

MULTI-LAYER NETWORKS
(FOR VECTORS)

ML.1

by

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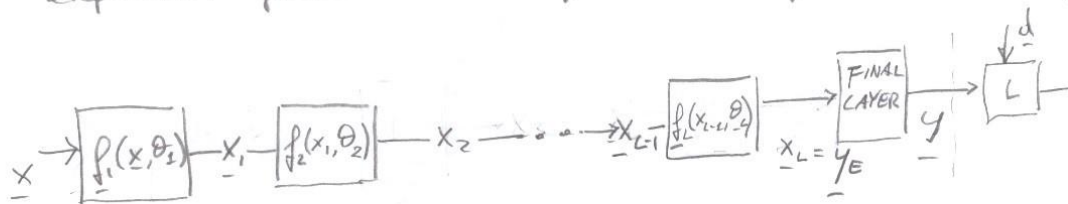
Artificial
 Neural networks have been originally inspired by biological networks where one of the main features is massive connectivity. Many paradigms that try to explain the signal processing capabilities of biological brains are based on progressive unfolding of the information coming from ^{the} various sensor modalities. Think of visual processing where, after a first transformation provided by the retinal circuits, the visual cortex extracts relevant features such as lines, bars and various patterns. This seems to be a strategy that we find both in ^{the} relatively simple brains of insects and in much more complex mammal neural architectures.

Therefore, even if we have shown in a previous chapter that two-layer network can already provide universal functional capabilities, there must be intrinsic advantages in using multiple layers. The reason for the need of multiple-layer architectures is not yet fully understood. Constrained connectivity may be one of reasons why we need multiple layers because of the need to provide sufficient mixing of the input elements. Localized feature extraction may be another one.

Much experience has been gained in the last forty years in researching the appropriate architecture for each problem, and almost invariably, multi-layer neural networks have

provided effective solutions. We should not forget that ^{ML-3}
 a working system has to provide sufficient
 generalization and massive contained connections
 may provide after learning the necessary smoothness.

In this chapter we consider
 general multi-layer architectures and provide
 explicit gradient computation for learning.



The figure above shows the cascade of L progressive
 layers that "prepare" the embedding y_E for the final
 layer. Recall from the previous chapter, that
 the final layer can be ~~of three different types~~ and
 be of three different types: (1) linear for regression;
 (2) linear + squards for multiple binary classification;
 (3) linear + softmax for n -ary classification.

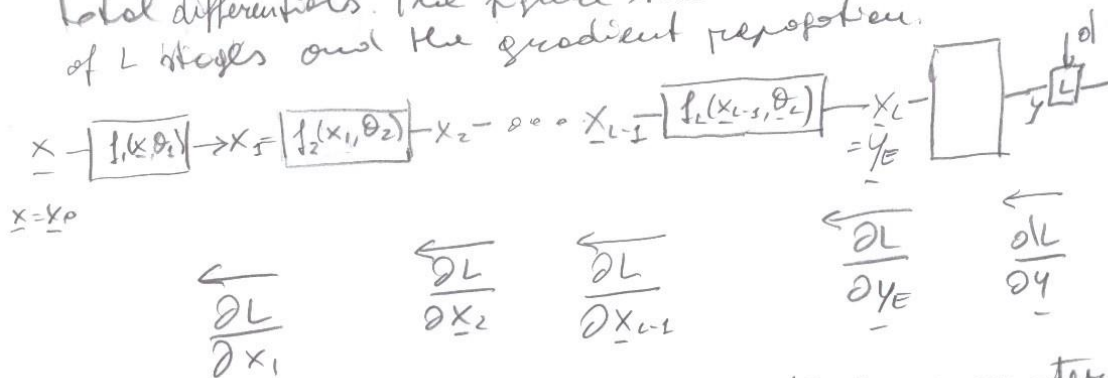
In all cases the multiple layers have to transform
 the input vector x into the embedding vector y_E
 in a way which is appropriate for the problem
 to be solved at the output y . Formally the
 transformation to the embedding space \mathcal{Y}_E is
 the nested function

$$y_E = f_L \left(f_{L-1} \left(f_{L-2} \left(\dots \left(f_2 \left(f_1(x, \theta_1), \theta_2 \right), \dots, \theta_{L-2} \right), \theta_{L-1}, \theta_L \right) \right) \right)$$

