Redundancy of Hidden Layers in Deep Learning: An Information Perspective

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Abstract

Although the deep structure guarantees the powerful expressivity of deep networks (DNNs), it also triggers serious overfitting problem. To improve the generalization capacity of DNNs, many strategies were developed to improve the diversity among hidden units. However, most of these strategies are empirical and heuristic in absence of either a theoretical derivation of the diversity measure or a clear connection from the diversity to the generalization capacity, which makes these strategies suspect. In this paper, from an information-theoretic perspective, we introduce a new definition of redundancy to describe the diversity of hidden units under supervised learning settings by formalizing the effect of hidden layers on the generalization capacity as the mutual information. We prove an opposite relationship existing between the defined redundancy and the generalization capacity, i.e., the decrease of redundancy generally improving the generalization capacity. The experiments show that the DNNs using the redundancy as the regularizer can effectively reduce the overfitting and decrease the generalization error, which well supports above points.

1 Introduction

Deep learning networks (DNNs) have achieved significant success in many practical applications owing to its strong expression capacity and powerful learning ability. However, deep structure of DNNs may lead to complicated nonlinear mappings from input to output, triggering serious overfitting problems. For this, many endeavors have been devoted to investigate how to improve the generalization capacity to settle the overfitting problem; to name a few, Dropout [Srivastava et al., 2014], weight decay [Krogh and Hertz, 1991], CIF [Zhao et al., 2018], etc. Despite the effectiveness of these methods, however, they do not leverage all the expression capacity of model since they reduced the effective number of model parameters.

Recently, many studies have explored the measures of diversity between hidden units and suggest improving the diversity between hidden units to reduce the generalization error but simultaneously to retain the expression capacity of DNNs [Cogswell et al., 2016; Gu et al., 2018]. Concretely, Cogswell et al. minimized the cross-covariance of hidden activations to encourage diverse or non-redundant representations in DNNs. Gu et al. extended the DeCov method, treating non overlapped groups of hidden units as component learners to avoid the bad influence of the breakdown of correlations. Impressively, by using mutual information among hidden units as the measure of diversity, Brakel et al. proposed a method to learn independent features [Brakel and Bengio, 2018]. Many other literatures also investigated the positive role of feature independence in the feature encoding [Bengio et al., 2017; Hjelm et al., 2019].

Actually, boosting up the diversity between hidden units of DNNs has been shown an effective way to reduce the redundancy in data thereby an feasible way to improve the generalization capacity in particular applications. However, the measure of diversity in the current set of these strategies was developed empirically and heuristically. The actual effect of the defined diversity on the generalization capacity is still not very clear, which make these methods suspect [Locatello et al., 2019]. Moreover, merely considering the diversity over the whole mixed data distribution but neglecting the subsistent local clustering feature of different classes may be harmful to the classification task [Grover and Ermon, 2019]. Hence, it is necessary to investigate the measure of diversity under supervised settings by examining the generalization error, so as to clarify the relationship between the diversity and the generalization error theoretically.

In this paper, we introduce a new definition of redundancy to describe the diversity among hidden units in one specified layer of DNNs under supervised learning settings by analyzing the effect of the relationship of hidden units on the generalization error. We follow the work of Xu et al. [Xu and Raginsky, 2017], getting a generalization error bound expressed as the activation values of the interested hidden layer of DNNs from the information theoretical perspective. Compared to the traditional generalization error bounds that are based on hypothesis space, e.g., the Rademacher complexity [Boucheron et al., 2005], or based on certain algorithm properties, e.g., the uniform stability [Bousquet and Elisseeff, 2002], the generalization error upper bound obtained here strongly depends on the input dataset, which would make the bound tighter [Kawaguchi et al., 2018] and make the analy-
sis on this bound credible and instructive. We decompose the generalization error bound and naturally introduce a new definition of redundancy, which is different from above diversity definitions as the local clustering feature is also considered by it. Intuitively, the introduced redundancy can be explained as the part of the total correlation information among hidden units, which is useless for classification.

To further clarify the relationship between the redundancy and the generalization capacity, we discuss this problem in different scenarios, including the scenarios with the small or large training dataset and the scenarios with the changeable distribution of classification parameters, where the classification parameters refer to the model parameters from the discussed hidden layer to the end layer. Nonetheless, based on the fluctuation theorem [Ito, 2013; Sagawa and Ueda, 2013], it is shown that the decrease of the redundancy can generally lead to the increase of the generalization capacity no matter which scenario is set.

