



Neural Networks

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Historical Notes on Neural Networks

- Introduced in the 1950s as models of low-level human brain functions
 - neurons, networks of neurons
- Suited to numerical attributes
- Current evolution: **deep neural networks**, widely used in
 - Computer vision
 - Speech recognition

Historical Notes on Neural Networks

- Inspired by findings in neuroanatomy and neurophysiology (19th – early 20th centuries)
- 1943: McCulloch and Pitts' model of neurons as *logic units*
- 1949: Hebb's model of changes in *synaptic strength* and *cell assemblies* as the origin of adaptation, learning and thinking
- 1957: Rosenblatt's **perceptron**:
 - network of McCulloch and Pitts' neural elements
 - *training procedures* for adjusting connection weights
 - applications to pattern recognition: *error-correction* training
 - perceptron learning algorithm

Historical Notes on Neural Networks

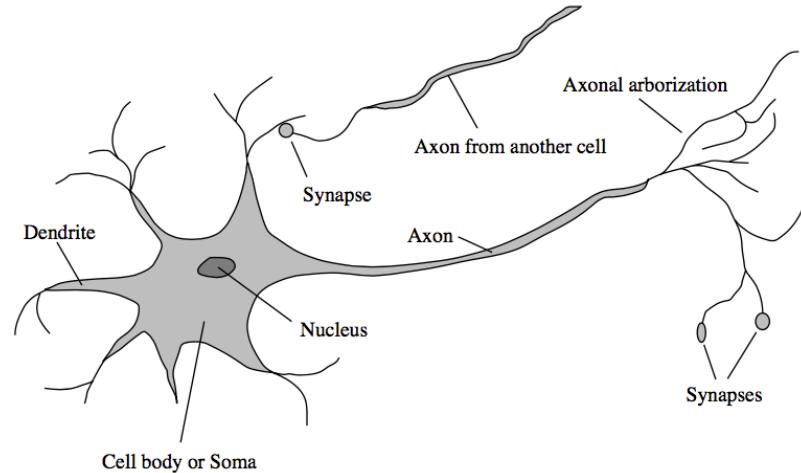
- 1970s:
 - limits of perceptrons (limited expressive power, lack of mathematical rigor)
 - drop of interest in neural networks [M.L. Minsky and S.A. Papert, *Perceptrons*, MIT Press, 1969]
- Mid-1980s:
 - renaissance of neural networks: the **connectionist** approach
 - learning algorithm: **back-propagation**
 - theoretical support: statistics, computational learning theory
 - Seminal work:
 - D.E. Rumelhart, J.L. McClelland (Eds.), *Parallel Distributed Processing*, MIT Press, 1986
 - D.E. Rumelhart, G.E. Hinton, R.J. Williams, *Learning representations by back-propagating errors*, Nature 323, 533-536, 1986

Historical Notes on Neural Networks

- Since the 1990s - different kinds of ANNs:
 - Feed-Forward Multi-Layer Perceptron
 - Radial Basis Networks
 - Recurrent networks:
 - Long Short-Term Memory (LSTM) networks
 - Hopfield networks, associative memories
 - Boltzmann machines
- Applications in several fields: computer vision, pattern recognition, control systems, etc.
- Today: great interest on **deep** neural networks

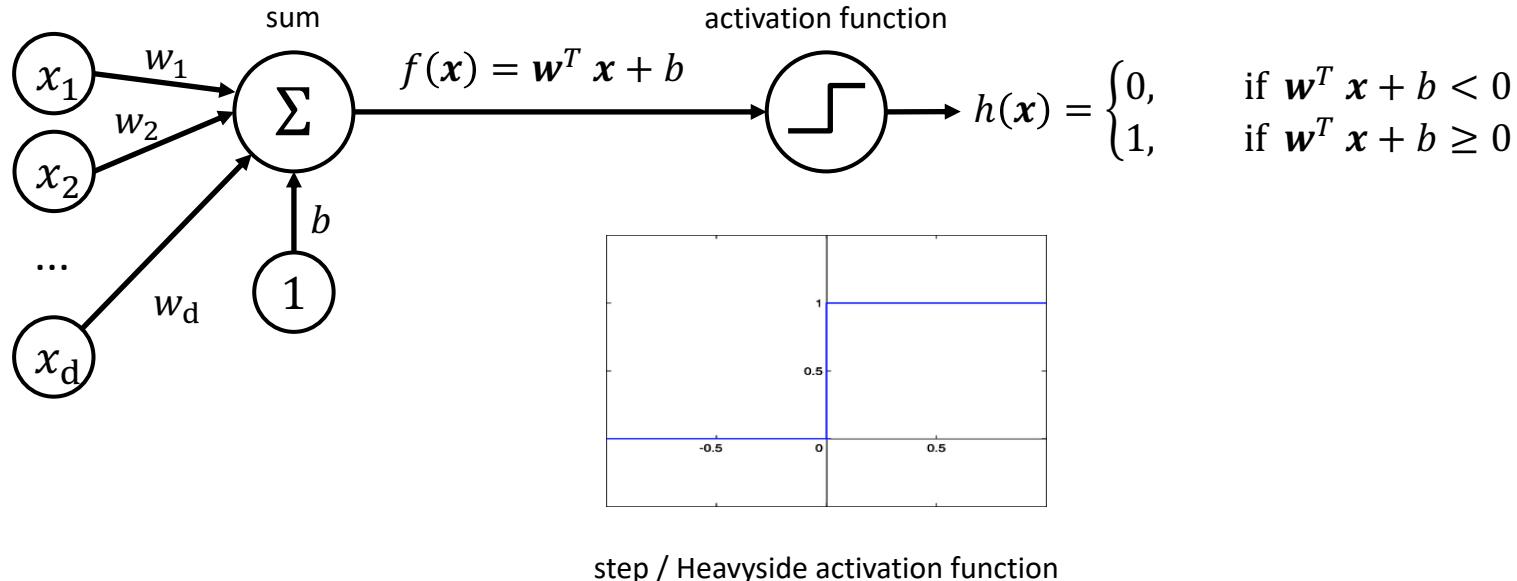
Brains and Neurons

- Basic unit: **neuron** (nerve cell)
- 10^{11} neurons, 10^{15} connections
- Apparently simple neuron behavior
 - firing (up to 103 Hz) in response to specific **patterns** of input signals
- Massive parallelism
- Robustness to noise
- Learning capability: novel connections between neurons and changing connection strength in response to external stimuli



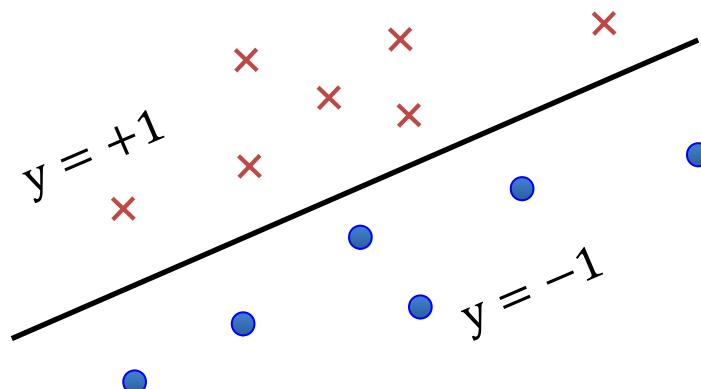
The Perceptron

- McCulloch and Pitts' model of neurons as *logic units* (1943):



Perceptron as a Linear Classifier

- $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$ corresponds to a linear discriminant function in feature space
- $f(\mathbf{x})$ is proportional to the distance of \mathbf{x} to the hyperplane
- $h(\mathbf{x})$ is equal to 1 in the positive-class region, and to 0 in the negative-class region



The Perceptron Learning Algorithm

- It is known that experience and learning change (among other things) the connection strength between neurons in the human brain
- Can the perceptron emulate this behaviour?
- To this end, the **connection weights** must be modified by some *learning algorithm* to reproduce a desired input-output behaviour, according to a given set of examples
- Such an algorithm was devised by F. Rosenblatt in 1960

The Perceptron Learning Algorithm

- Define a loss function (i.e., the perceptron loss)
$$L(\mathbf{w}, b) = \sum_i \max(0, -y_i f(\mathbf{x}_i)) = -\sum_{i:y_i f(\mathbf{x}_i) < 0} y_i f(\mathbf{x}_i)$$
 - i indexes the misclassified training samples