The input $x = x_0$ has size N , $x_1 \rightarrow N_1$, $x_2 \rightarrow N_2 \dots x_L \rightarrow N_L = N_E$

The layer functions can be of different types and each f_i may depend on a set of parameters θ_i to be learned. More generally some of the layer functions may be fixed with no free parameters as we will see in the following examples.

In all cases the parameters, to be learned, follow a gradient descent algorithm. The gradient is computed on the output loss function $L(y, y^d)$ and be "back propagated" following the rule of total differentials. The figure shows the cascade of L stages and the gradient propagation.



A parametric block $f_i(x_{i-1}, \theta_i)$ to update its parameters θ_i needs the gradient $\frac{\partial L}{\partial \theta_i}$, that can be computed from the back propagated gradient $\frac{\partial L}{\partial x_i}$ at its output x_i .

$$\text{as } \frac{\partial L}{\partial \theta_i} = \left(\frac{\partial x_i}{\partial \theta_i} \right)^T \frac{\partial L}{\partial x_i} \quad i = 1, \dots, L$$

Back propagation through layers consists in computing the Jacobian $\left(\frac{\partial x_{i+1}}{\partial x_i} \right)$ at each stage and propagate back word as follows:

$$\frac{\partial L}{\partial x_i} = \left(\frac{\partial x_{i+1}}{\partial x_i} \right)^T \frac{\partial L}{\partial x_{i+1}} \quad i = L-1, L-2, \dots, 1$$

Each layer may be of different type and also be non-parametric, i.e. with no parameters to be learned. In such a case we just backpropagate the gradient through it.

In the following we examine different kinds of blocks specifying the Jacobian for backpropagation and also the gradient for non-parametric learning.

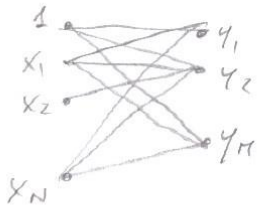
LINEAR LAYER

We have already discussed linear transformations both in the chapter on linear regression and classifiers and in the two-layer architecture. Linear layers (fully connected) can be inserted at any stage in the multi-layer architecture. They are usually followed by non-linearities, but we discuss them here separately as a potential building block of our code.

Recall that for a linear transformation we mean always an affine transformation, because we include biases to avoid to have to worry about

means and bias lines.
GENERIC LINEAR BLOCK

To facilitate notation, consider first a generic linear block $x \rightarrow y$



$$\underline{x} \xrightarrow{\underline{W}, \underline{b}} \underline{y}$$

$\frac{\partial L}{\partial \underline{x}} \longleftarrow$ $\frac{\partial L}{\partial \underline{y}} \longleftarrow$

$$\underline{W} = \begin{bmatrix} \underline{w}_1 & \underline{w}_2 & \dots & \underline{w}_M \end{bmatrix}$$

$$\underline{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_M \end{bmatrix}$$

Forward propagation can be written as

$$\underline{y} = \underline{W}^T \underline{x} + \underline{b} = \begin{bmatrix} \underline{w}_1^T \\ \underline{w}_2^T \\ \vdots \\ \underline{w}_M^T \end{bmatrix} \underline{x} + \underline{b}$$

or in the augmented form

$$\underline{y} = \begin{bmatrix} \underline{b} & \underline{W}^T \end{bmatrix} \begin{bmatrix} 1 \\ \underline{x} \end{bmatrix}$$

$$\underline{W}_a = \begin{bmatrix} \underline{b}^T \\ \underline{w}_1^T & \underline{w}_2^T & \dots & \underline{w}_M^T \end{bmatrix}$$

The Jacobian is defined and computed as

$$\frac{\partial \underline{y}}{\partial \underline{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_N} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_2}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_M}{\partial x_1} & \frac{\partial y_M}{\partial x_2} & \dots & \frac{\partial y_M}{\partial x_N} \end{pmatrix} = \begin{bmatrix} \underline{w}_1^T \\ \underline{w}_2^T \\ \vdots \\ \underline{w}_M^T \end{bmatrix} = \underline{W}^T$$

Note that it does not depend on the biases.

