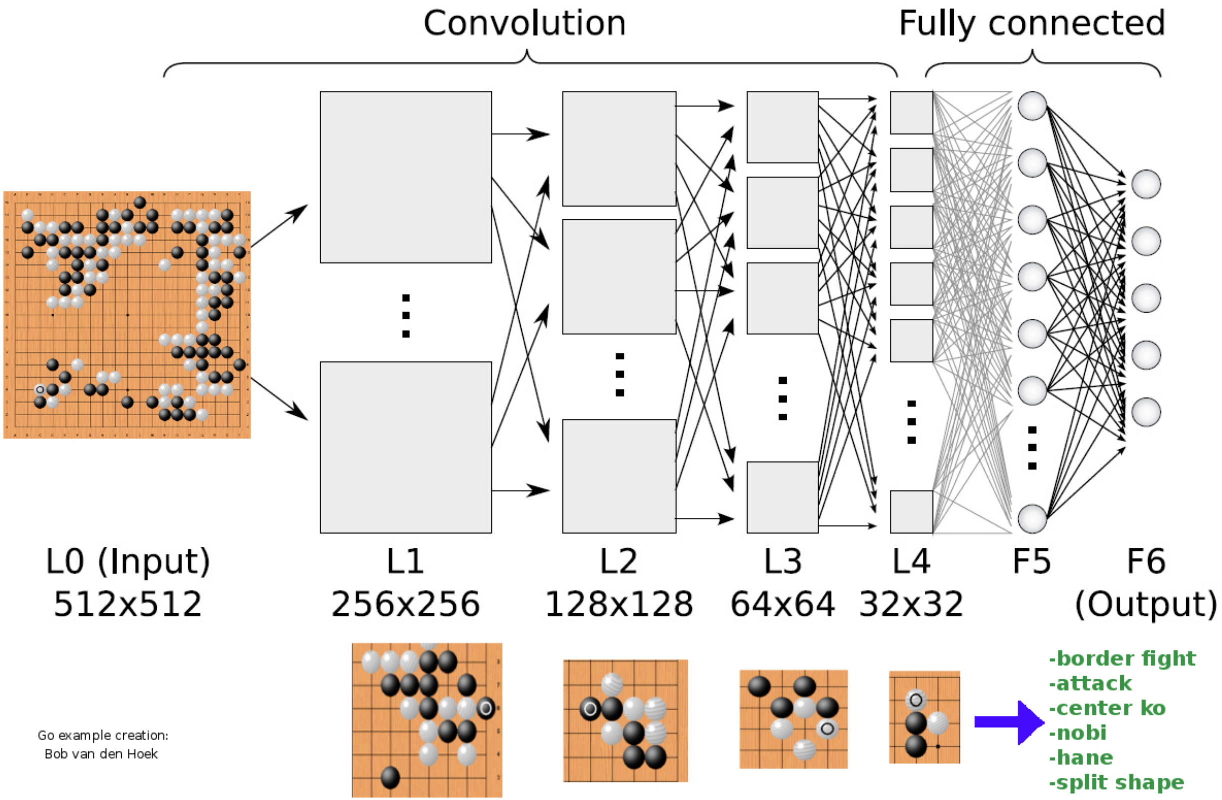
Angle = [-540°, 540°]



Classification:

