1. Introduction

A feed-forward neural network is a composition of alternating linear and coordinate-wise non-linear maps, where the matrices of linear maps are considered as adjustable (=optimizable) network parameters. Unlike the conventional regression models, the adjustable parameters enter the neural network non-linearly. To optimize (= to train) the neural network, we need to calculate, using the chain rule, the gradient of the network with respect to parameters. Formulas for the gradient were obtained by a number of authors (it is customary to refer to [WHF]), and the corresponding calculation were called the backpropagation algorithm. In the recursive-coordinate form we can find these formulas in any neural networks manual. Less often in these tutorials one can find an explicit (non-recursive) matrix version of the formulas, although the matrix representation for the neural network itself usually appears in books. Meanwhile, looking at the matrix representation for neural network, everyone (I think) wants to see in explicit matrix form both the final formula and entire calculation. In any case, when I began to teach students this subject, I was annoyed by the number of indices in the usual coordinate-recursive proof. To get rid of the indexes, I tried to apply the chain rule directly in matrix form. This undergraduate-level exercise turned out to be not too simple. Looking back at the result (see the text), I am not sure that the matrix-style proof has became simpler then in recursive-coordinate form. Still I hope that the text can be of some use.
2. Network functions

Everywhere further the vectors \( X \in \mathbb{R}^n \) are considered as columns \( X = [x_1, \ldots, x_n]^T \). The component-wise product (= Hadamard product) of matrices of the same dimension is denoted by \( A \circ B \). The coordinate-wise map \( \Sigma : \mathbb{R}^n \to \mathbb{R}^n \), defined by the formula

\[
\Sigma(X) = \Sigma([x_1, \ldots, x_n]^T) = [\sigma_1(x_1), \ldots, \sigma_k(x_n)]^T,
\]

i.e. the direct sum of \( n \) functions \( \sigma_i : \mathbb{R}^1 \to \mathbb{R}^1 \), is denoted by double arrow \( \Sigma : \mathbb{R}^n \Rightarrow \mathbb{R}^n \). The action of such a map on the vector \( X \) can be considered as an “operator” Hadamard product of columns \( \Sigma = [\sigma_1, \ldots, \sigma_k]^T \) and \( X = [x_1, \ldots, x_n]^T \), i.e. \( \Sigma(X) = \Sigma \circ X \). A (neural) network function \( f : \mathbb{R}^n \to \mathbb{R}^1 \) is a function of the form

\[
f(X) = f(X; W) = \Sigma_k(W_k \cdot \Sigma_{k-1}(W_{k-1} \cdot \Sigma_{k-2} \cdot \ldots \cdot \Sigma_2(W_2 \cdot \Sigma_1(W_1 \cdot X)) \ldots))
\]
or, alternatively, as the product

\[
f(X) = f(X; W) = \Sigma_k \circ W_k \cdot \Sigma_{k-1} \circ W_{k-1} \cdot \Sigma_{k-2} \cdot \ldots \cdot \Sigma_2 \circ W_2 \cdot \Sigma_1 \circ W_1 \cdot X
\]

(actions order is from the right to the left), where \( X = [x_1, \ldots, x_n]^T \in \mathbb{R}^n \) and \( W_i \) are matrices of the same name linear maps \( W_i \). These matrices are considered to be parameters of the map \( f(X; W) \), so the parameter vector \( W = (W_k, \ldots, W_1) \) consist of \( n_i \times n_{i-1} \) matrices \( W_i \) (\( n_k = 1, n_0 = n \)). We also set \( N_1(X) = W_1 \cdot X \) and \( N_{i+1}(X) = W_{i+1} \cdot \Sigma_i(N_i(X)) \), then

\[
f(X; W) = \Sigma_k(W_k \cdot \Sigma_{k-1}(W_{k-1} \cdot \Sigma_{k-2} \cdot \ldots \cdot \Sigma_2(W_2 \cdot \Sigma_1(W_1 \cdot X)) \ldots))
\]
and

\[ f(X; W) = \Sigma_k(N_k) = \Sigma_k(W_k \cdot \Sigma_{k-1}(N_{k-1})) = \ldots , \]

where \( N_k, \ldots, N_1 \) are the columns of dimensions \( n_k, \ldots, n_1 \). Note that for \( k = 1 \) and identity activation function \( \Sigma_k = \sigma_1 \) the network function is a homogeneous linear function of \( n \) variables.

