Model Fusion of Heterogeneous Neural Networks via Cross-Layer Alignment

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Abstract

Layer-wise model fusion via optimal transport, named OTFusion, applies soft neuron association for unifying different pre-trained networks to save computational resources. While enjoying its success, OTFusion requires the input networks to have the same number of layers. To address this issue, we propose a novel model fusion framework, named CLAFusion, to fuse neural networks with a different number of layers, which we refer to as heterogeneous neural networks, via cross-layer alignment. The cross-layer alignment problem, which is an unbalanced assignment problem, can be solved efficiently using dynamic programming. Based on the cross-layer alignment, our framework balances the number of layers of neural networks before applying layer-wise model fusion. Our synthetic experiments indicate that the fused network from CLAFusion achieves a more favorable performance compared to the individual networks trained on heterogeneous data without the need for any retraining. With an extra finetuning process, it improves the accuracy of residual networks on the CIFAR10 dataset. Finally, we explore its application for model compression and knowledge distillation when applying to the teacher-student setting.

1 Introduction

Deep neural networks have become ubiquitous recently due to the stark development of high-performance computational devices (e.g., GPUs, TPUs). Therefore, a natural question arises, “Can we combine the knowledge of two and more deep neural networks to improve performance?” As one of the earliest successful methods, ensemble learning leads to favorable performance in various tasks. Ensemble learning aggregates the output over a collection of trained base models, which is referred to as an ensemble, to improve the generalization ability [12, 43]. Despite the fact that ensemble learning improves the performance and robustness of neural networks, it is expensive in terms of computational resources. It requires storing and running a number of trained neural networks to produce a single prediction for a test sample. This approach, therefore, becomes infeasible in several applications where the limitation of computational resources and memory (e.g., edge devices, IoT devices) exists while the fast inference time still needs to be secure. To overcome the previous hardness, combining the knowledge of multiple networks into one appears as an elegant solution that has drawn attention from the community recently. In greater detail, we need to find a single neural network that can inherit the knowledge from multiple pre-trained neural networks and have a small size at the same time. To our best knowledge, there are two popular approaches for this purpose: knowledge distillation and model fusion.

The first approach, knowledge distillation, is a machine learning technique that transfers knowledge from large networks (teachers) into a smaller one (student) [14]. The smaller network is trained by the task-specific loss and additional distillation losses that encourage the student networks to
mimic the prediction of the teachers. Knowledge distillation is an efficient model compression and acceleration technique [11]. The distillation process, however, is computationally expensive because it trains the student network from scratch. In addition, knowledge distillation demands sharing the large training data between the teacher and student networks. In some situations sharing data is prohibited due to critical issues such as data security or network bandwidth constraints. To tackle this problem, various knowledge distillation methods have been proposed [28, 25, 17, 39, 36, 2].

The second line of works is called model fusion which is the problem of merging a collection of pre-trained networks into a unified network [7]. Although both approaches result in a single model, compression is not the absolute requirement of model fusion. Additionally, model parameters of the output are directly generated from model parameters of the input in model fusion.

The simplest technique in model fusion is vanilla averaging, which computes the weighted average of pre-trained network parameters without the need for retraining [35, 32]. Their methods fuse neural networks with the same architecture without considering the permutation invariance nature of neural networks. To mitigate this problem, the idea of solving a neuron alignment problem before applying weight averaging is discussed in [1, 24]. Recently, there are two concurrent works that benefit from the idea of neuron alignment [38] formulated and solved the assignment problem to find a permutation matrix that undoes the permutation of weight matrices. While Singh et al. [31] viewed the problem through the lens of optimal transport [26, 16] and utilized the transport map to align the weight matrices of pre-trained networks. Though both methods can fuse multiple neural networks, their applications are limited to networks with the same number of layers.

**Contributions.** In this paper, we propose a model fusion framework for fusing heterogeneous neural networks, namely, unequal width and unequal depth neural networks, which is named as Cross-Layer Alignment Fusion (CLAFusion). CLAFusion consists of three parts: cross-layer alignment, layer balancing method, and layer-wise model fusion method. Our framework provides a systematic way to combine the knowledge of pre-trained neural networks into a single fused network. In summary, our main contributions are two-fold:

1. First, we formulate the cross-layer alignment as an assignment problem using layer representation and layer similarity, then propose a dynamic programming-based algorithm to solve it. Next, we present two natural and fast methods to balance the number of layers between two networks. Overall, our framework can be generalized to fuse different types of neural network architectures by choosing the appropriate tools for each part.

