Machine/Statistical Learning

Introduction to Neural Networks, Back propagation principle

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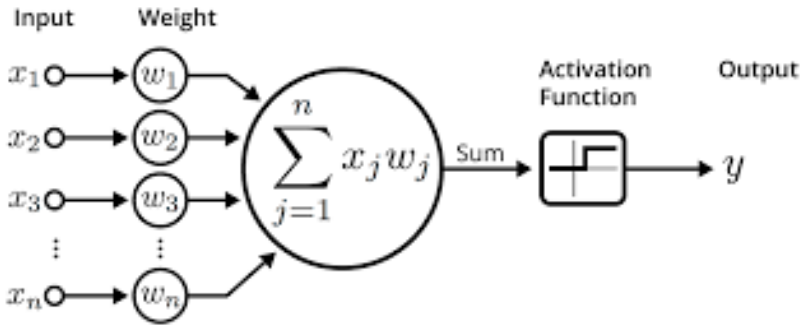
Motivation

- Build a Bio-inspired parametric model, with possibly high complexity.

Rosenblatt's perceptron, 1957



An illustration of an artificial neuron. Source: Becoming Human.

- Neural like structure, with a single unit
- n inputs

$w_j \overset{def}{=}$ *weight*, or *connecting weight*

Let $g(.)$ be the activation function, and $x = [x_1, \ldots, x_n]$ the input :

$$\begin{aligned} y &= g(a(x)) \\ a(x) &= \sum_{j=1}^{n} w_j x_x \end{aligned}$$

Remarks

- -for a (linear) classification problem, $g(a)$ is a threshold (or sigmoidal) functi
  for a (linear) regression problem, $g(a) = a$
- for binary classification,

$$g(a) = \begin{cases} -1 & \text{if } a \leq 0 \\ 1 & \text{if } a > 1 \end{cases}$$

- It is often convenient to introduce a bias to account for possible affine separating hyperplane : $[x_1, \dots x_n] \leftarrow [1, x_1, \dots, x_n] = x$
  $[w_1, \dots, w_n] \leftarrow [w_0, w_1, \dots, w_n] = w$
- In order to predict the probability of x to be in a given class :

$$g(a(x)) = \frac{1}{1 + \mathrm{e}^{a(x))}}$$

See MLPC_logical_example.ipynb

Training the perceptron

As for other ML approaches, minimize the empirical risk, i.e. an averaged cost function.

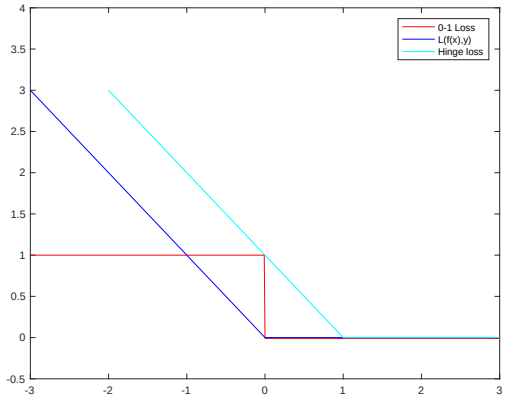
Online learning

The weights (parameters) $w_0, \ldots, w_n$ are updated to minimize the risk $L(f(x^i), y^i)$ each time that a new pair (x^i, y^i) is received, as opposed to batch learning. Gradient descent algorithm minimization :

$$w_j \leftarrow w_j - \nu \frac{\partial L(f(x^i), y^i)}{\partial w_j}$$

- ν is the learning rate. In practice, ν is often decreased when the risk is close to the minimum.
  - if ν is too large : possible instability
  - if ν is too small : slow convergence
- Many epochs may be performed on the whole training set.

historical example : binary classifier



- $y^i \in \{-1, +1\} \forall i \in [1, N]$
- $L(f(x^i, y^i) = \max(0, -y^i a(x^i)) = \max(0, -y^i w^T x^i)$

$$\Rightarrow w_j \leftarrow \begin{cases} w_j & if y^i w^T x^i > 0 \\ w_j - \nu y^i w^T x^i & if y^i w^T x^i \leq 0 \end{cases}$$

Albert Novikov theorem, 1962

Let $\mathcal{T} = \{(x^i, y^i), i = 1 \ldots, N\}$ be the training set. Let $D, \gamma \in \mathbb{R}^{+*}$, then