Gradient propagation through the block follows the rule

$$\frac{\partial L}{\partial \underline{x}} = \left(\frac{\partial \underline{y}}{\partial \underline{x}} \right)^T \frac{\partial L}{\partial \underline{y}} = \underline{W} \frac{\partial L}{\partial \underline{y}}$$

To form \underline{W} and \underline{b} we need the gradients

$$\frac{\partial L}{\partial \underline{w}} \quad \text{and} \quad \frac{\partial L}{\partial \underline{b}}$$

that can be computed from $\frac{\partial L}{\partial \underline{y}}$ as

$$\frac{\partial L}{\partial \underline{w}} = \left[\frac{\partial L}{\partial w_1} \frac{\partial L}{\partial w_2} \dots \frac{\partial L}{\partial w_H} \right] = \left[\frac{\partial L}{\partial y_1} \frac{\partial y_1}{\partial w_1}, \frac{\partial L}{\partial y_2} \frac{\partial y_2}{\partial w_2}, \dots, \frac{\partial L}{\partial y_H} \frac{\partial y_H}{\partial w_H} \right]$$

$$= \left[\frac{\partial L}{\partial y_1} x_1, \frac{\partial L}{\partial y_2} x_2, \dots, \frac{\partial L}{\partial y_H} x_H \right] = \left(\frac{\partial L}{\partial \underline{y}} \right)^T \otimes \underline{x}$$

$$\frac{\partial L}{\partial \underline{b}} = \begin{bmatrix} \frac{\partial L}{\partial b_1} \\ \frac{\partial L}{\partial b_2} \\ \vdots \\ \frac{\partial L}{\partial b_H} \end{bmatrix} = \begin{bmatrix} \frac{\partial L}{\partial y_1} \frac{\partial y_1}{\partial b_1} \\ \frac{\partial L}{\partial y_2} \frac{\partial y_2}{\partial b_2} \\ \vdots \\ \frac{\partial L}{\partial y_H} \frac{\partial y_H}{\partial b_H} \end{bmatrix} = \begin{bmatrix} \frac{\partial L}{\partial y_1} \cdot 1 \\ \frac{\partial L}{\partial y_2} \cdot 1 \\ \vdots \\ \frac{\partial L}{\partial y_H} \cdot 1 \end{bmatrix} = \frac{\partial L}{\partial \underline{y}}$$

In the augmented representation

$$\frac{\partial L}{\partial \underline{w}_n} = \left(\frac{\partial L}{\partial \underline{y}} \right)^T \otimes \underline{x}_n$$

$\underbrace{\left[\begin{matrix} w_{n1} & w_{n2} & \dots & w_{nH} \end{matrix} \right]}_{\underline{w}_n} \quad \underbrace{\left[\begin{matrix} x_{n1} \\ x_{n2} \\ \vdots \\ x_{nH} \end{matrix} \right]}_{\underline{x}_n}$

The above results are immediately applied to the i th linear stage

The forward propagation is $x_i = f_i(x_{i-1}, \theta_i) = \underline{w}_i^T x_{i-1} + b_i$ are in the augmented representation

$x_i = \underline{w}_i^T x_{i-1} + b_i$
 The Jacobian is $\frac{\partial x_i}{\partial x_{i-1}} = \underline{w}_i^T$ and the gradient backpropagation

$$\frac{\partial L}{\partial x_{i-1}} = \underline{w}_i \frac{\partial L}{\partial x_i}$$

