Towards Understanding Learning Representations: To What Extent Do Different Neural Networks Learn the Same Representation

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Abstract

It is widely believed that learning good representations is one of the main reasons for the success of deep neural networks. Although highly intuitive, there is a lack of theory and systematic approach quantitatively characterizing what representations do deep neural networks learn. In this work, we move a tiny step towards a theory and better understanding of the representations. Specifically, we study a simpler problem: How similar are the representations learned by two networks with identical architecture but trained from different initializations. We develop a rigorous theory based on the neuron activation subspace match model. The theory gives a complete characterization of the structure of neuron activation subspace matches, where the core concepts are maximum match and simple match which describe the overall and the finest similarity between sets of neurons in two networks respectively. We also propose efficient algorithms to find the maximum match and simple matches. Finally, we conduct extensive experiments using our algorithms. Experimental results suggest that, surprisingly, representations learned by the same convolutional layers of networks trained from different initializations are not as similar as prevalently expected, at least in terms of subspace match.

1 Introduction

It is widely believed that learning good representations is one of the main reasons for the success of deep neural networks [Krizhevsky et al., 2012, He et al., 2016]. Taking CNN as an example, filters, shared weights, pooling and composition of layers are all designed to learn good representations of images. Although highly intuitive, it is still illusive what representations do deep neural networks learn.

In this work, we move a tiny step towards a theory and a systematic approach that characterize the representations learned by deep nets. In particular, we consider a simpler problem: How similar are the representations learned by two networks with identical architecture but trained from different initializations. It is observed that training the same neural network from different random

\[^1\]The codes are available on https://github.com/MeckyWu/subspace-match

32nd Conference on Neural Information Processing Systems (NeurIPS 2018), Montréal, Canada.
initializations frequently yields similar performance [Dauphin et al., 2014]. A natural question arises:
do the differently-initialized networks learn similar representations as well, or do they learn totally
distinct representations, for example describing the same object from different views? Moreover,
what is the granularity of similarity: do the representations exhibit similarity in a local manner,
i.e. a single neuron is similar to a single neuron in another network, or in a distributed manner, i.e.
eurons aggregate to clusters that collectively exhibit similarity? The questions are central to the
understanding of the representations learned by deep neural networks, and may shed light on the
long-standing debate about whether network representations are local or distributed.

Li et al. [2016] studied these questions from an empirical perspective. Their approach breaks down
the concept of similarity into one-to-one mappings, one-to-many mappings and many-to-many
mappings, and probes each kind of mappings by ad-hoc techniques. Specifically, they applied linear
correlation and mutual information analysis to study one-to-one mappings, and found that some
core representations are shared by differently-initialized networks, but some rare ones are not; they
applied a sparse weighted LASSO model to study one-to-many mappings and found that the whole
correspondence can be decoupled to a series of correspondences between smaller neuron clusters;
and finally they applied a spectral clustering algorithm to find many-to-many mappings.

Although Li et al. [2016] provide interesting insights, their approach is somewhat heuristic, especially
for one-to-many mappings and many-to-many mappings. We argue that a systematic investigation
may deliver a much more thorough comprehension. To this end, we develop a rigorous theory
to study the questions. We begin by modeling the similarity between neurons as the matches of
subspaces spanned by activation vectors of neurons. The activation vector [Raghu et al., 2017]
shows the neuron’s responses over a finite set of inputs, acting as the representation of a single
neuron. Compared with other possible representations such as the weight vector, the activation
vector characterizes the essence of the neuron as an input-output function, and takes into consideration
the input distribution. Further, the representation of a neuron cluster is represented by the subspace
spanned by activation vectors of neurons in the cluster. The subspace representations derive from the
fact that activations of neurons are followed by affine transformations; two neuron clusters whose
activations differ up to an affine transformation are essentially learning the same representations.

In order to develop a thorough understanding of the similarity between clusters of neurons, we give a
complete characterization of the structure of the neuron activation subspace matches. We show the
unique existence of the maximum match, and we prove the Decomposition Theorem: every match
can be decomposed as the union of a set of simple matches, where simple matches are those which
cannot be decomposed any more. The maximum match characterizes the whole similarity, while
simple matches represent minimal units of similarity, collectively giving a complete characterization.
Furthermore, we investigate how to characterize these simple matches so that we can develop efficient
algorithms for finding them.

Finally, we conduct extensive experiments using our algorithms. We analyze the size of the maximum
match and the distribution of sizes of simple matches. It turns out, contrary to prevalently expected,
representations learned by almost all convolutional layers exhibit very low similarity in terms of
matches. We argue that this observation reflects the current understanding of learning representation
is limited.

Our contributions are summarized as follows.

1. We develop a theory based on the neuron activation subspace match model to study the
   similarity between representations learned by two networks with identical architecture
   but trained from different initializations. We give a complete analysis for the structure of
   matches.
2. We propose efficient algorithms for finding the maximum match and the simple matches,
   which are the central concepts in our theory.
3. Experimental results demonstrate that representations learned by most convolutional layers
   exhibit low similarity in terms of subspace match.

The rest of the paper is organized as follows. In Section 2 we formally describe the neuron activation
subspace match model. Section 3 will present our theory of neuron activation subspace match. Based
on the theory, we propose algorithms in Section 4. In Section 5 we will show experimental results

[Li et al., 2016] also implicitly used the activation vector as the neuron’s representation.
and make analysis. Finally, Section 5 concludes. Due to the limited space, all proofs are given in the supplementary.

2 Preliminaries

In this section, we will formally describe the neuron activation subspace match model that will be analyzed throughout this paper. Let $\mathcal{X}$ and $\mathcal{Y}$ be the set of neurons in the same layer of two networks with identical architecture but trained from different initializations. Suppose the networks are given $d$ input data $a_1, a_2, \ldots, a_d$. For $\forall v \in \mathcal{X} \cup \mathcal{Y}$, let the output of neuron $v$ over $a_i$ be $z_v(a_i)$. The representation of a neuron $v$ is measured by the activation vector $\text{ReLU}(\sum_{x \in \mathcal{X}} w_x z_v(a_i) + b)$, where $\{w_x : x \in \mathcal{X}\}$ are parameters.

We adopt the neuron activation subspace as the representation of a subset of neurons. The reason why we adopt the neuron activation subspace as the representation of a subset of neurons is that activations of neurons are followed by affine transformations. For any neuron $v$, $\forall a_i$, $\sum_{x \in \mathcal{X}} w_x z_v(a_i) = \sum_{y \in \mathcal{Y}} w_y z_v(a_i)$, and vice versa. Essentially $x$ and $y$ receive the same information from either $X$ or $Y$.

We now give the formal definition of a match.

**Definition 1** ($\epsilon$-approximate match and exact match). Let $X \subseteq \mathcal{X}$ and $Y \subseteq \mathcal{Y}$ be two subsets of neurons. $\forall \epsilon \in [0,1]$, we say $(X,Y)$ forms an $\epsilon$-approximate match in $(\mathcal{X}, \mathcal{Y})$, if
1. $\forall x \in X$, $\text{dist}(z_x, \text{span}(z_Y)) \leq \epsilon |z_x|$, 
2. $\forall y \in Y$, $\text{dist}(z_y, \text{span}(z_X)) \leq \epsilon |z_y|$, 

Here we use the $L_2$ distance: for any vector $z$ and any subspace $S$, $\text{dist}(z, S) = \min_{z' \in S} \|z - z'\|_2$.

We call a 0-approximate match an exact match. Equivalently, $(X,Y)$ is an exact match if $\text{span}(z_X) = \text{span}(z_Y)$.

