Mastering Deep Learning Within a Few Hours

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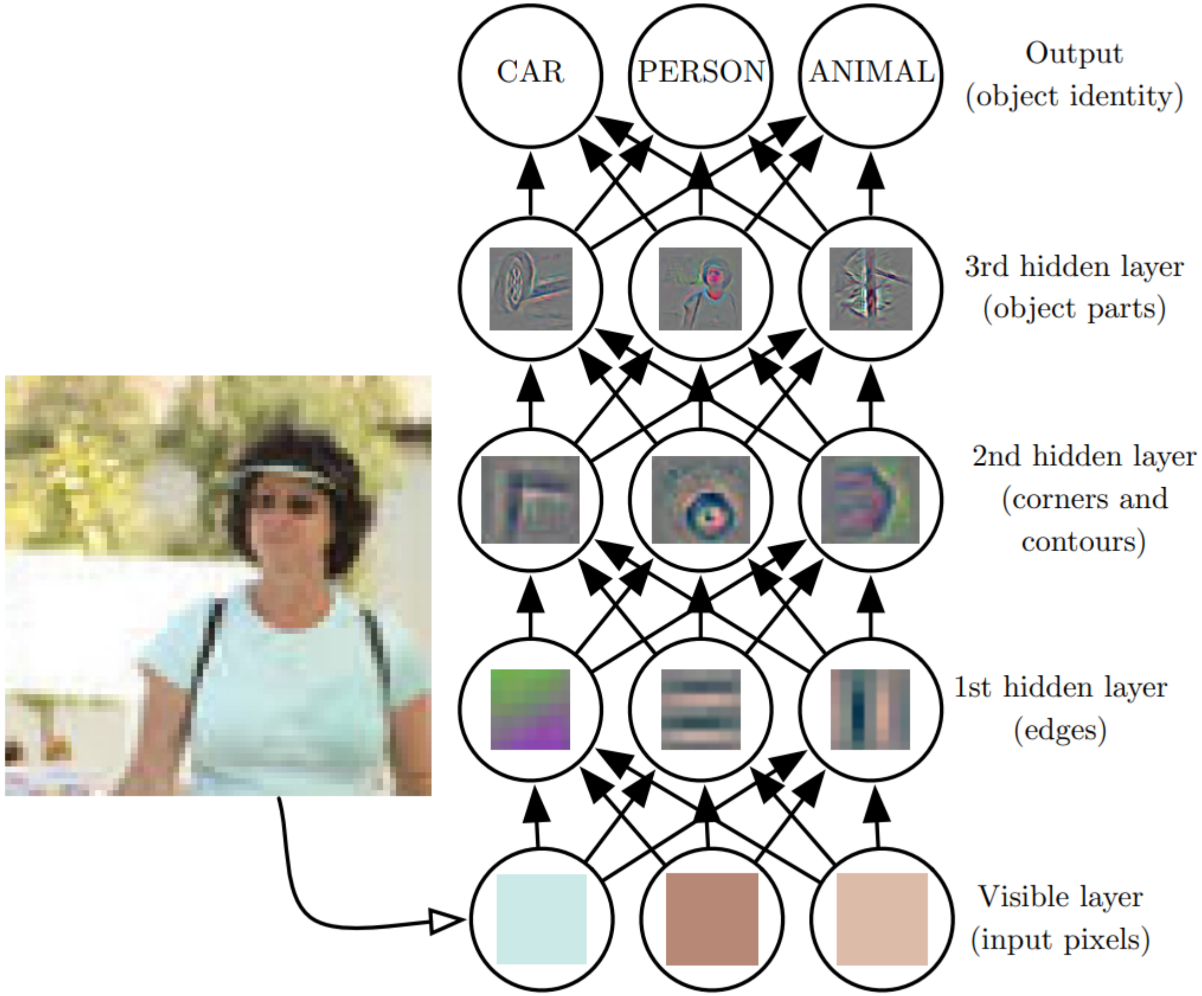
- Introduction
- Problem Formulation
- Implementation
- Experiments
- Advanced Topics

Introduction

Artificial v.s. Intelligence

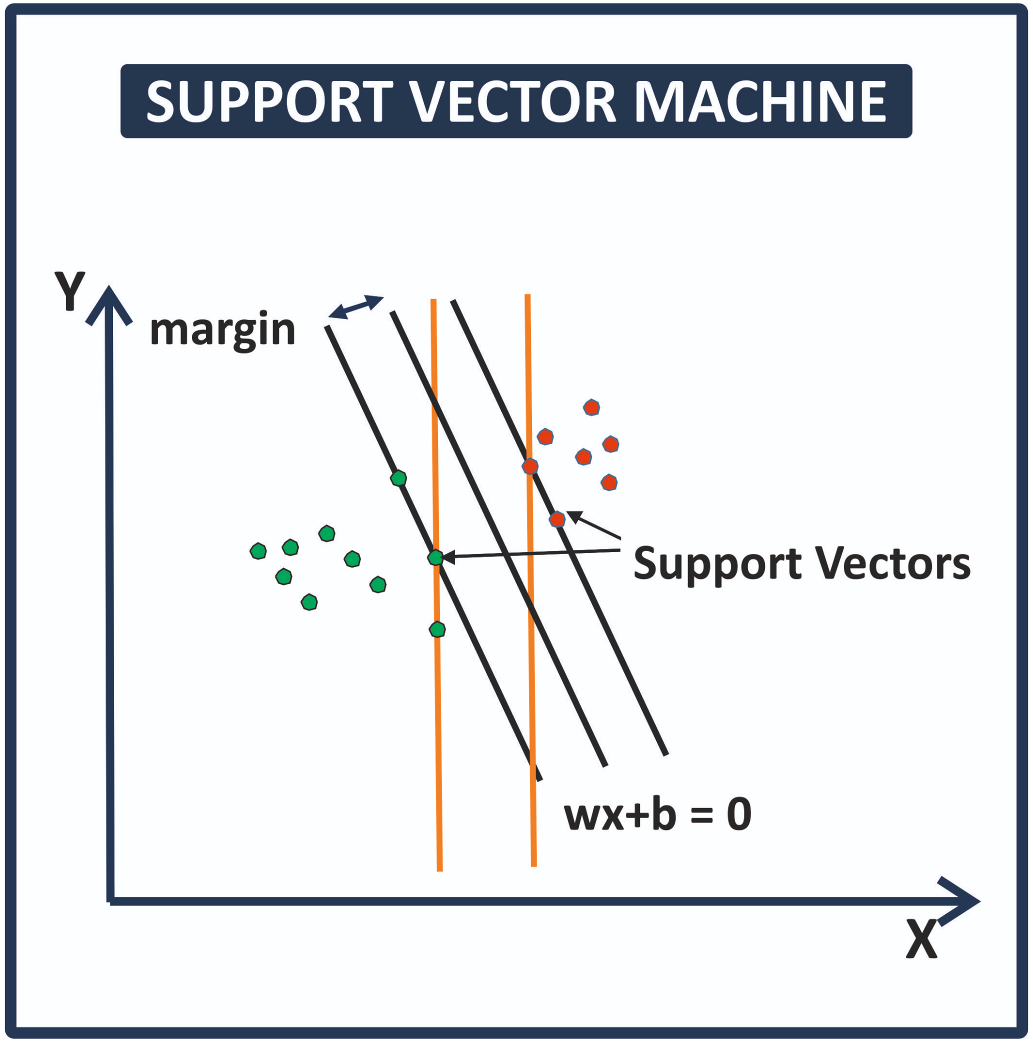
Intelligence

- Human Perception

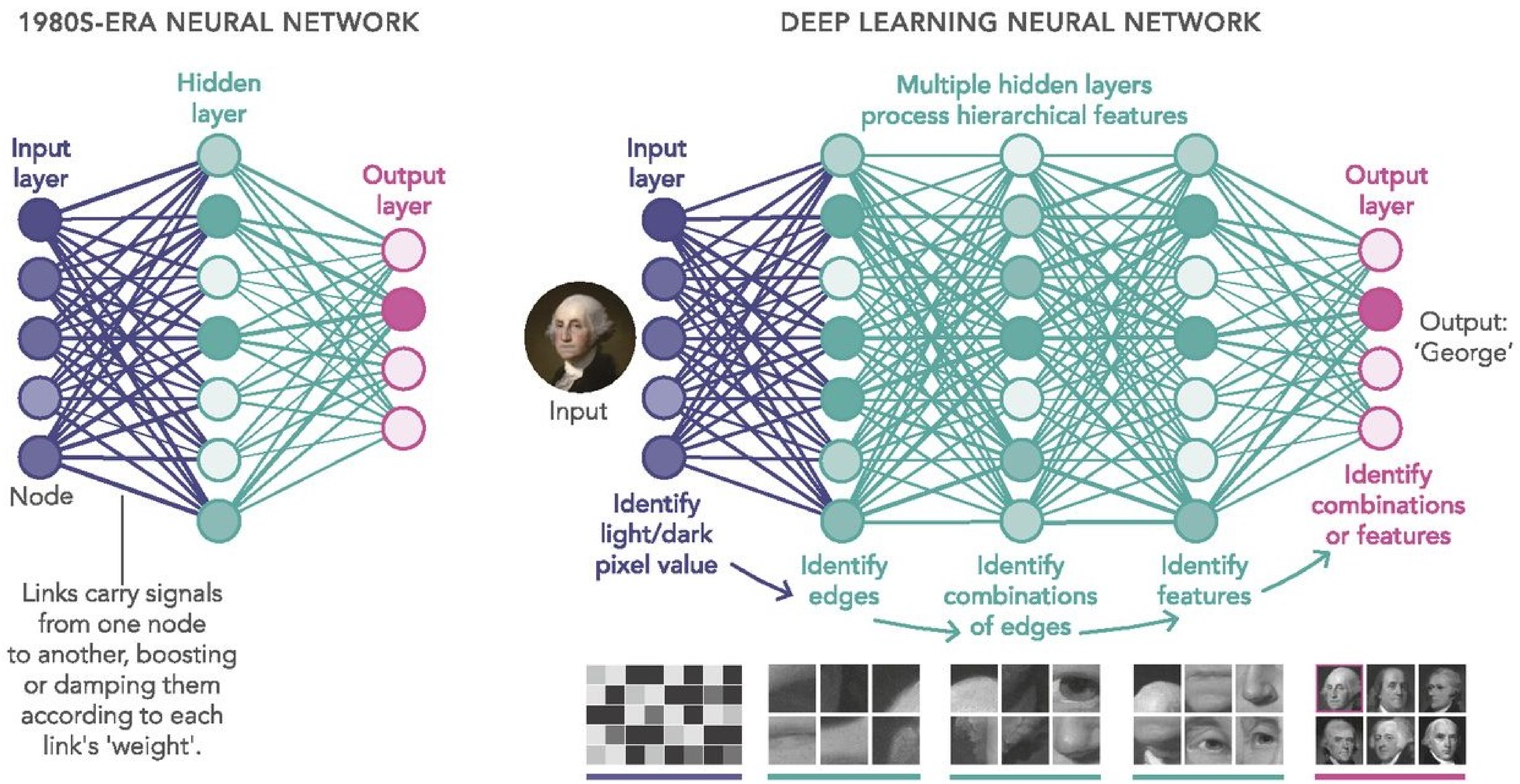


Artificial

- Machine Learning

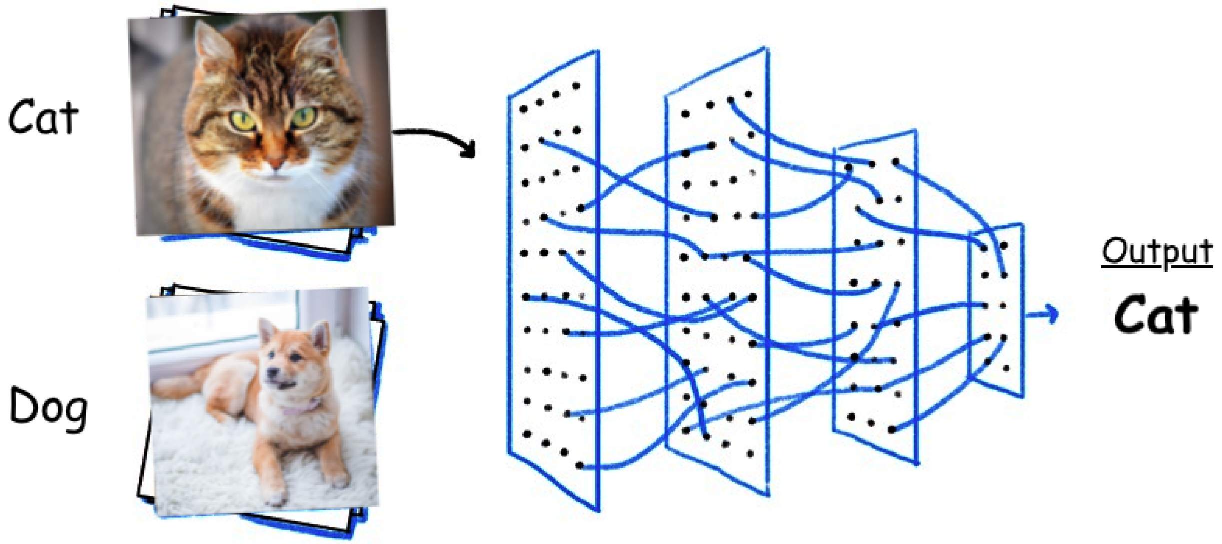


Deep Learning



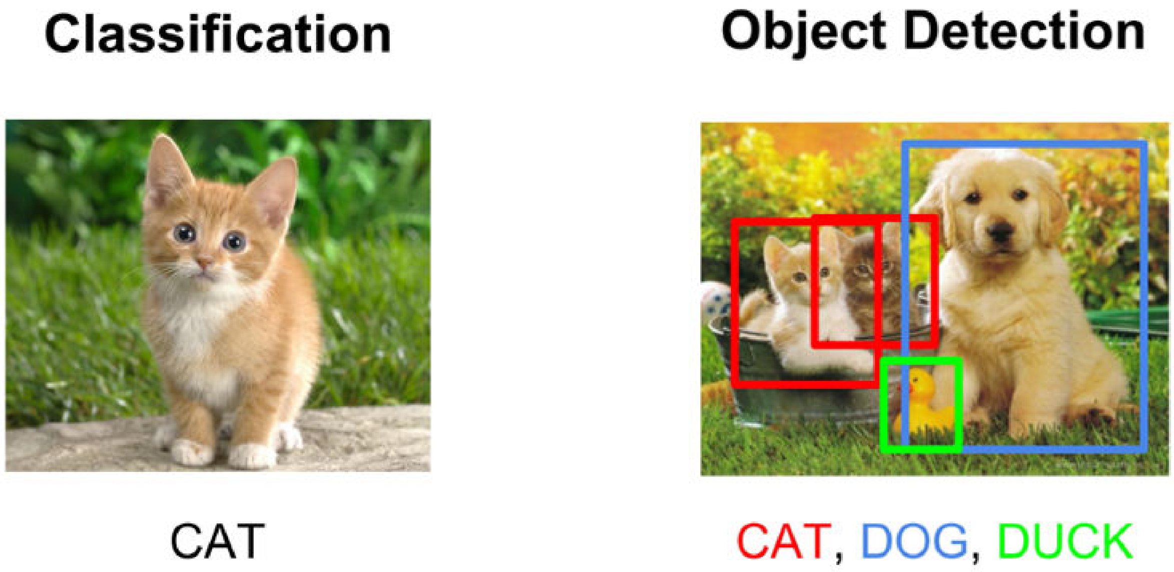
What Can Deep Learning Do?

- Classification
- What is this?



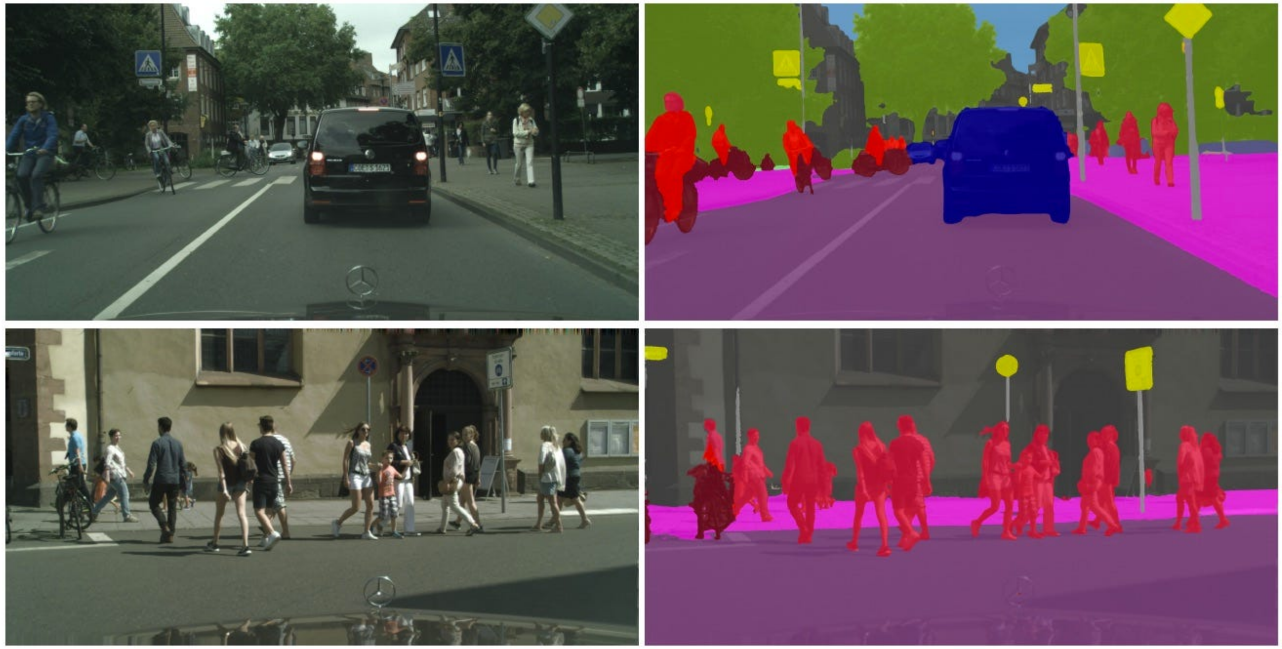
What Can Deep Learning Do?

- Objective Detection
- Where is it?



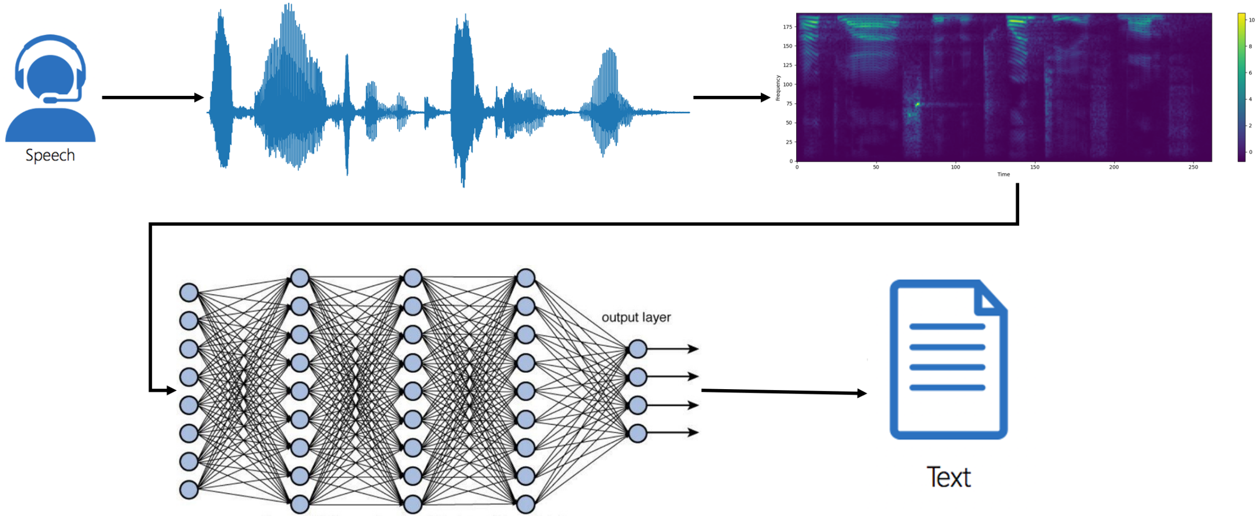
What Can Deep Learning Do?