IF

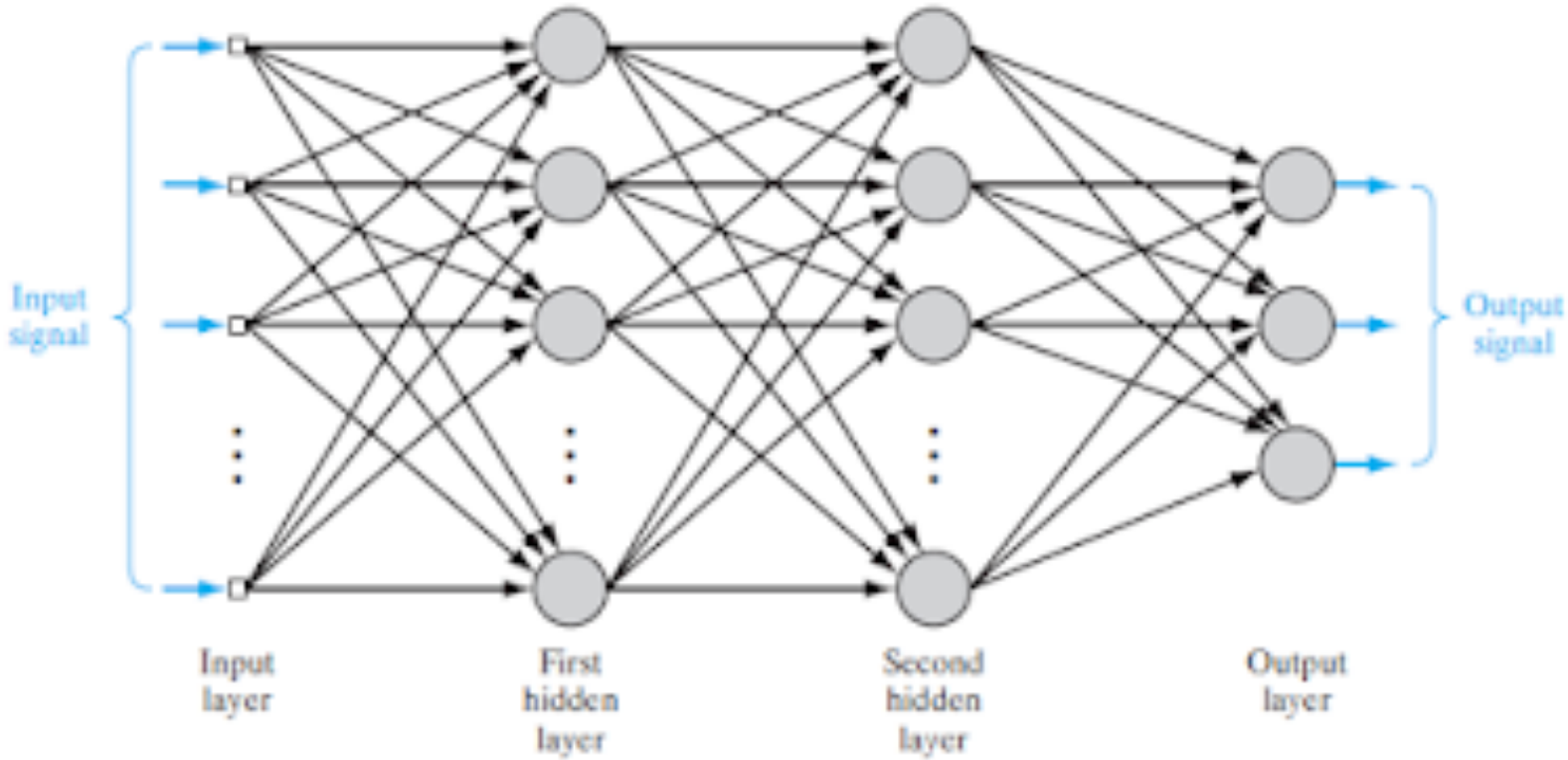
- $\forall x^i \in \mathcal{T}, ||x^i||^2 < D$ (← bounded support)
- $\exists u \in \mathbb{R}^{n+1} / \ ||u||^2 = 1$and $\forall (x^i, y^i) \in \mathcal{T}, y^i u^T x^i \geq \gamma$(← margin condition)

THEN the perceptron algorithm converges in less than $\left(\frac{D}{\gamma}\right)^2$ iterations.

