Quick review of Deep Learning

EE 5178

Kaushik Mitra

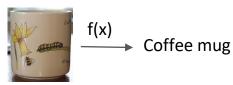
Depart. Of Electrical Engineering, IIT Madras

Machine learning

Goal: Learning from the data with minimal intervention from the user

Supervised learning:

 Learns a mapping b/w input and output pairs (x_i,y_i) e.g. image classification

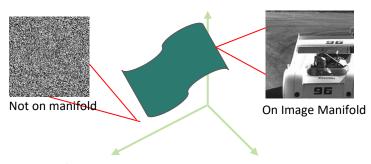




 Applications: image classification, object detection, scene recognition

Unsupervised learning:

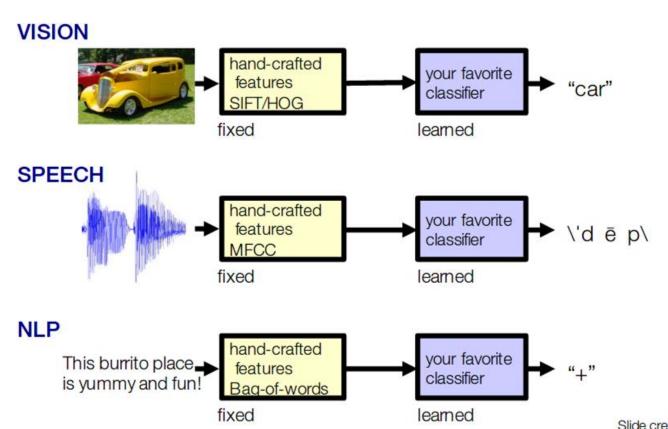
- Given only data 'x' learn the inherent underlying structure
- Consider a 64x64 binary image



 Applications: clustering, dimensionality reduction, density estimation

Traditional approaches

- Manual feature extraction (SIFT/HOG)
- Classifier is learned independent of feature extraction



Traditional approaches vs Deep learning

What's wrong with the traditional approaches?

 Compositional feature abstraction is missing

3 key ideas of deep learning

- (Hierarchical) Compositionality
 - Cascade of nonlinear functions
 - Multiple layers of abstractions
- End-to-End learning
 - Learning (task-driven) representations
 - Learning to extract features
- Distributed Representation
 - No single neuron encodes everything
 - Group of neurons work together

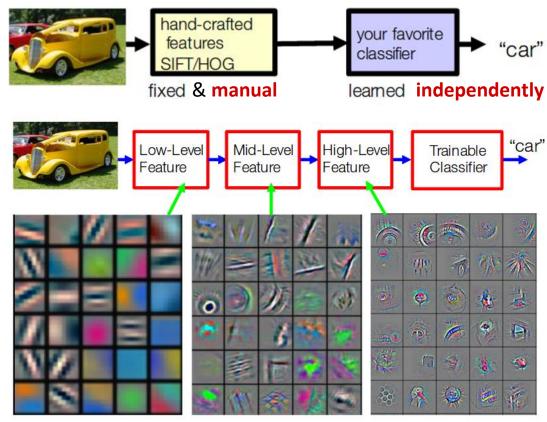
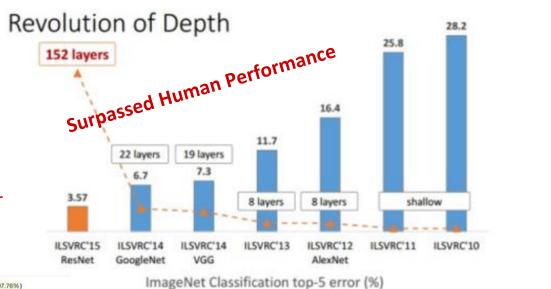


Image Classification

LeNet by Lecun et al. 1998 (MNIST)
AlexNet by Krish et al. NIPS' 12
VGGNet by Simonyan et al. ICLR' 15
GoogLeNet by Szegedy et al. CVPR' 15
ResNet by He et al., CVPR' 17 best paper





Animal (97,76%)
Wildlife (92,16%)
Tiger (90,11%)
Terrestrial animal (68,17%)
Bengal tiger (64,77%)
Whiskers (63,30%)
Zoo (58,16%)
Roaring cats (56,41%)
Cat (44,12%)

Kaiming He, Xiangyu Zhang, Shaoqing Ren, & Jian Sun. "Deep Residual Learning for Image Recognition". arXiv 2015.

*pic courtesy: Kaiming He

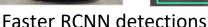
Object Detection

OverFeat by Sermanet et al., ICLR' 14 (NYU) R-CNN by Girshick et al., CVPR' 14 (UCB) SPP by He et al., ECCV' 14 (MSR) Fast R-CNN by Girshick et al., arxiv (MSR) Faster R-CNN by Ren et al., NIPS' 15 (MSR) YOLO by Redmon et al., arxiv 2015 YOLO 9000 by Redmon et al., CVPR' 17





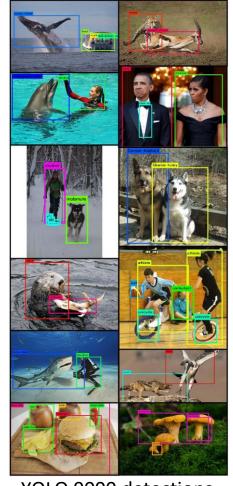








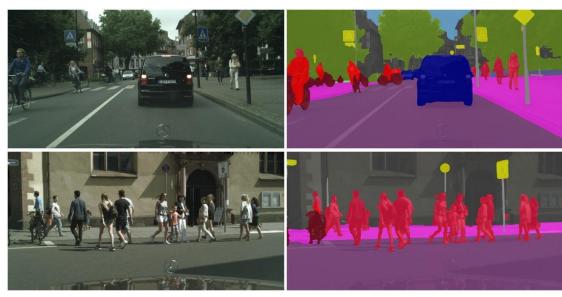




YOLO 9000 detections

Image Segmentation

FCN by Long et al. CVPR' 15
DeepLab by Chen et al. arxiv 2015
CRFS as RNNs by Zheng et al. ICCV' 15



*Pic courtesy: Kundu et al. CVPR 2016 on City scapes dataset

Style transfer

Neural style transfer by Gatys et al., CVPR' 16

Deep Photo Style Transfer by Luan et al., CVPR' 17

Actual

*Pic courtesy: http://deepart.io



Actual with style













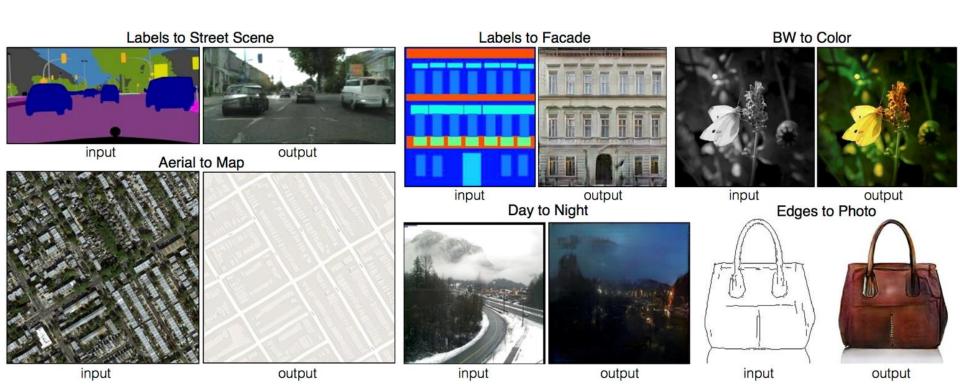




*Pic courtesy: Deep Photo Style Transfer, Luan et al. CVPR 2017

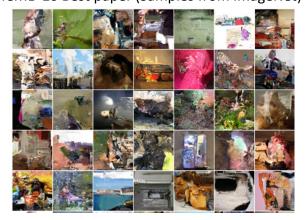
Artistic applications

Image-to-Image Translation with Conditional Adversarial Nets by Isola et al., CVPR' 17