The gradients for \underline{w}_i and b_i for learning are

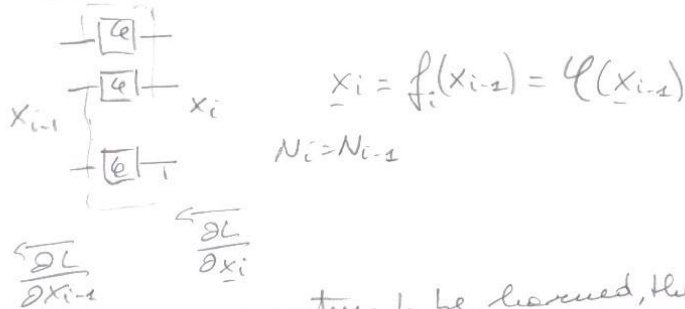
$$\frac{\partial L}{\partial \underline{w}_i} = \left(\frac{\partial L}{\partial x_i} \right)^T \otimes x_{i-1}, \quad \frac{\partial L}{\partial b_i} = \frac{\partial L}{\partial x_i}$$

In the augmented format

$$\frac{\partial L}{\partial \underline{w}_{i0}} = \left(\frac{\partial L}{\partial x_i} \right)^T \otimes x_{i-10}$$

SET OF NON LINEARITIES

ML.8



There are no parameters to be learned, therefore we have to provide only the propagation rule for gradients. The Jacobian is diagonal

$$\frac{\partial x_i}{\partial x_{i-1}} = \text{diag}(\varphi'(x_{i-1}))$$

and the gradient $\frac{\partial L}{\partial x_i}$ is backpropagated as

$$\frac{\partial L}{\partial x_{i-1}} = \left(\frac{\partial x_i}{\partial x_{i-1}} \right)^T \frac{\partial L}{\partial x_i} = \text{diag}(\varphi'(x_{i-1})) \frac{\partial L}{\partial x_i}$$

$\|N_{i-1} \times N_i\| \quad \left(\begin{matrix} N_i \\ \diagdown \\ N_i \end{matrix} \right) \quad \|N_i\|$

The nonlinearities could be sigmoids, RELUs or many others listed in Appendix x with their derivatives. To be specific consider as an example, logistics and RELUS.

For Logistics $\varphi(s) = \frac{1}{1+e^{-s}}$, $\varphi'(s) = \varphi(s)(1-\varphi(s))$

the vector of derivatives can be written as

$$\varphi'(\underline{x}) = \varphi(\underline{x}) \odot (\underline{1} - \varphi(\underline{x})) \quad \underline{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

Therefore

$$\frac{\partial L}{\partial x_{i-1}} = \text{diag}(x_i \odot (1 - x_i)) \frac{\partial L}{\partial x_i}$$

For RELUS $\varphi(s) = u(s)$, $\varphi'(s) = u'(s)$

the vector of derivatives can be written as

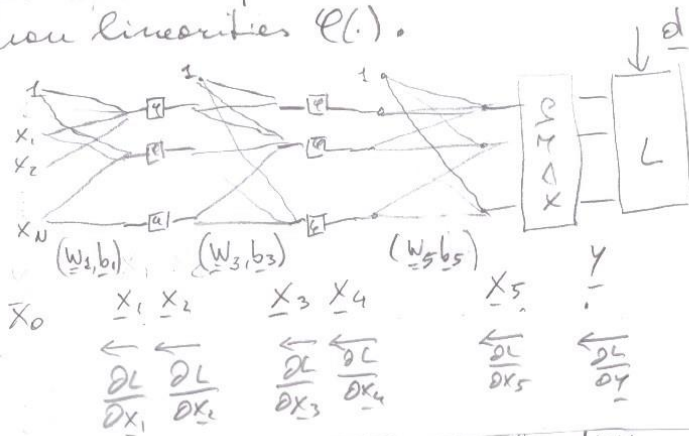
$$\varphi'(\underline{x}) = u'(\underline{x})$$

Therefore

$$\frac{\partial L}{\partial x_{i-1}} = \text{diag}(u'(x_{i-1})) \frac{\partial L}{\partial x_i}$$

The RELUS in the gradient backward flow act as gates because they do not propagate the output gradient if the input is negative.

