Constructing Basis Path Set by Eliminating Path Dependency

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Abstract: The way the basis path set works in neural network remains mysterious, and the generalization of newly appeared G-SGD algorithm to more practical network is hindered. The *Basis Path Set Searching* problem is formulated from the perspective of graph theory, to find the basis path set in a regular complicated neural network. Our paper aims to discover the underlying cause of path dependency between two independent substructures. Algorithm DEAH is designed to solve the *Basis Path Set Searching* problem by eliminating such path dependency. The path subdivision chain is proposed to effectively eliminate the path dependency inside the chain and between chains. The theoretical proofs and analysis of polynomial time complexity are presented. The paper therefore provides one methodology to find the basis path set in a more general neural network, which offers theoretical and algorithmic support for the application of G-SGD algorithm in more practical scenarios.

Key Words: substructure path, basis path, path subdivision chain, path dependency, neural network

1 Introduction

Neural network with ReLU activation function has been developed for a variety of tasks, such as distribution estimation in statistics, machine translation and language modeling etc. [1,2]. How to train the weights of ReLU neural network in appropriate space affects the network performance and efficiency. In order to handle the mismatch during optimizing neural networks in positively scale-invariant space [3,4], Meng et al. [5] proposed to optimize the values of basis path set in *G*-space of ReLU neural networks by stochastic gradient descent algorithm (SGD) [6]. The experiments turned out that this novel *G*-SGD algorithm [5] with attractive low dimensionality of basis path set significantly outperformed conventional SGD algorithm. In addition, the performance superiority was approved recently in language modeling and machine translation by adopting the concept of basis path set in transformer network [2]. It is promising for *G*-SGD algorithm to be generalized to more practical neural networks and be applied widely in applications.

In recent years many efforts have been invested into explaining and understanding the overwhelming success of neural network learning methods [7-11]. Despite the experimental success, G-SGD algorithm needs further theoretical investigation on how the inner mechanism of basis paths works in neural networks. For instance, how to analyze the structure relationship between the basis path set and the network and how does the different network structure affect the algorithm searching for basis path set? On the other hand, the generalization of G-SGD algorithm is currently hindered for the implementation of G-SGD algorithm [5] depends on the structure of neural network, because currently G-SGD algorithm can only heuristically find the basis path set in the simple fully connected network, which demands the width of all layer is the same and there is no edge-skipping over layers. However, there are varieties of structures in practical network such as ResNet and DenseNet with different combination of edge-skipping over layers and ununiform layer width.

We resort to graph theory for theoretical support to understand basis path set like the way explaining neural network in group operations and functional perspectives [12,13]. In the perspective of graph theory, Zhu et al.[14] defined basis path and proposed one hierarchical algorithm to find basis path set in each independent substructure. This hierarchical algorithm [14] can handle the network with ununiform layer width and edge-skipping but requires that there exist no shared layers between any two independent substructure paths, which is strict for practical network.

This paper considers the graph-theory-based Basis Path Set Searching problem how to find

maximal independent path set in the graph of regular fully connected neural network with any ununiform layer width and any edge-skipping without restriction. We first investigate the combinatoric possibility that maximal independent substructures will bring up path dependency. Then the paper proposes dependency eliminating algorithm based on hierarchical idea (DEAH) to solve *Basis Path Set Searching* problem. The hierarchical idea is employed to decompose the complicated neural network into maximally independent substructures and find basis path set for each independent substructure in parallel. Then we need to eliminate the paths which would cause the path dependency when we combine all these basis path sets together. To avoid the enumeration of all possible substructure path pairs for the shared layers, we take advantage of path subdivision chains in the algorithm designing. Lemmas and theorems are provided to guarantee the algorithm can solve *Basis Path Set Searching* problem in polynomial time.

The contributions of this paper are the following: (i) the paper explains the structure relationship of *Basis Path Set Searching* problem from graph theory perspective and provides one polynomial algorithm; (ii) Algorithm DEAH can help overcome the hurdle of current *G*-SGD algorithm and generalize *G*-SGD algorithm further; (iii) this paper provides one methodology to find the basis path set in more general neural network, and it can offer theoretical and algorithmic support for the application of *G*-SGD algorithm in more practical scenarios.

2 Preliminary

Regular fully connected neural network is a *L*-layer multi-layer perceptron with weighted edges that can skip over different layers [14]. We denote *i*-th node in *l*-th layer as O_i^l and the node set of the *l*-th layer as O^l . $(O_i^l, O_{i'}^{l+j})$ is denoted as the directed edge from layer *l* to layer l+j, which can skip layer l+1 till layer l+j-1 as shown in Fig. 1, where $1 \le j \le L-l$, $1 \le i \le |O^l|$ and $1 \le i' \le |O^{l+j}|$. Within the same layers, the edges are fully connected. Since graph theory provides one effective platform to investigate the paths in the graph intuitively and theoretically [15-17], the paper would interpret neural network as a triple graph G = (V, E, w), where the finite node set $V = O^0 \cup ... \cup O^l ... \cup O^L$ comprising all nodes in neural network *G* and finite edge set $E = \{(O_i^l, O_{i'}^{l+j})| \ 0 \le l \le L-1 \$ and $1 \le j \le L-l\}$ consisting of all directed fully connected edges between different layers. $w(O_i^l, O_{i'}^{l+j})$ is the weight of edge $(O_i^l, O_{i'}^{l+j}) \in E$, and m = |E| is the number of edges in graph *G*. Let set $P = \{(O_{i^*}^0, O_{i'}^{1'}, ..., O_{i^*}^{j}, ..., O_{i^*}^{L})| \ 0 \le 1' \le L^{-1}\}$ consist of all paths from the input layer in network *G*[15,16], where O_i^l is denoted as some node without specified position in the *l*-th layer for simplicity.

Definition 1 (independent path set)[14] Given path set $B \subseteq P$, if there exists one path $p \in B$ and another path $q \in B \setminus \{p\}$ such that we can reach path p from path q through finite steps of path addition and path removal within B, we call path set B is dependent. Otherwise, we call path set B is independent.

Definition 2 (maximal independent path set) [14] A path set $B \subseteq P$ of neural network *G* is maximally independent, if including any other path $p^* \in P \setminus B$ would make $B \cup p^*$ dependent. Hence, a basis path set *B* of neural network *G* is a maximal independent subset of *P*.

The definitions of basic path operations such as path addition and path removal [14] can be found in Appendix A.

Definition 3 (substructure path)[14] Given fully connected neural network G and induced subgraph G' with $V(G') = (O^0, O^{1'}, ..., O^{i'}, ..., O^L)$, where $1 \le i' \le L - 1$. Let P(G') be the path set from the input layer to the output layer in G'. If all paths in P(G') from the input to the output pass through the same layers homogenously, then any path $p \in P(G')$ can be called as the substructure path of neural network G. Substructure path p can express the structure information about sub-graph G' in network G.

Definition 4 (substructure path set) Define one induced sub-graph $G^S = (V^S, E^S)$ of fully connected neural network G, which is a simplified network with only one node neach layer, where $V^S = \{$ one randomly selected $O_{i^*}^l \in O^l | l = 0, ..., L \}$ and $E^S = \{(O_{i^*}^l, O_{i^*}^k) \in E | O_{i^*}^l \in V^S, O_{i^*}^k \in V^S, 0 \le l < k \le L \}$. By breadth first search, we can get all substructure paths starting from node $O_{i^*}^0$ to node $O_{i^*}^L$ in G^S . Denote this substructure path set as P^S , which can represent all substructure information of network G.

Definition 5 (maximal independent substructure path set) Given fully connected neural network *G* and substructure path set P^S . The substructure path set $P_{ind}^S \subset P^S$ is called dependent, if there is one substructure path $p \in P_{ind}^S$ and another path $q \in P_{ind}^S \setminus \{p\}$ such that we can reach path p from path q through finite steps of path addition and path removal within P_{ind}^S . Otherwise, we call P_{ind}^S is independent. A substructure path set P_{ind}^S of P^S is maximally independent, if including any other path $p^* \in P^S \setminus P_{ind}^S$ would make $P_{ind}^S \cup p^*$ dependent.