See Perceptron_sonar_example.ipynb

Motivation

Allow to deal with non linear frontiers between classes by inserting hidden layers, within a FEED FORWARD network.

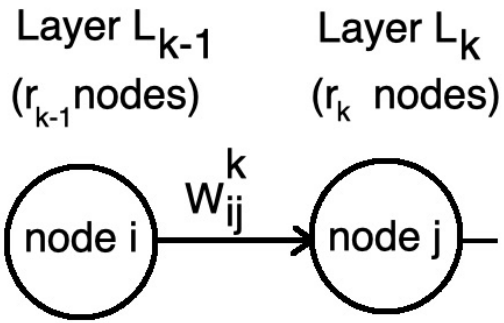


Notations

w_{ij}^k : weight for node j in layer l_k for incoming node i
b_i^k : bias for node i in layer l_k
a_i^k : product sum plus bias (activation) for node i in layer l_k
o_i^k : output for node i in layer l_k
r_k : number of nodes in layer l_k
g : activation function for the hidden layer nodes
g_o : activation function for the output layer nodes

Then

$$a_j^k = b_j^k + \sum_{i=1}^{r_{k-1}} w_{ij}^k o_i^{k-1} = \sum_{i=0}^{r_{k-1}} w_{ij}^k o_i^{k-1}$$



$$o_j^k = g(a_j^k) = g(\sum_{i=0}^{r_{k-1}} w_{ij}^k o_i^{k-1})$$

Gradient backpropagation algorithm

Backpropagation attempts to minimize the empirical risk (or loss)

$$L(X, \theta) = \frac{1}{N} \sum_i L(f(x^i), y^i)$$

with respect to the neural network's weights (gathered in θ) :
$\rightarrow$ for each weight w_{ij}^k, evaluate $\frac{\partial E}{\partial w_{ij}^k}$. By decomposing into a sum over individual error terms for each individual input-output pair

$$\frac{\partial L(X, \theta)}{\partial w_{ij}^k} = \frac{1}{N} \sum_{d=1}^{N} \frac{\partial L(f(x^d), y^d)}{\partial w_{ij}^k} = \frac{1}{N} \sum_{d=1}^{N} \frac{\partial L_d}{\partial w_{ij}^k}.$$

Loss function derivatives (index d is omitted hereafter

Remind the expression of output at node N_j :

$$o_j^k = g(a_j^k) = g(\sum_{i=0}^{r_{k-1}} w_{ij}^k o_i^{k-1})$$

L depends on w_{ij}^k trough a_j^k : Apply the chain rule to the loss function partial derivative

$$\frac{\partial L}{\partial w_{ij}^k} = \frac{\partial E}{\partial a_j^k} \frac{\partial a_j^k}{\partial w_{ij}^k}$$

$$\begin{cases} \delta_j^k & \stackrel{def}{=} \frac{\partial L}{\partial a_j^k} \\ \frac{\partial a_j^k}{\partial w_{ij}^k} & = \frac{\partial}{\partial w_{ij}^k} \left(\sum_{l=0}^{r_{k-1}} w_{lj}^k o_l^{k-1} \right) = o_i^{k-1} \end{cases} \Rightarrow \frac{\partial L}{\partial w_{ij}^k} = \delta_j^k o_i^{k-1}.$$

Output Layer (MLP with $m+1$ layers)

Assume a one-output neural network, so there is only one output node $j = 1$). Expressing L in terms of the value a_1^m $\big($since δ_1^m is a partial derivative with respect to $a_1^m\big)$ gives

$$L(f(x), y) = L\big(g_o(a_1^m), y\big)$$

where $g_o(x)$ is the activation function for the output layer.
thus,

$$\delta_1^m = L'\left(g_0(a_1^m), y\right) g_o'(a_1^m)$$

and finaly

$$\frac{\partial E}{\partial w_{i1}^m} = \delta_1^m o_i^{m-1} = L'\left(g_0(a_1^m), y\right) g_o'(a_1^m)\ o_i^{m-1}.$$

Backpropagation for hidden layers -cont'd- :

