Supplementary Material of Optimal Gradient Checkpoint Search for Arbitrary Computation Graphs

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1. Extra Examples

1.1. Extra Examples for Linear Computation Graph

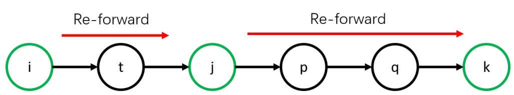


Figure 1: Example linear network for gradient checkpoint training. Letter denotes index of vertex and green vertices denotes gradient checkpoints.

Fig. 1 is an example linear network for gradient checkpoint training. Vertices v_i, v_j, v_k are stored in the first forward. During backward from v_k to v_j, a local forward is conducted starting from v_j to recompute v_p and v_q. During backward from v_j to v_i, v_t is recomputed from v_i. The recomputed vertices are used to compute gradients for backward.

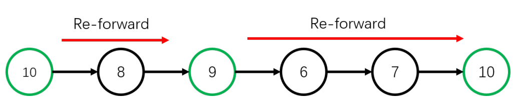


Figure 2: Example of memory cost function for Linear Computation Graph. Number in the vertex denotes its memory cost, and green vertices denotes gradient checkpoints.

Fig. 2 explains how we compute memory loss on the linear computation graph with gradient checkpoint training. Recall that the loss function is as follows:

$$\min_{V^R}(\sum_i l(v_i^R) + \max_i l(v_i^R, v_{i+1}^R)), \quad (1)$$

In Fig. 2, V^R is the GCs set (green vertices). $\sum_i l(v_i^R)$ is simply the sum of loss of these stored vertices: $10+9+10 = 29$. $\max_i l(v_i^R, v_{i+1}^R))$ describes the maximum re-forward loss. In this example, there are two local re-forwarding. Loss for the second re-forward: $6 + 7 = 13$. Loss for the first re-forward is 8. For each re-forwarding, the loss of it is simply the sum of all the vertices in between. Therefore, maximal Re-forward loss is $\max\{13, 8\} = 13$, and total Loss is $29 + 13 = 42$.

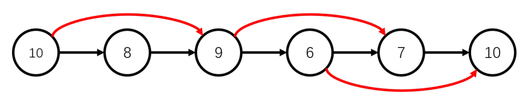


Figure 3: Denote $C = \max_i l(v_i^R, v_{i+1}^R)$. Given $C = 8$, this is an example of Accessibility Graph. Number in the vertex denotes its loss. The red edges are newly added accessibility edges in the accessibility graph.

Fig. 3 shows an example of accessibility graph. Given a certain $C = \max_i l(v_i^R, v_{i+1}^R)$, in the accessibility graph, two vertex have accessibility edge as long as their Re-forwarding loss is not greater than C. For example, the first vertex (loss 10) and the third vertex (loss 9) has accessibility edge because the re-forwarding loss (8) is not greater than C

1.2. Extra Examples for Arbitrary Computation Graph

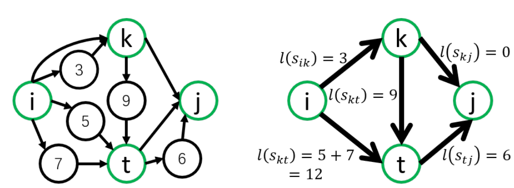


Figure 4: Example of gradient checkpointing for non-linear computation graph. Letter denotes vertex index, number denotes vertex memory cost and green vertices denote gradient checkpoints. The edges in the right graph are folded Independent Segment in the left graph.

Fig. 4 shows an example of gradient checkpoint training for a non-linear computation graph. Suppose we select vertices $\{v_i, v_k, v_t, v_j\}$ as gradient checkpoints. Based on the gradient checkpoints, the computation graph has IS $\{s_{ik}, s_{it}, s_{kt}, s_{kj}, s_{tj}\}$. If we view these IS as edges and fold the details within IS, we will get another ACG shown in the right of Fig. 4, where the vertices are GCs and the edges are IS in the original graph . During the first forward, only GCs $\{v_i, v_k, v_t, v_j\}$ are stored. Re-forwarding and backward are conducted independently in each IS.

2. Proof

2.1. Definitions and Lemmas

Definition 1. ***Independent Segment(IS):*** *An IS $s_{ij} = (V^{ij}, E^{ij}))$ satisfies the following three properties: 1. All the vertices in V^{ij} have a common ancestor v_i and a common descendent v_j; 2. Denote the set of edges between two arbitrary vertices in V^{ij} is E', the edge from v_i to v_j (if exists) as e_{ij}. E must either be E' or $E' - \{e_{ij}\}$; 3. An arbitrary $v_k \in (V^{ij} - \{v_i, v_j\})$ doesn't have edge with another arbitrary $v_t \notin V^{ij}$. For multiple valid IS between v_i and v_j, we denote the largest one as s_{ij}*

Definition 1 is to clarify properties of IS in maths for the following proof.