Finally, we develop a new regularization method named redundancy decrease method (RDM) by using the redundancy as the regularizer. The experiments show that RDM can effectively reduce the overfitting and decrease the generalization error compared to the methods without the redundancy regularizer. Further, the redundancy between hidden units is demonstrated as a crucial factor for reducing the generalization error in DNNs.

2 Background

This section briefly reviews some basics of information theory, i.e., the entropy and the mutual information. Hereinafter, we shall use the following notations. \( P_Z(z) \) (written as \( P_Z \) or \( P(z) \) sometimes for short) is used to denote either a probability mass function (PMF), or a probability density function (PDF) of random variable \( Z \), depending on the random variable having either discrete or continuous support, respectively. The symbol \( \mathbb{E}_X[\cdot] \) denotes expectation of the random object within the brackets w.r.t the subscript random variable \( X \). Then for a stochastic variable \( X \), its entropy is defined as

\[
H(X) = -\mathbb{E}_X[\log P_X(X)]
\]  

(1)

The mutual information of two stochastic variables is

\[
I(Z_1; Z_2) = \mathbb{E}_{(Z_1, Z_2)} \left[ \log \frac{P_{Z_1 Z_2}(Z_1, Z_2)}{P_{Z_1}(Z_1) P_{Z_2}(Z_2)} \right],
\]

(2)

which capturing the non-linear statistical dependencies between variables can be reformulated as the Kullback-Leibler (KL-) divergence between the joint density and the product of the marginal densities, i.e.,

\[
I(Z_1; Z_2) = D_{KL}(P_{Z_1 Z_2} \parallel P_{Z_1} \otimes P_{Z_2}),
\]

(3)

For more than two variables, the multivariate mutual information is defined as

\[
I(Z_1; Z_2, \ldots, Z_n) = D_{KL}(P_{Z_1 Z_2 \ldots Z_n} \parallel P_{Z_1} \otimes P_{Z_2} \otimes \ldots \otimes P_{Z_n})
\]

\[
= \mathbb{E}_{(Z_1, Z_2, \ldots, Z_n)} \left[ \log \frac{P_{Z_1 Z_2 \ldots Z_n}(Z_1, Z_2, \ldots, Z_n)}{P_{Z_1}(Z_1) P_{Z_2}(Z_2) \ldots P_{Z_n}(Z_n)} \right],
\]

(4)

which is an extension of mutual information. We will use it to measure the dependence of hidden units later and still call it the mutual information in the following content for the sake of consistency.

3 Information Redundancy

This section derives the generalization error which is associated with the specified hidden layer from the information theoretical perspective and presents the new definition of the redundancy of hidden units as well as the corresponding results.

3.1 Generalization error

As the analysis in the introduction, under supervised settings, a properly defined concept of diversity of the hidden units should have a clear connection to the generalization error. Based on this view of point, we follow the information-theoretic framework proposed by Xu et al. [Xu and Raginsky, 2017] and formulate the generalization error as a function of the values of the specified hidden layer, where it is convenient to think of each unit in the hidden layer as a component learner or a map from the data features to its activation value since the generalization error is initially related to the input rather than the values of hidden units; and we are actually more interested in the mechanism that produces the activation value than the activation value itself. Let \( Z = (X, Y) \) be the instance space, where \( X \) is the feature space and \( Y \) is the label space. The dataset \( S \) of size \( n \) is an \( n \)-tuple, i.e.,

\[
S = (Z_1, Z_2, \ldots, Z_n)
\]

(5)

of i.i.d random elements of \( Z \in Z \) with an unknown PDF \( P_Z(z) \). Given a neural net work with multilayers, let \( \hat{h} \) be the hidden layer to be discussed with \( m \) hidden units \( h_i \), i.e., \( \hat{h} = (h_1, h_2, \ldots, h_m) \), where each \( h_i \) is looked as a base learner. Consequently, the whole neural net work can be seen as an ensemble classifier. Let \( W \) be the hypothesis space of the ensemble classifier, where \( W \in \mathcal{W} \) called the classification parameter is the collection of model parameters from the specified hidden layer to the top layer. Let \( f(Z) = (\hat{h}(X), Y) \), then given \( W \in \mathcal{W} \), the loss function \( l \) on the sample \( Z \) can be restated as the function of \( f(Z) \) and \( W \), i.e., \( l : W \times f(Z) \rightarrow \mathbb{R}_+ \), where \( Z = (X, Y) \). Accordingly, let \( f(S) = (f(Z_1), \ldots, f(Z_n)) \). Now we are ready to obtain the generalization error.