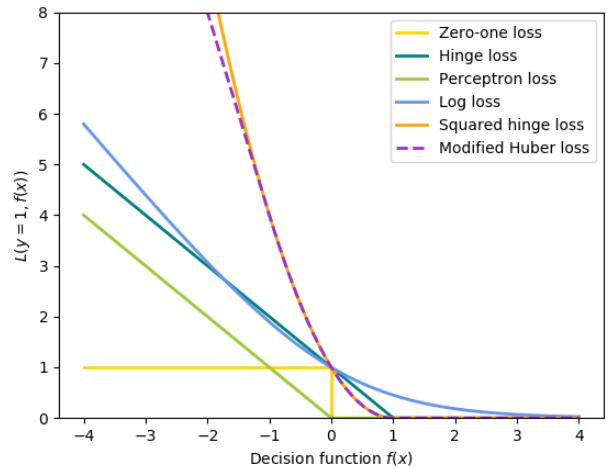
- Minimize it through gradient descent to find the hyperplane parameters (as in Ch. 6)

$$\mathbf{w}^*, b = \operatorname{argmin}_{\mathbf{w}, b} L(\mathbf{w}, b)$$

- Gradient computation (used to update the parameters)

$$\nabla_{\mathbf{w}} L(\mathbf{w}, b) = -\sum_{i:y_i f(\mathbf{x}_i) < 0} y_i \mathbf{x}_i$$

$$\nabla_b L(\mathbf{w}, b) = -\sum_{i:y_i f(\mathbf{x}_i) < 0} y_i$$



The Perceptron Learning Algorithm

```
function Perceptron-Learning( $\{x_i, y_i\}_{i=1}^n$ )
    returns weight values  $w$ , bias  $b$ 
        randomly initialize  $w, b$ 
        repeat
            for i=1, ..., n
                if  $y_i f(x_i) < 0$ 
                     $w \leftarrow w - \eta \nabla_w L(w, b)$ 
                     $b \leftarrow b - \eta \nabla_b L(w, b)$ 
            until a stopping condition is satisfied
        return w
```

The parameter η is called **learning rate**

Each for loop over the set of training samples is named **epoch**

Perceptron Convergence Theorem

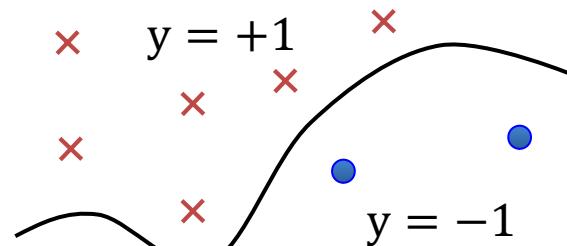
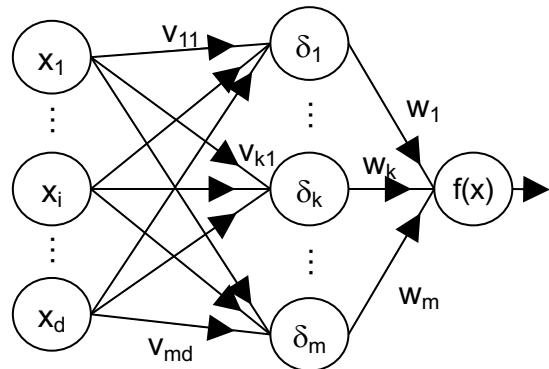
- **Perceptron convergence theorem** (F. Rosenblatt, 1960):
If the training set is **linearly separable**, the perceptron learning algorithm **always** converges to a consistent hypothesis after a **finite** number of epochs, for **any** $\eta > 0$.
- As convergence is guaranteed for any $\eta > 0$, usually $\eta = 1$ is set
- In practice we do not know in advance whether the training data is linearly separable
 - a suitable stop condition has thus to be used
- For instance, if the *training set* is **not** linearly separable, after a certain number of epochs the weights typically start *oscillating*
 - the detection of this behavior can be used as a stop condition

Limits of the Perceptron

- The perceptron turned out to be an **oversimplified** model of neurons, not useful for understanding the human brain
- More accurate models are still being developed by neuroscientists
 - See, e.g., the Human Brain EU Project at <https://www.humanbrainproject.eu/en/>
- **Main limitation:** The perceptron can not represent non-linear functions of \mathbf{x}

Perceptron Networks

- Neurons in the human brain are highly interconnected, yielding very complex *input-output* behaviors
- **Artificial neural networks** (ANN) made up of interconnected perceptrons can implement non-linear discriminant functions



Issues with Perceptron Networks (prior to the 70s)

- No target output can be defined for **hidden** units
- Rosenblatt's algorithm cannot be applied to set the weights of their input connections
 - alternative algorithms devised in the 1970s exhibited a too high **computational complexity**
- How to define a suitable network **architecture**, i.e., the number of perceptrons and the connections among them, for a given application?
- Can the architecture itself be chosen by the learning algorithm, together with connection weights?
- These difficulties contributed to a drop of interest in neural networks in the 1970s

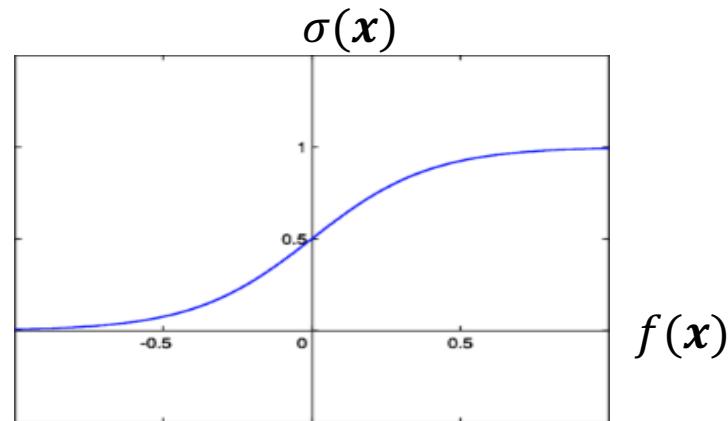
The Renaissance of Neural Networks

- A practical solution to the aforementioned issues was found in the 1980s
- Learning the network architecture is too difficult
 - it is better to use a predefined architecture, and to learn only the connection weights
- Efficient learning algorithms can be devised for
 - specific architectures, like **feed-forward** networks
 - **continuous** activation functions, instead of the step function

Continuous Activation Functions

- Sigmoid (or Logistic)

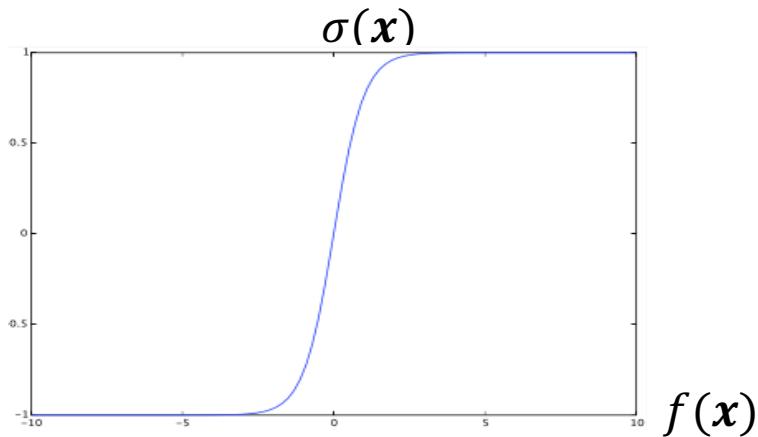
$$\sigma(x) = \frac{1}{1 + e^{-f(x)}} \in (0,1)$$



Continuous Activation Functions

- Hyperbolic Tangent (tanh)

$$\sigma(x) = \frac{e^{f(x)} - e^{-f(x)}}{e^{f(x)} + e^{-f(x)}} \in (-1,1)$$

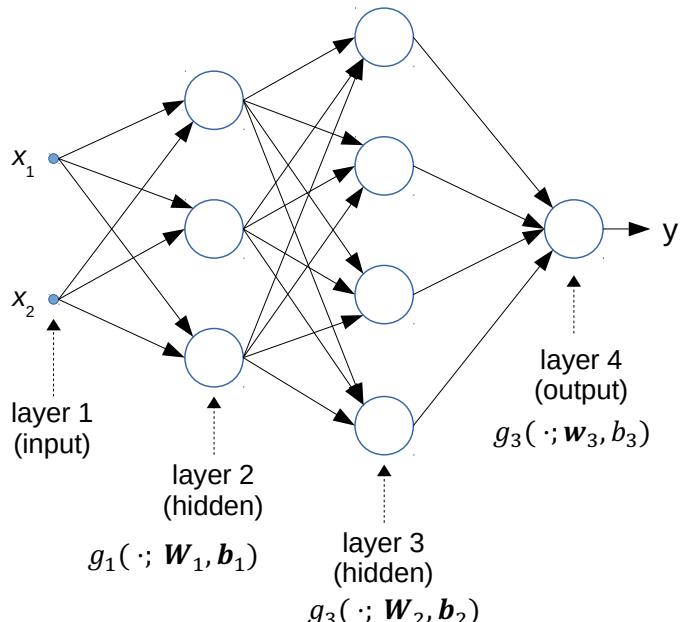


Feed-forward Multi-layer Perceptron (MLP)