Definition 2. $[s_{ij}) = (V^{ij} - \{v_j\}, E^{ij})$. $(s_{ij}] = (V^{ij} - \{v_i\}, E^{ij})$. $(s_{ij}) = (V^{ij} - \{v_i, v_j\}, E^{ij})$.

For convenience, we define notations for IS s_{ij} excluding v_i, or v_j or both.

Lemma 1. *If $(s_{ij}) \cap (s_{kt}) \neq \emptyset$ and $(s_{ij}) \not\subset (s_{kt})$ and $(s_{kt}) \not\subset (s_{ij})$, then $(s_{ij}) \cap (s_{kt}) = (s_{kj})$ or $(s_{ij}) \cap (s_{kt}) = (s_{it})$*

Proof. Let $s_{ij} \cap s_{kt} = s_{pq} = \{V^{pq}, E^{pq}\}$. If $v_p \neq v_i$ and $v_p \neq v_k$ and $v_q \neq v_j$ and $v_q \neq v_t$, then v_i, v_k has path to v_p and v_j, v_t has path from v_q. Therefore, v_p has at least 2 immediate parents v_a, v_b with $v_a \in s_{ij}, v_a \notin s_{kt}, v_b \in s_{kt}, v_b \notin s_{ij}$. If so, the independence of s_{ij} and s_{kt} is violated. Therefore, v_p must be v_i or v_k.

Same on v_q, v_q must be v_j or v_t.

If $v_p = v_i, v_q = v_j$, then $s_{ij} \subset s_{kt}$. If $v_p = v_k, v_q = v_t$, then $s_{kt} \subset s_{ij}$. Therefore, $v_p = v_i, v_q = v_t$ or $v_p = v_k, v_q = v_j$. Suppose $v_p = v_k, v_q = v_j$, let's prove s_{pq} is an IS.

With $s_{pq} \subset s_{kt}$, $\forall v_1 \in (s_{pq})$, v_1 has no edge with $v_2 \notin (s_{kt})$. With $s_{pq} \subset s_{ij}$, $\forall v_1 \in (s_{pq})$, v_1 has no edge with $v_2 \notin (s_{ij})$. Therefore, $\forall v_1 \in (s_{pq})$, v_1 has no edge with $v_2 \notin s_{pq}$. The independence of s_{pq} is guaranteed.

In the discussion before, we can see the source vertex v_p of s_{pq} must be either v_i or v_k. If v_i and v_k are both the source vertices of s_{pq}, then $v_i \in s_{kt}$ and $v_k \in s_{ij}$, v_i has path to v_k and v_k has path to v_i, which will force $v_i = v_k$ because the s_{ij}, s_{kt} is acyclic. Same on v_q, s_{pq} can only have 1 source vertex and 1 target vertex. Therefore, s_{pq} is an IS.

Therefore, $(s_{ij}) \cap (s_{kt}) = (s_{kj})$ or $(s_{ij}) \cap (s_{kt}) = (s_{it})$. □

Lemma 2. *The intersection of IS $s_{pq} = s_{ij} \cap s_{kt} \neq \emptyset$ is also an IS*

Proof. Given the independence of s_{ij} and s_{kt}, the independence of s_{pq} is obvious. The remaining thing is whether s_{pq} only has 1 source vertex and 1 target vertex. In the proof of Lemma 1, we can see any source or target vertex of s_{pq} will eventually become source or target vertex of s_{ij} and s_{kt}. With simple discussion, we can have this lemma. □

Lemma 3. *If $s_{ij} \cap s_{kt} = s_{kj} \neq \emptyset$, then v_k is the linear splitting vertex of s_{ij} and v_j is the linear splitting vertex of s_{kt}*

Proof. Let's first prove that v_k is the linear splitting vertex of s_{ij}.

Let $s_{ik} = s_{ij} - s_{kj} + \{v_k\}$. Obviously, $s_{ij} = s_{ik} \cup s_{kj}$ and $s_{ik} \cap s_{kj} = \{v_k\}$. We only need to prove that s_{ik} is IS.

v_i is obviously the only source vertex of s_{ik} because v_i is source vertex of s_{ij}. We discuss the target vertex here. If v_k is not the target vertex of s_{ik}, as $v_k \in s$, v_k must have path to the target vertex v of s_{ik} and v also has path to v_j as $v \in s_{ij}$. Because $v \notin s_{kj}$, in the path from v to v_j, there exists an edge that connects a vertex $v_1 \in s_{ik}$ with a vertex $v_2 \in s_{kt}$ which violates the independence of s_{kt}. Therefore, the target vertex of s_{ik} can only be v_k.

As $s_{ik} \subset [s_{ij})$, $\forall v_1 \in s_{ik}$, v_1 has no edge with $v_2 \notin [s_{ij})$. As s_{kj} is IS, $\forall v_1 \in (s_{ik})$, v_1 has no edge with $v_2 \in (s_{kj})$. $\forall v_1 \in (s_{ik})$, v_1 can only have edge with $v_2 \in s_{ik}$. Thus the independence of s_{ik} is guaranteed. Therefore, s_{ik} is IS, v_k is the linear splitting vertex of s_{ij}.