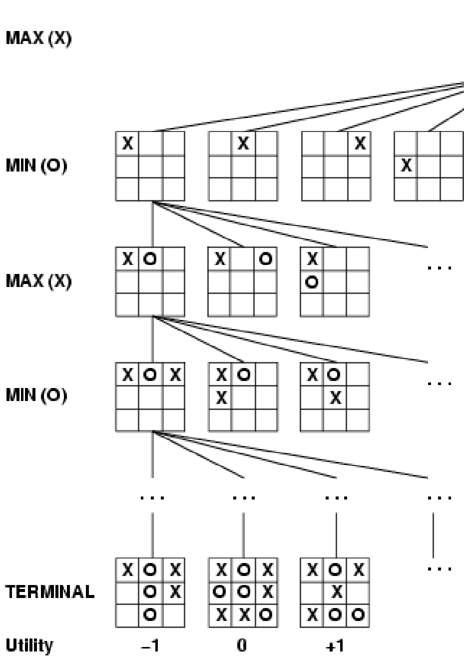
- Turn left
- Turn right
- Stay Still

Which Move

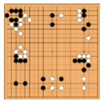


Go example creation:
Bob van den Hoek

Design Utility Function



We can train a CNN to replace the manual utility function

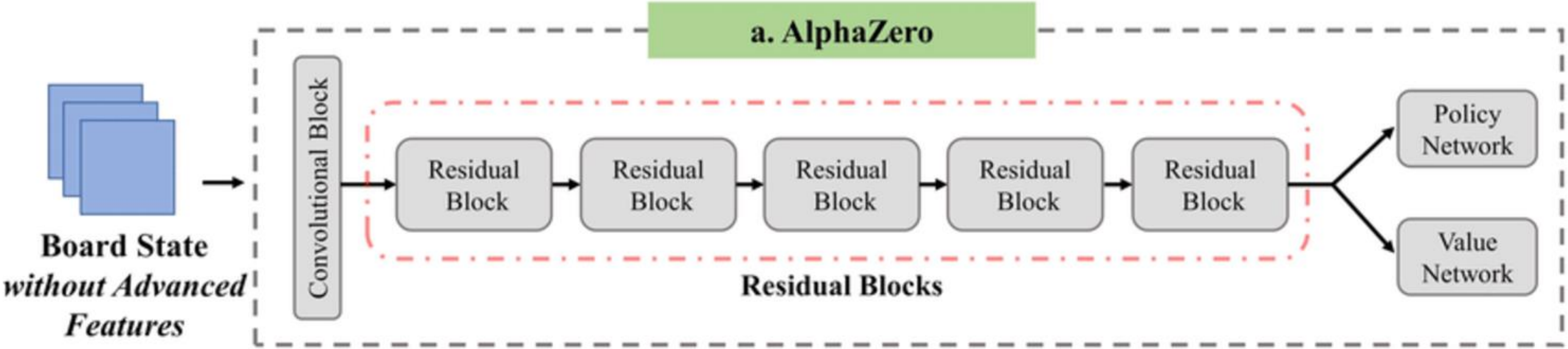
Utility = CNN()