EXAMPLE Consider the following multi-layer M.L.G architecture for classification. Assume logistic non-linearities $\phi(\cdot)$.



The network implements the function $\underline{y} = f(\underline{x}, \underline{\theta})$ where $0 \leq y_i \leq 1 \quad i=1, \dots, M$ represent the estimated posterior associated to the sample \underline{x} . The parameters to be learned are $\{(W_1, b_1), (W_3, b_3), (W_5, b_5)\}$

The forward flow is

$$\underline{x}_0 = \underline{x} \rightarrow \underline{x}_1 = W_1^T \underline{x}_0 + b_1 \rightarrow \underline{x}_2 = \phi(\underline{x}_1) \rightarrow \underline{x}_3 = W_3^T \underline{x}_2 + b_3 \rightarrow \underline{x}_4 = \phi(\underline{x}_3) \rightarrow \underline{x}_5 = W_5^T \underline{x}_4 + b_5$$

$$\rightarrow \underline{y} = S_{\max}(\underline{x}_5)$$

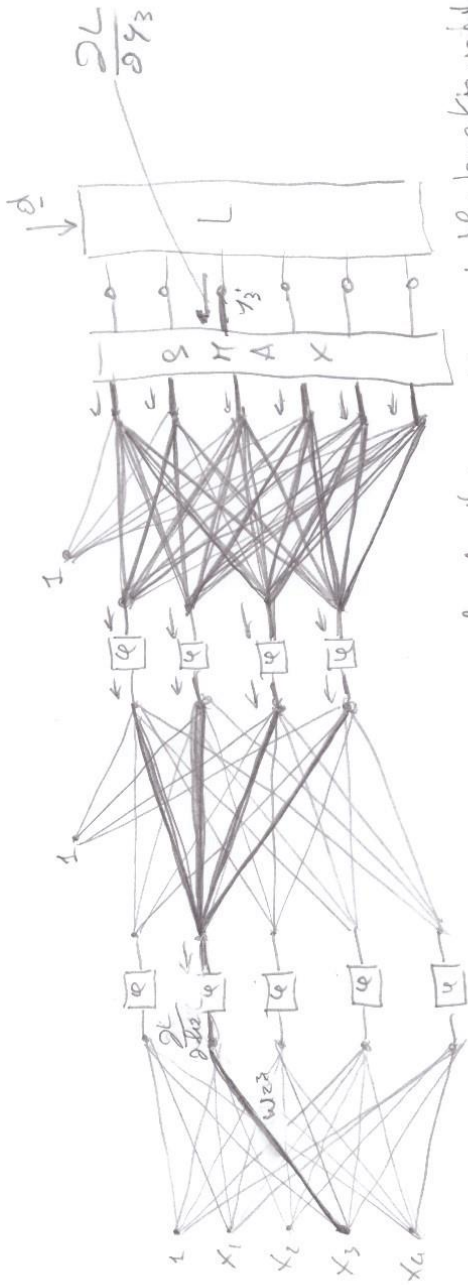
Using the cross-entropy as the loss function, the gradients vectors backpropagated are.

$$\frac{\partial L}{\partial \underline{y}} = -\frac{\underline{d}}{\underline{y}} \rightarrow \frac{\partial L}{\partial \underline{x}_5} = (\text{diag}(\underline{y}) - \underline{y}\underline{y}^T) \frac{\partial L}{\partial \underline{y}} \rightarrow \frac{\partial L}{\partial \underline{x}_4} = W_5 \frac{\partial L}{\partial \underline{x}_5} \rightarrow$$

$$\frac{\partial L}{\partial \underline{x}_3} = \text{diag}(\underline{x}_4 \circ (1 - \underline{x}_4)) \frac{\partial L}{\partial \underline{x}_4} \rightarrow \frac{\partial L}{\partial \underline{x}_2} = W_3 \frac{\partial L}{\partial \underline{x}_3} \rightarrow \frac{\partial L}{\partial \underline{x}_1} = \text{diag}(\underline{x}_3 \circ (1 - \underline{x}_3)) \frac{\partial L}{\partial \underline{x}_2}$$