Image, Video and Audio Generation

PixelRNN/CNN by Gregor et al., ICML' 16 Best paper (Samples from ImageNet)



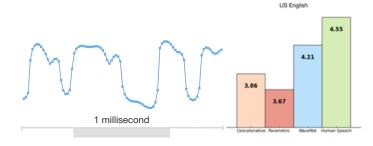
DCGAN Chintala et al. ICLR' 16 Sample bedroom images



Generating **videos** with scene dynamics, by Vondrick et al., NIPS' 16



WaveNet for **audio** synthesis by Oord et al. 2016, Deepmind



Check out wavenet's generated music piano clips

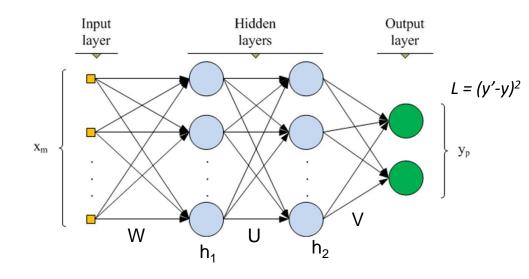
1. Basic Neural Networks

Multi-layer perceptrons (MLP) is a feed forward neural network with hidden layers

$$h_1 = f(Wx + b_1), f$$
 is an activation function
 $h_2 = g(Uh_1 + b_2)$
 $y' = Vh_2 + b_3$



 hence, better to have more hidden layers than a single layer with large number of neurons



Universal Approximation Theorem:

1. Basic Neural Networks

What we will learn in the course about Neural Networks?

Introduction

- McCulloch and Pits model
- Rosenblatt's perceptron

Perceptrons

- Geometry and linear separability
- XoR problem
- Multi-layer perceptron (MLP)

Training MLPs

- Error back propagation
- Loss functions

Regularization and optimization

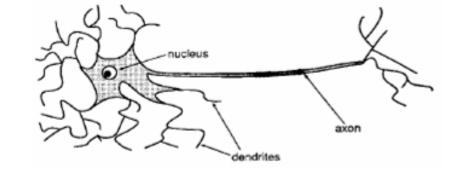
- Over fitting / Under fitting
- Regularization
- Various algorithm

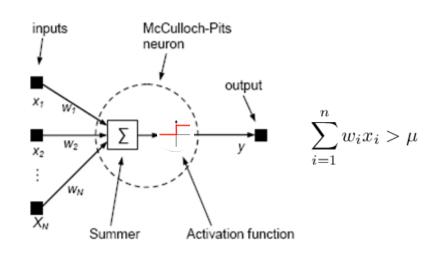


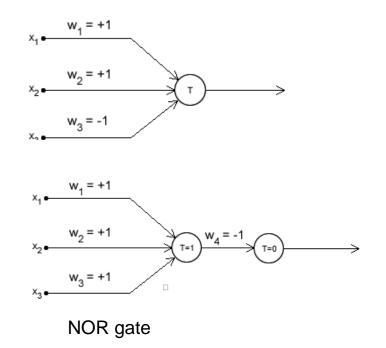
Perceptron, XOR Problem, Multi-layer Perceptron (MLP), Cost Functions, Activation functions and Output units

Xetwo

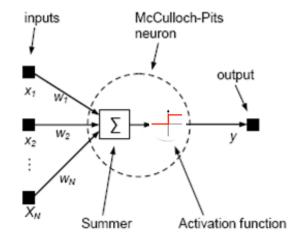
McCulloch - Pits model



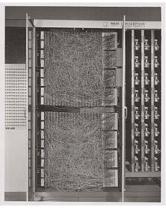




The Perceptron - Rosenblatt (1953)







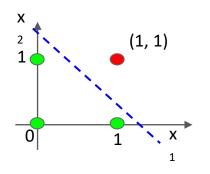
*Pic courtesy, wikipedia

The Mark 1 Perceptron
By Rosenblat
for digit recognition

Perceptron - geometrical interpretation

$$\sum_{i=1}^n w_i x_i > \mu$$
 , What does this inequality imply in 2D case? Half plane

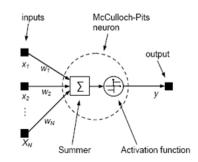
X	AND
(0, 0)	0
(0, 1)	0
(1, 0)	0
(1, 1)	1

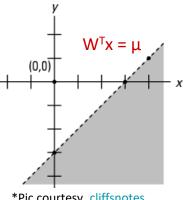


Solve for W, μ:

$$x_1 + x_2 > 1.5$$

 $w_1 = 1$, $w_2 = 1$ and $\mu = 1.5$





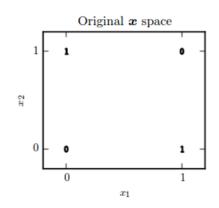
*Pic courtesy, cliffsnotes

Any function that is linearly separable can be computed by a perceptron

Perceptron - Limitations

Goal: learn the XoR function (f^*)

X	f*
(0, 0)	0
(0, 1)	1
(1, 0)	1
(1, 1)	0



The data is not linearly separable

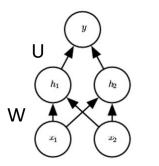
How to tackle this problem?

- Can we use more than one line?
- Yes, but how?

Perceptron - Limitations

How to tackle this problem?

Add a hidden layer with two units



$$y = f^{(2)}(h; U, c)$$

$$y = f^{(2)}(f^{(1)}(x))$$

$$h = f^{(1)}(x; W, b)$$

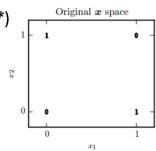
What should f:(1) compute?

If its linear again the composition still remains linear

$$f^{(2)}(h) = U^{T}h \text{ and } h = Wx$$

 $V = U^{T}Wx = W'x$

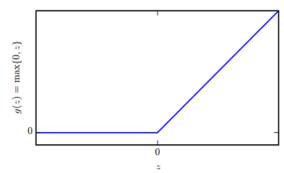
Goal: learn the XoR function (f^*)



- $f^{(1)}$ should be nonlinear to extract useful features

$$h = f^{(1)}(x; W, b) = g(Wx+b)$$

- g is referred as activation function commonly
- We will use ReLU here
 - ☐ Rectified Linear Unit (widely used)

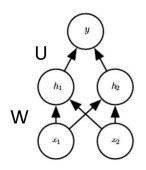


*Slide courtesy, Ian Goodfellow et al., deep learning book

Perceptron - Limitations

How to tackle this problem?