- Semantic Segmentation
- Classify every pixel



What Can Deep Learning Do?

- Speech Recognition
- Voice to text

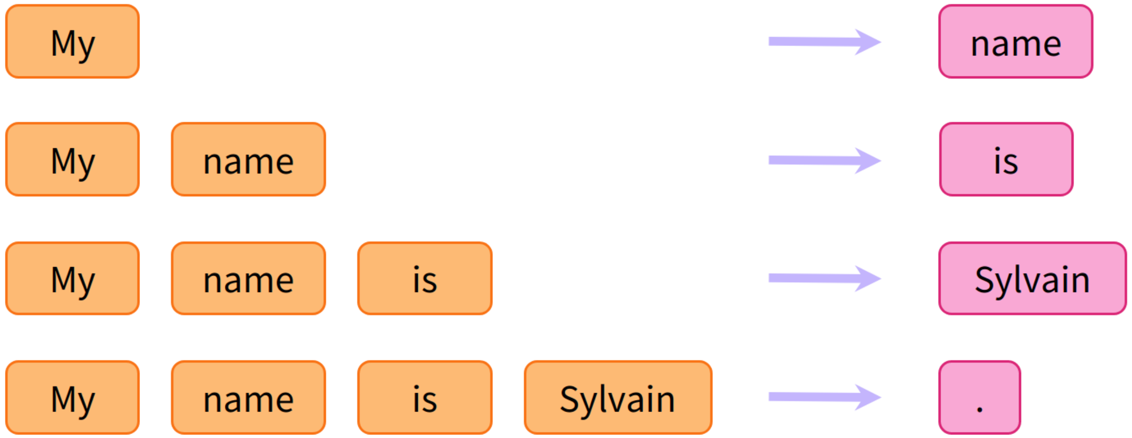


What Can Deep Learning Do?

- AIGC: AI-Generated Content
- Text-to-image/image-to-image

What Can Deep Learning Do?

- GPT: Generative Pre-trained Transformer
- Autoregressive model



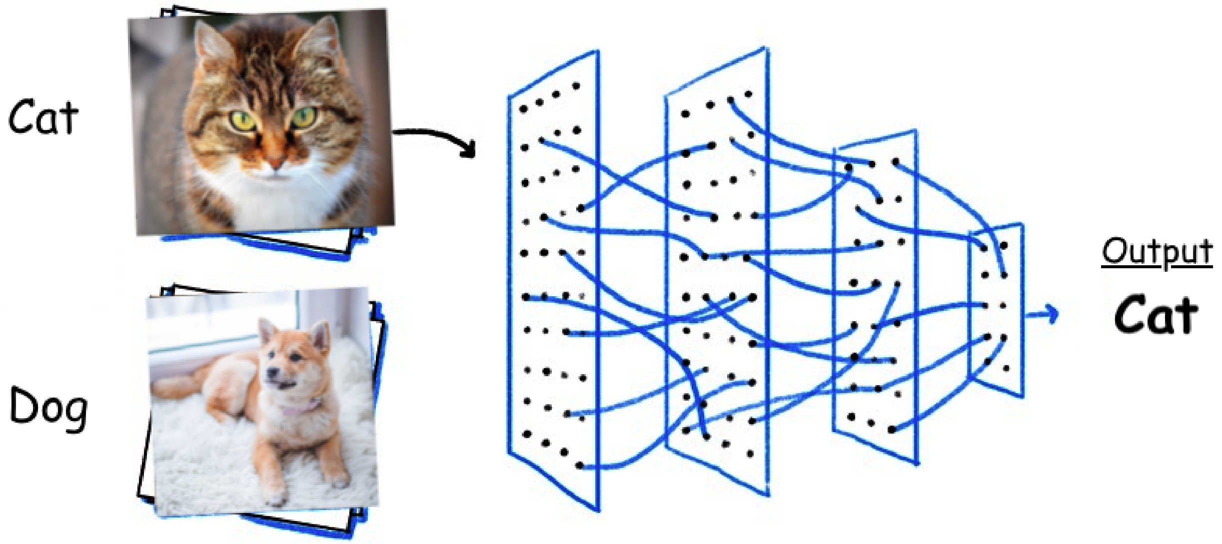
Problem Formulation

$$\overline{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{W}, \boldsymbol{x}) = \boldsymbol{f}_M(\boldsymbol{W}_M, \boldsymbol{f}_{M-1}(\boldsymbol{W}_{M-1}, \ldots\ldots \boldsymbol{f}_1(\boldsymbol{W}_{\mathbf{1}}, \boldsymbol{x})))$$

$$\boldsymbol{W} = \arg\min_{\boldsymbol{W}} \sum_{i=1}^{N} L(\overline{\boldsymbol{y}}, \boldsymbol{y})$$

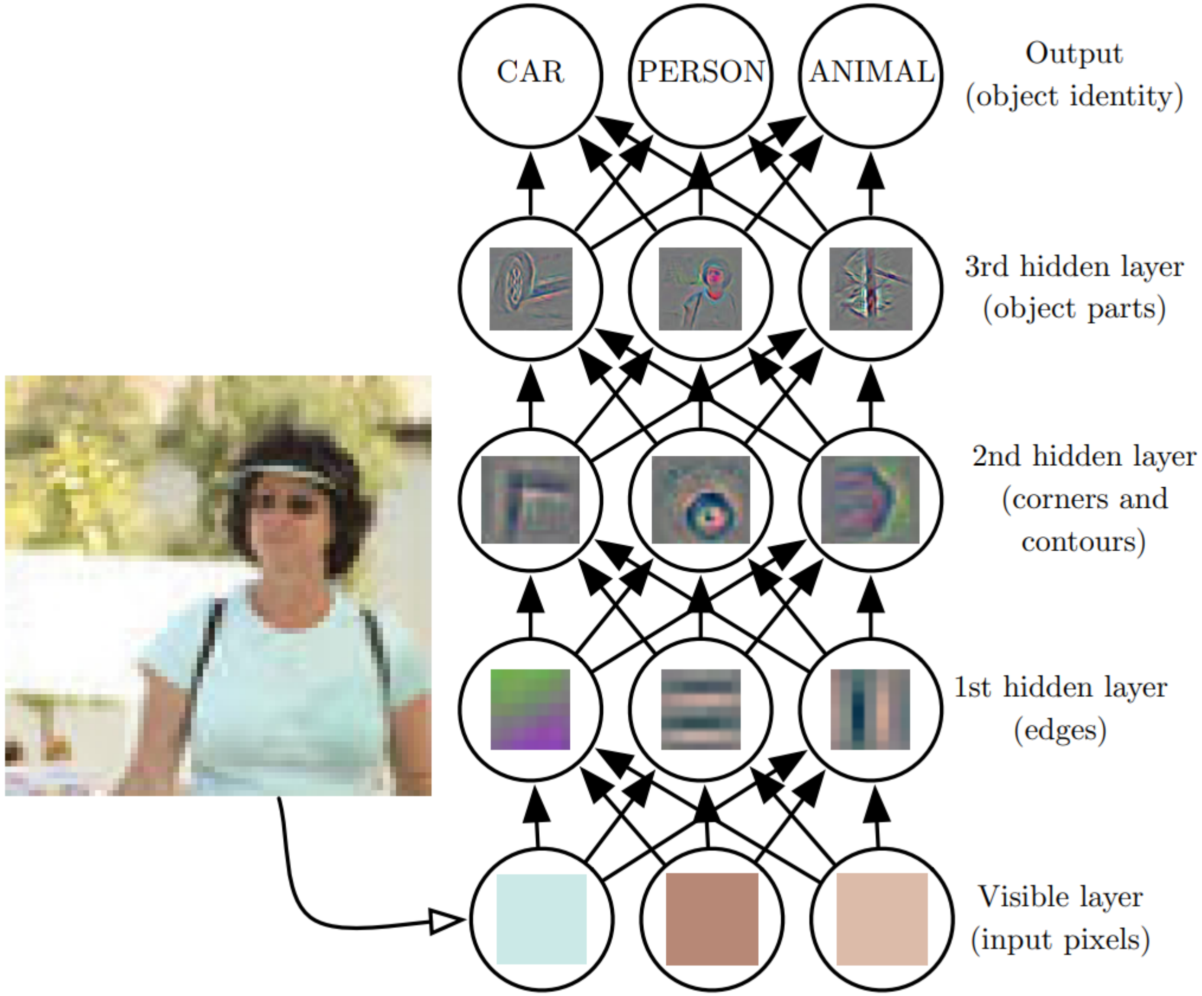
Revisiting Classification

- Input: $\boldsymbol{x}$ is the image (RGB)
- Output: cat: $\boldsymbol{y}=[1,0]$; dog: $\boldsymbol{y}=[0,1]$
- $\overline{\boldsymbol{y}}=\boldsymbol{f}(\boldsymbol{W},\boldsymbol{x})$



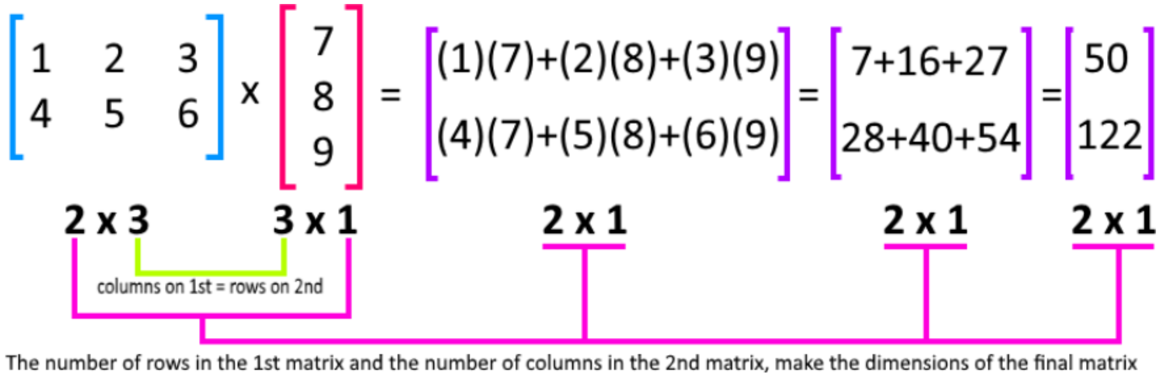
Imitating Human Perception

- Input: $\boldsymbol{x}$ is the image (RGB)
- 1st hidden layer:
  $\boldsymbol{x}_1 = \boldsymbol{f}_1(\boldsymbol{x}) = \sigma(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$
- 2nd hidden layer:
  $\boldsymbol{x}_2 = \boldsymbol{f}_2(\boldsymbol{x}) = \sigma(\boldsymbol{W}_2\boldsymbol{x}_1 + \boldsymbol{b}_2)$
- … …



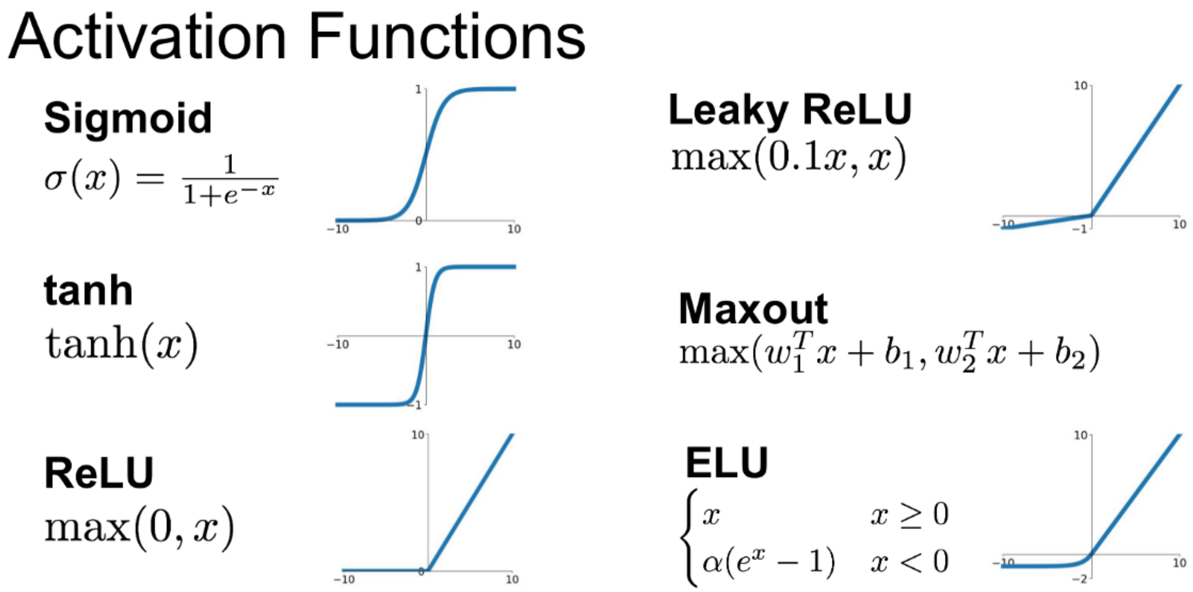
Matrix Multiplication

- $\boldsymbol{W}_1\boldsymbol{x}$



Activation Function

- $\boldsymbol{f}_1(\boldsymbol{x}) = \sigma(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$



Imitating Human Perception

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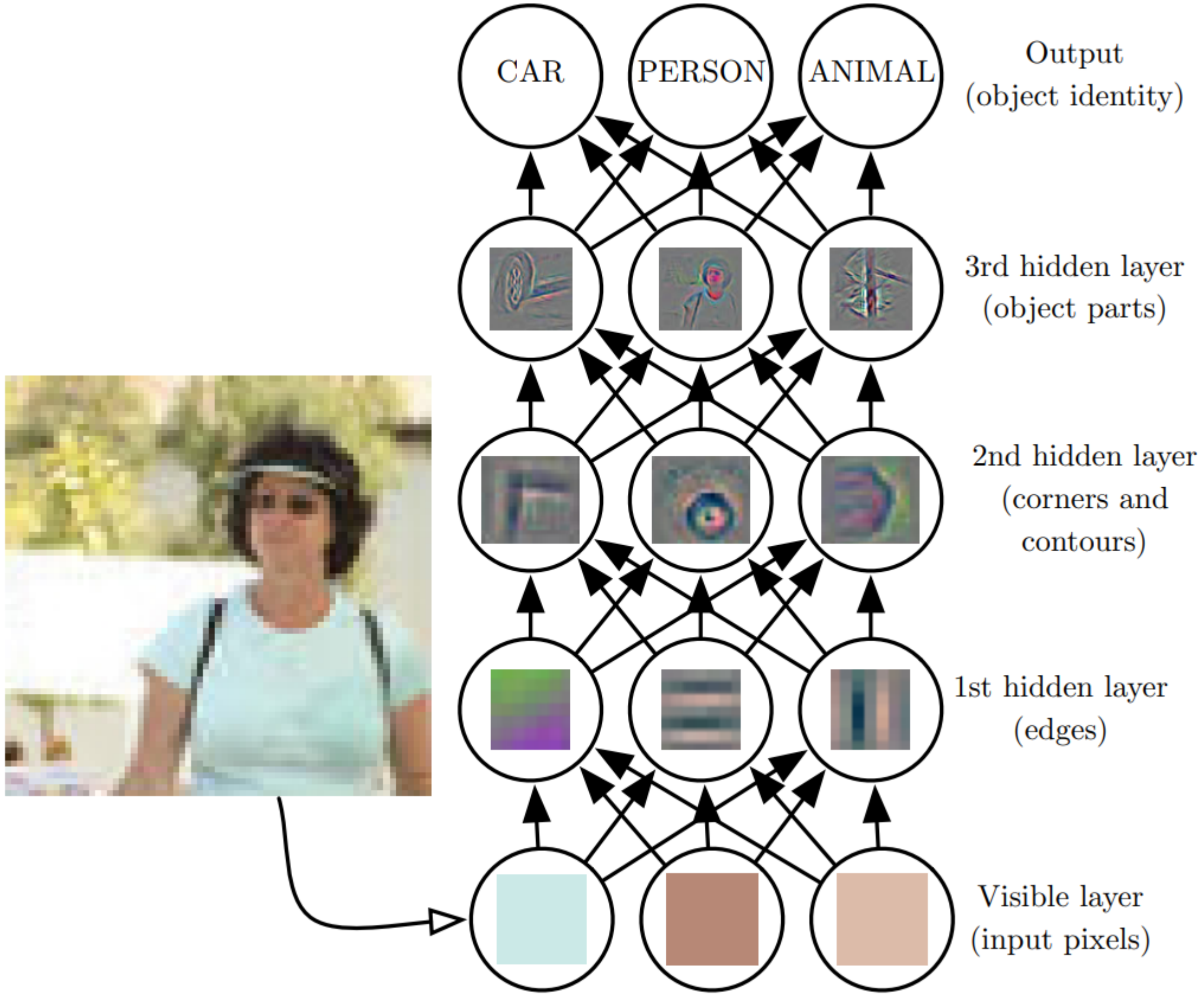
- … …



Output Function

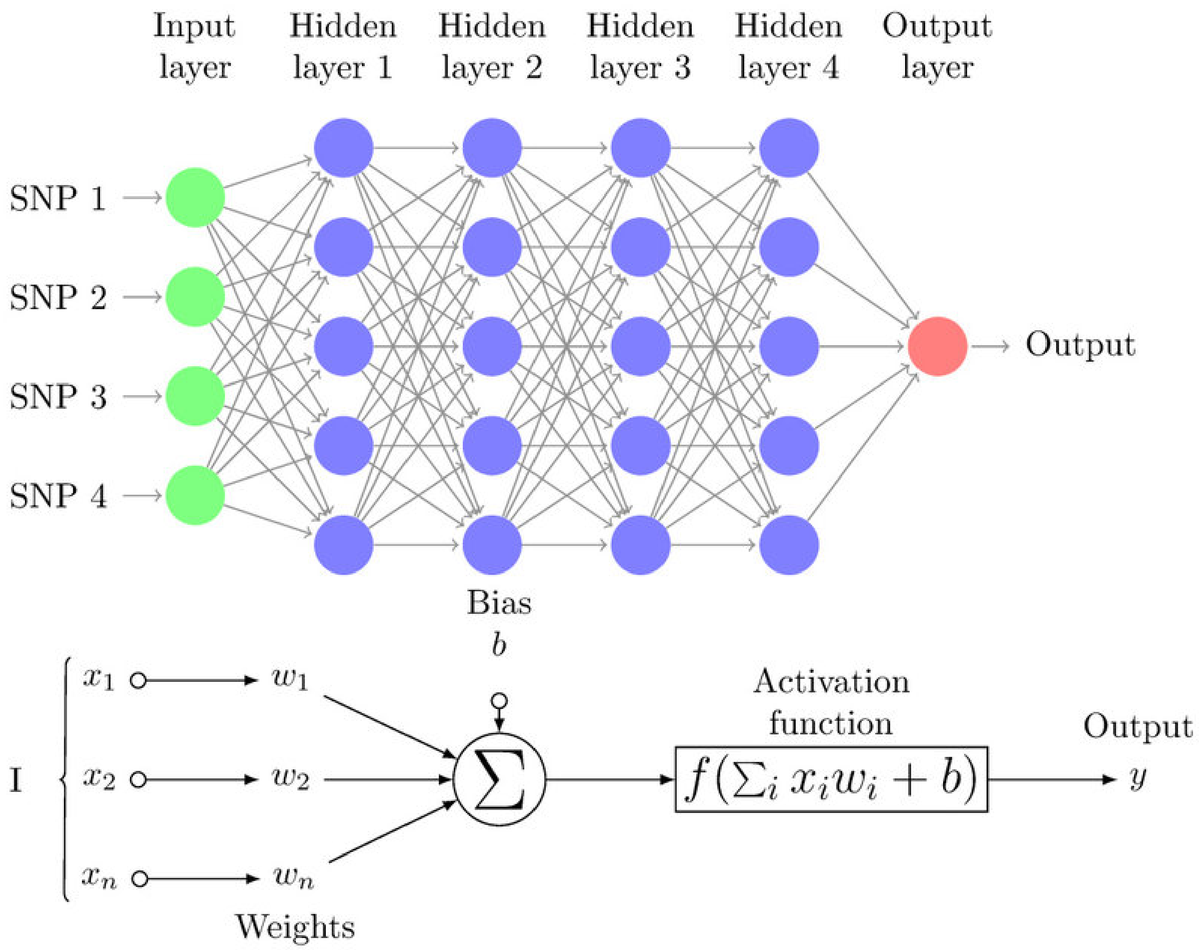
- $\boldsymbol{x}_M = \mathrm{softmax}(\boldsymbol{W}_M \boldsymbol{x}_{M-1} + \boldsymbol{b}_M)$
- $\mathrm{softmax}(\boldsymbol{x}_M)_i = \frac{e^{x_{M,i}}}{\sum_j e^{x_{M,j}}}$
- Regarded as probabilities

$$\begin{bmatrix} \frac{e^{x1}}{e^{x1}+e^{x2}+e^{x3}+e^{x4}} \\ \frac{e^{x2}}{e^{x1}+e^{x2}+e^{x3}+e^{x4}} \\ \frac{e^{x3}}{e^{x1}+e^{x2}+e^{x3}+e^{x4}} \\ \frac{e^{x4}}{e^{x1}+e^{x2}+e^{x3}+e^{x4}} \end{bmatrix} = \begin{bmatrix} e^{x1} \\ e^{x2} \\ e^{x3} \\ e^{x4} \end{bmatrix} /(e^{x1} + e^{x2} + e^{x3} + e^{x4})$$

$$\Longrightarrow e^{x}/sum(e^{x})$$

Multi-layer Perceptrons (MLP)