Similarly, v_j is the splitting vertex of s_{kt} □

Lemma 4. *If s_{ij} has n splitting vertices $\{v_1, v_2, ..., v_n\}$, then $s_{ij} = s_{i1} \cup s_{12} \cup ... \cup s_{nj}$*

Proof. If $n = 2$, the splitting vertices are v_1, v_2, $s_{ij} = s_{i1} \cup s_{1j} = s_{i2} \cup s_{2j}$. Let $v_1 \in s_{i2}, v_1 \neq v_2$, then $s_{1j} \cap s_{i2} = s_{12} \neq \emptyset$. According to Lemma 3, v_1 is linear splitting vertex of s_{i2} and v_2 is linear splitting vertex of s_{1j}. Therefore, $s_{ij} = s_{i1} \cup s_{12} \cup s_{2j}$.

For $n > 2$, the lemma can be proved by repetitively using the conclusion in $n = 2$.

□

Lemma 5. *If the Complicate IS s_{ij} has division $\{s_{pq}\}$, and $|\{s_{pq}\}| > 2$, denote $\{v\}$ as all the connecting vertices of $s \in \{s_{pq}\}$. Then $\forall v \in \{v\}, v \neq v_i, v_j$, v is the connecting vertex of at least 3 member IS of the division.*

Proof. If v_b is the connecting vertex of only 2 member IS, suppose the 2 members are s_{ab} and s_{bc}. If so, s_{ab} and s_{bc} can be merged into s_{ac}. If $s_{ac} \neq s_{ij}$, this violates the definition of divison of Complicate IS. Otherwise, it violates the condition that s_{ij} is not a Branch IS and $|\{s_{pq}\}| > 2$. It is impossible that the 2 members are s_{ab} and s_{cb} because in this way v_b has no path to v_j and violates the definition of IS. If v_b is the connecting vertex of only 1 member IS of the division, then v_b must be either v_i or v_j. Therefore, this lemma is proved. □

Lemma 6. *For Complicate IS s_{ij}, any member IS s_{pq} of its division can not be the subset of another IS s_{kt}, i.e. $s_{pq} \subsetneqq s_{kt} \subsetneqq s_{ij}$.*

Proof. The source vertex of s_{kt} is v_k and target vertex is v_t. Suppose a member IS $s_{pq} \subsetneqq s_{kt}$.

Suppose another member IS s_{ab} of the division has its source vertex v_a inside s_{kt} and target vertex v_b outside s_{kt}. Then the boundary vertex (the vertex that has edges to the non-overlapping parts of both sets) must be v_t, otherwise the independence of s_{kt} will be violated. Notice that v_t is inside s_{ab} and the independence of s_{ab} needs to be guaranteed, for $\forall v_x \in s_{kt}, v_x \notin s \cap s_{ab}, v_y \in s_{kt} \cap s_{ab}$, v_x has no edge with v_y. Therefore, v_a is a splitting vertex of s_{kt}.

Similarly, if s_{ba} has its target vertex v_a inside s_{kt} and source vertex v_b outside s_{kt}, the boundary vertex must be v_k and v_a is a splitting vertex of s_{kt}.

For the member IS s_{kt}, from the discussion above, we know that there are at most 2 members in the division that can overlap with s_{kt}. Other members must be either completely inside s_{kt} or completely outside s_{kt}. Let's discuss the number of members that overlaps with s_{kt}.

If there are 0 member that overlaps with s_{kt}, s_{kt} is the union of a subset of members of the division, which violates the definition of division.

If there is 1 member that overlaps with s_{kt}, suppose the corresponding splitting vertex is v_b, and the boundary vertex is actually v_t. Then s_{kb} is an IS containing s_{pq} and corresponds to the situation of 0 member overlapping. s_{kb} is the union of a subset of members of the division, and violates the definition of maximal split.

If there are 2 members that overlaps with s_{kt}, suppose they generate two different splitting vertex v_a and v_b. Then s_{ab} is an IS containing s_{pq} and corresponds to the situation of 0 member overlapping. s_{ab} is the union of a subset of members of the division, and violates the definition of the division.

If they generate the same splitting vertex v_b, from lemma 5, v_b is also the connecting vertex of at least 1 other member s_{ab} which has to be inside s_{kt}. Suppose the two overlapping members are s_{cb} that contains v_k, and s_{bd} that contains v_t. As the source vertex of s_{kt}, v_k has path to v_b and v_k has path to v_a, which implies v_b has path to v_a. As the target vertex of s_{kt}, v_t has path from v_b and v_t has path from v_a, which implies v_b has path from v_a. This conflicts with the fact that s_{kt} is acyclic. Therefore, this case is not possible.