AlphaZero

ResNet backbone

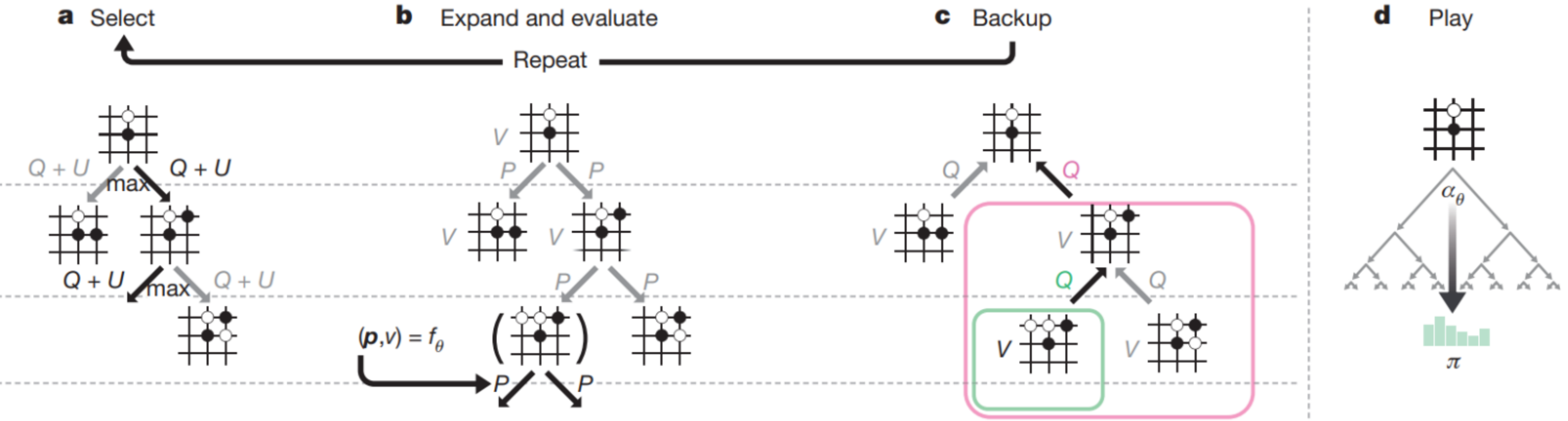
Policy Network

Value Network

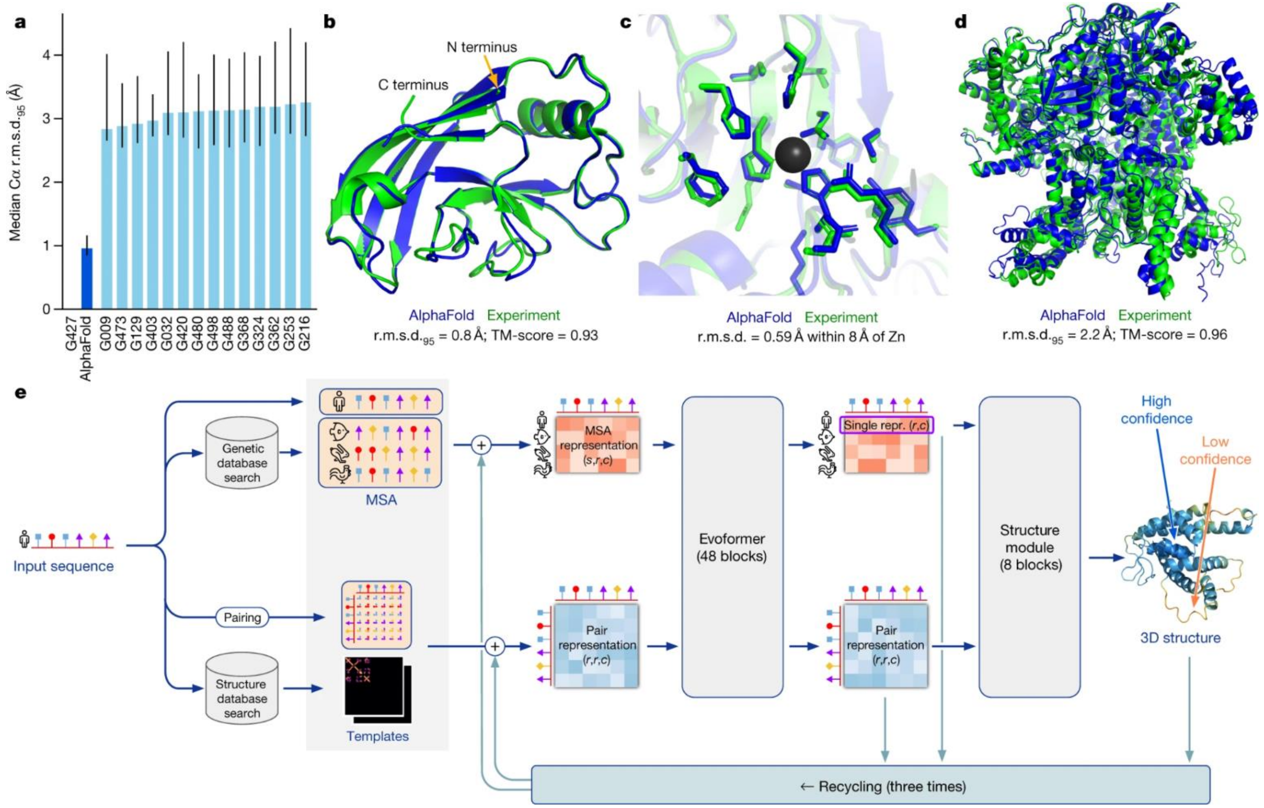


Monte Carlo Tree Search

Active Learning to balance Exploration v.s. Exploitation

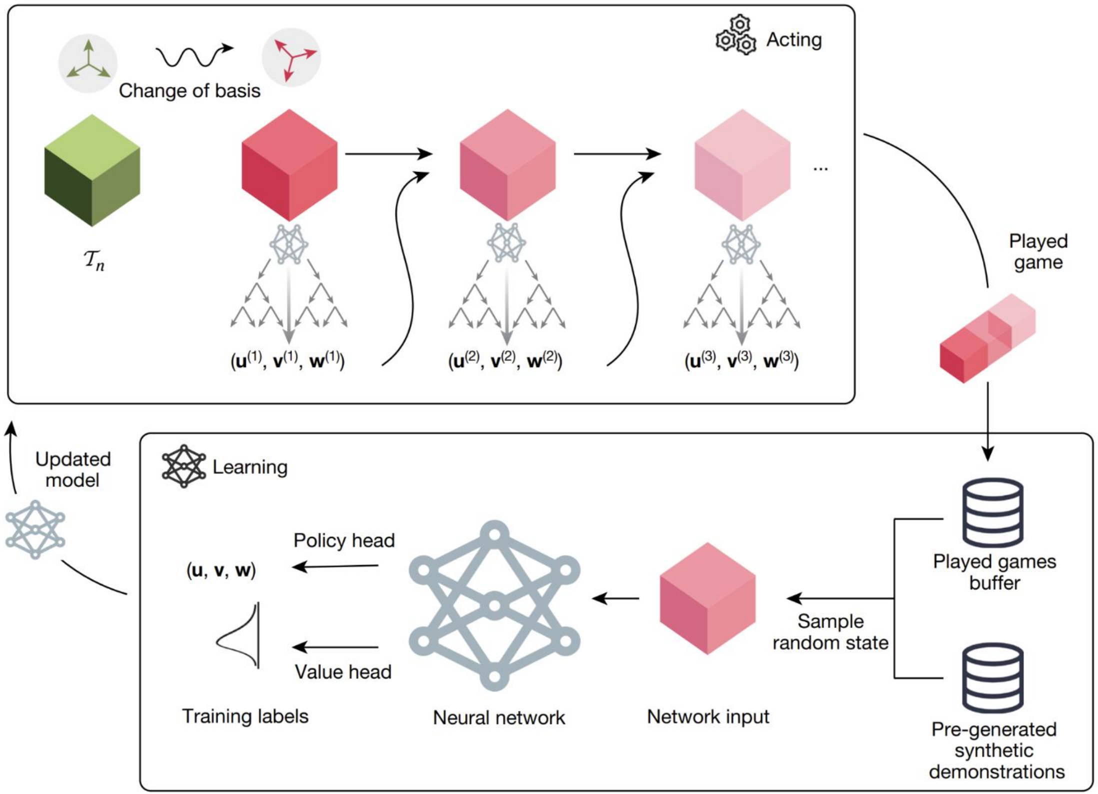


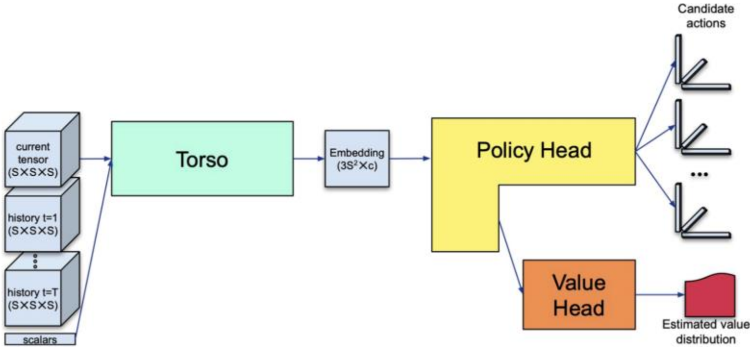
Alpha Fold



a
Median Cα r.m.s.d.95 (Å)
G427
AlphaFold
G009
G473
G129
G403
G032
G420
G480
G498
G488
G368
G324
G362
G253
G216
b
N terminus
C terminus
AlphaFold Experiment
r.m.s.d.95 = 0.8 Å; TM-score = 0.93
c
AlphaFold Experiment
r.m.s.d. = 0.59 Å within 8 Å of Zn
d
AlphaFold Experiment
r.m.s.d.95 = 2.2 Å; TM-score = 0.96
e
Input sequence
Genetic database search
MSA
Pairing
Structure database search
Templates
MSA representation (s,r,c)
Pair representation (r,r,c)
Evoformer (48 blocks)
Single repr. (r,c)
Pair representation (r,r,c)
Structure module (8 blocks)
High confidence
Low confidence
3D structure
← Recycling (three times)