There exists one special structure relationship between two independent substructure paths, *i.e.*, path subdivision, which is the adaptation of graph subdivision [18-20] to the path.

Definition 6 (path subdivision) Given a substructure path set P^S and one substructure path $p \in P^S$ with one edge $e = (u, v) \in E(p)$. If there exists one substructure path $p' \in P^S$ with sub-path $(u, x_1, x_2, ..., x_k, v)$, sub-path $(u, x_1, x_2, ..., x_k, v)$ is called the edge subdivision of edge e. We call e the subdivided edge and $x_1, x_2, ..., x_k$ the subdivision vertices. Furthermore, if $p - e = p' - (u, x_1, x_2, ..., x_k, v)$, we call path p' the path subdivision of path p and path p the subdivided path. Especially, we denote by p' the path obtained from p by subdividing the edges $e_1, ..., e_t, ..., e_{T'}$, where each edge $e_t \in E(p)$ is subdivided once for $t \in \{1, ..., T'\}$.



There is no edge subdivision in P^S in Fig. 1(a). In Fig. 1(b), edge (O^0, O^2) is a subdivided edge, because there exists sub-path (O^0, O^1, O^2) between O^0 and O^2 . Let $p_1 = (O^0, O^1, O^2, O^3, O^4)$, $p_2 = (O^0, O^2, O^3, O^4)$, $p_3 = (O^0, O^1, O^2, O^4)$ and $p_4 = (O^0, O^2, O^4)$. Substructure path p_1 is the path subdivision of path p_2 , p_3 and p_4 . Paths p_2 and p_3 are the path subdivision of path p_4 but p_2 and p_3 are not path subdivision of each other. Note we use the layer to represent the random node in the layer when discussing the substructure path, which is different from regular path expression.

Definition 7 (underlying substructure path) Given the substructure path set P^S , subset $P' \subset P^S$ and one substructure path $p_0 \in P'$. We call p_0 the underlying substructure path of P' if

 p_0 is the path subdivision of any substructure path $p \in P' \setminus \{p_0\}$.

3 Problem Statement

3.1 Basis Path Set Searching Problem

To solve the challenge related to basis path set in more general neural network mentioned in section Introduction, this paper focuses on *Basis Path Set Searching* Problem, which is defined as follows.

Given graph G representing the regular fully connected network, we aim to find maximal independent path set (basis path set) B in graph G.

Here the regular fully connected network can be a network with unbalanced layers (the widths of different layers are not equal) and with edges jumping over different layers.

3.2 Path Dependency between Two Independent Substructures

In graph theory, any path $p \in P$ in fully connected network G from the input layer to the output layer can be represented by the basis path set B with smaller cardinality [14]. One hierarchical algorithm has been proposed [14] to decompose the fully connected network into maximal independent substructures P_{ind}^S , where each sub-graph G_r induced from $p_r \in P_{ind}^S$ can be treated as a fully connected graph without any edge-skipping. Here G_r is the sub-graph of G by taking all edges from G with the same layers as substructure path p_r , in which Algorithm Subroutine [14] (in Appendix C) can find basis path set B_r accordingly. It is wellknown that hierarchical idea usually decomposes the complicated combinatorial optimization problem into several independent and simpler sub-optimization problems [21-24] and solves each sub-optimization problems separately. Since P_{ind}^{S} is the maximal independent substructure set and each independent substructure $p_r \in P_{ind}^S$ has unique structure, intuitively we would consider to simply combine these basis path sets B_r together to form basis path set B for network G. However, the basis paths from two independent substructures p_r and p_s in our regular graph G couldn't guarantee they are path dependent, though their structures are unique. After investigation, we found the underlying cause of path dependency is $E(p_r) \cap$ $E(p_s) \neq \emptyset$ $(r \neq s)$, *i.e.*, there exist shared edges (layers) between p_r and p_s . The shared edges offer the chance for basis paths to exchange the locations of the shared layers between substructures and to cancel same unshared layers within the substructure for the structure uniqueness. There are three typical cases to illustrate this combinatoric possibility, and we also notice that the basis paths from each substructure must appear in pair to cancel the unique unshared layers.

Case 1

In Fig. 2, substructure path p_2 is the path subdivision of substructure path p_1 in the layers of I. p_1 and p_2 share layers of S and S', and p_1 and p_2 are independent. Given basis paths $p_{1,1}, p_{1,2} \in B_1$, and $p_{2,1}, p_{2,2} \in B_2$. Any path can be represented by the remaining three paths, such as $p_{1,1} = p_{2,1} - p_{2,2} + p_{1,2}$. The same sub-path I' in $p_{1,1}$ and $p_{1,2}$ in the unshared layers can be cancelled inside substructure p_1 , and the same sub-path I in $p_{2,1}$ and $p_{2,2}$ can be cancelled inside substructure p_2 too. In the shared layers, sub-path S of $p_{1,1}$ and $p_{2,2}$.

Case 2

In Fig. 3, both substructure paths p_2 and p_3 have edge subdivision in each other but they are not path subdivision to each other. p_2 and p_3 share layers at S and S', so sub-path S' in $p_{2,1}$ and $p_{3,1}$ can be swapped and S in $p_{2,2}$ and $p_{3,2}$ can be swapped. In the unshared layers, sub-path I' + J' in $p_{2,1}$ and $p_{2,2}$ can be cancelled, and I + J in $p_{3,1}$ and $p_{3,2}$ can be cancelled too.



Case 3

In Fig. 4, substructure paths p_2 and p_1 have no edge subdivision in each other, but p_1 and p_2 have layers of S and S' in common. In the unshared layers, same sub-path I in $p_{1,1}$ and $p_{1,2}$ can be cancelled from each other, and sub-path I' in $p_{2,1}$ and $p_{2,2}$ can be cancelled too. In the shared layers, sub-path S in $p_{1,1}$ and $p_{2,1}$ and S' in $p_{1,2}$ and $p_{2,2}$ can be swapped.



Property 1 If $E(p_r) \cap E(p_s) \neq \emptyset$ $(r \neq s)$, then the path set $B_r \cup B_s$ is not path independent.

Claim 1 Given two independent substructure paths p_1 and p_2 with their shared layers $S^* = E(p_1) \cap E(p_2)$, basis paths $p_{1,1}, p_{1,2} \in B_1$ with $S \in E(p_{1,1})$ and $S' \in E(p_{1,2})$ at the shared layers S^* . If $p_{1,1} - \sum_{e \in S} e = p_{1,2} - \sum_{e \in S'} e$ at the unshared layers, then there must exist basis paths $p_{2,1}, p_{2,2} \in B_2$ such that $S \in E(p_{2,1})$ and $S' \in E(p_{2,2})$ at the layers of S^* and $p_{2,1} - \sum_{e \in S'} e = p_{2,2} - \sum_{e \in S'} e$.

Proof: We will prove this claim from two cases.

Case 1. Unshared layers of I appear at the top of shared layers of S^* . As shown in Fig. 4, let $I = p_{1,1} - \sum_{e \in S} e = p_{1,2} - \sum_{e \in S'} e$. According to the properties of the direct path [14], the first edge in I must be direct path, because it accepts two different sub-paths S and S' from its incident node, denoted as $O_{j^*}^{i^*}$. Moreover, there must exist one direct path starting from $O_{j^*}^{i^*}$ in B_2 regarding p_2 . Pick up one sub-path starting with this direct path, denoted as I'. Here we demand the rule to randomly select paths in **Algorithm Subroutine** be the same while constructing all basis path set. So sub-paths S and S' ending at $O_{j^*}^{i^*}$ must be included in some basis paths of p_2 and I' will accept both S and S' in $p_{2,1}$ and $p_{2,2}$ as shown in Fig. 4.

Case 2. If the shared layers of S^* is at the top of unshared layers of I as shown in Fig. 2, S and S' are two different sub-paths starting from $O_{j'}^{i'}$ in B_1 . According to the same rule to randomly select paths, S and S' must exist as layers of two basis paths in B_2 . We can pick

up the direct path ending at $O_{i'}^{i'}$ which can be concatenated by S and S' at $O_{i'}^{i'}$.