- Add a hidden layer with two units
- Use ReLU activation in 1st layer



$$y = U^Th + c$$
; $y = U^T \max\{0, Wx+b\} + c$

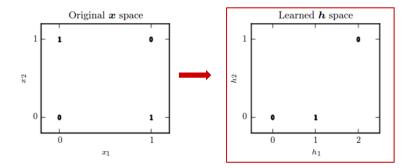
$$h = g(Wx+b)=max\{0, Wx+b\}$$

Let,

$$\mathsf{W} = \left[\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right], \quad \mathsf{b} = \left[\begin{array}{c} 0 \\ -1 \end{array} \right], \quad \mathsf{U} = \left[\begin{array}{c} 1 \\ -2 \end{array} \right],$$

$$c = 0$$

Goal: learn the XoR function (f^*)



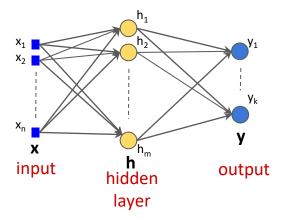
$$X = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \qquad WX = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 1 & 1 & 2 \end{bmatrix}$$

WX + b =
$$\begin{bmatrix} 0 & 1 & 1 & 2 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$
 $h = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix}$

$$h = \begin{bmatrix} 0 & 1 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \begin{array}{c} \text{Upon} \\ \text{ReLU} \end{array}$$

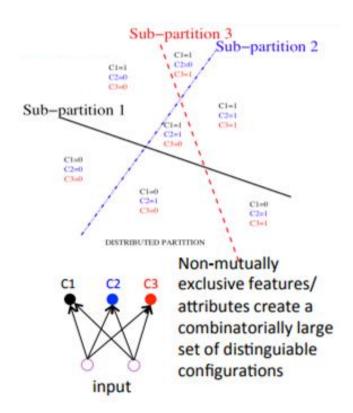
Multi-layer Perceptrons (MLP)

A typical feed forward neural network



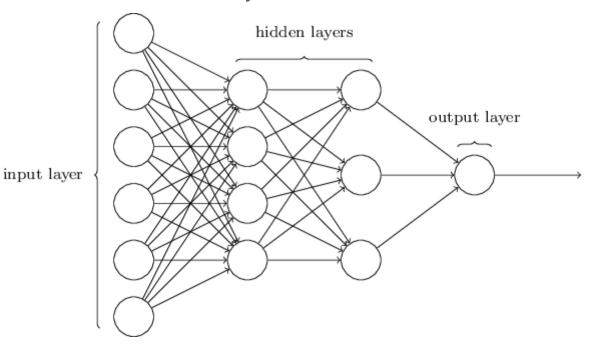
$$\mathbf{h} = f(\mathbf{W}\mathbf{x} + \mathbf{b}_1); \quad \mathbf{y} = g(\mathbf{U}\mathbf{h} + \mathbf{b}_2)$$

With more hidden units network is more expressible

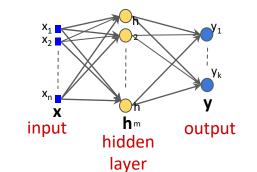


Specification of a MLP

- Number of hidden layers and units in each layer
- Activation function for
 - > Hidden layers
 - Output layers
- Cost function



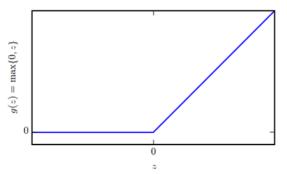
Activation functions for hidden layers



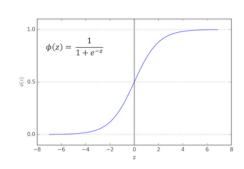
h = g(Wx+b); Affine transformation followed by activation function, g

Very important factor in learning features

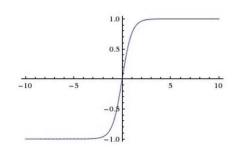
$$g(z) = \max\{0,z\}, ReLU$$



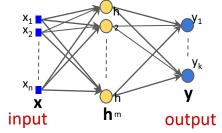
$$g(z) = \sigma(z)$$
, sigmoid



$$tanh(z) = 2\sigma(2z) - 1$$



Activation functions for Output units



- Linear units for real valued outputs
 - Activation function is left to be linear
 - Given features h,

$$y' = Wh+b$$

Most commonly used with regression tasks

- Say you want to do binary classification
 - ☐ What kind of distribution describes output?

Bernouli

☐ How to constrain the output - valid probability? Can you use linear activation?

$$P(y = 1 \mid \boldsymbol{x}) = \max \{0, \min \{1, \boldsymbol{w}^{\mathsf{T}} \boldsymbol{h} + b\}\}.$$

- What is the problem? Not amenable for gradient based learning
- ☐ Instead, use sigmoid unit output ∈ [0,1]

$$\hat{y} = \sigma \left(\boldsymbol{w}^{\top} \boldsymbol{h} + b \right)$$

Activation functions for Output units

- Now, say we want to do multi-class classification (K classes)
 - Output should be K probabilities, $p_k = p(class = k \mid x) \forall k = 1 \text{ to } K$
 - ☐ Can we use K sigmoid units?

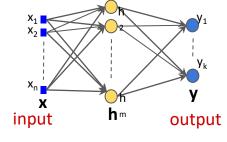
Won't be sufficient, since probabilities are not constrained to sum to 1

$$\sum_{k} p_{k} = 1$$

- ☐ We will look at softmax unit for this
 Idea is to convert a vector of real values to valid probabilities,
 ☐ Haw? Make all the elements positive
 - Normalize the values

- Let,
$$\mathbf{z} = [z_1, ..., z_K]^T$$
; $\mathbf{z} = \mathbf{Wh} + \mathbf{b}$

$$\operatorname{softmax}(\mathbf{z})_i = \frac{\exp(z_i)}{\sum_i \exp(z_i)}.$$



Cost functions

For regression,

$$J(\theta) = \frac{1}{2} \mathbb{E}_{\mathbf{x}, \mathbf{y} \sim \hat{p}_{\text{data}}} ||\mathbf{y} - f(\mathbf{x}; \boldsymbol{\theta})||^2$$
$$\frac{1}{2} \sum_{\{x_i, y_i\}} ||y_i - f(x_i, \theta)||^2$$

For classification,

- Typically outputs a probability vector $q(c = k | x) \forall k$
- How do you compare two distributions?
 - \Box KL divergence, KL($p \parallel q$)

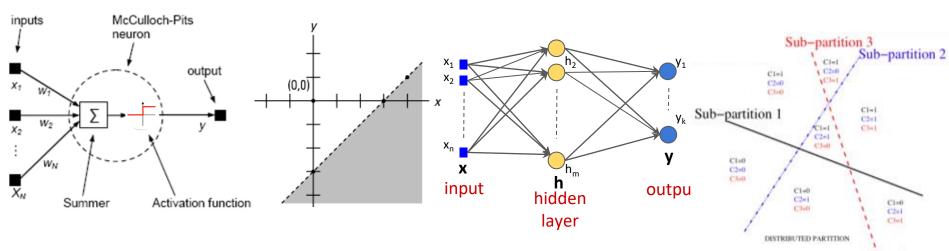
$$D_{KL}(p(x)||q(x)) = \sum_{x \in X} p(x) \ln \frac{p(x)}{q(x)}$$

$$= \sum_{x \in X} p(x) \ln p(x) - p(x) \ln q(x)$$

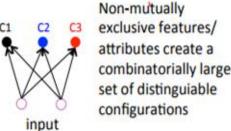
$$= -H(p) + H(p,q)$$
Entropy cross-entropy

$$J(\theta) = \sum_{x_i, y_i} H(p(x_i), q(x_i))$$

What we learnt till now:

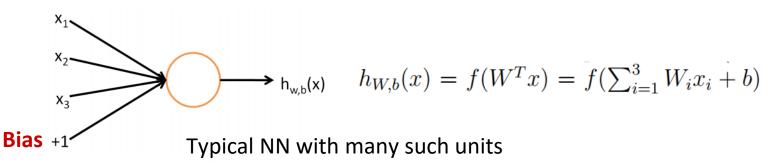


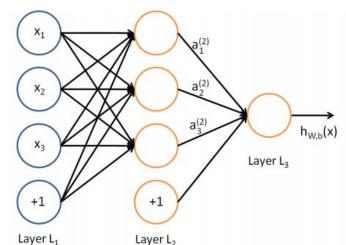
- Network specification
 - Number of hidden layers and units in each layer
 - Activation function for
 - Hidden layers
 - Output layers
 - Cost function



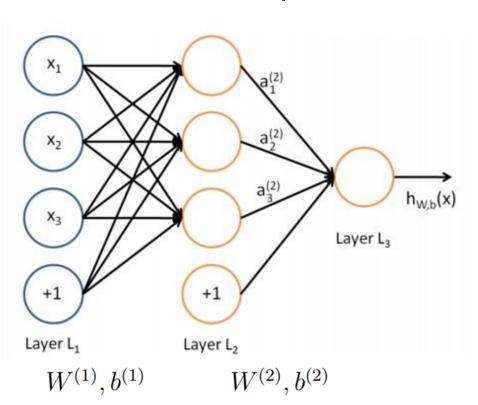
How to learn the network parameters?

Error back propagation





- One hidden layer
 - 3 neuron units
- One output



$$L_l$$
 – Layer l

$$a_i^{(l)}$$
 – activation of unit i in layer l

$$W_{ij}^{(l)}$$
 – Weight from $j^{ ext{th}}$ unit in l to $i^{ ext{th}}$ unit in $l+1$

$$b_i^{(l)}$$
 - bias to unit i in layer $l+1$

Parameters:

$$(W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$$

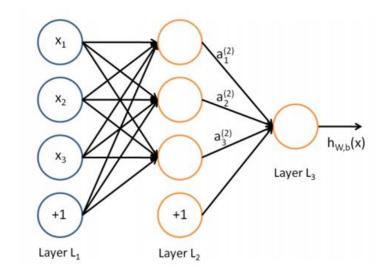
$$W^{(1)} \in \mathbb{R}^{3\times3}, W^{(2)} \in \mathbb{R}^{1\times3}$$

Layer 2,

$$a_{1}^{(2)} = f(W_{11}^{(1)}x_{1} + W_{12}^{(1)}x_{2} + W_{13}^{(1)}x_{3} + b_{1}^{(1)})$$

$$a_{2}^{(2)} = f(W_{21}^{(1)}x_{1} + W_{22}^{(1)}x_{2} + W_{23}^{(1)}x_{3} + b_{2}^{(1)})$$

$$a_{3}^{(2)} = f(W_{31}^{(1)}x_{1} + W_{32}^{(1)}x_{2} + W_{33}^{(1)}x_{3} + b_{3}^{(1)})$$



Layer 3,

$$h_{W,b}(x) = a_1^{(3)} = f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)})$$

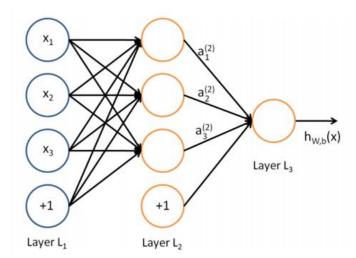
Simplification

Let, $z_i^{(l)}$ denote weighted sum for the activation $a_i^{(l)}$ $a_i^{(l)} = f(z_i^{(l)}) \quad \textit{f(.)} \text{ applies the function point wise}$

$$a_1^{(2)} = f(W_{11}^{(1)}x_1 + W_{12}^{(1)}x_2 + W_{13}^{(1)}x_3 + b_1^{(1)})$$

$$a_2^{(2)} = f(W_{21}^{(1)}x_1 + W_{22}^{(1)}x_2 + W_{23}^{(1)}x_3 + b_2^{(1)})$$

$$a_3^{(2)} = f(W_{31}^{(1)}x_1 + W_{32}^{(1)}x_2 + W_{33}^{(1)}x_3 + b_3^{(1)})$$



$$h_{W,b}(x) = a_1^{(3)} = f(W_{11}^{(2)}a_1^{(2)} + W_{12}^{(2)}a_2^{(2)} + W_{13}^{(2)}a_3^{(2)} + b_1^{(2)})$$

Let, $z_i^{(l)}$ denote weighted sum for the activation $a_i^{(l)}$

$$z^{(2)} = W^{(1)}x + b^{(1)}$$

$$a^{(2)} = f(z^{(2)})$$

$$z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$$

$$a^{(l+1)} = W^{(l)}a^{(l)} + b^{(l)}$$

$$a^{(l+1)} = f(z^{(l+1)})$$

$$h_{W,b}(x) = a^{(3)} = f(z^{(3)})$$

Given *m* training examples

$$\{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$$

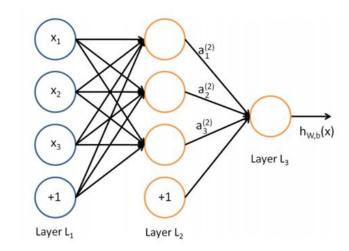
Minimize:

$$J(W, b; x, y) = \frac{1}{2} \|h_{W,b}(x) - y\|^2$$

Assume we are solving a regression problem

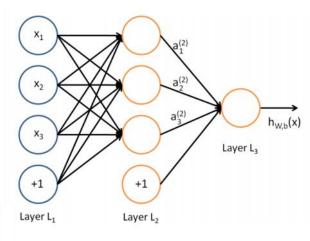
$$J(W, b) = \left[\frac{1}{m} \sum_{i=1}^{m} J(W, b; x^{(i)}, y^{(i)})\right]$$

$$= \left[\frac{1}{m} \sum_{i=1}^{m} \left(\frac{1}{2} \left\| h_{W,b}(x^{(i)}) - y^{(i)} \right\|^{2} \right) \right]$$



Minimize:
$$J(W, b) = \left[\frac{1}{m} \sum_{i=1}^{m} J(W, b; x^{(i)}, y^{(i)}) \right]$$

$$= \left[\frac{1}{m} \sum_{i=1}^{m} \left(\frac{1}{2} \left\| h_{W,b}(x^{(i)}) - y^{(i)} \right\|^{2} \right) \right]$$



Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$

$$b_i^{(l)} := b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W, b)$$

How to evaluate these partial derivatives?

Error back-propagation

Error back propagation

Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b) \qquad J(W, b) = \left[\frac{1}{m} \sum_{i=1}^{m} J(W, b; x^{(i)}, y^{(i)}) \right]$$

$$b_{i}^{(l)} := b_{i}^{(l)} - \alpha \frac{\partial}{\partial b_{i}^{(l)}} J(W, b) \qquad = \left[\frac{1}{m} \sum_{i=1}^{m} \left(\frac{1}{2} \left\| h_{W, b}(x^{(i)}) - y^{(i)} \right\|^{2} \right) \right]$$

$$\frac{\partial}{\partial W_{ij}^{(l)}} J(W, b) = \frac{\partial}{\partial W_{ij}^{(l)}} \left[\frac{1}{m} \sum_{i=1}^{m} J(W, b; x^{(i)}, y^{(i)}) \right]$$

- Overall gradient can be computed by computing gradients wrt individual data terms
- Perform back propagation for computing individual data gradients
- Average them to get the overall gradient

Back-propagation algorithm

Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$

Idea:

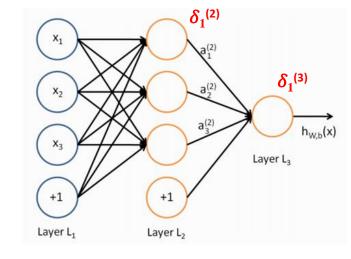
First, forward pass the data to calc. all responses

In backward pass, for each unit i in layer l calculate error term $\delta_i^{(l)}$ - measures how much unit i is responsible for output error

- For output unit in last layer (n_l) , this is easy

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z_i^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$

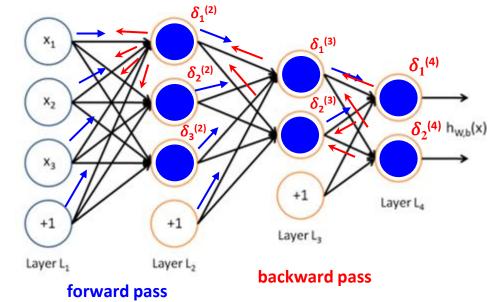
– How to measure $\delta_i^{(l)}$ for hidden units?