Therefore, this lemma is proved. □

Lemma 7. *If Complicate IS s_{ij} has at least 1 vertex excluding v_i and v_j, then its division has length > 2*

Proof. As s_{ij} is Complicate, the members IS of its division cannot have the source vertex as v_i and target vertex as v_j at the same time. If s_{ij} has at least 1 vertex excluding v_i and v_j, and its division has length 2, then its division must be $\{s_{ik}, [s_{kj}\}$, and v_k will be the linear splitting vertex of s_{ij}, which violates that s_{ij} has no splitting vertex.

If s_{ij} has no splitting vertex, it has at least 2 edges and cannot have a trivial length 1 maximal split. Therefore, its maximal split has length > 2 □

2.2. Uniqueness of Division Tree

To prove this uniqueness, we simply discuss the uniqueness of division of Linear IS, Branch IS and Complicate IS.

2.2.1 Uniqueness of Division of Linear IS

Proof. By the definition of Linear IS division and Lemma 4, the uniqueness of the division is equivalent to the uniqueness of the linear splitting vertex set of a Linear IS. The linear splitting vertex set is obviously unique. □

2.2.2 Uniqueness of Division of Branch IS

Proof. If there exists another division, there must be a branch member s_{ij}^1 in division 1 and a branch member s_{ij}^2 in division 2, where $s_{ij}^1 \cap s_{ij}^2 \neq \{v_i, v_j\}$ and $s_{ij}^1 \neq s_{ij}^2$.

Denote $s_{ij}^3 = s_{ij}^1 \cap s_{ij}^2$. By Lemma 1 and 2, s_{ij}^3 is also an IS. From the definition of the division, we know s_{ij}^1 and s_{ij}^2 cannot be divided into more branches, $s_{ij}^3 = s_{ij}^1 = s_{ij}^2$. Therefore, the division of Branch IS is unique. □

2.2.3 Uniqueness of Division of Complicate IS

Proof. As the IS in the division tree has at least 1 vertex excluding source and target vertex, with Lemma 7, we know that the division of Complicate IS s_{ij} will have length > 2. Denote this division as $\{s_{pq}\}$, we only need to prove this division is unique.

Suppose there is a another different division $\{s'_{pq}\}$, let us only check the difference between $\{s_{pq}\}$ and $\{s'_{pq}\}$. Denote $\{s_{kt}\}$ and $\{s'_{kt}\}$ with $\{s_{pq}\} - \{s_{kt}\} = \{s'_{pq}\} - \{s'_{kt}\}$ and $\nexists s \in \{s_{kt}\}, s' \in \{s'_{kt}\}, s = s'$. As $\{s_{pq}\} - \{s_{kt}\} = \{s'_{pq}\} - \{s'_{kt}\}$, we have $\cup\{s_{kt}\} = \cup\{s'_{kt}\}$

Obviously, $|\{s_{kt}\}| \geq 2$ and $|\{s'_{kt}\}| \geq 2$. Denote $\{v\}$ as all the connecting vertices of $s \in \{s_{kt}\}$, and $\{v'\}$ for $\{s'_{kt}\}$. Obviously $\{v\} \neq \emptyset$ and $\{v'\} \neq \emptyset$. As s_{ij} is not Branch IS, $\{v\} \cup \{v_i, v_j\} - \{v_i, v_j\} \neq \emptyset$ and $\{v'\} \cup \{v_i, v_j\} - \{v_i, v_j\} \neq \emptyset$.

Suppose $s_{ab}, s_{bc} \in \{s_{kt}\}$, according to Lemma 5, there's at least 1 other member IS that has v_b as connecting vertex. Suppose the other connecting vertex of this member IS is v_d. Let's discuss whether $v_b \in \{v'\}$ and whether $v_d \in \cup\{s_{kt}\}$.

If $v_d \notin \cup\{s_{kt}\}$, then v_b must occur in $\{v'\}$. Otherwise, v_b would be inside an IS which would be violated by v_d. Given $v_b \in \{v'\}$, as $s_{ab} \notin \{s'_{kt}\}$, suppose $s_{eb} \in \{s'_{kt}\}$ and $s_{ab} \cap s_{eb} \neq \emptyset$. If $v_a \in s_{eb}$, from Lemma 1, s_{eb} is invalid IS. If $v_e \in s_{ab}$, from Lemma 5, s_{ab} is invalid IS. In this case, there cannot exist another different division.

If $v_d \in \cup\{s_{kt}\}$, then $s_{bd} \in \{s_{kt}\}$. If $v_b \in \{v'\}$, we can use the same logic above to show this is impossible. Therefore, $v_b \notin \{v'\}$ and s_{bd} is contained by an IS s. From Lemma 6, this is impossible. In this case, there cannot exist another division.

In all the cases, there cannot exist another division. Therefore, the division of Complicate IS is unique. ☐

2.3. Completeness of Division Tree

Similar with the uniqueness, the completeness of division tree is equivalent to the completeness of the division of an IS. To prove this completeness, we simply discuss the completeness of division of Linear IS, Branch IS, and Complicate IS.