2. Second, we demonstrate the efficiency of CLAFusion on three different setups. In skill transfer, our framework successfully fuses two heterogeneous neural networks trained on heterogeneous data and improves the performance over the individual networks without retraining. In addition, the result from CLAFusion serves as an efficient initialization when training residual networks. Furthermore, CLAFusion shows potential applications for model compression and knowledge distillation in the teacher-student setting.

**Organization.** The rest of the paper is organized as follows. After reviewing some background in Section 2, we introduce CLAFusion in Section 3. We study their performance in Section 4 on the image classification task with various settings and followed by discussions in Section 5. Finally, experimental settings and additional experiments are deferred to the supplementary material.
2 Background

In this section, we first recall the layer representation and layer similarity that have been widely used in applications. Then, we review available model fusion methods and their limitations. Finally, we discuss OTFusion and the challenge of applying this framework to heterogeneous neural networks.

2.1 Layer Representation and Layer Similarity

A common layer representation is the matrix of activations [19]. Activation matrix, also known as activation map, can be used as a type of knowledge to guide the training in knowledge distillation [11]. However, this representation may lead to the loss of information about weights and biases [27]. Hence, Neill et al. [27] choose the weight matrix as the layer representation of neural networks. One limitation of the mentioned paper is that they only perform the intra-network comparison. When comparing layers across two models, the matrix of activations works better. Because the weight matrix is strongly dependent on the training data of each model, it is incomparable in case of heterogeneous training datasets. On the other hand, the matrix of activations computed using the same samples is a more meaningful representation.

The neural network exhibits the same output when its neurons in each layer are permuted, this is so-called the permutation invariance nature of neural network parameters. Recall that, the permutation of neurons can be done by multiplying the weight matrix by a transport map (another matrix). Due to the permutation invariance property, a meaningful layer similarity index should be invariant to orthogonal transformations [19]. The proposed Centered Kernel Alignment (CKA) in [19] effectively identifies the relationship between layers of different architectures when the layer representation is the matrix of activations. For layer representation using the weight matrix, the Wasserstein distance along with the cosine distance and Kullback–Leibler divergence can be used to measure the dissimilarity between two layers [27].

2.2 Model fusion

It was empirically found that vanilla averaging combines the knowledge contained in several neural networks into a single fused model [35, 32]. The simple vanilla averaging, however, only works in the case when the weights of individuals networks are relatively close in the weight space. Because vanilla averaging did not study the permutation invariance nature of neural networks. As an effective remedy, several works on model fusion considered performing permutation of neurons in hidden layers before applying vanilla averaging. FBA-Wagging [1], Elastic Weight Consolidation [23], and FedMA [38] formulate the neuron association problem as an assignment problem and align the neurons. Nevertheless, those variants are not generalized to heterogeneous neural networks.

There is limited literature devoted to the discussion of fusing heterogeneous neural networks. NeuralMerger [6] is one of the few attempts to deal with this setting. Although NeuralMerger also contains a cross-layer alignment step, there are two key differences in NeuralMerger from our CLAFusion. First, their one-to-one mapping between hidden layers of two networks is hand-crafted and dedicated to specific neural network architectures. Secondly, they decompose weights into lower dimensions and use vector quantization to merge the weights of two networks. On the other hand, we introduce a systematic way to solve the cross-layer alignment problem and combining weights is done using the layer-wise model fusion method.
Figure 1: CLAFusion strategy: In the first step, the cross-layer alignment problem is solved for two pre-trained models. Two corresponding layers are surrounded by two rounded rectangles of the same color. Based on the optimal mappings obtained in the previous step, CLAFusion balances the number of layers (adding layers in this figure). The red circles and lines indicate the newly added neurons and weights (Zero weights are omitted). Finally, CLAFusion applies a layer-wise model fusion method to produce the final output.

2.3 Model fusion via Optimal Transport

Recently, Singh et al. [31] proposed OTFusion, which solves the neuron association problem based on free-support barycenters [8]. OTFusion leads to a noticeable improvement over vanilla averaging when all individual networks have the same architecture. One advantage of OTFusion over other vanilla averaging-based model fusion methods is that it can fuse networks with different widths (i.e., number of neurons) thanks to the nature of optimal transport.