The empirical risk of a hypothesis \( W \in \mathcal{W} \) over the dataset \( S \) is

\[
L_f(S)(W) \triangleq \frac{1}{n} \sum_{i=1}^{n} l(f(Z_i), W).
\]

(6)

The expected risk of \( W \) on \( P_S \) is

\[
L_{\mathbb{E}_S}(W) \triangleq \mathbb{E}_S \left[ \frac{1}{n} \sum_{i=1}^{n} l(f(Z_i), W) \right]
\]

(7)

where \( F_i = f(Z_i) \) (\( 1 \leq i \leq n \)) are i.i.d random variables. Taking expectation on the difference between \( L_f(S)(W) \) and
The generalization error is defined as the absolute value of the expectation, i.e.,

$$g(P_S, P_{W|S}) \triangleq |E_{(S, W)}[L_{f,W}(S) - L_f(S)]|$$

$$= |E_{f(S,W)}[L_{f,W}(S) - E_{f(S)}[L_f(S)]]|$$

(8)

where $E_{f(S,W)}$ means taking expectation w.r.t the product of the marginal PDFs of $f(S)$ and $W$. Xu and Raginsky have justified that given two random variables $X$ and $Y$ with the joint PDF $P_{XY}$ and the product of the marginal PDFs $P_X \otimes P_Y$, if the function $f(X, Y)$ is a $\sigma$-subgaussian function under $P_{XY}$, then

$$|E_{(X, Y)}[f(X, Y)] - E_{X \otimes Y}[f(X, Y)]| \leq 2\sigma^2 I(X; Y),$$

(9)

where a random variable $U$ is $\sigma$-subgaussian if $\log E[e^{\lambda(U-E[U])}] \leq \lambda^2 \sigma^2/2$ for all $\lambda \in \mathbb{R}$. Generally, if the loss function in the Eqs. (6) and (7) is restricted as a function bounded in $[a, b]$ thereby being a $\sigma$-subgaussian function, then $L_{f(S)}(W)$ in Eq. (8) is consequently a $\sigma/\sqrt{n}$-subgaussian function for $W$ due to the independence among $f_i(S)(1 \leq i \leq n)$, where $\sigma = (b-a)/2$. Then according to the Eq. (9), by setting $X$ and $Y$ in the Eq. (9) as $f(S)$ and $W$ respectively, we obtain the following Lemma.

**Lemma 1.** If the loss function $l$ is $\sigma$-subgaussian, then the generalization error is upper-bounded in terms of the mutual information between $f(S)$ and $W$, i.e.,

$$g(P_S, P_{W|S}) \leq \frac{1}{n} 2\sigma^2 \sqrt{nI(f(S); W)}.$$

(10)

### 3.2 Measure of redundancy

We will further introduce a new definition of the redundancy among the hidden units in this subsection. As mentioned in the introduction, since the decrease of the redundancy could empirically reduce the generalization error, it would be nature to derive the measure of the redundancy directly from the upper bound of the generalization error. Based on this view of point, we decompose the upper bound of generalization error and obtain the following theorem.

**Theorem 1.** Decomposing the upper bound of the generalization error obtains

$$\frac{1}{n} \sqrt{nI(f(S); W)} =$$

$$\frac{1}{n} \sqrt{nI(f(S); W)} =$$

$$\sqrt{I(h_1(X); \ldots; h_m(X)} + \sqrt{H(W) - H(S_y, W | h(S_x))},$$

where $S_x = \{X_1, \ldots, X_n\}$, $S_y = \{Y_1, \ldots, Y_n\}$ and $h(S_x) = \{h(X_1), \ldots, h(X_n)\}$.