- $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{f}_M \circ \boldsymbol{f}_{M-1} \circ \ldots\ldots \circ \boldsymbol{f}_1(\boldsymbol{x})$
- $\boldsymbol{W}_1, \boldsymbol{b}_1$, … …, $\boldsymbol{W}_M, \boldsymbol{b}_M$ are trainable



Loss Function

- $L(\overline{\boldsymbol{y}}, \boldsymbol{y})$, indicates the quality
- Smaller is better $\downarrow$
- Cross entropy is for classification
- e.g. $\boldsymbol{p} = [1, 0]$; $\boldsymbol{q} = [0.8, 0.2]$
- $CE(\boldsymbol{p}, \boldsymbol{q}) = -log(0.8)$

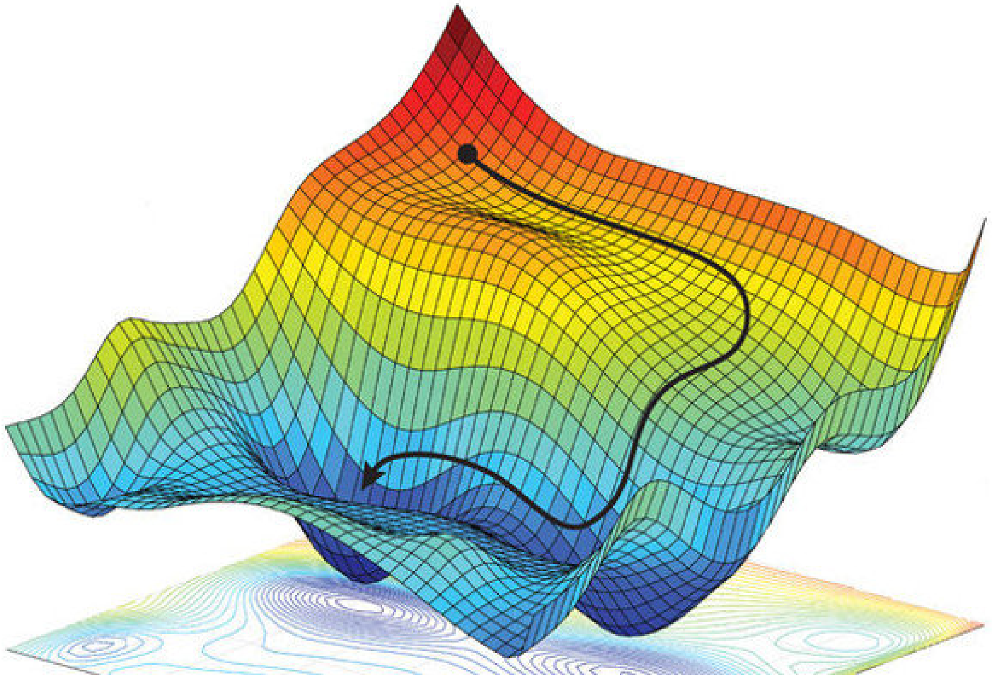
True probability distribution (one-hot)

$$H(p, q) = -\sum_{x \in \text{classes}} p(x) \log q(x)$$

Your model's predicted probability distribution

Gradient Descent

- Iterative algorithm
- $\boldsymbol{W}^{(t)} = \boldsymbol{W}^{(t-1)} - \gamma \frac{\partial L}{\partial \boldsymbol{W}^{(t)}}$
- γ is the learning rate
- Chain rule $\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$

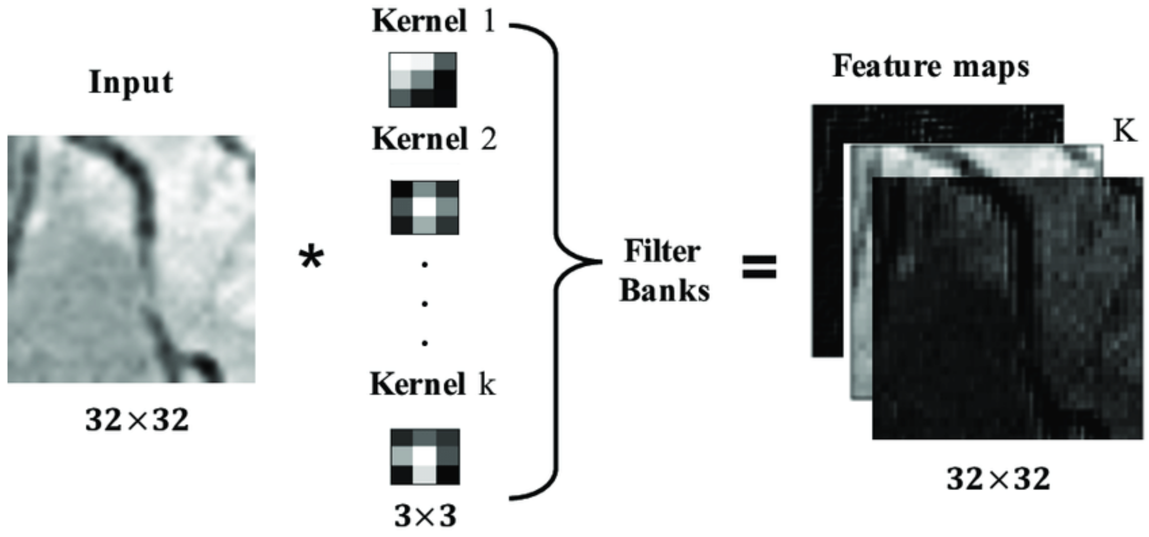


Implementation

- Convolutional Neural Networks
- Training and Testing
- PyTorch

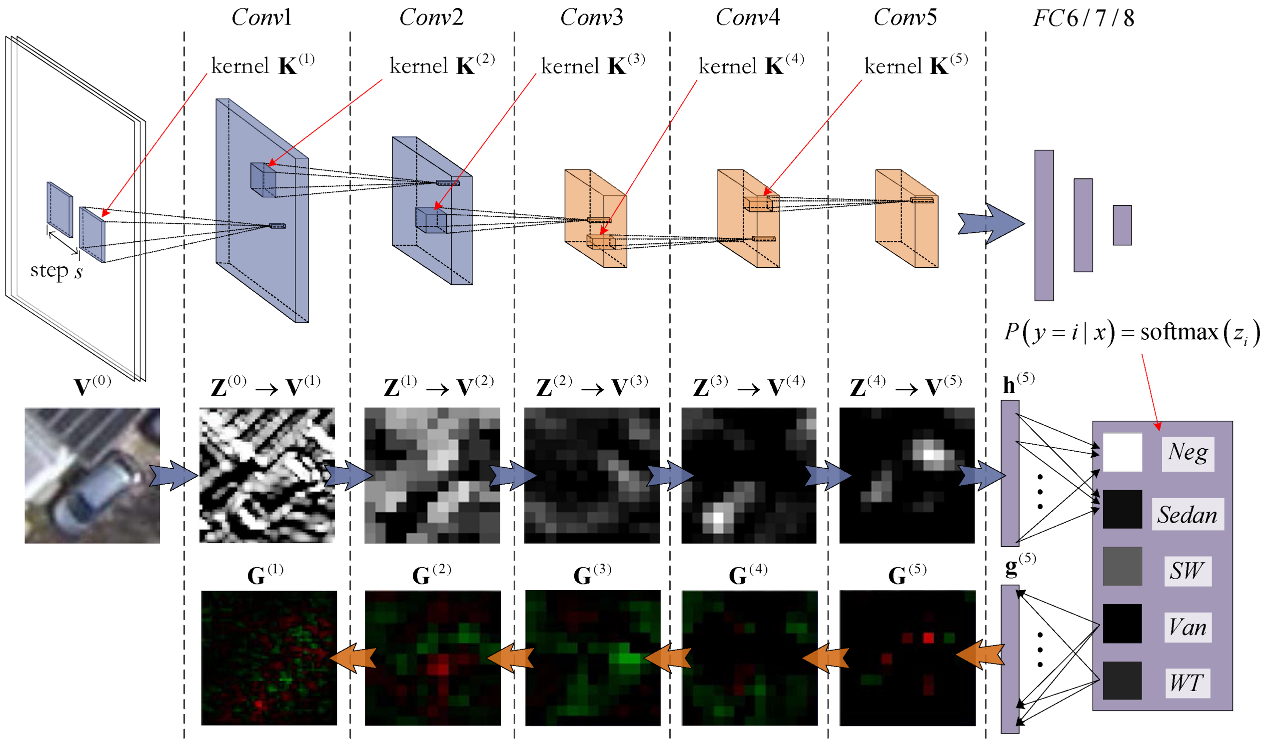
Convolution

- From signal processing
- For feature extraction



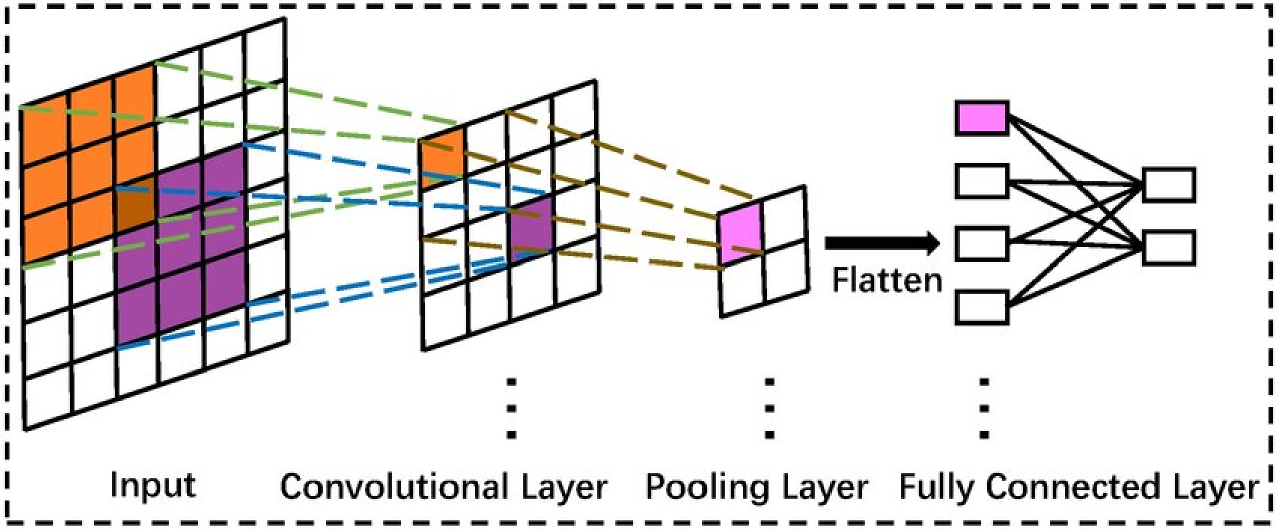
Convolutional Layers

- Convolutional layer
- Preserve 2D structure
- Local perception
- Less weights



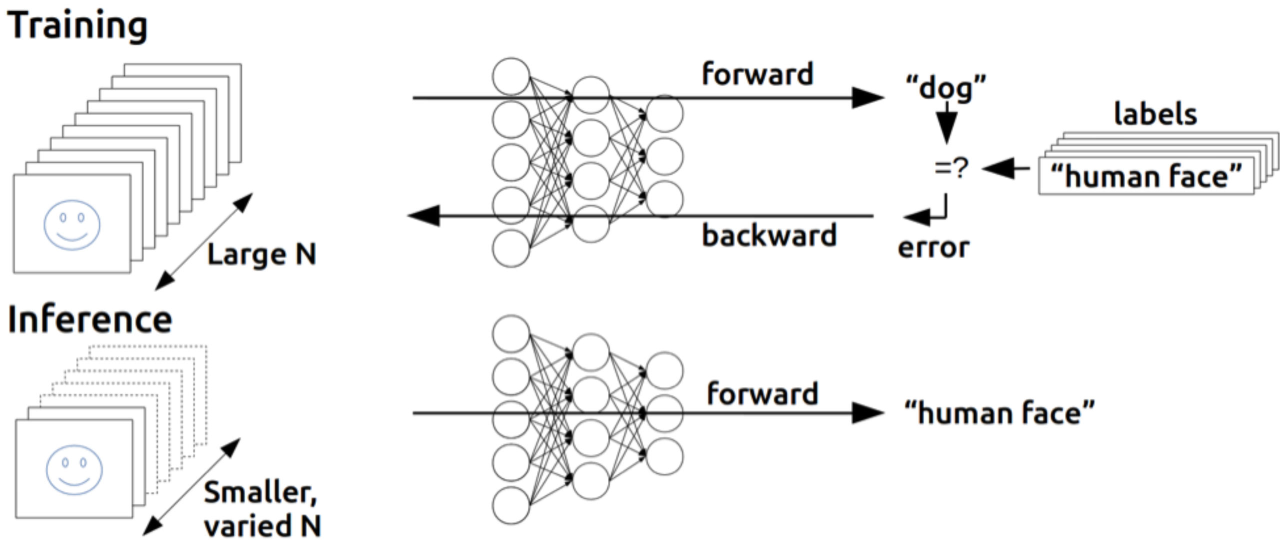
Convolutional Neural Networks

- Convolutional layer
- Max/avg. pooling layer
- Fully connected layer (MLP)



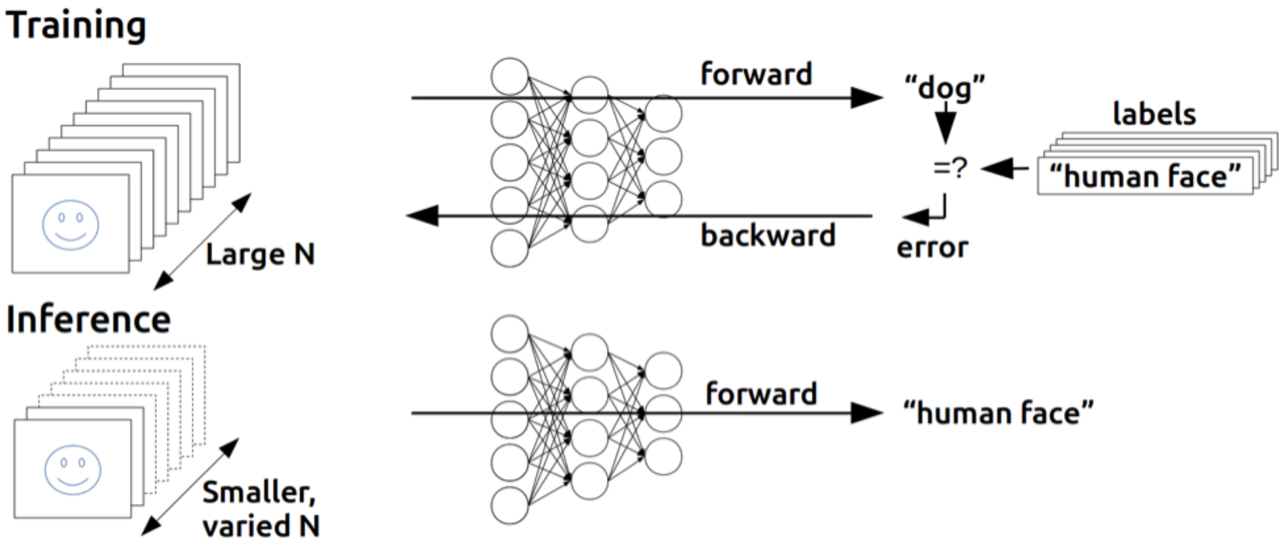
Training Neural Networks

- Sample a batch of data
- Forward: compute the loss
- Backward: update the weights
- $\boldsymbol{W}^{(t)} = \boldsymbol{W}^{(t-1)} - \gamma \frac{\partial L}{\partial \boldsymbol{W}^{(t)}}$



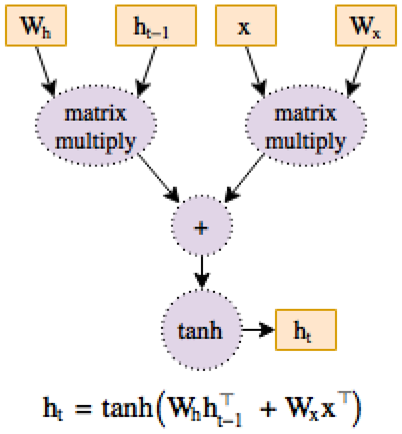
Testing Neural Networks

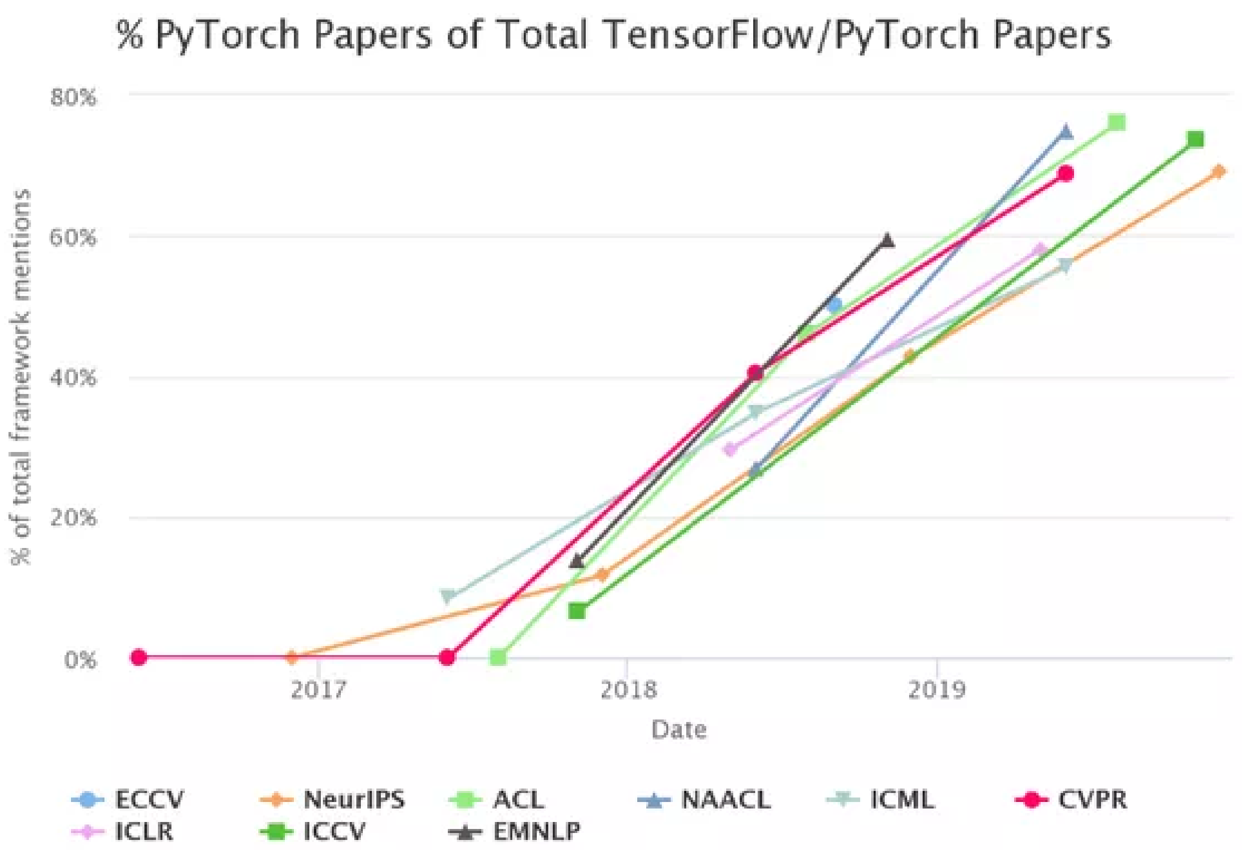
- Sample a batch of data
- Compute the loss and accuracy



