#### Basic Feedforward Network

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15th April 2018

Adapted from Prof. Fuxin Li's slides.



## Linear Classifier and the Perceptron Algorithm

- $f(x) = \sigma(w^T x + b)$
- Note: vector or matrix can be judged by context, e.g., here w and x is vector.
- $\sigma$ : Sigmoid function  $\sigma(x) = \frac{1}{1+e^{-x}}$
- The connection to logistic regression:
  - Assume binomial distribution with parameter  $\hat{p}$
  - Assume the logit transform is linear:

$$\log \frac{\hat{p}}{1 - \hat{p}} = w^T x + b$$

$$\Rightarrow \hat{p} = \sigma(f(x))$$

## Maximum Log-Likelihood

• MLE of the binomial likelihood:

$$\begin{split} \sum_{i=1}^n y_i^* \log \hat{p} + (1 - y_i^*) \log(1 - \hat{p}) \\ \text{where } y_i^* \in \{0, 1\} &= \frac{1 + y_i}{2} \\ & \log \hat{p} = -\log(1 + e^{-f(x)}) \\ & \log(1 - \hat{p}) = -\log(1 + e^{f(x)}) \\ y_i^* \log \hat{p} + (1 - y_i^*) \log(1 - \hat{p}) &= -\log(1 + e^{-yf(x)}) \end{split}$$

## Gradient descent optimization

Optimize w, b with gradient descent

$$\min_{w,b} \sum_{i} \log(1 + e^{-y_i(w^T x_i + b)})$$

$$\nabla w = \sum_{i} \frac{-y_i e^{-y_i (w^T x_i + b)}}{1 + e^{-y_i (w^T x_i + b)}} x_i = \sum_{i} -y_i^* (1 - \hat{p}(x_i)) - (1 - y_i^*) \hat{p}(x_i) x_i$$

$$\nabla b = \sum_{i} \frac{-y_{i} e^{-y_{i}(w^{T} x_{i} + b)}}{1 + e^{-y_{i}(w^{T} x_{i} + b)}}$$

## XOR problem and linear classifier

- 4 points: X = [(-1, -1), (-1, 1), (1, -1), (1, 1)]
- Y = [-1, 1, 1, -1]
- Try using binomial log-likelihood loss:

$$\min_{w} \sum_{i} \log(1 + e^{-y_i(w^T x_i + b)})$$

Gradient:

$$\nabla w = \sum_{i} \frac{-y_{i} e^{-y_{i}(w^{T} x_{i} + b)}}{1 + e^{-y_{i}(w^{T} x_{i} + b)}} x_{i}$$

$$\nabla b = \sum_{i} \frac{-y_{i} e^{-y_{i}(w^{T} x_{i} + b)}}{1 + e^{-\dagger i(w^{T} x_{i} + b)}}$$

• Try w = 0, b = 0, what do you see?



## With 1 hidden layer

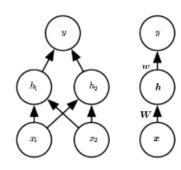
 A hidden layer makes a nonlinear classifier

$$f(x) = w^T g(W^T x + c) + b$$

- g needs to be nonlinear
- Sigmoid:  $\sigma(x) = 1/(1-x)$

$$\sigma(x) = 1/(1 + e^{-x})$$

• RELU:  $g(x) = \max(0, x)$ 



## Taking gradient

$$\min_{W,w} E(f) = \sum_{i} L(f(x_i), y_i)$$
$$f(x) = w^T g(W^T x + c) + b$$

- What is  $\frac{\partial E}{\partial W}$  ?
- Consider chain rule:  $\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$

## Note: Vectorized Computations

• The computations performed by a network.

$$z_{i} = \sum_{i} W_{ij}x_{j}$$

$$h_{i} = \sigma(z_{i})$$

$$y = \sum_{i} v_{i}h_{i}$$

- Write them in terms of matrix and vector operations.
- Note: judge vector or matrix by context