**Proof.** Only a belief proof is given herer (see the supplementary material for the detail).

$$I(f(S); W) = I(h(S_x), S_y; W)$$

$$= H(h(S_x), h(S_x), S_y) - H(h(S_x), S_y, W) + H(W)$$

(12)

By adding $\sum_{i=1}^{m} H(h_i(S_x)) - \sum_{i=1}^{m} H(h_i(S_x) | S_y) - \sum_{i=1}^{m} I(h(S_x), S_y)$ to the right-hand side of above equation, it follows that

$$I(f(S); W) = \sum_{i=1}^{m} I(h_i(S_x); S_y) + H(W)$$

$$+ [H(S_y) - I(h_1(S_x); \ldots; h_m(S_x))],$$

(13)

By the fact that the samples $(X_i, Y_i)$ in $S$ are sampled in an i.i.d. fashion, we have $I(h_1(S_x); h_2(S_x); \ldots; h_m(S_x)) = nI(h_1(X); h_2(X); \ldots; h_m(X)|Y)$, $I(h_1(S_x); h_2(S_x); \ldots; h_m(S_x)) = nI(h_1(X); h_2(X); \ldots; h_m(X))$ and $\sum_{i=1}^{m} I(S_y; h_i(S_x)) + H(S_y) = n(\sum_{i=1}^{m} I(h_i(X); Y) + H(Y)).$ Combining above equations gives the Eq. (11), which completes the proof.

Let us focus on the Eq. (11). There are five terms under the square root. The last term that is a function of the classification parameters $W$ and the sample size $n$ corresponds to the training process of the ensemble of the component learners $h_i(1 \leq i \leq m)$. The fourth term is a constant w.r.t. the model parameters. The third term is the sum of respective relevancy of component learner $h_i(1 \leq i \leq m)$ to the labels $Y$. Only the first two terms purely are unrelated to the sample size $n$ and the model parameters $W$, reflecting the relationships among the hidden units. We argue that the two terms naturally quantify the divergence or redundancy among the hidden units.

**Definition 1.** The information redundancy among the hidden units is defined as

$$R_h(S) = I(h_1(X); \ldots; h_m(X)) - I(h_1(X); \ldots; h_m(X)|Y).$$

(14)

The first term in the redundancy definition is independent of the label, which is similar to the most diversity measure concepts proposed in the present literatures for improving the generality or for learning the better feature representation. It is common accepted that reducing such term would lead to the decrease of the correlations among the hidden units. The second term in Eq. (14) is label-dependent. It reflects the local clustering feature captured by the hidden units. Improving this term may strengthen the class-conditional correlation and make the activations of the same class more consistent, which is usually important for a classification task. However, there is currently very little discussion on it.

The difference between the two terms is referred to as the information redundancy, as it can be intuitively understood as the part of the total correlation information among hidden units, which is useless for classification task. Note that according to the definition of redundancy, by reducing only its first term without the labels $Y$ being considered, the value of redundancy would not go down since the second term always equals to the first in this case and then has no effect on the generalization error, which implies that the endeavor that focuses only on the unsupervised diversity measure, i.e., the first term here, might be noneffective for the classification task if there is no extra input information. We also notice that this redundancy definition has been proposed by [Brown,
However, they focused on the ensemble learning and derived the redundancy definition in the Bayesian learning framework from the upper bound of the probability of classification error, where only 0-1 loss is permitted. Nonetheless, according to their work, we can directly obtain the following equation
\[
I(\hat{h}(X);Y) = \sum_{i=1}^{m} I(h_i(X);Y) - R_h(S) \tag{15}
\]
and obtain the upper bound of the probability of classification error for any given classification function \(g\).
\[
P(g(\hat{h}(X)) \neq Y) \leq \frac{H(Y) - I(\hat{h}(X);Y)}{2}, \tag{16}
\]
which implies that the decrease of the redundancy may well lead to a decrease of the classification error.

## 3.3 The effect of redundancy

We have introduced the definition of the information redundancy. However, due to the existence of the other terms in Eq. (11), the effect of the redundancy is still not very clear. In this subsection, we will clarify the effect of the redundancy on the generalization error and answer the question that whether the learning algorithm could always benefit from the decrease of the redundancy; i.e., whether the decrease of the redundancy leads to the improvement of the generalization capacity.