3 A Theory of Neuron Activation Subspace Match

In this section, we will develop a theory which gives a complete characterization of the neuron activation subspace match problem. For two sets of neurons $\mathcal{X}, \mathcal{Y}$ in two networks, we show the structure of all the matches $(X,Y)$ in $(\mathcal{X}, \mathcal{Y})$. It turns out that every match $(X,Y)$ can be decomposed as a union of simple matches, where a simple match is an atomic match that cannot be decomposed any further.

Simple match is the most important concept in our theory. If there are many one-to-one simple matches (i.e. $|X| = |Y| = 1$), it implies that the two networks learn very similar representations at the neuron level. On the other hand, if all the simple matches have very large size (i.e. $|X|, |Y|$ are both large), it is reasonable to say that the two networks learn different representations, at least in details.

We will give mathematical characterization of the simple matches. This allows us to design efficient algorithms finding out the simple matches (Sec 3). The structures of exact and approximate match are somewhat different. In Section 3.1, we present the simpler case of exact match, and in Section 3.2, we describe the more general $\epsilon$-approximate match. Without being explicitly stated, when we say match, we mean $\epsilon$-approximate match.

We begin with a lemma stating that matches are closed under union.

**Lemma 2** (Union-Close Lemma). Let $(X_1, Y_1)$ and $(X_2, Y_2)$ be two $\epsilon$-approximate matches in $(\mathcal{X}, \mathcal{Y})$. Then $(X_1 \cup X_2, Y_1 \cup Y_2)$ is still an $\epsilon$-approximate match.

The fact that matches are closed under union implies that there exists a unique maximum match.
Definition 3 (Maximum Match). A match \((X^*, Y^*)\) in \((X', Y')\) is the maximum match if every match \((X, Y)\) in \((X', Y')\) satisfies \(X \subseteq X^*\) and \(Y \subseteq Y^*\).

The maximum match is simply the union of all matches. In Section 4 we will develop an efficient algorithm that finds the maximum match.

Now we are ready to give a complete characterization of all the matches. First, we point out that there can be exponentially many matches. Fortunately, every match can be represented as the union of some simple matches defined below. The number of simple matches is polynomial for the setting of exact match given \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) being both linearly independent, and under certain conditions for approximate match as well.

Definition 4 (Simple Match). A match \((\bar{X}, \bar{Y})\) in \((X', Y')\) is a simple match if \(\bar{X} \cup \bar{Y}\) is non-empty and there exist no matches \((X_i, Y_i)\) in \((X', Y')\) such that

1. \(\forall i, (X_i \cup Y_i) \subseteq (\bar{X} \cup \bar{Y})\);
2. \(\bar{X} = \bigcup_i X_i, \bar{Y} = \bigcup_i Y_i\).

With the concept of the simple matches, we will show the Decomposition Theorem: every match can be decomposed as the union of a set of simple matches. Consequently, simple matches fully characterize the structure of matches.

Theorem 5 (Decomposition Theorem). Every match \((X, Y)\) in \((X', Y')\) can be expressed as a union of simple matches. Formally, there are simple matches \((\bar{X}_i, \bar{Y}_i)\) satisfying \(X = \bigcup X_i\) and \(Y = \bigcup Y_i\).

3.1 Structure of Exact Matches

The main goal of this and the next subsection is to understand the simple matches. The definition of simple match only tells us it cannot be decomposed. But how to find the simple matches? How many simple matches exist? We will answer these questions by giving a characterization of the simple match. Here we consider the setting of exact match, which has a much simpler structure than approximate match.

An important property for exact match is that matches are closed under intersection.

Lemma 6 (Intersection-Close Lemma). Assume \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) are both linearly independent. Let \((X_1, Y_1)\) and \((X_2, Y_2)\) be exact matches in \((X', Y')\). Then, \((X_1 \cap X_2, Y_1 \cap Y_2)\) is still an exact match.

It turns out that in the setting of exact match, simple matches can be explicitly characterized by a \(v\)-minimum match defined below.

Definition 7 (\(v\)-Minimum Match). Given a neuron \(v \in X' \cup Y'\), we define the \(v\)-minimum match to be the exact match \((X_v, Y_v)\) in \((X', Y')\) satisfying the following properties:

1. \(v \in X_v \cup Y_v\);
2. any exact match \((X, Y)\) in \((X', Y')\) with \(v \in X \cup Y\) satisfies \(X_v \subseteq X\) and \(Y_v \subseteq Y\).

Every neuron \(v\) in the maximum match \((X^*, Y^*)\) has a unique \(v\)-minimum match, which is the intersection of all matches that contain \(v\). For a neuron \(v\) not in the maximum match, there is no \(v\)-minimum match because there is no match containing \(v\).

The following theorem states that the simple matches are exactly \(v\)-minimum matches.

Theorem 8. Assume \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) are both linearly independent. Let \((X^*, Y^*)\) be the maximum (exact) match in \((X', Y')\). \(\forall v \in X^* \cup Y^*\), the \(v\)-minimum match is a simple match, and every simple match is a \(v\)-minimum match for some neuron \(v \in X^* \cup Y^*\).

Theorem 8 implies that the number of simple exact matches is at most linear with respect to the number of neurons given the activation vectors being linearly independent, because the \(v\)-minimum match for each neuron \(v\) is unique. We will give a polynomial time algorithm in Section 4 to find out all the \(v\)-minimum matches.
3.2 Structure of Approximate Matches

The structure of \( \epsilon \)-approximate match is more complicated than exact match. A major difference is that in the setting of approximate matches, the intersection of two matches is not necessarily a match. As a consequence, there is no \( \nu \)-minimum match in general. Instead, we have \( \nu \)-minimal match.

**Definition 9 (\( \nu \)-Minimal Match).** \( \nu \)-minimal matches are matches \((X_v, Y_v)\) in \((X, Y)\) with the following properties:

1. \( v \in X_v \cup Y_v \);
2. if a match \((X, Y)\) with \( X \subseteq X_v \) and \( Y \subseteq Y_v \) satisfies \( v \in X \cup Y \), then \((X, Y) = (X_v, Y_v)\).

Different from the setting of exact match where \( \nu \)-minimum match is unique for a neuron \( v \), there may be multiple \( \nu \)-minimal matches for \( v \) in the setting of approximate match, and in this setting simple matches can be characterized by \( \nu \)-minimal matches instead. Again, for any neuron \( v \) not in the maximum match \((X^*, Y^*)\), there is no \( \nu \)-minimal match because no match contains \( v \).

**Theorem 10.** Let \((X^*, Y^*)\) be the maximum match in \((X, Y)\). \( \forall v \in X^* \cup Y^* \), every \( \nu \)-minimal match is a simple match, and every simple match is a \( \nu \)-minimal match for some \( v \in X^* \cup Y^* \).

**Remark 1.** We use the notion \( \nu \)-minimal match for \( v \in X \cup Y \). That is, the neuron can be in either networks. We emphasize that this is necessary. Restricting \( v \in X \) (or \( v \in Y \)) does not yield Theorem [10] anymore. In other word, \( \nu \)-minimal matches for \( v \in X \) do not represent all simple matches. See Remark A.1 in the Supplementary Material for details.

**Remark 2.** One may have the impression that the structure of match is very simple. This is not exactly the case. Here we point out the complicated aspect:

1. Matches are not closed under the difference operation, even for exact matches. More generally, let \((X_1, Y_1)\) and \((X_2, Y_2)\) be two matches with \( X_1 \subseteq X_2, Y_1 \subseteq Y_2 \). \((X_2 \setminus X_1, Y_2 \setminus Y_1)\) is not necessarily a match.
2. The decomposition of a match into the union of simple matches is not necessarily unique. See Section C in the Supplementary Material for details.