An equivalent statement of the completeness of the division is: there doesn't exist an IS whose source vertex is in one member IS of the division and whose target vertex is in another member IS of the division.

2.3.1 Completeness of Division of Linear IS

Proof. Suppose there exists an IS s_{pq} whose source vertex v_p is in one member IS s_1 and whose target vertex v_q is in another member IS s_2.

If v_p is not an endpoint vertex of s_1, then according to Lemma 3, v_p is also a linear splitting vertex in s_1 and can break s_1 into smaller IS, which makes v_p also the linear splitting vertex of the whole IS s_{ij}. However, v_p is not the splitting vertex of the whole IS s_{ij}. This also applies to v_q. Therefore, the division of Linear IS is complete. ☐

2.3.2 Completeness of Division of Branch IS

Proof. Suppose there exists an IS s_{pq} whose source vertex v_p is in one branch s^1_{ij} and whose target vertex v_q is in another branch s^2_{ij}. As s_{pq} crosses s^1_{ij} and s^2_{ij}, there exists a boundary vertex v in s_{pq}, which belongs to s^1_{ij} and has direct connection with a vertex outside s^1_{ij}. If v is not v_i or v_j, it will violate the independence of s_{ij}. If $v = v_i$, as v_i is the source vertex of both s^1_{ij} and s^2_{ij}, it cannot be the boundary vertex, same when $v = v_j$. Therefore, there cannot exist such an IS s_{ij}. The division of Branch IS is complete. ☐

2.3.3 Completeness of Division of Closed Set Type 3

Proof. Suppose there exists an IS s_{pq} whose source vertex v_p is in one member IS s_1 and whose target vertex v_q is in another member IS s_2. Same with Branch IS, the boundary vertex v has to be the endpoint vertex of s_1 or the independence of s_1 will be violated. According to Lemma 5, v is the connecting vertex of at least 3 members, meaning that v will at least have 1 connection with another IS s_3. To maintain the independence of s_{pq}, s_{pq} has to contain s_3 as well. However, s_3 also has its endpoint vertices. This will propagate until s_{pq} becomes the whole closed set s_{ij}. Therefore, there cannot exist such an IS s_{pq}. The division of Complicate IS is complete. ☐

3. Complexity Analysis

3.1. Algorithm 1

Suppose there are $|V|$ vertices and $|E|$ edges in the computation graph. There are $O(|V|^2)$ vertex pairs. For each vertex pair, the time cost is mainly on constructing accessibility graph and finding the shortest path. Denote the source vertex of the whole computation graph as v_0. To construct an accessibility graph, first we traverse the linear computation graph, record the accumulated sum $l(v_0, v_i)$ for each vertex v_i, and form a table of $l(v_i, v_j) = l(v_0, v_j) - l(v_0, v_i) - l(v_i)$. These steps will cost $O(|V|^2)$ and will only run once. Then we traverse each (v_i, v_j) pair to form the edges of the accessibility graph, which also cost $O(|E|)$. Solving the shortest path problem in accessibility graph will cost $O(|V|log|V| + |E|)$. Therefore, the overall time complexity of Algorithm 1 would be $O(|V|^2|E| + |V|^3 log|V|)$.

The space complexity would be $O(|V|^2)$ for the table of $l(v_i, v_j)$ and the accessibility graph itself.

3.2. Algorithm 2

Suppose there are $|V^{ij}|$ vertices and $|E^{ij}|$ edges in the IS s_{ij}. In step 2, getting $\{v_{in}\}$ and $\{v_{out}\}$ will cost $O(|V^{ij}|)$ time for traversing the ancestors and descendants of v_t. In our implementation, an array a of length $|V^{ij}|$ is used to represent $\{v_{in}\}$ and $\{v_{out}\}$: $a_i = 1$ indicates $v_i \in \{v_{in}\}$, $a_i = 2$ indicates $v_i \in \{v_{out}\}$ and $a_i = 0$ indicates $v_i \notin \{v_{in}\} \cup \{v_{out}\}$. Then the union check and intersection check in step 3 can be done in $O(|V^{ij}|)$. The connection check in step 3 traverses the edges and costs $O(|E^{ij}|)$. Other steps are $O(1)$. Therefore, the overall time complexity of Algorithm 2 would be $O(|V^{ij}|^3)$.

The space complexity would be $O(|V^{ij}|)$ for the array to represent $\{v_{in}\}$ and $\{v_{out}\}$.

3.3. Algorithm 3

Suppose there are $|V^{ij}|$ vertices in the IS s_{ij}. The most time consuming part will be from step 7 to step 18. Other steps are $O(1)$. In step 7 to step 18, every edge between two vertices in s_{ij} is at most visited once and there are $O(E^{ij})$ edges. Therefore, the overall time complexity of Algorithm 3 would be $O(E^{ij})$.

In our implementation, an array of length $|V^{ij}|$ is used to represent the vertex set $s = \{v_k\}$. Therefore, the space complexity would be $O(|V^{ij}|)$.