Preview of back-propagation

- 1. Perform a feedforward pass
 - Computing activations L_1 , L_2 and so on ...
- 2. For each output unit i in layer L_4 (output layer), set

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$



3. Starting from last but one layer to 2nd layer;

$$l = n_1 - 1, n_1 - 2, \ldots, 2$$

- For each node
$$i$$
 in layer l , set $\delta_i^{(l)} = \left(\sum_{i=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)}\right) f'(z_i^{(l)})$

4. Compute the desired partial derivatives, as:

$$\frac{\partial}{\partial W_{ii}^{(l)}}J(W,b;x,y) = a_j^{(l)}\delta_i^{(l+1)} \qquad \frac{\partial}{\partial b_i^{(l)}}J(W,b;x,y) = \delta_i^{(l+1)}.$$

*Slide courtesy, sparse autoencoder by Andrew Ng

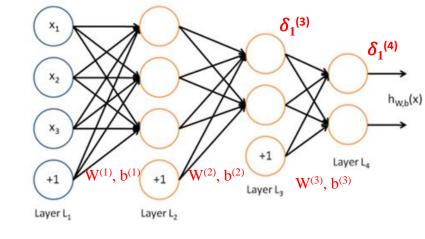
Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$
$$J(W, b; x, y) = \frac{1}{2} \|h_{W,b}(x) - y\|^2$$

For last layer:

$$\frac{\partial J}{\partial W_{ij}^{(3)}} = \frac{\partial J}{\partial z_i^4} \frac{\partial z_i^4}{\partial W_{ij}^{(3)}}$$
$$\frac{\delta_i^{(4)}}{a_j^{(3)}}$$

$$\frac{\partial J}{\partial W_{ii}^{(l)}} = \delta_i^{(l+1)} a_j^{(l)} \quad \frac{\partial J}{\partial b_i^{(l)}} = \delta_i^{(l+1)}$$



$$h_{W,b}(x) = a^{(4)} = f(z^{(4)}); \ z^{(4)} = W^{(3)}a^{(3)} + b^{(3)}$$

$$\frac{\partial J}{\partial z_i^4} = -(y_i - a_i^{(4)}) \cdot f'(z_i^4)$$

$$\frac{\partial z_i^4}{\partial W_{ij}^3} = a_j^{(3)}$$

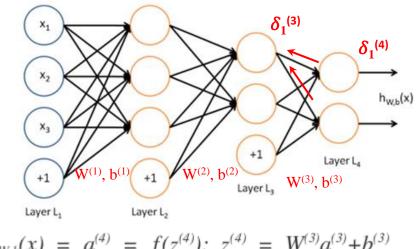
$$\delta_i^{(4)} \text{ error term}$$

Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$
$$J(W, b; x, y) = \frac{1}{2} \|h_{W,b}(x) - y\|^2$$

For layers other than last:

$$\begin{split} \frac{\partial J}{\partial W_{ij}^{(2)}} &= \begin{bmatrix} \frac{\partial J}{\partial z_i^{(3)}} & \frac{\partial z_i^{(3)}}{\partial W_{ij}^{(2)}} \\ \frac{\partial J}{\partial W_{ij}^{(l)}} & \frac{\partial J}{\partial y_i^{(l)}} \end{bmatrix} a_j^{(2)} \\ \frac{\partial J}{\partial W_{ii}^{(l)}} &= \delta_i^{(l+1)} a_j^{(l)} & \frac{\partial J}{\partial b_i^{(l)}} &= \delta_i^{(l+1)} \end{split}$$



$$h_{W,b}(x) = a^{(4)} = f(z^{(4)}); \ z^{(4)} = W^{(3)}a^{(3)} + b^{(3)}$$

 $a^{(3)} = f(z^{(3)}); \ z^{(3)} = W^{(2)}a^{(2)} + b^{(2)}$

error term
$$\frac{\delta_{i}^{(3)}}{\partial z_{i}^{(3)}} = \frac{\partial J}{\partial a_{i}^{(3)}} \frac{\partial a_{i}^{(3)}}{\partial z_{i}^{(3)}}$$

$$= \left(\sum_{j} \frac{\partial J}{\partial z_{j}^{(4)}} \frac{\partial z_{j}^{(4)}}{\partial a_{i}^{(3)}}\right) f'(z_{i}^{(3)})$$

$$\delta_{i}^{(4)} \qquad W_{ii}^{(3)}$$

Layer - (l+1)

*Slide courtesy, sparse autoencoder by Andrew Ng

- 1. Perform a feedforward pass
 - Computing activations L_1 , L_2 and so on ...
- 2. For each output unit i in layer L_4 (output layer), set

$$\delta_i^{(n_l)} = \frac{\partial}{\partial z_i^{(n_l)}} \frac{1}{2} \|y - h_{W,b}(x)\|^2 = -(y_i - a_i^{(n_l)}) \cdot f'(z_i^{(n_l)})$$

 $\delta_1^{(4)}$ $\delta_{2}^{(4)} h_{W,b}(x)$ Layer L4 Layer L₃ Layer L, Layer L, backward pass forward pass

3. Starting from last but one layer to 2nd layer;

$$l = n_1 - 1, n_1 - 2, \ldots, 2$$

- For each node
$$i$$
 in layer l , set $\delta_i^{(l)} = \left(\sum_{i=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)}\right) f'(z_i^{(l)})$

4. Compute the desired partial derivatives, as:

$$\frac{\partial}{\partial W_{ii}^{(l)}}J(W,b;x,y) = a_j^{(l)}\delta_i^{(l+1)} \qquad \frac{\partial}{\partial b_i^{(l)}}J(W,b;x,y) = \delta_i^{(l+1)}.$$

*Slide courtesy, sparse autoencoder by Andrew Ng

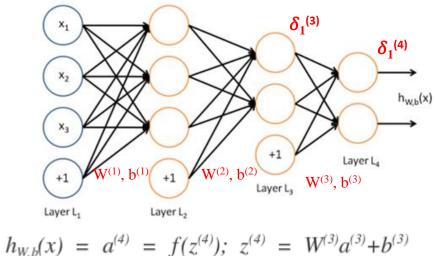
Gradient descent:

$$W_{ij}^{(l)} := W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W, b)$$
$$J(W, b; x, y) = \frac{1}{2} \|h_{W,b}(x) - y\|^2$$

