Deep Learning Fundamentals

Haozhe Xie

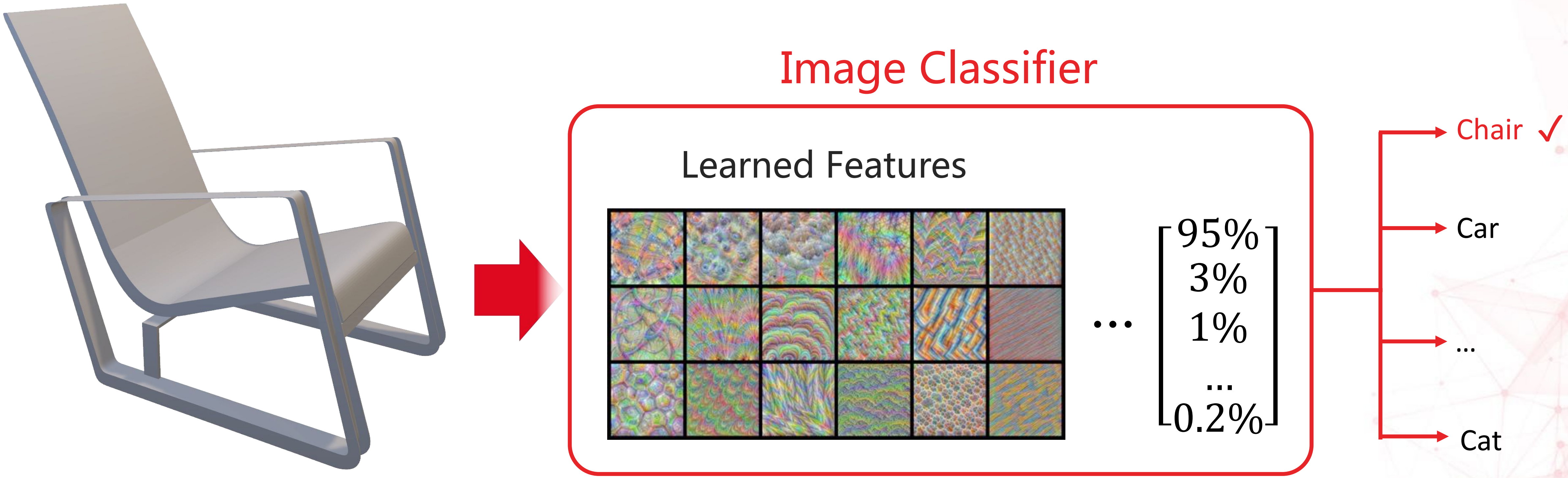
cshzxie@gmail.com

Outline

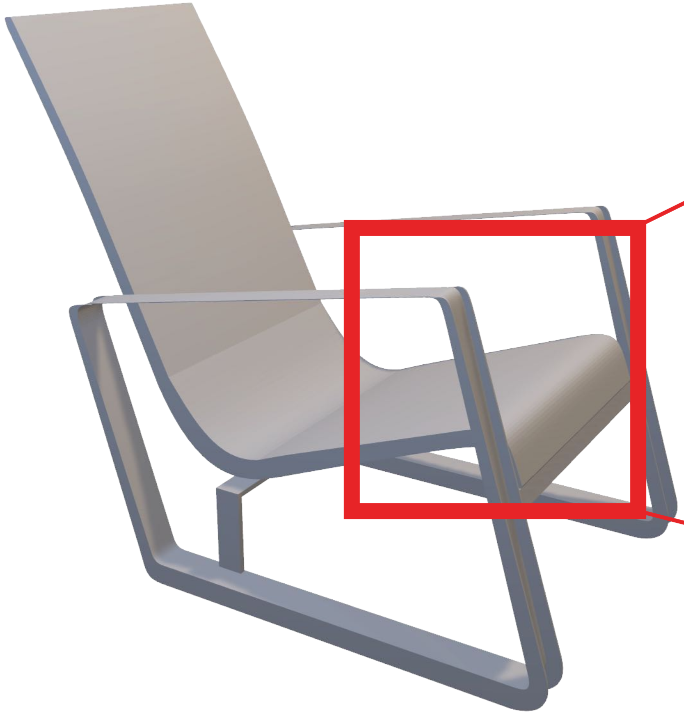
Part I

K-Nearest Neighbor

What is Image Classification?



The Problem: Semantic Gap



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 [ 99  81  81  93 120 131 127 100  95  98 102  99  96  93 101  94]
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 [122 121 102  80  82  86  94 117 145 148 153 102  58  78  92 107]
 [122 164 148 103  71  56  78  83  93 103 119 139 102  61  69  84]]
```

What the computer sees

Challenges: Viewpoint variation

Other Challenges

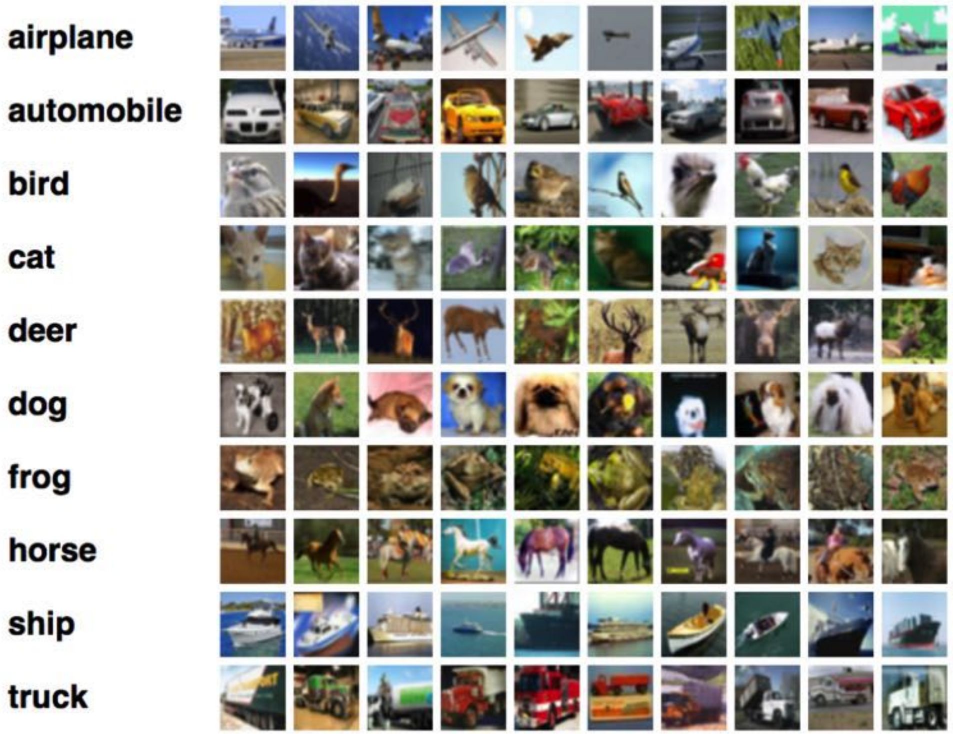
Illumination

Deformation

Occlusion

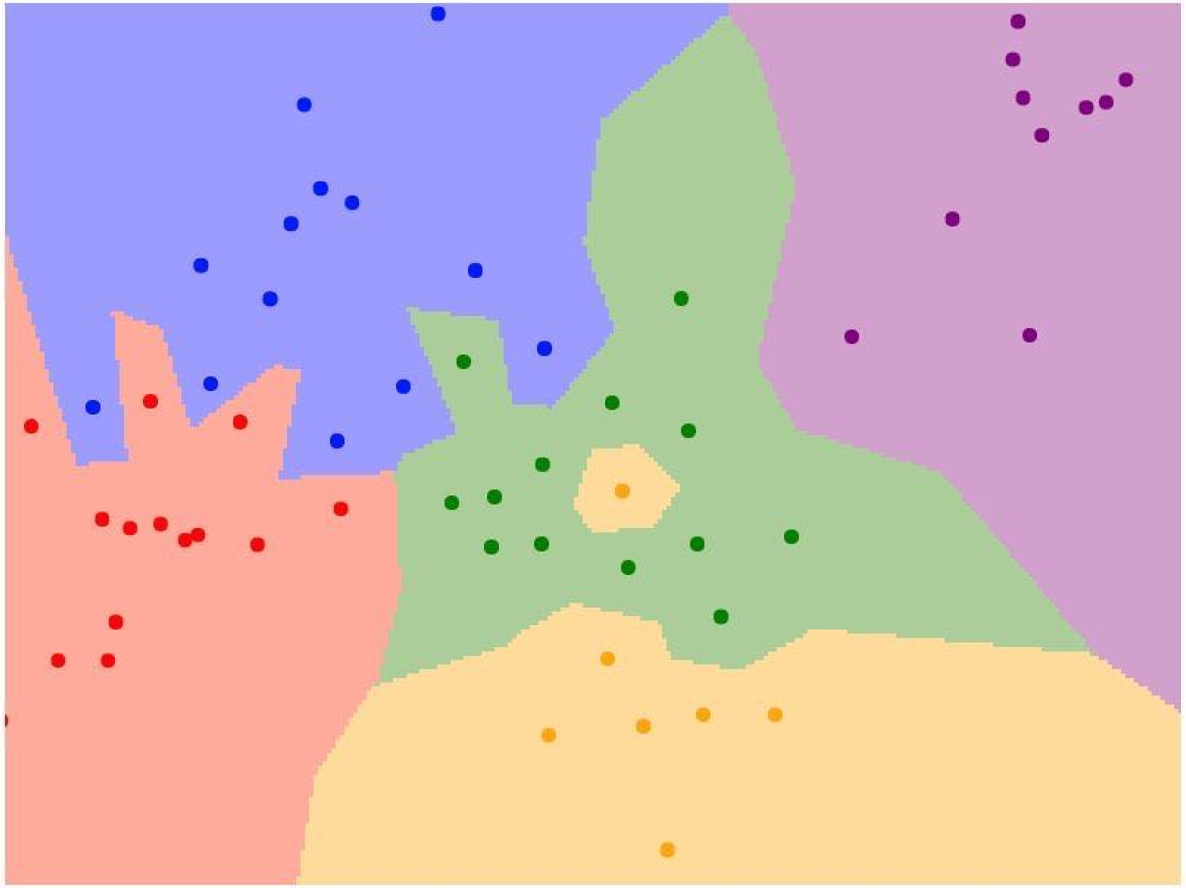
How to Classify Images?

- Data-Driven Approach
  - Collect a dataset of images and labels
  - Use Machine Learning to train a classifier
  - Evaluate the classifier on new images



Naïve Imager Classifier: Nearest Neighbor

```python
import numpy as np

class NearestNeighbor:
  def __init__(self):
    pass

  def train(self, X, y):
    """ X is N x D where each row is an example. Y is 1-dimension of size N """
    # the nearest neighbor classifier simply remembers all the training data
    self.Xtr = X
    self.ytr = y

  def predict(self, X):
    """ X is N x D where each row is an example we wish to predict label for """
    num_test = X.shape[0]
    # lets make sure that the output type matches the input type
    Ypred = np.zeros(num_test, dtype = self.ytr.dtype)

    # loop over all test rows
    for i in xrange(num_test):
      # find the nearest training image to the i'th test image
      # using the L1 distance (sum of absolute value differences)
      distances = np.sum(np.abs(self.Xtr - X[i,:]), axis = 1)
      min_index = np.argmin(distances) # get the index with smallest distance
      Ypred[i] = self.ytr[min_index] # predict the label of the nearest example

    return Ypred
```

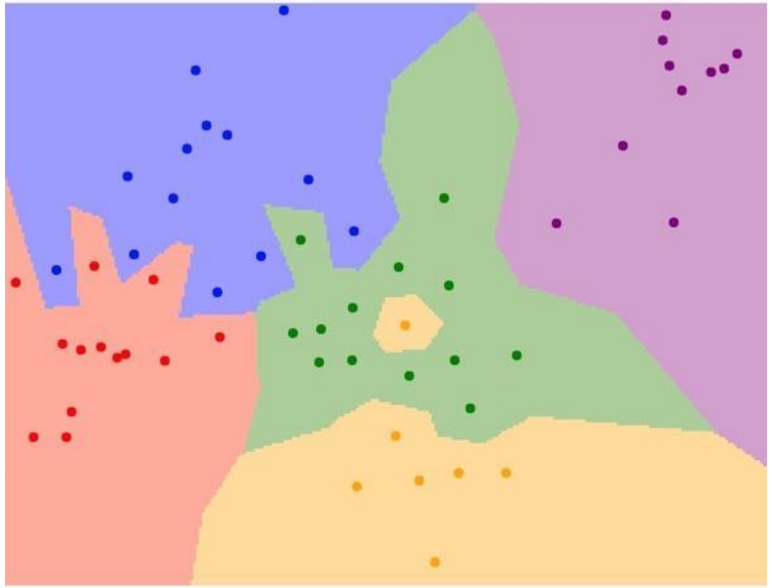


Distance Metric:

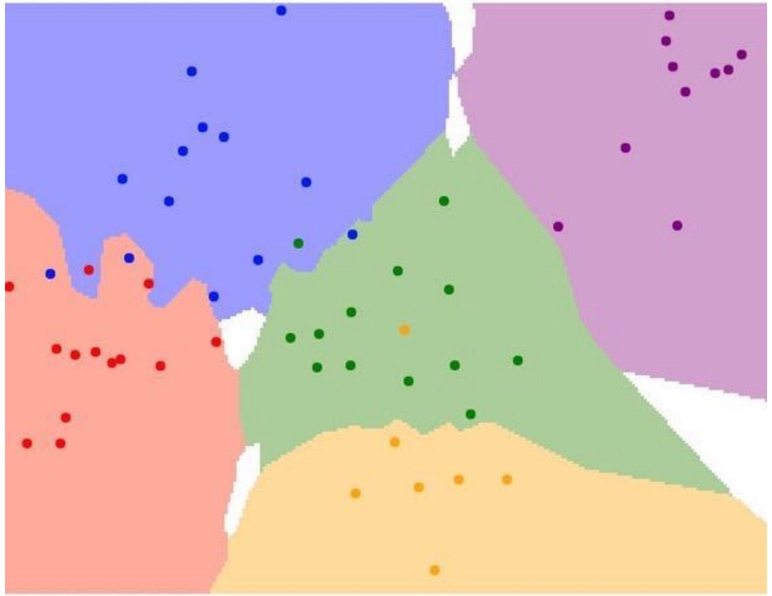
$$d_1(I_1, I_2) = \sum_p \left| I_1^p - I_2^p \right|$$

Naïve Imager Classifier: K-Nearest Neighbor

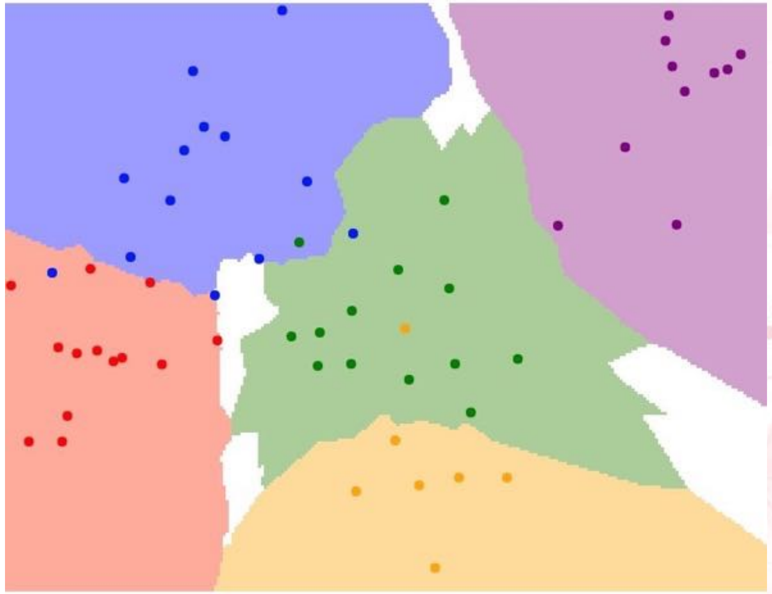
Instead of copying label from nearest neighbor, take majority vote from K closest points.