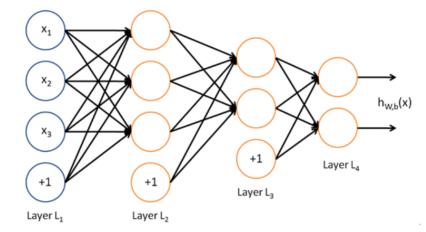
$$z = Wx$$
$$h = \sigma(z)$$
$$y = v^{T}h$$

• Where  $\sigma(v)$  denote the logistic sigma function applied elementwise to a vector v. Let W be a matrix where the (i,j) entry is the weight from visible unit j to hidden unit



## Backpropagation

- Save the gradients and the gradient products that have already been computed to avoid computing multiple times
- In a multiple layer network(Ignore constant terms)



## Backpropagation

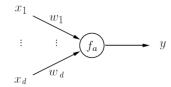
- Save the gradients and the gradient products that have already been computed to avoid computing multiple times
- In a multiple layer network(Ignore constant terms)

$$f(x) = w_n^T g(W_{n-1}^T g(W_{n-2}^T g(W_1^T g(x)))))$$
$$\frac{\partial E}{\partial W_k} = \frac{\partial E}{\partial f_k} g(f_{k-1}(x)) = \frac{\partial E}{\partial f_{k+1}} \frac{\partial f_{k+1}}{\partial f_k} g(f_{k-1}(x))$$

• Define:  $f_k(x) = w_k^T g(f_{k-1}(x)), f_0(x) = x$ 

### Modules

- Each layer can be seen as a module
- Given input, return
- Output  $f_a(x)$ 
  - Network gradient  $\frac{\partial f_a}{\partial x}$
  - Gradient of module parameters  $\frac{\partial f_a}{\partial w_a}$



- During backprop, propagate/update
  - Backpropagated gradient  $\frac{\partial E}{\partial t_a}$

$$\frac{\partial E}{\partial W_k} = \frac{\partial E}{\partial f_k} g(f_{k-1}(x)) = \frac{\partial E}{\partial f_{k+1}} \frac{\partial f_{k+1}}{\partial f_k} g(f_{k-1}(x))$$

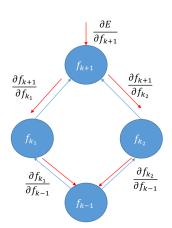
- Three term above are respectively Backprop signal; Network Gradient; gradient of parameters

  Note:  $\frac{\partial E}{\partial f_{t}} = \frac{\partial E}{\partial f_{t+1}} \frac{\partial f_{k+1}}{\partial f_{t}}$



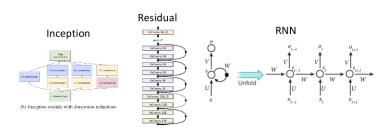
## Multiple Inputs and Multiple Outputs

$$\frac{\partial E}{\partial f_{k-1}} = \frac{\partial E}{\partial f_{k+1}} \frac{\partial f_{k+1}}{\partial f_{k_1}} \frac{\partial f_{k_1}}{\partial f_{k-1}} + \frac{\partial E}{\partial f_{k+1}} \frac{\partial f_{k+1}}{\partial f_{k_2}} \frac{\partial f_{k_2}}{\partial f_{k-1}}$$



#### Different DAG structures

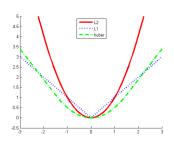
- The backpropation algorithm would work for any DAGs
- So one can imagine different architectures than the plain layerwise one



#### Loss functions

- Regression:
  - Least squares  $L(f) = (f(x) y)^2$
  - L1 loss L(f) = |f(x) y|
  - Huber loss

$$L(f) = \begin{cases} \frac{1}{2}(f(x) - y)^2 &, |f(x) - y| \le \delta \\ \delta(|f(x) - y| - \frac{1}{2}\delta) &, \text{ otherwise} \end{cases}$$