One has for the error term δ_j^k in layer $1 \leq k < m$:

$$\delta_j^k = \frac{\partial L}{\partial a_j^k} = \sum_{l=1}^{r^{k+1}} \frac{\partial L}{\partial a_l^{k+1}} \frac{\partial a_l^{k+1}}{\partial a_j^k},$$

where l ranges from 1 to r^{k+1}
(The bias input o_0^k corresponds to w_{0j}^{k+1} is fixed, does not depend on the outputs of previous layers, thus l does not take on the value 0.)
Plugging in the error term :

$$\delta_j^k = \sum_{l=1}^{r^{k+1}} \delta_l^{k+1} \frac{\partial a_l^{k+1}}{\partial a_j^k}.$$

From the definition of a_l^{k+1}

$$a_l^{k+1} = \sum_{j=1}^{r^k} w_{jl}^{k+1} g(a_j^k),$$

where $g(x)$ is the activation function for the hidden layers,

$$\frac{\partial a_l^{k+1}}{\partial a_j^k} = w_{jl}^{k+1} g'(a_j^k).$$

Backpropagation -cont'd- :

Plugging this into the latter equation yields a final equation for the error term δ_j^k in the hidden layers, called the *backpropagation* formula :

$$\delta_j^k = \sum_{l=1}^{r^{k+1}} \delta_l^{k+1} w_{jl}^{k+1} g'\left(a_j^k\right) = g'\left(a_j^k\right) \sum_{l=1}^{r^{k+1}} w_{jl}^{k+1} \delta_l^{k+1}.$$

And putting all equations together :

$$\frac{\partial L}{\partial w_{ij}^k} = \delta_j^k o_i^{k-1} = g'\left(a_j^k\right) o_i^{k-1} \sum_{l=1}^{r^{k+1}} w_{jl}^{k+1} \delta_l^{k+1}.$$

$\Rightarrow$ gradient values for updating weights at layer k are computed from the gradient $\frac{\partial L_d}{\partial a_l^{k+1}}$ used for updating layer $k+1$

Computation principle

For each pair (x_d^i, y_d^i), compute the output of each neuron by going forward long the network. Then , during a of back propagation of the errors, update all the weights going from the last hidden layer toward the first one.

BACKPROPAGATION ALGO, Main equations

For the partial derivatives,

$$\frac{\partial L_d}{\partial w_{ij}^k} = \delta_j^k o_i^{k-1}$$

where, for the final layer's error term,

$$\delta_1^m = g_o'(a_1^m) L'(f(x_d), y_d)$$

where, for the hidden layers' error terms,

$$\delta_j^k = g'\left(a_j^k\right) \sum_{l=1}^{r^{k+1}} w_{jl}^{k+1} \delta_l^{k+1}.$$

For combining the partial derivatives for each input-output pair,

$$\frac{\partial L(X,\theta)}{\partial w_{ij}^k} = \frac{1}{N} \sum_{d=1}^{N} \frac{\partial L_d}{\partial w_{ij}^k}.$$

For updating the weights,

$$\Delta w_{ij}^k = -\nu \frac{\partial L(X,\theta)}{\partial w_{ij}^k}.$$

Backpropagation algorithm summary

1) Calculate the **forward phase** for each (x_d, y_d); store the results $\hat{y_d}$, a_j^k, and o_j^k for each node j in layer k by proceeding from layer 0, to layer m, the output layer.
2) Calculate the **backward phase** for each (x_d, y_d); store $\frac{\partial L_d}{\partial w_{ij}^k}$ for each weight w_{ij}^k. Proceed from output layer m, to layer 1, the input layer.

a) Evaluate δ_1^m

b) Backpropagate the error terms for the hidden layers δ_j^k, working backwards

c) Evaluate the partial derivatives of the individual error L_d with respect to w_{ij}^k

3) Combine the individual gradients for each input-output pair to get the total gradient for the entire set $X = \{(x_1, y_1), \ldots, (x_N, y_N)\}$ (a simple average of the individual gradients).
4) Update the weights according to the learning rate α and total gradient $\frac{\partial L(X,\theta)}{\partial w_{ij}^k}$

Remarks

In the classic formulation,
for hidden nodes $\big(g(x) = \sigma(x)\big)$ (sigmoidal function)
and the output activation function is $\big(g_o(x) = x\big)$

$$g'(x) = \frac{\partial \sigma(x)}{\partial x} = \sigma(x)\big(1 - \sigma(x)\big).$$

$$g'_o(x) = \frac{\partial g_o(x)}{\partial x} = \frac{\partial x}{\partial x} = 1.$$

$\rightarrow$ No need to remember the activation values a_1^m and a_j^k in addition to the output values o_1^m and o_j^k, greatly reducing the memory footprint of the algorithm.