- Units are arranged into **layers** (hence the name *multi-layer*)
 - **input** layer: fictitious units corresponding to inputs
 - **output** layer: one unit for two-class problems, c units for c -class problems with $c > 2$
 - one or more **hidden** layers
- No recurrent connections (hence the name *feed-forward*)
 - every hidden and output unit receives **inputs** only from units of the **previous** layer
 - every input and hidden unit sends its **output** only to units in the **next** layer
- Usually these networks are **fully-connected**
 - every input and hidden unit is connected to **all** units in the next layer

MLP: An Example

- Fully-connected MLP with two inputs, two hidden layers of three and four neurons each, and one output unit (suitable for two-class classification)



$$\begin{aligned}f(\mathbf{x}; \boldsymbol{\theta}) &= g_3(\cdot; \mathbf{w}_3, b_3) \circ g_2(\cdot; \mathbf{W}_2, \mathbf{b}_2) \circ g_1(\mathbf{x}; \mathbf{W}_1, \mathbf{b}_1) \\&= g_3(g_2(g_1(\mathbf{x}; \mathbf{W}_1, \mathbf{b}_1); \mathbf{W}_2, \mathbf{b}_2); \mathbf{w}_3, b_3)\end{aligned}$$

$$g(\cdot; \mathbf{W}, \mathbf{b}) = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$$

$$\mathbf{W}_1 \in \mathbb{R}^{3 \times 2}, \quad \mathbf{b}_1 \in \mathbb{R}^3$$

$$\mathbf{W}_2 \in \mathbb{R}^{4 \times 3}, \quad \mathbf{b}_2 \in \mathbb{R}^4$$

$$\mathbf{w}_3 \in \mathbb{R}^4, \quad b_3 \in \mathbb{R}$$

MLP Output Layer

- $\sigma(\mathbf{x})$ is a continuous output, it has to be converted to a class label
- For two-class problems, it can be thresholded
 - For example, if the sigmoid is used,
 $\sigma(\mathbf{x}) < 0.5$ corresponds to label -1, and +1 otherwise
- For multi-class problems with $c>2$ classes, c output neurons can be used and combined in a one-vs-all manner
- A softmax layer can also be used to estimate the class posterior probabilities as:

$$p(y = j|\mathbf{x}) = \frac{e^{f_j(\mathbf{x})}}{\sum_{k=1}^c e^{f_k(\mathbf{x})}}$$

- The softmax function generalizes the logistic/sigmoid function to the multi-class case

Selecting the Neural Network Architecture

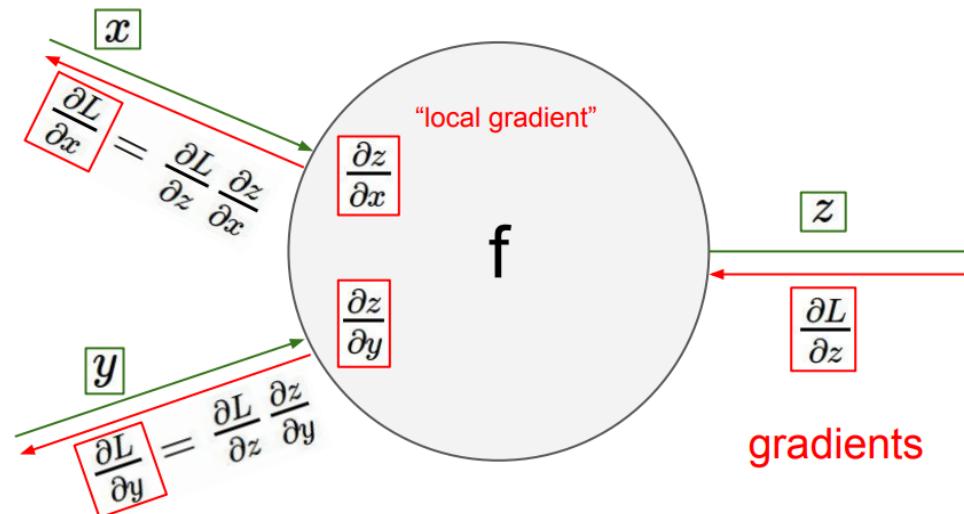
- In practical classification problems the target function (i.e., the relationship between feature values and class label) is **unknown**
- This means that also the best MLP architecture (in terms of number of hidden layers and of hidden units) is unknown
- An iterative trial-and-error design approach is usually adopted
 - start with a small network (e.g., one hidden layer and a few hidden units)
 - evaluate increasingly complex architectures (by increasing the number of hidden units and/or hidden layers) until a desired generalization capability is attained
- This agrees with the Occam's razor, promoting simpler solutions over complex ones

Back-Propagation Learning

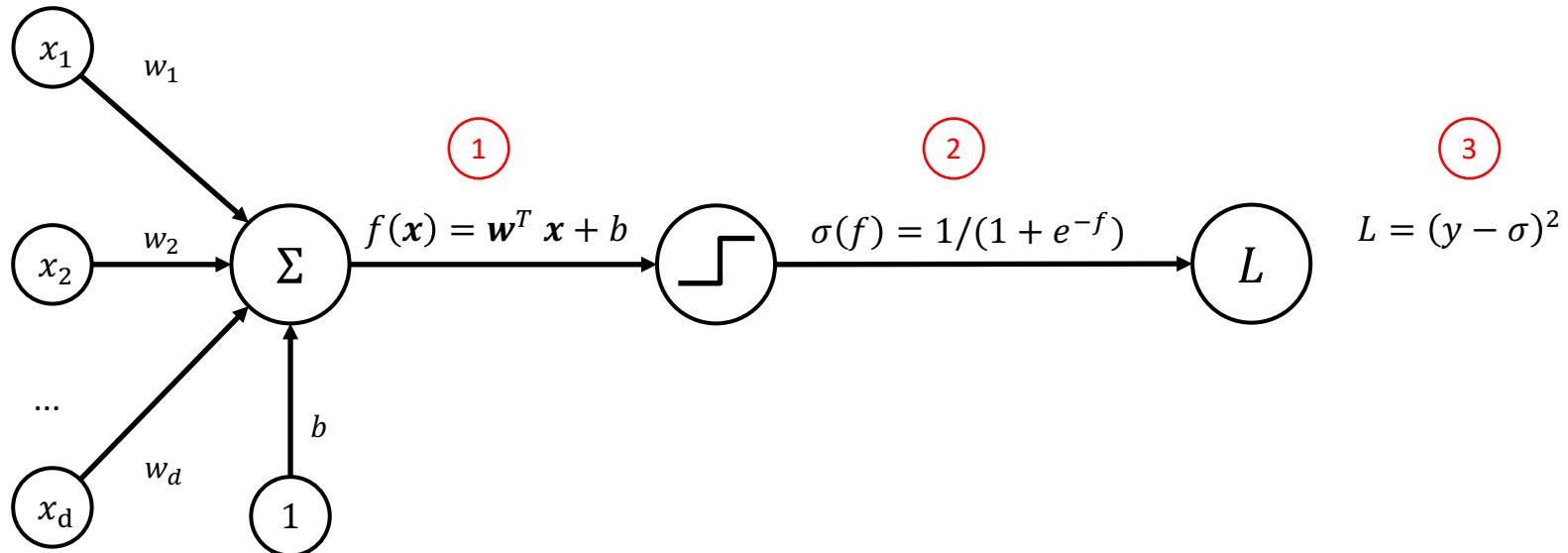
- Efficient learning algorithm devised in the 1980s for feed-forward MLP networks
- It exploits the continuous, differentiable activation function of each unit, which makes the network output a **continuous** and **differentiable** function of the network inputs
- To this end:
 - a **continuous, differentiable loss function** is used to evaluate the difference between the network output and the target output of a given example (e.g., MSE)
 - the loss function can be minimized over a training set using a gradient-based procedure

