Basic Feedforward Network

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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.
- σ: 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:

$$\sum_{i=1}^{n} y_i^* \log \hat{p} + (1 - y_i^*) \log(1 - \hat{p})$$

where $y_i^* \in \{0, 1\} = \frac{1+y_i}{2}$

$$\log \hat{p} = -\log(1 + e^{-f(x)})$$

$$\log(1 - \hat{p}) = -\log(1 + e^{f(x)})$$

$$y_i^* \log \hat{p} + (1 - y_i^*) \log(1 - \hat{p}) = -\log(1 + e^{-yf(x)})$$

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:

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

- Gradient:

$$\nabla w = \sum_i \frac{-y_i e^{-y_i(w^T x_i + b)}}{1 + e^{-y_i(w^T x_i + b)}} x_i$$

$$\nabla b = \sum_i \frac{-y_i e^{-y_i(w^T x_i + b)}}{1 + e^{-y_i(w^T x_i + b)}}$$

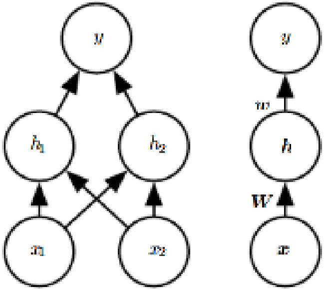
- Try $w = 0, b = 0$, what do you see?

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

$$z = Wx$$

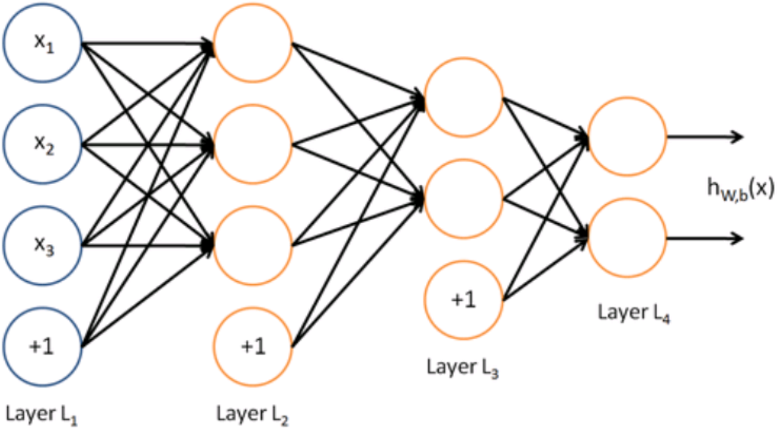
$$h = \sigma(z)$$

$$y = v^T h$$

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

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)

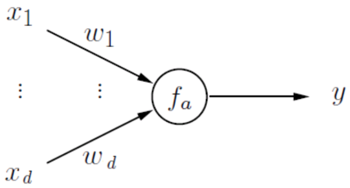
$$f(x) = w_n^T g\left(W_{n-1}^T g\left(W_{n-2}^T g\left(W_1^T g(x)\right)\right)\right)$$

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

- 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 $\frac{\partial f_a}{\partial w_a}$



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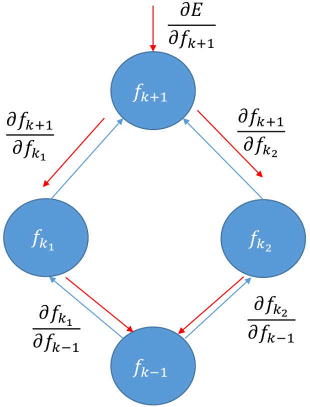
- During backprop, propagate/update
  - Backpropagated gradient $\frac{\partial E}{\partial f_a}$

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

  - Backprop signal   Network Gradient   gradient of parameters
  - Note: $\frac{\partial E}{\partial f_k} = \frac{\partial E}{\partial f_{k+1}} \frac{\partial f_{k+1}}{\partial f_k}$

Multiple Inputs and Multiple Outputs

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



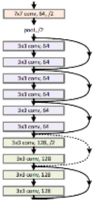
Different DAG structures

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

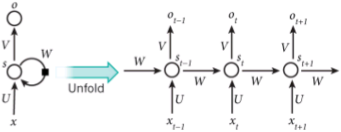
Inception

(b) Inception module with dimension reductions

Residual



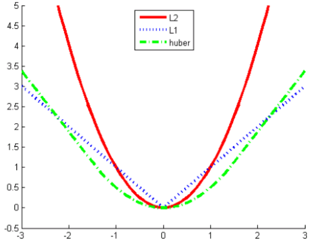
RNN



Loss functions

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

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



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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

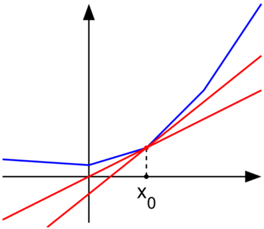
$$P(y=j|x) = \frac{e^{x^T w_j}}{\sum_{k=1}^{K} e^{x^T w_k}}$$

- Log-likelihood:
- Loss function is minus $\log$-likelihood

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

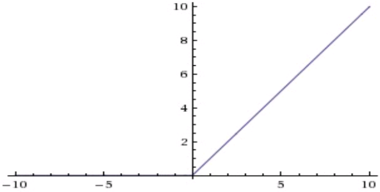
Subgradients

- What if the function is non-differentiable?
- Subgradients:
  - For convex $f(x)$ at x_0:
  - If for any y
$$f(y) \geq f(x) + g^T(y - x)$$
  - g is called a subgradient
- Subdifferential: ∂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:
    $\alpha_k \geq 0, \sum_{k=1}^{\infty} \alpha_k^2 < \infty, \sum_{k=1}^{\infty} \alpha_k = \infty$
  - 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 φ; 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,

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

Thank you!