BUT gradient descent algorithm may be infeasible when the training data size is huge. Thus, a stochastic version of the algorithm is often used instead.

Remarks -cont'd-

• Empirical risk minimization for multilayer perceptron is an ill-posed and ill-conditioned NON CONVEX problem.

• Gradient values in the first hidden layers often takes either too large (explosion) or too low values (vanishing gradient, leading to slow down learning convergence).

• Weights initialization values, learning rate, choice of $g()$, m, r_m do all influence the result ! first results date back to Hinton, 2006

• To avoid saturation effects of node outputs (either to 0 or to 1), l_2 regularization of $L(f(x), y)$ may beapplied on θ.

Stochastic Gradient method

At each iteration, rather than computing

$$\nabla_\theta L(\mathbf{X}) = \nabla_\theta(\sum_{d=1}^{N} L(x_d)) = \sum_{d=1}^{N} \nabla_\theta L(x_d)$$

stochastic gradient descent randomly samples d at uniform and computes $\nabla_\theta L(x_d)$ instead :
SGD uses $\nabla L(x_d)$ as an unbiased estimator of $\nabla L(\mathbf{X})$;

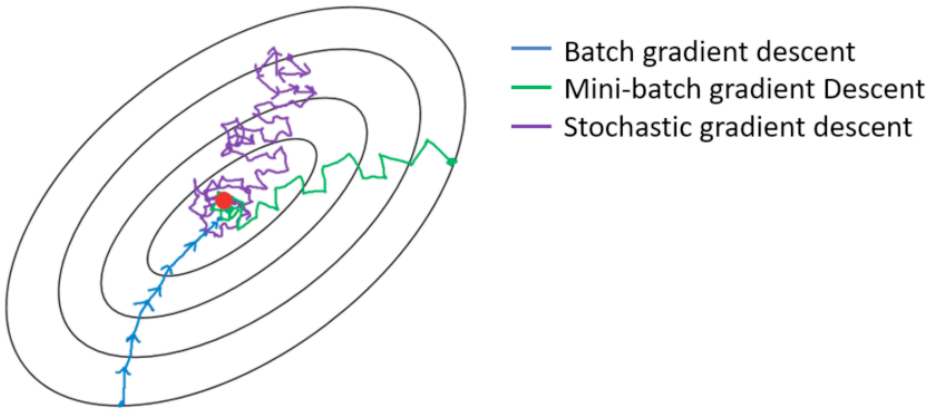
$$\mathbb{E}\left[\nabla_\theta L(x_d)\right] = \mathbb{E}\left[\frac{1}{k}\sum_{i=1}^{k} \nabla L(x_k)\right] = \nabla L(\mathbf{X}).$$

In a generalized case, at each iteration a mini-batch $\mathcal{B}$ that consists of indices for training data instances may be sampled at uniform with replacement.

$$\nabla L_{\mathcal{B}}(\mathbf{X}) = \frac{1}{|\mathcal{B}|}\sum_{d\in\mathcal{B}} \nabla L(x_d)$$

update θ as

$$\theta := \theta - \eta \nabla L_{\mathcal{B}}(\mathbf{X})$$



- The per-iteration computational cost is $\mathcal{O}(|\mathcal{B}|)$. Thus, when the mini-batch size is small, the computational cost at each iteration is light.
- If the training data set has many redundant data instances, stochastic gradients may be so close to the true gradient $\nabla_\theta L(\mathbf{X})$ that a small number of iterations will find useful solutions to the optimization problem.
- Stochastic gradient descent can be considered as offering a regularization effect especially when the mini-batch size is small due to the randomness and noise in the mini-batch sampling.
- Certain hardware processes mini-batches of specific sizes more efficiently.

See MLPC_sonar_example.ipynb

Backprop in Practice

Y LeCun

- Use ReLU non-linearities
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples (← very important)
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization on the weights (or a combination)
  - But it's best to turn it on after a couple of epochs
- Use "dropout" for regularization
- Lots more in [LeCun et al. "Efficient Backprop" 1998]
- Lots, lots more in "Neural Networks, Tricks of the Trade" (2012 edition) edited by G. Montavon, G. B. Orr, and K-R Müller (Springer)
- More recent: Deep Learning (MIT Press book in preparation)

AutoEncoder