Other locations of shared layers S^* are the combination of Case 1 and Case 2.

Claim 2 The path dependency couldn't happen among three or more than three independent substructures, if we eliminate the paths which cause path dependency when combing the basis path sets of two independent substructures.

Proof: The analysis of path dependency indicates that basis paths from one substructure must appear in pair to cancel unshared layers for the structure uniqueness. Suppose the path dependency happens among three independent substructure paths, *i.e.*, p_1, p_2 and p_3 as shown in Fig.5. Assume $p_{1,1} - p_{1,2} + p_{2,1} - p_{2,2} = p_{3,1} - p_{3,2}$, where $p_{1,1}, p_{1,2} \in B_1$, $p_{2,1}, p_{2,2} \in B_2$, and $p_{3,1}, p_{3,2} \in B_3$. The common layers $E(S) \subset E(p_{1,1})$ and $E(S) \subset E(p_{2,1})$ must appear in pair for swapping. The same for $E(S') \subset E(p_{2,2})$ and $E(S') \subset E(p_{3,1})$, and $E(S'') \subset E(p_{1,2})$ and $E(S'') \subset E(p_{3,2})$. The unshared layers $p_{1,1} - \sum_{e \in S} e$ and $p_{1,2} - \sum_{e \in S'} e$ must appear the same to cancel the unique structure. So do $p_{2,1} - \sum_{e \in S} e$ and $p_{2,2} - \sum_{e \in S'} e$ pair and $p_{3,1} - \sum_{e \in S'} e$ and $p_{3,2} - \sum_{e \in S'} e$ pair. When we consider eliminating the paths which cause path dependency between two independent substructures, we must delete at least one basis path from corresponding two pairs. For example, if $p_{1,1}$ and $p_{3,2}$ stay, $p_{1,2}$ must be discarded when considering p_1 and p_3 . Therefore, it is impossible to either take swapping for the shared layers or cancel the unshared layers for the basis path from the third substructure such as p_2 . So, the assumption couldn't happen and Claim 2 holds.

Claim 2 indicates that we only need to consider the path dependency between any two independent substructures. However, it would be expensive if we enumerate all two substructure path pairs with the shared layers in graph G. In Case 2 of analysis of path dependency, the maximal independent substructure path set could be $\{p_0, p_1, p_2, p_3\}$ in Fig. 3(a) and it can also be $\{p_0, p_4, p_5, p_6\}$ as in Fig. 3(c), where p_5 is the path subdivision of p_4 , p_6 is the path subdivision of p_5 and the underlying substructure path p_0 is the path subdivision. Motivated by this, path subdivision chain is proposed to avoid complicated enumeration.

Definition 8 (path subdivision set) Given the substructure path set P^S of fully connected network G and subset $P' \subset P^S$, the path subdivision set U_r of substructure path $p_r \in P'$ is defined as $\{p \in P' | p \text{ is the subdivision of } p_r\}$.

Definition 9 (path subdivision chain) Given set $\{U_r | r = 1, ..., |P'|\}$ of path subdivision sets on $P' \subset P^S$. Based on set containment relationship, we can get T path subdivision chains, *i.e.*, the *t*-th chain $U_{t_1} \supset U_{t_2} ... \supset U_{t_j} ... \supset U_{t_{s_t}}$, where $\sum_{t=1}^T s_t \ge |P'|$ and $U_{t_j} \in \{U_r | r = 1, ..., R\}$ is the *j*-th set of the *t*-th chain.

Fig.3(c) can form one path subdivision chain $U_4 \supset U_5 \supset U_6 \supset U_0$ but Fig.3(a) needs 3 chains such as $U_1 \supset U_0$, $U_2 \supset U_0$ and $U_3 \supset U_0$, though p_1, p_2 and p_3 have subdivision layers in each other. Obviously, path subdivision set $U_0 = \emptyset$. Some properties and lemmas about the path subdivision chain can be found in Appendix B.

4 Dependency Eliminating Algorithm Based on Hierarchical Idea (DEAH)

Algorithm HBPS [14] initiated one inspiring hierarchical idea to decompose the complicated graph G into several independent substructures but the restriction is there doesn't exist shared layers between any two maximal independent substructures, which may cause the path

dependency. However, one practical fully connected network allows edge-skipping over different layers and shared layers between different substructures. To solve *Basis Path Set Searching* problem in regular graph G, we propose Algorithm DEAH to overcome the restriction of Algorithm HBPS to find basis path set in more practical network by eliminating path dependency.

Step 1 of Algorithm DEAH employs hierarchical idea to decompose the complicated network G into $|P_{ind}^{S}|$ maximal independent substructures. Compute path subdivision set U_r for $p_r \in P^S$ and sort $\{U_r\}$ with $|U_r|$ in descending order as $\{U_{r_i}|i = 0, 1 \dots, |P^S| - 1\}$ with $U_{r_0} = U_0$. Starting from i = 0, get the first $|P_{ind}^{S}|$ substructure paths from $\{p_{r_i}|i = 0, 1 \dots, |P^S| - 1\}$ such that they are independent. The purpose of this step is to avoid Case 2 in path dependency analysis and stretch the path subdivision chains as long as possible in Step 3. We must pay attention to $|U_{r_{i-1}}| = |U_{r_i}|$ when $Rank(\{U_{r_0}, U_{r_{1'}}, \dots, U_{r_{k'}}, \dots, U_{r_{i-1}}, U_{r_i}\}) > Rank$ $(\{U_{r_0}, U_{r_1'}, \dots, U_{r_{k'}}, \dots, U_{r_{i-1}}, U_{r_i}\})$. In this case, if there exists some $U_{r_j}(j < i - 1)$ such that $U_{r_{i-1}} \subset U_{r_j}$ and $U_{r_i} \subset U_{r_j}$ and substructure paths $p_{r_{i-1}}$ and p_{r_i} have edge subdivision in each other, we skip U_{r_i} and go to $U_{r_{i+1}}$. This step rules out the possibility of Case 2 of path dependency (shown in Fig. 3(a)). This is because the chain with $U_{r_{i-1}}$ would split into two chains but we can manipulate to form one chain instead by simply skipping U_{r_i} .

Step 2 finds basis path set B_r by calling Algorithm Subroutine for each G_r induced by $p_r \in$ P_{ind}^{S} in parallel, which can be treated as a simple network without edge-skipping. Step 3 is to eliminate the path dependency between different substructure path pairs, by constructing multiple path subdivision chains to avoid enumeration as discussed in Section 3. We scan the selected path subdivision sets in $\{U_r | r = 0, 1, ..., |P_{ind}^S| - 1\}$ with $|U_r|$ in descending order to stretch the *t*-th chain $U_{t_1} \supset U_{t_2} ... \supset U_{t_j} ... \supset U_{t_{s_t}} \supset U_0$ as long as possible, and start one new chain starting from U_r if U_r couldn't be contained in some ready chain. Once the multiple chains are established, the next step is to eliminate the path dependency. Algorithm DEAH divides the selected path subdivision sets into two groups. The first group includes the sets which are not the first set in any chain. The second group consists of the first set in all chain. For each set $U_{t_{i+1}}$ in the first group in t-th chain, call Algorithm SDVChain (in Appendix C) to discard the paths from path set $B'_{t_{j+1}}$ based on original basis path set B_{t_j} . Here we emphasize $B'_{t_{i+1}}$ instead of original $B_{t_{i+1}}$ because $U_{t_{i+1}}$ may appear in different chains and paths in $B'_{t_{j+1}}$ can be discarded from multiple chains. For U_0 , what we should do is to keep discarding paths from B'_0 based on $U_{t_{s_t}}$ for all t-th chain. The rule for Algorithm **SDVChain** to keep one path in $B'_{t_{j+1}}$ is that the shared layers with B_{t_j} have the most concurrency and the unshared layers appear at least twice in $B'_{t_{i+1}}$ according to **Claim 1**. For U_{t_1} in some t-th chain from the second group, enumerate all t'-th chain to find the last set $U_{t'_{i^*}}(t' \neq t)$ such that $p_{t'_{i^*}}$ shares layers with p_{t_1} and discard the paths from B'_{t_1} based on original $B_{t'_{**}}$. The aim of stretching path subdivision chain as long as possible is to reduce the enumeration as much as possible and the trick of path subdivision chain is that we only have to consider the path dependency between the consecutive sets in the chain.