k=1



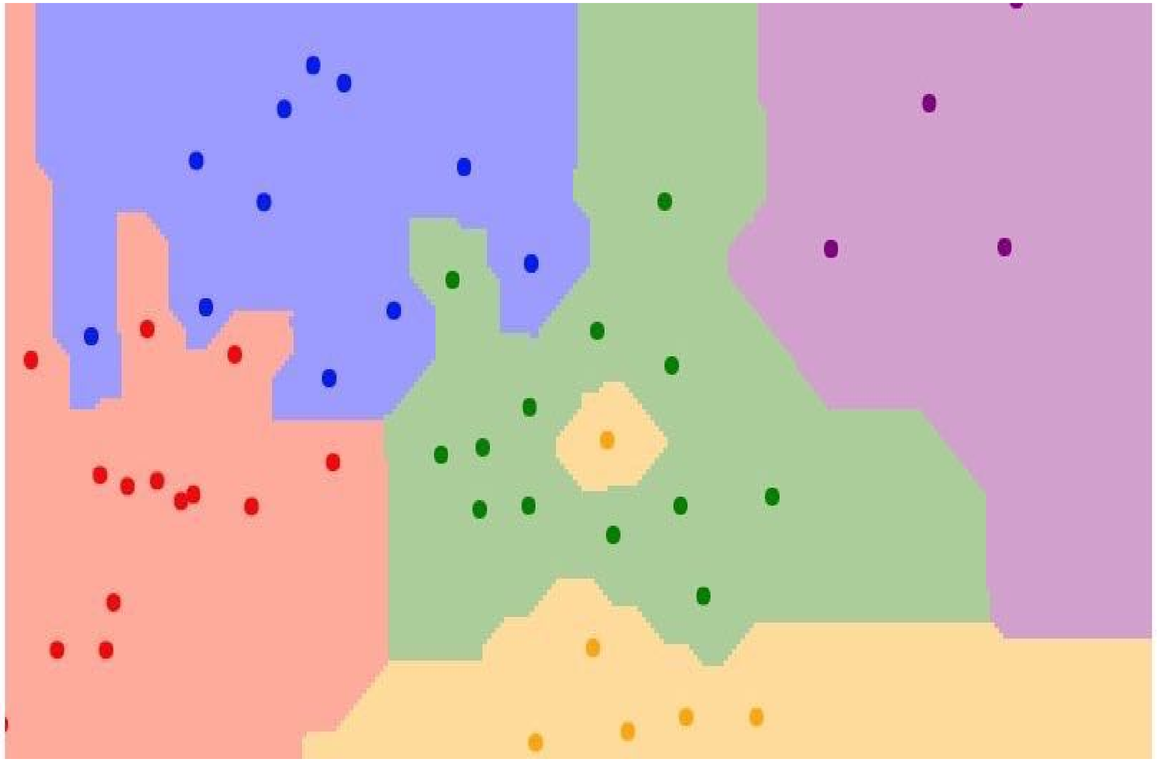
k=3

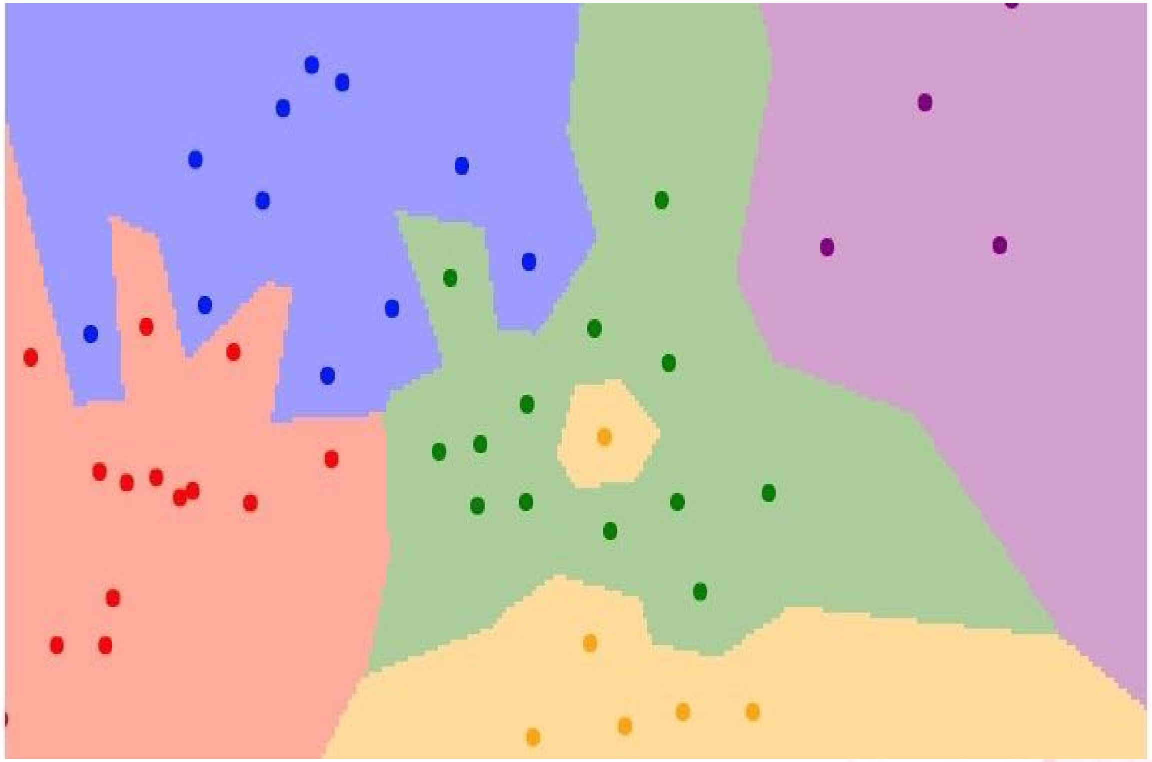


k=5

Naïve Imager Classifier: Nearest Neighbor

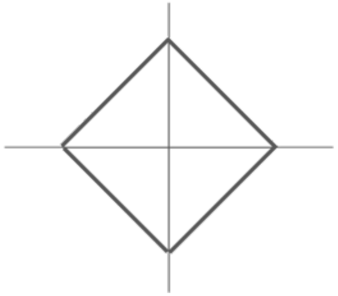
K-Nearest Neighbors: Distance Metrics





L1 (Manhattan) distance

$$d_1(I_1, I_2) = \sum_p |I_1^p - I_2^p|$$



L2 (Euclidean) distance

$$d_2(I_1, I_2) = \sqrt{\sum_p (I_1^p - I_2^p)^2}$$

K-Nearest Neighbors: Hyperparameters

- What is the best value of k to use?
- What is the best distance to use?

- These are **hyperparameters**: choices about the algorithm that we set rather than learn
- Very problem-dependent.
- Must try them all out and see what works best.

K-Nearest Neighbors: Hyperparameters

- Idea #1: Choose hyperparameters that work best on the data

  BAD: K = 1 always works perfectly on training data

- Idea #2: Split data into train and test, choose hyperparameters that work best on test data

  BAD: No idea how algorithm will perform on new data

- Idea #3: Split data into train, validation, and test; choose hyperparameters on validation and evaluate on test

  Better!

K-Nearest Neighbors: Hyperparameters

- Idea #4: Cross-Validation: Split data into folds, try each fold as validation and average the results

Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Fold 6	Test
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Fold 6	Test
Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Fold 6	Test

Note: Useful for small datasets, but not used too frequently in deep learning

Drawbacks of K-Nearest Neighbors

- k-Nearest Neighbor on images never used
  - Very slow at test time
  - Distance metrics on pixels are not informative

Original

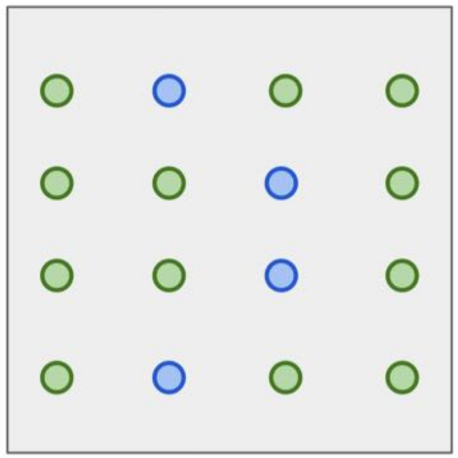
Shifted

Tinted

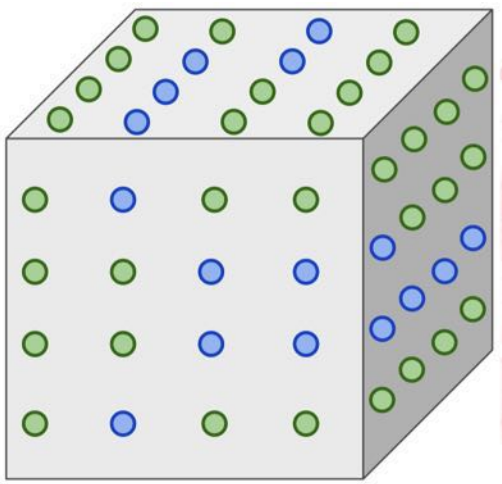
Drawbacks of K-Nearest Neighbors

- k-Nearest Neighbor on images never used
  - Very slow at test time
  - Distance metrics on pixels are not informative
  - Curse of dimensionality

Dimension = 1
Points = 4



Dimension = 2
Points = 4^2



Dimension = 3
Points = 4^3

K-Nearest Neighbors: Summary

- In image classification we start with a **training set** of images and labels, and must predict labels on the **test set**;
- The K-Nearest Neighbors classifier predicts labels based on nearest training examples;
- Distance metric and K are hyperparameters;
- Choose hyperparameters using the validation set; only run on the test set once at the very end.

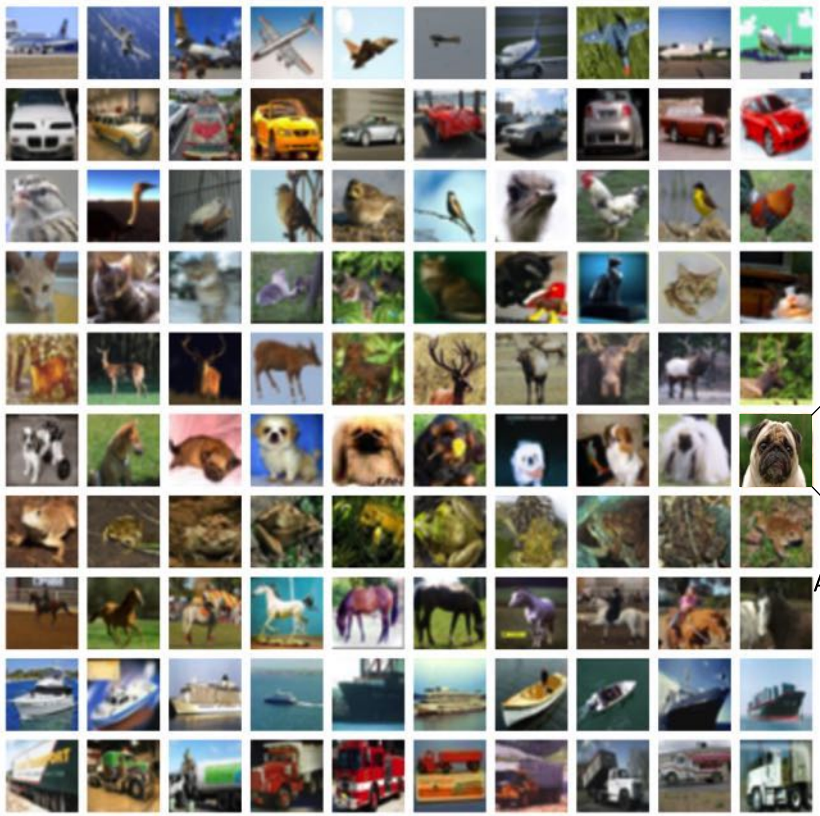
Part II

Linear Classifier

Linear Classifier

Recall CIFAR 10

airplane
automobile
bird
cat
deer
dog
frog
horse
ship
truck



50,000 training images of sizes 32x32x3
10,000 test images.

Image

Array of 32x32x3 numbers
3072 numbers in total

$$f(x, W)$$

10 numbers giving class scores

Parameters or weights

Linear Classifier

$$\overset{10 \times 1}{\boxed{f(x, W)}} = \underset{10 \times 3072}{\boxed{W}}\,\overset{3072 \times 1}{\boxed{x}} + \underset{10 \times 1}{b}$$

Image

Array of 32x32x3 numbers
3072 numbers in total

$$\text{Image} \rightarrow f(x, W) \rightarrow \text{10 numbers giving class scores}$$

Parameters
or weights

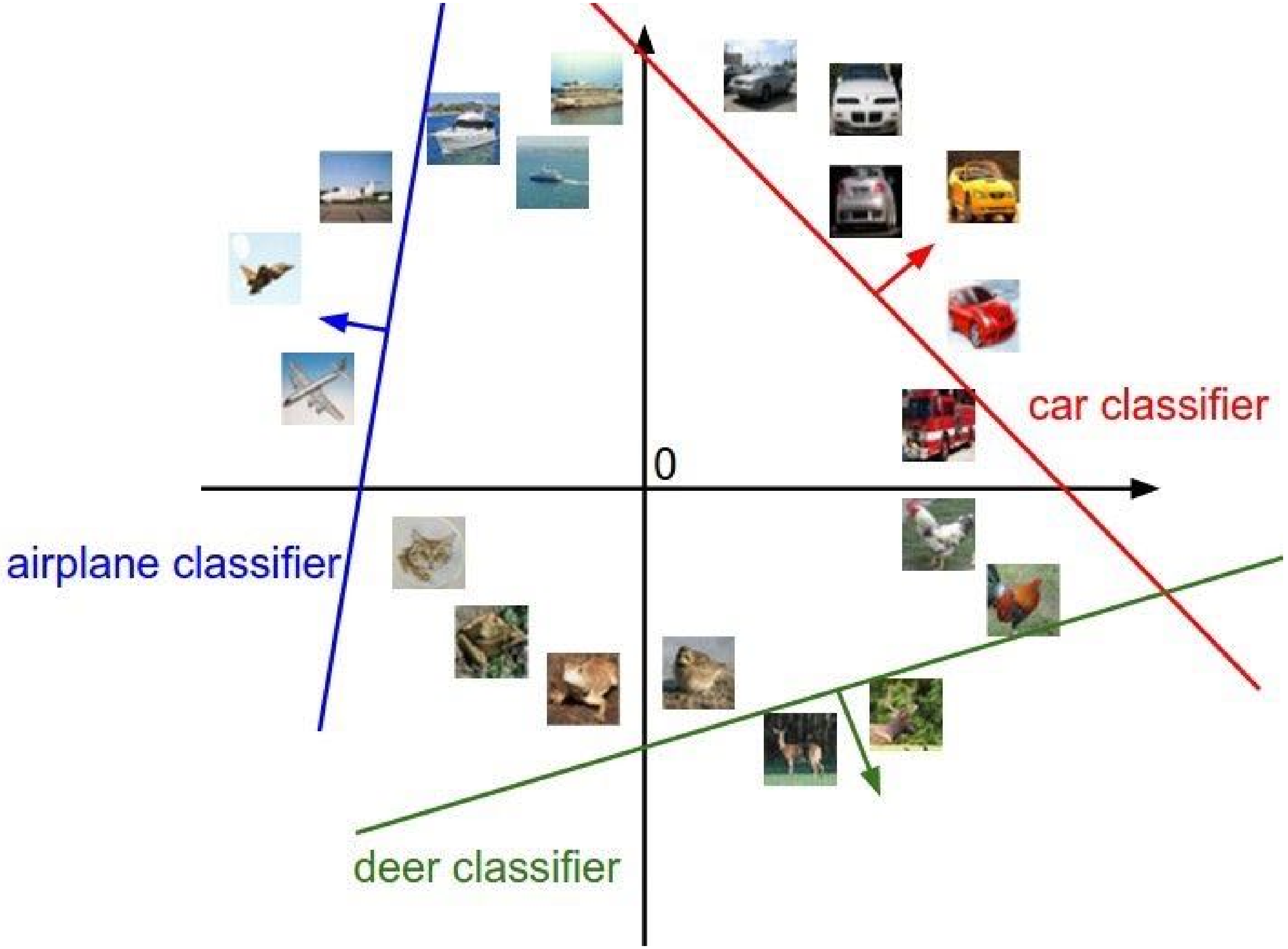
An Example of Linear Classifier

Example with an image with 4 pixels, and 3 classes (cat/dog/ship)

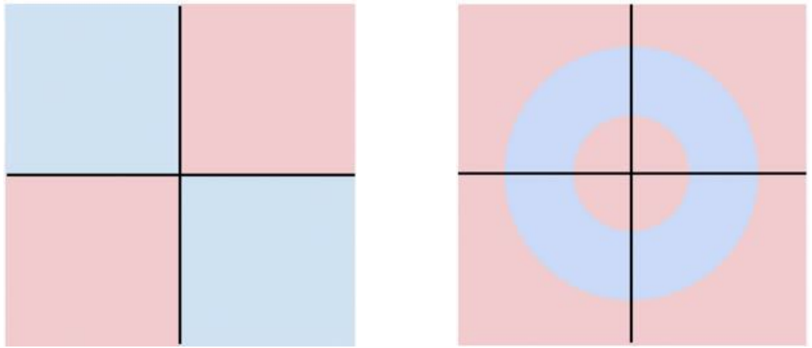
56	231
24	2

$$
\begin{bmatrix} 0.2 & -0.5 & 0.1 & 2.0 \\ 1.5 & 1.3 & 2.1 & 0.0 \\ 0 & 0.25 & 0.2 & -0.3 \end{bmatrix}
\times
\begin{bmatrix} 56 \\ 231 \\ 24 \\ 2 \end{bmatrix}
+
\begin{bmatrix} 1.1 \\ 3.2 \\ -1.2 \end{bmatrix}
=
\begin{array}{c} \begin{bmatrix} -96.8 \\ 437.9 \\ 61.95 \end{bmatrix} \end{array}
\begin{array}{l} \text{Cat Score} \\ \text{Dog Score} \\ \text{Ship Score} \end{array}
$$

Linear Classifiable



- Not Linearly Classifiable Cases



Part III

Loss Functions and Optimization

Things TODO in Linear Classifier

- Quantify the Classification Scores
  - Loss Function
- Find the Parameters Effectively
  - Optimization

Loss Functions

- What is Loss Function?