4 Algorithms

In this section, we will give an efficient algorithm that finds the maximum match. Based on this algorithm, we further give an algorithm that finds all the simple matches, which are precisely the \( \nu \)-minimum/minimal matches as shown in the previous section. The algorithm for finding the maximum match is given in Algorithm 1. Initially, we guess the maximum match \((X^*, Y^*)\) to be \( X^* = X, Y^* = Y \). If there is \( x \in X^* \) such that \( \text{dist}(z_x, \text{span}(z_{Y^*})) > \epsilon \), then we remove \( x \) from \( X^* \). Similarly, if for some \( y \in Y^* \) such that \( y \) cannot be linearly expressed by \( z_{X^*} \) within error \( \epsilon \), then we remove \( y \) from \( Y^* \). \( X^* \) and \( Y^* \) are repeatedly updated in this way until no such \( x, y \) can be found.

**Algorithm 1 max_match\((z_v)_{v \in X \cup Y}; \epsilon)\)

1: \((X^*, Y^*) \leftarrow (X, Y)\)
2: changed \leftarrow true
3: while changed do
4: changed \leftarrow false
5: for \( x \in X^* \) do
6: if \( \text{dist}(z_x, \text{span}(z_{Y^*})) > \epsilon \) then
7: \( X^* \leftarrow X^* \setminus \{x\} \)
8: changed \leftarrow true
9: if changed then
10: changed \leftarrow false
11: for \( y \in Y^* \) do
12: if \( \text{dist}(z_y, \text{span}(z_{X^*})) > \epsilon \) then
13: \( Y^* \leftarrow Y^* \setminus \{y\} \)
14: changed \leftarrow true
15: return \((X^*, Y^*)\)
Theorem 11. Algorithm \[\text{Algorithm 2}\] outputs the maximum match and runs in polynomial time.

Our next algorithm (Algorithm \[\text{Algorithm 2}\]) is to output, for a given neuron \( v \in X \cup Y \), the \( v \)-minimum match (for exact match given the activation vectors being linearly independent) or one \( v \)-minimal match (for approximate match). The algorithm starts from \((X_v, Y_v)\) being the maximum match and iteratively finds a smaller match \((X_v, Y_v)\) keeping \( v \in X_v \cup Y_v \) until further reducing the size of \((X_v, Y_v)\) would have to violate \( v \in X_v \cup Y_v \).

Algorithm 2 \text{min\_match}((z_{v'}), v' \in X \cup Y \cup Y, v, \epsilon)

1: \((X_v, Y_v) \leftarrow \text{max\_match}((z_{v'}), v' \in X \cup Y \cup Y, \epsilon)\)
2: if \( v \notin X_v \cup Y_v \) then
3: return “failure”
4: while there exists \( u \in X_v \cup Y_v \) unchecked do
5: Pick an unchecked \( u \in X_v \cup Y_v \) and mark it as checked
6: if \( u \in X_v \) then
7: \((X, Y) \leftarrow (X_v \setminus \{u\}, Y_v)\)
8: else
9: \((X, Y) \leftarrow (X_v, Y_v \setminus \{u\})\)
10: \((X^*, Y^*) \leftarrow \text{max\_match}((z_{v'}), v' \in X \cup Y \cup Y, \epsilon)\)
11: if \( v \in (X^*, Y^*) \) then
12: \((X_v, Y_v) \leftarrow (X^*, Y^*)\)
13: return \((X_v, Y_v)\)

Theorem 12. Algorithm \[\text{Algorithm 2}\] outputs one \( v \)-minimal match for the given neuron \( v \). If \( \epsilon = 0 \) (exact match), the algorithm outputs the unique \( v \)-minimum match provided \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) are both linearly independent. Moreover, the algorithm always runs in polynomial time.

Finally, we show an algorithm (Algorithm \[\text{Algorithm 3}\]) that finds all the \( v \)-minimal matches in time \( L^O(N_v) \). Here, \( L \) is the size of the input \((L = (|X| + |Y|) \cdot d)\) and \( N_v \) is the number of \( v \)-minimal matches for neuron \( v \). Note that in the setting of \( \epsilon = 0 \) (exact match) with \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) being both linearly independent, we have \( N_v \leq 1 \), so Algorithm \[\text{Algorithm 3}\] runs in polynomial time in this case.

Algorithm 3 \text{all\_min\_match}((z_{v'}), v' \in X \cup Y \cup Y, v, \epsilon)

1: \( S \leftarrow \emptyset \)
2: found \( \leftarrow \text{true} \)
3: while found do
4: found \( \leftarrow \text{false} \)
5: Let \( S = \{(X_1, Y_1), (X_2, Y_2), \ldots, (X_{|S|}, Y_{|S|})\}\)
6: while \(!\text{found}\) and there exists \((u_1, u_2, \ldots, u_{|S|}) \in (X_1 \cup Y_1) \times (X_2 \cup Y_2) \times \cdots \times (X_{|S|} \cup Y_{|S|})\) unchecked do
7: Pick the next unchecked \((u_1, u_2, \ldots, u_{|S|}) \in (X_1 \cup Y_1) \times (X_2 \cup Y_2) \times \cdots \times (X_{|S|} \cup Y_{|S|})\) and mark it as checked
8: \((X, Y) \leftarrow (X, Y)\)
9: for \( i = 1, 2, \ldots, |S|\) do
10: if \( u_i \in X \) then
11: \( X \leftarrow X \setminus \{u_i\}\)
12: else
13: \( Y \leftarrow Y \setminus \{u_i\}\)
14: if \text{min\_match}((z_{v'}), v' \in X \cup Y \cup Y, v, \epsilon)\) doesn’t return “failure” then
15: \((X_v, Y_v) \leftarrow \text{min\_match}((z_{v'}), v' \in X \cup Y \cup Y, v, \epsilon)\)
16: \( S \leftarrow S \cup \{(X_v, Y_v)\}\)
17: found \( \leftarrow \text{true} \)
18: return \( S \)
Theorem 13. Algorithm 3 outputs all the $N_v$ different $\epsilon$-minimal matches in time $O(N_v)$. With Algorithm 3, we can find all the simple matches by exploring all $v \in X \cup Y$ based on Theorem 10.

In the worst case, Algorithm 3 is not polynomial time, as $N_v$ is not upper bounded by a constant in general. However, under assumptions we call strong linear independence and stability, we show that Algorithm 3 runs in polynomial time. Specifically, we say $(z_x)_{x \in X}$ satisfies $\theta$-strong linear independence for $\theta \in (0, \frac{\pi}{2})$ if $0 \notin z_X$ and for any two non-empty disjoint subsets $X_1, X_2 \subseteq X$, the angle between $\text{span}(z_{X_1})$ and $\text{span}(z_{X_2})$ is at least $\theta$. Here, the angle between two subspaces is defined to be the minimum angle between non-zero vectors in the two subspaces. We define $\theta$-strong linear independence for $(z_y)_{y \in Y}$ similarly. We say $(z_x)_{x \in X}$ and $(z_y)_{y \in Y}$ satisfy $(\epsilon, \lambda)$-stability for $\epsilon \geq 0$ and $\lambda > 1$ if $\forall x \in X, \forall y \in Y \subseteq Y, \text{dist}(z_x, \text{span}(z_Y)) \notin \{\epsilon |z_x|, \lambda |z_x|\}$ and $\forall y \in Y, \forall X \subseteq X, \text{dist}(z_y, \text{span}(z_X)) \notin \{\epsilon |z_y|, \lambda |z_y|\}$. We prove the following theorem.