3.4. Algorithm 4

Suppose there are $|V^{ij}|$ vertices and $|E^{ij}|$ edges in the IS s_{ij} and there are $O(|V^{ij}|^2)$ vertex pairs. For each vertex pair, the connection check in step 2-4 will cost $O(|E^{ij}|)$, similar to the connection check in Algorithm 2. Thus step 1-4 will cost $O(|V^{ij}|^2|E^{ij}|)$. In our implementation, for each vertex in the IS s_{ij}, we select the largest formed IS s_{kt} that contains this vertex. The IS number is then reduced to $O(|V^{ij}|)$ and step 5-6 can be done in $O(|V^{ij}|^3)$. Therefore, the overall time complexity of Algorithm 4 would be $O(|V^{ij}|^2|E^{ij}| + |V^{ij}|^3)$

As $O(|V^{ij}|^2)$ IS can be formed in step 1-4 and each closed set is a smaller DAG with $O(|V^{ij}|)$ vertices and cost $O(|V^{ij}|^2)$ space, the space complexity would be $O(|V^{ij}|^4)$ for all these closed sets.

3.5. Algorithm 5

Given a max term C, the actual time consuming part in the recursion will be step 9 which calls the LCG solver under constraint C, and other steps would be $O(1)$. Suppose the LCG solver is called k times, solving problems of $a_1, a_2, ..., a_k$ vertices and $e_1, e_2, ..., e_k$ edges. The total complexity of this would be $O(a_1 log a_1 + e_1) + O(a_2 log a_2 + e_2) + ... + O(a_k log a_k + e_k)$. Notice that $a_1 + a_2 + ... + a_k \leq |V|$ for the fact that any vertex in the computation graph would not be solved twice by LCG solver, and $e_1 + e_2 + ... + e_k \leq |E|$, we have $a_1 log a_1 + e_1 + a_2 log a_2 + e_2 + ... + a_k log a_k + e_k \leq |V| log |V| + |E|$. Therefore the time complexity of Algorithm 5 is $O(|V| log |V| + |E|)$.

3.6. Algorithm 6

Step 1 is similar to step 1-4 in Algorithm 4 with s_{ij} being the whole computation graph. Therefore, the overall time complexity for step 1 is $O(|V^{ij}|^2|E^{ij}| + |V^{ij}|^3)$.

In step 2, the complexity of building division tree is related to the complexity of getting the division of an IS. For Linear IS, getting the division cost $O(|V|^3)$ time. For Branch IS, Algorithm 3 is used to get its division and costs $O(|E|)$ time. For Complicate IS, Algorithm 4 is called to solve for its division. Notice that we have already stored all possible IS in step 1, step 1-4 in Algorithm 4 can be skipped and thus the time complexity of getting the division of Complicate IS is reduced to $O(|V|^3)$. Therefore, getting the division of an arbitrary IS costs $O(|V|^3)$ time. In depth i of the division tree, suppose there are k IS, and the number of vertices of jth closed sets is a_j. To build depth $i+1$ of the division tree, we need to get the division of all these IS, which will cost $\sum_j O(a_j^3)$. As $\sum_j a_j \leq |V|$, we have $\sum_j O(a_j^3) \leq O(|V|^3)$. As the depth of division tree is $log|V|$, the overall time complexity of step 2 would be $O(|V|^3 log|V|)$.

For the loop, the length of $\{c\}$ would be $O(|V|^2)$ for there are $O(|V|^2)$ vertex pair, and the recursion costs $O(|V| log|V| + |E|)$. Therefore the time complexity of the loop is $O(|V|^2|E| + |V|^3 log|V|)$.

Step 1 would cost $O(|V|^4)$ space to store all the possible closed sets. Step 2 would cost $O(|V|^2)$ space for the division tree. the loop would cost $O(|V|^2)$ space for calling LCG solver.

In conclusion, the overall time complexity of Algorithm 6 is $O(|V|^2|E| + |V|^3 log|V|)$ and the overall space complexity of Algorithm 6 is $O(|V|^4)$.

4. Runtime Analysis

The number of vertices in the computation graph and the preprocess time of ACG Solver (Algorithm 6) for each network are listed in Table 1. All the preprocess time were measured on a desktop.

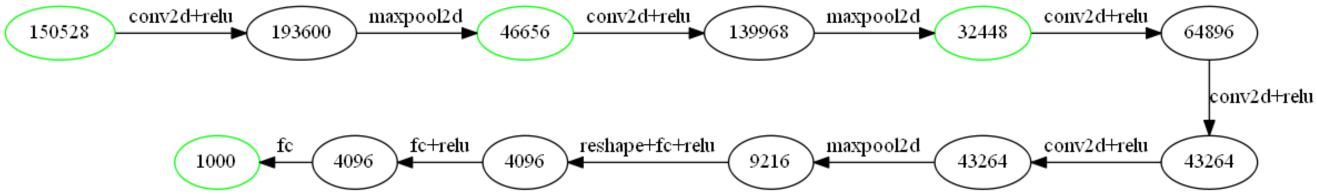
Although it might be concerning that the preprocess time is too much for some deep networks, it is still relatively small compared to training processes which might cost days or even weeks. More importantly, solving the optimal solution for a network is an one-time effort. The optimal solutions for all popular networks will be released online for people to use without taking the time to run ACG solver.