RL Applications: Alpha Tensor





Intro to PyTorch

Deep Learning Libraries

mxnet

TensorFlow

theano

scikit learn

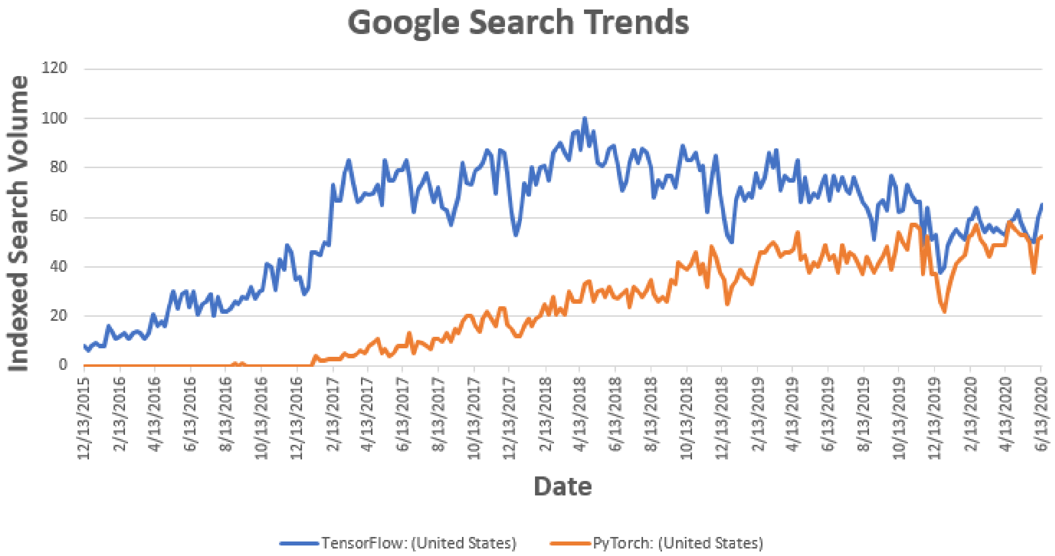
Caffe2

Keras

PYTORCH

Deep Learning Frameworks

- Before 2012: custom C++, MatLab, R, Lua, … code.
  - Only limited libraries/functions
  - You need to do most things yourself
- MXNet (2015)
- TensorFlow (2015)
- Caffee (2015)
- Torch (2002): Lua
- PyTorch (2016)



Why PyTorch

- Autograd
- Dynamic computational graph
- Debugging is easier!
- Data Parallelism (multiple GPU)
- Pythonic-syntax (Python)
- Multiple language support: Python, C++, Java
- Many more!

Model Definition

```
import torch.nn as nn
import torch.nn.functional as F


class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.pool = nn.MaxPool2d(2, 2)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1 = nn.Linear(16 * 5 * 5, 120)
        self.fc2 = nn.Linear(120, 84)
        self.fc3 = nn.Linear(84, 10)

    def forward(self, x):
        x = self.pool(F.relu(self.conv1(x)))
        x = self.pool(F.relu(self.conv2(x)))
        x = x.view(-1, 16 * 5 * 5)
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        x = self.fc3(x)
        return x


net = Net()
```

Training a model

```
running_loss = 0.0
for i, data in enumerate(trainloader, 0):
    # get the inputs
    inputs, labels = data

    # zero the parameter gradients
    optimizer.zero_grad()

    # forward + backward + optimize
    outputs = net(inputs)
    loss = criterion(outputs, labels)
    loss.backward()
    optimizer.step()

    # print statistics
    running_loss += loss.item()
    if i % 2000 == 1999:    # print every 2000 mini-batches
        print('[%d, %5d] loss: %.3f' %
              (epoch + 1, i + 1, running_loss / 2000))
        running_loss = 0.0
```