Theorem 14. Suppose $\exists \theta \in (0, \frac{\pi}{2})$ such that $(z_x)_{x \in X}$ and $(z_y)_{y \in Y}$ both satisfy $\theta$-strong linear independence and $(\epsilon, \sin \theta + 1)$-stability. Then, $\forall v \in X \cup Y, N_v \leq 1$. As a consequence, Algorithm 3 finds all the $\epsilon$-minimal matches in polynomial time, and we can find all the simple matches in polynomial time by exploring all $v \in X \cup Y$ based on Theorem 10.

5 Experiments

We conduct experiments on architectures of VGG [Simonyan and Zisserman, 2014] and ResNet [He et al., 2016] on the dataset CIFAR10 [Krizhevsky et al.] and ImageNet [Deng et al., 2009]. Here we investigate multiple networks initialized with different random seeds, which achieve reasonable accuracies. Unless otherwise noted, we focus on the neurons activated by ReLU.

The activation vector $z_v$ mentioned in Section 2 is defined as the activations of one neuron $v$ over the validation set. For a fully connected layer, $z_v \in \mathbb{R}^d$, where $d$ is the number of images. For a convolutional layer, the activations of one neuron $v$, given the image $x$, is a feature map $z_v(a_i) \in \mathbb{R}^{h \times w}$. We vectorize the feature map as $\text{vec}(z_v(a_i)) \in \mathbb{R}^{h \times w}$, and thus $z_v := (\text{vec}(z_v(a_1)), \text{vec}(z_v(a_2)), \ldots, \text{vec}(z_v(a_d))) \in \mathbb{R}^{h \times w \times d}$.

5.1 Maximum Match

We introduce maximum matching similarity to measure the overall similarity between sets of neurons. Given two sets of neurons $X, Y$ and $\epsilon$, algorithm 1 outputs the maximum match $X^*, Y^*$. The maximum matching similarity $s$ under $\epsilon$ is defined as $s(\epsilon) = \frac{|X^*| + |Y^*|}{|X| + |Y|}$.

Here we only study neurons in the same layer of two networks with same architecture but initialized with different seeds. For a convolutional layer, we randomly sample $d$ from $h \times w \times d$ outputs to form an activation vector for several times, and average the maximal matching similarity.

Different Architecture and Dataset

We examine several architectures on different dataset. For each experiment, five differently initialized networks are trained, and the maximal matching similarity is averaged over all the pairs of networks given $\epsilon$. The similarity values show little variance among different pairs, which indicates that this metric reveals a general property of network pairs. The detail of network structures and validation accuracies are listed in the Supplementary Section E.2.

Figure 3 shows maximal matching similarities of all the layers of different architectures under various $\epsilon$. From these results, we make the following conclusions:

1. For most of the convolutional layers, the maximum match similarity is very low. For deep neural networks, the similarity is almost zero. This is surprising, as it is widely believed that the convolutional layers are trained to extract specific patterns. However, the observation shows that different CNNs (with the same architecture) may learn different intermediate patterns.

2. Although layers close to the output sometimes exhibit high similarity, it is a simple consequence of their alignment to the output: First, the output vector of two networks must be well aligned because they both achieve high accuracy. Second, it is necessary that the layers before output are similar because if not, after a linear transformation, the output vectors will not be similar. Note that in Figure 3(b) layers close to the output do not have similarity. This is because in this experiment the accuracy is relatively low. (See also in Supplementary
Figure 1: Maximal matching similarities of different architectures on different datasets under various $\epsilon$. The x-axis is along the propagation. (a) shows ResNet18 on CIFAR10 validation set, we leave other classical architectures like VGG in Supplementary material; (b) shows VGG16 on ImageNet validation set; (c) shows a deeper ResNet on CIFAR10.

materials that, for a trained and an untrained networks which have very different accuracies and therefore layers close to output do not have much similarity.)

3. There is also relatively high similarity of layers close to the input. Again, this is the consequence of their alignment to the same input data as well as the low-dimension nature of the low level layers. More concretely, the fact that each low-level filter contains only a few parameters results in a low dimension space after the transformation; and it is much easier to have high similarity in low dimensional space than in high dimensional space.

5.2 Simple Match

The maximum matching illustrates the overall similarity but does not provide information about the relation of specific neurons. Here we analyze the distribution of the size of simple matches to reveal the finer structure of a layer. Given $\epsilon$ and two sets of neurons $\mathcal{X}$ and $\mathcal{Y}$, algorithm 5 will output all the simple matches.

For more efficient implementation, given $\epsilon$, we run the randomized algorithm 2 over each $v \in \mathcal{X} \cup \mathcal{Y}$ to get one $v$-minimal match for several iterations. The final result is the collection of all the $v$-minimal matches found (remove duplicated matches), which we use to estimate the distribution.

Figure 2 shows the distribution of the size of simple matches on layers close to input or output respectively. We make the following observations:

1. While the layers close to output are similar overall, it seems that they do not show similarity in a local manner. There are very few simple matches with small sizes. It is also an evidence that such similarity is the result of its alignment to the output, rather than intrinsic similar representations.

2. The layer close to input shows lower similarity in the finer structure. Again, there are few simple matches with small sizes.

In sum, almost no single neuron (or a small set of neurons) learn similar representations, even in layers close to input or output.
6 Conclusion

In this paper, we investigate the similarity between representations learned by two networks with identical architecture but trained from different initializations. We develop a rigorous theory and propose efficient algorithms. Finally, we apply the algorithms in experiments and find that representations learned by convolutional layers are not as similar as prevalently expected.

This raises important questions: Does our result imply two networks learn completely different representations, or subspace match is not a good metric for measuring the similarity of representations? If the former is true, we need to rethink not only learning representations, but also interpretability of deep learning. If from each initialization one learns a different representation, how can we interpret the network? If, on the other hand, subspace match is not a good metric, then what is the right metric for similarity of representations? We believe this is a fundamental problem for deep learning and worth systematic and in depth studying.

7 Acknowledgement

This work is supported by National Basic Research Program of China (973 Program) (grant no. 2015CB352502), NSFC (61573026) and BJNSF (L172037) and a grant from Microsoft Research Asia.

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Theorem 10. Let \((X_1, Y_1)\) and \((X_2, Y_2)\) be two \(\epsilon\)-approximate matches in \((\mathcal{X}, \mathcal{Y})\). Then \((X_1 \cup X_2, Y_1 \cup Y_2)\) is still an \(\epsilon\)-approximate match.

Proof. The lemma follows immediately from the definition of \(\epsilon\)-approximate match.

Theorem 5 (Decomposition Theorem). Every match \((X, Y)\) in \((\mathcal{X}, \mathcal{Y})\) can be expressed as a union of simple matches. Formally, there are simple matches \((\hat{X}_i, \hat{Y}_i)\) satisfying \(X = \bigcup_i \hat{X}_i\) and \(Y = \bigcup_i \hat{Y}_i\).

Proof. We prove by induction on the size of the match, \(|X \cup Y|\). When \(|X \cup Y|\) is the smallest among all non-empty matches, we know \((X, Y)\) is itself a simple match, so the theorem holds. For larger \(|X \cup Y|\), \((X, Y)\) may not be a simple match, and in this case we know \((X, Y)\) is the union of smaller matches \((X_i, Y_i)\): \(X_1 \cup Y_1 \subseteq X \cup Y\) and \(X = \bigcup_i X_i\), \(Y = \bigcup_i Y_i\), and thus by the induction hypothesis that every \((X_i, Y_i)\) is a union of simple matches, we know \((X, Y)\) is a union of simple matches.

Lemma 6 (Intersection-Close Lemma). Assume \((z_x)_{x \in \mathcal{X}}\) and \((z_y)_{y \in \mathcal{Y}}\) are both linearly independent. Let \((X_1, Y_1)\) and \((X_2, Y_2)\) be exact matches in \((\mathcal{X}, \mathcal{Y})\). Then, \((X_1 \cap X_2, Y_1 \cap Y_2)\) is still an exact match.