3. Network functions and neural networks

The network function of the form (1) defines a homogeneous \( k \)-layered feed-forward neural network with \( n \)-dimensional input and one-dimensional output. The number of hidden (internal) layers is \( k - 1 \) and the \( i \)-th layer contains \( n_i \) neurons. The word homogeneous in this context is not generally accepted and means that all intermediate linear maps are homogeneous. The conventional affine network, in which linear maps are supplemented with biases, can be obtained from the homogeneous one if:

(a) all input vectors have the form \( X = [x_1, \ldots, x_{n-1}, 1]^T \);

(b) the last rows of all matrices \( W_i \) with \( i < k \) have the form \([0, \ldots, 0, 1] \);

(c) the last functions \( \sigma_{in_i} \) in the columns \( \Sigma_i \) with \( i < k \) are identical.

In this instance, the homogeneous network will be equivalent to a \( k \)-layered affine neural network with \((n - 1)\)-dimensional input and one-dimensional output. Each hidden layer of such a network will contain \( n_i - 1 \) “genuine” neurons and one (last) “formal”, responsible for the bias; the last column of the matrix \( W_i \), except the last element, will be the bias vector for the \( i \)-th layer. For \( k = 1 \) and identical activation function \( \sigma_1 = \text{id} \) the described adjustment corresponds to the standard transition from a homogeneous multiple regression to a non-homogeneous by adding to the set of independent variables (predictors) an additional formal predictor, always equal to one.

4. Gradient \( \nabla_W f(X; W) \) in one-dimensional case

Let \( n = n_1 = \ldots = n_k = 1 \). Then all matrices \( W_i \) are numbers \( w_i \), all columns \( \Sigma_i \) are functions \( \sigma_i \) and

\[ f(x) = f(x; W) = \sigma_k(w_k\sigma_{k-1}(w_{k-1}\sigma_{k-2}(w_{k-2}\sigma_{k-3}\ldots\sigma_2(w_2\sigma_1(w_1x))\ldots))). \]

The application of the chain rule does not cause difficulties, and for the gradient

\[ \nabla_W f = (\nabla_{w_k}f, \nabla_{w_{k-1}}f, \nabla_{w_{k-2}}f, \ldots, \nabla_{w_1}f) \]
we obtain

\[
\begin{align*}
\nabla_{w_k} f &= \sigma'_k(N_k) \sigma_{k-1}(N_{k-1}) \\
\nabla_{w_{k-1}} f &= \sigma'_k(N_k) w_k \sigma'_{k-1}(N_{k-1}) \sigma_{k-2}(N_{k-2}) \\
\nabla_{w_{k-2}} f &= \sigma'_k(N_k) w_k \sigma'_{k-1}(N_{k-1}) w_{k-1} \sigma'_{k-2}(N_{k-2}) \sigma_{k-3}(N_{k-3}) \\
\n\end{align*}
\]  

(1)

\[ \]

or, omitting the arguments \( N \) for brevity,

\[
\begin{align*}
\nabla_{w_k} f &= \sigma'_k \sigma_{k-1} \\
\nabla_{w_{k-1}} f &= \sigma'_k w_k \sigma'_{k-1} \sigma_{k-2} \\
\nabla_{w_{k-2}} f &= \sigma'_k w_k \sigma'_{k-1} w_{k-1} \sigma'_{k-2} \sigma_{k-3} \\
\n\end{align*}
\]  

(2)

Here the braces emphasize the periodicity in the structure of the formulas. In order to write down the recursive formula we set, omitting again the arguments in the notations,

\[ \Delta_i = \Delta_{i+1} w_{i+1} \sigma'_i, \]

where \( i = k, \ldots, 1 \) and \( \Delta_{k+1} = w_{k+1} = 1 \). Then

\[ \nabla_{w_1} f = \Delta_i \sigma_i \]

where \( \sigma_0 = x \).