The challenge of applying OTFusion to heterogeneous neural networks. OTFusion, however, is still a layer-wise approach that cannot be directly employed in heterogeneous neural networks setting. We need to find two corresponding layers, matching their neurons before averaging weight matrices. There are two challenges to this scheme. Firstly, the one-to-one mapping between layers is not available in advance. A naive one-to-one mapping of layers with the same index as layer-wise approach may cause a mismatch when the numbers of layers are different. For example, we analyze two VGG configurations [30, Table 1] with different depths: VGG11 and VGG13. The second convolution layer of VGG11 has 128 channels and an input image of size $112 \times 112$. While that of VGG13 has 64 channels and an input image of size $224 \times 224$. Secondly, assume that we have successfully found a one-to-one mapping, there still necessitates a special treatment for remaining layers that has no counterparts. Simply removing those layers has an adverse effect on the deeper network, this may cumulatively degrades the performance of the fused model.

3 Cross-layer Alignment Model Fusion

To overcome the challenges of OTFusion, in this section, we propose Cross-layer Alignment Model Fusion (in short, CLAFusion) framework for fusing heterogeneous neural networks (generally speaking, unequal width and unequal depth).

Notation. We define $[n]$ as a set of integers $\{1, \ldots, n\}$ and $I_n$ as an identity matrix of size $n \times n$. We use $A$, $B$ to denote the individual models and $F$ to denote the fused model. $l$ indicates the layer index. Layer $l$ of model $A$ has $p_A^{(l)}$ neurons and an activation function $f_A^{(l)}$. The pre-activation and activation vector at layer $l$ of model $A$ are denoted as $z_A^{(l)}$, $x_A^{(l)} \in \mathbb{R}^{p_A^{(l)}}$, respectively. The weight matrix between layers $l$ and $l-1$ of model $A$ is $W_A^{(l, l-1)}$. The following equations hold between two
We stack the pre-activation vector over $t$ samples to form a $t$-row pre-activation matrix. Let $Z_A^{(l)} \in \mathbb{R}^{t \times p_A^{(l)}}$ denote a matrix of pre-activations at layer $l$ of model A for $t$ samples, and $Z_B^{(l)} \in \mathbb{R}^{t \times p_B^{(l)}}$ denote a matrix of pre-activations at layer $l$ of model B for the same $t$ samples. The activation matrices $X_A^{(l)}, X_B^{(l)} \in \mathbb{R}^{t \times p_B^{(l)}}$ are obtained by applying the corresponding activation functions element-wise to the pre-activation matrices.

**Problem setting.** Hereafter, we consider fusing two feed-forward neural networks A and B of the same architecture family (e.g., VGG, RESNET). Two networks have the same input and output dimension but a different number of hidden layers. In each network, the hidden layer has an activation function of ReLU, which is the general setting in a lot of modern architectures. Additional work is required to handle bias terms and the batch normalization layer properly so we leave them for future work. Let $m$ and $n$ be the number of hidden layers of models A and B, respectively. Taking the input and output layers into account, the numbers of layers are $m + 2$ and $n + 2$, respectively. Without loss of generality, assume that $m \geq n$. The layer index of model A and B are \{0, 1, ..., $m + 1$\} and \{0, 1, ..., $n + 1$\}, respectively.

**General strategy.** Our framework has three components, which are illustrated in Figure 1. The first part is a cross-layer alignment which is a one-to-one mapping from hidden layers of model B to hidden layers of model A. The second part is a layer balancing method that equalizes the number of layers of two models based on the cross-layer alignment. The last part is a layer-wise model fusion method that is applied to same-sized models. The third part of our framework adopts any model fusion methods that can fuse two neural networks with the same number of layers. Next, we give more details about the first and second parts as well as providing some concrete methods.

### 3.1 Cross-layer alignment

Cross-layer alignment (CLA) is a nontrivial problem that also arises in the context of the feature-based knowledge distillation approach [41, 34, 4]. CLA requires finding a one-to-one function that matches similar layers between two models. Out of a few model fusion approaches considering CLA, NeuralMerger is based on the hand-crafted layer association, which causes a lack of generalization. To address this matter, we introduce an efficient method for solving the CLA problem.

Because the input and output layers of the two models are identical in both dimension and functionality, we only align their hidden layers. In addition, the first and last hidden layers usually play a critical role in the model performance [42]. Therefore, we directly match the first and last hidden layers of the two models. The importance of this constraint in CLA is studied in Appendix C. Furthermore, two networks are feed-forward, so the mapping is necessary to keep the sequential order of layers. Taking all into consideration, we formulate the CLA problem as follows.