Lemma 6 is a direct corollary of the following claim.

Claim 15. Assume \((z_x)_{x \in \mathcal{X}}\) is linearly independent. Then \(\forall X_1, X_2 \subseteq \mathcal{X}, \text{span}(z_{X_1 \cap X_2}) = \text{span}(z_{X_1} \cap \text{span}(z_{X_2}))\).

Proof. \(\text{span}(z_{X_1 \cap X_2}) \subseteq \text{span}(z_{X_1}) \cap \text{span}(z_{X_2})\) is obvious. To show \(\text{span}(z_{X_1}) \cap \text{span}(z_{X_2}) \subseteq \text{span}(z_{X_1 \cap X_2})\), let's consider a vector \(z \in \text{span}(z_{X_1}) \cap \text{span}(z_{X_2})\). Note that \((z_x)_{x \in \mathcal{X}}\) is linearly independent, so there exists unique \(\lambda_x \in \mathbb{R}\) for each \(x \in \mathcal{X}\) s.t. \(z = \sum_{x \in \mathcal{X}} \lambda_x z_x\). The uniqueness of \(\lambda_x\) and the fact that \(z \in \text{span}(z_{X_1})\) shows that \(\forall x \in \mathcal{X} \setminus X_1, \lambda_x = 0\). Similarly, \(\forall x \in \mathcal{X} \setminus X_2, \lambda_x = 0\). Therefore, \(\lambda_x \neq 0\) only when \(x \in X_1 \cap X_2\), so \(z \in \text{span}(z_{X_1 \cap X_2})\).

Theorem 8. Assume \((z_x)_{x \in \mathcal{X}}\) and \((z_y)_{y \in \mathcal{Y}}\) are both linearly independent. Let \((X^*, Y^*)\) be the maximum (exact) match in \((\mathcal{X}, \mathcal{Y})\). \(\forall v \in X^* \cup Y^*, \text{the v-minimum match is a simple match, and every simple match is the v-minimum match for some neuron v \in X^* \cup Y^*\).

Proof. We show that under the assumption of Theorem 8, the concept of v-minimum match and the concept of v-minimal match (Definition 9) coincide so Theorem 8 is a special case of Theorem 10.

According to Lemma 5, \(\forall v \in X^* \cup Y^*\) has a unique v-minimum match \((X_v, Y_v)\) being the intersection of all the matches containing \(v\). Therefore, for any v-minimal match \((X'_v, Y'_v)\), it holds that \(X_v \subseteq X'_v, Y_v \subseteq Y'_v\), and according to Definition 9 we have \((X_v, Y_v) = (X'_v, Y'_v)\).

Theorem 10. Let \((X^*, Y^*)\) be the maximum match in \((\mathcal{X}, \mathcal{Y})\). \(\forall v \in X^* \cup Y^*, \text{every v-minimal match is a simple match, and every simple match is a v-minimal match for some v} \in X^* \cup Y^*\).

Proof. We start by showing the first half of the lemma. To prove by contradiction, let’s assume that a v-minimal match \((\hat{X}_v, \hat{Y}_v)\) can be written as the union of smaller matches \((X_i, Y_i)\), i.e., \((X_1 \cup Y_1) \subseteq (X_v \cup Y_v), X_v = \bigcup_i X_i, Y_v = \bigcup_i Y_i\). In this case, one of the matches \((X_i, Y_i)\) contains \(v\), which is contradictory with the definition of v-minimal match.

Now we show the second half of the lemma. For any neuron \(v\) in a simple match \((\hat{X}, \hat{Y})\), we consider one of the smallest matches \((X_v, Y_v)\) in \((\hat{X}, \hat{Y})\) containing \(v\). Here, “smallest” means that \(|X_v \cup Y_v|\) is the smallest among all matches in \((\hat{X}, \hat{Y})\) containing \(v\). Note that \((\hat{X}, \hat{Y})\) is itself a match.
Algorithm 3, we can find all the simple matches by exploring all $S$ we put a match into $X$ with $v$. Theorem 11. Algorithm 1 outputs the maximum match and runs in polynomial time. Theorem 13. Algorithm 3 outputs all the $v$-minimal matches for the given neuron $v$. To prove by contradiction, let’s suppose $\hat{X} \neq \hat{Y}$ and $\hat{Y}$ is a simple match, one of $(X_v, Y_v)$ has to be equal to $(\hat{X}, \hat{Y})$, which proves the second half of the lemma.

Remark 3. One important thing to note is that “$v \in X^* \cup Y^*$” in the second half of Lemma 10 cannot be replaced by “$v \in X^*$”. For example, let $z_x = \{(\sqrt{1/2}, \sqrt{1/2}, 0), (\sqrt{1/2}, -\sqrt{1/2}, 0)\}$ and $z_y = z_x \cup \{(\sqrt{1/2}, \sqrt{1/2}, 0), (\sqrt{1/2}, -\sqrt{1/2}, 0)\}$. In this case, the entire match $(X, Y)$ cannot be expressed as a union of $x$-minimal matches for $x \in X$ because no $x$-minimal match contains the vector in $z_y \setminus z_x$. However, in the case of Theorem 12 when $\epsilon = 0$ and $(z_x)_{x \in X}, (z_y)_{y \in Y}$ are both linearly independent, we can perform the replacement. That is because in this case, every match $(X, Y)$ satisfies $|X| = |Y|$, so we know $\hat{X} = \bigcup_{v \in X} X_v$ and $\hat{Y} = \bigcup_{v \in X} Y_v$ imply $(X, Y) = (\bigcup_{v \in X} X_v, \bigcup_{v \in X} Y_v)$.

B Omitted Proofs in Section 4

Theorem 11. Algorithm 1 outputs the maximum match and runs in polynomial time.

Proof. Every time we delete a neuron $x$ (or $y$) from $X^*$ (or $Y^*$) at Line 7 (or Line 13), we make sure that the activation vector $z_x$ (or $z_y$) cannot be linearly expressed by $z_y \cdot (z_x \cdot) \cdot$ within error $\epsilon$, so $(X^*, Y^*)$ always contains the maximum match. On the other hand, when the algorithm terminates, we know $\forall x \in X^*, z_x$ is linearly expressible by $z_y \cdot$ within error $\epsilon$ and $\forall y \in Y^*, z_y$ is linearly expressible by $z_x \cdot$ within error $\epsilon$, so $(X^*, Y^*)$ is a match by definition. Therefore, the output $(X^*, Y^*)$ of Algorithm 1 is a match containing the maximum match, which has to be the maximum match itself.

Before entering each iteration of the algorithm, we make sure that at least a neuron is deleted from $X^*$ or $Y^*$ in the last iteration, so there are at most $|X \cup Y|$ iterations. Therefore, the algorithm runs in polynomial time.

Theorem 12. Algorithm 2 outputs one $v$-minimal match for the given neuron $v$. If $\epsilon = 0$ (exact match), the algorithm outputs the unique $v$-minimum match provided $(z_x)_{x \in X}$ and $(z_y)_{y \in Y}$ are both linearly independent. Moreover, the algorithm always runs in polynomial time.

Proof. Clearly, Algorithm 2 runs in polynomial time. If there exist at least one $v$-minimal matches, then $v$ has to be in the maximum match and thus the algorithm doesn’t return “failure”. Therefore, the remaining is to show that the match $(X_v, Y_v)$ returned by the algorithm is indeed a $v$-minimal match.