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- Binary Classification
  - Hinge loss  $L(f) = \max(1 yf(x), 0)$
  - Binomial log-likelihood  $L(f) = \ln(1 + \exp(-2yf(x)))$
  - Cross-entropy  $L(f) = -y^* \ln \sigma(f) (1-y^*) \ln (1-\sigma(f))$  ,
  - $y^* = (y+1)/2$

## Multi-class: Softmax layer

Multi-class logistic loss function

$$P(y = j|x) = \frac{e^{x^T w_j}}{\sum_{k=1} K e^{x^T w_k}}$$

- {Log}-likelihood:
- Loss function is minus log-likelihood

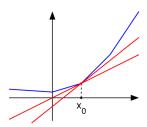
$$-\log P(y=j|x) = -x^T w_j + \log \sum_k e^{x^T w_k}$$

## Subgradients

- What if the function is non-differentiable?
- Subgradients:
  - For convex f(x) at  $x_0$ :
  - If for any y

$$f(y) \ge f(x) + g^T(y - x)$$

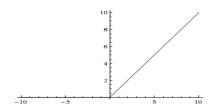
- g is called a subgradient
- Subdifferential:  $\partial f$ : set of all subgradients
- Optimality condition:  $0 \in \partial f$



### The RELU unit

- $f(x) = \max(x, 0)$
- Convex
- Non-differentiable

• Subgradient: 
$$\frac{\partial f}{\partial x} = \begin{cases} 1 & , x > 0 \\ [0,1] & , x = 0 \\ 0 & , x < 0 \end{cases}$$



## Subgradient descent

Similar to gradient descent

$$x^{(k+1)} = x^{(k)} - \alpha_k g^{(k)}$$

- Step size rules:
  - Constant step size:  $\alpha_k = \alpha$
  - Square summable:

$$\alpha_k \ge 0, \sum_{k=1}^{\infty} \alpha_k^2 < \infty, \sum_{k=1}^{\infty} \alpha_k = \infty$$

• Usually, a large constant that drops slowly after a long while . e.g.  $\frac{100}{100-k}$ 

## Universal Approximation Theorems

- Many universal approximation theorems proved in the 90s
- Simple statement: for every continuous function, there exist a function that can be approximated by a 1-hidden layer neural network with arbitrarily high precision

#### Formal statement [edit]

The theorem[2][3][4][5] in mathematical terms:

Let  $\varphi(\cdot)$  be a nonconstant, bounded, and monotonically-increasing continuous function. Let  $I_m$  denote the m-dimensional unit hypercube  $[0,1]^m$ . The space of continuous functions on  $I_m$  is denoted by  $C(I_m)$ . Then, given any function  $f\in C(I_m)$  and  $\varepsilon>0$ , there exists an integer N and real constants  $v_i,b_i\in\mathbb{R}$ , where  $i=1,\cdots,N$  such that we may define:

$$F(x) = \sum_{i=1}^{N} v_i \varphi \left( w_i^T x + b_i \right)$$

as an approximate realization of the function f where f is independent of arphi; that is,

$$|F(x) - f(x)| < \varepsilon$$

for all  $x \in I_m$ . In other words, functions of the form F(x) are dense in  $C(I_m)$ .

It obviously holds replacing  $I_m$  with any compact subset of  $\mathbb{R}^m$ .

## Universal Approximation Theorems

 The approximation does not need many units if the function is kinda nice. Let

$$C_f = \int_{R_d} ||\omega|| |\tilde{f}(\omega)| d\omega$$

 Then for a 1-hidden layer neural network with n hidden nodes, we have for a finite ball with radius r,

$$\int_{B_n} (f(x) - f_n(x))^2 d\mu(x) \le \frac{4r^2 C_f^2}{n}$$

# Thank you!