To find the maximal independent substructure path set P_{ind}^S from P^S in Step 1, we borrow the concept of adjacent matrix in graph theory [15-17] and define adjacent matrix M_r for path $p_r \in P^S$ as

 $M_r(j,l) = \begin{cases} 1, & \text{if there is edge from } j - \text{th layer to the } l - \text{th layer } j = 0,1,\dots,L \\ 0, & \text{otherwise} \\ l = 0,1,\dots,L \end{cases}$

Reshape M_r to substructure path vector $\alpha_r = [M_r(0,:), ..., M_r(j,:), ..., M_r(L,:)]$, so each p_r can be expressed as a 0-1 substructure path vector α_r with $(L + 1)^2$ elements. It is easy to

calculate the maximal independent path set P_{ind}^S from P^S by implementing linear algebra method, but it is infeasible to get basis path set B in P in this way, because G^{S} is the simplest network with only one node in each layer and the size of regular network G is too huge. To find the path subdivision and edge subdivision between two independent substructure paths, straightforward L + 1-dimensional incident vector β_r for substructure path p_r is defined as

 $\beta_r(l) = \begin{cases} 1, & \text{if } p_r \text{ passes through the } l - th \text{ layer} \\ 0, & \text{otherwise} \end{cases}, \text{ where } l = 0, 1, \dots, L.$ For p_r and p_t , let $X = \beta_r - \beta_t$. If X contains 1 and -1, then p_r and p_t are not path

subdivision to each other. If X contains only 0 and -1, p_t is path subdivision of p_r .

Algorithm DEAH

Input: Fully connected neural network G = (V, E) with L + 1 layers **Output:** Path set *B* of neural network *G*

% Step 1. (The upper level) %

Select randomly node $O_{i^*}^l$ at the *l*-th (l = 0, ..., L) layer of graph G. Set node subset $V^S =$ $\{O_{i^*}^0, \dots, O_{i^*}^l, \dots, O_{i^*}^L\}$ and edge subset $E^S = \{(O_{i^*}^j, O_{i^*}^l) \in E | O_{i^*}^j \in V^S, O_{i^*}^l \in V^S\}$. Let P^S be the path set from $O_{i^*}^0$ to $O_{i^*}^L$ by breadth-first searching in $G^S = (V^S, E^S)$. For each path $p_r \in P^S$ do

Construct substructure path vector α_r and incident vector β_r .

End For

Calculate $R = Rank(\{\alpha_r\})$ by numerical linear algebra method.

For $r = 1: |P^S|$ do

Let $U_r = \emptyset$. For each $t \in \{1, ..., |P^S|\}$, let $X = \beta_r - \beta_t$. If X contains only 0 and -1, set $U_r = U_r \cup \{t\}.$

End For

Pick up $p_{r_0} \in P^S$ with $U_{r_0} = \emptyset$. Sort $|U_{r_1}| \ge |U_{r_2}| \dots \ge |U_{r_{R-1}}| \dots \ge |U_{r_{|P^S|-1}}| \ge |U_{r_0}|$.

Set i = 1 and $A = \{\alpha_{r_0}\}$.

While |A| < R do % Rule out the possibility of Case 2 in the cause analysis of path dependency.

If $Rank(A \cup \{\alpha_{r_i}\}) = Rank(A) + 1$ and $|U_{r_{i-1}}| \neq |U_{r_i}|$, let $A = A \cup \{\alpha_{r_i}\}$. If $Rank(A \cup \{\alpha_{r_i}\}) = Rank(A) + 1$ $\{\alpha_{r_i}\} = Rank(A) + 1$ but $|U_{r_{i-1}}| = |U_{r_i}|$, let $X = \beta_{r_{i-1}} - \beta_{r_i}$. If there is no 0 between any 1 and -1 in X or no U_{r_i} (j < i - 1) such that $r_i, r_{i-1} \in U_{r_i}$, let $A = A \cup \{\alpha_{r_i}\}$.

Let i = i + 1.

End While

Output A as $\{U_r | r = 0, 1, ..., R - 1\}$ with $U_0 = \emptyset$ and $|U_r|$ in descending order, $\{\beta_r\}$ and $P_{ind}^S = \{p_r\}.$

%Step 2. (The lower level) % Get basis path set B_r for p_r .

For each $p_r \in P_{ind}^S$ do % Induce sub-graph G_r with the same structure as p_r .

Let $L_r = \{l | O_{i^*}^l \in p_r\}, V_r = \{O^l \subset V | l \in L_r\}$ and $E_r = \{(O_i^{l_j}, O_{i'}^{l_{j+1}}) \in E | O_i^{l_j} \in O^{l_j}, U_r \in V\}$

 $O_{i'}^{l_{j+1}} \in O^{l_{j+1}}$ }. Set $G_r = (V_r, E_r)$. Call **Subroutine** (G_r) and output basis path set B_r . **End For**

%Step 3. % Eliminate path dependency from the union of basis paths. Set $X = \emptyset$ and let t = 0.

For r = 1: R do % If U_r doesn't belong to any chain, start a new chain.

If $r \notin X$, let t = t + 1 and $U_{t_1} = U_r$. Find path subdivision chain $U_{t_1} \supset U_{t_2} \dots \supset$ $U_{t_i} \dots \supset U_{t_{s_*}} \supset U_0$ by searching $\{U_r | r = r + 1, \dots, R - 1\}$ in order, till we couldn't stretch the chain further. Let $Y_t = \{t_1, ..., t_j, ..., t_{s_t}\}$ and $X = X \cup Y_t$. **End For** Let T = t.

For t = 1:T do

Let $B'_0 = B_0$ and $B'_{t_i} = B_{t_i}$ for all *j*. % Initialization for Algorithm SDVChain.

Let $Sh_t = \{r | E(p_{r_1}) \cap E(p_{t_1}) \neq \emptyset, r < t\}$ and $Q_t = \{t_j^* |$ the last t_j^* satisfying $E(p_{t_1}) \cap E(p_{t_j^*}) \neq \emptyset, j \neq 1, t' \neq t\}$. Let $Q_t = Q_t \setminus Y_t$. % One element may appear in multiple chains **End For**

For t = 1:T do

Call **SDVChain**($\{B'_{t_j}\}_{j=1}^{s_t}, \{B_{t_j}\}_{j=1}^{s_t}, \{p_{t_j}\}_{j=1}^{s_t}, \{\beta_{t_j}\}_{j=1}^{s_t}, B'_0, p_0, \beta_0, G\}$, and output updated shrunk path set $\{B'_{t_j}\}_{j=2}^{s_t}$ and discarded path set D'_0 . Let $B'_0 = B'_0 \setminus D'_0$.

For each $k \in \{1, ..., |Q_t|\}$, call **SDVChain** $(B'_{Q_t(k)}, B_{Q_t(k)}, p_{Q_t(k)}, \beta_{Q_t(k)}, B'_{t_1}, p_{t_1}, \beta_{t_1}, G)$, output discarded path set D_{t_1} and let $B'_{t_1} = B'_{t_1} \setminus D_{t_1}$.% $Q_t(k)$ is the k-th element of Q_t . **End For**

Output path set $B = \bigcup_{t=1}^{T} (\bigcup_{j=1}^{s_t} B'_{t_j}) \cup B'_0$.

Theorem 1 Given fully connected neural network G and T path subdivision chains from Algorithm DEAH in G, *i.e.*, $U_{t_1} \supset U_{t_2} ... \supset U_{t_j} ... \supset U_{t_{s_t}} \supset U_0$ with t = 1, ..., T. B_{t_j} is the original basis path set of substructure path p_{t_j} and B'_{t_j} is the shrunk path set of B_{t_j} after path discarding from Algorithm DEAH. Then the set $B = \bigcup_{t=1}^{T} (\bigcup_{j=1}^{S_t} B'_{t_j}) \cup B'_0$ is path independent and any path $p \in B_{t_j} \setminus B$ or $p \in B_0 \setminus B$ can be represented by B.