PyTorch

- PyTorch is famous
- Computation graph





Import Libaries

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

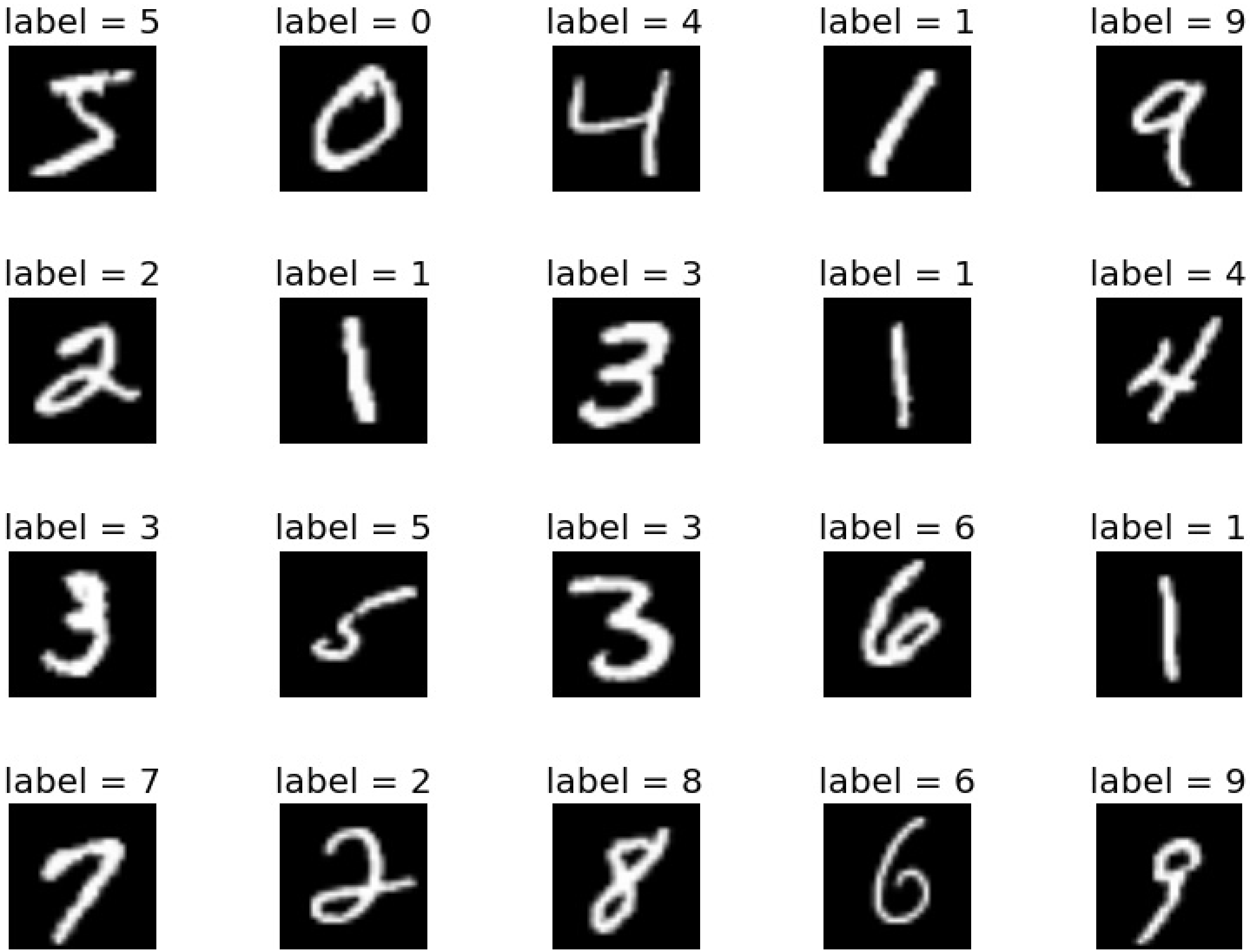
- "torch.nn" for neural network layers (Conv2D, Linear, ...)
- "torch.nn.functional" for basic functions (sigmoid, max_pool2d, ...)
- "torch.optim" for optimizers (gradient descent)
- "torchvision" for data preparation

Load Data

```
batch_size_train = 100 # Size of a batch of data for training
batch_size_test = 100 # Size of a batch of data for testing
train_loader = torch.utils.data.DataLoader(
    torchvision.datasets.MNIST('data/', train=True, download=True,
                               transform=torchvision.transforms.Compose([
                                   torchvision.transforms.ToTensor(),
                                   torchvision.transforms.Normalize((0.1307,), (0.3081,))
                               ])),
    batch_size=batch_size_train, shuffle=True)

test_loader = torch.utils.data.DataLoader(
    torchvision.datasets.MNIST('data/', train=False, download=True,
                               transform=torchvision.transforms.Compose([
                                   torchvision.transforms.ToTensor(),
                                   torchvision.transforms.Normalize((0.1307,), (0.3081,))
                               ])),
    batch_size=batch_size_test, shuffle=True)
```

MNIST Handwritten Digit Dataset



Define the Model

```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 10, kernel_size=5)
        self.conv2 = nn.Conv2d(10, 20, kernel_size=5)
        self.fc1 = nn.Linear(320, 50)
        self.fc2 = nn.Linear(50, 10)

    def forward(self, x):
        x = F.relu(F.max_pool2d(self.conv1(x), 2))
        x = F.relu(F.max_pool2d(self.conv2(x), 2))
        x = x.view(-1, 320)
        x = F.relu(self.fc1(x))
        x = F.dropout(x, training=self.training)
        x = self.fc2(x)
        return x
```

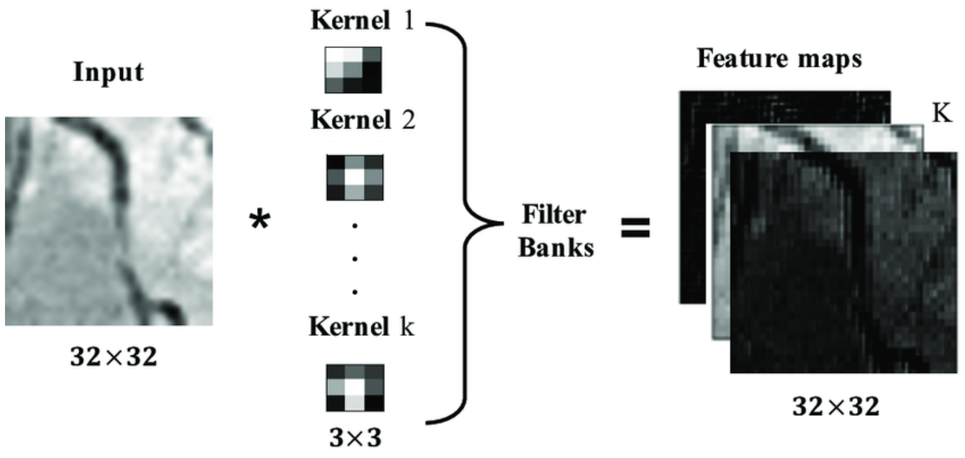
Define the Model

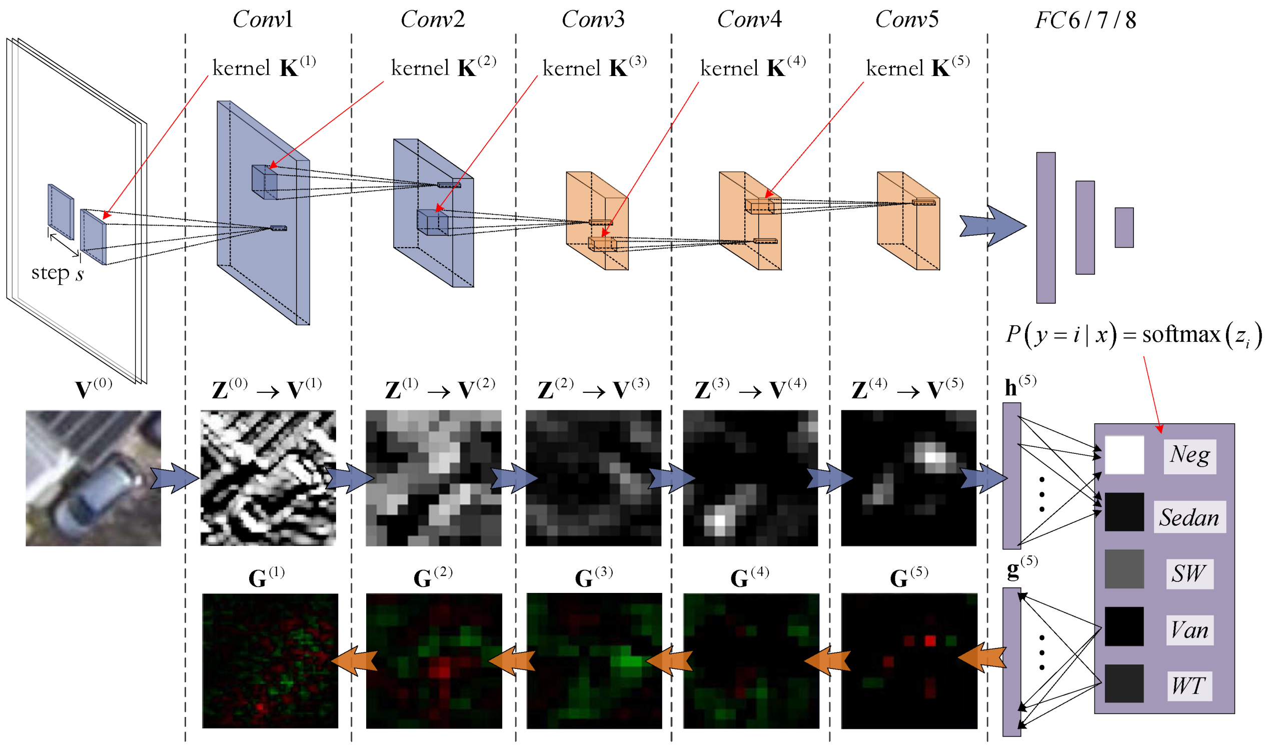
- Define the layers
- "self.conv1": convolution layer, input channel 1, output channels 10, kernel size 5
- "self.conv2": convolution layer, input channel 10, output channels 20, kernel size 5

```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 10, kernel_size=5)
        self.conv2 = nn.Conv2d(10, 20, kernel_size=5)
        self.fc1 = nn.Linear(320, 50)
        self.fc2 = nn.Linear(50, 10)
```

Convolution Layer

- Channels and kernel size





Define the Model

- "self.fc1": fully connected layer, input size 320, output size 50
- "self.fc2": fully connected layer, input size 50, output size 10
- How to get the input size of self.fc1 ?

```
class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 10, kernel_size=5)
        self.conv2 = nn.Conv2d(10, 20, kernel_size=5)
        self.fc1 = nn.Linear(320, 50)
        self.fc2 = nn.Linear(50, 10)
```

Define the Forward Pass

- conv1 $\rightarrow$ pooling $\rightarrow$ ReLU
- conv2 $\rightarrow$ pooling $\rightarrow$ ReLU
- fc1 $\rightarrow$ ReLU $\rightarrow$ fc2

```python
class Net(nn.Module):
    def forward(self, x):
        x = F.relu(F.max_pool2d(self.conv1(x), 2))
        x = F.relu(F.max_pool2d(self.conv2(x), 2))
        x = x.view(-1, 320) # flatten
        x = F.relu(self.fc1(x))
        x = self.fc2(x)
        return x
```

Define the Forward Pass

- conv1 $\rightarrow$ pooling $\rightarrow$ ReLU $\rightarrow$ conv2 $\rightarrow$ pooling $\rightarrow$ ReLU $\rightarrow$ fc1 $\rightarrow$ ReLU $\rightarrow$ fc2

```python
class Net(nn.Module):
    def forward(self, x):
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        x = x.view(-1, 320) # flatten
        x = F.relu(self.fc1(x))
        x = self.fc2(x)
        return x
```

Instantiate the Model

- "network" is the model
- "optimizer" is for gradient descent
- Gradients are derived automatically

```
learning_rate = 0.01
# Instantiate the model
network = Net()
# Instantiate the optimizer
optimizer = optim.SGD(network.parameters(), lr=learning_rate)
```

Training and Testing

- Epoch: a pass of training on **the dataset**
- Step: an iteration of gradient descent on **a batch of data**

```
for epoch in range(n_epochs):
    # Training
    for step, (data, target) in enumerate(train_loader):
        # A training step
    # Testing
    for step, (data, target) in enumerate(test_loader):
        # A testing step
```

A Training Step

- "output" is the inferred results
- "loss" is the loss value
- "loss.backward()" computes the gradients
- "optimizer.step()" do gradient descent

```
# Inference
output = network(data)
# Compute the loss
loss = F.cross_entropy(output, target)
# Gradient descent
optimizer.zero_grad()
loss.backward()
optimizer.step()
```

A Testing Step

- "F.cross_entropy" computes the loss
- "pred" is the prediction (the class with the maximum probability)
- "(pred == target).sum()" computes the accuracy

```
# Inference
output = network(data)
# Compute the loss
test_loss += F.cross_entropy(output, target).item()
# Get the prediction
pred = output.max(dim=1)[1]
# Count correct predictions
correct += (pred == target).sum()
```

Experiments

- See classifiction.ipynb
- https://github.com/shelljane/dl_tutorial

Advanced Topics -- Deep Learning in Practice

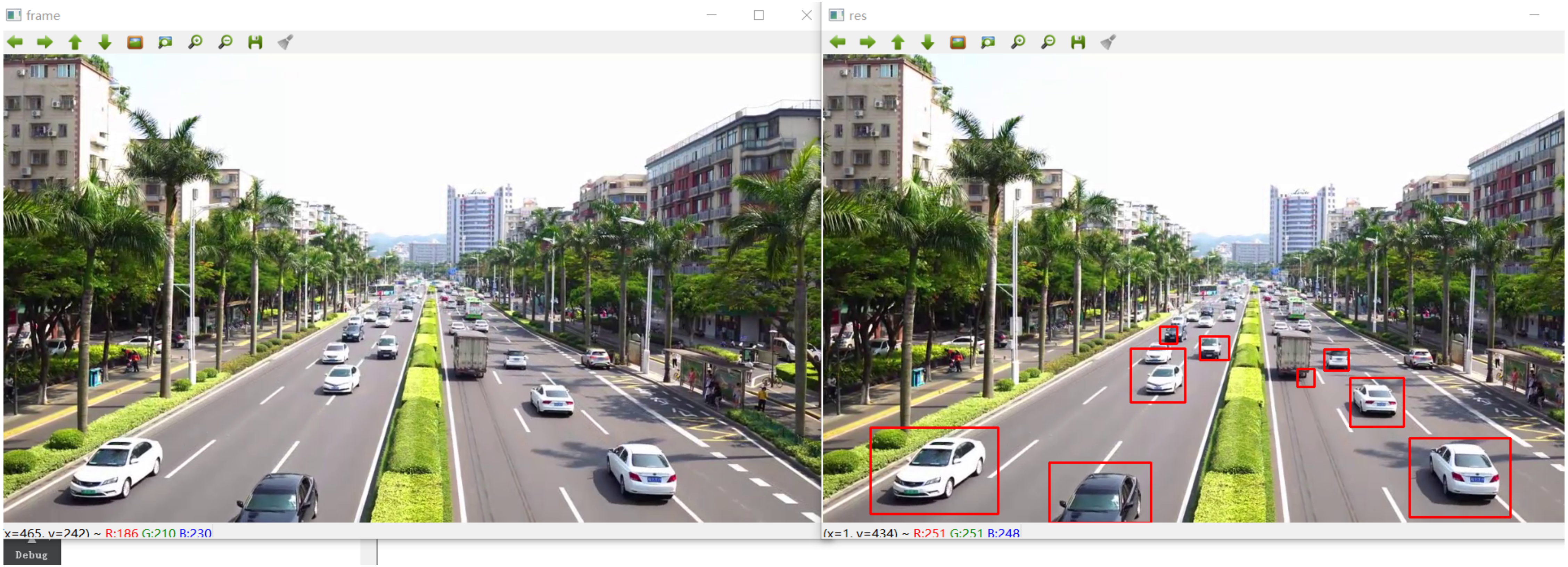
- Network as a black box
- Layer as a black box
- Useful tricks

Deep Learning in Practice

- Network as a black box
- (a) Formulate the task
  -> classification, detection, segmentation, image-to-image, ...
- (b) Find a state-of-the-art model
  -> Carefully choose the input size (32x32, 256x256, 1024x1024, ...)
- (c) Change the dataset to fit your task
  -> Pay attention to the data format

Deep Learning in Practice

- Example: Car Detection



Deep Learning in Practice

- Formulate the task:
  -> *Objective detection*
- Find a state-of-the-art model:
  -> *YOLO-X*

Deep Learning in Practice

- Find it on Github
  -> https://github.com/Megvii-BaseDetection/YOLOX

YOLOX

Exceeding YOLO series in 2021

Deep Learning in Practice

- Change the dataset to fit your task
  -> YOLOX/docs/train_custom_data.md

1. Create your own dataset

Step 1 Prepare your own dataset with images and labels first. For labeling images, you can use tools like Labelme or CVAT.

Step 2 Then, you should write the corresponding Dataset Class which can load images and labels through `__getitem__` method. We currently support COCO format and VOC format.

Step 3 Prepare the evaluator. We currently have COCO evaluator and VOC evaluator. If you have your own format data or evaluation metric, you can write your own evaluator.

Step 4 Put your dataset under `$YOLOX_DIR/datasets`, for VOC:

```
ln -s /path/to/your/VOCdevkit ./datasets/VOCdevkit
```

Deep Learning in Practice

- Go training

Except special cases, we always recommend to use our COCO pretrained weights for initializing the model.