5. Gradient \( \nabla_W f(X; W) \) in general case

In general case, the components \( \nabla_W f(X; W) \) of the gradient \( \nabla_W f(X; W) \) can be written in a form, analogous to (1). Recall that \( W_i \) is \( n_i \times n_{i-1} \) matrix and hence \( \nabla_{W_i} f(X; W) \) is also \( n_i \times n_{i-1} \) matrix. The application of the chain rule in such notation can not be called a quite simple problem. Nevertheless, using the analogy with (1), one can guess the result. To write down the formulas, we need three kind of
matrix product: the usual column-by-row product $A \cdot B$, the Hadamard column-by-column product $A \circ B$ and the “inverted” column-by-matrix product $A \bullet B = B \cdot A$ of the column $A$ by the matrix $B$. As in the formulas (2), we omit, for brevity, the arguments $N_i$ in $\Sigma_i(N_i)$ and $\Sigma_i'(N_i)$.

For the network function

$$f(X; W) = \Sigma_k(W_k \cdot \Sigma_{k-1}(W_{k-1} \cdot \Sigma_{k-2} \cdots \Sigma_2(W_2 \cdot \Sigma_1(W_1 \cdot X)) \cdots))$$

we have

$$\nabla_{W_k} f = \Sigma_k' \cdot \Sigma_{k-1}^T$$

$$\nabla_{W_{k-1}} f = \Sigma_k' \cdot W_k^T \circ \Sigma_{k-1}' \cdot \Sigma_{k-2}^T$$

$$\nabla_{W_{k-2}} f = \Sigma_k' \cdot W_k^T \circ \Sigma_{k-1}' \cdot W_{k-1}^T \circ \Sigma_{k-2}' \cdot \Sigma_{k-3}^T$$

$$\nabla_{W_{1}} f = \Sigma_k' \cdot W_k^T \circ \Sigma_{k-1}' \cdot W_{k-1}^T \circ \Sigma_{k-2}' \cdot W_{k-2} \cdots \Sigma_2' \cdot W_2^T \circ \Sigma_1' \cdot X^T.$$  

Remarks.

1. The braces indicate the periodicity in the structure of formulas (rather than the order of multiplications). The actions order in (3) is from the left to the right.

2. One can replace the product $\Sigma_k \bullet W_k^T$ by $\Sigma_k' \cdot W_k^T$, (because $\Sigma_k'$ is a scalar) and the bullet is used in this case only in order to emphasize the periodicity in the structure of formulas.

3. In order to write down the recursive formula, we set, omitting again the arguments in the notations,

$$\Delta_i = \Delta_{i+1} \bullet W_{i+1}^T \circ \Sigma_i' = (W_{i+1}^T \cdot \Delta_{i+1}) \circ \Sigma_i',$$

where $i = k, \ldots, 1$ and $\Delta_{k+1} = W_{k+1}^T = 1$. Then

$$\nabla_{W_i} f = \Delta_i \cdot \Sigma_{i-1}^T$$

where $\Sigma_0 = X$.

4. $\Delta_i$ is a $n_i$-column and $\Sigma_i^{T}$ is a $n_{i-1}$-string, thus $\nabla_{W_i} f$ is, as expected, a $n_i \times n_{i-1}$-matrix.
5. By reversing the order of factors, one can get rid of bullets and rewrite (3) as

$$
\begin{align*}
\nabla W_k f &= \Sigma_{k-1}^T \otimes \Sigma'_{k+1} \\
\nabla W_{k-1} f &= \Sigma_{k-2}^T \otimes (\Sigma'_{k-1} \circ W_k \cdot \Sigma_k' \cdot \Sigma_k) \\
\nabla W_{k-2} f &= \Sigma_{k-3}^T \otimes (\Sigma'_{k-2} \circ W_k \cdot \Sigma_k' \circ W_k \cdot \Sigma_k') \\
\n\vdots
\end{align*}
$$

(4)

The actions order in (4) is from the right to the left, \( \otimes \) is the Kronecker product, and, as before, the braces are not related to the order of operations.

