Distant generalization by feedforward neural networks

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Abstract

This paper discusses the notion of generalization of training samples over long distances in the input space of a feedforward neural network. Such a generalization might occur in various ways, that differ in how great the contribution of different training features should be.

The structure of a neuron in a feedforward neural network is analyzed and it is concluded, that the actual performance of the discussed generalization in such neural networks may be problematic – while such neural networks might be capable for such a distant generalization, a random and spurious generalization may occur as well.

To illustrate the differences in generalizing of the same function by different learning machines, results given by the support vector machines are also presented.

keywords: supervised learning, generalization, feedforward neural network, support vector machine

1 Introduction

Generalization is one of the basic notions in machine learning. Yet, in the existing literature, usually only the indicators of generalization quality like the mean square error over the test samples are presented, without a more detailed study of the characteristics of the generalization functions produced by different learning machines.

In this paper, a special kind of generalization is analyzed, on the example of classic feedforward neural networks with linear weight functions. In the discussed generalization type, generalized samples exist which are distant to any training samples. The distance of two samples is defined as the distance $d$ between the independent variables of the samples, in the input space of a feedforward learning machine $L$. For example, let the sample $s_i$ be $(x_{i1}, x_{i2}, y_i)$ where the independent variables are $x_{i1}$ and $x_{i2}$, and the dependent variable is $y_i$. Then, the discussed distance $d$ between two samples $s_p$ and $s_q$ might be defined as the Euclidean distance...
between the points in the input space of \( L \), whose coordinates are the independent variables \((x_{p1}^i, x_{p2}^i)\) and \((x_{q1}^i, x_{q2}^i)\). If a generalized sample \( s_g \) is distant from any training samples, it means that there are different groups of training samples, that might be expected to compete in generalizing \( s_g \).

\[ \begin{array}{c}
\text{‘0’:} & y^i = 0 & \diamond \\
\text{‘1’:} & y^i = 1 & + \\
\text{C:} & y^i = a & \bullet \\
\text{D:} & y^i = b & \bullet \\
\end{array} \]

Figure 1: An example of a close sample \( C \) and a distant sample \( D \) in an input space of a feedforward learning machine.

Let us discuss examples of the distant and, conversely, close samples. Fig. 1 illustrates an input space of a feedforward learning machine. Let the learning machine has two inputs \( x_1 \) and \( x_2 \). Let there be some samples in the space, whose independent variables \((x_1^i, x_2^i)\) determine the respective position in the input space, and which have a dependent variable \( y^i \). Let the training samples have the values of \( y^i \) equal to either 0 or 1, and let us call these samples ‘0’ or ‘1’ samples, respectively. Let there be also two generalized samples absent in the training set, whose dependent variables are unknown, and thus their \( y^i \) values are denoted by \( a \) and \( b \). The sample with \( y^i = a \), let us call it \( C \), can be regarded as a close one – it is near only to a cluster of ‘1’ samples, and it is likely that the user of the learning machine expects that the dependent variable of the sample should be estimated to a value that is close to 1. Let the sample with \( y^i = b \) be called \( D \). At least three obvious ways of generalization of \( D \) can be thought of:

- In the surrounding of \( D \), there are some ‘0’ samples and some ‘1’ samples in an approximate balance, thus, the dependent variable of \( D \) should be equal to about 0.5.

- All samples ‘1’ create together a single horizontal stripe–shaped feature, and \( D \) is inside the feature. Additionally, ‘0’s create two horizontal stripe–shaped features and \( D \) is outside each one. Thus, the dependent variable of \( D \) should be equal to about 1.

- The closest training sample to \( D \) is ‘0’, so, the dependent variable of \( D \) should be equal to about 0.

Thus, groups of samples of different type were discerned around \( D \), that can compete in generalizing of \( D \). The sample \( D \) is thus regarded as a distant sample.
It will be shown, that such alternate ways of generalization, in the case of
the feedforward neural networks, may sometimes produce a random and spurious
generalization. That is, the problem of long distance generalization may sometimes
be solved well by the neural network, but in some other cases the network may
give quite unexpected results, being the artifacts revealing an internal structure of
the learning machine rather than a likely estimation hypothesis.