Proof: We now study the path independency between p_k and p_l from three cases.

Case 1 $k = t_j$ $(j \neq 1)$, $l = t'_i$ $(i \neq 1)$ and $t \neq t'$. In this case U_k and U_l are not the first sets in the t-th and t'-th chain respectively. Let B'_{t_i} be the shrunk path set of B_{t_i} based on $B_{t_{j-1}}$ and $B'_{t'_i}$ be the shrunk path set of $B_{t'_i}$ based on $B_{t'_{i-1}}$ from the algorithm. We will prove that $B'_{t_j} \cup B'_{t'_j}$ from two different chains is path independent. Because of no path dependency within the same chain according to Lemma 1 (in Appendix B), assume that one path $p_{t_{j,1}}$ such that $p_{t_{j,1}} = p_{t'_{i,1}} - p_{t'_{i,2}} + p_{t_{j,2}}$, where $p_{t_{j,1}}, p_{t_{j,2}} \in B'_{t_j}$ and $p_{t'_{i,1}}, p_{t'_{i,2}} \in B'_{t'_j}$. Apparently, neither U_{t_i} nor U_{t_i} could take U_0 , otherwise U_{t_i} and U_{t_i} are in the same chain. Let the layers I' of substructure path $p_{t'_i}$ be the edge subdivision of the layers I of p_{t_i} , as shown in Fig. 3(b). And the layers of J in p_{t_i} is the edge subdivision of J' in $p_{t'_i}$. As for the structure uniqueness, paths $p_{t'_i,1}$ and $p_{t'_i,2}$ must have the same layers I' and J' to cancel each other, and paths $p_{t_i,1}$ and $p_{t_i,2}$ have the same layers I and J. For the shared layers, $p_{t'_{i},1}$ and $p_{t_{j},1}$ must have S' and $p_{t'_{i},2}$ and $p_{t_{j},2}$ have S to swap between different substructures. No overlap between I and J. Exchange edge set J' and edge set J in $p_{t'_{i,1}}$ and $p_{t_i,1}$ and exchange part J' and part J in $p_{t'_i}$ and p_{t_i} . Interestingly, we get two new substructure paths p1 and p2 (in Fig. 6). However, we notice that $p1, p_{t_i}$ and $p_{t'_i}$ (in Fig.3) are the path subdivisions of p2. It contradicts the way we select the maximal independent substructure path set.

Case 2 $k = t_1$ and $l = t'_i$ $(i \neq 1)$. In this case, U_k is the first set in the *t*-th and U_l is inside the *t'*-th chain, where $t \neq t'$. $B'_{t'_i}$ is the shrunk path set of $B_{t'_i}$ based on $B_{t'_{i-1}}$ and B'_{t_1} is shrunk from B_{t_1} . We prove that $B'_{t_1} \cup B'_{t'_i}$ is path independent. Lemma 2 (in Appendix

B) indicates that no path dependency would be produced for any $U_{t'_i}$ if we calculate B'_{t_1} based on $p_{t'_i}$, which is the last substructure path in the chain $U_{t'_1} \supset U_{t'_2} \supset \cdots \cup U_{t'_i} \supset \cdots \cup U_{t'_i} \supset \cdots \cup U_{t'_{i'+1}} \supset U_{t'_{i'+1}} \supset U_{t'_{i'+1}} \supset U_{t'_{i'+1}}$ to have shared layers with p_{t_1} . If $i \le i^*$, $B'_{t_1} \cup B'_{t'_i}$ is path independent from Lemma 2. If $i > i^*$, $B'_{t_1} \cup B'_{t'_i}$ is path independent, because p_{t_1} and $p_{t'_i}$ don't share common edges.



Case 3 $k = t_1$ and $l = t'_1$. In this case, both U_k and U_l are the first sets in their chains, where $t \neq t'$. In order to calculate B'_{t_1} , Algorithm **SDVChain** needs to find $p_{t'_{i^*}}$ in each t'-th chain and discard the corresponding paths from B'_{t_1} based on $B_{t'_{i^*}}$. This procedure guarantees the path independency for $B'_{t_1} \cup B'_{t'_1}$, according to Lemma 2.

According to Algorithm **SDVChain**, D'_0 is the path set which will be discarded from B'_0 , based on original $B_{r_{s_t}}$ in the *t*-th chain. B'_0 is initialized as original B_0 and is updated as $B'_0 = B'_0 \setminus D'_0$ iteratively for $t = 1 \dots T$. And any $p \in B_0 \setminus B'_0$ can be represented by $B'_0 \cup B_{r_{s_t}}$ for some *t*. Since $U_{t_1} \supset U_{t_2} \dots \supset U_{t_j} \dots \supset U_{t_{s_t}} \supset U_0$ is path subdivision chain, so $B'_0 \cup B_{r_j}$ is path independent for $j = 1, \dots, s_t$ in the *t*-th chain. Therefore, $B = \bigcup_{t=1}^T (\bigcup_{j=1}^{s_t} B'_{t_j}) \cup B'_0$ is path independent based upon Claim 1 and Claim 2.

Note set $U_{t_j}(j \neq 1)$ can appear in multiple chains but the first set U_{t_1} can only appear in exactly t-th chain. Lemma 1 proves that any path $p \in B_{t_j} \setminus B'_{t_j}$ can be represented by $B_{t_{j-1}} \cup B'_{t_j}$ recursively till B_{t_1} . If U_{t_j} belongs to the t'-th chain and the t-th chain, *i.e.*, $U_{t_1'} \supset \cdots \cup U_{t_i'} \supset U_{t_j}$, $p \in B_{t_j} \setminus B'_{t_j}$ can be represented either by $B_{t_{j-1}} \cup B'_{t_j}$ or by $B_{t_i'} \cup B'_{t_j}$. Hence, any path $p \in B_{t_j} \setminus B'_{t_j}$ ($j \neq 1$) can be represented by B. Moreover, any path $p \in B_{t_1} \setminus B'_{t_1}$ can be represented by B, because Lemma 2 concludes p can be represented by some $B_{t_{i'}'} \cup B'_{t_1}$ and any path in $B_{t_{i''}}$ can be represented by B. Furthermore, any $p \in B_0 \setminus B'_0$ can be represented by $B'_0 \cup B_{r_{s_t}}$ for some t.

Theorem 2 Given fully connected neural network G and independent path set $B = \bigcup_{t=1}^{T} (\bigcup_{j=1}^{S_t} B'_{t_j}) \cup B'_0$ output from Algorithm DEAH, where T is the number of path subdivision chains and B'_{t_j} is the shrunk path set of B_{t_j} in G_{t_j} . Then any path $p \in P$ from the input layer to the output layer in G can be represented by B.

Proof: Any path $p \in P$ can be represented in the hierarchical way, first at substructure level and then at basis path level. If the structure of p is $p_r \in P_{ind}^S$ but $p \notin B_r$, it is trivia that path p can be represented by B_r . If the structure of p is out of the structure range of P_{ind}^S , the structure of p can be expressed as $p_{r_1} \dots + p_{r_j} \dots + p_{r_d} - p_{s_1} \dots - p_{s_h} \dots - p_{s_m}$, where $r_1, \dots, r_d, s_1, \dots, s_m$ are distinct, $p_{r_j} \in P_{ind}^S$ and $p_{s_h} \in P_{ind}^S$ $(1 \le j \le d, 1 \le h \le m)$. Suppose the randomly node set is $V^S = \{O_i^{0}, \dots, O_i^{l}, \dots, O_i^{L}\}$ and target path p passes

 $\{O_{i'}^0, \dots, O_{i'}^l, \dots, O_{i'}^L\}$ sequentially. Define new node set $V' = \{O_{i''}^0, \dots, O_{i''}^l, \dots, O_{i''}^L\}$, where $l = 0, 1, \dots, L$. If p skips over the l-th layer, set $O_{i''}^l = O_{i^*}^l$. If p passes through the l-th layer and $O_{i'}^l \neq O_{i^*}^l$, set $O_{i''}^l = O_{i'}^l$. For each p_{r_j} and p_{s_h} , construct new path p'_{r_j} and p'_{s_h} passing through node set V' but p'_{r_j} and p'_{s_h} keep the same structure as p_{r_j} and p_{s_h} under V^S . V' covers all nodes of path p, and node $O_{i^*}^l \in V^S$ corresponds to $O_{i''}^l \in V'$. In original graph G, path p therefore can be accordingly expressed as $p = p'_{r_1} \dots + p'_{r_j} \dots + p'_{r_d} - p'_{s_1} \dots - p'_{s_h} \dots - p'_{s_m}$. Moreover, new path p'_{r_j} can be represented by basis path set B_{r_j} and p'_{s_h} can be represented by $B = \bigcup_{t=1}^T (\bigcup_{j=1}^{s_t} B'_{t_j}) \cup B'_0$ according to Theorem 1. Therefore, B is a basis path set for neural network G.