Clearly, the first requirement of $v$-minimal match that $v \in X_v \cup Y_v$ is obviously satisfied by the algorithm. Now we prove that the second requirement is also satisfied. Consider a match $(X_0, Y_0)$ with $X_0 \subseteq X_v$ and $Y_0 \subseteq Y_v$ that satisfies $v \in X_0 \cup Y_0$. We want to show that $(X_0, Y_0) = (X_v, Y_v)$. To prove by contradiction, let’s suppose $u \in (X_v \cup Y_v) \setminus (X_0 \cup Y_0)$. Let’s consider $(X, Y)$ and $(X^*, Y^*)$ at Line 11 in the iteration when $u$ is being picked by the algorithm at Line 5. Since $u \notin X_0 \cup Y_0$, we know $X_0 \subseteq X_v \setminus \{u\} \subseteq X$ and $Y_0 \subseteq Y_v \setminus \{u\} \subseteq Y$. In other words, $(X_0, Y_0)$ is a match in $(X, Y)$. Moreover, since $u \notin X_v \cup Y_v$, we know the “if” condition at Line 11 is not satisfied, i.e., $v \notin (X^*, Y^*)$. Therefore, $(X_0 \cup X_v, Y_0 \cup Y_v)$ is a match in $(X, Y)$ that is strictly larger than $(X^*, Y^*)$ (note that $v \in X_0 \cup Y_0$), a contradiction with $(X^*, Y^*)$ being the maximum match in $(X, Y)$.

Theorem 13. Algorithm 3 outputs all the $N_v$ different $v$-minimal matches in time $L^{O(N_v)}$. With Algorithm 3, we can find all the simple matches by exploring all $v \in X \cup Y$ based on Theorem 10.

Proof. The fact that we remove all $u_t$ from $X$ and $Y$ in each iteration implies that every time we put a match into $S$, the match is different from the existing matches in $S$. Moreover, every time we put a match into $S$, the match is a $v$-minimal match, so $|S| \leq N_v$ during the whole algorithm. Therefore, the running time of the algorithm is $L^{O(N_v)}$. The remaining is to show that $S$ returned by the algorithm contains all the $v$-minimal matches. To prove by contradiction, suppose $S = \{(X_1, Y_1), (X_2, Y_2), \cdots, (X_k, Y_k)\}$ while there exists a $v$-minimal match $(X_{k+1}, Y_{k+1})$ that is
not in $S$. By the fact that $(X_{k+1}, Y_{k+1})$ is minimal, we know $X_i \cup Y_i$ is not a subset of $X_{k+1} \cup Y_{k+1}$ for $i = 1, 2, \ldots, k$. Therefore, there exists $u_j \in (X_i \cup Y_i) \setminus (X_{k+1} \cup Y_{k+1})$ for $i = 1, 2, \ldots, k$. Consider the iteration when we pick $(u_1, u_2, \ldots, u_k)$ at Line 7. We know the “if” condition at Line 14 is satisfied because of $(X_{k+1}, Y_{k+1})$, which then implies that $(X_{k+1}, Y_{k+1}) \in S$, a contradiction. 

**Theorem 14.** Suppose \( \theta \in (0, \frac{\pi}{2}] \) such that \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) both satisfy \( \theta \)-linear independence and \((\epsilon, \frac{2}{\sin \theta} + 1)\)-stability. Then, \( \forall v \in X \cup Y, N_v \leq 1 \). As a consequence, Algorithm 3 finds all the \( v \)-minimal matches in polynomial time, and we can find all the simple matches in polynomial time by exploring all \( v \in X \cup Y \) based on Theorem 10.

Theorem 14 is a direct corollary of the following lemma.

**Lemma 16.** Suppose \((z_x)_{x \in X}\) and \((z_y)_{y \in Y}\) both satisfy \( \theta \)-linear independence and \((\epsilon, \frac{2}{\sin \theta} + 1)\)-stability. Let \( (X_1, Y_1), (X_2, Y_2) \) be two matches in \((X, Y)\). Then, \( (X_1 \cap X_2, Y_1 \cap Y_2) \) is also a match.

**Proof.** \( \forall x \in X_1 \cap X_2 \), let \( |z_x - \sum_{y \in Y_2} \mu_y z_y| \leq c|z_x| \) and \( |z_x - \sum_{y \in Y_2} \mu_y z_y| \leq c|z_x| \). Therefore, \( |z_x - \sum_{y \in Y_2} \mu_y z_y + (\sum_{y \in Y_1 \setminus Y_2} (\mu_y - \mu_y') z_y - \sum_{y \in Y_1 \setminus Y_2} \mu_y' z_y)| \leq 2c|z_x| \), which implies that \( \text{dist}(\sum_{y \in Y_1 \setminus Y_2} \mu_y z_y, \text{span}(z_{Y_2})) \leq 2c|z_x| \). Note that by \( \theta \)-linear independence, we have the angle between \( \text{span}(z_{Y_1 \setminus Y_2}) \) and \( \text{span}(z_{Y_2}) \) is at least \( \theta \). Therefore, \( |\sum_{y \in Y_1 \setminus Y_2} \mu_y z_y| \leq \frac{2c|z_x|}{\sin \theta} \). Together with \( |z_x - \sum_{y \in Y_1} \mu_y z_y| \leq c|z_x| \), we know \( |z_x - \sum_{y \in Y_1 \setminus Y_2} \mu_y z_y| \leq c|z_x| + \frac{2c|z_x|}{\sin \theta} = \left(\frac{2}{\sin \theta} + 1\right)c|z_x| \). By \((\epsilon, \frac{2}{\sin \theta} + 1)\)-stability, we know \( \text{dist}(z_y, \text{span}(z_{Y_1 \cap Y_2})) \leq c|z_x| \). Similarly, we can prove \( \text{dist}(z_y, \text{span}(z_{X_1 \cap X_2})) \leq c|z_y| \) for every \( y \in Y_1 \cap Y_2 \).

**C Complicated Aspects of the Structure of Matches**

**Matches are not closed under the difference operation.** Let’s consider the case where \( d = 2, X = \{x_1, x_2\}, Y = \{y_1, y_2\}, z_{x_1} = z_{y_1} = (1, 0), z_{x_2} = (0, 1), z_{y_2} = (1, 1) \). When \( \epsilon \) is sufficiently small, there are two non-empty matches in total: \( \{x_1\}, \{y_1\} \) and \( \{x_1, x_2\}, \{y_1, y_2\} \). The difference of the two matches, \( \{x_2\}, \{y_2\} \), is not a match.

An **simple match might be a proper subset of another simple match.** In the example given in the last paragraph, \( \{x_1\}, \{y_1\} \) and \( \{x_1, x_2\}, \{y_1, y_2\} \) are both simple matches, while \( \{x_1\} \subseteq \{x_1, x_2\} \) and \( \{y_1\} \subseteq \{y_1, y_2\} \).

The **decomposition of a match into a union of simple matches might not be unique.** A trivial example is a simple match \( (X_1, Y_1) \) being a proper subset of another simple match \( (X_2, Y_2) \), where \((X_2, Y_2)\) can also be decomposed as the union of \((X_1, Y_1)\) and \((X_2, Y_2)\), a different decomposition from the natural decomposition using only \((X_2, Y_2)\). A more non-trivial example is when \( X = \{x_1, x_2, x_3\}, Y = \{y_1, y_2, y_3\}, z_{x_1} = (0, 1), z_{y_1} = (1, 0), z_{x_2} = z_{y_2} = (1, 1), z_{x_3} = z_{y_3} = (1, -1) \). When \( \epsilon \) is sufficiently small, the entire match \((X, Y)\) can be decomposed as the union of simple matches in two different ways: the union of \( \{x_1, x_2\}, \{y_1, y_2\} \) and \( \{x_3\}, \{y_3\} \), or the union of \( \{x_1, x_2\}, \{y_1, y_2\} \) and \( \{x_2\}, \{y_2\} \).