  - A loss function tells how good our current classifier is.

- Given a dataset of examples: $\{(x_i, y_i)\}_{i=1}^{N}$
- Loss over the dataset is a sum of loss over examples:

$$L = \frac{1}{N}\sum_{i} L_i(f(x_i, W), y_i)$$

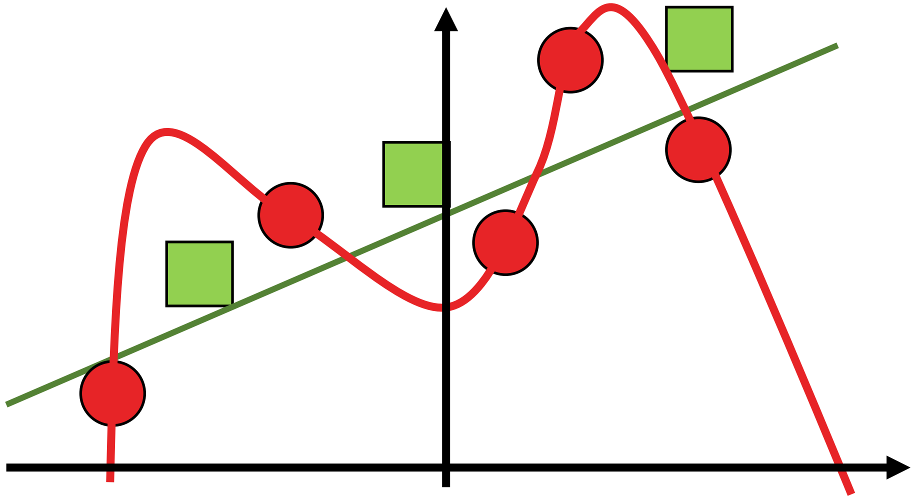
Regularization

$$\underbrace{L = \frac{1}{N}\sum_i L_i(f(x_i, W), y_i)}_{} + \lambda R(W)$$

Regularization: Model should be "simple", so it works on test data

Occam's Razor:
"Among competing hypotheses, the simplest is the best"
William of Ockham, 1285 - 1347

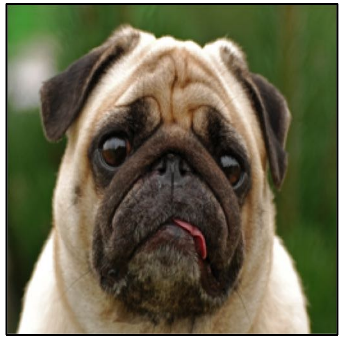
Data Loss: Model predictions should match training data



Regularization

- Common Regularization
  - L2 Regularization: $R(W) = \sum_{j=0}^{p} \beta_j^2$
  - L1 Regularization: $R(W) = \sum_{j=0}^{p} |\beta_j|$
  - Elastic net (L1 + L2): $R(W) = \alpha \sum_{j=0}^{p} \beta_j^2 + \sum_{j=0}^{p} |\beta_j|$
  - Max norm regularization
  - Dropout
  - Fancier: Batch normalization, stochastic depth

Softmax Classifier



3.2	Cat Score
5.1	Dog Score
-1.7	Ship Score

- Scores = unnormalized log probabilities of the classes

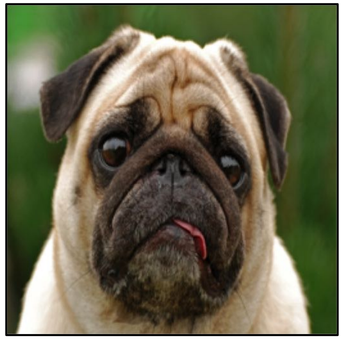
$$P(Y=k|X=x_i)=\frac{e^{s_k}}{\sum_j e^{s_j}} \qquad \text{where } s=f(x_i,\mathbf{W})$$

Want to maximize the log likelihood (loss function) to minimize the negative log likelihood of the correct class:

$$L_i=-\log P(Y=y_i|X=x_i)$$

- In Summary: $L_i=-\log(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}})$

Softmax Classifier



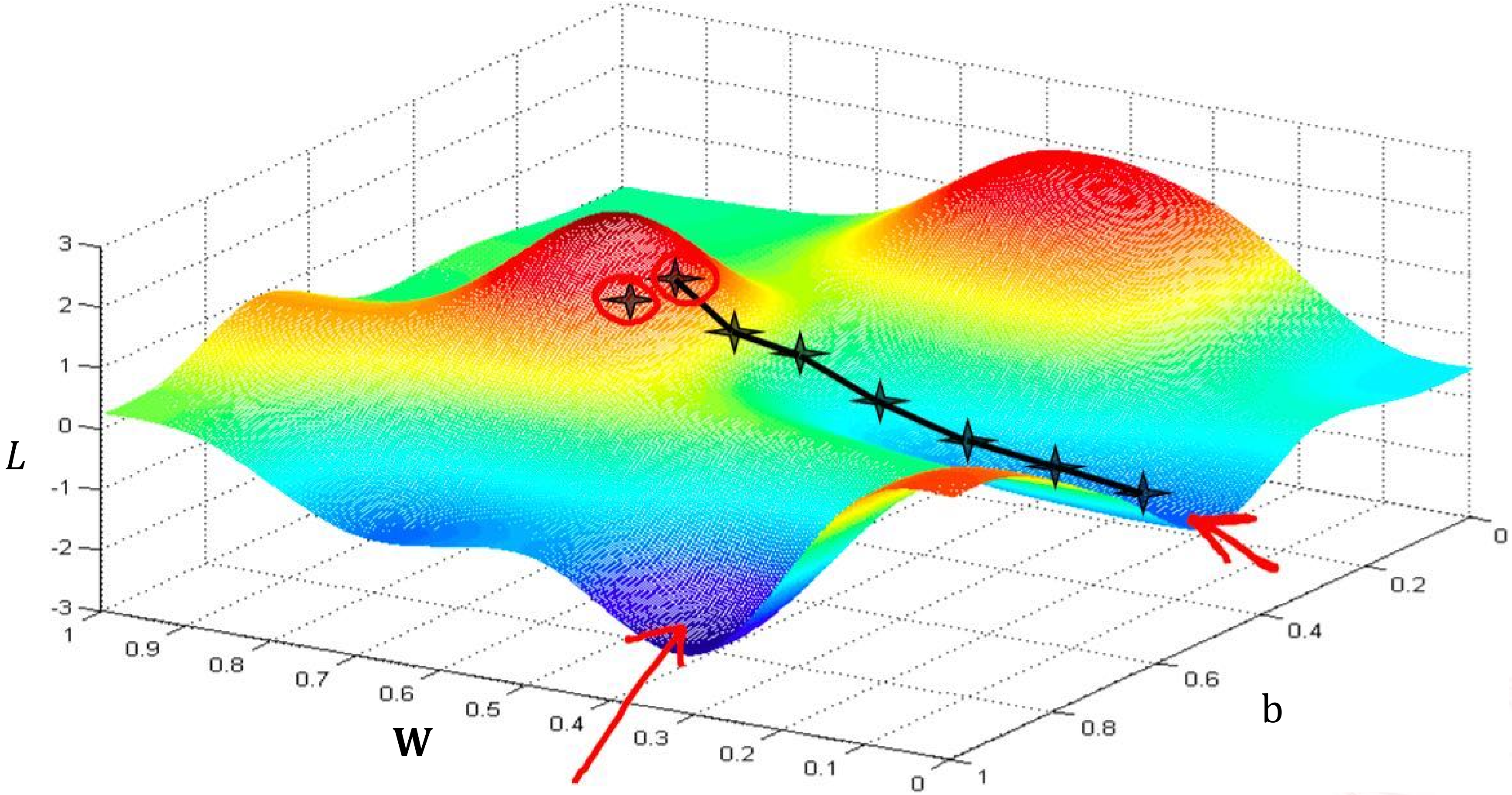
$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	normalized probabilities
Cat	3.2		24.5		0.13
Dog	5.1		164.0		0.87
Ship	-1.7		0.18		0.00

$$L_i = -\log(0.87) = 0.06$$

Optimization

- How to find the best **W** and b?



Optimization: Gradient Decent

- Stochastic Gradient Descent (SGD)
  - $L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$
  - $\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$

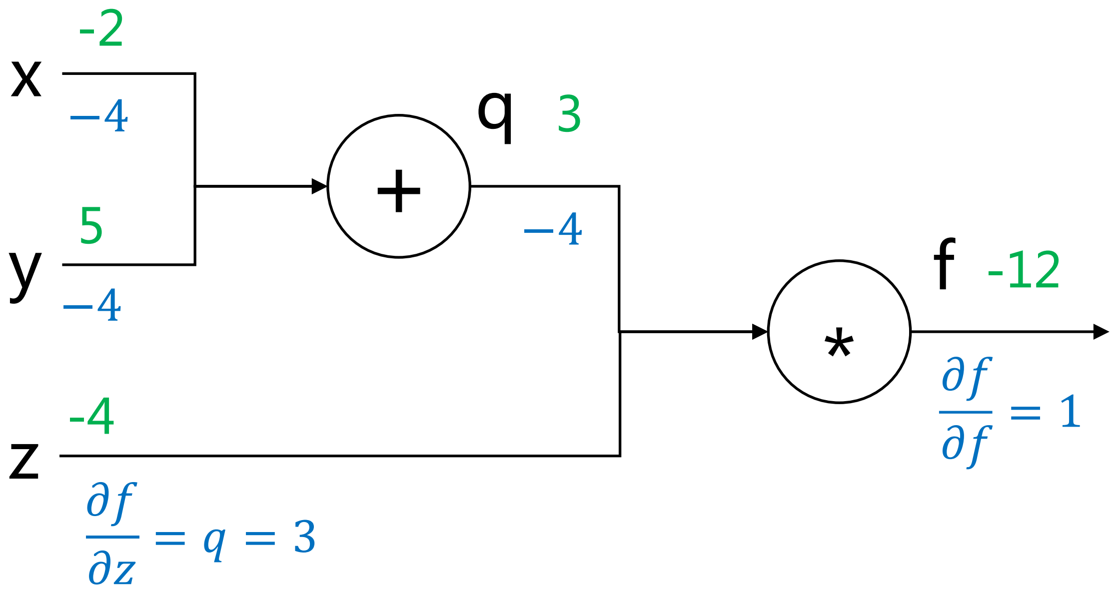
```
# Vanilla Minibatch Gradient Descent
while True:
    data_batch = sample_training_data(data, 64)
    weights_grad = eval_gradient(loss_func, data_batch, weights)
    weights -= weights_grad * learning_rate
```

Part IV

Backpropagation and Neural Networks

Backpropagation

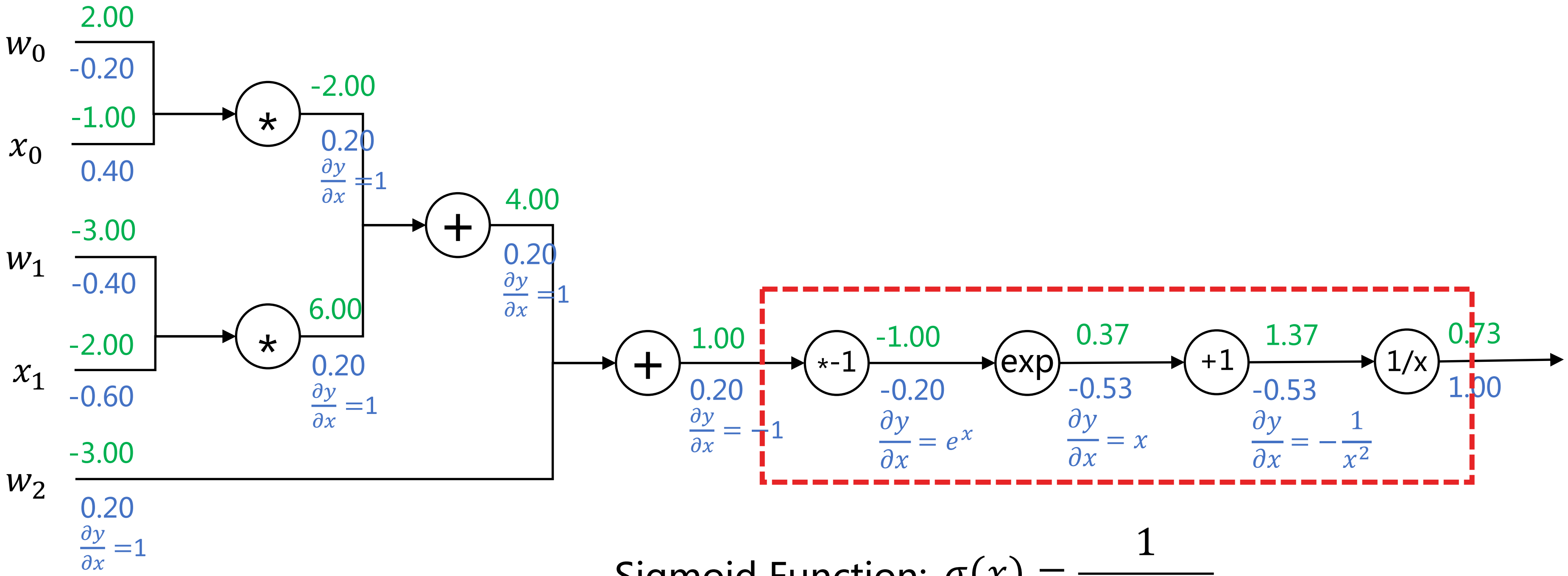
- How to get the gradient?