6. We can also get rid of Hadamard product by replacing the columns \( \Sigma_i' \) with square diagonal matrices \( \hat{\Sigma}_i' \) where \( \Sigma_i' \) is the diagonal. Then (4) turns into

$$
\begin{align*}
\nabla W_k f &= X^T \otimes (\hat{\Sigma}_{11} \circ W_{22} \circ \ldots \circ W_{k-1} \circ \hat{\Sigma}_{k-1} \cdots \circ W_{k-1} \circ \hat{\Sigma}_k) \\
\n\nabla W_{k-1} f &= X^T \otimes (\hat{\Sigma}_{11} \cdots \circ W_{22} \circ \ldots \circ W_{k-1} \circ \hat{\Sigma}_{k-1} \cdots \circ W_{k-1} \circ \hat{\Sigma}_k) \\
\n\nabla W_{k-2} f &= X^T \otimes (\hat{\Sigma}_{11} \cdots \circ W_{22} \circ \ldots \circ W_{k-1} \circ \hat{\Sigma}_{k-1} \cdots \circ W_{k-1} \circ \hat{\Sigma}_k) \\
\n\vdots
\end{align*}
$$

(5)

Note that \( W_k^T \) is a column and \( \hat{\Sigma}_k = \Sigma_k' \) is a scalar.

6. **Proof of (3)**

The formulas (3) follow immediately from the equalities

$$
\begin{align*}
\nabla W_r f &= (\nabla \Sigma_r f) \circ \Sigma_r' \cdot \Sigma_{r-1}^T \\
\n\nabla \Sigma_r f &= (\nabla \Sigma_{r+1} f) \circ \Sigma_{r+1}' \cdot W_{r+1}^T \\
\end{align*}
$$

(6) (7)

and we will prove (6) and (7). We need the following rule for calculating the gradient, consistent with our agreement on the matrix representation of matrix derivatives: if \( A \) is a string and \( B \) is a column, then

$$
\nabla_A (A \cdot B) = B^T.
$$
Denote by \( W^i_r \) the \( i \)-th raw of the matrix \( W_r = \{W_r^i\}_i \) and by \( \Sigma^i_r \) the \( i \)-th element of the column \( \Sigma_r = \{\Sigma_r^i\}_i \). In particular, \( \nabla_{W_r} = \{\nabla_{W_r^i}\}_i \) and \( \nabla_{\Sigma_r} = \{\nabla_{\Sigma_r^i}\}_i \). Let us verify now (6):

\[
\nabla_{W_r} f = \{\nabla_{W_r^i} f\}_i = \{\nabla_{\Sigma_r^i} f \cdot \nabla_{W_r^i} \Sigma_r^i\}_i = \{\nabla_{\Sigma_r^i} f \cdot \nabla_{W_r^i} (\Sigma_r^i (W_r^i \cdot \Sigma_{r-1}))\}_i = \\
= \{\nabla_{\Sigma_r^i} f \cdot \Sigma_r^i \cdot \Sigma_{r-1}^T\}_i = (\nabla_{\Sigma_r} f) \circ \Sigma_r^i \cdot \Sigma_{r-1}^T.
\]

Next, the equation (7) in coordinate-wise form is

\[
\{\nabla_{\Sigma_r^i} f\}_i = \{(\nabla_{\Sigma_r+1} f) \circ \Sigma_{r+1}^i \cdot (W_r^{T+1})^i\}_i.
\]

Let us verify the equality of the corresponding coordinates:

\[
\nabla_{\Sigma_r^i} f = \langle \nabla_{\Sigma_r+1} f \circ \Sigma_{r+1}^i, \nabla_{\Sigma_r^i} (\Sigma_{r+1}(W_{r+1}\Sigma_r)) \rangle = \\
= \langle \nabla_{\Sigma_r+1} f, \Sigma_{r+1}^i \circ (W_r^{T+1})^i \rangle = \langle \nabla_{\Sigma_r+1} f \circ \Sigma_{r+1}^i, (W_r^{T+1})^i \rangle = (\nabla_{\Sigma_r+1} f) \circ \Sigma_{r+1}^i \cdot (W_r^{T+1})^i
\]

(here \( \langle , \rangle \) is the scalar product).

References

[RHW] Rumelhart D.E., Hinton G.E., Williams R.J., *Learning Internal Representations by Error Propagation*. In: Parallel Distributed Processing, vol. 1, pp. 318362. Cambridge, MA, MIT Press. 1986