Once you get the Exp file and the COCO pretrained weights we provided, you can train your own model by the following below command:

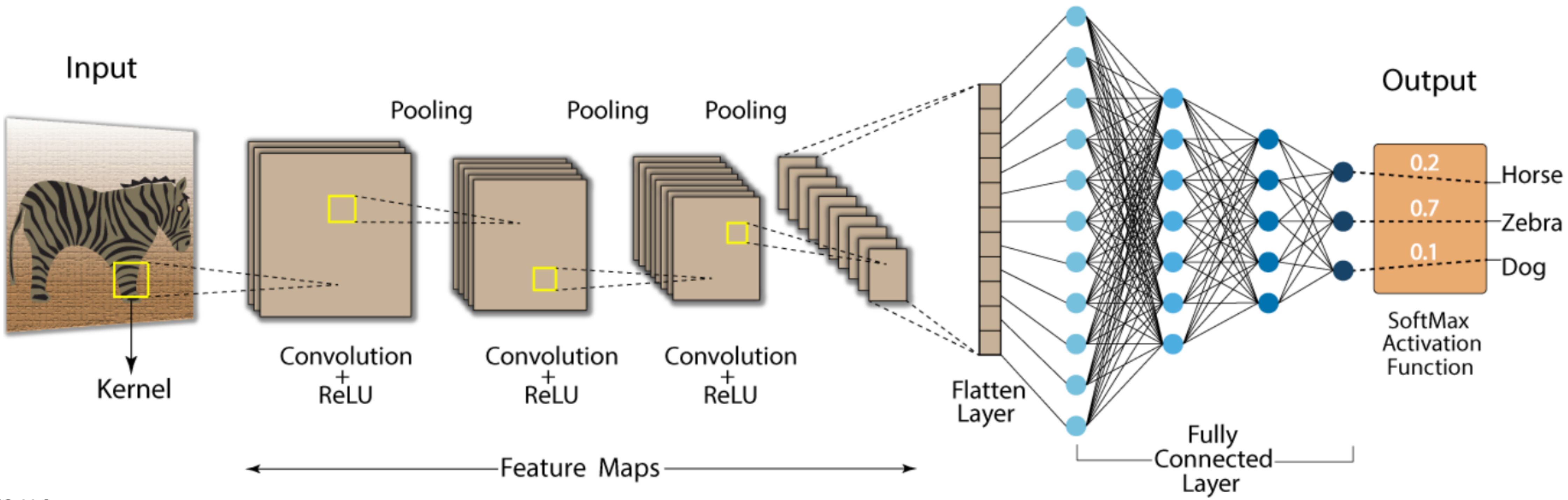
```
python tools/train.py -f /path/to/your/Exp/file -d 8 -b 64 --fp16 -o -c /path/to/the/pretrained/weights [--cache]
```

Deep Learning in Practice

- Layer as a black box
- (1) Find a backbone network
- (2) Design add-on layers or modify it

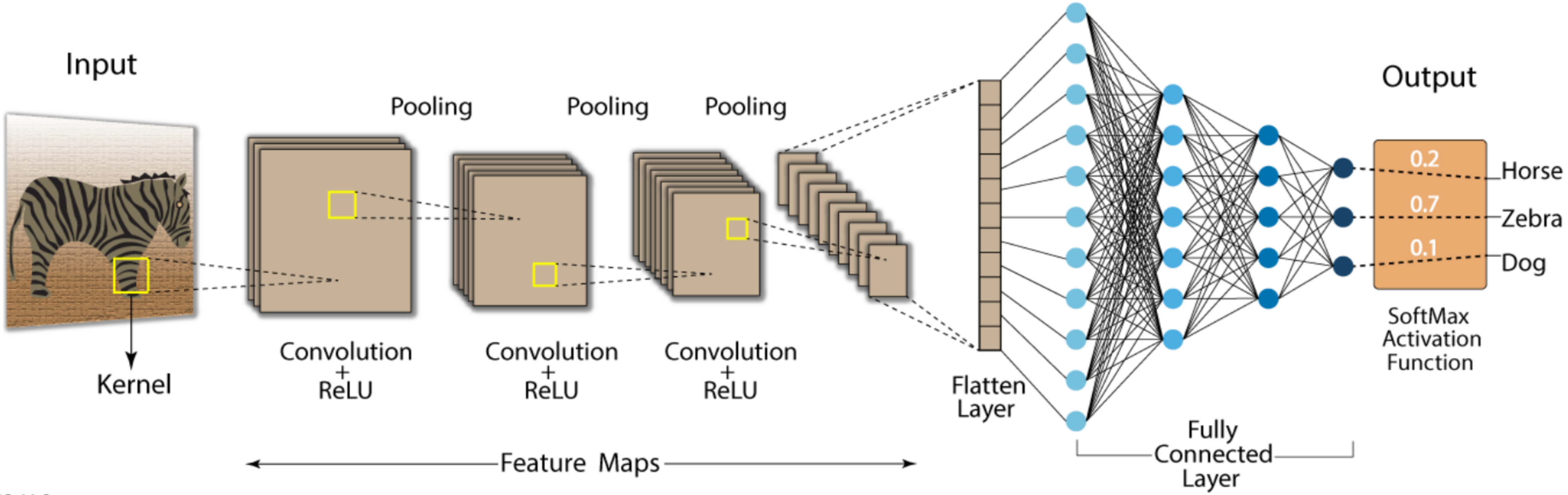
Deep Learning in Practice

- Care about the input/output size!
- Batched inputs:
- (a) One image: CxHxW array (C=3 for RGB)
- (b) A batch of N images: NxCxHxW array



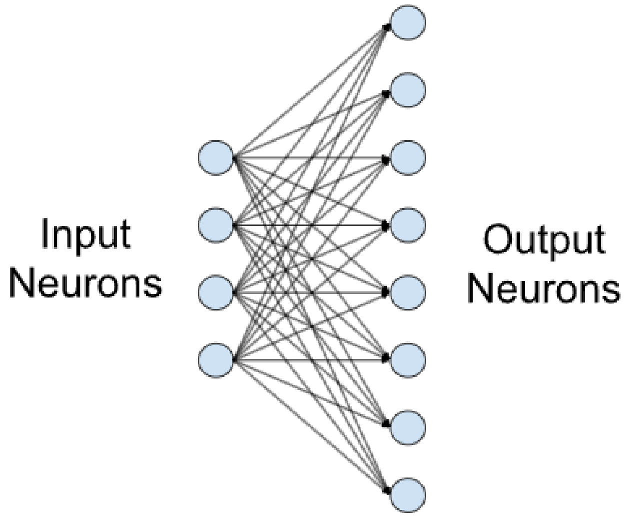
Deep Learning in Practice

- Care about the input/output size!
- Convolutional layer (Conv.):
- (a) Input size: $[N, C_{i-1}, H_{i-1}, W_{i-1}]$
- (b) Output size: $[N, C_i, H_i, W_i]$



Deep Learning in Practice

- Care about the size!
- Fully connected layer (FC)
- (a) Input size: $[N, M_{i-1}]$
- (b) Output size: $[N, M_i]$
- Flattening is needed between Conv. and FC layers

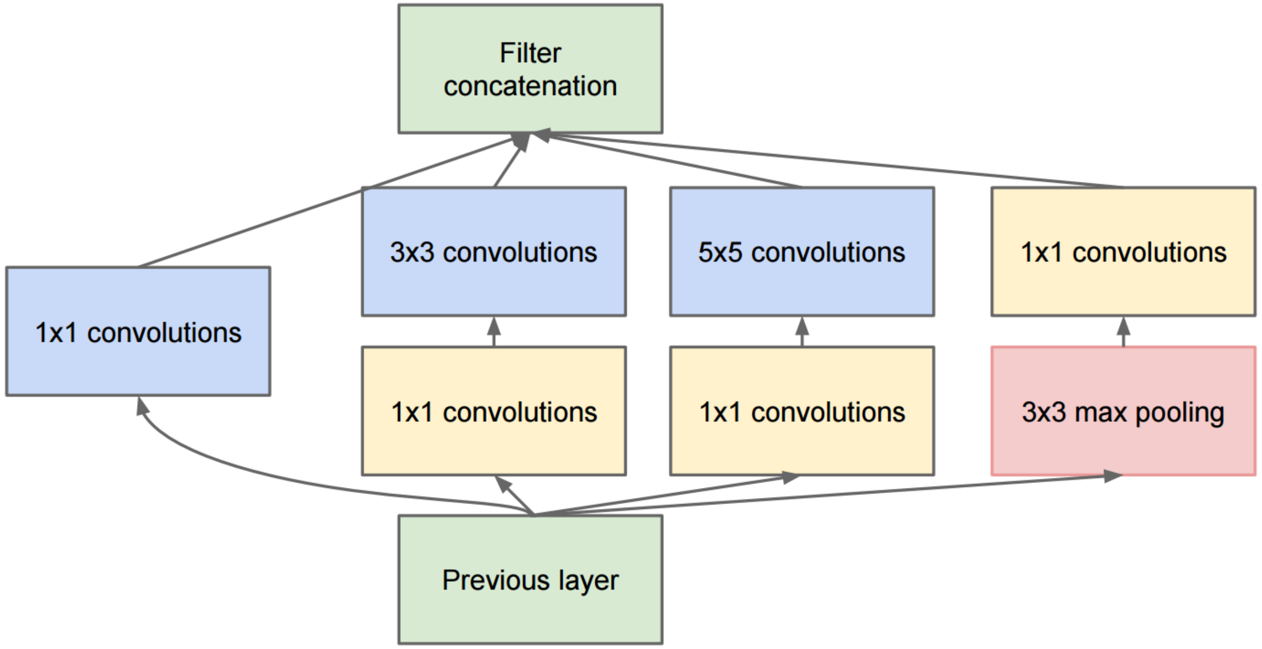


Deep Learning in Practice

- Then use them as LEGO blocks!

Deep Learning in Practice

- Inception Block



Deep Learning in Practice

- Inception V3 Network

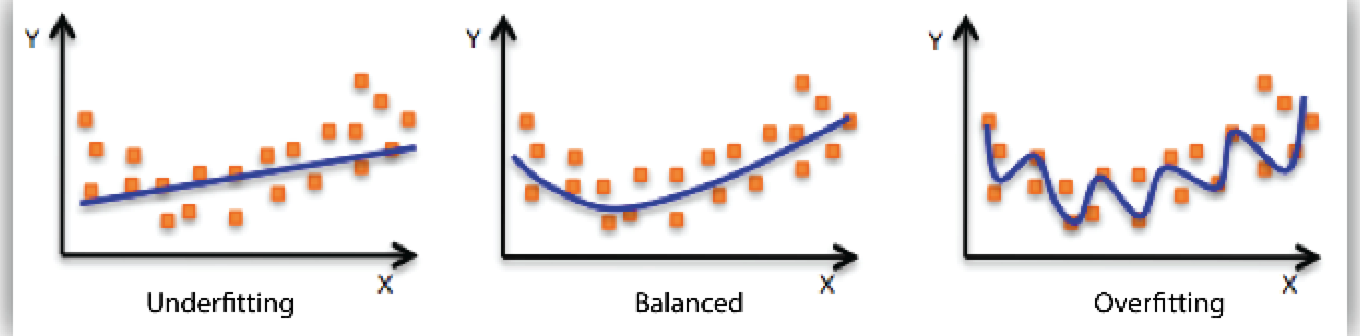
Type	Kernel size/stride	Input size
Convolution	$3 \times 3/2$	$299 \times 299 \times 3$
Convolution	$3 \times 3/1$	$149 \times 149 \times 32$
Convolution	$3 \times 3/1$	$147 \times 147 \times 32$
Pooling	$3 \times 3/2$	$147 \times 147 \times 64$
Convolution	$3 \times 3/1$	$73 \times 73 \times 64$
Convolution	$3 \times 3/2$	$71 \times 71 \times 80$
Convolution	$3 \times 3/1$	$35 \times 35 \times 192$
Inception module	Three modules	$35 \times 35 \times 288$
Inception module	Five modules	$17 \times 17 \times 768$
Inception module	Two modules	$8 \times 8 \times 1{,}280$
Pooling	8×8	$8 \times 8 \times 2{,}048$
Linear	Logits	$1 \times 1 \times 2{,}048$
Softmax	Output	$1 \times 1 \times 1{,}000$

Deep Learning in Practice

- Useful tricks
- (1) Number of parameters
- (2) Normalization
- (3) Other tricks

Deep Learning in Practice

- Underfitting and overfitting
- (a) Underfitting: low training accuracy
- (b) Overfitting: low testing accuracy but high training accuracy



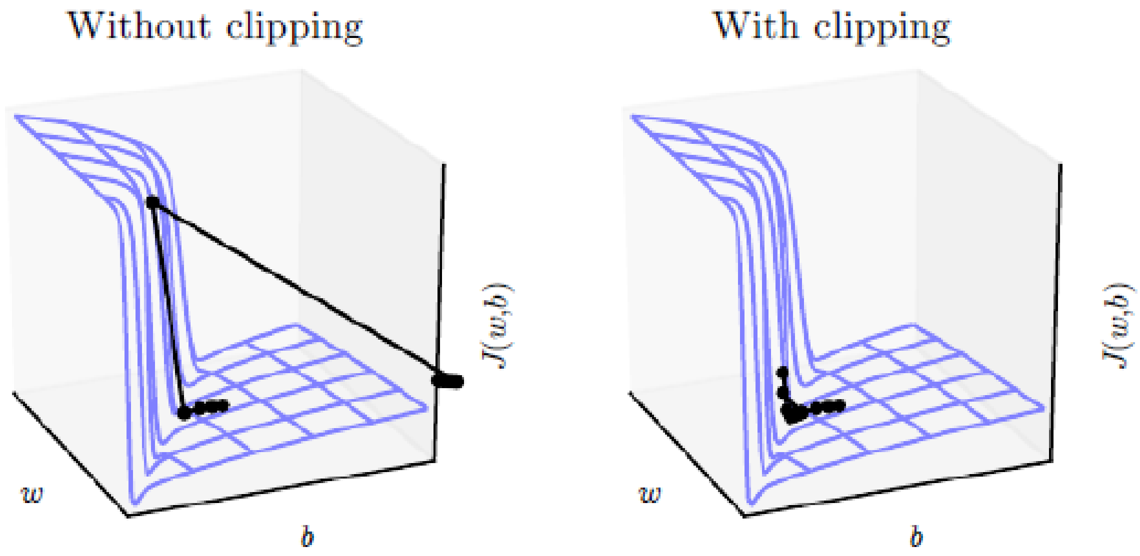
Deep Learning in Practice

- Convolutional layer
- (a) Kernel size: 3x3, 5x5, 11x11, … …
- (b) Channel width: 16, 32, 64, … …
- Principles
- (a) Larger kernel and channel sizes => more parameters to train
- (b) More parameters => higher capacity, overfitting, harder to train

Deep Learning in Practice

- Abnormal gradients
- (a) Gradient vanishing
- (b) Gradient explosion

1. ***Vanishing gradient*** $\left\| \frac{\partial h_i}{\partial h_{i-1}} \right\|_2 < 1$
2. ***Exploding gradient*** $\left\| \frac{\partial h_i}{\partial h_{i-1}} \right\|_2 > 1$



Deep Learning in Practice

- Batch normalization
  -> Stablize the training by normalizing the outputs of each layer

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

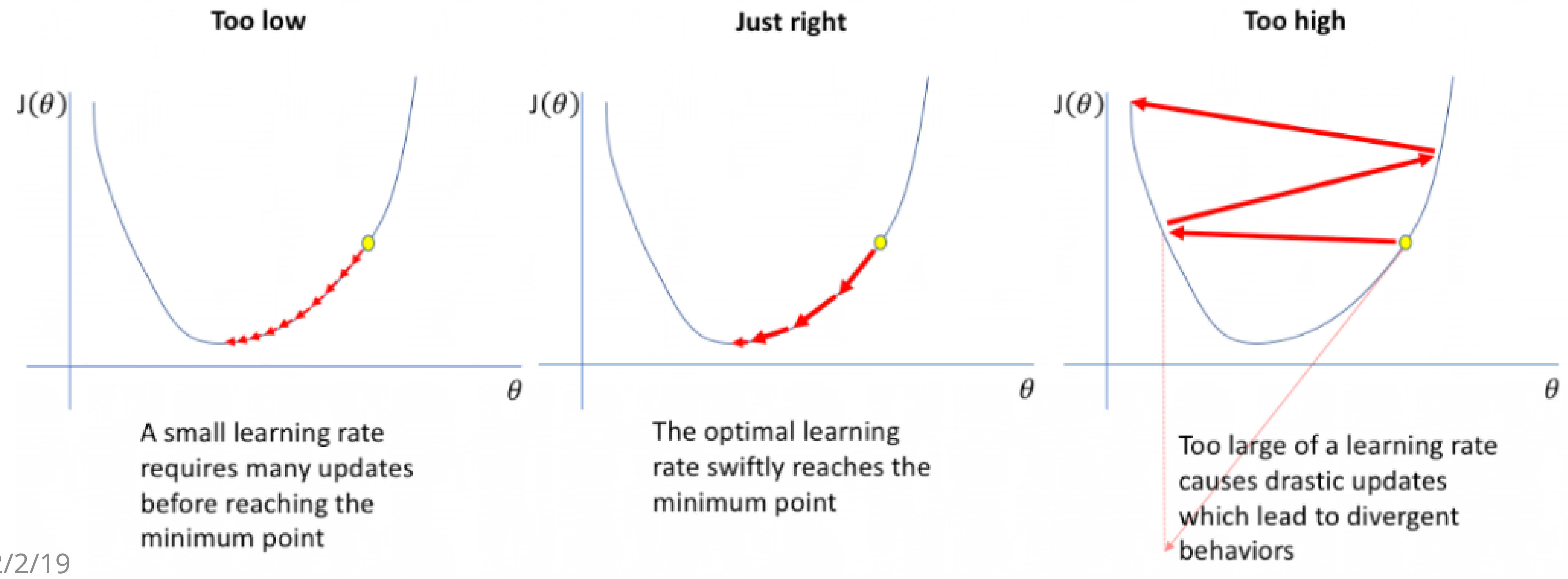
$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m} (x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

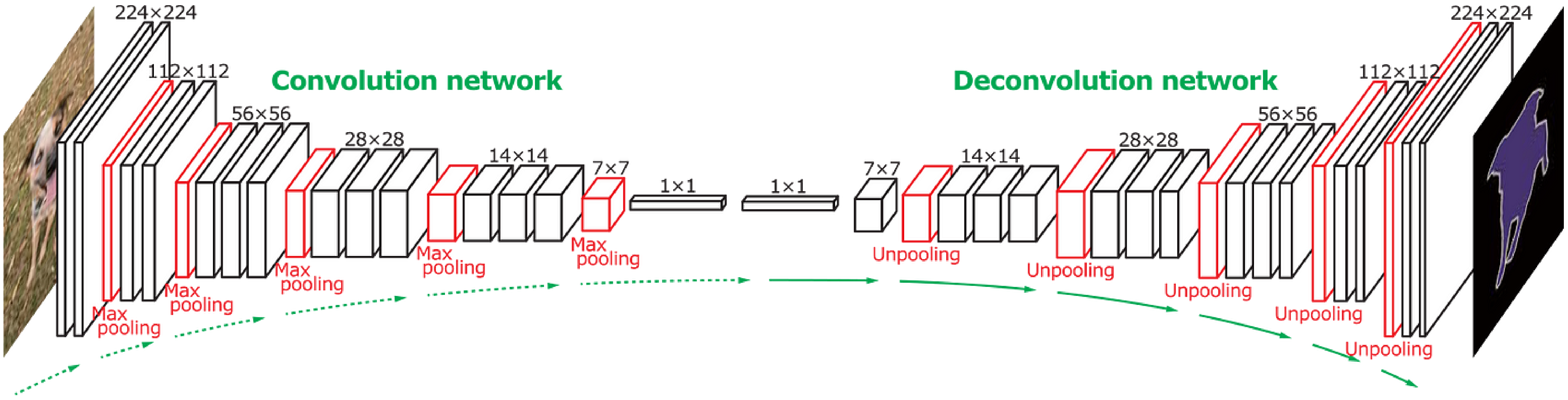
Deep Learning in Practice

- Other tricks, e.g.
- (a) Adjust the learning rate
- (b) Weight regularization
- (c) Dropout