Let us first have a relaxation of the generalization error upper bound. In view of the Eq. (11), the last term is associated with the training process of classification parameters \(W\). If the size \(n\) is large and \(|H(W) - H(S_{y}, W|h(S_{x}))| \leq \delta\) with \(\delta\) a constant, then the generalization is mainly determined by the first four terms. By omitting the last term, we obtain a relaxation of the upper bound, i.e.,
\[
g(P_{S}, P_{W|S}) \leq \sqrt{2} \sigma^2 \left[ R_h(S) - \sum_{i=1}^{m} I(h_i(X);Y) + H(Y) \right], \tag{17}
\]
where the decrease of the information redundancy actually improves the generality.

However, if above conditions cannot be satisfied, e.g., a relatively small sample size, then ignoring the influence of the last term on the generalization error may not be appropriate. Notice that by Eqs. (15), (17) and (18), the increase of \(R_h(S)\) implies a decrease of \(I(\hat{h}(S_{x}); S_{y})\) if the total relevance of respective component learner to the labels, i.e., \(\sum_{i=1}^{m} I(h_i(X);Y)\), keeps unchanged. Then, in the following discussion, we convert the problem to justify whether the increase of \(I(\hat{h}(S_{x}); S_{y})\) leads to the decrease of \(I(f(S);W)\). Nonetheless, before dealing with the general case, consider an extreme case first, where \(\hat{h}(S_{x})\) is moved to \(S_{y}\), so as to be almost identical to \(S_{y}\). In this case, \(I(\hat{h}(S_{x}); S_{y})\) is close to its maximum, whereby \(R_h(S)\) arrives at its minimum if the relevancy sum of respective component learners to labels stays the same; and consequently, \(I(f(S);W) \approx I(S_{y};W)\). By \(I(f(S);W) \geq I(S_{y};W)\), given \(W\), the upper bound of the generalization error also reaches its minimum. This extreme case gives a coarse picture about what happens when we reduce the value of the information redundancy.

Next we discuss the general case, where it turns out that the reduction of the redundancy also leads to the decrease of the generalization error. Note there are infinite trajectories to make \(R_h(S)\) decrease. Only focusing on some special trajectories generally makes no sense. Then we need a tool that can cover all the possible trajectories and describe the complex interaction behaviour between \(\hat{h}(S_{x}), W\) and \(S_{y}\). Fortunately, the fluctuation theorem in the presence of information [Ito, 2013; Sagawa and Ueda, 2013; Lahiri et al., 2012; Jinwoo, 2019] can well meet these needs. To this end, we first introduce the conclusion based on the fluctuation theorem of [Ito, 2013], where some necessary changes are made to adapt it to the current problem.

**Theorem 2.** Adapting \(\hat{h}(S_{x})\) as well as \(W\) in terms of \(S_{y}\) along the prescribed trajectories, then
\[
\langle \Delta H(\hat{h}(S_{x})) \rangle + \langle \Delta H(W) \rangle - \langle \Delta I(\hat{h}(S_{x});S_{y}) \rangle + \langle I_{ini}(f(S);W) \rangle \geq \langle I_{fin}(f(S);W) \rangle, \tag{21}
\]
where the marginal distribution of \(S_{y}\) does not change during the adaption process; \(I_{ini}\) and \(I_{fin}\) are the mutual information at the initial time and the final time respectively.

**Lemma 2.** Let \(T_1\) and \(T_2\) denote two systems, where \(T_1\) evolves under only the influence of the value of \(T_2\) along with the prescribed trajectories, and the marginal distribution of \(T_2\) does not change during the evolution. Then, in the average sense (averaging over evolution trajectories), the lower bound of the entropy increase of \(T_1\) denoted by \(\sigma\) is given by the change of the mutual information between \(T_1\) and \(T_2\), i.e.,
\[
\langle \sigma \rangle \geq \langle \Delta I(T_1; T_2) \rangle, \tag{18}
\]
where \(\langle \cdot \rangle\) describes the ensemble average over all trajectories.