Theorem 1 and Theorem 2 prove that Algorithm DEAH can find the basis path set B for Basis Path Set Searching problem in regular graph G. Next, we will prove that Algorithm DEAH can be completed in polynomial time.

Theorem 3 The time complexity of **Algorithm DEAH** to solve *Basis Path Set Searching* problem in regular graph *G* is $O(RL^2W_{max}^2) + O\left(\max(R, T^2) \cdot (L + B_{max}^3)\right)$, where $R = |P_{ind}^S|$, $W_{max} = \max_{0 \le l \le L} \{|O^l|\}$ and $B_{max} = \max_{r \in \{1,2,\dots,R\}} |B_r|$. **Proof:** There are three major steps in Algorithm DEAH.

Step 1 of Algorithm DEAH finds V^S in $\mathcal{O}(L)$ time, and searches E^S in $\mathcal{O}(m)$ time and P^S in at most $\mathcal{O}(m)$ time. In order to get P_{ind}^S , we compute all U_r in at most $\mathcal{O}(m^2)$ time and compute Rank(A) by searching $\{U_{r_1}, U_{r_2}, ..., U_{r_{|P^S|-1}}\}$ in at most $\mathcal{O}(m)$ time, since $|P^S| \leq m$. So, Step 1 runs in $\mathcal{O}(3m + m^2 + L) = \mathcal{O}(m^2)$ time.

Step 2 calls **Subroutine** (G_r) to find basis path set B_r of substructure $p_r(r = 1, 2, ..., R)$. **Lemma 3** (in Appendix C) proves that **Algorithm Subroutine**(G) runs in time $O(L^2 W_{max}^2)$ in fully connected graph G without edge-skipping. Let $W_{max} = \max_{0 \le l \le L} \{|O^l|\}$ in network G. Therefore, the time complexity of Step 2 is $O(RL^2 W_{max}^2)$.

In Step 3, there are two parts for the computation of shrunk path sets. One part is to compute $B'_{t_{i+1}}$ $(j \neq 0)$. In every t-th chain we call **SDVChain** to compute $B'_{t_{i+1}}$ based on B_{t_i} iteratively. It takes $\mathcal{O}(L)$ time to find common layers between p_{t_j} and $p_{t_{j+1}}$, $\mathcal{O}(|B_{t_j}|)$ time to separate the shared layers and unshared layers in B_{t_i} and $\mathcal{O}\left(|B_{t_{i+1}}|\right)$ time to separate the layers of $B_{t_{j+1}}$. To get unique unshared layers $\{Ep_{t_j,i}\}$ needs $\mathcal{O}\left(|B_{t_j}|^2\right)$ time. For each $Ep_{t_j,i}$, it needs at most $\mathcal{O}\left(|B_{t_j}|\right)$ time to compute UCP_i and UCP_i^* in B_r and $O\left(\left|B_{t_j}\right|\left|B_{t_{j+1}}\right|\right)$ time to get unshared layers set IEp_i in B'_{r+1} . Since there are at most $\mathcal{O}\left(|B_{t_j}|\right)$ elements in $\left\{Ep_{t_j,i}\right\}$, so this phase needs at most $\mathcal{O}\left(|B_{t_j}| \cdot \left(|B_{t_j}| + C_{t_j}|\right)\right)$ $|B_{t_j}||B_{t_{j+1}}|) = \mathcal{O}(B_{max}^3)$ time, where $B_{max} = \max_{r \in \{1,2,\dots,R\}} |B_r|$. Furthermore, there are T chains, every t-th chain needs to call SDVChain for s_t times, some $U_{t_{j+1}}$ may appear in most T chains and the path set after $U_{t_{j+1}}$ in the chain only needs computing once. Hence, we at most $\mathcal{O}(R+T) \cdot \mathcal{O}\left(L + \left|B_{t_i}\right| + \left|B_{t_{i+1}}\right| + \left|B_{t_i}\right|^2 + B_{max}^3\right) = \mathcal{O}\left((R+T)\left(L + C_{t_i}\right)^2\right)$ need $B_{max}^{3}) = O(R(L + B_{max}^{3}))$ time. In the other part of Step 3, every U_{t_1} needs to enumerate all elements in Q_t to call **SDVChain** to update B'_{t_1} based on $B_{Q_t(k)}$ iteratively. This simple version of **SDVChain** would take at most $O(L + B_{max}^{3})$ time for each iteration

and there are at most *T* elements in $B_{Q_t(k)}$, *i.e.*, totally $\mathcal{O}(T(L + B_{max}^3))$ time. Because there are *T* chains, so this phase takes $\mathcal{O}(T^2(L + B_{max}^3))$ time. Therefore, Step 3 takes totally $\mathcal{O}(R(L + B_{max}^3)) + \mathcal{O}(T^2(L + B_{max}^3)) = \mathcal{O}(\max(R, T^2)(L + B_{max}^3))$ time.

In sum, the total time complexity of Algorithm DEAH is $\mathcal{O}(m^2) + \mathcal{O}(RL^2W_{max}^2) + \mathcal{O}\left(\max(R,T^2)(L+B_{max}^3)\right) = \mathcal{O}(RL^2W_{max}^2) + \mathcal{O}\left(\max(R,T^2)(L+B_{max}^3)\right).$

It is obvious that the computation complexity of **Algorithm DEAH** to solve *Basis Path Set Searching* problem depends heavily on the structure of the network, *i.e.*, the maximal layer width and edge-skipping over layers. Usually B_0 is the basis path set taking B_{max} . Each $p_r \in P_{ind}^S$ represents one type of substructure information about edge-skipping over layers in network *G*, and different types of substructures can be combined in a variety of ways. Thus, there is no constraint about the graph structure levying on our Algorithm DEAH, which breaks the bottleneck of the algorithm in [14] and generalizes it to more practical networks. Though Algorithm DEAH considers only one underlying structure path, but it can be easily extended to the network with multiple underlying structure paths.

5 Conclusion

In regular fully connected network G, the shared layers between two independent substructure paths bring up the combinatoric possibility of path dependency when combining the basis path sets from these substructures. Algorithm DEAH is designed to eliminate such path dependency and the trick of effective elimination is the path subdivision chain. The theoretical proofs guarantee the feasibility of Algorithm DEAH for *Basis Path Set Searching* problem. The paper generalizes the specific network structure with equal layer and without edge-skipping to more practical network and provides one methodology to solve *Basis Path Set Searching* problem in more general neural network. This work can help facilitate the theoretic research and applications of G-SGD algorithm in more practical scenarios.

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Appendix A

Some definitions may be referred.

Definition 10 (path addition to a graph)[14] Given a graph H and a path p, we denote the path addition by H + p with $V(H + p) = V(H) \cup V(p)$ and E(H + p) being the disjoint union of E(G) and E(p) (Parallel edges may arise).

Definition 11 (path removal from a graph)[14] Given a graph *H* and one path $p \subseteq E(H)$, the removal of the path *p* from the graph *H* is defined as H - p with $E(H - p) = E(H) \setminus E(p)$ and $V(H - p) = V(H) \setminus \{v \in V(H) | v \text{ is an isolated vertex after } E(H) \setminus E(p)\}$.

Definition 12 (structure path)[14] Given fully connected neural network *G*, if all paths in *P* from the input layer to the output layer passes through the same layers consecutively, any path $p \in P$ can be called as the structure path of neural network *G*, since it can express the structure

information of G.