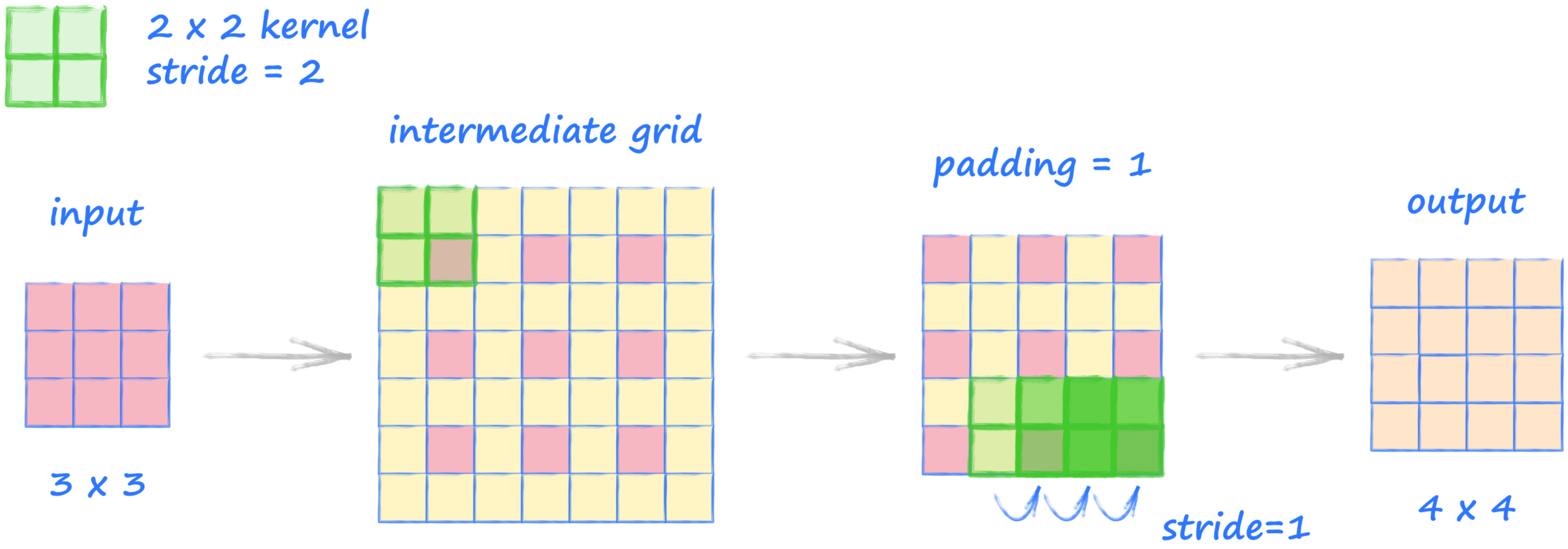
Advanced Topics -- Beyond Classification

- Semantic segmentation
- Image-to-image translation
- Deep learning for OPC



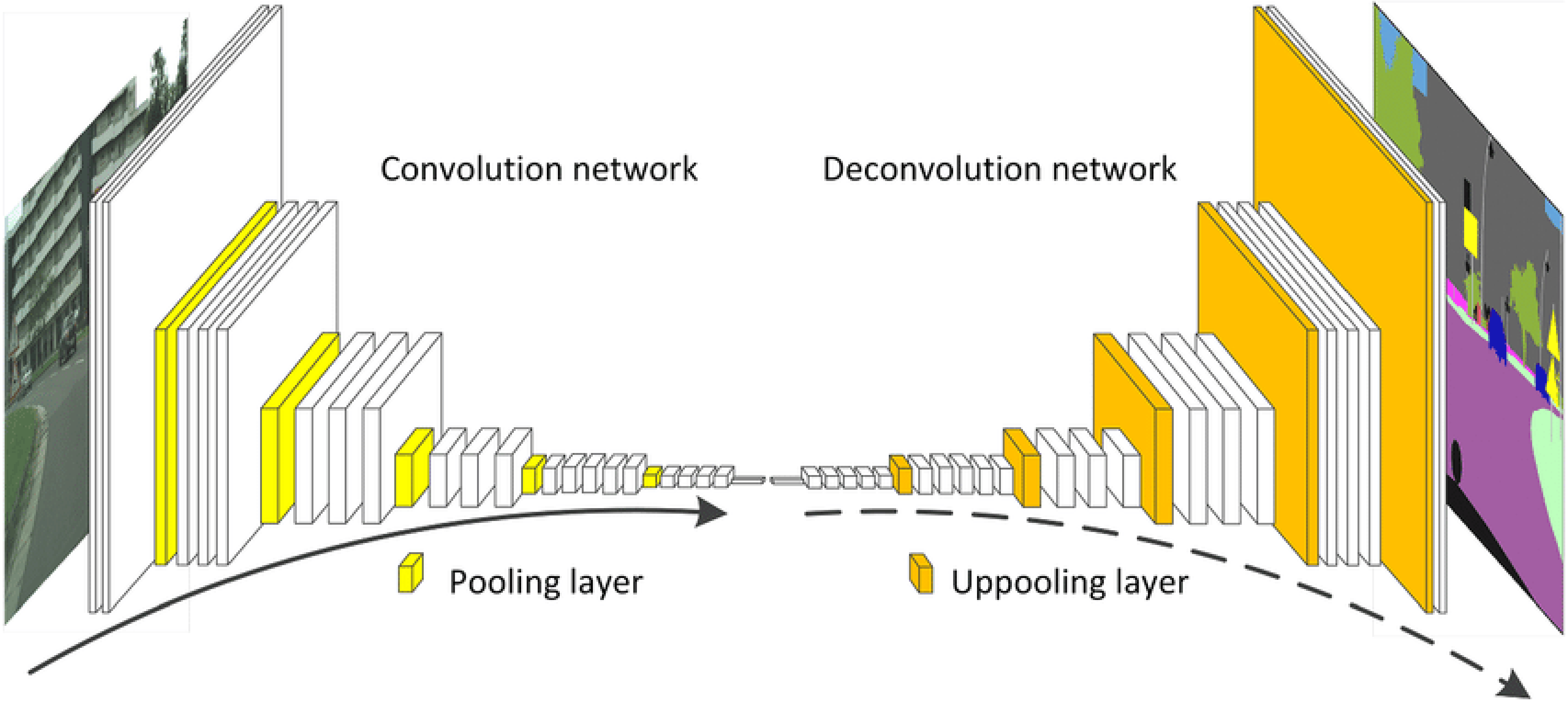
Semantic Segmentation

- Deconvolutional Layer



Semantic Segmentation

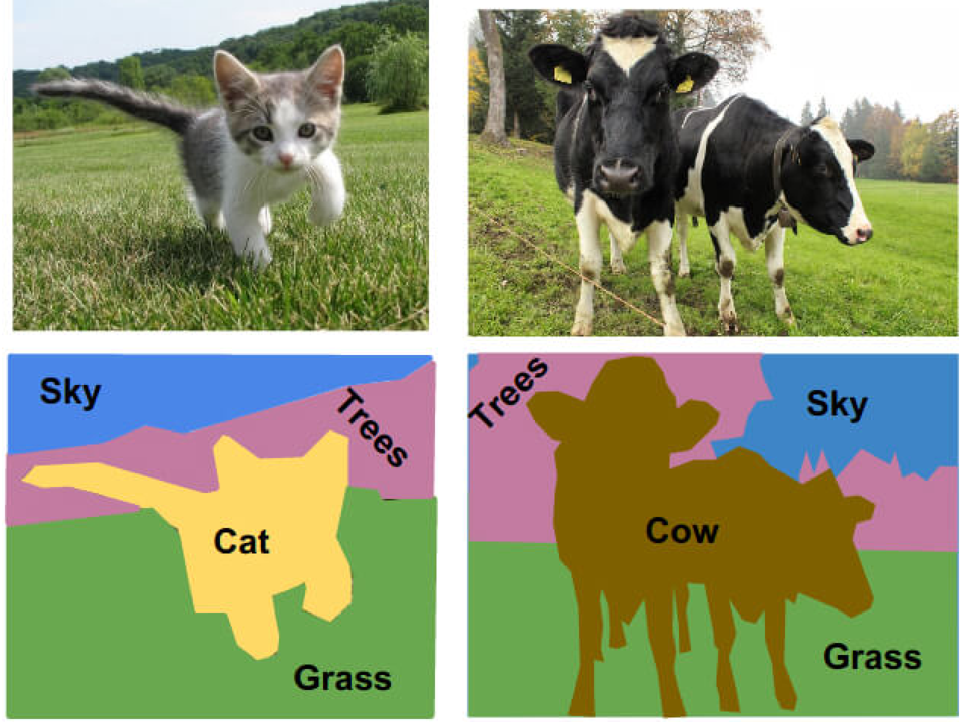
- Fully Convolutional Network (FCN)

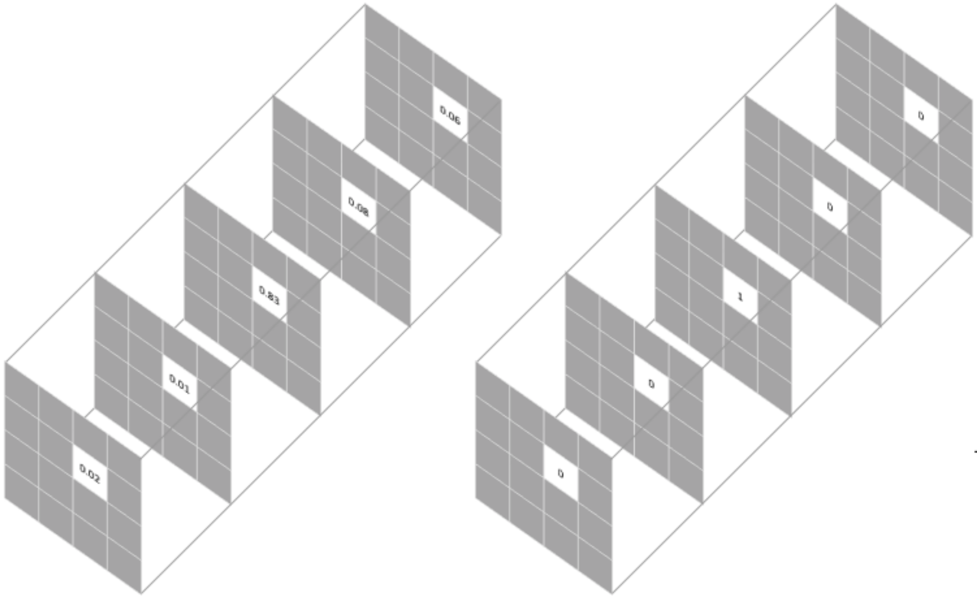


Semantic Segmentation

- The last layer

This image is CC0 public domain





Prediction for a selected pixel

Target for the corresponding pixel

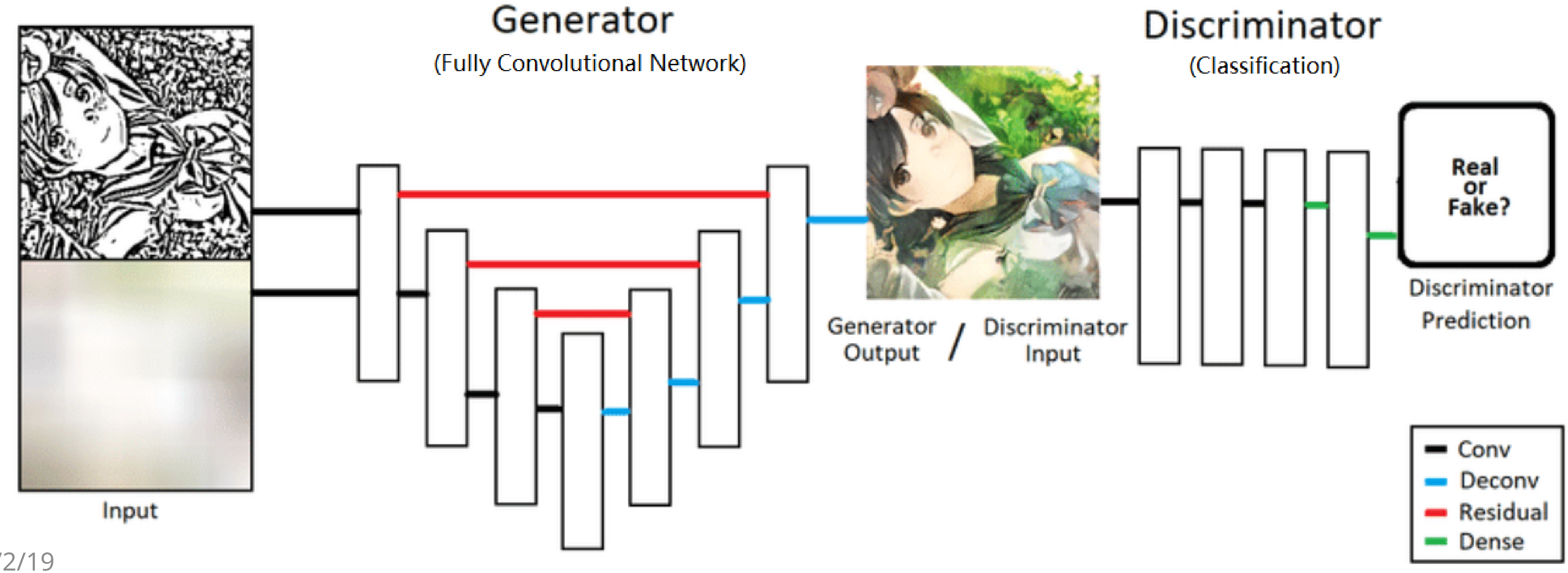
Pixel-wise loss is calculated as the log loss, summed over all possible classes

$$-\sum_{classes} y_{true} \log\left(y_{pred}\right)$$

This scoring is repeated over all **pixels** and averaged

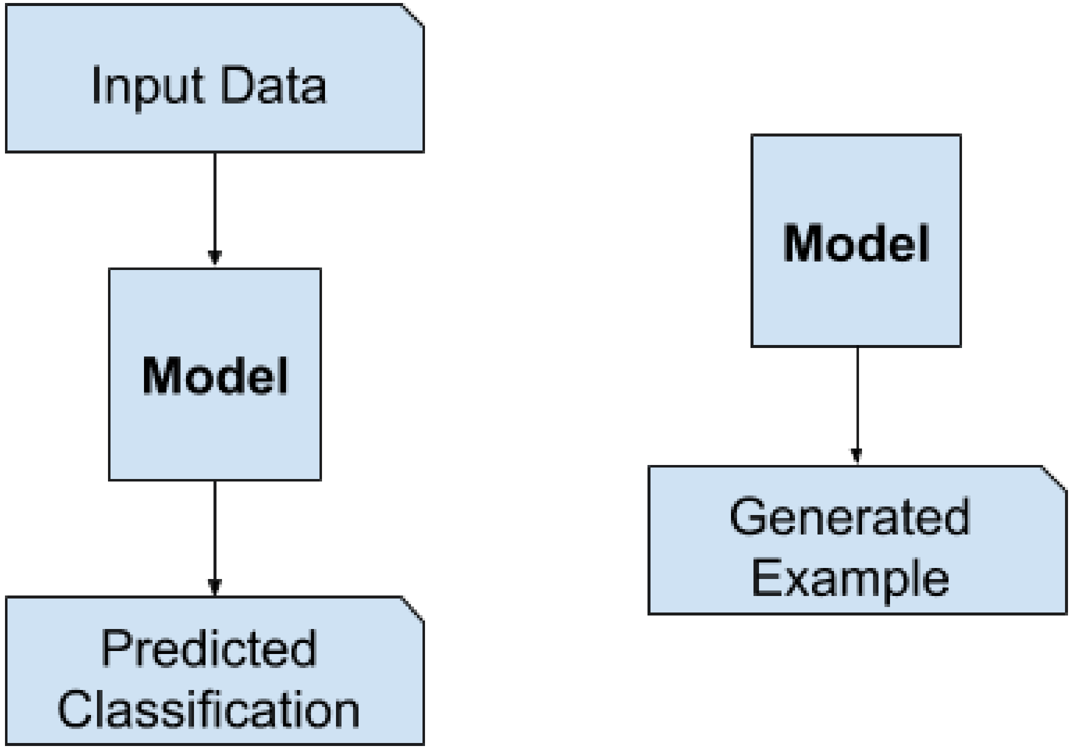
Image-to-image Translation

- Generative Adversarial Network (GAN)
- Generator: generate "fake" image
- Descriminator: distinguish real and "fake" images



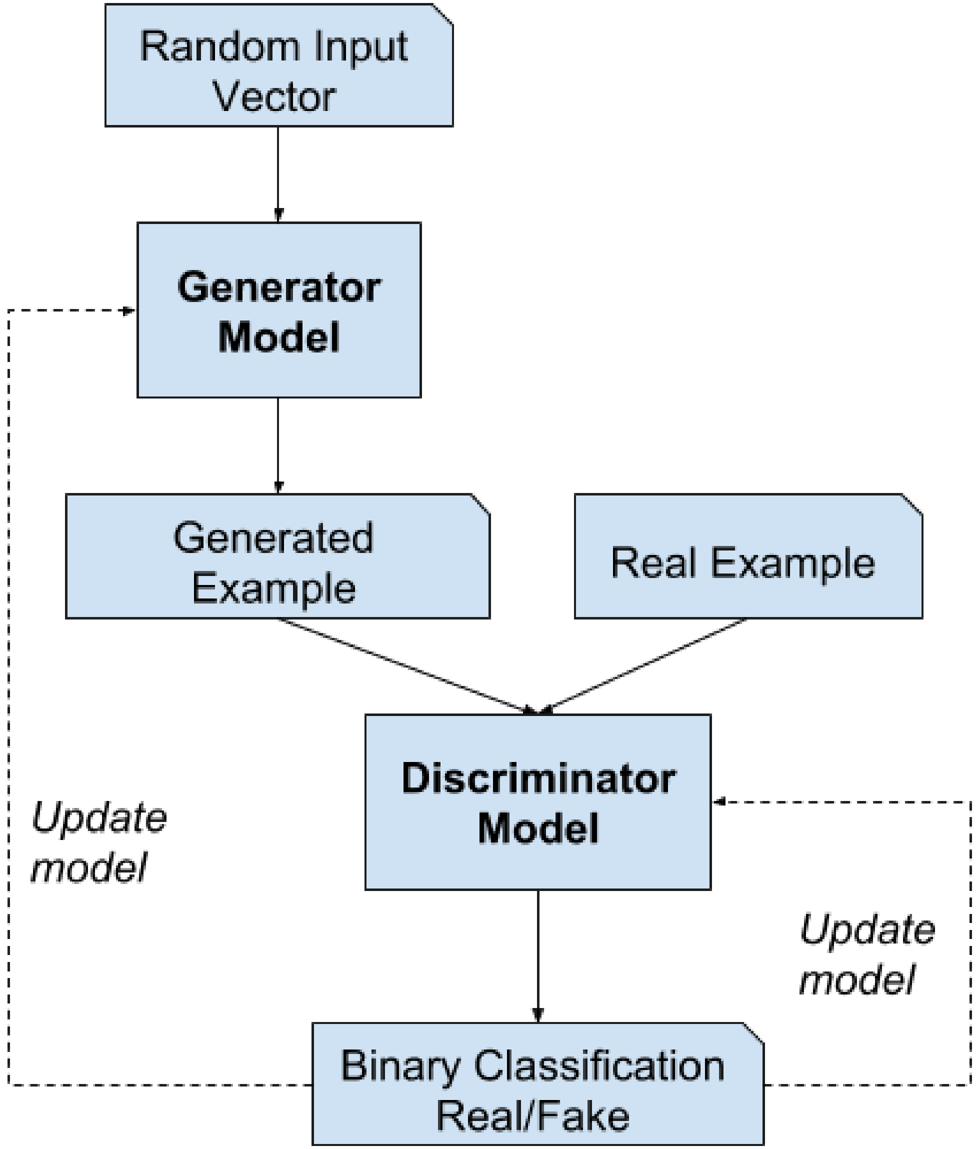
Generative Adversarial Network (GAN)

- Discriminative vs. Generative Modeling



Generative Adversarial Network (GAN)