The above lemma can be directly derived from the main result presented in [Ito, 2013], where Ito et al. discussed the dynamics of causal networks between two systems \(T_1\) and \(T_2\) and gave the following result:
\[
\langle \exp[-\sigma + \Theta] \rangle = 1, \tag{19}
\]
Here, \(\sigma\) is the entropy production in \(T_1\); the quantity \(\Theta\) is characterized by the topology of causal networks (see Fig. 1):
\[
\Theta = I_{fin}(T_1; T_2) - I_{ini}(T_1; T_2) - I_{tr}(T_1; T_2), \tag{20}
\]
where \(I_{ini}\) and \(I_{fin}\) are the mutual information between \(T_1\) and \(T_2\) before and after the evolution in the presence of feedback control; \(I_{tr}\) is the information transfered into \(T_2\) from \(T_1\), which equals to zero as \(T_2\) is unchanged during the evolution (see Eq. (5) in [Ito, 2013] for the detail). Then, by the Jensen inequality, we obtain the Eq. (18) immediately. Moreover, we stress that since there is no heat flow in the lemma’s setup, the positive entropy production \(\sigma\) originates actually only from the change of the correlation of systems [Jinwoo, 2019; Sagawa and Ueda, 2012]. That is, \(\sigma\) is the increment of the entropy of \(T_1\), i.e., \(\sigma = \Delta H(T_1)\).

By setting \(T_1 = \{\hat{h}(S_{x}), W\}\) and \(T_2 = S_{y}\), the process of reducing \(R_h(S)\) or equivalently improving \(I(\hat{h}(S_{x}); S_{y})\) can be cast as a special case of Lemma 2. Then, we obtain the following theorem.

**Theorem 2.** Adapting \(\hat{h}(S_{x})\) as well as \(W\) in terms of \(S_{y}\) along the prescribed trajectories, then
\[
\langle \Delta H(\hat{h}(S_{x})) \rangle + \langle \Delta H(W) \rangle - \langle \Delta I(\hat{h}(S_{x});S_{y}) \rangle + \langle I_{ini}(f(S);W) \rangle \geq \langle I_{fin}(f(S);W) \rangle, \tag{21}
\]
where the marginal distribution of \(S_{y}\) does not change during the adaption process; \(I_{ini}\) and \(I_{fin}\) are the mutual information at the initial time and the final time respectively.
Figure 1: (a) A Venn diagram representation of the interactions between \(\hat{h}(S_x), S_y\) and \(W\), where the shaded area represents the mutual information \(I(f(S); W)\). (b) Representation of the dynamics as a causal network, where \(T_1 = \{\hat{h}(S_x), W\}\) evolves only under the influence of \(T_2 = S_y\).

Proof. Since

\[
\langle \Delta H(\hat{h}(S_x), W) \rangle \geq \langle \Delta I(\hat{h}(S_x), W; S_y) \rangle,
\]

we obtain

\[
\langle \Delta H(\hat{h}(S_x), W) \rangle \geq \langle \Delta I(\hat{h}(S_x); S_y) \rangle + \langle \Delta I(S_y; W|\hat{h}(S_x)) \rangle.
\]

Then,

\[
\langle \Delta H(\hat{h}(S_x)) \rangle + \langle \Delta H(W) \rangle - \langle \Delta I(\hat{h}(S_x); S_y) \rangle \\
\geq \langle \Delta I(\hat{h}(S_x); W) \rangle + \langle \Delta I(S_y; W|\hat{h}(S_x)) \rangle,
\]

and finally

\[
\langle \Delta H(\hat{h}(S_x)) \rangle + \langle \Delta H(W) \rangle - \langle \Delta I(\hat{h}(S_x); S_y) \rangle \\
\geq \langle \Delta I(\hat{h}(S_x), S_y; W) \rangle,
\]

which completes the proof. \(\square\)

We note that above discussions are in the average sense over all trajectories. Thus, according to the Eq. (21), we prove the stated conclusion: in the general cases, e.g., with a small sample size or changeable model parameters, reducing the information redundancy among the hidden units can usually bring down the final generalization error, due to the positivity of \(\Delta I(\hat{h}(S_x); S_y)\) under the prescribed protocol. Moreover, as a byproduct, Eq. (21) also implies that the decrease of \(H(\hat{h}(S_x))\) or \(H(W)\) can also make the generalization error decrease, which is consistent with some regularization methods. For example, the L1 [Zhang et al., 2011] and L2 [Krogh and Hertz, 1991] regularization methods and the Dropout method [Srivastava et al., 2014] can be seen as the means of reducing the joint entropy of hidden units or network’s weights.