Partial derivatives:

$$\delta_i^{(l)} = \left(\sum_{j=1}^{s_{l+1}} W_{ji}^{(l)} \delta_j^{(l+1)}\right) f'(z_i^{(l)})$$

$$\frac{\partial J}{\partial W_{ii}^{(l)}} = \delta_i^{(l+1)} a_j^{(l)} \quad \frac{\partial J}{\partial b_i^{(l)}} = \delta_i^{(l+1)}$$



$$h_{W,b}(x) = a^{(4)} = f(z^{(4)}); \ z^{(4)} = W^{(3)}a^{(3)} + b^{(3)}$$

Matrix notation:

$$\delta^{(l)} = ((W^{(l)})^T \delta^{(l+1)}) \bullet f'(z^{(l)})$$

$$\frac{\partial J}{\partial W^{(l)}} = \delta^{(l+1)} (a^{(l)})^T \qquad \frac{\partial J}{\partial b^{(l)}} = \delta^{(l+1)}$$

- 1. Perform a feedforward pass
 - Computing activations L_1 , L_2 and so on ...
- 2. For each output unit i in layer L_4 (output layer), set

$$\delta^{(n_l)} = -(y - a^{(n_l)}) \bullet f'(z^{(n)})$$

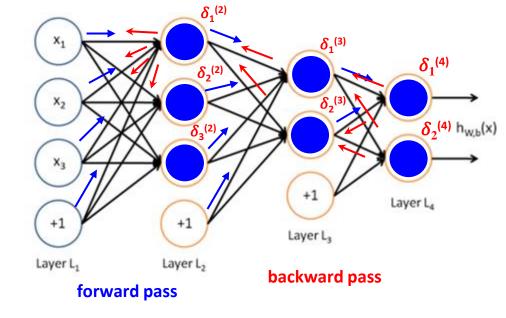
3. Starting from last but one layer to 2^{nd} layer; $l = n_l - 1, n_l - 2, \dots, 2$

$$\delta^{(l)} = ((W^{(l)})^T \delta^{(l+1)}) \bullet f'(z^{(l)})$$

4. Compute the desired partial derivatives, as:

$$\nabla_{W^{(l)}} J(W, b; x, y) = \delta^{(l+1)} (a^{(l)})^T,$$

 $\nabla_{b^{(l)}} J(W, b; x, y) = \delta^{(l+1)}.$



Summary: Error back propagation

Gradient descent:

$$\begin{split} W_{ij}^{(l)} &:= W_{ij}^{(l)} - \alpha \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b) \\ b_i^{(l)} &:= b_i^{(l)} - \alpha \frac{\partial}{\partial b_i^{(l)}} J(W,b) \\ \frac{\partial}{\partial W_{ij}^{(l)}} J(W,b) &= \frac{\partial}{\partial W_{ij}^{(l)}} \left[\frac{1}{m} \sum_{i=1}^m J(W,b;x^{(i)},y^{(i)}) \right] \end{split}$$

- Perform back propagation for computing individual gradient wrt each data
- Average them to get the overall gradient

Basic Neural Networks

What we will learn in the course about Neural Networks?

Introduction

- McCulloch and Pits model
- Rosenblatt's perceptron

Perceptrons

- Geometry and linear separability
- XoR problem
- Multi-layer perceptron (MLP)

Training MLPs

- Error back propagation
- Loss functions

Regularization and optimization

- Over fitting / Under fitting
- Regularization
- Various algorithm

Regularization

Overfitting and underfitting, L2 and L1 norm regularizations, Bagging, Dropout

Generalization

The central challenge of machine learning is to perform well on the - unseen test data, not just the training data

While training the model

What we actually want

Train err
$$\frac{1}{m^{(\text{train})}}||oldsymbol{X}^{(\text{train})}oldsymbol{w} - oldsymbol{y}^{(\text{train})}||_2^2,$$

Test err (or)
Generalization err

$$\frac{1}{m^{(\text{test})}}||\boldsymbol{X}^{(\text{test})}\boldsymbol{w}-\boldsymbol{y}^{(\text{test})}||_2^2.$$

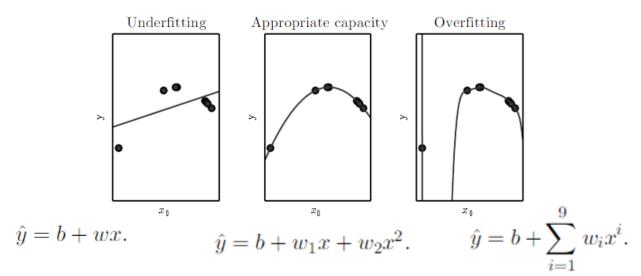
How can we say something about the test data by only seeing the train data?

Statistical learning theory

- Training and Test sets are not arbitrary
- Underlying data generating distribution is same

Capacity, Overfitting and Underfitting

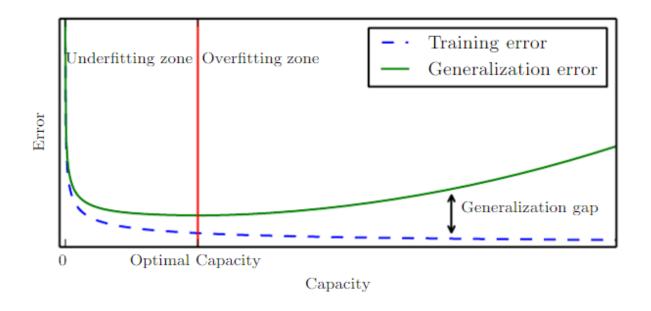
The central challenge of machine learning is to perform well on the *unseen test* data, not just the *training data*



Occam's razor: This principle states that among competing hypotheses that explain known observations equally well, one should choose the "simplest" one.

Capacity, Overfitting and Underfitting

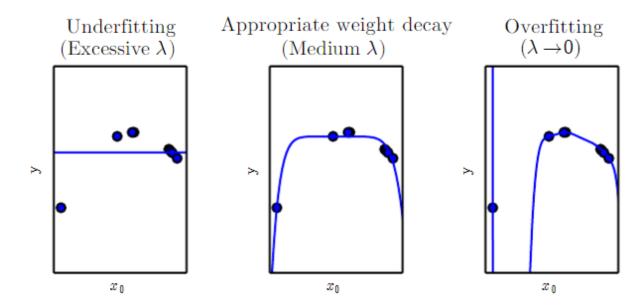
The central challenge of machine learning is to perform well on the *unseen test* data, not just the *training data*



Regularization

Regularization is any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error

$$J(\boldsymbol{w}) = \text{MSE}_{\text{train}} + \lambda \boldsymbol{w}^{\top} \boldsymbol{w},$$



^{*}Slide courtesy, Ian Goodfellow et al., deep learning book

Regularization - parameter norm penalties

L_2 norm regularization

(weight decay, ridge regression)

$$\tilde{J}(\boldsymbol{\theta};\boldsymbol{X},\boldsymbol{y}) = J(\boldsymbol{\theta};\boldsymbol{X},\boldsymbol{y}) + \alpha \Omega(\boldsymbol{\theta})$$

$$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \frac{\alpha}{2} \boldsymbol{w}^{\top} \boldsymbol{w} + J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}),$$

Parameter update:

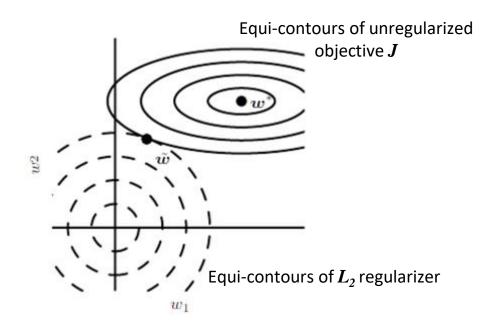
$$\nabla_{\boldsymbol{w}} \tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \alpha \boldsymbol{w} + \nabla_{\boldsymbol{w}} J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}).$$