**D Instances without Strong Linear Independence or Stability**

In this section, we prove Lemmas 17 and 18 to show that neither of the two assumptions in Theorem 14 can be removed. Specifically, Lemma 17 shows that we cannot remove the strong linear independence assumption, even for \( \epsilon = 0 \) where the stability assumption is trivial. Lemma 18 shows that we cannot remove the stability assumption, even when the instance satisfies \( \frac{2}{\pi} \)-strong linear independence (orthogonality).
Lemma 17. There exist instances \((z_s)_{s \in X \cup Y}\), where there are more than polynomial number of simple exact matches. Moreover, the number of linear subspaces formed by these simple exact matches is also more than polynomial.

Proof. Suppose \(k, c \geq 2\) are positive integers and \(d > \binom{ck}{k}\) is the dimension of the space \(\mathbb{R}^d\) we are considering. Suppose we have a set \(S = d - \binom{ck}{k} + ck\) subspaces of dimension \(d - 1\) in general position. In other words, the normal vectors \(n_s\) for all \(s \in S\) are linearly independent.\footnote{Note that when \(k, c \geq 2\), we have \(d - \binom{ck}{k} + ck < d\).}

Let \(X = \{x_1, x_2, \ldots, x_N\}\) and \(Y = \{y_1, y_2, \ldots, y_N\}\) for \(N = \left(\frac{d - \binom{ck}{k} + ck}{d - \binom{ck}{k} + (c-1)k}\right)\). For each \(d - \binom{ck}{k} + (c-1)k\)-sized subset \(S_i \subseteq S\), we independently pick two random unit vectors \(z_{x_i}, z_{y_i}\) in the subspace \(t_i := \bigcap_{s \in S_i} s\), i.e., \(z_{x_i}, z_{y_i}\) are independently picked uniformly from \(B_0(1) \cap t_i\).

Here, the size of \(X\) and \(Y\) are both \(\left(\frac{d - \binom{ck}{k} + ck}{d - \binom{ck}{k} + (c-1)k}\right)\), which is roughly \(d^k\) when \(d\) is very large. We are going to show that, almost surely, there are roughly \(d^k\) simple matches in this case. Note that \(c\) and \(k\) are arbitrary at the very beginning and \(d\) can grow arbitrarily large for any fixed \(c\) and \(k\), this leads to the correctness of Lemma 17.

First, for any \(S' \subseteq S\) with size \(|S'| > d - \binom{ck}{k}\), we show that the number of neurons \(x \in X\) with \(z_x \in h := \bigcap_{s \in S'} s\) is almost surely less than \(d - |S'|\), and by symmetry, this claim also holds for neurons \(y \in Y\). The claim is obvious for \(|S'| > d - \binom{ck}{k} + (c-1)k\), because in this case, almost surely, there isn’t any neuron \(x \in X\) with \(z_x \in h\), while \(d - |S'| \geq d - |S| = \binom{ck}{k} - ck > 0\). Now we consider the case where \(d - \binom{ck}{k} < |S'| \leq d - \binom{ck}{k} + (c-1)k\). Let \(\ell := |S'| - (d - \binom{ck}{k}) \in \{1, 2, \ldots, (c-1)k\}\). According to our procedure, \(S_i\) are \(\binom{ck}{k} + (c-1)k\) sized subsets of \(S\), so there are \(\binom{ck}{k-\ell}\) different \(S_i\) containing \(S'\). Therefore, almost surely, the number of neurons \(x \in X\) with \(z_x \in h\) is exactly \(\binom{ck}{k-\ell}\). The rest is to show that \(\binom{ck}{k-\ell} < d - |S'|\). In fact, \(d - |S'| - \binom{ck}{k-\ell} = -\ell + \binom{ck}{k} - \binom{ck}{k-\ell} = -\ell + \sum_{i=0}^{\ell-1} \binom{ck}{k-i} > -\ell + \sum_{i=0}^{\ell-1} 1 = 0\). The last inequality is based on the fact that \(0 < k - 1 < ck - \ell\).

The claim we showed above implies that for any \(S' \subseteq S\) with size \(|S'| > d - \binom{ck}{k}\), almost surely, \(h := \bigcap_{s \in S'} s\) is not the subspace formed by any match, because there are not enough vectors in \(h\) to span the \(d - |S'|\) dimensional space \(h\).

Next, we show that, almost surely, there is no match spanning a linear subspace of dimension \(0 < \ell < \binom{ck}{k}\). Otherwise, by permuting the indices and considering only linearly independent vectors in a match, we can assume without loss of generality that with non-zero probability, \(\{x_1, x_2, \ldots, x_\ell\}, \{y_{\sigma(1)}, y_{\sigma(2)}, \ldots, y_{\sigma(\ell)}\}\) is a match spanning an \(\ell\) dimensional space. In our procedure, \(z_{x_i}\) is a unit vector randomly picked from the space \(t_i = \bigcap_{s \in S_i} s\) where \(S_i\) is a subset of \(S\). Note that if \(t_i\) is not a subspace of \(\hat{Y} := \text{span}\{y_{\sigma(1)}, y_{\sigma(2)}, \ldots, y_{\sigma(\ell)}\}\), then almost surely, \(z_{x_i}\) doesn’t belong to \(\hat{Y}\). Therefore, ignoring the event of probability zero, we know that with non-zero probability every \(t_i\) is a subspace of \(\hat{Y}\) for \(i = 1, 2, \ldots, \ell\), i.e., \(\bigcap_{i=1}^{\ell} t_i \subseteq \hat{Y}\).

Here, the summation is over linear subspaces and the sum of linear subspaces is defined to be the linear space spanned by the subspaces. Using the fact that \(A^\perp + B^\perp = (A \cap B)^\perp\), we have \(t_i = \bigcap_{s \in S_i} s^\perp = (\bigcap_{s \in S_i} s^\perp)^\perp = (\bigcap_{i=1}^\ell \bigcap_{s \in S_i} s_i^\perp)^\perp = (\bigcap_{i=1}^\ell s_i^\perp s_i^\perp)^\perp\). The correctness of the last equality is because \(s_i^\perp = \text{span}\{n_s\}\) are linearly independent for different \(s\) (see Claim 15). Therefore, \(\sum_{i=1}^\ell t_i = \bigcap_{i=1}^\ell s_i\), so the dimension of \(\sum_{i=1}^\ell t_i = d - \bigcap_{i=1}^\ell S_i\) while the dimension
of \( \hat{Y} \) is \( \ell \), and thus \( d - \sum_{i=1}^{\ell} S_i \leq \ell < \binom{ck}{k} \). According to the claim we showed before, the number of neurons in \( X \) with \( z_x \) belonging to \( \sum_{i=1}^{\ell} t_i \) is almost surely less than \( d - \sum_{i=1}^{\ell} S_i \leq \ell \), which is a contradiction.

Then, we show that, almost surely, \((z_x)_{x \in X}\) for \( X \subseteq X' \) with size \( |X| \leq \binom{ck}{k} \) is linearly independent, and by symmetry this also holds for \( Y \subseteq Y' \). Otherwise, the smallest subset \( X \) making \((z_x)_{x \in X}\) not linearly independent with non-zero probability has size \( \ell \leq \binom{ck}{k} \). Without loss of generality, we assume \( X = \{x_1, x_2, \ldots, x_\ell\} \). \( X \) has the minimum size implies that, almost surely conditioned on \((z_x)_{x \in X}\) being not linearly independent, \( z_{x_i} \in \text{span}(\{z_x : x \in X \setminus \{x_i\}\}) = \text{span}(\{z_x : x \in X\}) \) for every \( 1 \leq i \leq \ell \). According to our procedure, \( z_{x_i} \) is randomly picked from \( t_i \), and as before, we know that every \( t_i \) is a subspace of \( \text{span}(\{z_x : x \in X \setminus \{x_i\}\}) = \text{span}(\{z_x : x \in X\}) \) for \( i = 1, 2, \ldots, \ell \) with non-zero probability. Therefore, we know with non-zero probability,

\[
\sum_{i=1}^{\ell} t_i \subseteq \text{span}(\{z_x : x \in X\}) \text{ has dimension at most } \ell - 1 < \binom{ck}{k},
\]

which leads to the same contradiction as before.

