Machine/Statistical Learning

Introduction to Neural Networks,
Back propagation principle

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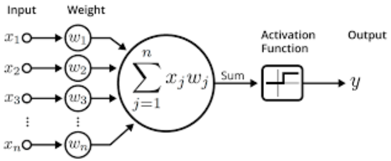
Motivation

- 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,

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

- It is often convenient to introduce a bias to account for possible affine separating hyperplane : $\begin{array}{l} [x_1, \ldots x_n] \leftarrow [1, x_1, \ldots, x_n] = x \\ [w_1, \ldots, w_n] \leftarrow [w_0, w_1, \ldots, w_n] = w \end{array}$
- 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

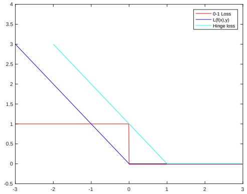
The weights (parameters) $w_0, \ldots, w_n$ are updated to minimize the risk $L(f(x^i), y^i)$ each time that a new pair (x^i, y^i) is received, as opposed to batch learning. Gradient descent algorithm minimization :

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

- 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

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



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

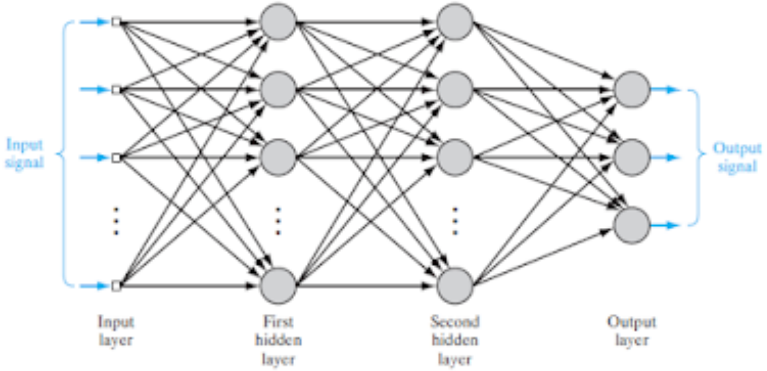
Albert Novikov theorem, 1962

Let $\mathcal{T} = \{(x^i, y^i), i = 1 \dots, N\}$ be the training set. Let $D, \gamma \in \mathbb{R}^{+*}$, then
IF
• $\forall x^i \in \mathcal{T}, ||x^i||^2 < D$ ($\leftarrow$ bounded support)
• $\exists u \in \mathbb{R}^{n+1} / \ ||u||^2 = 1$and $\forall (x^i, y^i) \in \mathcal{T}, y^i u^T x^i \geq \gamma$($\leftarrow$ 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.

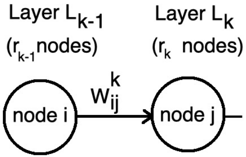


Notations

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 $\frac{\partial L}{\partial w_{ij}^k}$. 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

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

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

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

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

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 $\nabla L(\mathbf{X})$;

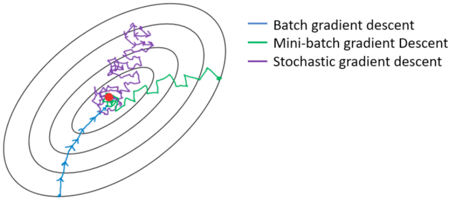
$$\mathbb{E}\left[\nabla_\theta L(x_d)\right] = \mathbb{E}\left[\frac{1}{k}\sum_{i=1}^{k} \nabla L(x_k)\right] = \nabla L(\mathbf{X}).$$

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.

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

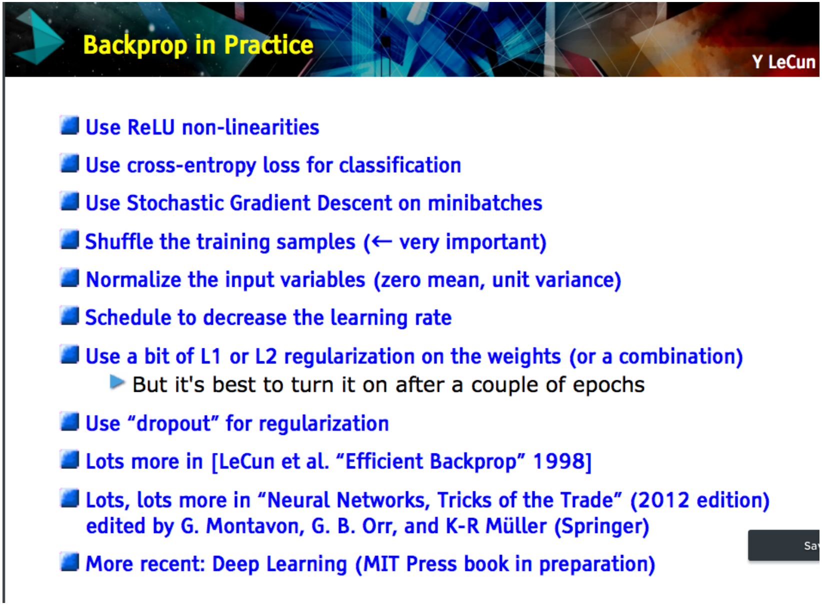
update θ as

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



- 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

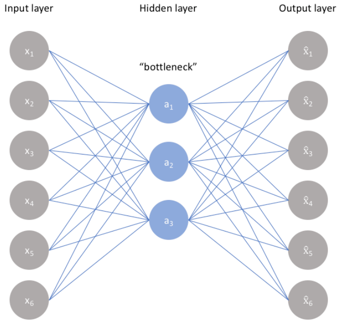
- Use ReLU non-linearities
- Use cross-entropy loss for classification
- Use Stochastic Gradient Descent on minibatches
- Shuffle the training samples (← very important)
- Normalize the input variables (zero mean, unit variance)
- Schedule to decrease the learning rate
- Use a bit of L1 or L2 regularization 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