**Definition 1.** Assume that we have two layer representations for hidden layers of two models as, $L_A = \{L_A^{(1)}, ..., L_A^{(n)}\}$ and $L_B = \{L_B^{(1)}, ..., L_B^{(n)}\}$. Let $C_{i,j}$ denote the cost $d$, layer dissimilarity, between two representations $L_A^{(i)}$ and $L_B^{(j)}$, i.e., $C_{i,j} = d(L_A^{(i)}, L_B^{(j)})$. The optimal CLA is a strictly increasing mapping $a : \{n\} \rightarrow \{m\}$ satisfying $a(1) = 1, a(n) = m$ and minimizing $\sum_{i=1}^{n} C_{a(i),i}$. 

$$x^{(l)} = f_A^{(l)}(z_A^{(l)}) = f_A^{(l)}(W_A^{(l,l-1)} x^{(l-1)}).$$
Figure 2: Cross-layer alignment example: Two pre-trained neural networks are given in (a). Model A has 4 hidden layers of size 4, 4, 2, 1 while model B has 3 hidden layers of size 4, 2, 1. (b) shows the cost matrix (squared Euclidean distance) between layer representations (number of neurons) for hidden layers of two networks. Three color cells represent the solution of the CLA problem. Note that the upper-left and lower-right cells are automatically chosen by the constraints on the first and last hidden layers. (c) visualizes the optimal mapping. Two rounded rectangles of the same colors represent two corresponding layers in the optimal CLA.

**Discussion.** The above problem is a special case of the (linear) unbalanced assignment problem [29]. The condition of strictly increasing ensures the sequential order of layers when matching. If we have two increasing layer representations in 1-D, the problem can be interpreted as the Partial Optimal Transport in 1-D problem with uniform weights. It can be solved efficiently in \(O(mn)\) using the proposed method in [3]. However, the increasing constraint on layer representations is quite strict and layer representations might not be in 1-D in general. On the other hand, the unbalanced assignment problem can be solved using the generalization of the Hungarian algorithm [21]. The time complexity of the Hungarian algorithm in our CLA problem is \(O(mn^2)\). Therefore, we propose an efficient algorithm based on dynamic programming to solve the CLA problem. Details are described in Algorithm 1 in Appendix A. Given the cost matrix, the time complexity of Algorithm 1 is only \(O(mn)\). Note that the optimal alignment from Definition 1 is not necessarily unique so we choose one which is obtained by backtracking. Due to space constraints, we provide the discussion on the layer representation in Appendix A.

**CLA for Convolutional neural network (CNN).** Following NeuralMerger, we do not match fully connected layers and convolution layers. It is natural that a convolution layer has different functionality from a fully connected layer. In addition, there is a lack of an appropriate way to combine the weights of a fully connected layer and a convolution layer. To the rest of this paper, we consider CNN architecture which consists of consecutive convolution layers followed by fully connected layers such as VGG [30] and RESNET [13]. The key idea is to solve the CLA for same-type layers separately then combine two mappings. Note that the combination of two strictly increasing mappings is also a strictly increasing mapping, thus it satisfies the strictly increasing requirement. We further break the convolution layers part into smaller groups and find the mapping for each pair of groups. In particular, we divide into 5 groups separated by the max-pooling layers in VGG. In RESNET, we group consecutive blocks with the same number of channels, also known as stage, and in each stage, align blocks instead of layers. For the block representation, we choose the (pre-)activation matrix of the second convolution layer in each block.
3.2 Layer balancing methods

As mentioned above, some layers in model A may have no counterparts in model B in the optimal mapping. Naturally, we have two opposite directions: reduce layers in model A or add layers into model B. But we do not know the locations of layers to reduce or add. Hence, the optimal alignment obtained in the first part comes to help us. Assume that we have already balanced the number of layers up to layer $l$ of model B. At layer $l + 1$ of model B, there are two possibilities. If $a(l + 1) - a(l) = 1$, the layer-wise fusion method is ready to apply up to layer $l + 1$. If $a(l + 1) - a(l) > 1$, we can either merge layers between $a(l)$ and $a(l + 1)$ of model A or add layers between $l$ and $l + 1$ of model B. Next, we discuss two approaches in the case $a(l + 1) - a(l) = 2$. When $a(l + 1) - a(l) > 2$, we can repeat the same approach $(a(l + 1) - a(l) - 1)$ times.