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \epsilon \left(\alpha \boldsymbol{w} + \nabla_{\boldsymbol{w}} J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) \right).$$

$$\boldsymbol{w} \leftarrow (1 - \epsilon \alpha) \boldsymbol{w} - \epsilon \nabla_{\boldsymbol{w}} J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}).$$

Illustration of Weight decay

$$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \frac{\alpha}{2} \boldsymbol{w}^{\top} \boldsymbol{w} + J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}),$$



Regularization - parameter norm penalties

L_1 norm regularization

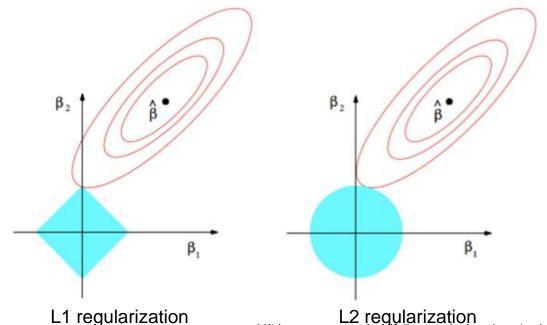
$$\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) + \alpha \Omega(\boldsymbol{\theta})$$

$$\Omega(\boldsymbol{\theta}) = ||\boldsymbol{w}||_1 = \sum |w_i|,$$

$$\tilde{J}(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y}) = \alpha ||\boldsymbol{w}||_1 + J(\boldsymbol{w}; \boldsymbol{X}, \boldsymbol{y})$$

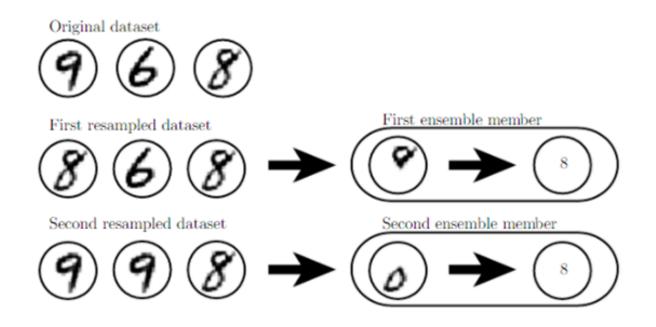
L1 regularization results in sparser solution

Feature selection



L2 regularization
*Slide courtesy, Ian Goodfellow et al., deep learning book

Bagging - bootstrap aggregating (Breiman, 1994)



Bagging - bootstrap aggregating

- Say k regression models
 - Say each of them makes ϵ_i error
 - Error is drawn from Multivariate normal distribution

$$\mathbb{E}[\epsilon_i^2] = v; \quad \mathbb{E}[\epsilon_i \epsilon_j] = c$$

• Avg. error by $m{k}$ models

$$(1/k) \sum_{i} \epsilon_{i}$$

 Expected squared error of the ensemble predictor

$$\mathbb{E}\left[\left(\frac{1}{k}\sum_{i}\epsilon_{i}\right)^{2}\right] = \frac{1}{k^{2}}\mathbb{E}\left[\sum_{i}\left(\epsilon_{i}^{2} + \sum_{j\neq i}\epsilon_{i}\epsilon_{j}\right)\right]$$
$$= \frac{1}{k}v + \frac{k-1}{k}c.$$

- If perfectly uncorrelated, c = 0, error reduces to v/k
- If the models are perfectly correlated and c = v, error remains at v

Disadvantage: Need to train multiple networks. Not very feasible for deep learning

Drop-out (Srivastava et al., 2014)

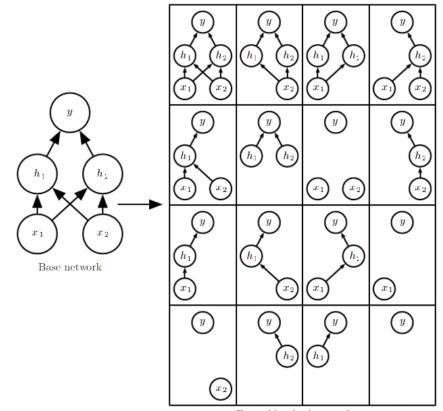
Stochastically turn the activation of the hidden unit off with a probability, *p*

$$h^{(k)} = f(Wh^{(k-1)} + b^{(k-1)})$$
$$\hat{h}^{(k)} = \mu^{(k)} \odot h^{(k)}$$

 How to train it? Each batch of data sees a sampled sub-network

Inference: Weight rescaling (Hinton et al., 2012)

 Multiply weights going out of unit i with probability of including unit i



Ensemble of subnetworks

Dataset augmentation



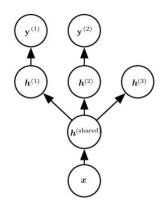
Flipping the image for classification

*pic courtesy, web

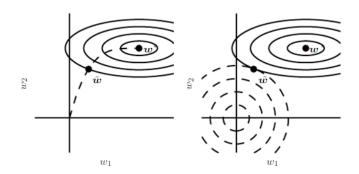
Parameter sharing and tying

Most extensively employed with Convolutional Neural Nets (CNN)

Multi-task learning



Early stopping



What we covered in Regularization

- Overfitting and underfitting
- ❖ L2 and L1 norm regularization
- Bagging
- Drop-out
- Other methods

Optimization

Minibatch optimization, Stochastic Gradient Descent, Momentum, Algorithms (AdaGrad, RMSProp, Adam)

Cost function to optimize

While training the model

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x}, y) \sim \hat{p}_{\text{data}}} L(f(\boldsymbol{x}; \boldsymbol{\theta}), y),$$

 \hat{p}_{data} distribution of training data

What we actually want

$$J^*(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x}, \mathbf{y}) \sim p_{\text{data}}} L(f(\boldsymbol{x}; \boldsymbol{\theta}), y).$$

 P_{data} distribution of actual data

Empirical risk minimization

$$\mathbb{E}_{\boldsymbol{x}, \mathbf{y} \sim \hat{p}_{\text{data}}(\boldsymbol{x}, y)}[L(f(\boldsymbol{x}; \boldsymbol{\theta}), y)] = \frac{1}{m} \sum_{i=1}^{m} L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), y^{(i)})$$

Batch and Minibatch algorithms

Loss function

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x}, y) \sim \hat{p}_{\text{data}}} L(f(\boldsymbol{x}; \boldsymbol{\theta}), y),$$

Training by backpropagation

$$\nabla_{\theta} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \nabla_{\theta} L(f(x_i; \theta), y_i)$$

It requires you to evaluate gradients w.r.t all the training examples for gradient estimation

Is this efficient?

- Variance in the estimation with m samples $\sqrt[\sigma]{\sqrt{m}}$
- By calculating grads over all samples, we get only sub-linear performance

Batch and Minibatch algorithms

Loss function

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x}, \mathbf{y}) \sim \hat{p}_{\text{data}}} L(f(\boldsymbol{x}; \boldsymbol{\theta}), y),$$

Training by backpropagation

$$\nabla_{\theta} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \nabla_{\theta} L(f(x_i; \theta), y_i)$$

By calculating grads over all samples, we get only **sub-linear** performance

What is the alternative?