- $f(x, y, z) = (x + y)z$



- Given x = -2, y = 5, z = -4
- $q = x + y \qquad \frac{\partial q}{\partial x} = 1 \quad \frac{\partial q}{\partial y} = 1$
- $f = qz \qquad \frac{\partial f}{\partial q} = z \quad \frac{\partial f}{\partial z} = q$
- $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} \qquad \frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y}$

Backpropagation

- $f(\mathrm{W},\mathrm{x}) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



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

Backpropagation

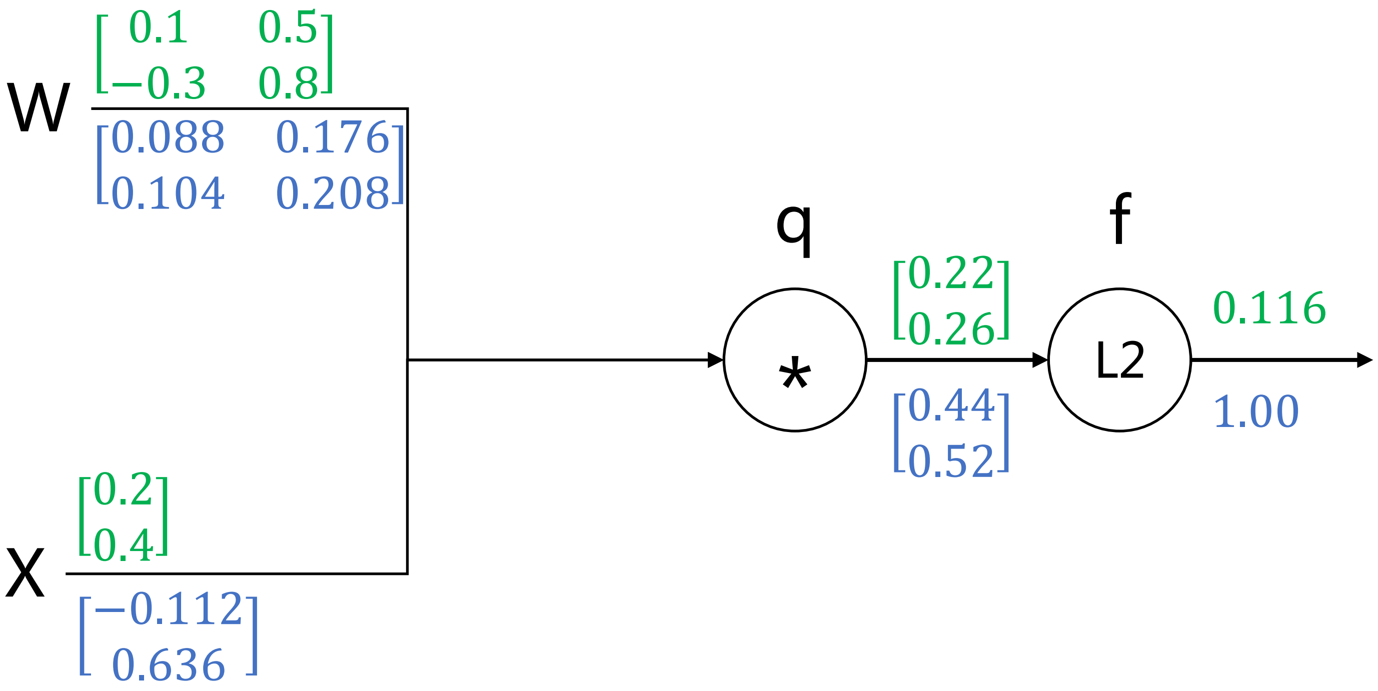
- Let $z = x + y$. What if x and y are vectors?
  - $x = (x_1, x_2)$, $y = (y_1, y_2)$
  - $z = (x_1 + y_1, x_2 + y_2)$
  - $\frac{\partial z_1}{\partial x_1} = 1$, $\frac{\partial z_1}{\partial x_2} = 0$, $\frac{\partial z_2}{\partial x_1} = 0$, $\frac{\partial z_1}{\partial x_2} = 1$
  - $\boxed{\frac{\partial z}{\partial x} = \begin{bmatrix} \frac{\partial z_1}{\partial x_1} & \frac{\partial z_1}{\partial x_2} \\ \frac{\partial z_2}{\partial x_1} & \frac{\partial z_1}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}$ Jacobian matrix

Backpropagation

- Let $y = \max(0, x)$ and x is a vector of size 4096. What is the size of the Jacobian matrix?
  - 4096×4096
- What the size of the Jacobian matrix if we use a minibatch of size 100?
  - 409600×409600
- What does the Jacobian matrix look like?
  - $\begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}$

Backpropagation