**Add layers into model B.** We add a layer $l'$ between layer $l$ and $l + 1$ of model B. The new weight matrices are defined as $W^{(l',l)}_B \leftarrow I_p$ and $W^{(l+1,l')}_B \leftarrow W^{(l+1,l)}_B \in \mathbb{R}^{p_{l+1} \times p_l}$. The new activation function is defined as $f^{(l')}_B \leftarrow f^{(a(l)+1)}_A$, which is ReLU. Because $x^{(l)}_B \succeq 0$ for all $l \in [n]$, from Equation 1 we have

$$x^{(l')}_B = f^{(l')}_B(W^{(l',l)}_B x^{(l)}_B) = ReLU(x^{(l)}_B) = x^{(l)}_B.$$ 

Therefore, the information of model B remains unchanged after adding layer $l'$. Note that the new layer is just an identity mapping, which is a trick that has been used in RESNET and NET2NET [5]. Also discussed in NET2NET, the adding layers method is a function-preserving transformation that allows us to generate an valuable initialization for training a larger network. We later examine this hypothesis in our experiments.

**Merge layers in model A.** We merge layer $a(l) + 1$ into layer $a(l)$ of model A by directly connecting layer $a(l)$ to layer $a(l + 1)$. Because $f^{(a(l)+1)}_A$ is ReLU, the new weight matrix can be
written as
\[ W_A^{(a(l+1),a(l))} = W_A^{(a(l+1),a(l)+1)} D_A^{(a(l)+1)} W_A^{(a(l)+1,a(l))}, \]

where \( D_A^{(a(l)+1)} \in \mathbb{R}^{p_A^{(a(l)+1)} \times p_A^{(a(l)+1)}} \) is an input-dependent diagonal matrix with 0s and 1s on its diagonal. The \( i^{th} \) entry in the diagonal has a value of 1 if the \( i^{th} \) entry of \( z_A^{(a(l)+1)} \) is positive and 0 otherwise. Because the actual sign of neuron \( i \) at layer \( a(l) + 1 \) varies by the input, we provide a simple estimation. Given that the neuron \( i \in [p_A^{(a(l)+1)}] \) has a pre-activation vector over \( t \) samples as \( z_{i,:} \in \mathbb{R}^t \), which is the \( i^{th} \) column of the pre-activation matrix \( Z_A^{(a(l)+1)} \). We estimate the sign of neuron \( i \) using either sign of sum (\( \text{sgn} \sum_{j=1}^{t} z_{j,i} \)) or sign of majority (i.e., 1 if at least \( t/2 \) samples have positive activation values, 0 otherwise).

**Pros and cons of balance methods.** An advantage of merging layers is that the fused model has fewer layers. However, merging layers degrades the accuracy of model A and it is slower than adding layers method that does not involve any complex calculations. On the flip side, adding layers does not affect the accuracy of model B but results in a deeper fused model. Surprisingly, merging layers shows comparatively better performance than adding layers in our experiments on MLP. Performance comparison between the two methods will be provided in Appendix C and D.1. Note that we can use more sophisticated model compression methods instead of the merging layers method. Similarly, it is possible to replace the adding layers method with a more network expanding technique [40]. Here, we just introduce two natural and fast ways to demonstrate our framework.

**Balancing the number of layers for CNN.** The same merging method does not work in the case of CNN. On the other hand, the adding layers method can be easily applied for convolution layers. For VGG, we can set all filters of a new convolution layer to identity kernels. For RESNET, we add a new block in which all filters of two convolution layers become zero kernels while the short-cut connection remains as the identity mapping. A block without short-cut connection can be simply replaced by two identity convolution layers as in VGG.

4 Experiments

To investigate the performance of our CLAFusion, we conduct experiments on three standard architectures including MLP, RESNET, and VGG. Those networks are trained to do classification on two datasets which are MNIST [22] and CIFAR10 [20]. After aligning layers of two target networks, adding layers and OTFusion are chosen to be the layer balancing method and layer-wise model fusion method in all experiments. In this section, we focus on three setups. Our method is first applied for two MLPs trained on the synthetic MNIST dataset. We then fuse a RESNET34 and a RESNET18 trained on the CIFAR10 dataset. The last one is a teacher-student setting in which VGG architecture is utilized. The detailed settings including training hyperparameters, used assets, and computational resources are specified in Appendix B. We further conduct ablation studies to validate the effectiveness of cross-layer alignment and compare two layer balancing methods in Appendix C. The experimental results for different seeds can be found in Appendix D.