Table 1: Preprocess time by ACG Solver

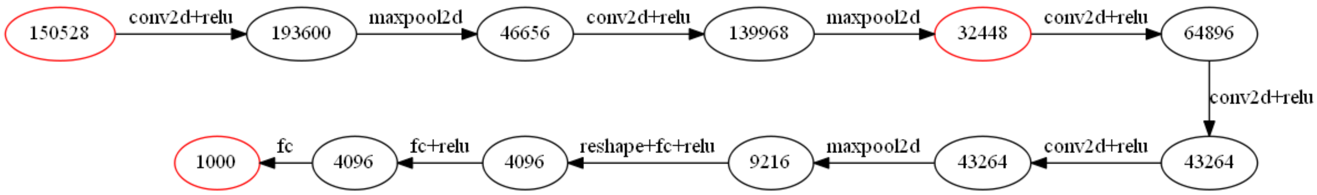
Linear network	Number of vertices	Preprocess Time (s)
Alexnet	12	0.097
Vgg11	17	0.198
Vgg13	19	0.274
Vgg16	22	0.416
Vgg19	25	0.531
Non-linear network	Number of vertices	Preprocess Time (s)
Resnet18	51	0.200
Resnet34	91	0.502
Resnet50	125	0.910
Resnet101	244	2.690
Resnet152	363	6.576
Densenet121	306	35.024
Densenet161	406	79.754
Densenet169	426	87.111
Densenet201	506	160.808
Inceptionv3	219	4.344
NASNet	1149	39.098
AmoebaNet	1015	30.250
DARTS	1073	28.483

5. Visualization

We visualize the computation graph of Alexnet, vgg11, vgg13, vgg16 ,vgg19 and CustomNet and the solution of our approach (in green) and the solution of Chen's approach (in red). In the computation graphs, the cost of each vertex and the actual operation of each edge are also marked. The cost of each vertex is the size of this tensor during forward given the input as $[1, 3, 224, 224]$ ($[1, 3, 300, 300]$ for inception v3). For example, in Alexnet, the input is $[1, 3, 224, 224]$ and thus the source vertex has the cost $150528 = 1 \times 3 \times 224 \times 224$. After 2D convolution and relu, the tensor becomes $[1, 64, 55, 55]$ and thus the second vertex has the cost $193600 = 1 \times 64 \times 55 \times 55$.