Appendix B

Some properties and theoretical proofs related to path subdivision chains are given in this section. Suppose *T* path subdivision chains $\{U_{t_1} \supset U_{t_2} ... \supset U_{t_j} ... \supset U_{t_{s_t}} \supset U_0 | t = 1, ..., T\}$ are output from Algorithm DEAH.

Lemma 1 Given path subdivision chain $U_{t_1} \supset U_{t_2} \dots \supset U_{t_j} \dots \supset U_{t_{s_t}} \supset U_0$ in fully connected neural network G, where path subdivision set U_{t_j} and basis path set B_{t_j} correspond to maximal independent substructure path p_{t_j} . Especially U_0 and B_0 correspond to the underlying substructure path p_0 . Then, $B_{t_1} \cup B'_{t_2} \cup \dots B'_{t_{s_t}}$ is path independent, where B'_{t_j} output from Algorithm SDVChain is the shrunk path set of B_{t_j} based on original basis path set $B_{t_{j-1}}$ for $j = 2, 3, \dots, s_t$.

Proof: We use induction on the *j*-th subdivided substructure path to prove that $B_{t_1} \cup B'_{t_2} \cup \cdots B'_{t_j} \dots \cup B'_{t_{s_t}}$ is path independent. The inputs of Algorithm **SDVChain** are $\{B'_{t_j}\}_{j=1}^{s_t}, \{B_{t_j}\}_{j=1}^{s_t}$, $\{p_{t_j}\}_{j=1}^{s_t}, \{\beta_{t_j}\}_{j=1}^{s_t}, B'_0, p_0$ and β_0 , where $B'_{t_j} = B_{t_j}$ and $B'_0 = B_0$ for algorithm initiation.

Basis step: j = 1 and $U_{t_1} \supset U_{t_2}$. Step 1 of Algorithm **SDVChain** picks up UCP_j^* with the most frequent occurrence in UCP_j for each unique $Ep_{t_1,j}$ of B_{t_1} . The trick is that the edge between every two common layers with the most frequency must be the direct path according to the construction rule [14] of basis path. Step 2 of the algorithm searches the unshared layers set IEp_j in B_{t_2} which has the shared layers from UCP_j and discard the element with frequency less than 2 from IEp_j . According to Claim 1, the paths with multiple repetition at unshared layers in IEp_j can cause path dependency. Next, the algorithm outputs B'_{t_2} by discarding the paths from B_{t_2} whose unshared layers are from IEp_j element and shared layers are not UCP_j^* . Hence, any path $p \in B_{t_1} \cup B'_{t_2}$ couldn't be represented by $B_{t_1} \cup B'_{t_2} \setminus \{p\}$ and any path $p_{t_2u'} \in B_{t_2} \setminus B'_{t_2}$ can be represented by $B_{t_1} \cup B'_{t_2}$. So, $B_{t_1} \cup B'_{t_2}$ is path independent for the basic step.

Induction step: $j \ge 2$. Suppose that $B_{t_1} \cup B'_{t_2} \cup \dots B'_{t_j}$ is an independent path set and any path $p \in B_{t_{j-1}} \setminus B'_{t_j}$ can be represented by $B_{t_{j-1}} \cup B'_{t_j} \setminus \{p\}$. Let $B'_{t_{j+1}}$ be the shrunk path set of $B_{t_{j+1}}$ based on original B_{t_j} from Algorithm. We will prove that any path $p \in B_{t_1} \cup B'_{t_2} \cup \dots B'_{t_j} \cup B'_{t_{j+1}} \setminus \{p\}$. Assume path $p' \in B_{t_1} \cup B'_{t_2} \cup \dots B'_{t_j} \cup B'_{t_{j+1}} \setminus \{p\}$. Assume path $p' \in B_{t_1} \cup B'_{t_2} \cup \dots B'_{t_j} \cup B'_{t_{j+1}} \setminus \{p'\}$. According to Claim 2, consider the simplest form that $p' = p_{t_{j+1},1-p_{t_{j+1},2}} + p''$, where $p_{t_{j+1},1} \in B'_{t_{j+1}}$ and $p'' \in B'_{t_m}$ and $p'' \in B'_{t_m}$ with $m \le j - 1$. Similar to basic step, any path $p \in B_{t_j} \setminus B'_{t_{j+1}}$ can be represented by $B_{t_j} \cup B'_{t_{j+1}} \setminus \{p\}$, so it is obvious that $p', p'' \notin B'_{t_{j+1}}$ and $p', p'' \notin B'_{t_j}$.



Fig. 7 Edge operation in subdivided unshared layers

Among the specific chain $U_{t_m} \supset U_{t_j} \supset U_{t_{j+1}}$, substructure path $p_{t_{j+1}}$ is the path subdivision of p_{t_j} , and p_{t_j} is the path subdivision of p_{t_m} . So $p_{t_{j+1}}$ is the most subdivided path. As shown in Fig. 7, $p_{t_{j+1},1}$ and $p_{t_{j+1},2}$ must have same sub-path I and paths p' and p'' must have J to cancel the unique sub-paths, since $p_{t_{j+1}}$ is the path subdivision of p_{t_m} at the layers of J. For the shared layers of p_{t_m} and $p_{t_{j+1}}$, p' and $p_{t_{j+1}1}$ share sub-path S and p''and $p_{t_{j+1}2}$ share S'. p_{t_j} should be the path subdivision of p_{t_m} in some part of J, *i.e.*, the dashed lowest part J^* of J. Hence, the dashed part I^* in J^* of p_{t_j} subdivided by $p_{t_{j+1},1}$ and $p_{t_{j+1,2}}$ are the same. However, the shared layers such as $I - I^* + S$ in $p_{t_{j+1}1}$ and $I - I^* + S'$ in $p_{t_{j+1}2}$ are different as shown in Fig. 7. This contradicts the Algorithm **SDVChain** which keeps only the most frequent shared layers from B_{t_j} to $B'_{t_{j+1}}$.

Repeat this induction step till $j = s_t$.

The trick of Lemma 1 is that we can construct path subdivision chain to avoid the enumeration within the chain. Furthermore, if U_{t_j} belongs to more than one chain, *i.e.*, $U_{t'_i} \supset U_{t_j}$ in the t'-th chain and U_{t_j} is the nearest path subdivision of $U_{t'_i}$, Algorithm **SDVChain** will shrink B'_{t_j} iteratively by discarding the paths from B'_{t_j} based on $B_{t'_i}$. In this case, it is trivia that path set $B_{t_1} \cup B'_{t_2} \cup \dots B'_{t_j} \dots \cup B'_{t_{s_t}}$ is an independent path set and any path $p \in B_{t_j} \setminus B'_{t_j}$ can be represented by either $B_{t_{j-1}} \cup B'_{t_j}$ or $B_{t'_j} \cup B'_{t_j}$.

Lemma 2 Given the first set U_{t_1} in the *t*-th chain and some $i^* \in Q_t$, where $p_{t'_{i^*}}$ is the last substructure path in the *t'*-th chain to have shared layers with $p_{t_1}(t' \neq t \text{ and } t'_{i^*} \neq 0)$. B'_{t_1} is the shrunk path set output from Algorithm **SDVChain** by deleting the paths from B_{t_1} based on all $B_{t'_{i^*}}$ iteratively. Then $B'_{t_1} \cup B'_{t'_i}$ is path independent for any $i \in \{1, ..., i^* - 1\}$ in the *t'*-th chain.