- $f(x, \mathbf{W}) = \|\mathbf{W}x\|^2 = \sum_{i=1}^{n}(\mathrm{W}x)_i^2$



$$f(q) = \|q\|^2 = q_1^2 + q_2^2 + \cdots + q_n^2$$

$$\frac{\partial f}{\partial q_i} = 2q_i$$

$$q = \begin{bmatrix} q_1 \\ \vdots \\ q_n \end{bmatrix} = \mathbf{W}x = \begin{pmatrix} W_{(1,1)}x_1 + \cdots + W_{(1,n)}x_n \\ \vdots \\ W_{(n,1)}x_1 + \cdots + W_{(n,n)}x_n \end{pmatrix}$$

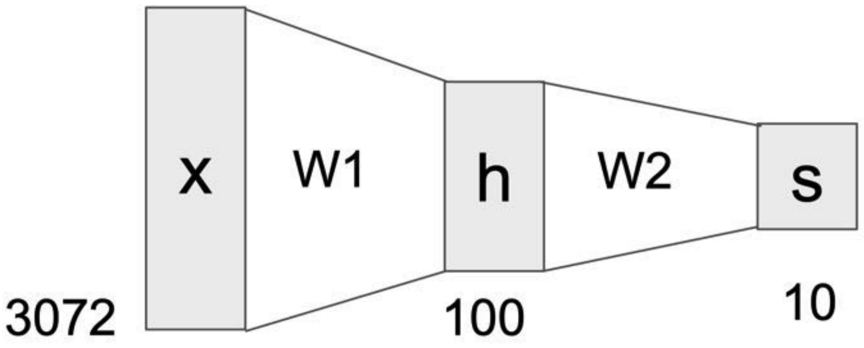
$$\frac{\partial q_k}{\partial W_{(i,j)}} = \mathbf{1}_{k=i}x_j \quad \frac{\partial f}{\partial W_{(i,j)}} = \mathbf{1}_{k=i}x_j \cdot 2\mathrm{q_i}$$

$$\frac{\partial q_k}{\partial x_i} = W_{(k,i)} \qquad \frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k}\frac{\partial q_k}{\partial x_i}$$

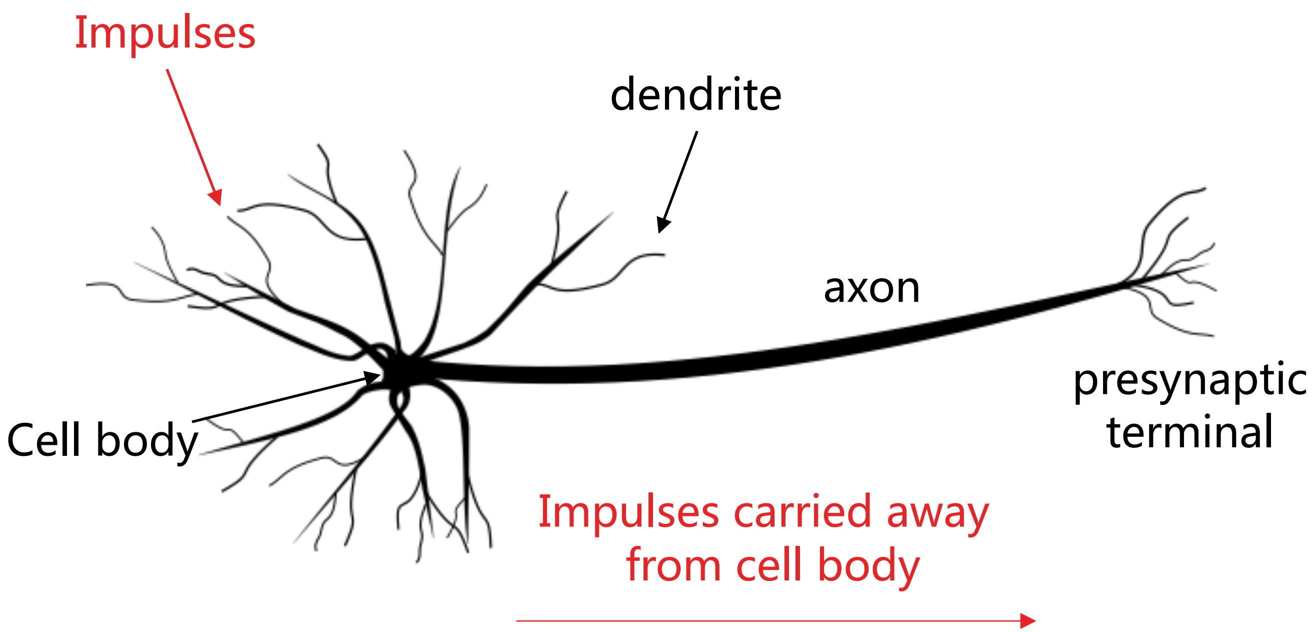
$$= \sum_k 2q_k W_{(k,i)}$$

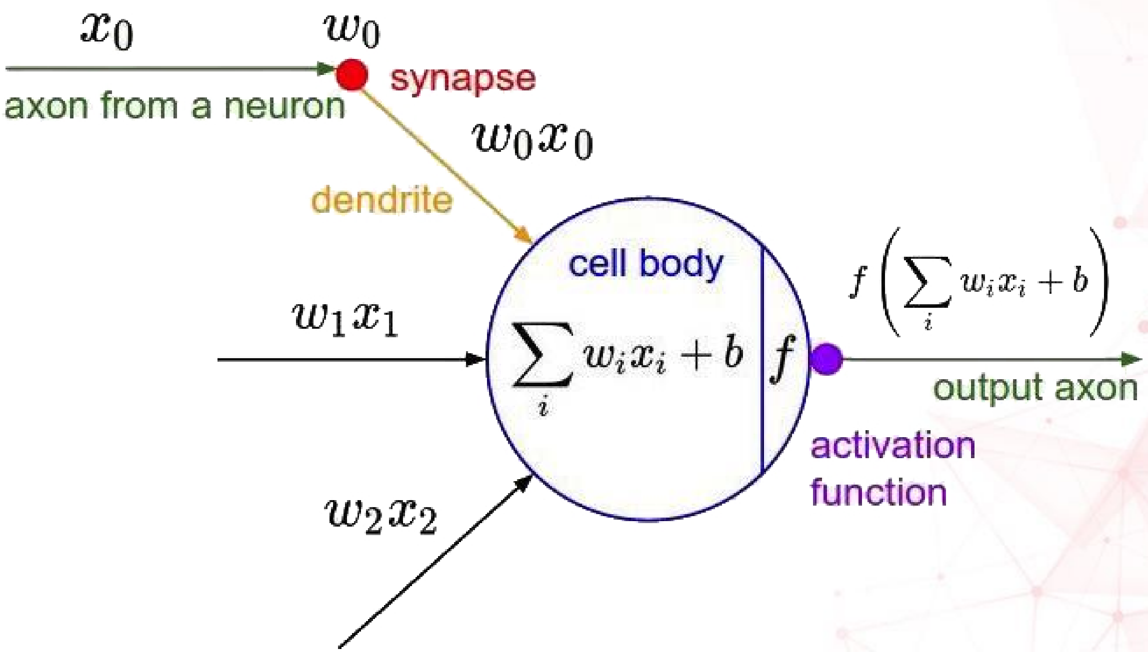
Neural Networks

- Linear Score Function
  - $f = \mathbf{W}x$
- 2-Layer Neural Network
  - $f = \mathbf{W_2} \max(0, \mathbf{W_1}x)$
- 3-Layer Neural Network
  - $f = \mathbf{W_3} \max(\mathbf{W_2} \max(0, \mathbf{W_1}x))$

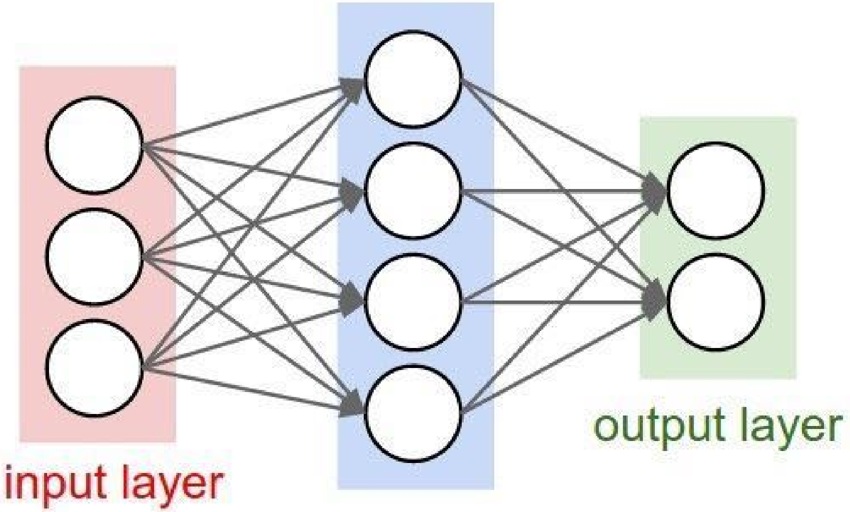


Neural Networks

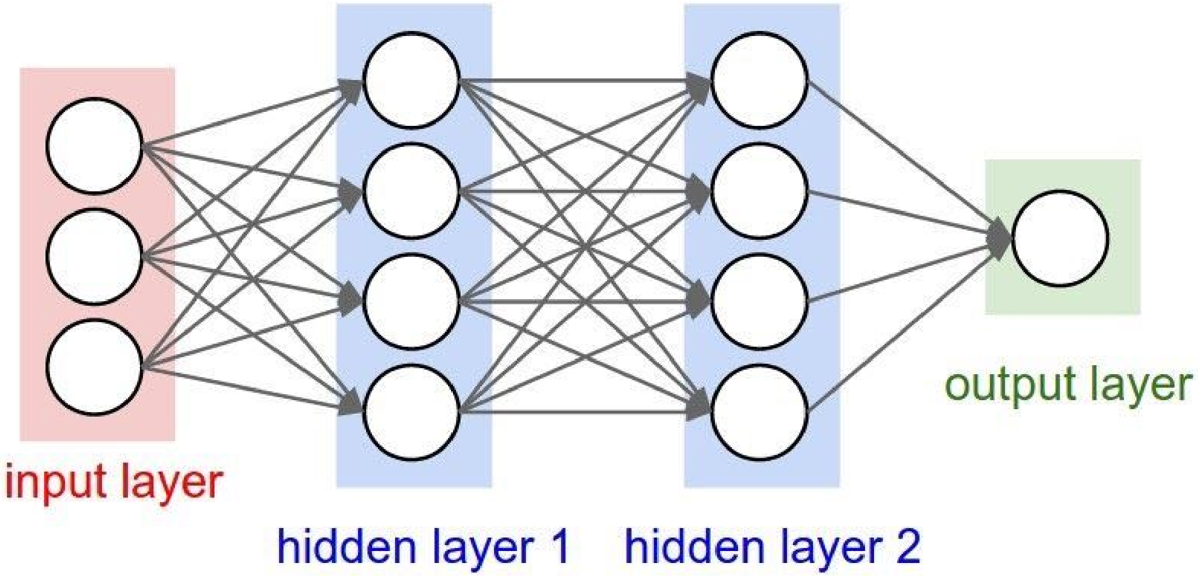




Neural networks: Architectures



Fully Connected Layers



- “2-layer Neural Net”
- “1-hidden-layer Neural Net”

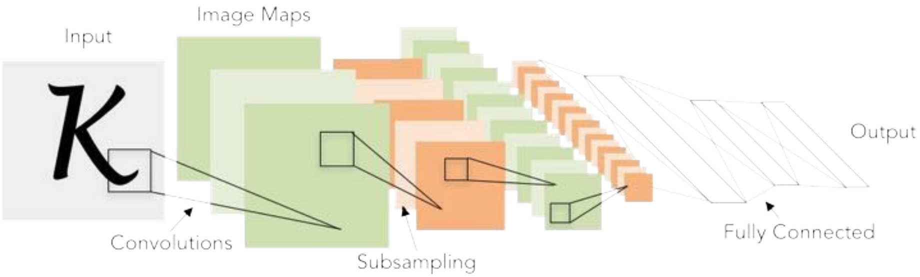
- “3-layer Neural Net”
- “2-hidden-layer Neural Net”

Part V

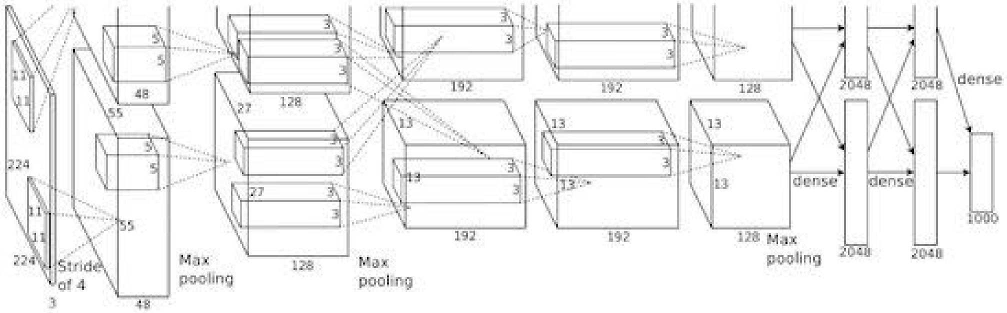
Convolutional Neural Networks

Important Events of CNNs

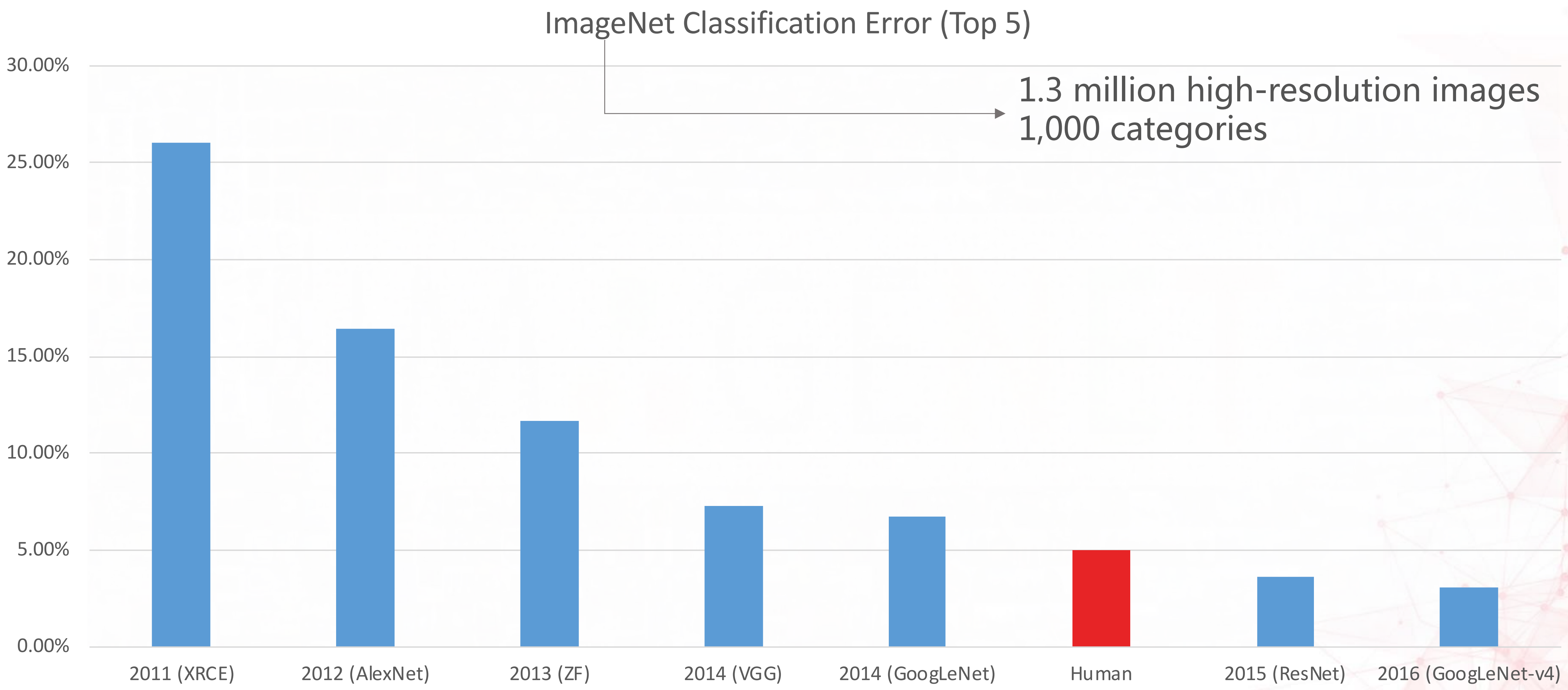
- LeNet-5