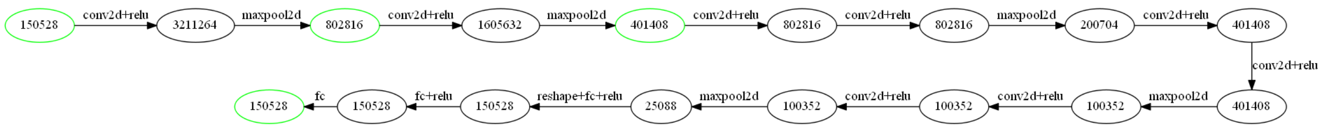


(a) Gradient checkpoints (green) of our approach

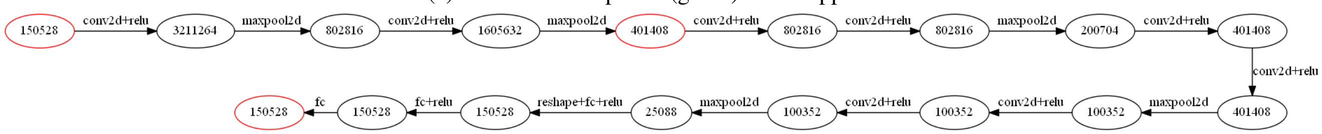


(b) Gradient checkpoints (red) of Chen's approach

Figure 5: Gradient checkpoints found on Alexnet

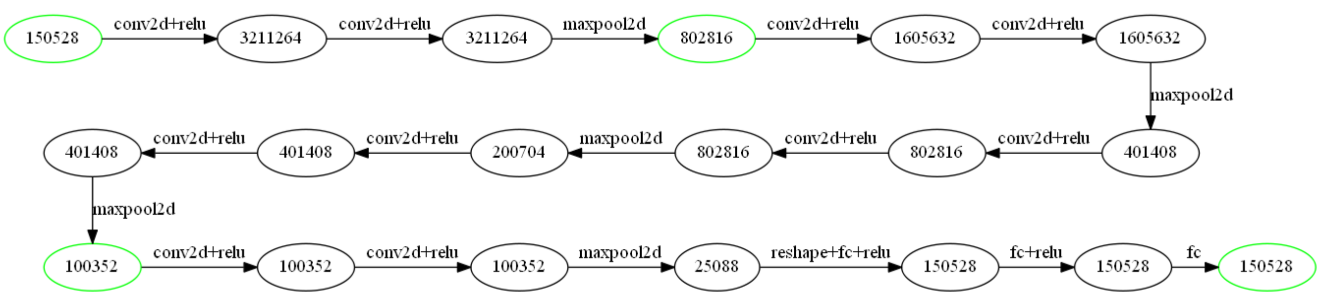


(a) Gradient checkpoints (green) of our approach

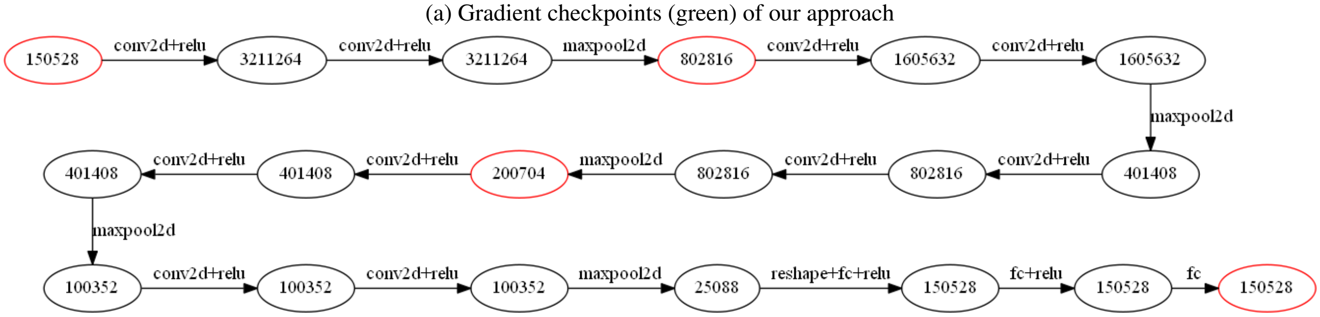


(b) Gradient checkpoints (red) of Chen's approach

Figure 6: Gradient checkpoints found on vgg11

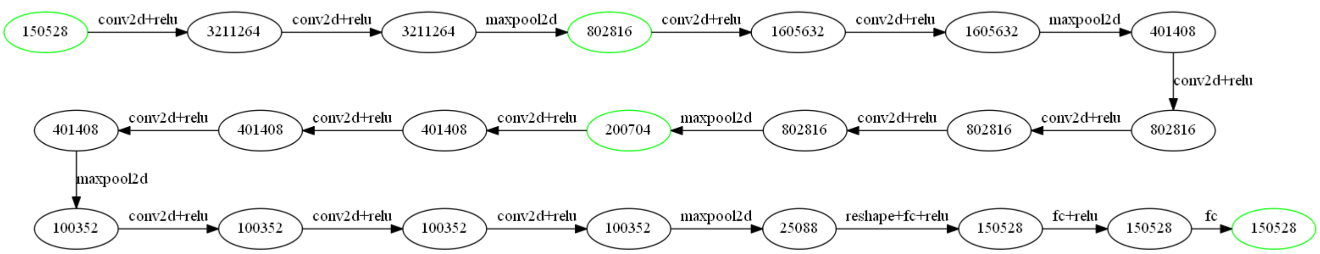


(a) Gradient checkpoints (green) of our approach

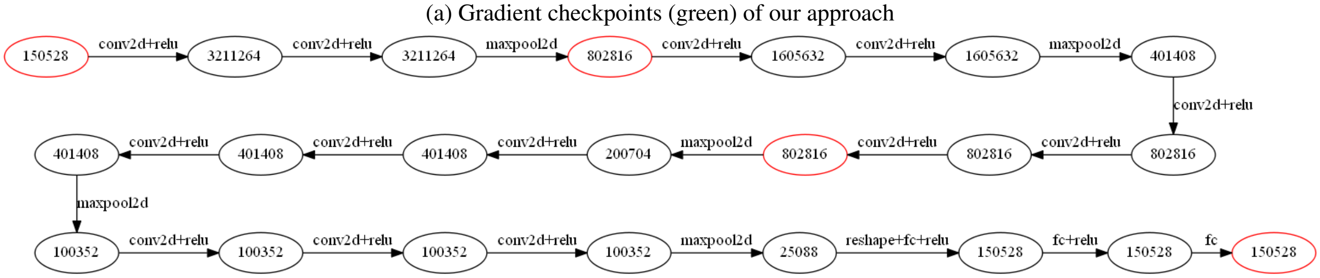


(b) Gradient checkpoints (red) of Chen's approach

Figure 7: Gradient checkpoints found on vgg13



(a) Gradient checkpoints (green) of our approach



(b) Gradient checkpoints (red) of Chen's approach

Figure 8: Gradient checkpoints found on vgg16