- Simple solution, don't use all the samples for gradient estimation
- At each update iteration, randomly chose B samples and use them for estimating gradients Minibatch training
- Also, does as unbiased estimate of gradients

$$\nabla_{\theta} J(\theta) = \frac{1}{\mathbf{B}} \sum_{i=1}^{\mathbf{B}} \nabla_{\theta} L(f(x_i; \theta), y_i)$$

Stochastic Gradient Descent (SGD)

```
Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

Require: Learning rate \epsilon_k.

Require: Initial parameter \boldsymbol{\theta}

while stopping criterion not met do

Sample a minibatch of m examples from the training set \{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\} with corresponding targets \boldsymbol{y}^{(i)}.

Compute gradient estimate: \hat{\boldsymbol{g}} \leftarrow +\frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_{i} L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})

Apply update: \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}

end while
```

Stochastic Gradient Descent (SGD) with momentum

Parameter update step of SGD

Apply update:
$$\theta \leftarrow \theta - \epsilon \hat{g}$$

- Depending on ϵ , learning can be very slow or have drastic oscillations
- Momentum is designed to accelerate SGD
- The momentum algorithm accumulates a weighted avg.
 of past gradients and continues to move in their direction.

Figure showing effect of momentum ----- path with momentum

→ direction that SGD would take

$$\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \nabla_{\boldsymbol{\theta}} \left(\frac{1}{m} \sum_{i=1}^{m} L(\boldsymbol{f}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)}) \right),$$

Velocity v accumulates the past gradients

$$\theta \leftarrow \theta + v$$
.

The larger α is relative to ϵ , the effect of past gradients is more

Stochastic Gradient Descent (SGD) with momentum

Parameter update step now

$$\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \nabla_{\boldsymbol{\theta}} \left(\frac{1}{m} \sum_{i=1}^{m} L(\mathbf{f}(\mathbf{x}^{(i)}; \boldsymbol{\theta}), \mathbf{y}^{(i)}) \right),$$

 $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mathbf{v}.$

- In SGD, update step size was ϵ ||g||
- With momentum, depends on how large and how aligned a sequence of gradients are
- Its largest, when successive gradients are same

If momentum repeatedly observes gradient as ${m g}$, it accelerates by a factor of $\frac{1}{1-\alpha}$, resulting in $\frac{\epsilon||{m g}||}{1-\alpha}$.

For α = 0.9, the descent is 10 times normal SGD

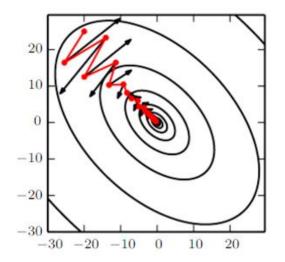


Figure showing effect of momentum ----- path with momentum

→ direction that SGD would take

Stochastic Gradient Descent (SGD) with momentum

```
Algorithm 8.2 Stochastic gradient descent (SGD) with momentum Require: Learning rate \epsilon, momentum parameter \alpha.

Require: Initial parameter \boldsymbol{\theta}, initial velocity \boldsymbol{v}.

while stopping criterion not met do

Sample a minibatch of m examples from the training set \{\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(m)}\} with corresponding targets \boldsymbol{y}^{(i)}.

Compute gradient estimate: \boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_{i} L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}),\boldsymbol{y}^{(i)})

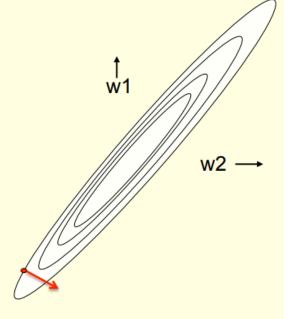
Compute velocity update: \boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \boldsymbol{g}

Apply update: \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}

end while
```

Why learning can be slow

- If the ellipse is very elongated, the direction of steepest descent is almost perpendicular to the direction towards the minimum!
 - The red gradient vector has a large component along the short axis of the ellipse and a small component along the long axis of the ellipse.
 - This is just the opposite of what we want.



Algorithms for optimization - adaptive learning rate

AdaGrad (Duchi et al., 2011)

Parameter update

Scales the learning rate with square root of sum of past gradients

 Larger partial derivatives reduced learning rates (viceversa)

Algorithm 8.4 The AdaGrad algorithm

Require: Global learning rate ϵ Require: Initial parameter θ

Require: Small constant δ , perhaps 10^{-7} , for numerical stability

Initialize gradient accumulation variable r=0

while stopping criterion not met do

Sample a minibatch of m examples from the training set $\{x^{(1)}, \ldots, x^{(m)}\}$ with corresponding targets $y^{(i)}$.

Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_{i} L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$

Accumulate squared gradient: $r \leftarrow r + g \odot g$

Compute update: $\Delta \theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{r}} \odot g$. (Division and square root applied

element-wise)

Apply update: $\theta \leftarrow \theta + \Delta \theta$

end while

Algorithms for optimization - adaptive learning rate

RMSProp(Hinton et al., 2012)

Parameter update

Scales the learning rate with weighted average of square of past gradients

Algorithm 8.5 The RMSProp algorithm

Require: Global learning rate ϵ , decay rate ρ .

Require: Initial parameter θ

Require: Small constant δ , usually 10^{-6} , used to stabilize division by small numbers.

Initialize accumulation variables r = 0

while stopping criterion not met do

Sample a minibatch of m examples from the training set $\{x^{(1)}, \dots, x^{(m)}\}$ with corresponding targets $y^{(i)}$.

Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_{i} L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$

Accumulate squared gradient: $r \leftarrow \rho r + (1 - \rho)g \odot g$

Compute parameter update: $\Delta \theta = -\frac{\epsilon}{\sqrt{\delta + r}} \odot g$. $(\frac{1}{\sqrt{\delta + r}})$ applied element-wise

Apply update: $\theta \leftarrow \theta + \Delta \theta$

end while

Algorithms for optimization - adaptive learning rate

Adam (Kingma et al., 2014)

Parameter update

Combines RMSProp and momentum methods

Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)

Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in [0,1).

(Suggested defaults: 0.9 and 0.999 respectively) Require: Small constant δ used for numerical stabilization. (Suggested default:

 10^{-8}) Require: Initial parameters θ

Initialize 1st and 2nd moment variables s = 0, r = 0

Initialize time step t = 0

while stopping criterion not met do

Sample a minibatch of m examples from the training set $\{x^{(1)}, \dots, x^{(m)}\}$ with

corresponding targets $\mathbf{y}^{(i)}$. Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_{i} L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta}), \mathbf{y}^{(i)})$

 $t \leftarrow t + 1$

Update biased first moment estimate: $s \leftarrow \rho_1 s + (1 - \rho_1) g$

Update biased second moment estimate: $r \leftarrow \rho_2 r + (1 - \rho_2) g \odot g$

Correct bias in first moment: $\hat{s} \leftarrow \frac{s}{1-\rho_1^t}$ Correct bias in second moment: $\hat{r} \leftarrow \frac{r}{1-\rho_2^t}$

Compute update: $\Delta \theta = -\epsilon \frac{\hat{s}}{\sqrt{\hat{r}} + \delta}$ (operations applied element-wise)

Apply update: $\theta \leftarrow \theta + \Delta \theta$

end while

*Slide courtesy, Ian Goodfellow et al., deep learning book

What we covered in Optimization

- Minibatch optimization
- Stochastic Gradient Descent (SGD)
- Momentum method
- Adaptive learning rate algorithms
 - ➤ AdaGrad
 - > RMSProp
 - > Adam

Summary: Basic Neural Networks

Introduction

- McCulloch and Pits model
- Rosenblatt's perceptron

Perceptrons

- Geometry and linear separability
- XoR problem
- Multi-layer perceptron (MLP)

Training MLPs

- Error back propagation
- Loss functions

Regularization and optimization

- Over fitting / Under fitting
- Regularization
- Various algorithm