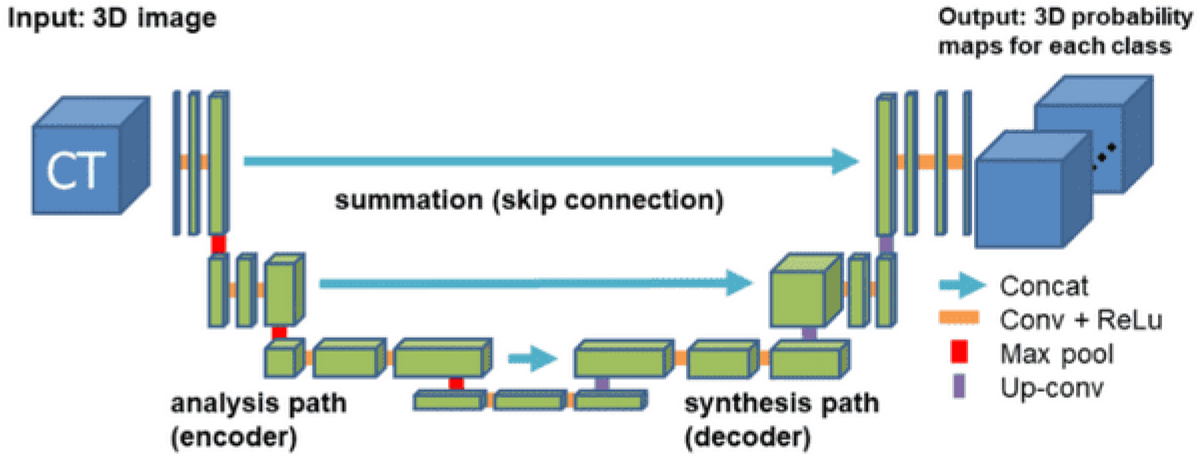
- Generator: generate "fake" image
- Descriminator: distinguish real and "fake" images



Generative Adversarial Network (GAN)

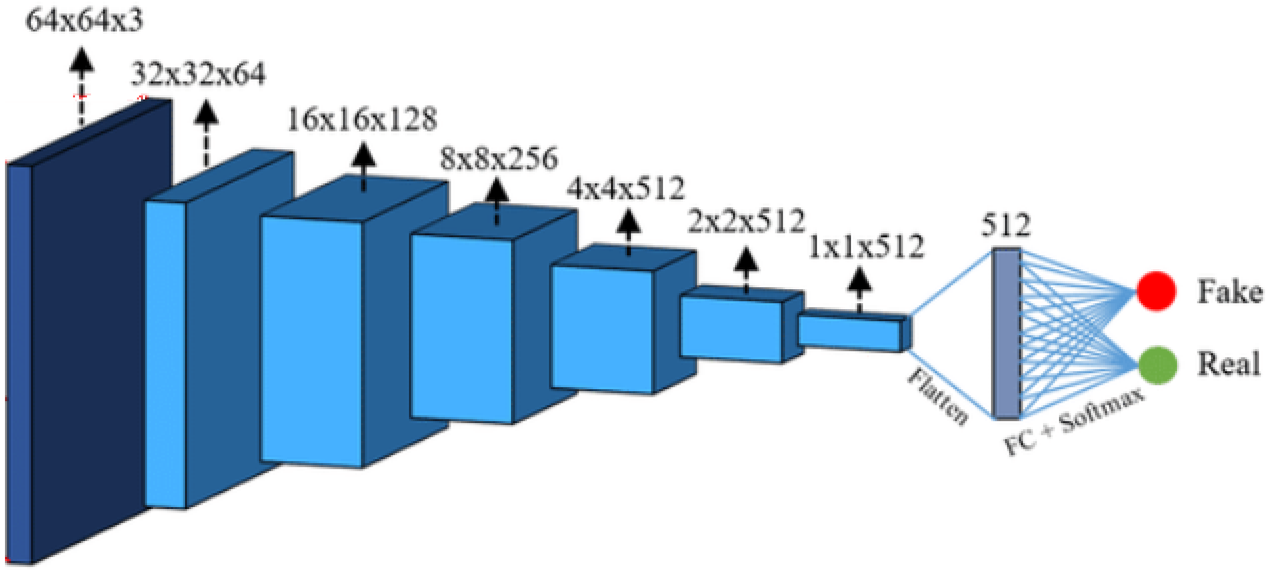
- Generator: U-Net

```
def forward(self, x):
    x1 = self.inc(x)
    x2 = self.down1(x1)
    x3 = self.down2(x2)
    x4 = self.down3(x3)
    x5 = self.down4(x4)
    x = self.up1(x5, x4)
    x = self.up2(x, x3)
    x = self.up3(x, x2)
    x = self.up4(x, x1)
    x = self.outc(x)
    return x
```



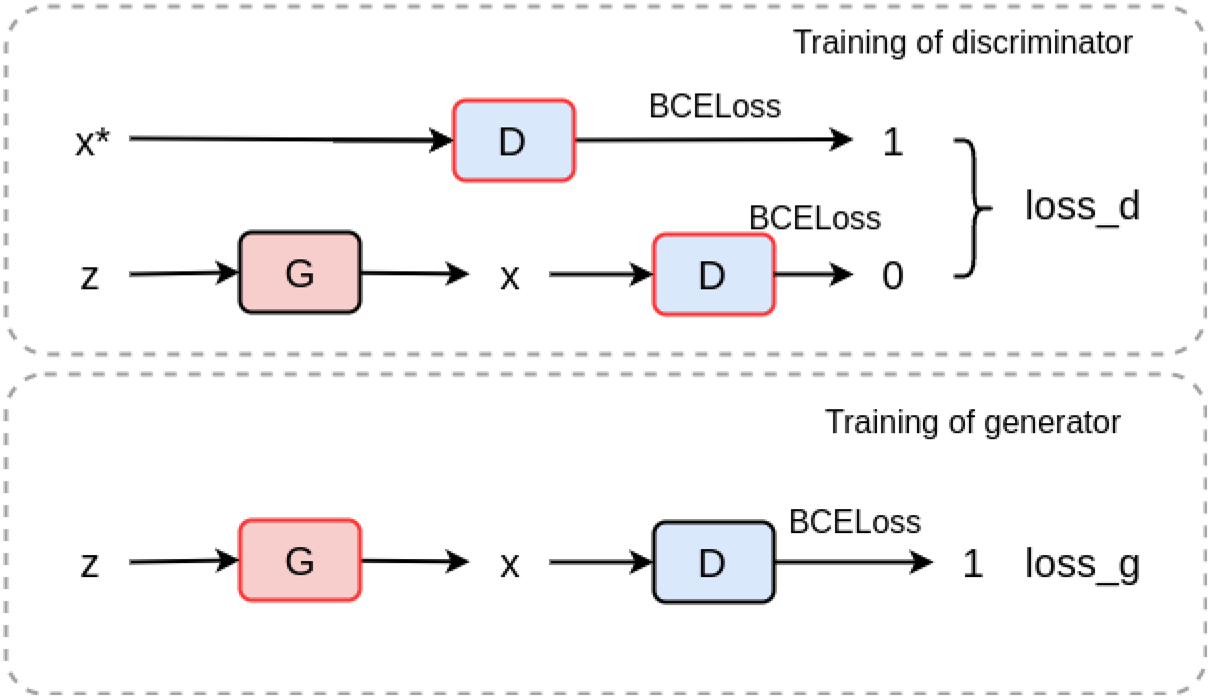
Generative Adversarial Network (GAN)

- Discriminator: convolutional neural network (CNN)



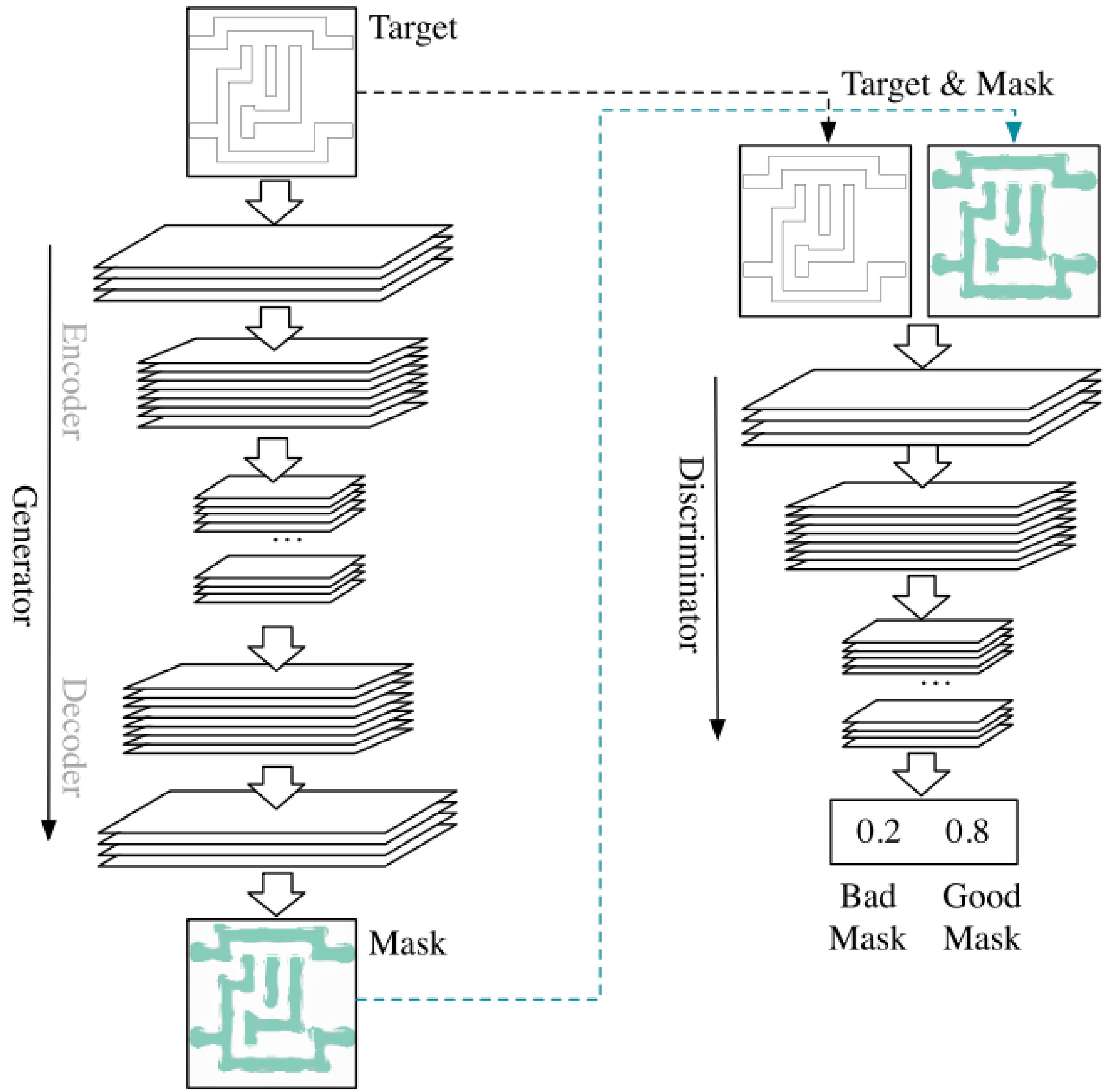
Generative Adversarial Network (GAN)

- Generator: generate "fake" image
- Descriminator: distinguish real and "fake" images



Deep Learning for OPC

- Imag-to-image translation
- Input: target image Z_t
- Output: OPC image Z^*
- Target: $\|Litho(Z^*) - Z_t\|_2^2$
- Can be guided by ILT methods



Deep Learning for OPC

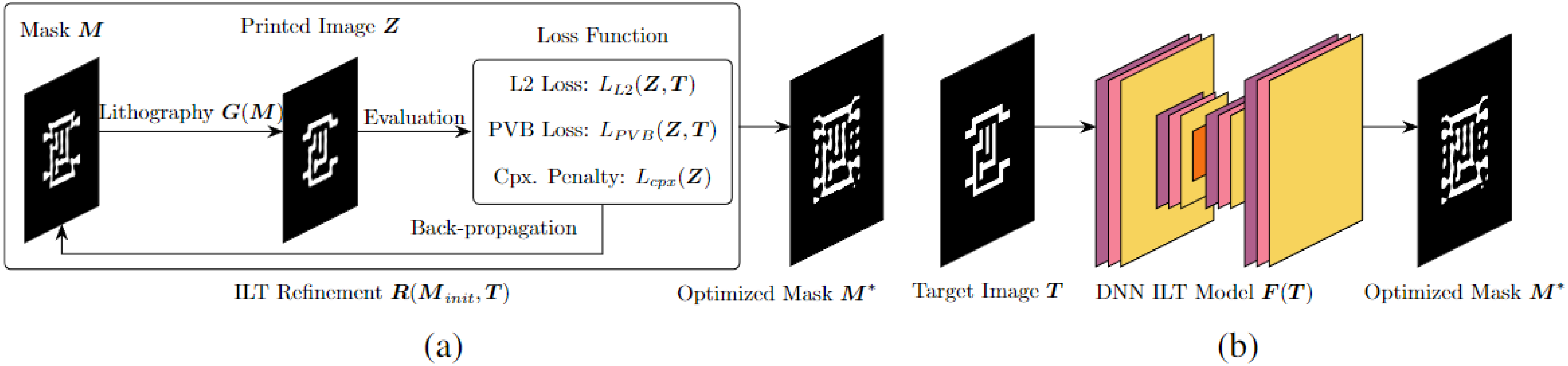


Figure 1: Overview of (a) traditional ILT and (b) DNN-based ILT.

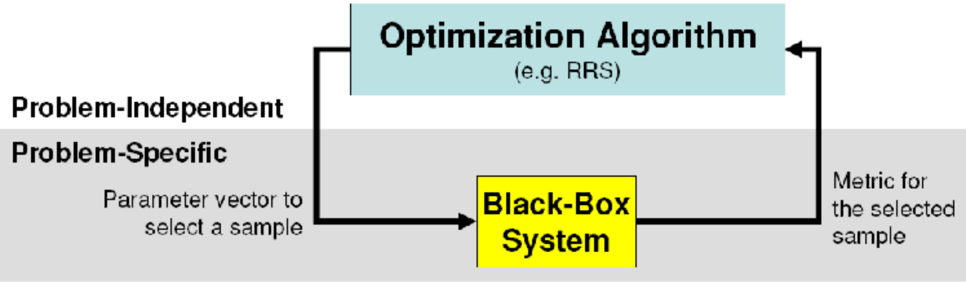
Deep Learning for OPC

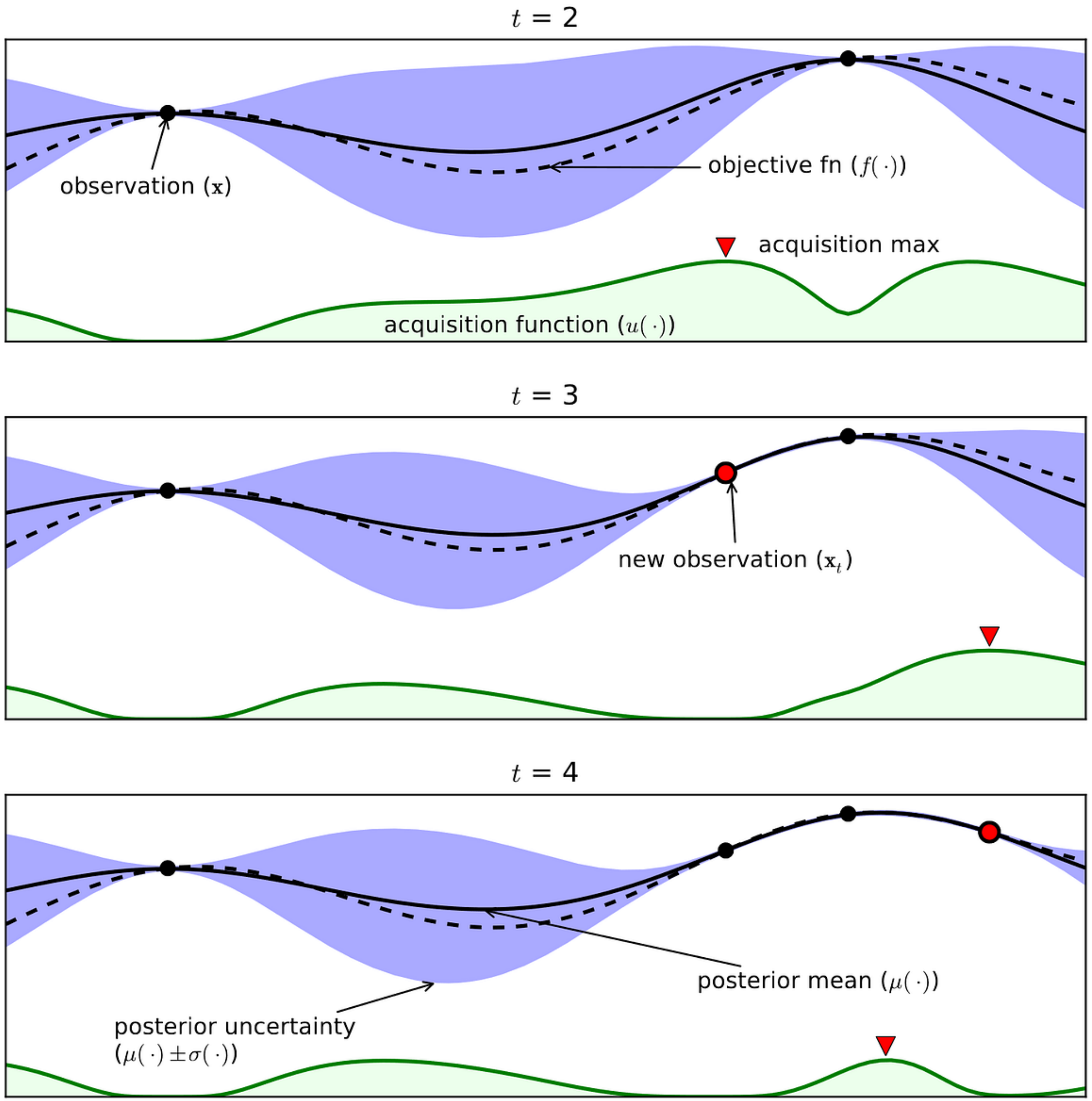
(a) (b) (c) (d) (e)

Figure 5: Mask optimization samples. (a)Ref.,(b)GAN-OPC,(c)Neural-ILT,(d)DAMO,(e)CFNO.

What's Next?