Homework 4
Convolutional Neural Networks
In PyTorch

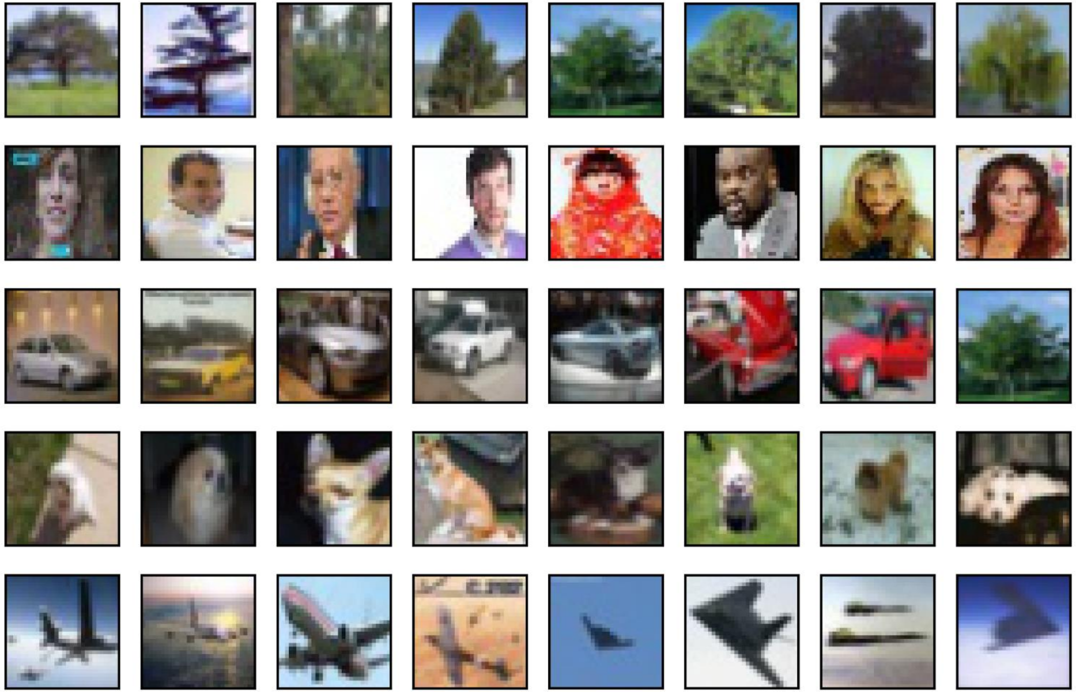
Which Object?

Image Classification:

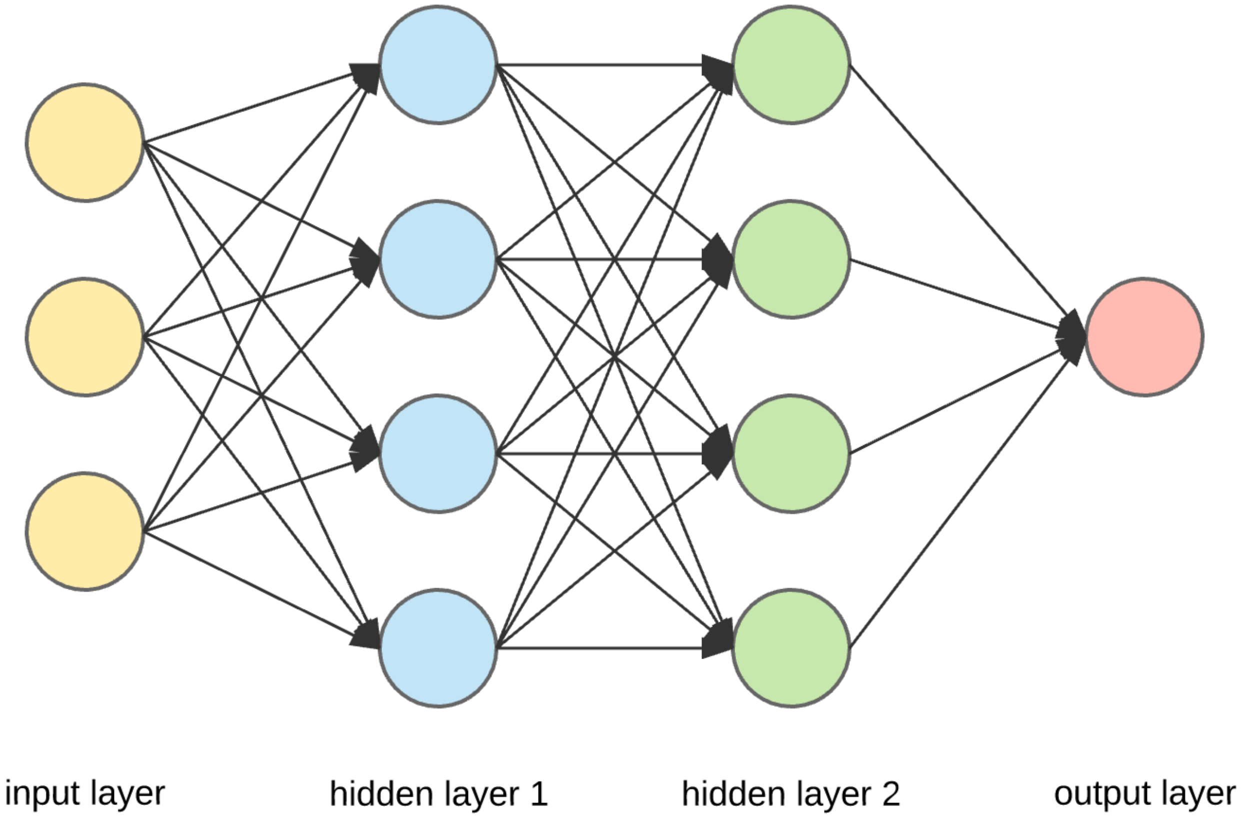
- Tree
- Face
- Car
- Dog
- Plane

Training set: 90 images per cls

Testing set: 10 images per cls



Neural Network (Q1)



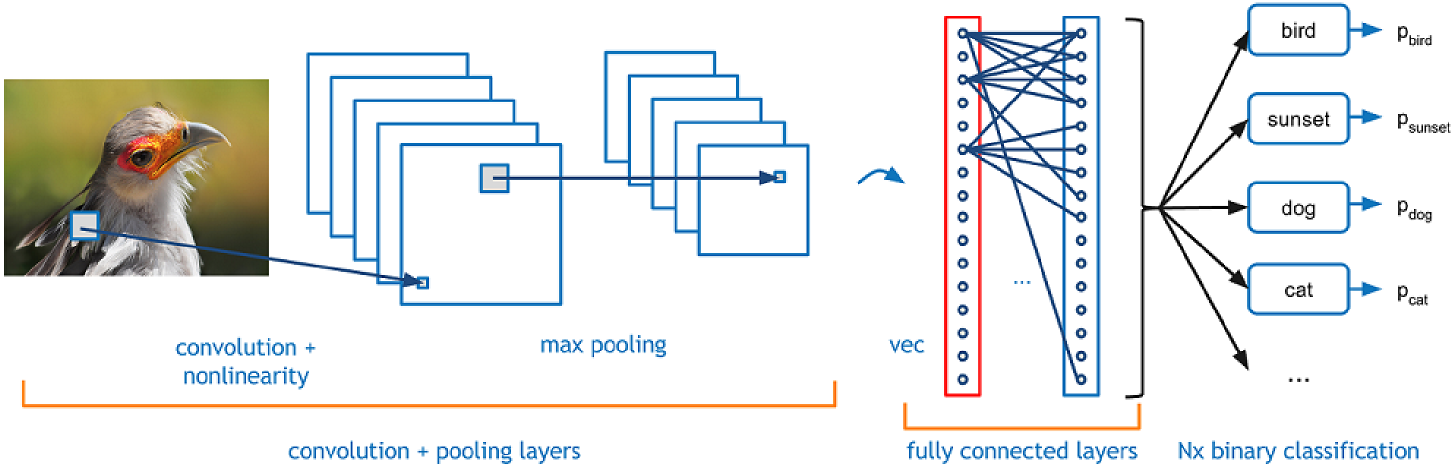
Convolutional Neural Network (Q2)