Proof: Suppose the t' -th path subdivision chain be $U_{t_1'} \supset U_{t_2'} \supset \cdots U_{t_i'} \supset \cdots U_{t_{i^{*-1}}} \supset U_{t_{i^{*}}} \ldots \supset U_{t_{s_{t'}}}$. Q_t would rules out some substructure paths: 1) substructure path after $p_{t_{i^{*}}}$ because it doesn't share layers with p_{t_1} . 2) the sets from the t-th chain because of Lemma 1. 3) $p_{r_1}(r < t)$ which shares edges with p_{t_1} , because the algorithm only run one direction. Assume there exist two paths $p_{t_{i'},1}, p_{t_{i'},2} \in B'_{t_i'}$ with $i < i^*$ and two paths $p_{t_{1,1},1}, p_{t_{1,2}} \in B'_{t_1}$ such that $p_{t_{i',1}} - p_{t_{i',2}} = p_{t_{1,1}} - p_{t_{1,2}}$. Since Step 2 of Algorithm DEAH demands the substructure path be subdivided in the unshared layers by the next substructure path when forming the t'-th chain, there must be corresponding $p_{t_{i',1}}$ and $p_{t_{i',2}}$ in $B_{t_{i'}}$ such that $p_{t_{i',1}} - p_{t_{i,2}} = p_{t_{1,1}} - p_{t_{i',2}}$ for $p_{t_{i'}}$ shares layers with $p_{t_i'}$. But, Algorithm SDVChain discards $p_{t_{1,1}}$ or $p_{t_{1,2}}$ based on original $B_{t_{i'}}$ already. This contradicts the assumption. So $B'_{t_1} \cup B'_{t_i'}$ is path independent. On the other hand, any path $p \in B_{t_1} \setminus B'_{t_1}$ can be represented by $B'_{t_i'}$. And any path $p \in B_{t_{i'}}$ can be represented by $B'_{t_i'} \cup B_{t_{i'+1}}$.

Lemma 2 indicates that no path dependent would be produced for any $U_{t'_i}$ if we calculate B'_{t_1} based on $B_{t'_{i'}}$, though some $p_{t'_i}$ (*i*<*i*^{*}) shares common layers with $p_{t'_{i'}}$. The second trick of substructure path subdivision chain is to avoid enumerating the full chain for the first set of another chain.

Appendix C

Lemma 3 The time complexity of Algorithm Subroutine(G) in fully connected graph G

without edge skipping is $\mathcal{O}(L^2 W_{max}^2)$, where $W_{max} = \max_{\substack{0 \le l \le L}} \{|O^l|\}$. **Proof:** Algorithm **Subroutine** takes at most totally $\mathcal{O}(W_{max}^2 L)$ time to construct all sub-graph G(k) (k = 0: L - 1). It takes $\mathcal{O}(W_{max}^2)$ time to search direct path set $P_{dir}^{(k)}$ and cross path set $P_{cross}^{(k)}$ in G(k), so total running time for all G(k) is $\mathcal{O}(W_{max}^2L)$. When updating $P_{dir}^{(k)}$ and $P_{cross}^{(k)}$, the average number of paths from the lower layer is at most $O(kW_{max})$ for each node O_i^k and there are at most W_{max} nodes for k-th layer, so the total time complexity for updating is $\mathcal{O}(\frac{L(L-1)}{2}W_{max}^2)$. The time for classifying paths to k+1-th layer is the same as for updating $P_{dir}^{(k)}$ and $P_{cross}^{(k)}$. So the total running time for Algorithm Subroutine is $\mathcal{O}(W_{max}^2L + W_{max}^2L + W_{max}^2$ $2 \times \frac{L(L-1)}{2} W_{max}^2) = \mathcal{O}(L^2 W_{max}^2).$

SDVChain $(\{B'_r\}_{r=1}^s, \{B_r\}_{r=1}^s, \{p_r\}_{r=1}^s, \{\beta_r\}_{r=1}^s, B_0, p_0, \beta_0, G)$:

Input: Shrunk path set B'_r , basis path set B_r and β_r regarding p_r , independent path set B_0 and β_0 regarding p_0 in fully connected network G.

% p_r is subdivided by p_{r+1} and p_s is subdivided by p_0

Output: Updated shrunk path set $\{B'_r\}_{r=2}^s$ and discarded path set D'_0 .

Let $B'_{s+1} = B_0, p_{s+1} = p_0$ and $\beta_{s+1} = \beta_0$. For r = 1:s do

Search shared layers $\{(O^{l'_k}, O^{l''_k})\}_{k=1}^K$ for p_r and p_{r+1} , according to β_r and β_{r+1} . Find unique unshared layers $\{Ep_{r,j}\}$ in B_r . Let $DiscardPat\hbar = \emptyset$.

For each unique $Ep_{r,i}$ do

Find shared layers set UCP_i in B_r with $Ep_{r,i}$ as the unshared layers. Calculate UCP_i^* with the most frequent occurrence for each element in UCP_i . % Find the most frequent edge set in the shared layers.

Construct the unshared layers set IEp_i in B'_{r+1} which has the shared layers from UCP_i . Discard the element with frequency less than 2 from IEp_i . % Get rid of the path whose unshared layers appears only once, which couldn't cause path dependency.

Let $DiscardPath = DiscardPath \cup \{p_{r+1,i} \in B'_{r+1} | \text{the unshared layers of } p_{r+1,i} \text{ is}$ from IEp_i and the shared layers are not UCP_i^* , $i \in \{1, ..., |IEp_i|\}$. % Discard the path which brings up dependency when combining B_r with B'_{r+1} .

End For

Update $B'_{r+1} = B'_{r+1} \setminus DiscardPath$ and set $D'_{r+1} = DiscardPath$. **End For** Set $D'_0 = D'_{s+1}$.

Subroutine(G):

Input: Fully connected neural network G = (V, E) without any edge-skipping over layers. **Output:** Basis path set *B* in graph *G*

For k = 0: L - 1 do

Let $E^k = \{e \in G | e \text{ leaves from } k\text{-th layer and enters } k + 1\text{-th layer } \}.$ % Step 1. Construct the direct path set. Let sub-graph $G(k) = (O^k \cup O^{k+1}, E^k)$. If $|O^k| \ge |O^{k+1}|$ do

Find $|O^{k+1}|$ direct vertex disjoint paths by depth-first searching, and let the direct path set be $P_{dir}^{(k)}$

For $v \in O^k \setminus V(P_{dir}^{(k)})$ do

Pick up one node $O_{i'}^{k+1} \in O^{k+1}$ randomly and construct path $(v, O_{i'}^{k+1})$. Set $P_{dir}^{(k)} = P_{dir}^{(k)} \cup (v, O_{i'}^{k+1}).$

End For

Else do

Find $|O^k|$ direct vertex disjoint paths by depth-first searching, and let the direct path set be $P_{dir}^{(k)}$.

End If For $i = 1, 2, ..., |O^k|$ do Let the path set $P_{dir}(O_i^k) = \{ p \in P_{dir}^{(k)} | \text{the tail of } p \text{ is node } O_i^k \}.$ **End For** % Step 2. Construct the cross path. Set cross path set $P_{cross}^{(k)} = E^k \setminus E(P_{dir}^{(k)})$ For $i = 1, 2, ..., |O^k|$ Let the path set $P_{cross}(O_i^k) = \{p \in P_{cross}^{(k)} | \text{the tail of } p \text{ is node } O_i^k\}$. **End For** % Step 3. Concatenate the direct paths and cross paths from the k - 1-th layer. If $k \neq 0$ % If k = 0, there is no concatenation for any path and go to Step 4 directly. **For** $i = 1, 2, ..., |O^k|$ do % Form $|P(O_i^k)|$ direct paths and extend all cross paths. Let $P_{dir}(O_i^k) = \{p_0 + p_1 | p_1 \in P_{dir}(O_i^k), p_0 \in P(O_i^k)\}$ for node $O_i^k \in O^k$. Select one path $p^* \in P(O_i^k)$ randomly and let $P_{cross}(O_i^k) = \{p^* + p_1 | p_1 \in P_{cross}(O_i^k)\}$. **End For** Update direct path set $P_{dir}^{(k)} = \bigcup_{O_i^k \in O^k} P_{dir}(O_i^k)$ and cross path set $P_{cross}^{(k)} = \bigcup_{O_i^k \in O^k} P_{cross}(O_i^k).$ End If % Step 4. Classify the paths for the nodes in the k + 1-th layer. For $i = 1, 2, ..., |0^{k+1}|$ do Set the path set $P(O_i^{k+1}) = \{ p \in P_{dir}^{(k)} \cup P_{cross}^{(k)} | \text{ the head of } p \text{ is node } O_i^{k+1} \}.$

End For

End for

Output basis path set $B = P_{dir}^{(L-1)} \cup P_{cross}^{(L-1)}$