Back-Propagation Learning: Intuition

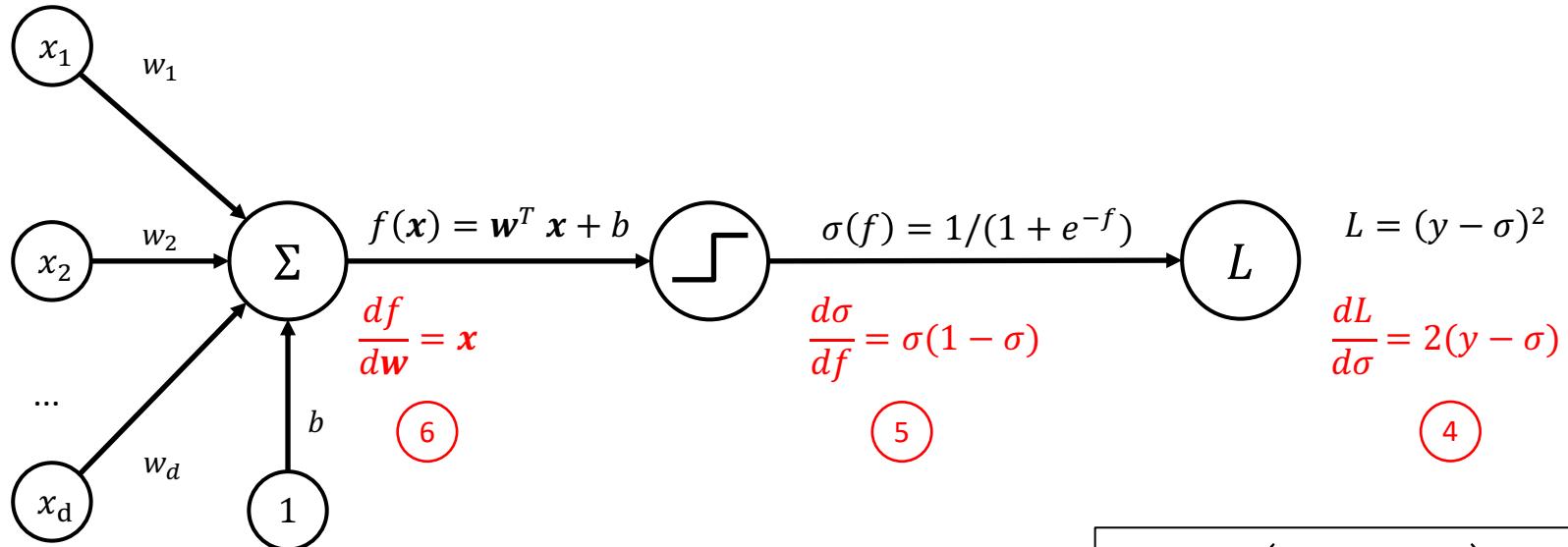
- **Forward step:** compute output function (e.g., loss) given input (e.g., one sample)
- **Backward step:** compute gradient in reverse-mode automatic differentiation, via the chain rule; e.g., $dL/dx = dL/dz * dz/dx$



Forward Pass



Backward Pass



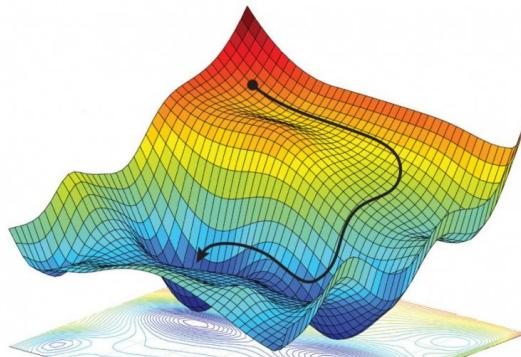
$$\frac{dL}{d\mathbf{w}} = \left(\left(\frac{dL}{d\sigma} \right) \cdot \frac{d\sigma}{df} \right) \cdot \frac{df}{d\mathbf{w}}$$

Back-Propagation Learning

```
function BACK-PROPAGATION ( $T$ )
returns weight values  $w$ 
    randomly choose the initial weight values  $w$ 
    repeat
        for each  $(x^k, t_k) \in T$  do
            compute the network output  $y(x^k)$  (forward-propagation)
            update the weights  $w$  (back-propagation)
        end for
        until a stopping condition is satisfied
    return  $w$ 
```

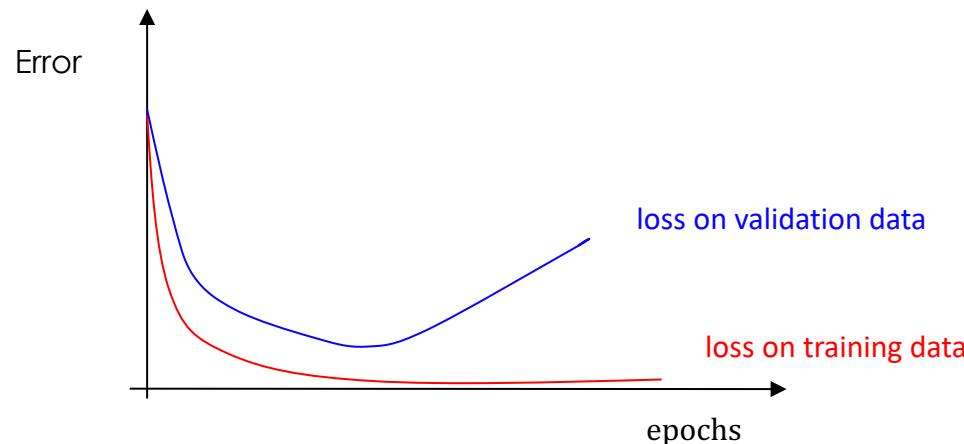
Back-Propagation Learning: Issues

1. The error function usually has many **local minima**
 - gradient descent does not guarantee convergence to the smallest error on training examplesA **multi-start** strategy can be used to mitigate this problem
 - the algorithm is run several times starting from **different** random weights, and the solution with minimum error is chosen
2. Like all classifiers also NNs are prone to **over-fitting**
Early-stopping can be used to tackle this issue



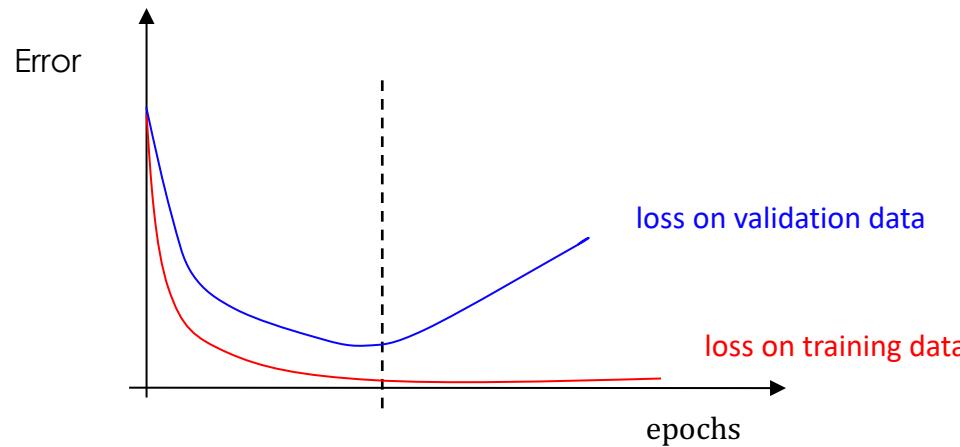
Overfitting

- Overfitting can be detected by running the back-propagation algorithm on a training set made up of a **subset** of the available examples, and by evaluating the error function also on (a subset of) the remaining examples, called **validation set**
- If the loss on validation data starts increasing, overfitting is occurring



Early Stopping

- The back-propagation algorithm is stopped when the error function starts increasing on validation examples



Regularization

- Another way of mitigating overfitting is to use a **regularized** objective function

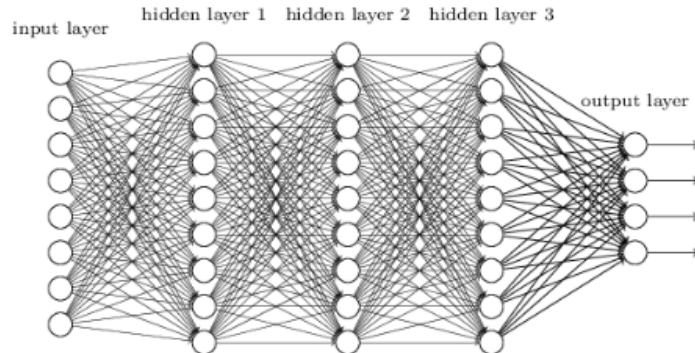
$$E(\mathbf{w}) = \frac{1}{2n} \sum_{i=1}^n (a(\mathbf{x}_i) - y_i)^2 + \lambda \underbrace{\Omega(\mathbf{w})}_{\text{regularization term}}$$

- λ is a trade-off parameter between loss on training data and weight regularization
 - L1 and L2 norms are typically used for weight regularization

Deep Learning

Deep Neural Networks (DNNs)

- DNNs are a recent popular extension of NNs (but early ideas date back to the 1970s), inspired by the structure of the brain
- Basically, they are multi-layer networks with **many** hidden layers



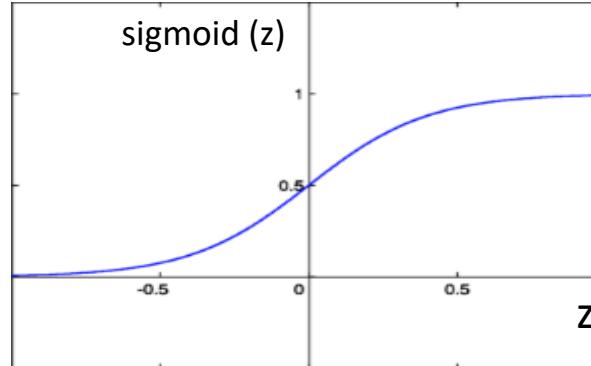
taken from <http://neuralnetworksanddeeplearning.com>