The performance of support vector machines will be presented as well, to show
the generalization differences that exist between different types of learning ma-
chines.

2 Distant generalization in feedforward neural
networks

In a feedforward neural network (FNN), the combination function in a neuron of
the McCulloch type [5] is a linear combination of the input values of the neuron.
To obtain the output value of the neuron, the value of the combination function is
non-linearly transformed, typically using a sigmoidal or hyperbolic tangent activa-
tion function. It means that the neuron acts the same for arguments that create
hyperplanes in the space of the domain of the neuron. For example, there is a
hyperplane $P_i$, for which the output value of the neuron is constant and equal to
$i$. The partial derivatives of the neuron function against each of the inputs of the
neuron are constant for $P_i$ as well. It might be said, thus, that a trained neuron
transfers the properties of some samples, that it learned during the training process,
over infinitely large regions in the input space of the neuron, because hyperplanes
are infinite. The infinity of the transfer might make FNNs good for distant gen-
eralizations, as it will be further shown in tests. On the other hand, though, the
infinite transfer may sometimes produce wrong results, because a training sample
$s_i$ may influence on the generalization of some sample $s_g$ even if these samples are
very distant from each other. But, intuitively, samples that are very far from each
other might have nothing in common.

3 Tests

Let us discuss a real process of training a FNN with two kinds of data – the first
one, $\theta_l$, deliberately constructed to simplify the distant generalization, and the
second one, $\theta_c$, constructed to make the generalization complex to solve by the
FNN. The two three-dimensional sets are illustrated in Fig. 2(a) and Fig. 2(b),
respectively. The sets are $64 \times 64$ images. Let the coordinates of the pixels be
the two independent variables, and the brightnesses of the pixels be the dependent
variable.

Let the pixel at the lower left corner has the coordinates $(-0.5, -0.5)$ and let
the pixel at the upper right corner has the coordinates $(0.5, 0.5)$. Let the brightness
of the pixels represents the range from $-0.5$ for black to $0.5$ for white.

Let the feedforward layered densely connected networks with two inputs and
a single neuron in the output layer be used. Let the sizes of the FNNs be such
that they can comfortably fit to both of the generalized sets – it was tested that it is sufficient if each of the networks has two hidden layers of 16 neurons each. Let the FNNs have classic hyperbolic tangent activation functions. Let there be a weight decay at a rate of $2 \cdot 10^{-7}$ to improve generalization [4]. Let an online backpropagation training be used [6] with a fixed learning step of 0.02.

The training subsets of both the set $\theta_l$ and the set $\theta_c$ are represented by the image in Fig. 2(c) – the black pixels in the image mean that the corresponding pixels in Fig. 2(a) and Fig. 2(b) represent the training subsets of the respective sets. Thus, the white region in Fig. 2(c) is the unknown one during training. Because the unknown region is relatively large in comparison to the sizes of the features in the training sets, it can be told that the generalization to the region employs the distant generalization.

Let four of these neural networks, $N^l_i, i = 0 \ldots 3$, be trained with the training subset of $\theta_l$, and let the other four of these neural networks $N^c_i, i = 0 \ldots 3$, be trained with the training subset of $\theta_c$. During the training, the generalizing functions of the networks and the weights of the neurons in the first hidden layer were sampled, at the iterations 10000000th, 31622777th and 100000000th. The results are illustrated in Fig. 3. In the figure, there is a two row table for each of the iterations at which the sampling was done. The sampled generalization functions are placed the upper row and the diagrams representing the input spaces of neurons in the first hidden layer are placed respectively in the lower row. The representation of the generalization functions is analogous to that of the sets $\theta_l$ and $\theta_c$. Each of the input space diagrams shows with translucent lines the zeroes of the outputs of the first hidden layer neurons, that is, it shows the hyperplanes $P_0$ in the input space of the tested FNNs. The lower left corner of the dotted rectangles drawn within the diagrams represents the input values at $(-0.5, -0.5)$ and the upper right corner of the rectangles represents the input values at $(0.5, 0.5)$.