The updates on $(W_1, b_1), (W_3, b_3), (W_5, b_5)$ are based on the gradients

$$\frac{\partial L}{\partial W_1} = \left(\frac{\partial L}{\partial \underline{x}_1}\right)^T \otimes \underline{x}_0, \quad \frac{\partial L}{\partial b_1} = \frac{\partial L}{\partial \underline{x}_1}, \quad \frac{\partial L}{\partial W_3} = \left(\frac{\partial L}{\partial \underline{x}_3}\right)^T \otimes \underline{x}_2, \quad \frac{\partial L}{\partial b_3} = \frac{\partial L}{\partial \underline{x}_3}, \quad \frac{\partial L}{\partial W_5} = \left(\frac{\partial L}{\partial \underline{x}_5}\right)^T \otimes \underline{x}_4$$



The figure shows an example in which it is evidenced the backpropagation flow for a specific weight w_{23} in the first layer and a specific gradient $\frac{\partial L}{\partial y_3}$ in the output layer. The network across the network weights and non-linearities to w_{23} . The effect of $\frac{\partial L}{\partial y_3}$ is transmitted in an update on w_{23} proportional to

$$\frac{\partial L}{\partial y_3} \cdot x_3.$$

SUMMARY OF THE BACKPROPAGATION ALGORITHM ML.11

The following steps are the standard gradient updates for the backpropagation algorithm. The procedures presented in the "batch" version. "Minibatch" and "stochastic" versions are easy modifications.

Our training set $\mathcal{Z} = \{(x^{[n]}, d^{[n]})\}, n=1, \dots, n_2$ will be used many times for learning the system parameters. Each time the training set is used, we say that we perform one "EPOQUE". Typically the parameters obtained at the end of each epoch, are used as initial conditions for the following one.

INITIALIZATION

At the beginning of each training session, the network parameters are usually initialized to random values. Means and variances are usually determined heuristically and may depend on the problem at hand. Loss and gradients are set to zero

$$L_0 = 0 \quad \underline{g}_0 = \underline{0}$$

EPOQUE K

Keep from the previous epoch only the network parameters θ_{k-1} ; set epoch loss and gradients to zero: $L_0 = 0, \underline{g}_0 = \underline{0}$.

EXAMPLE $n=1:n_2$

- get example $(x^{[n]}, d^{[n]})$ from the training set;
- Propagate forward $x^{[n]}$ computing all the activations in the network.
- Compute the instantaneous loss $L^{[n]} = L(y^{[n]}, d^{[n]})$ of the output.
- Compute all instantaneous gradients $\frac{\partial L^{[n]}}{\partial \theta^{[n]}}$ for every parameter backpropagating $\frac{\partial L^{[n]}}{\partial y^{[n]}}$.
- Update the loss with a running mean

$$L^{[n]} = \frac{n-1}{n} L^{[n-1]} + \frac{1}{n} L^{[n]}$$

- update the gradient for each parameter with a running mean ML.12

$$g_{\theta} [n] = \frac{n-1}{n} g_{\theta} [n-1] + \frac{1}{n} \frac{\partial L(n)}{\partial \theta [n]}$$

END OF EPOCH K .

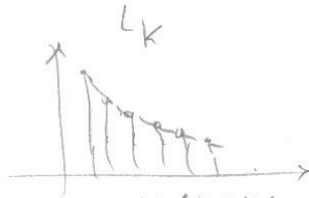
If the loss $L = L[n_k]$ has reached a satisfactory value \rightarrow EXIT
 Otherwise update the parameters

$$\theta_k = \theta_{k-1} - \mu g_{\theta}(n_k)$$

and start a new epoch.

Note that the total loss after each epoch could be computed separately using the parameters obtained at the end of that epoch. We presented the algorithm in a combined way ^{with the gradients} to present the training set to the network only once for each epoch. The only disadvantage is a useless computation of the gradients in the last epoch.