- Ad-hoc modifications to activation functions and training procedures have been introduced to avoid drawbacks of standard ones (e.g., very slow convergence)

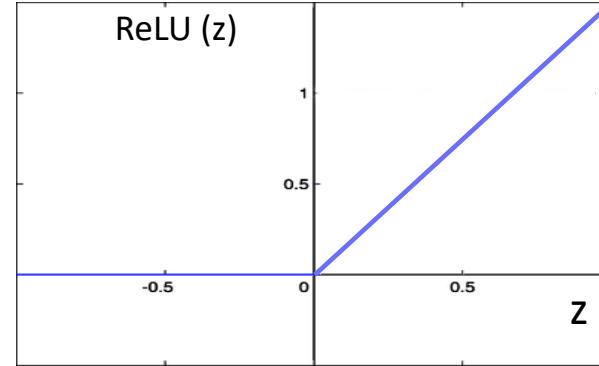
ReLU Activations

- **Problem:** sigmoid takes on values in $(0,1)$. Its gradient $z(1-z)$ is closer to 0 than z .
 - The net effect is that, propagating the gradient back to the initial layers, it tends to become 0 (**vanishing gradient problem**).
 - From a practical perspective, this slows down the training procedure of the initial layers
- Rectified Linear Unit (**ReLU**) activations can overcome this issue

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

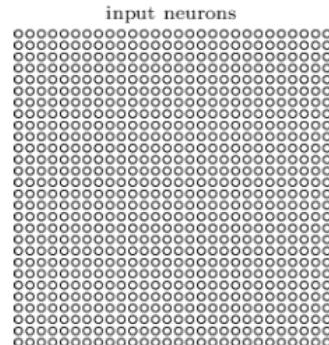


$$\text{ReLU}(z) = \max(0, z)$$



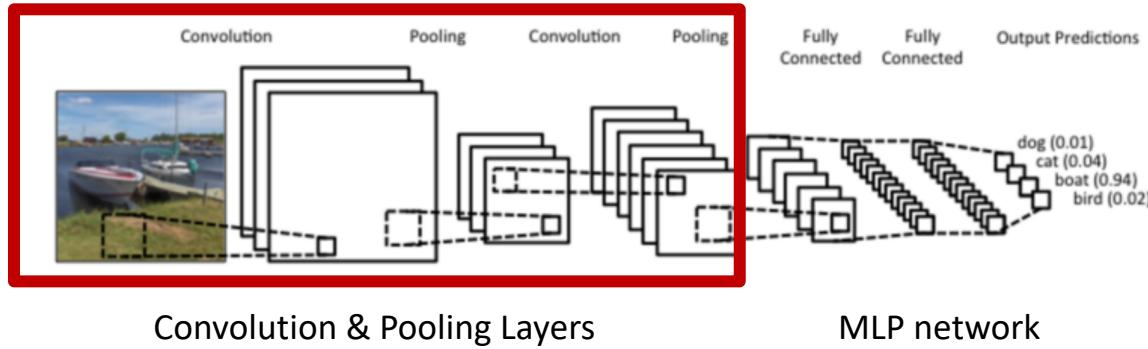
Convolutional Neural Networks

- DNNs are widely employed for computer vision tasks, for which specialized architectures have been proposed, named ***convolutional neural networks*** (CNNs)
- In this case the CNN input is a raw image. Accordingly, the CNN architecture is not fully connected, but it exploits the **spatial adjacency** between pixels. Input units are arranged into an array



taken from <http://neuralnetworksanddeeplearning.com>

Convolutional Neural Networks



Convolutional Neural Networks

- CNNs hidden layers carry out specific image processing operations. They basically alternate two kinds of layers:
 - **filtering** layers, whose connection weights (that determine the filter implemented), are **learnt**
 - **pooling** layers, which have predefined connection weights, and carry out a downsampling operation on the outputs of the previous layer
- The upper layers consist of a standard, fully-connected feed-forward network
- A key difference between standard (*shallow*) and deep networks is that the connection weights of the DNN hidden layers (including CNNs) are usually learnt with **no** supervision, which makes such layers to work as powerful, unsupervised **feature extractors**

Filtering (Convolutional Units)



I

-1	-1	-1
2	2	2
-1	-1	-1

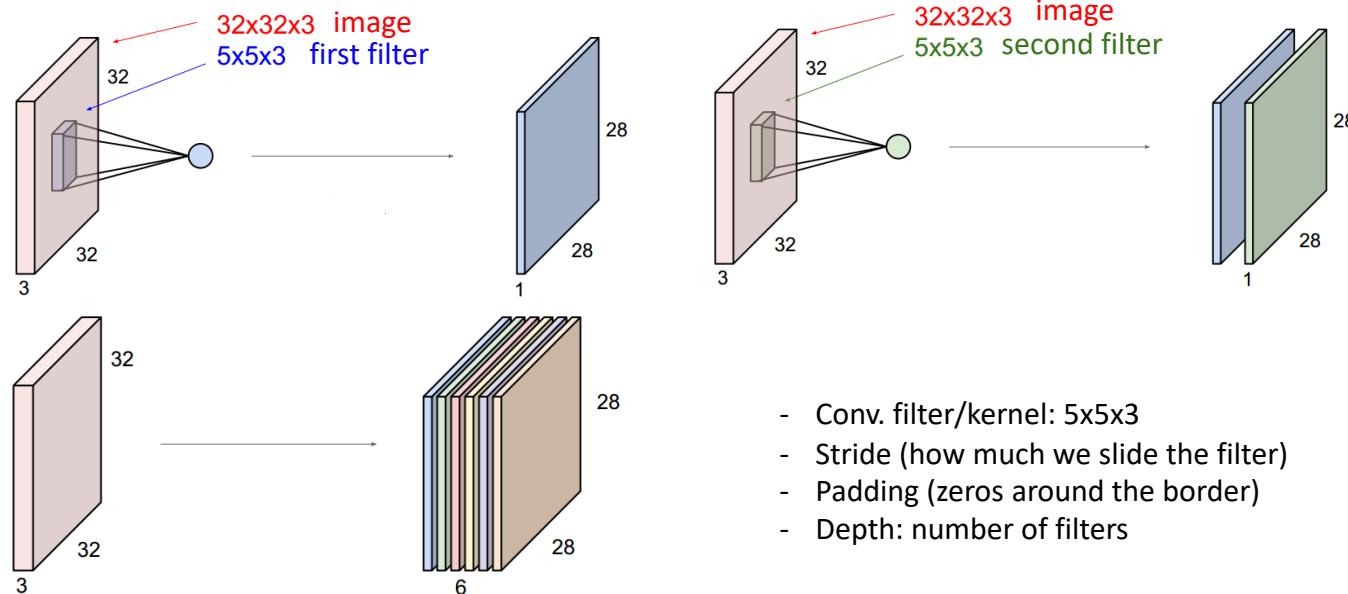
K



I * K

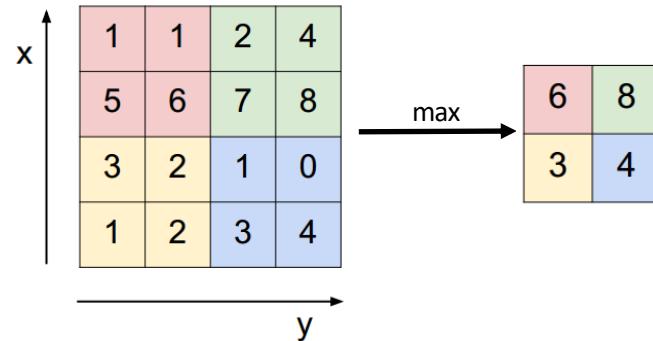
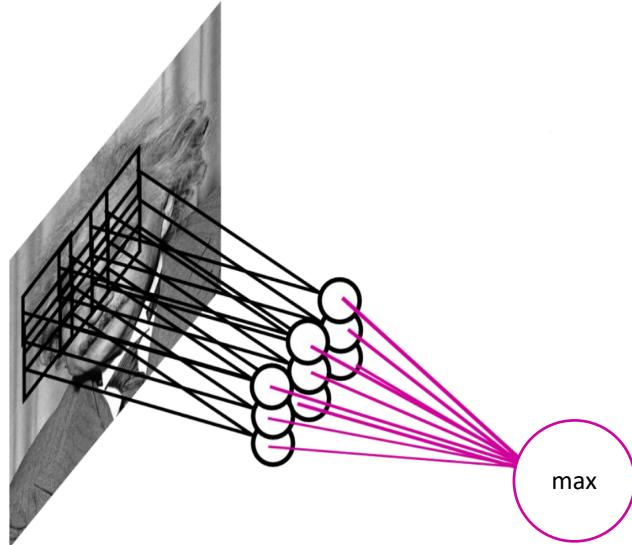
Filtering (Convolutional Units)