Let us divide the features in the training sets into the linear ones $f_l$ being the three white lines, and the circular ones $f_c$ being the four white circles. It is visible in Fig. 3 that in the case of $N^l_i$ most hyperplanes concentrate near the linear features $f_l$, and in the case of $N^c_i$ generally some hyperplanes concentrate near the linear features $f_l$ and some concentrate near the circular features $f_c$. In the latter case, in effect, the hyperplanes concentrated near $f_c$ cross the hyperplanes concentrated near $f_l$. Additionally, the crossings occur partially in the unknown region, i.e. in the region marked in Fig. 2(c) by white. These are exactly the conditions showing the discussed notion of competing groups of samples. While in

![Figure 2: The data sets (a) $\theta_l$, (b) $\theta_c$ and (c) the mask of the training subsets.](image)
the case of $\mathcal{N}_i^l$ the neurons transferred only the properties of $f_l$ over the unknown region, in the case of $\mathcal{N}_i^c$ some neurons extend their hyperplanes onto the unknown region from the region of $f_l$, and some other from the region of $f_c$. Thus, properties of both $f_l$ and $f_c$ are transmitted to the unknown region.

The differences between $\mathcal{N}_i^l$ and $\mathcal{N}_i^c$ are clearly visible. $\mathcal{N}_i^l$ finely generalized $f_l$ over the unknown region, while $\mathcal{N}_i^c$ produced in the unknown region some features that look like random artifacts. Thus, it might be told that the discussed distant generalization was resolved in some cases in a fine way, and in some cases in a rather spurious way by the tested FNNs. An example alternate solution without the artifacts might be to generalize to the unknown region in the case of the set $\theta_c$ in the same way as it happened in the tests in the case of the set $\theta_l$, that is, just generalize the features $f_l$ over the unknown region, because $f_l$, and not $f_c$, are directly neighboring to the unknown region.

Let us compare the FNNs to SVMs [1, 3]. SVMs give very different results for both sets. Example results are illustrated in Fig. 4. The particular example used $\nu$-SVC [7] trained using LIBSVM [2].

In the particular examples, SVMs solved the problem of distant generalization in a different way than the tested FNNs in the case of both the set $\theta_l$ and the set $\theta_c$. The SVMs were able to produce a generalization with minimal artifacts if their learning coefficients allowed for a proper fitting to the training data, as seen in

Figure 3: The generalizing functions and diagrams of the zeroes of the first hidden layer neurons.
Figure 4: Examples of generalization using $\nu$–SVC with the radial basis kernel with $\nu = 0.2$, $\epsilon = 0.001$ and: for the binarized $\theta_l$ set with a threshold at 0.5 (a) $c = 0.3$, $\gamma = 3$, (b) $c = 1$, $\gamma = 10$, (c) $c = 3$, $\gamma = 30$, for the binarized $\theta_c$ set with a threshold at 0.5 (d) $c = 1$, $\gamma = 10$, (e) $c = 3$, $\gamma = 30$, (f) $c = 10$, $\gamma = 100$.

Fig. 4(c) and (f). The SVMs have a large test error for both sets, though, as they did not fuse $f_i$ into a single set of parallel bars.

Thus, FNNs have a smaller test error for $\theta_l$, because they could fuse the features $f_i$, and both FNNs and SVMs have a relatively large test error for $\theta_c$, but for different reasons.

4 Conclusions

The distant generalization may work quite differently for different training sets and for different learning machines. In particular, the resulting generalizing functions may contain artifacts, related to the internal structure of the learning machine.

Study of these differences might give more clues for using a particular learning machines for a particular task, than the comparison of the test MSE alone would give.

For example, the classic FNNs with linear combination functions and hyperbolic tangent activation functions may introduce substantial random artifacts to the generalizing functions. In some applications where the stability of the results is important, usage of such FNNs might thus be discouraged. But, conversely, the tested FNNs, thanks to the structure of neurons, can be capable of generalizing by extending and fusing together elongated features that exist in the training set.

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