  - Used for Document Classification (1998)



- AlexNet
  - Used for Image Classification (2012)

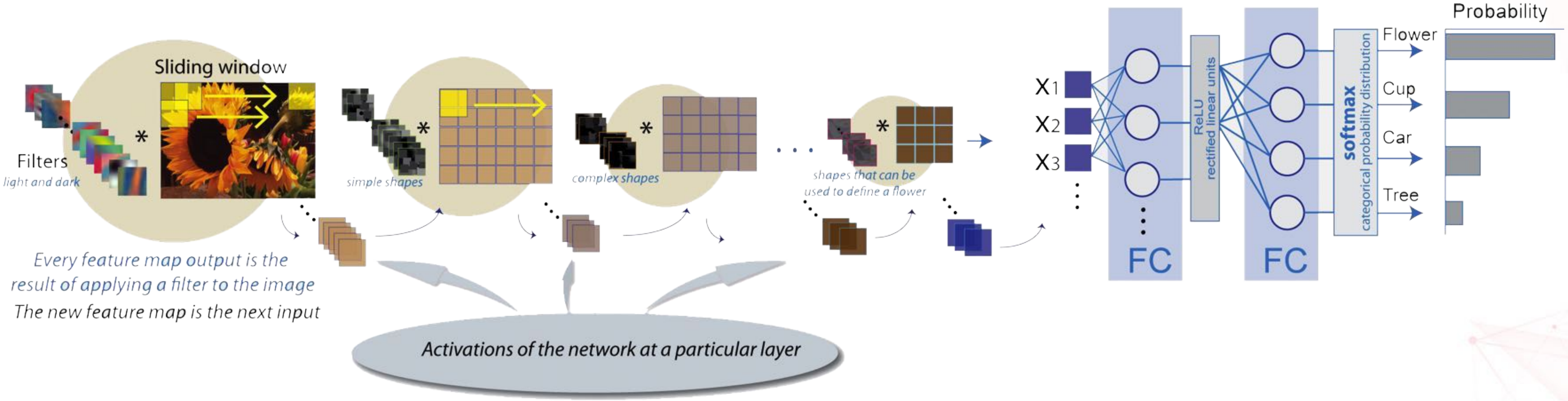


Fast-forward to Today: CNNs are Everywhere



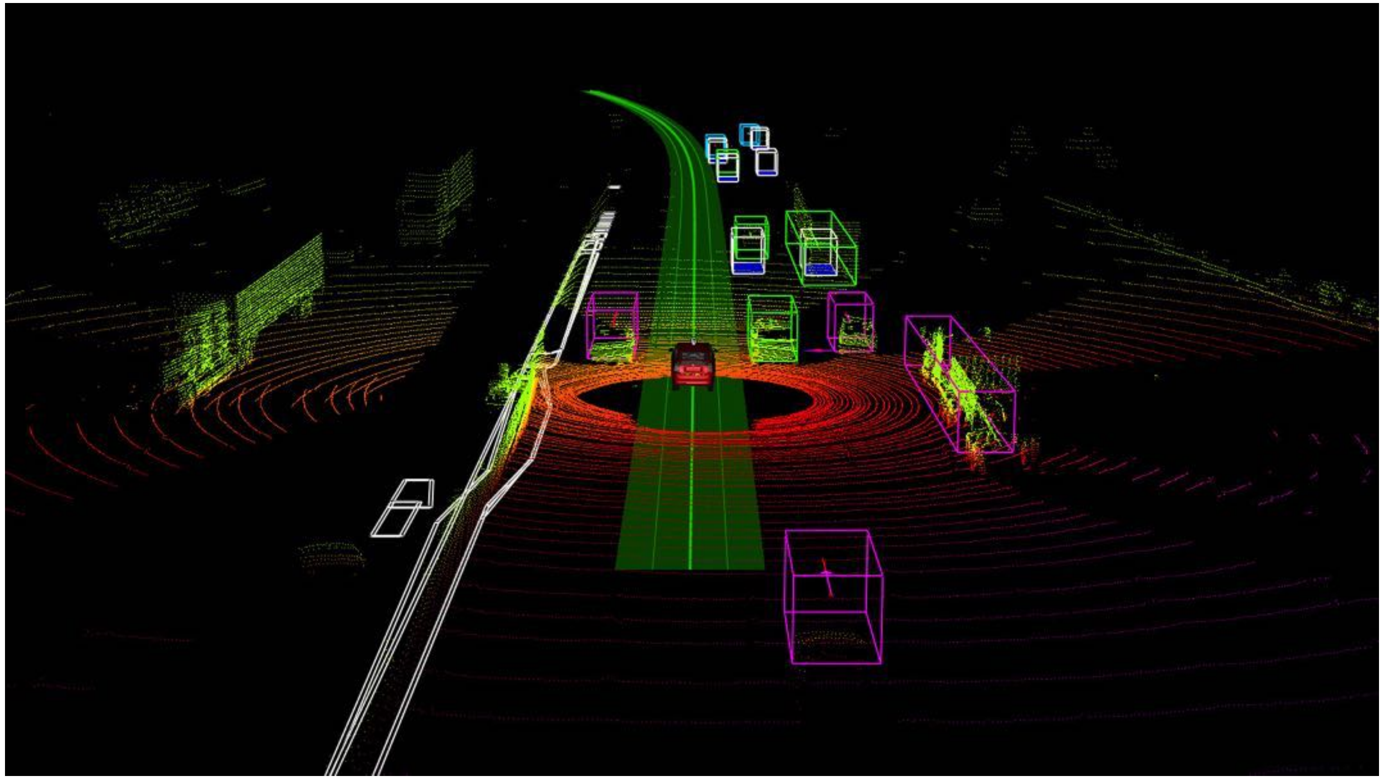
Fast-forward to Today: CNNs are Everywhere

- Image Classification



Fast-forward to Today: CNNs are Everywhere

- Object Detection in 2D/3D



Fast-forward to Today: CNNs are Everywhere

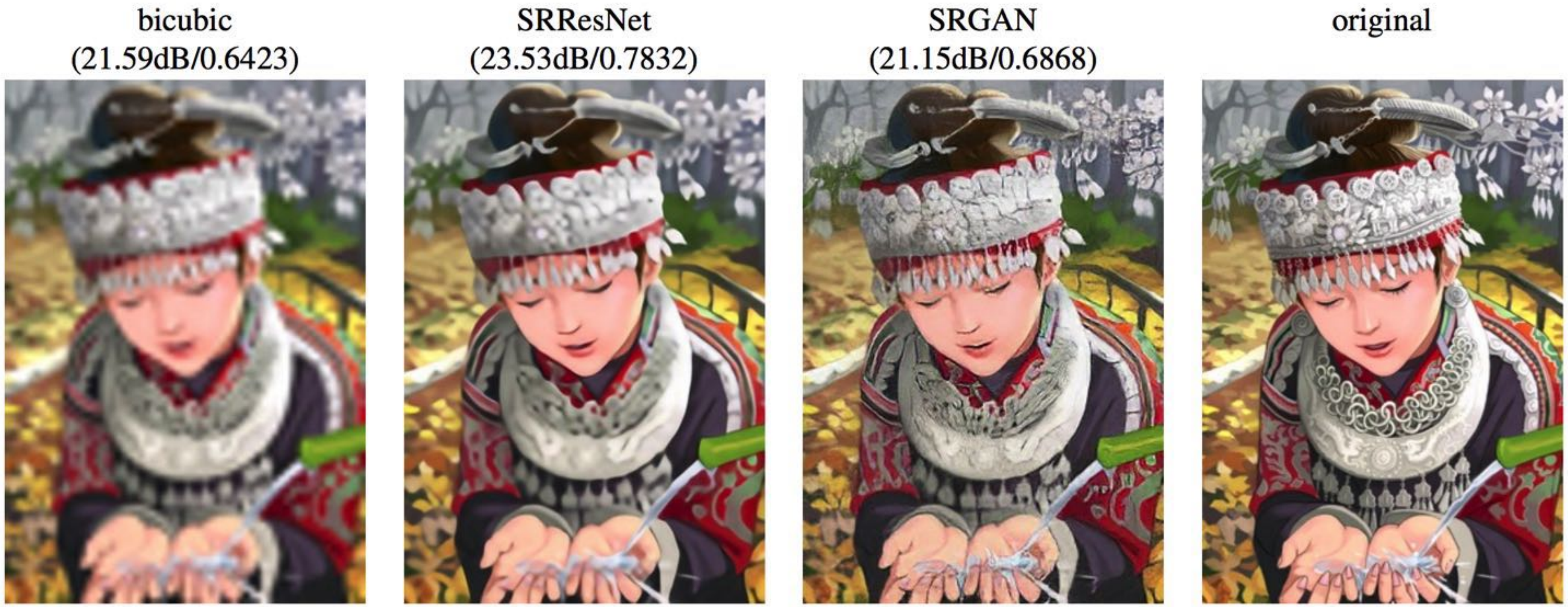
- Semantic Segmentation

Fast-forward to Today: CNNs are Everywhere

- Pose Estimation

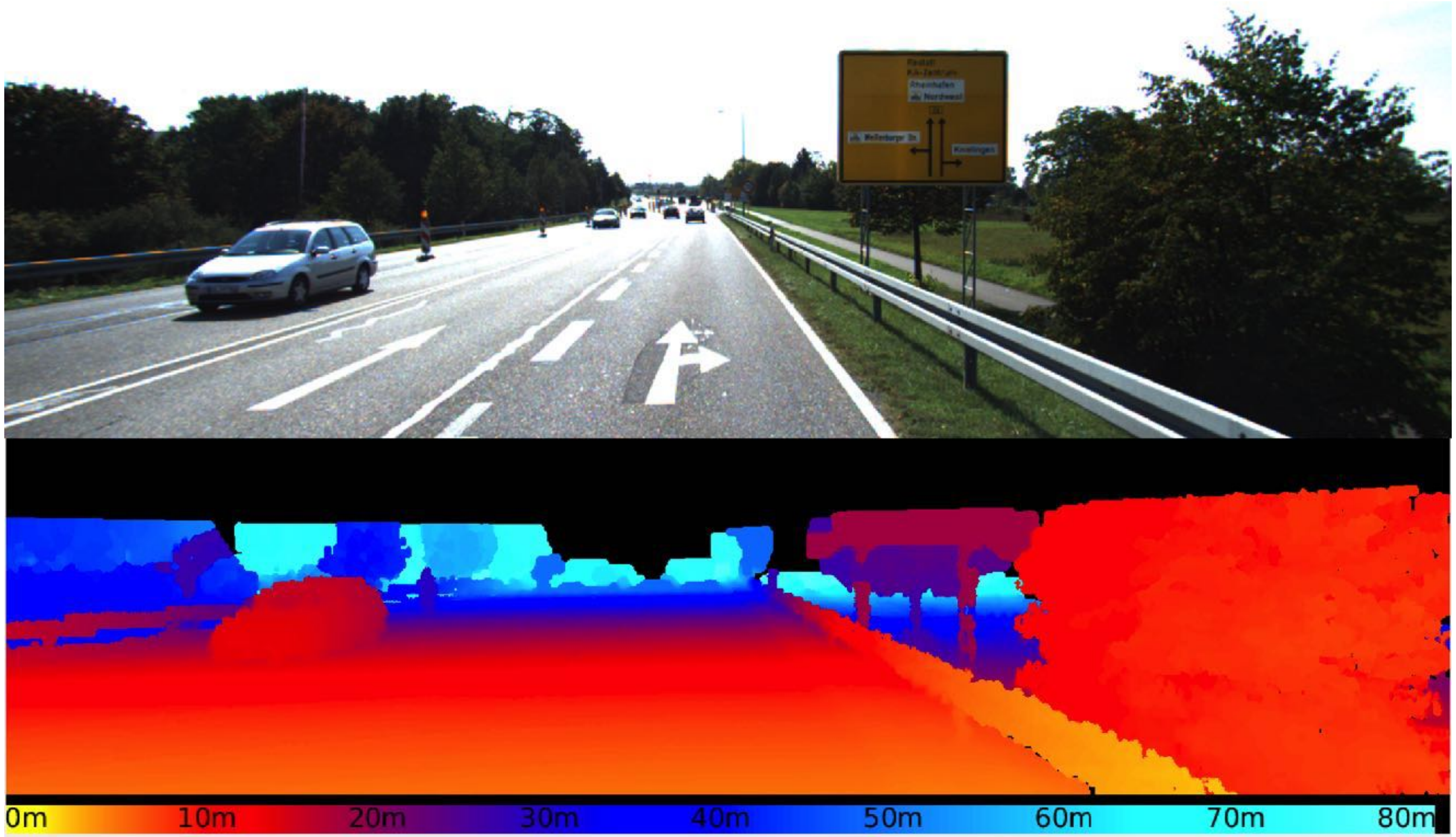
Fast-forward to Today: CNNs are Everywhere

- Image Super Resolution



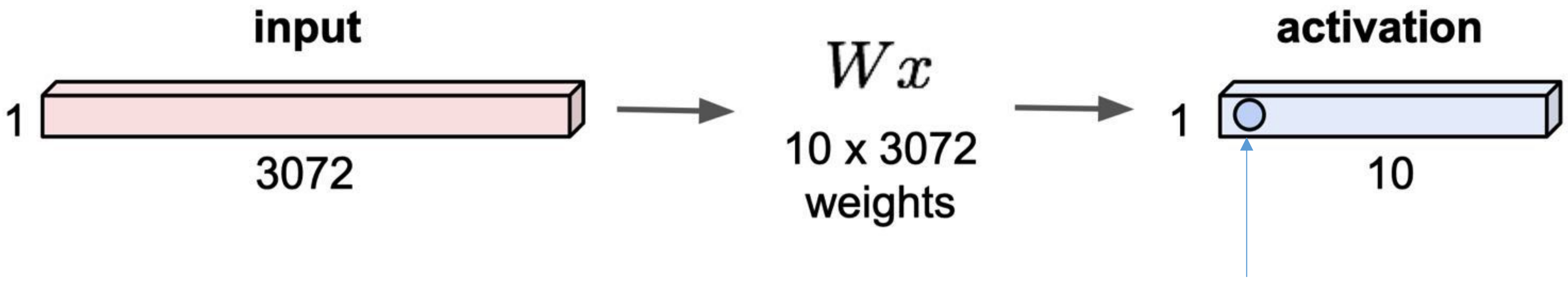
Fast-forward to Today: CNNs are Everywhere

- Depth Estimation



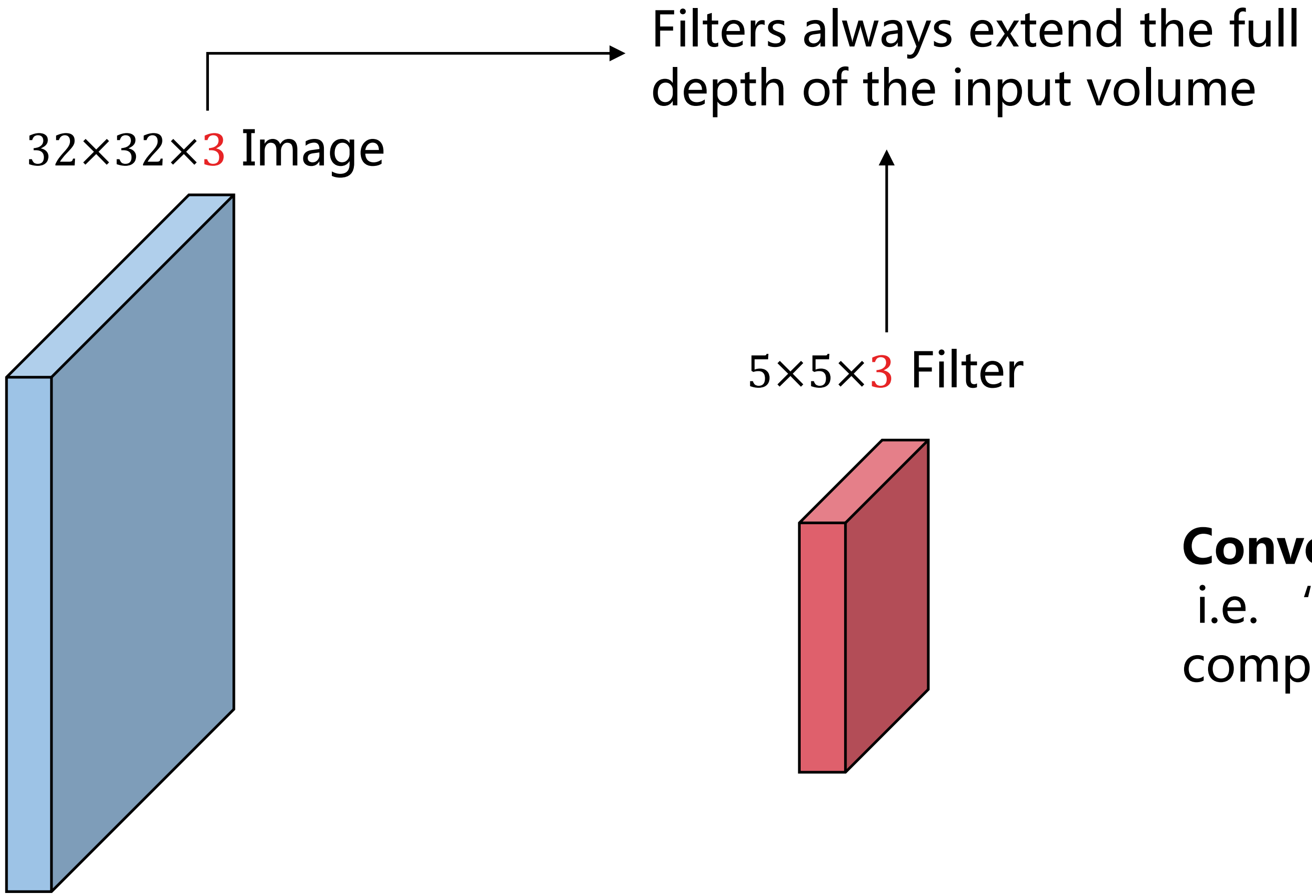
Recap: Fully Connected Layer

- Given an image of size $32 \times 32 \times 3$



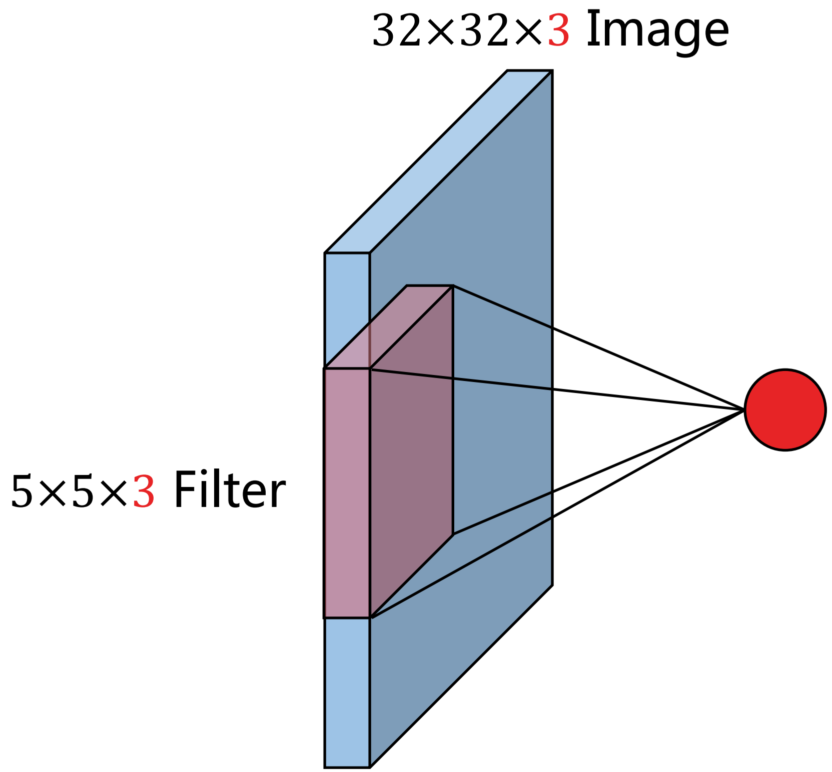
1 number
the result of taking a dot product between a row of W and the input (a 3072-dimensional dot product)

Convolutional Layer



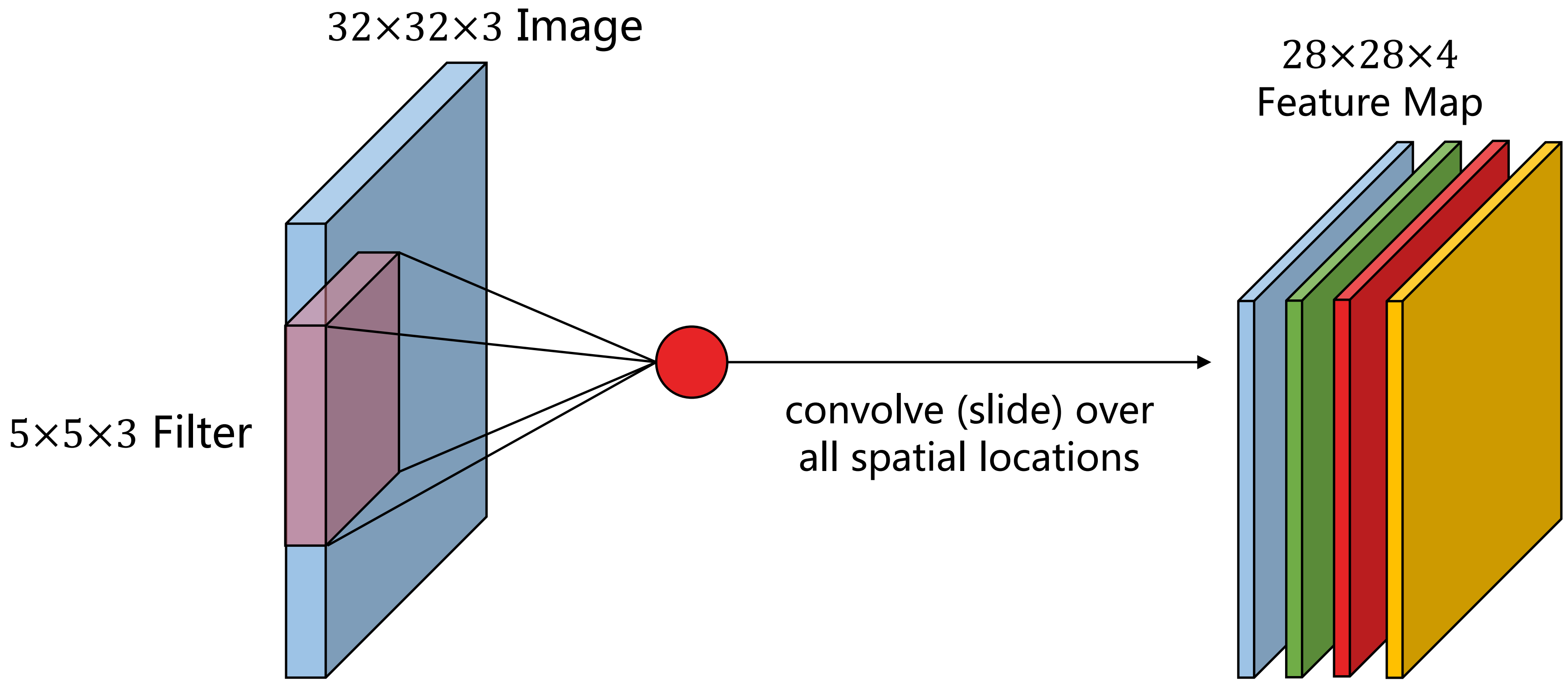
Convolve the filter with the image
i.e. “slide over the image spatially, computing dot products”

Convolutional Layer



1 number
the result of taking a dot product between the filter and a small 5×5×3 chunk of the image
(i.e. 75-dimensional dot product + bias)

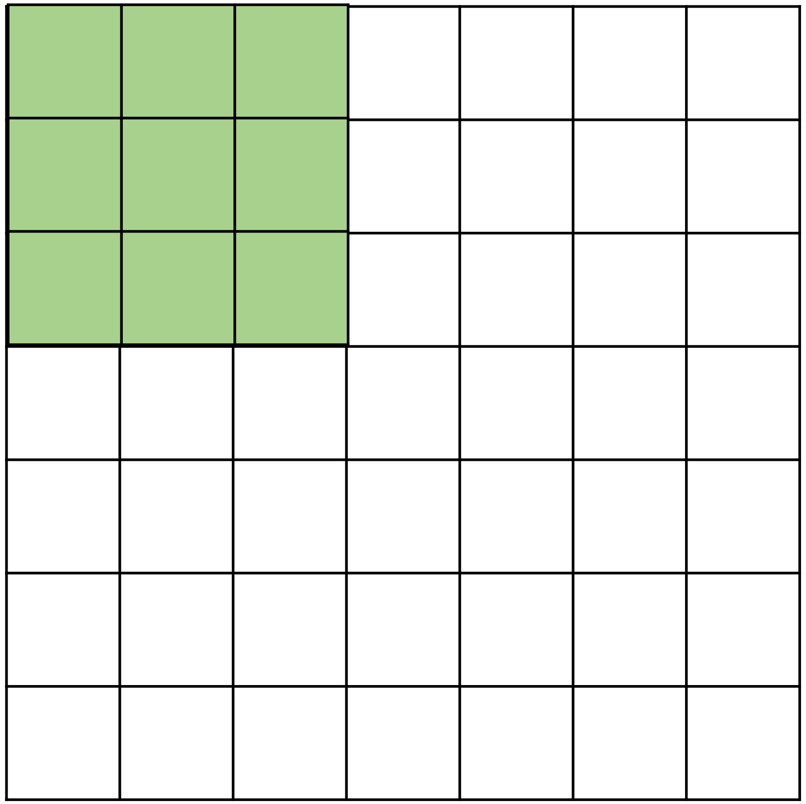
Convolutional Layer



Conclusion: If we have 4 $5\times5\times3$ filters, we can get 4 separate feature maps.