- Normally, several filters are packed together and learnt automatically during training
 - For more details on convolutions, see: <https://cs231n.github.io/convolutional-networks/>



Pooling

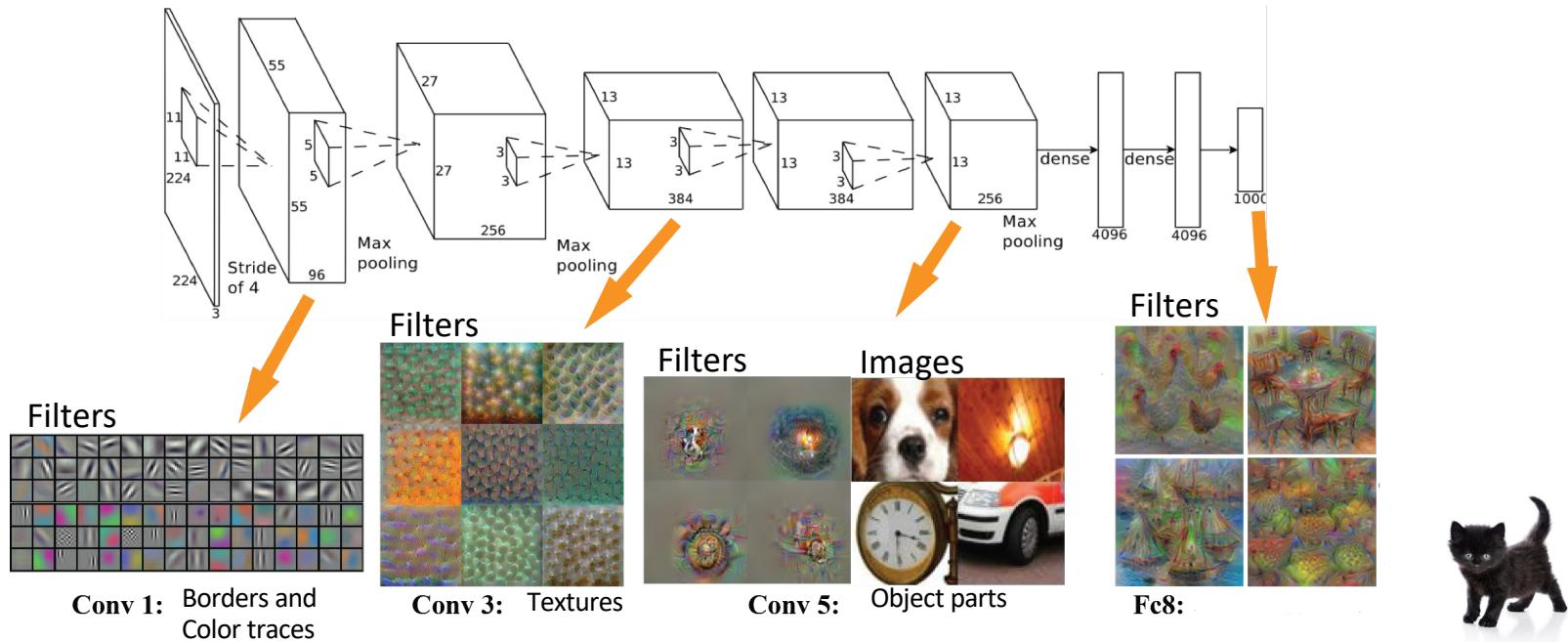
- Max pooling is a way to simplify the network architecture, by downsampling the number of neurons resulting from filtering operations



Slide credits: M. A. Ranzato e Fei Fei Li

Convolutional Neural Networks

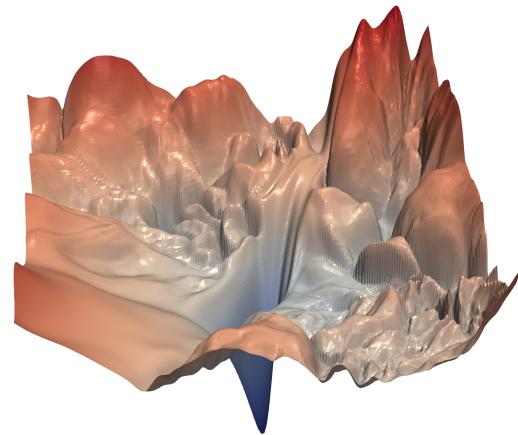
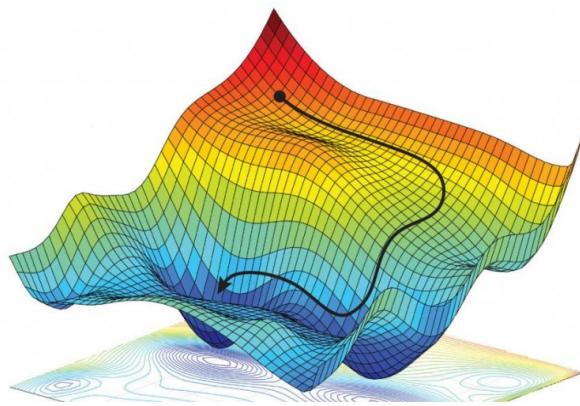
- The deep network gradually learns more complex and abstract notions



Optimization

Optimizing Deep Networks

- Neural networks aim to learn a mapping function $f(x; \boldsymbol{\theta}) = g_k \circ g_{k-1} \circ \dots \circ g_1(x; \mathbf{W}_1, \mathbf{b}_1)$ which is typically not convex w.r.t. $\boldsymbol{\theta} = (\mathbf{W}_1, \mathbf{b}_1 \dots, \mathbf{W}_k, \mathbf{b}_k)$
- Learning the classifier parameters (e.g., via cross-entropy loss minimization) is then much more challenging, as it requires solving a non-convex optimization problem



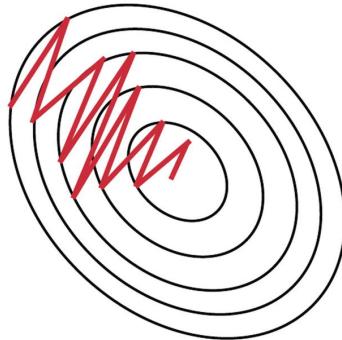
Visualizing the loss landscape of NNs, <https://arxiv.org/pdf/1712.09913.pdf>

Optimizing Deep Networks

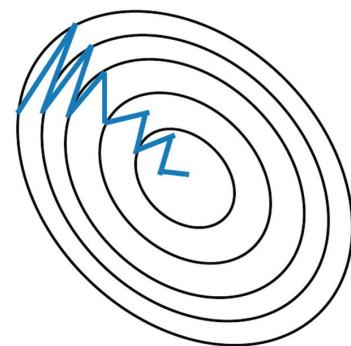
- Non-convex problem with large number of parameters and data points (up to millions)
 - The data may not even fit in memory
 - Easy to get stuck in bad local minima, slow convergence rates for gradient-based methods
- For this reason, many variants of *online* gradient-based optimizers have been proposed
 - Data is loaded in batches
 - Gradient is computed for the current batch and used to update the parameters (similarly to Stochastic Gradient Descent, SGD)
- **Most popular ones:** Momentum, Adam, Adagrad, RMSProp, etc.
 - https://d2l.ai/chapter_optimization/index.html

Momentum

- The gradient \mathbf{g}_k is averaged across iterations, with weight β
 - $\mathbf{v}_k = \beta\mathbf{v}_{k-1} + \mathbf{g}_k$
 - $\theta_k = \theta_{k-1} - \eta_k \mathbf{v}_k$
- With $\beta=0$, it is equivalent to the steepest descent method
- Momentum works as a smoothing operator on the objective function, facilitating convergence



Stochastic Gradient Descent **without** Momentum



Stochastic Gradient Descent **with** Momentum

More at: https://d2l.ai/chapter_optimization/momentum.html

Dropout and Batch Normalization

- Techniques/regularizers to facilitate training
- **Dropout:** randomly de-activate some neurons during training (to prevent overfitting)
- **Batch Normalization:** normalize inputs to have zero mean and unit variance
 - mean and variance are estimated for each batch separately

Open-source Frameworks

- Good news: DNN learning is widely automated nowadays
 - Many available open-source frameworks (Tensorflow, PyTorch, Keras, MXNet, ...)
- Basic idea: model as a computational graph (i.e., a sequence of instructions!)
 - Each node represents a function that transforms the input data (tensors)
 - Autodifferentiation is readily available – we can differentiate through computer programs!
- Computational advantages
 - Gradients are computed efficiently and readily available
 - Parallel computation via GPUs (very efficient for parallel matrix multiplication)
 - Horizontal scalability / cloud computing
- Models can be served in production