Images for this section were adapted from https ://www.jeremyjordan.me/autoencoders/

- Autoencoders are Unsupervised Neural Networks, designed for Representation learning and/or dimension reduction.
- main idea : impose a bottleneck in the network to compressed knowledge representation of the input.

rk : This assumes that the data are structured (input features are correlated) as for e.g. iid data, such compression will be very difficult if not impossible without loosing much information.



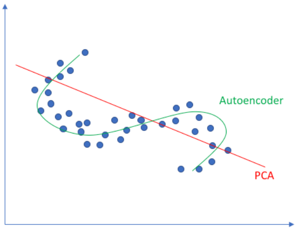
AutoEncoder principle

⇒ Formulate the problem as a supervised learning problem whose output is $\{x^i\}$

⇒ The empirical risk to minimize is thus $L(f(x), x)$: the bottleneck plays a key role (otherwise the network simply passes the values to the output.

⇒ if linear activation function were used, that would perform PCA like dimension reduction

Linear vs nonlinear dimensionality reduction



The AutoEncoder must be :

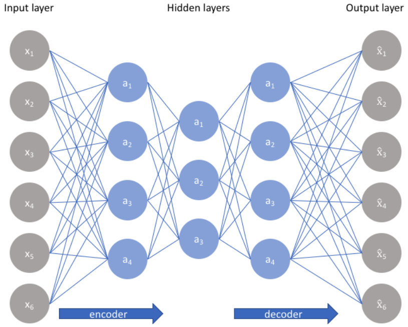
- sensitive enough to the inputs, to built an accurate reconstruction
- insensitive enough to the inputs to avoid overfitting

This requires to regularize the loss function of the form

$$L(f(x), x) + regularization$$

UnderComplete AE

Limit of the flow of information going through the NN by limiting the nb of nodes in the hidden layers :



No explicit regularization term is required here.
If too many nodes, i.e. high capacity -in the sense of Vapnik-, the AE may be capable of learning a way to simply memorize the data. The primary aim to discover latent variable cannot be attained !

Sparse AE

Idea is to keep the number of nodes in hidden layers quite large, but regularize the loss function by penalizing activations within a layer ($\neq$ weights regularisation) $\Rightarrow$ only a small nb of neurons are activated.

l_1 regularization

For layer k :

$$(f(x), x) + \lambda \sum_{j=1}^{r_k} |o_j^k|$$

Remind that in the notation of the previous section, activation of a neuron was noted $o_j^k = g(a_j^k)$. Activations are in $[0, 1]$ or $[-1, 1]$, depending on the choice of $g()$. Below, we assume $o_j^k \in [0, 1]$.

Sparse AE - cont'd-

Kullback-Leibler regularization

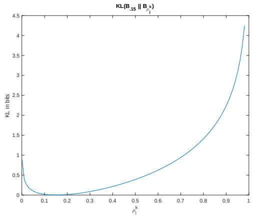
Let $\hat{\rho}_j^k \overset{def}{=} \frac{1}{n}\sum_{i=1}^n o_j^k(x)$ be the average activation of neuron i in layer k, estimated over a collection of n samples $\{x^i, i = 1 \dots n\}$.

$$L(f(x), x) + \lambda \sum_{k=1}^{m} \sum_{j=1}^{r_k} \mathrm{KL}(\mathcal{B}_\rho || \mathcal{B}_{\hat{\rho}_j^k})$$

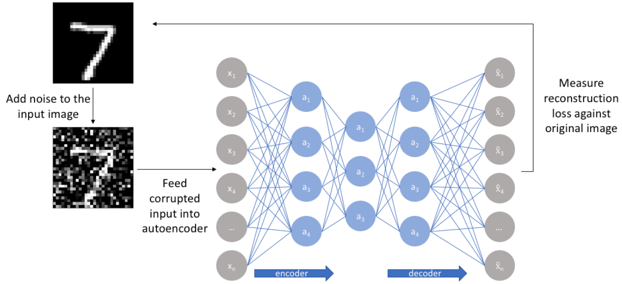
where $\mathcal{B}_\rho$ is the Bernoulli process of parameter ρ, thus

$$\mathrm{KL}(\mathcal{B}_\rho || \mathcal{B}_{\hat{\rho}_j^k}) = \rho \log \frac{\rho}{\hat{\rho}_{j^k}} + (1-\rho) \log \frac{1-\rho}{1-\hat{\rho}_{j^k}}$$

$\Rightarrow$ ρ acts as a "sparsity parameter" ; small values of ρ correspond to low probability for the neuron to fire.



AE for denoising : principle



Alternate approach for denoising

Force the activation of the hidden layer to be weakly sensitive to small deviations of the inputs

$$L(f(x),x) + \lambda \sum_{k=1}^{m} \sum_{j=1}^{r_k} ||\nabla_x o_j^k(x)||^2$$