The number of parameters of the convolutional layer is $5\times5\times3\times4+5\times3\times4=360$.

Convolutional Layer



Assume the input is of size 7×7,

and the filter is of size 3×3.

With Stride = 1:

Output size is 5×5.

With Stride = 2:

Output size is 3×3.

With Stride = 3:

Cannot apply 3×3 filter on 7×7 input with stride 3.

Output Size= (Input Size – Filter Size) / Stride + 1

Convolutional Layer

0	0	0	0	0	0	0	0	0	0
0									0
0									0
0									0
0									0
0									0
0									0
0									0
0	0	0	0	0	0	0	0	0	0

Sometimes, we pad zeros to the border.

Assume the input is of size 7×7,

and the filter is of size 3×3.

With Stride = 3 and pad = 1

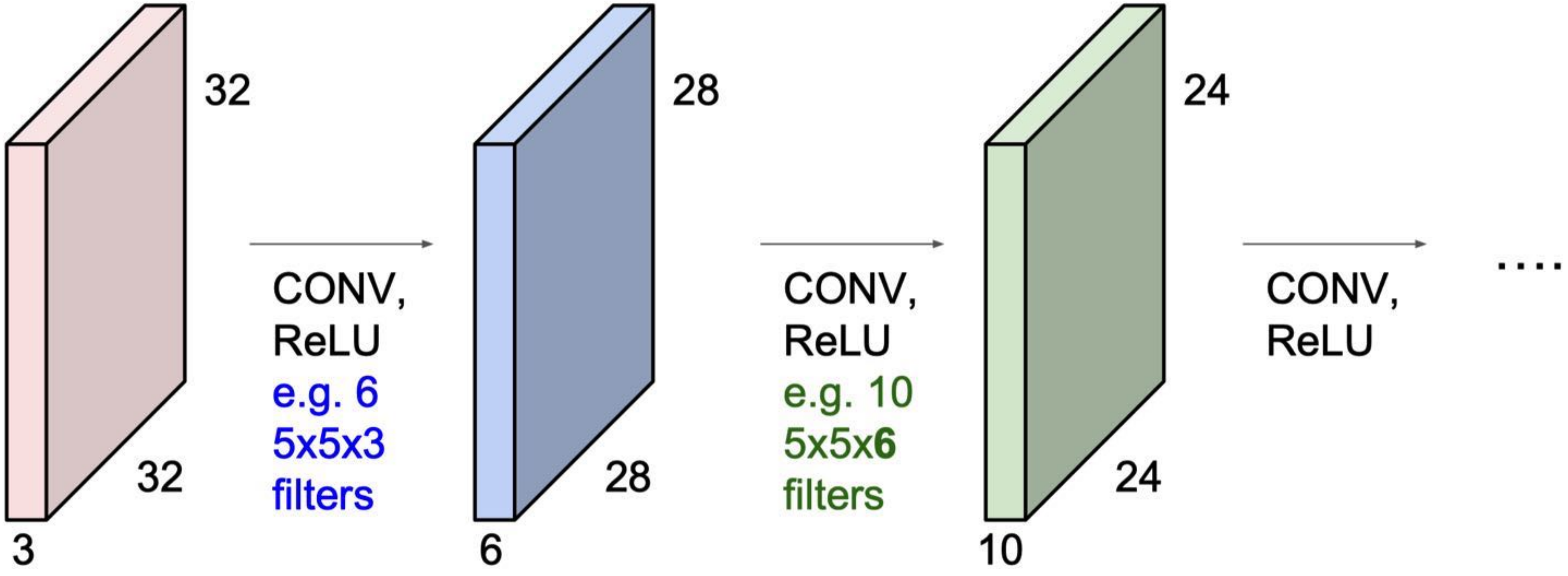
Output size is 3×3.

UPDATE:

Output Size =

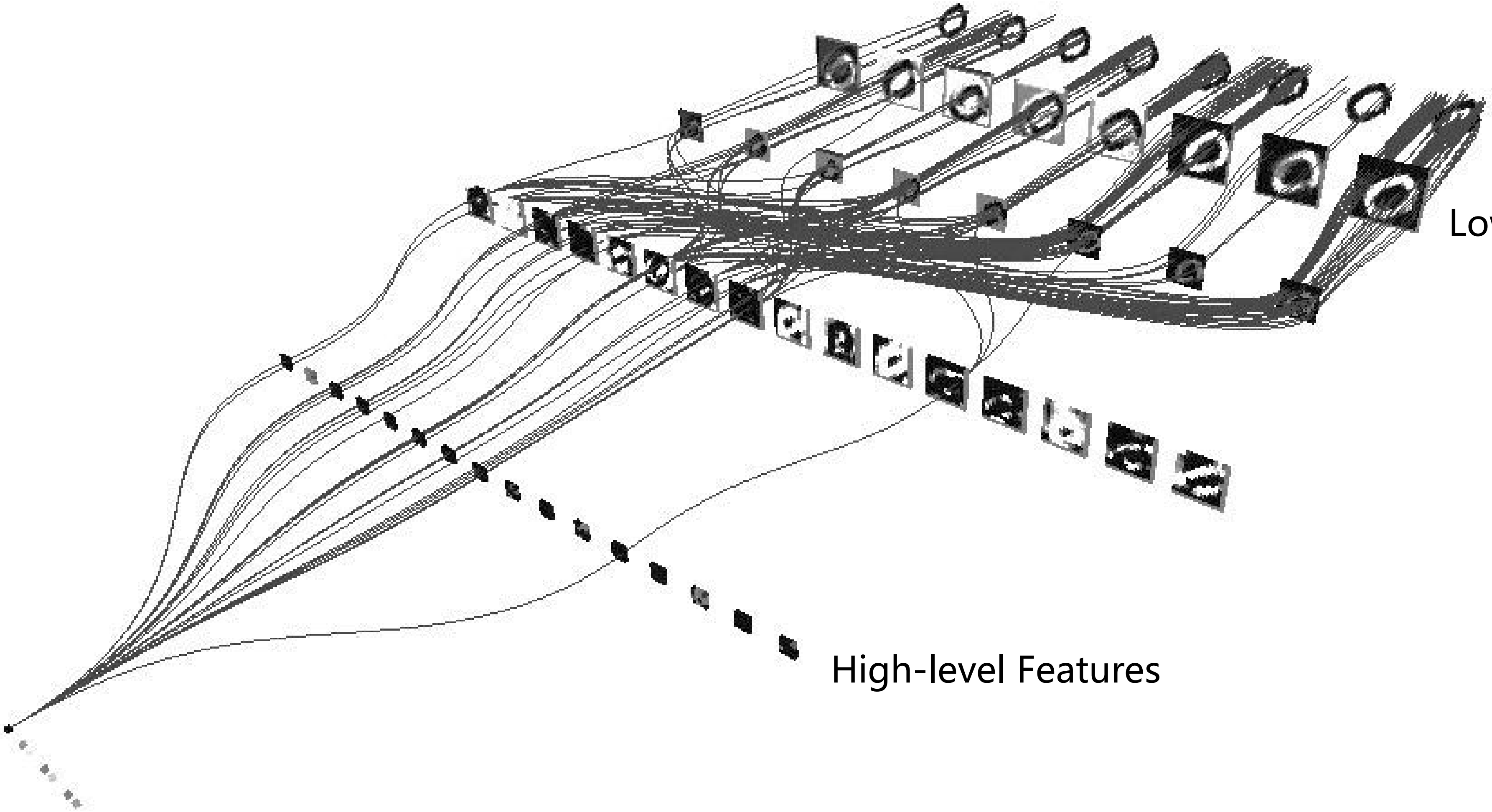
(Input Size – Filter Size + 2 * Padding) / Stride + 1

Convolutional Neural Networks



- ConvNet is a sequence of Convolutional Layers, interspersed with activation functions
- Shrinking too fast is not good, doesn’ t work well.

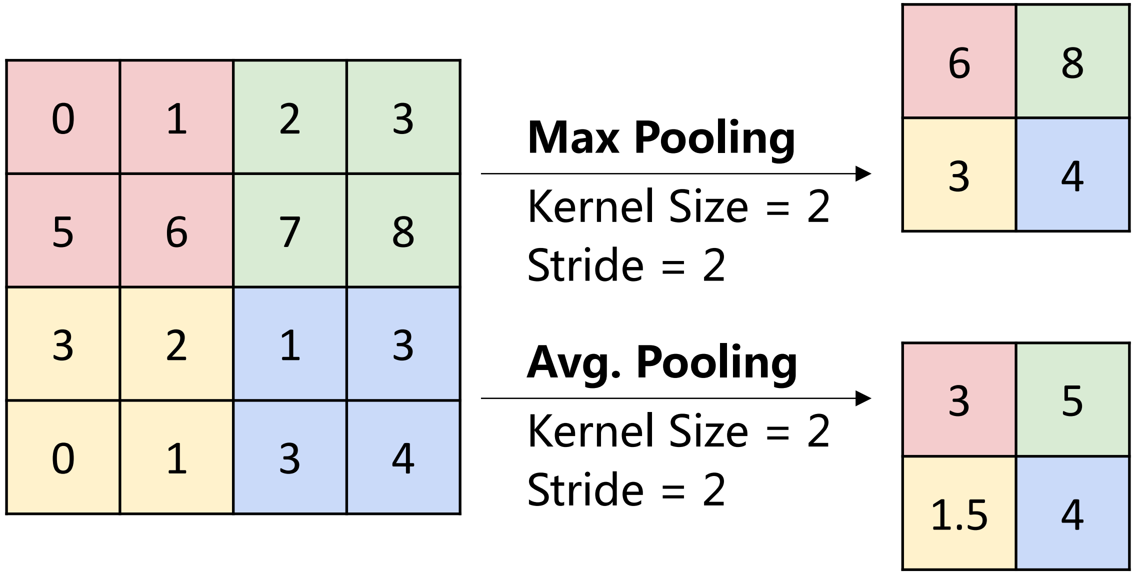
Convolutional Neural Networks

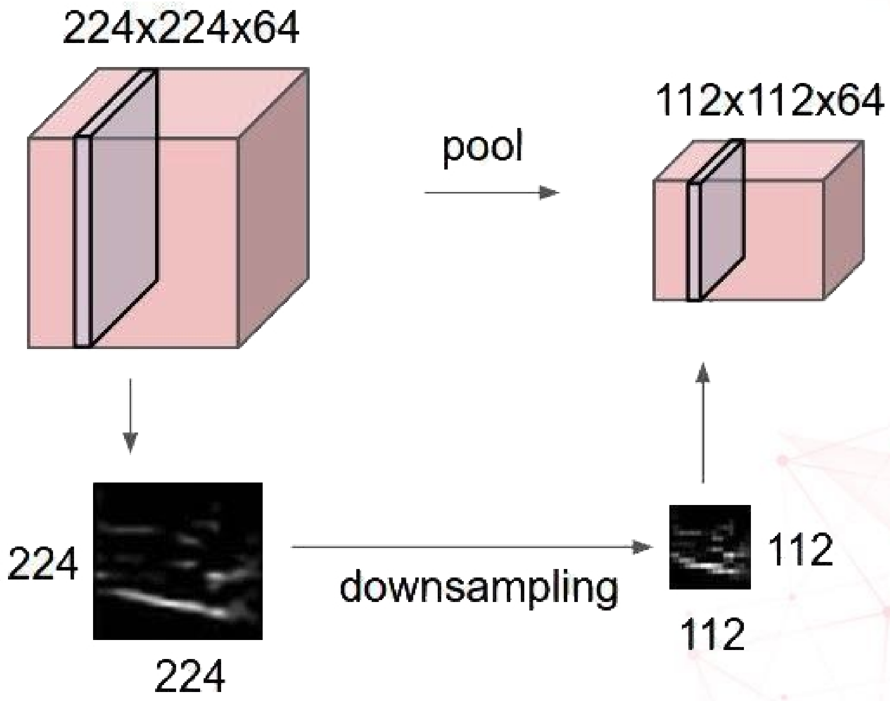


Low-level Features

High-level Features

Pooling Layer



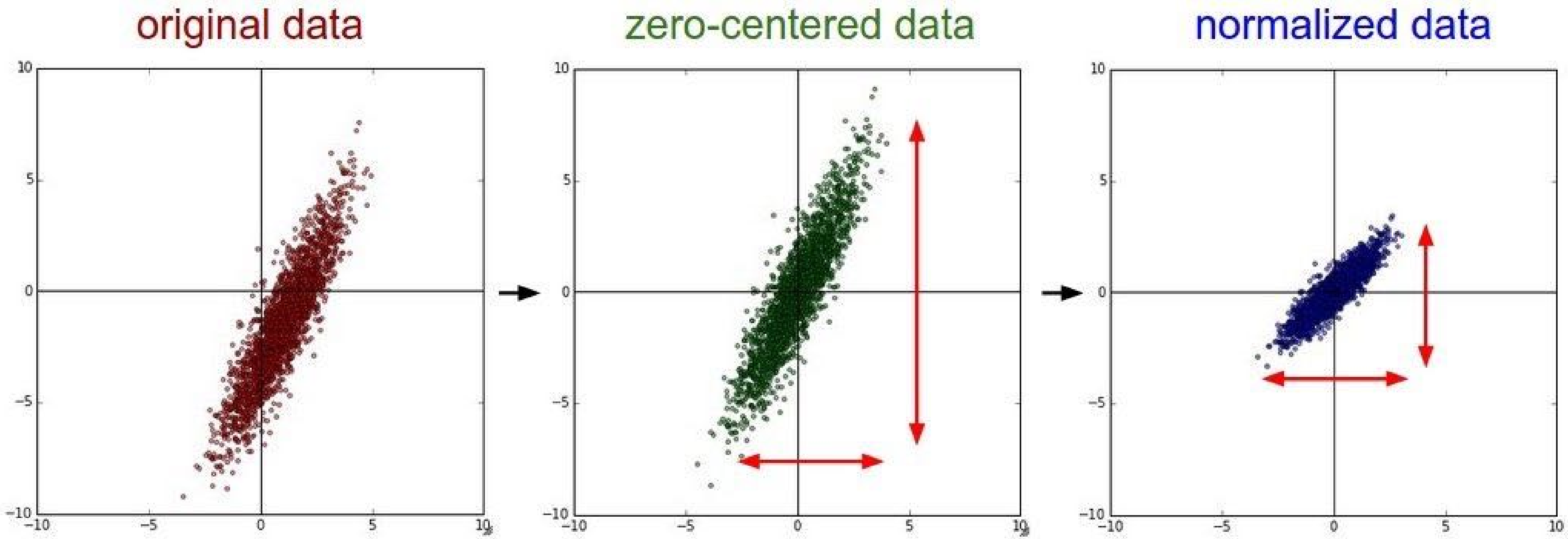


How to Train a Neural Network?