TensorFlow

 TensorFlow

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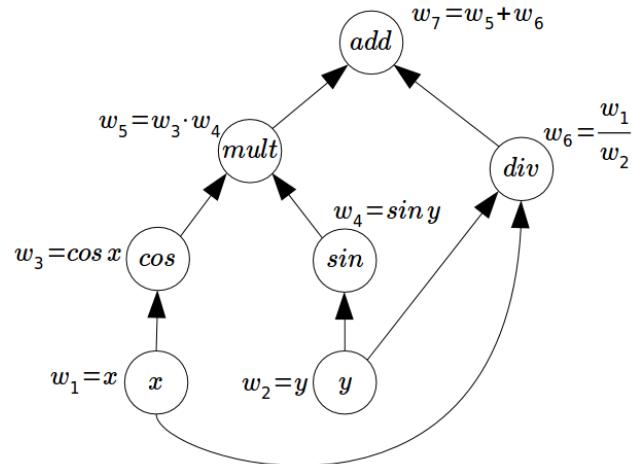
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KEY FEATURES & CAPABILITIES

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Automatic/Algorithmic Differentiation

- Gradients are readily available from the computation graph
 - Dual numbers: each node evaluates the function along with its gradient
 - Derivative of output w.r.t inputs is obtained through the chain rule
- Forward-mode autodifferentiation
 - accumulates derivatives going forward, initializing x and y
 - convenient when $n_{\text{inputs}} \ll n_{\text{outputs}}$
- Reverse-mode autodifferentiation
 - accumulates derivatives going backward, initializing the output
 - convenient when $n_{\text{outputs}} \ll n_{\text{inputs}}$



$$f(x,y) = \cos x \sin y + x/y$$

Read more at: <http://jmlr.org/papers/volume18/17-468/17-468.pdf>
<https://mathematical-tours.github.io/book-sources/optim-ml/OptimML.pdf>

Deep Learning with PyTorch

https://pytorch.org/tutorials/beginner/blitz/cifar10_tutorial.html

1. Load data

```
transform = transforms.Compose(  
    [transforms.ToTensor(),  
     transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))])  
  
trainset = torchvision.datasets.CIFAR10(root='./data', train=True,  
                                         download=True, transform=transform)  
trainloader = torch.utils.data.DataLoader(trainset, batch_size=4,  
                                         shuffle=True, num_workers=2)  
  
testset = torchvision.datasets.CIFAR10(root='./data', train=False,  
                                         download=True, transform=transform)  
testloader = torch.utils.data.DataLoader(testset, batch_size=4,  
                                         shuffle=False, num_workers=2)  
  
classes = ('plane', 'car', 'bird', 'cat',  
          'deer', 'dog', 'frog', 'horse', 'ship', 'truck')
```

2. Define network

```
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
```

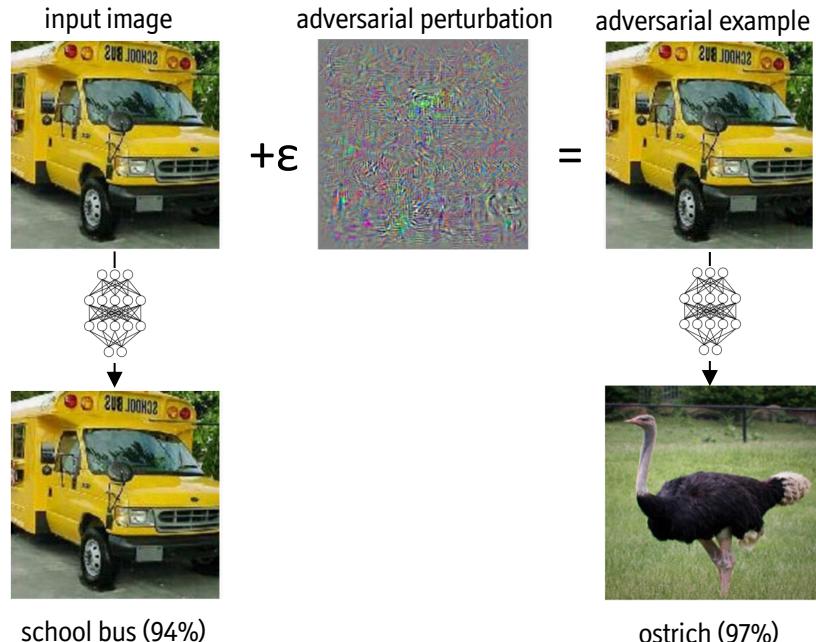
3. Optimization

```
criterion = nn.CrossEntropyLoss()  
optimizer = optim.SGD(net.parameters(), lr=0.001, momentum=0.9)
```

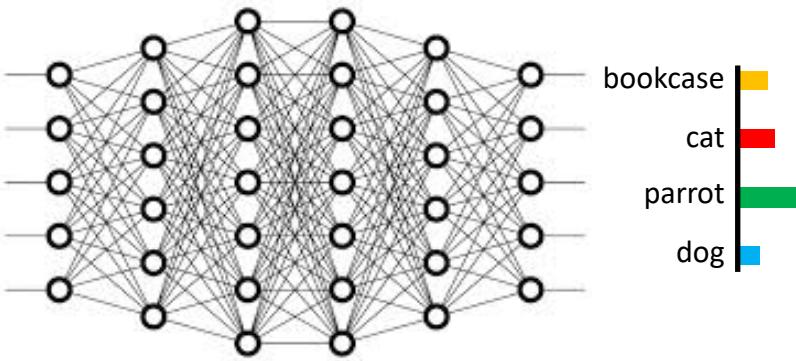
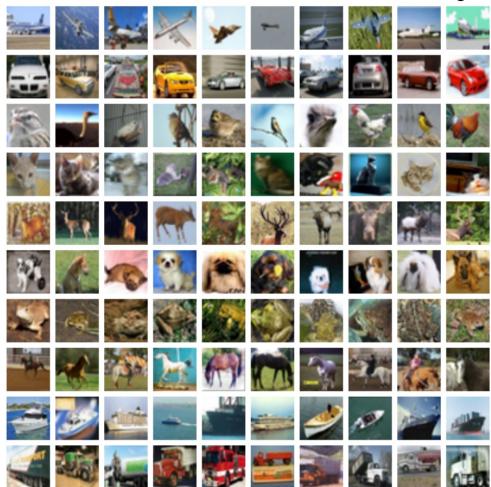
Do DNNs Really Learn Like Humans?

Do DNNs Really Learn Like Humans?

- DNNs (and machine learning, in general) can be easily fooled by **adversarial examples**
 - Biggio *et al.*, Evasion attacks against machine learning at test time, **ECML-PKDD 2013**
 - Szegedy *et al.*, Intriguing properties of neural networks, **ICLR 2014**
- **How do these attacks work?**



Modern AI is Optimization + Big Data

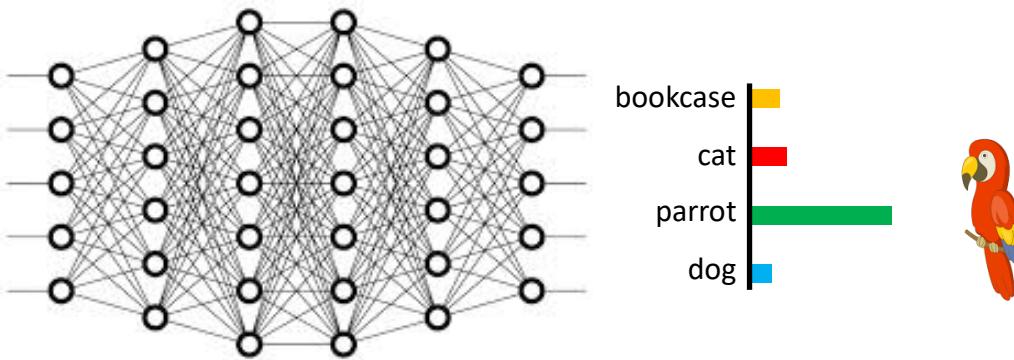


$$\min_w L(D; \mathbf{w})$$

The goal is to minimize
the fraction of
classification errors

... by iteratively updating the classifier
parameters \mathbf{w} along the gradient
direction $\nabla_{\mathbf{w}} L(D; \mathbf{w})$

Adversarial Attacks

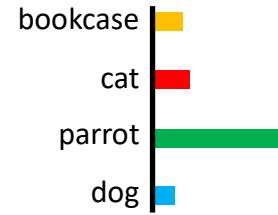
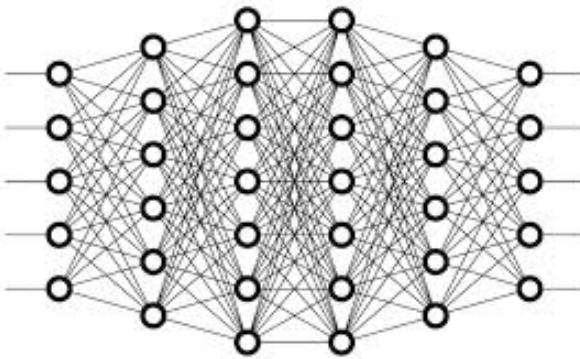


Adversarial attacks exploit the same underlying mechanism of learning, but aim to maximize the probability of error on the input data: $\max_D L(D; \mathbf{w})$

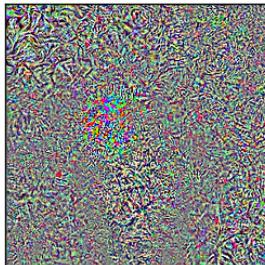
This problem can also be solved with gradient-based optimizers

(*Biggio et al., ICML 2012; Biggio et al., ECML 2013; Szegedy et al., ICLR 2014*)

How Do These Attacks Work?