Finally, for any \( S' \subseteq S \) with size \( |S'| = d - \binom{ck}{k} \), we show that, almost surely, \( h := \bigcap_{s \in S'} s \) is the subspace spanned by a match. In this case, the dimension of \( h \) is \( \binom{ck}{k} \) and there are \( \binom{ck}{k} \) vectors in \((v_x)_{x \in X}\) (and in \((v_y)_{y \in Y}\) belonging to \( h \) according to our procedure. These vectors are almost surely linearly independent as we have shown before, so they span \( h \), forming a match.

As we showed above, almost surely, every \( S' \subseteq S \) with size \( |S'| = d - \binom{ck}{k} \) is a simple match, so there are \( \binom{d - \binom{ck}{k}}{d - \binom{ck}{k}} \) simple matches, which is roughly \( d^{ck} \) when \( d \) is very large.

The following lemma shows that we cannot remove the stability assumption, even when the instance satisfies \( \frac{c}{2} \)-strong linear independence (orthogonality).

**Lemma 18.** \( \forall \epsilon \in (0, \frac{1}{2}], \text{there exist instances } (z_x)_{x \in X \cup Y} \text{satisfying } \frac{c}{2} \text{-strong linear independence with exponential number of simple } \epsilon \text{-approximate matches.} \)

**Proof.** Let \( X = \{x_1, x_2, \ldots, x_n\} \) and \( Y = \{y_1, y_2, \ldots, y_n\} \). Suppose the dimension \( d \) is equal to \( n \). (If we want \( d > n \), we can append zeros to the coordinate of every vector.) Let \( z_{x_i} = (0, 0, \ldots, 0, 1, 0, 0, \ldots, 0) \in \mathbb{R}^n \). Before we construct \( z_{y_i} \), we first consider a sequence of matrices \( A_{2m}, A_{2m+1}, A_{2m+2}, \ldots \) defined in the following way:

1. \( A_1 = [1] \);
2. \( A_{2m} = \begin{bmatrix} A_m & A_m \\ -A_m & A_m \end{bmatrix} \).

We choose \( n \) to be a power of 2. It’s easy to show by induction that \( A_n A_n^T = A_n^T A_n = nI, A_n + A_n^T = 2I \) and every element on the diagonal of \( A_n \) is 1. Now we define \( w_i \in \mathbb{R}^n \) to be the vector whose coordinate is the \( i \)-th column of \( A_n \) for \( i = 1, 2, \ldots, n \). We have the following:

1. \( |w_i| = \sqrt{n} \);
2. \( w_i \cdot w_j = 0 \) for \( i \neq j \);
3. \( w_i z_{x_i} = 1 \);
4. \( w_i z_{x_j} = \pm 1 \);
5. \( w_i z_{x_j} + w_j z_{x_i} = 0 \) for \( i \neq j \).

Let \( \delta = \sqrt{\frac{2\epsilon^2}{n}} \). We define \( z_{y_i} = (\sqrt{1 - (n - 1)\delta^2} - \delta) z_{x_i} + \delta w_i \). Now we have the following:
1. $|z_{y_i}| = 1$;
2. $z_{y_i} \cdot z_{y_j} = 0$ for $i \neq j$;
3. $z_{x_i} \cdot z_{y_i} = \sqrt{1 - (n - 1)\delta^2}$;
4. $z_{x_i} \cdot z_{y_j} = \pm \delta$ for $i \neq j$.

Now, let’s consider an $\epsilon$-approximate match $(X,Y)$ in $(\mathcal{X},\mathcal{Y})$. Suppose $y_i \in Y$. We show by contradiction that $x_i \notin X$. Suppose $x_i \notin X$. Then $\text{dist}(z_{y_i}, \text{span}(z_X)) = \sqrt{1 - |X|\delta^2} \geq \sqrt{1 - n\delta^2} = \sqrt{1 - 2\epsilon^2} > \epsilon$, which is a contradiction. Therefore, as long as $y_i \in Y$, we know $x_i \in X$. For the same reason, as long as $x_i \in X$, we know $y_i \in Y$. Therefore, $\exists S \subseteq \{1, 2, \cdots, n\}$ s.t. $X = \{x_i : i \in S\}, Y = \{y_i : i \in S\}$.

Now we show that $(\{x_i : i \in S\}, \{y_i : i \in S\})$ is an $\epsilon$-approximate match if and only if $|S| \geq \frac{n}{2}$. Actually, we have $\forall j \in S, \text{dist}(z_{x_j}, \text{span}(\{z_{y_i} : i \in S\})) = \text{dist}(z_{y_j}, \text{span}(\{z_{x_i} : i \in S\})) = \sqrt{|n - |S||\delta^2} = \sqrt{2|n - |S||\epsilon^2}$, and we know $\sqrt{2|n - |S||\epsilon^2} \leq \epsilon$ if and only if $|S| \geq \frac{n}{2}$. Therefore, the number of simple matches is $\left(\binom{n}{\frac{n}{2}}\right)$, which is exponential in $n$. □

E Additional Experiment Results

E.1 Different Architectures

Besides ResNet18, VGG16 and ResNet34, we also train differently initialized neural networks like VGG11 and VGG13. Figure 3 shows the maximum matching similarities of all the layers of VGG13 and ResNet10. The result is similar to what is mentioned in Section 5, which implies that our conclusions might apply on most modern deep networks.

![Figure 3: Maximum matching similarities of all the layers of different architectures under various $\epsilon$.](image-url)
E.2 Details of Architecture

| Architecture | Stage 1 | Stage 2 | Stage 3 | Stage 4 | Stage 5 | Accuracy |
|--------------|--------|--------|--------|--------|--------|----------|
| VGG11        | conv×1 | conv×1 | conv×1 | conv×1 | conv×1 | 91.10%   |
| VGG13        | conv×2 | conv×2 | conv×2 | conv×2 | conv×3 | 92.78%   |
| VGG16        | conv×2 | conv×2 | conv×3 | conv×3 | conv×3 | 92.84%   |
| ResNet18     | block×2| block×2| block×2| block×2| block×3| 94.24%   |
| ResNet34     | block×3| block×4| block×6| block×3|         | 95.33%   |

Table 1: Structure of architecture (fully connected layers are omitted) and validation accuracy

E.3 Max Match during Training

As can be seen in Figure 4, after initialization, two untrained networks show similarity to some extent, while the untrained network and the trained network are much more different with each other. We believe the similarity between two untrained networks is due to the fact that the initialized networks take all its parameters from the same distributions like Xaiver initialization. Since we have many neurons that can be seen as drawn from the same distribution, we may observe phenomenon like this. Meanwhile, after training, the network turns to be quite different.

E.4 Neuron Visualization

Our experiments show that there exist a few simple matches of small size. We randomly choose a pair of networks to produce two simple matches for two fully connected layers and visualize them following the common practice. Figure 5 and 6 visualize top 9 images that maximize the activation of each neuron in simple matches.
Figure 5: Visualization of neurons in $fc_2$. Each row includes top 9 images that maximize the activation of one neuron. The neurons in the same network are illustrated on the same side.

Figure 6: Visualization of neurons in $fc_1$. Each row includes top 9 images that maximize the activation of one neuron. The neurons in the same network are illustrated on the same side.