- Babysitting the Learning Process
  - Data Preprocessing
  - Choose the architecture (Convolutional Layers, Activation functions, Losses)
  - Weights initialization
  - Optimizers used for updating parameters
- Optional
  - Data Augmentation
  - Batch Normalization
  - Dropout

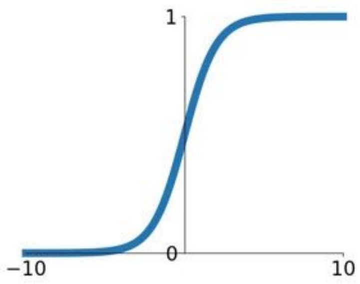
Data Preprocessing

- Normalize

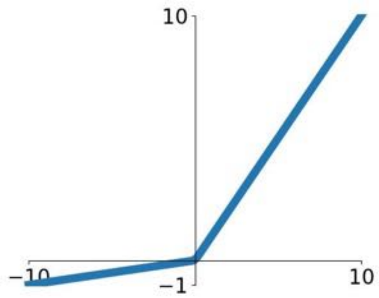


Activation Functions

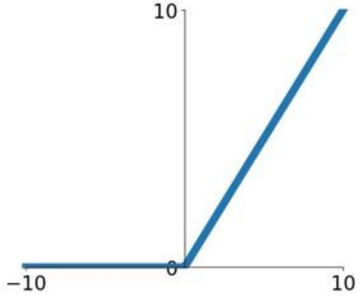
- Sigmoid
  - $\sigma(x) = \frac{1}{1+e^{-x}}$
- ReLU
  - $f(x) = \max(0, x)$
- Leaky ReLU
  - $f(x) = \max(0.01x, x)$
- ELU
  - $f(x) = \begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$



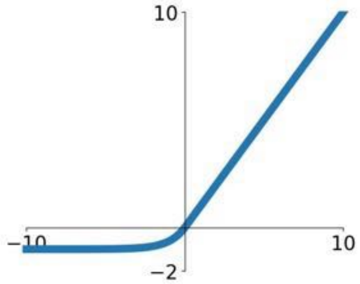
Sigmoid



Leaky ReLU



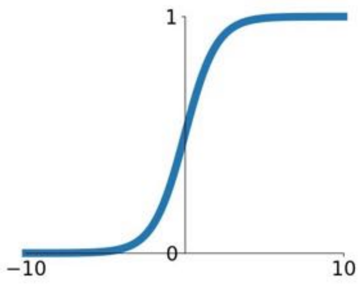
ReLU



ELU

Activation Functions

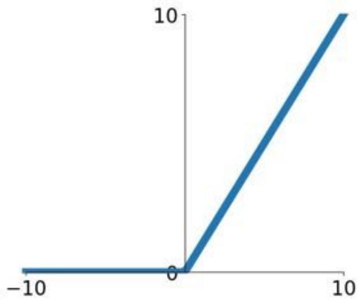
- Sigmoid
  - $\sigma(x) = \frac{1}{1+e^{-x}}$
  - Squashes numbers to range $[0,1]$



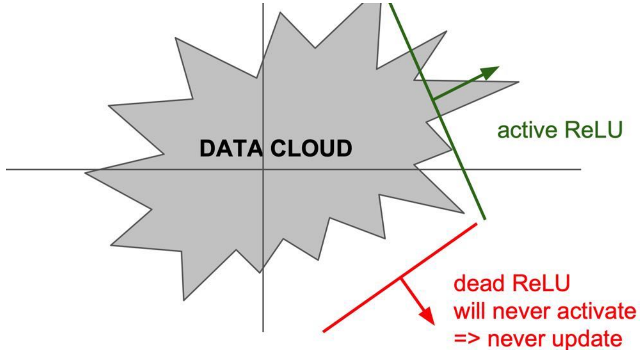
- Issues
  - Saturated neurons "kill" the gradients
  - Sigmoid outputs are not zero-centered
  - exp() is a bit compute expensive

Activation Functions

- ReLU
  - $f(x) = \max(0, x)$

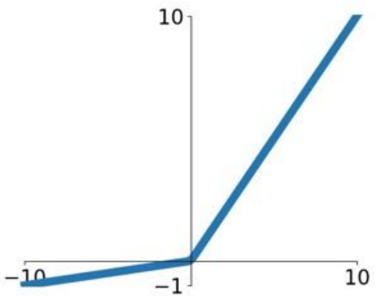


- Characteristics
  - Very computationally efficient
  - Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Issues
  - Not zero-centered output
  - dead ReLU



Activation Functions

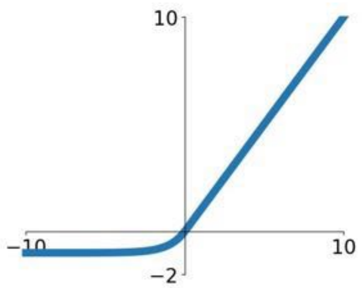
- Leaky ReLU
  - $f(x) = \max(0.01x, x)$



- Characteristics
  - Does not saturate
  - Very computationally efficient
  - Converges much faster than sigmoid/tanh in practice (e.g. 6x)
  - will not “die”

Activation Functions

- ELU
  - $f(x) = \begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$



- Characteristics
  - All benefits of ReLU
  - Closer to zero mean outputs
  - Negative saturation regime compared with Leaky ReLU adds some robustness to noise
- Issues
  - Computation requires exp()

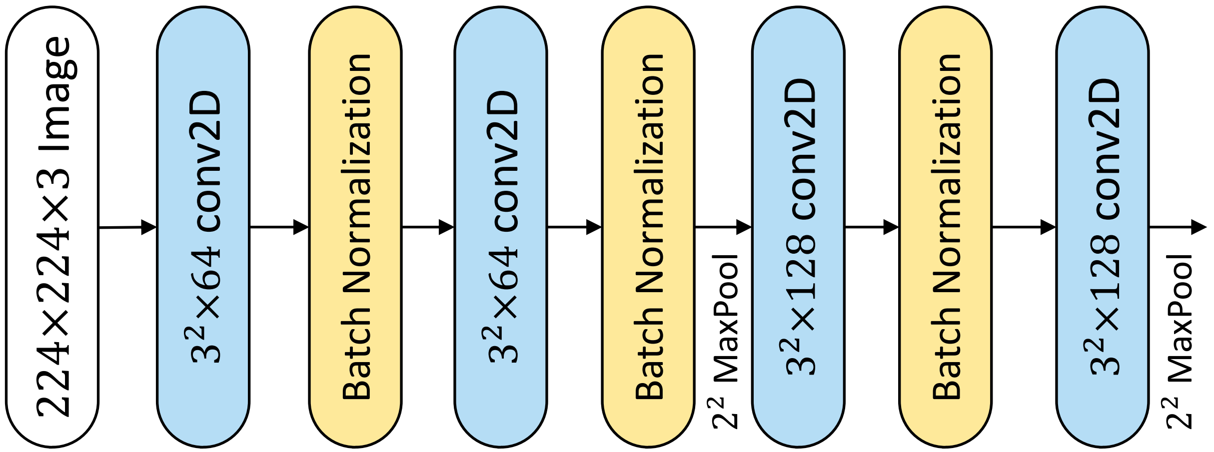
Weights Initialization

- What if all the initial values are set to 0?
  - Output the same thing and have the same gradient.
- What if initial values are samples from a Gaussian distribution $\sigma(0, 0.01)$?
  - Works small for small networks, but problems with deeper networks.
- How to solve the problem?
  - Xavier initialization
  - Kaiming initialization
  - …

Batch Normalization

- "Do you want unit gaussian activations? just make them so."
- Consider a batch of activations at some layer. To make each dimension unit gaussian, apply:

$$\hat{x}^k = \frac{x^k - \mathrm{E}[x^k]}{\sqrt{\mathrm{Var}[x^k]}}$$



Note: BNs are usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

Batch Normalization

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

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

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

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

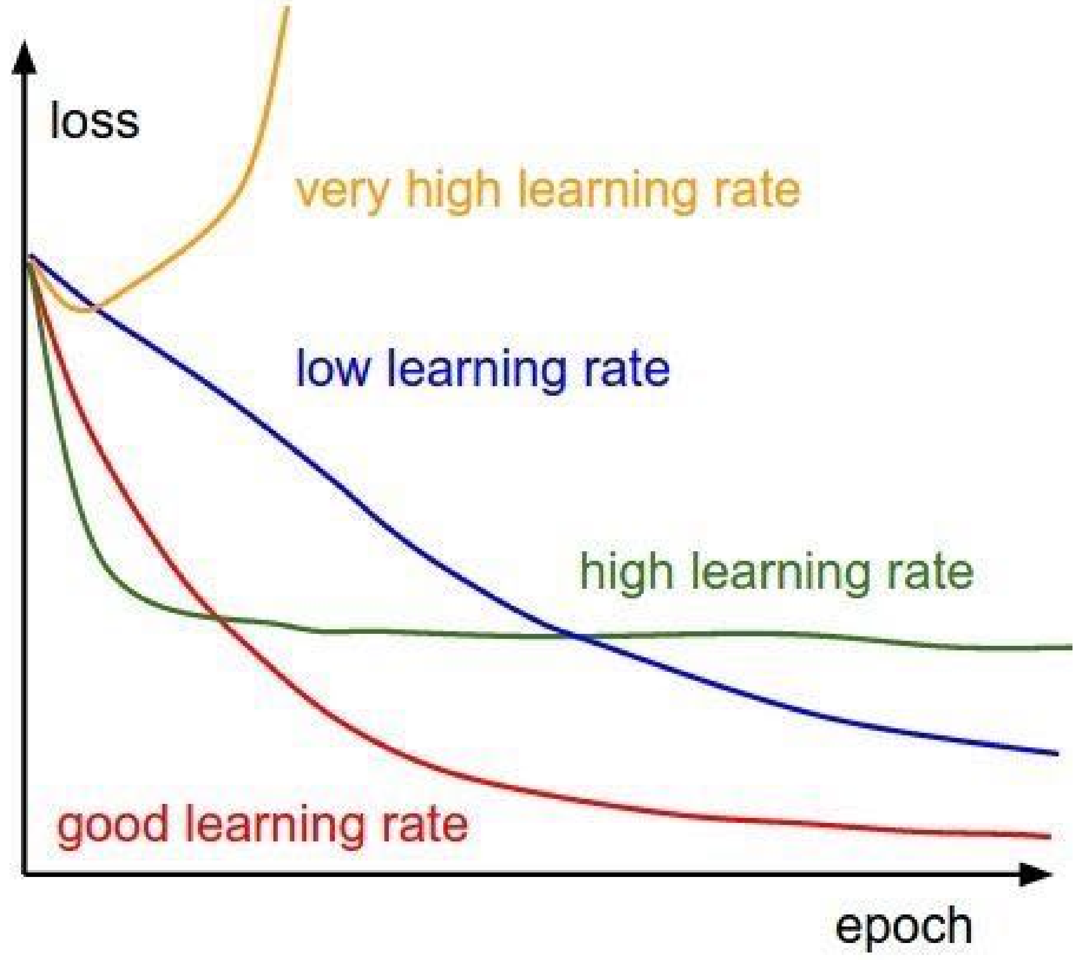
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

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

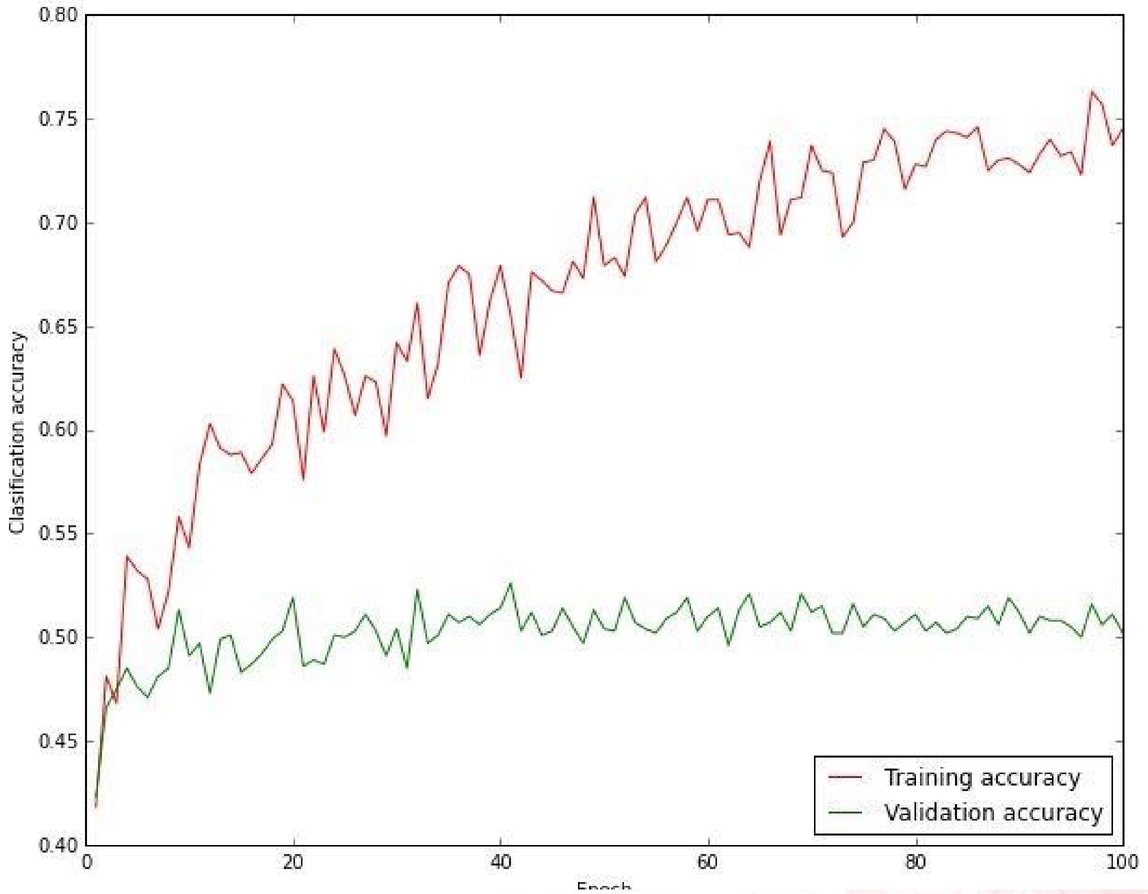
- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

Babysitting the Training Process

- Choose a Proper Learning Rate

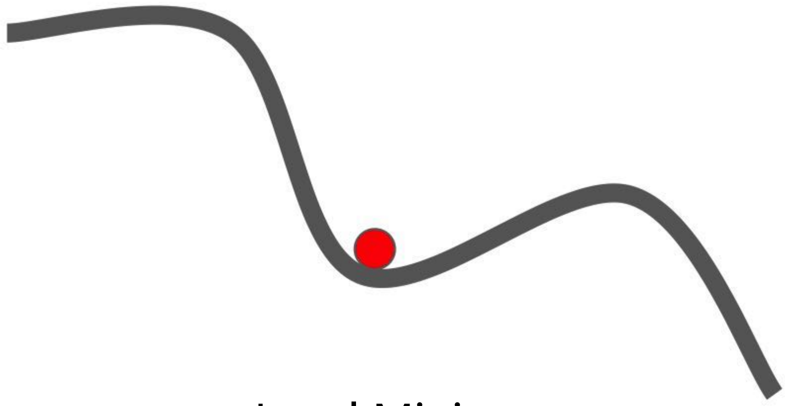


- Overfitting



Optimizers

- SGD
  - $g_t = \nabla_{\theta_{t-1}} f(\theta_{t-1})$
  - $\nabla_{\theta_t} = -\eta g_t$
- SGD + Momentum
  - $m_t = \mu m_{t-1} + g_t$
  - $\nabla \theta_t = -\eta m_t$
  - Typically, $\mu = 0.9$ or 0.99
- Problems with SGD



Local Minima

Saddle Point

Optimizers

- AdaGrad
  - $n_t = n_{t-1} + g_t^2$
  - $\nabla\theta_t = -\frac{\eta}{\sqrt{n_t + \epsilon}} \cdot g_t$
- RMSProp
  - $n_t = v n_{t-1} + (1 - v) g_t^2$
  - $\nabla\theta_t = -\frac{\eta}{\sqrt{n_t + \epsilon}} \cdot g_t$
- Adam
  - $m_t = \mu m_{t-1} + (1 - \mu) g_t$
  - $n_t = v n_{t-1} + (1 - v) g_t^2$
  - $\widehat{m_t} = \frac{m_t}{1 - \mu^t}$
  - $\widehat{n_t} = \frac{n_t}{1 - v^t}$
  - $\nabla\theta_t = -\frac{\widehat{m_t}}{\sqrt{\widehat{n_t} + \epsilon}} \cdot \eta$

Thank You!