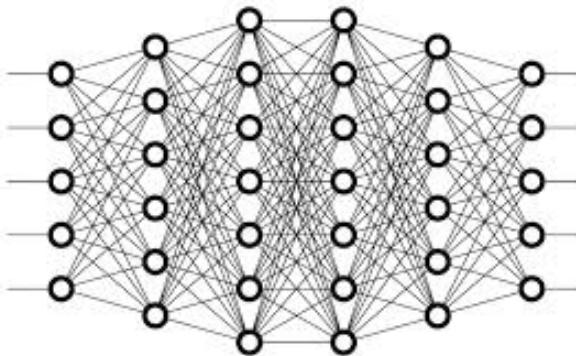


$$\max_D L(D; \mathbf{w})$$



The gradient of the objective allows us to compute an *adversarial perturbation*...

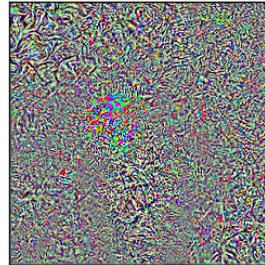
How Do These Attacks Work?



bookcase
cat
parrot
dog



... which is then added to the input image to cause misclassification



Evasion Attacks against Machine Learning at Test Time

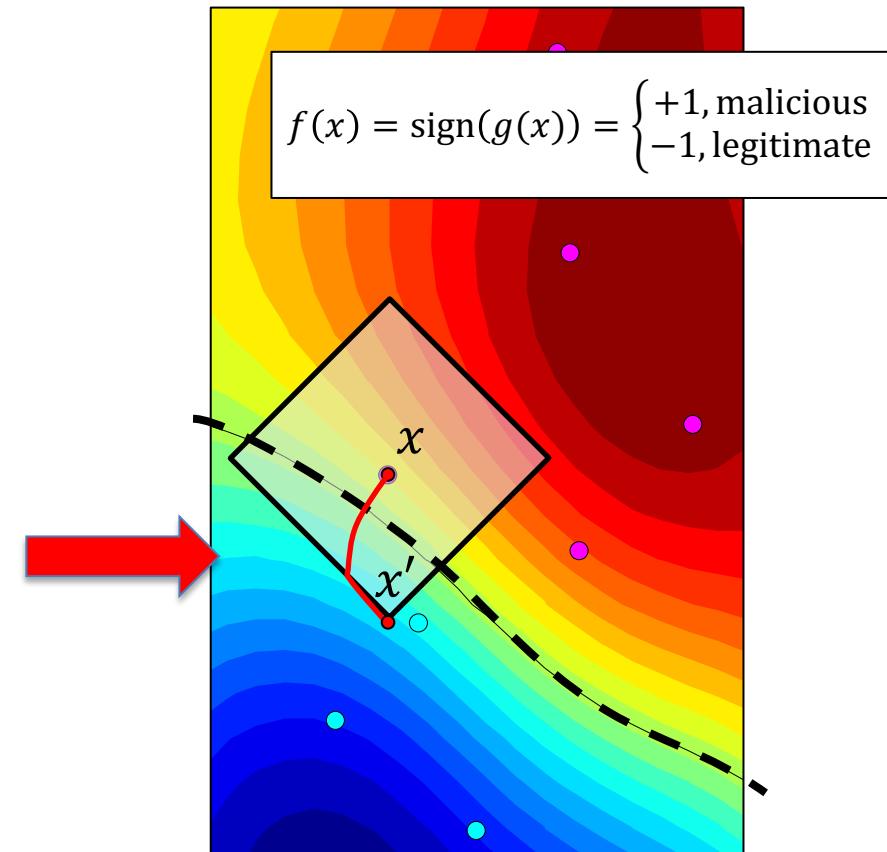
Biggio et al., ECML PKDD 2013

- **Main idea:** to formalize the attack as an optimization problem

$$\min_{x'} g(x')$$

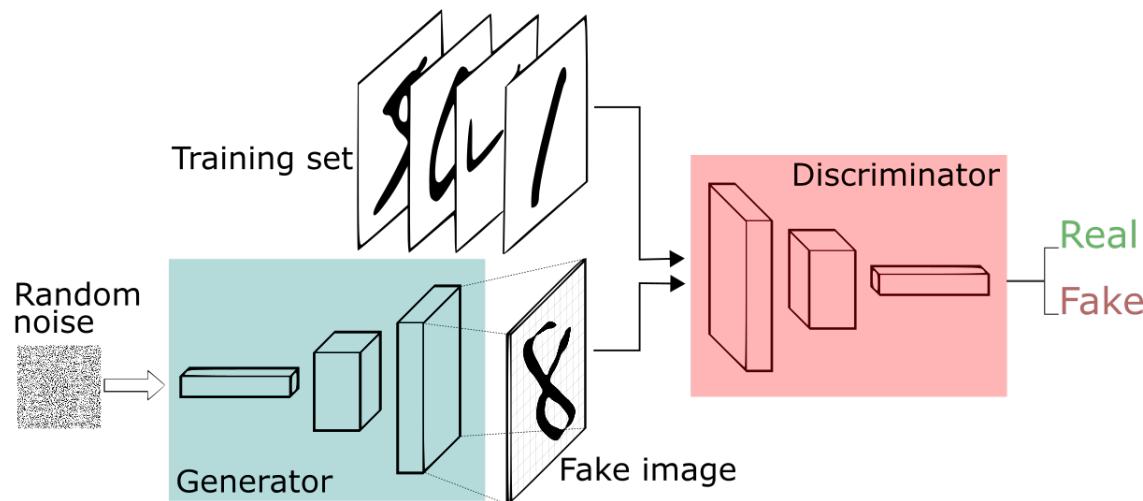
$$\text{s. t. } \|x - x'\| \leq \varepsilon$$

- Non-linear, constrained optimization
 - **Projected gradient descent:** approximate solution for smooth functions
- Gradients of $g(x)$ can be analytically computed in many cases
 - SVMs, Neural networks



Beyond DNNs for Classification

Generative Adversarial Networks (GANs)

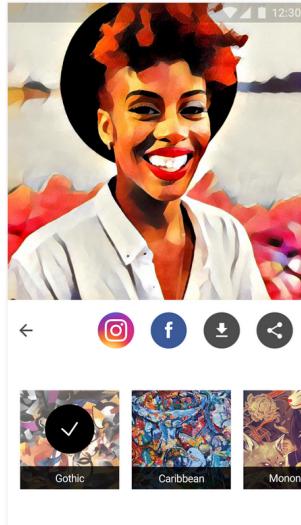
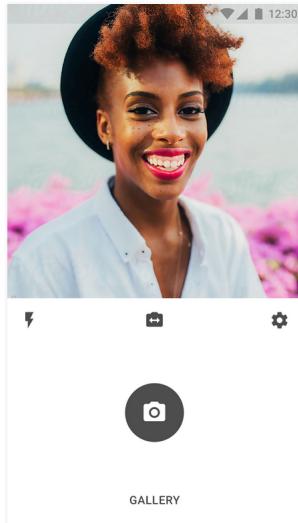


$$\min_G \max_D V(D, G) = \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})} [\log(1 - D(G(\mathbf{z})))].$$

Ian Goodfellow et al., GANs <https://arxiv.org/pdf/1406.2661.pdf>

Applications of Generative DNNs

- Gatys et al. Image Style Transfer Using Convolutional Neural Networks, CVPR 2016
 - Prisma (Android): <https://play.google.com/store/apps/details?id=com.neuralprisma>
 - Prisma (iOS): <https://itunes.apple.com/us/prisma-art-filters-photo-effects/id1122649984?mt=8>



Applications of Generative DNNs

this small bird has a pink breast and crown, and black primaries and secondaries.



this magnificent fellow is almost all black with a red crest, and white cheek patch.



the flower has petals that are bright pinkish purple with white stigma



this white and yellow flower have thin white petals and a round yellow stamen



Reed et al., Generative Adversarial Text to Image Synthesis <https://arxiv.org/pdf/1605.05396.pdf>

References

- <http://neuralnetworksanddeeplearning.com>
- <http://deeplearning.stanford.edu/tutorial/>
- <http://www.deeplearningbook.org/>
- <http://deeplearning.net/>
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