To keep track of convergence we look at the sequence $\{L_k\}$



Also global statistics about coefficients and performance metrics may be tracked during learning.

We have discussed the method with reference to a batch approach. The strategy is easily modified for mini batches simply considering n epochs (subepochs) subsets of the training set. Recall at the end of each subset, we keep only the network parameters for the new batch. The stochastic version simply updates the parameters after each example.

CONSIDERATIONS ABOUT THE BACKPROPAGATION ALGORITHM ML.13

The backpropagation algorithm being a gradient search on a nonconvex cost function, will converge inevitably to a local minimum. To reach a global minimum is generally a rather hopeless task because in theory global convergence can be obtained starting from sufficiently many initial conditions. Therefore we have to rely on solutions that represent satisfactory local minimum.

Obviously the solutions obtained must be verified on the validation set for generalization.

In practice a neural network, to be useful in an application, has to go through various cycles of learning perhaps adjusting parameters to obtain a good ^{comparison between} performances on the training set and generalization.

Generalization is a crucial feature, as pointed out many times before, and can be thought as a sort of smoother: if the training set samples are exactly modeled the obtained function may be overfitting the data because it interpolates the training points too finely. A smoother function may do a better job in capturing the variations outside the training set. Therefore the problem of obtaining a smooth solution may be posed as a regularization problem

$$\hat{\theta}^0 = \underset{\theta}{\operatorname{argmin}} \left(\sum_{n=1}^{N_2} L(y^{[n]}, d^{[n]}) + \lambda R(\theta) \right)$$

where $R(\theta)$ is a function of the parameters and λ is

The Lagrange multiplier λ that regulates the effect of the added term
be $R(\theta) = \sum_{i=1}^M \theta_i^2$ (Tikhonov regularization). ML14

The constraint usually lead to a decaying term that encourages smaller weights. Smaller weights that contribute the input of a sigmoidal function should give a smoother function. Regulating λ to larger values favors smoother at the expense of accuracy in the cost function. Vice-versa small λ offset less the cost function encouraging smoother.

There are other regularization strategies, also on the gradient, to encourage smoother.

The most popular strategies to encourage generalization are based on simple heuristics:

Heuristic 1: EARLY STOPPING

This strategy suggests to stop training before reaching convergence. This provides solutions that are less accurate, but that perhaps are smoother.

Heuristic 2: ENSEMBLING

We train different networks, using different initial conditions, and combine the predictions (results). In regression we could use the mean or the median. Max rule could be used for classification (the classification that gets the largest score). This is sometimes called the committee machine.

Another strategy could be to train the system on different subsets of the training set obtaining different networks. The predictions from the networks are then combined (averaged or mixed out).

This strategy in statistics is known as
BOOTSTRAP AGGREGATION or BAGGING.

ML.15

The models are expected to be smoother.

Heuristic 3 : DROPOUT

In this strategy during training some hidden units are randomly set to zero at each gradient backpropagation. The number of censored units is usually 50% or less.

In this way the gradient estimates become noisy and may make the system more robust against overfitting. The evolution during training is a more scattered pattern that may lead to better minima and better generalization. Dropout has allowed a major leap in performance for convolutional networks in solving image recognition tasks.

Heuristic 4 : ADD NOISE

Dropout discussed above can be seen as applying bernoulli noise to the hidden units during training. The idea can be extended by applying noise during gradient calculations. In regression it can be shown to be equivalent to regularization. Noise can be also added to the weights.

CONVERGENCE SPEED

The gradient updates are controlled by the stepsize parameter $\mu[k]$ that can be made adaptive.

Clearly, large μ correspond to faster updates that may overshoot the valleys of the cost function. Vice versa small μ may be slow and more precise in catching the minima, but they may be bad (high cost) local minima.

Generally, at the beginning of training μ is kept large with progressive decay around convergence. A good compromise that tracks the evolution of the gradient is ADAM widely used and already presented in one of our previous chapters. Also ADAM has some free parameters that are determined by trial-and-error.