4 Regularization method

In this section, a new regularization method named redundancy decrease method (RDM) is proposed, which uses the information redundancy \(R_h\) as the regularizer. Typically, the redundancy regularizer is applied to an interested hidden layer to learn a new feature representation of the data. The total loss of this method is formulated as

\[
T_{loss} = E_{loss} + \lambda R_h
\]

where \(E_{loss}\) is the premier loss function of the DNNs without any regularizer, for instance, the cross entropy between the data empirical distribution and the model distribution; \(\lambda > 0\) is the balance parameter.

The redundancy regularizer \(R_h\) is actually the difference of two mutual information terms. The estimation of the mutual information has been recognized as a very difficult thing due to the continuity and high dimensions of data. Fortunately, recent researches [Belghazi et al., 2018; Brakel and Bengio, 2018; Hjelm et al., 2019] show that this problem can be settled by using the Donsker-Varadhan representation [Donsker and Varadhan, 1975] of KL-based mutual information. Here, we follow the work of [Brakel and Bengio, 2018; Hjelm et al., 2019] and use the Jensen-Shannon divergence (JSD)-based mutual information to replace KL-based mutual information since JSD-based methods are often more stable than the KL-based mutual information. Now, for the first term of the redundancy, i.e., \(I(h_1; h_2; \ldots; h_m)\), it is estimated by

\[
J_u = \text{JSD}(P_{h_1, h_2, \ldots, h_m}, P_{h_1} \otimes P_{h_2} \otimes \ldots \otimes P_{h_m}) \\
\geq \sup \{E[\log[\sigma(T(h_1, \ldots, h_m))] + E[\log[1 - \sigma(T(h_1, \ldots, h_m))] ]\}
\]

(27)

where \(T\) is a neural network and hereinafter \(\sigma\) is a sigmoid function; the vector of \((h_1, \ldots, h_m)\) is an instance sampled from the product of the marginal densities. It is produced by combining the extracted features in the corresponding dimensions of the randomly selected different instances from the joint PDF. This part of work has actually been completed by [Brakel and Bengio, 2018].

Similarly, the second term of \(R_h\), i.e., the conditional mutual information \(I(h_1; \ldots; h_m|Y)\), can be estimated by

\[
J_L = \mathbb{E}_{Y}[\text{JSD}(P_{h_1, h_2, \ldots, h_m}, P_{h_1} \otimes P_{h_2} \otimes \ldots \otimes P_{h_m}|Y)]
\]

(28)

However, \(J_L\) is an expectation of JSD with respect to \(Y\). To get the expectation, for each given label, the JSD w.r.t. the label is needed to be estimated. For example, given \(Y = i\), the corresponding JSD is estimated by

\[
J_{Y=i} \geq \sup_{T} \{E[\log[\sigma(T(h_1, \ldots, h_m))] \}
\]

\[
+ E[\log[1 - \sigma(T(h_1, \ldots, h_m))] ]\}
\]

(29)

where \(T\) in Eq. (27) is reused; all the vectors of \((h_1, \ldots, h_m)\) have the label \(Y = i\); the process to obtain the vector of \((h_1, \ldots, h_m)\) is similar to the producing of \((h_1, \ldots, h_m)\) except that the features are drawn from the samples with the same label \(Y = i\). After obtaining \(J_{Y=i}\) for all labels \(i\), taking an expectation over \(Y\) gives the estimation of \(J_L\).

The learning algorithm is finally turned out as an iterative min-max process, where the maximizations of the right hand side of Eqs. (27) and (28) guarantee a sufficient approximation to the information redundancy \(R_h\); and the minimization of Eq. (26), i.e.,

\[
\theta = \arg \min_{\theta} \{E_{loss} + \lambda(J_U - J_L)\}
\]

(30)
is actually the training process of regularization DNNs to obtain the model parameters, where $\theta$ is the set of model parameters.

5 Experiments

We aim to check whether the regularizer can reduce the information redundancy of the data and whether the decrease of the information redundancy may bring an improvement to the generalization capacity.

Dataset. The experiments were conducted on the MNIST dataset [LeCun et al., 2010] and the forest cover types (CTYPES) dataset [Gama et al., 2003]. MNIST contains a training set of 60000 samples and a test set of 10000 samples. CTYPES contains 7 classes and 581012 samples with 54 features, from which 4000 samples were randomly sampled to combine the train set and the others combining the test set. Moreover, in order to increase the difficulty of the classification problem, the Gaussian noise with the mean value 0 and the variance 1, multiplied by 2, was added to the original two datasets.