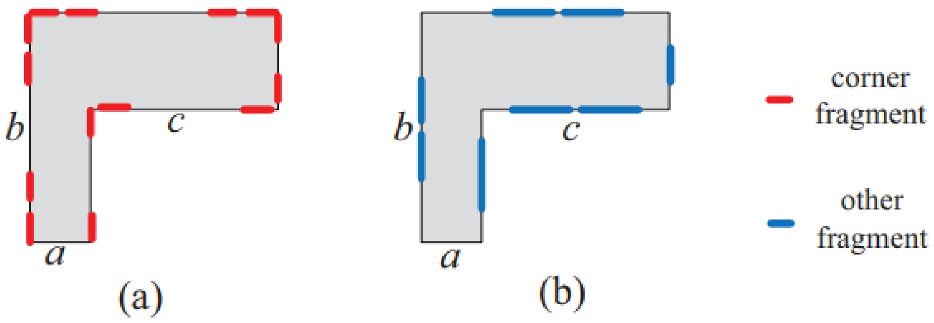
- Black-box optimization
- $min_x f(x)$, f is a black-box

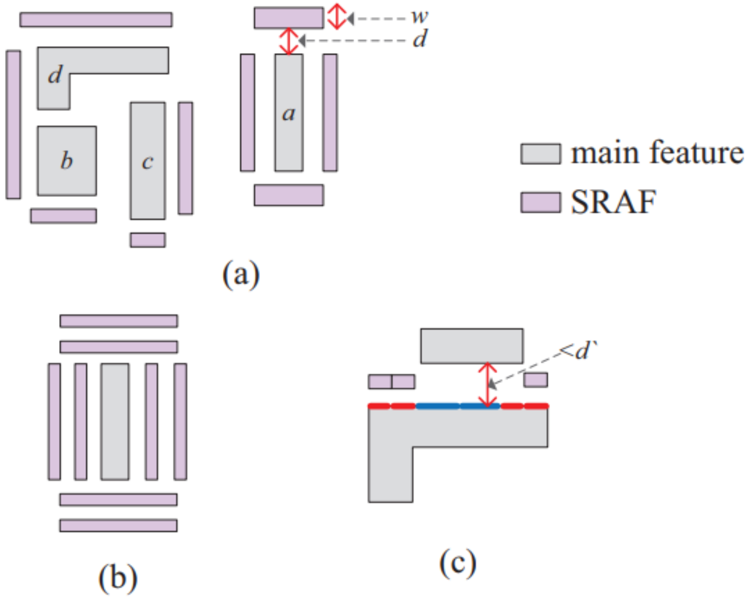




Black-box Optimization

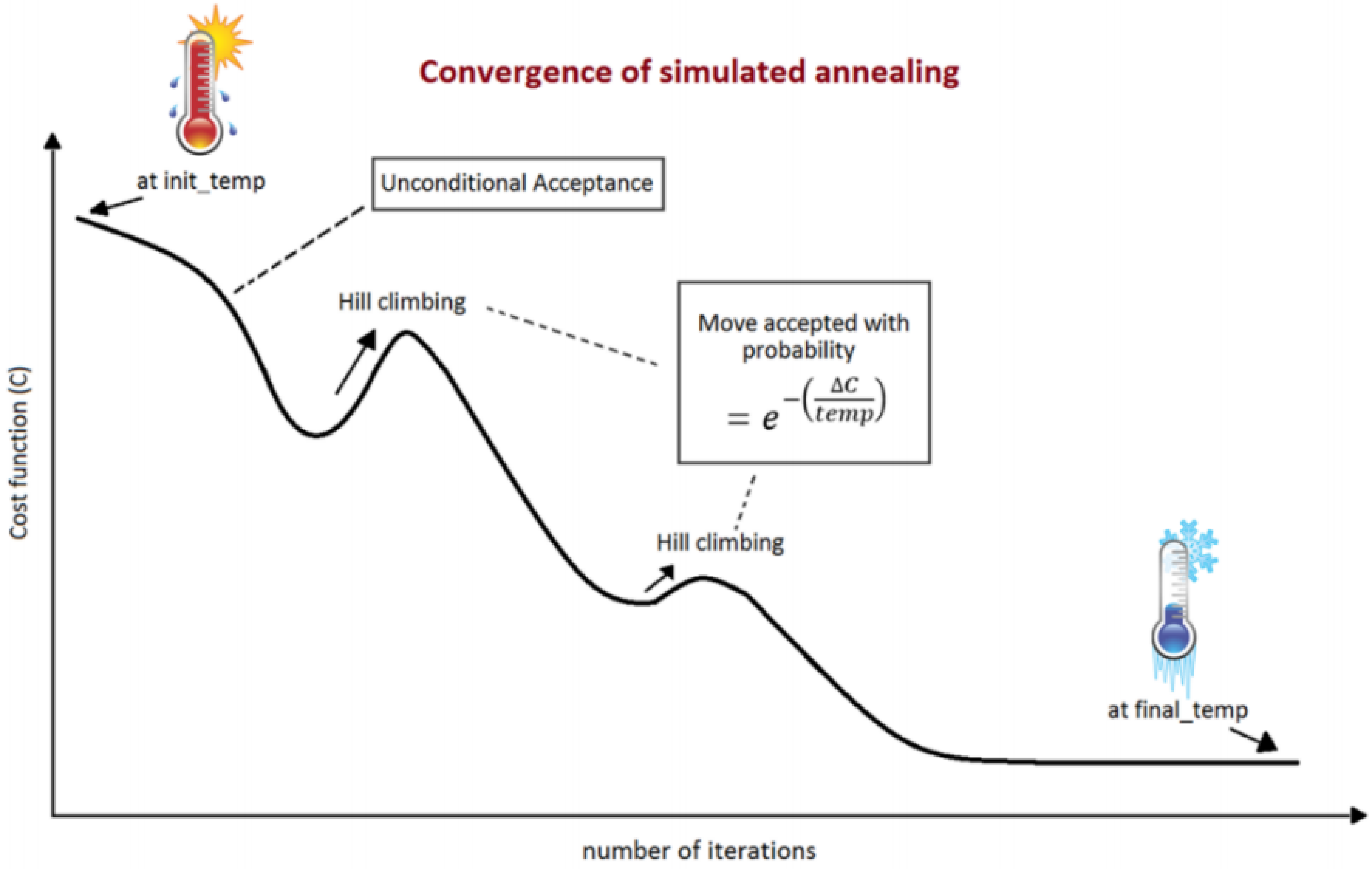
- Example: rule-based OPC
  -> Fragments: lengths of corner/other fragments
  -> SRAF: distance, length, width





Black-box Optimization

- Simulated annealing (SA)



Simulated Annealing, an Example

- Initial parameter: d=50, w=100, l=200, cost=10, temperature=10
- 1st iteration: d=40, w=100, l=200, cost=5, $\Delta_{cost} < 0$ => **accept**
- 2nd iteration: d=40, w=120, l=200, cost=15, $\Delta_{cost} > 0$ => accept with a probability of $e^{-\frac{\Delta_{cost}}{temperature}} = e^{-1}$
- ... ...

Pros & Cons

- Pros: low computation complexity, fast convergence
- Cons: local and sequential search, sensitive to the initial point

Concerns for Practical Applications

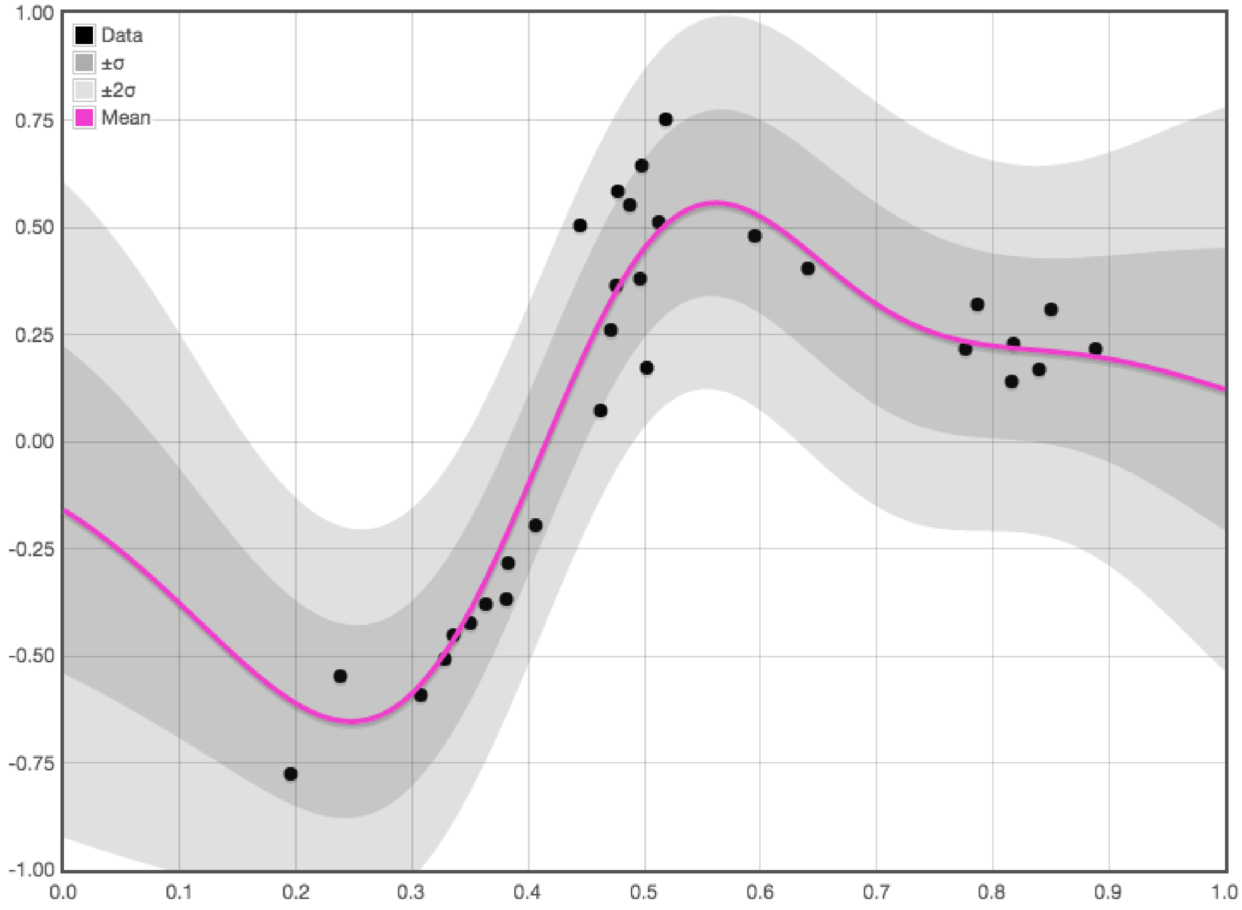
- Long evaluation time (e.g. calibre, innovus, … …)
  => Only a small number of iterations is allowed
- Search space is super large
  => many variables, many possible values

Exploration and Exploitation

- Exploration: get more unknown/uncertain knowledge => need more iterations
- Exploitation: make use of known/certain knowledge => trapped by local optima
- *A good search method should balance exploration and exploitation*
- Problem 1: how to represent the certainty?
- Problem 2: how to utilize the certainty?

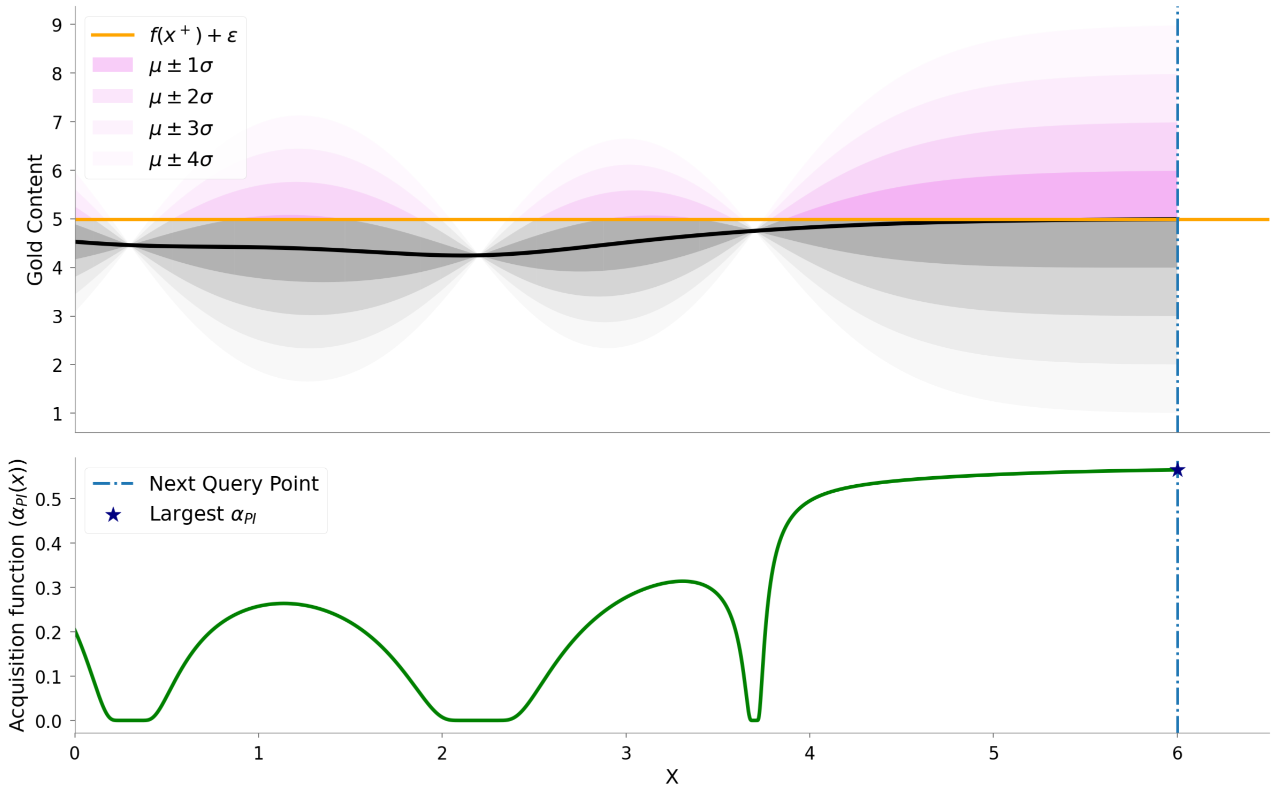
How to Represent the Certainty?

- Gaussian Process (GP)
  $\mu, \sigma = GP(x), s.t.\, y \sim \mathcal{N}(\mu, \sigma)$
- Input: variables x
- Outputs: mean μ and variance σ of the prediction y
- *Variance is the uncertainty*



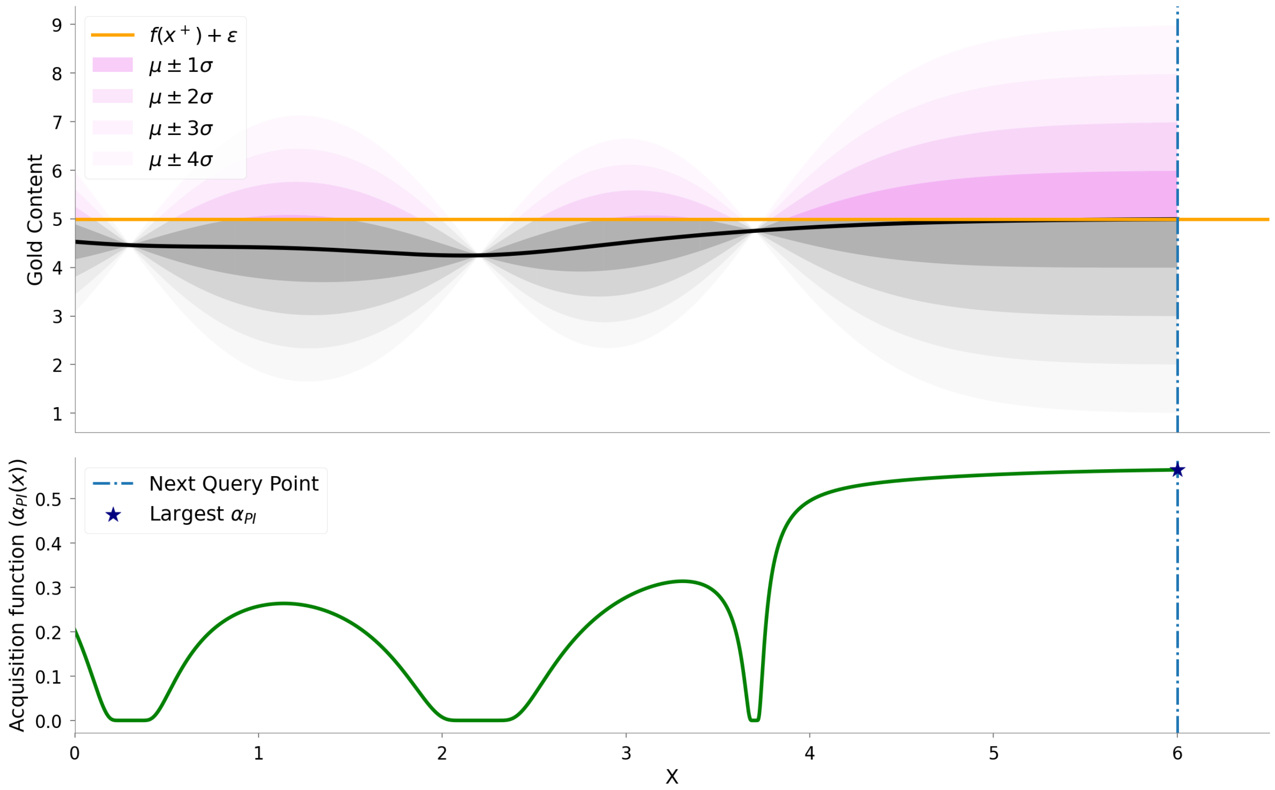
How to Utilize the Certainty?

- Expected Improvement (EI)
- $x^* = \arg\max_x E[GP(x)]$
- EI selects a point with a high μ or a large σ



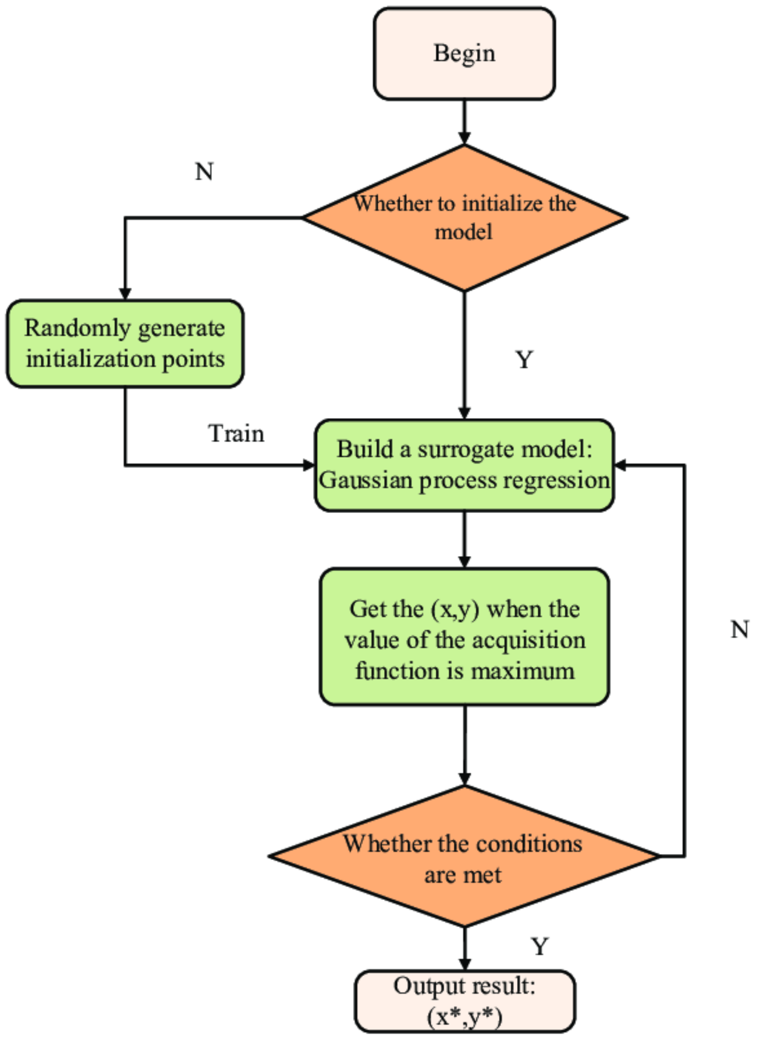
Bayesian Optimization

- Surrogate model: GP
- Acquisition function: EI
- Other models/functions are also applicable



Bayesian Optimization

- (1) Sample initial points and evaluate them
- (2) Train the GP with the data
- (3) Sample a new point by maximizing EI



Bayesian Optimization, an Example

- **Initialization**
- Randomly generate 16 recipes
  e.g. {d=50, w=100, l=200}, {d=100, w=120, l=70}, ...
- Evaluate the recipes and get the quality of results (QoRs)
  e.g. using the parameters to run a full-chip OPC
- Obtain the data: x: recipes, y: QoRs

Bayesian Optimization, an Example

- **Optimization**
- Train a GP with known data
- Sample a new recipe by maximizing EI
- Evaluate the recipe and get its QoRs
- Repeat these steps for N iterations

Bayesian Optimization Toolbox

- Optuna: https://optuna.readthedocs.io/en/stable/