Conv

Pool

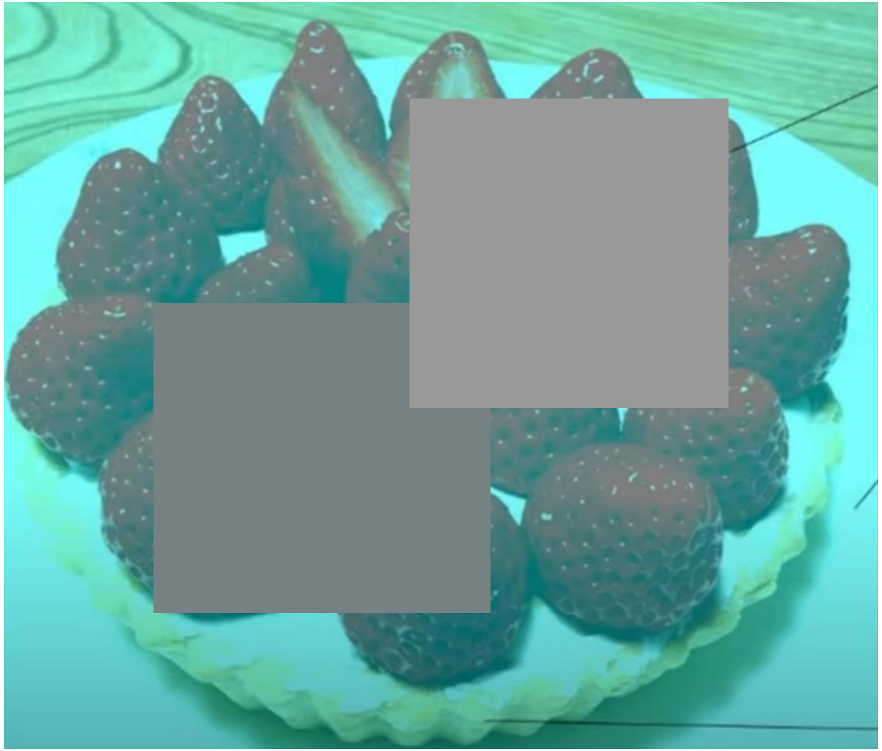
FC

Cross Entropy

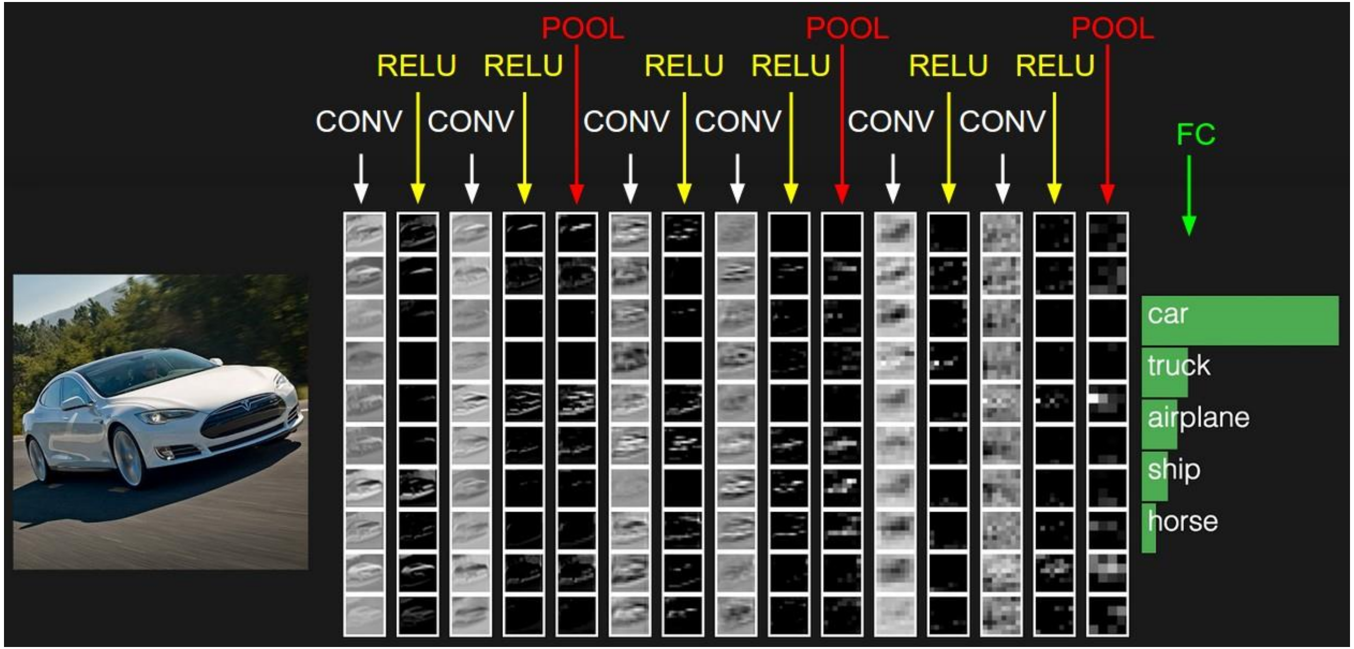


Color Normalization (Q3)

What’s the Color of the Strawberry



Deep Convolutional Neural Network (Q4)



Make the Design More Flexible

Input:

[8, 16, 32, "pool"]

Layer	Output Size	Output Channels
Input	30 x 30	3
Conv	28 x 28	8
ReLU	28 x 28	8
Conv	26 x 26	16
ReLU	26 x 26	16
Conv	24 x 24	32
ReLU	24 x 24	32
Max Pool	12 x 12	32
Linear	5	

Data Augmentation (Q5)

Random Affine Transformation