Method. We use a 11-layer fully connected neural network, including 9 hidden layers with 32 ReLU units and a single input and output layer. The batch size of data is 128. The learning rate is 0.001. Moreover, to compare with the unsupervised learning method, the training processes were separated into the representation learning step and the classifier training step. In the representation learning step, the loss function was set to the reconstruction error with the RDM being applied to the second hidden layer (the input layer is the 0 layer) to get the new data representations. To compute the information redundancy of the hidden layer, an additional network $T$ (see Eqs. (27), (29)) is needed, which is equivalent to the discriminator in the GAN network [Goodfellow et al., 2014]. The balance parameter (see Eq. (30)) was set to 1. $T$ has there layers with the hidden layer containing 200 units. Its training settings are the same as the main network except that its update number for each update of main network is set to 15. Additionally, in the classifier training step, only 500 randomly selected samples are retained for the preceeding training. The training iteration number is set to 2000. All the experiments are implemented by Tensorflow [Abadi et al., 2016].

Reduction of Redundancy. To investigate the effectiveness of the proposed method RDM, we compared it with the method that has no regularizer (none), and the independence learning method, called ILM here [Brakel and Bengio, 2018], which actually uses the first term of the information redundancy as the regularizer. Every experiment was repeated for five times. The evaluation metric is the information redundancy proposed by us, which is estimated by the score on the discriminator network $T$. And the average result is shown in Fig. 2 (a) and 3 (a). It can be seen from the Fig. 2(a) and 3 (a) that the information redundancy of RDM is much smaller than the other methods as the number of iterations increases, which indicates that RDM encourages the reduction of the redundancy in the hidden units. Oppositely, the method of ILM has an almost unchanged information redundancy owing to its regularizer only reflecting the global diversity over the whole feature distribution, reducing the global diversity and meanwhile the valuable class-conditional dependencies. The none method keeps relatively high information redundancy, which implies that the features learned by it tend to be coadapted and to influence each other. It generally means a bad classification performance on these features. Moreover, to show that RDM can at least remove the linear redundancy, we check the correlation gap between the class-independent correlation and the class-conditional correlation.

Information Redundancy and Generalization Error. We have experimentally testified that the regularization method RDM can leads to the reduction of the information redundancy or the correlation gap. Further, we check the empirical generalization error of these methods to show whether there exists a clear and stable relationship between the information redundancy and the generalization error. The experiment results are shown in the Fig. 4 and the Table 1. From Fig. 4, we can observe that RBM has the minimal empirical generalization error than the other methods. Since RBM differs from the other methods only by the used regularizer and achieves the significantly lower information redundancy and
In this paper, by investigating the upper bound of the generalization error from the information perspective, we naturally derive a measure of the redundancy among the hidden units of DNNs. Moreover, we theoretically prove that the proposed information redundancy has a clear connection to the generalization capacity of DNNs. Based on this insight, we design a regularization method, which formalizes the information redundancy as the regularizer and uses an additional network to estimate and minimize the information redundancy as the regularizer and unsing an additional net work to estimate and minimize the information redundancy. Our experiments testified the effectiveness of the proposed method in term of the information redundancy can avoid such problems.

6 Conclusion

In this paper, by investigating the upper bound of the generalization error from the information perspective, we naturally derive a measure of the redundancy among the hidden units of DNNs. Moreover, we theoretically prove that the proposed information redundancy has a clear connection to the generalization capacity of DNNs. Based on this insight, we design a regularization method, which formalizes the information redundancy as the regularizer and unsing an additional network to estimate and minimize the information redundancy. Our experiments testified the effectiveness of the proposed method and gave an empirical evidence for our point view.

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| Methods | MNIST | | Covertypes | | |
|---------|-------|---|---|---|---|---|
| RDM     | 1     | 0.960 | 0.040 | 4545 | 444 | sss |
| ILM     | 1     | 0.906 | 0.094 | 4545 | 444 | sss |
| None    | 1     | 0.941 | 0.059 | 4545 | 444 | sss |

Table 1: The classification results of all methods on MNIST and Forest Covertypes Datasets.

Figure 4: Comparison of the empirical generalization error of different methods with iterations on MNIST dataset.
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