4.1 Skill transfer

In skill transfer, we aim to obtain a single model that can inherit both overall and specialized skills from the two individual models. We adopt the same heterogeneous data-split technique as in [31,
Section 5.1] for two MLPs A and B. The MNIST dataset is separated into two datasets. One dataset has all images of label 4 and 10% images of other labels while the other contains the rest. The further details of skill transfer are given in Appendix D.1. We change the weight proportion of model B (also known as fusion rate in [32]) to find the weight combination that has the best performance.

**Results.** Figure 4 shows that when the weight proportion of model B is small (0.1 or 0.2), the fused model improves over both individual models. The reason for this phenomenon is that the specialist model A has higher accuracy than the generalist model B. When distributing the weight proportion fairly (0.5), the fused model performs worst due to the effect of heterogeneous training data. The fused model has the best accuracy of 91.31%, which is higher than those of models A (90.76%) and B (87.58%). This claims that the knowledge from both models has been transferred successfully to the fused model without retraining.

### 4.2 CLAFusion as an efficient initialization

Inspired by NET2NET, we use CLAFusion to generate an initialization when training the larger neural network. We apply CLAFusion to pre-trained RESNET34 and RESNET18, then finetune the fused model. The details of fusing and finetuning are described in Appendix D.2. The term $M_B$ aligned is referred to the model state after adding layers into the shallower model but before fusing with the deeper model. $M_B$ aligned can be considered as a function-preserving initialization when applying NET2NET to transform RESNET18 into RESNET34. We further finetune the pre-trained models, $M_B$ aligned and a RESNET34 from scratch to compare with our result. As another baseline, we conduct ensemble learning that calculates the average predictions over all individual models.

**Results.** Table 1 summarizes the average performance across 5 seeds, the detailed results are reported in Table 11. Retraining from the fused model gains an accuracy of 93.60, which is the highest among all initializations. This demonstrates the advantage of CLAFusion over NET2NET when initializing a large model from a pre-trained small model. Our method allows combining the
knowledge from the pre-trained large model to generate a better initialization, rather than solely relying on the knowledge of the small model. Although the result is still lower than the accuracy of ensemble learning, the fused model almost halves the computational resources.

**Applications to heterogeneous model transfer.** Heterogeneous model transfer [37] is a branch of model transfer that deals with heterogeneous neural networks. It is contrasted to homogeneous model transfer, also known as transfer learning, in which the same network architecture is used in both the pre-training and finetuning phase. In this experiment, we apply CLA in combination with OTFusion to the heterogeneous model transfer method (in short, HMT). We transfer the pre-trained RESNET18 to the pre-trained RESNET34 using different methods, then finetune and compare their performance. Details of different methods and their performance are provided in Appendix D.3. Table 2 demonstrates the average performance of different transfer methods. Using CLA improves the performance of model transfer significantly. After finetuning, the combination of CLA and OTFusion leads to an improvement of 0.77 compared to using HMT only.

### 4.3 Teacher-student fusion

In this experiment, we transfer the knowledge from the pre-trained teacher model to the student model. The teacher model has more layers and more neurons in each layer than the student model. Therefore, the teacher model usually has higher accuracy than the student one. On the other hand, the student model requires less storage and less computational resources, thus it is more suitable to deploy on resource-constrained devices. We train two VGG models on CIFAR10 dataset, then finetune the fused model. The network architectures and finetuning details can be found in Appendix D.4.

**Results.** The classification accuracies are summarized in Table 3. After retraining, the fused model yields a better performance than retraining other student models. The compression ratio between the fused model and the teacher is about 11 at a cost of reducing 1.74% accuracy. This
suggests that CLAFusion can act as a network pruning method to compress a heavy model into a lightweight one.

**Knowledge distillation.** As discussed in OTFusion, the fused model is an efficient initialization for knowledge distillation. To examine the same application of CLAFusion, we perform knowledge distillation to the above pretrained VGG models. We employ the method in [14] to match the logit distribution of the student model to the teacher model. For initialization, we consider five different choices for the student model: (a) randomly initialized $M_B$, (b) $M_B$, (c) $M_F$, (d) $M_B$ aligned, (e) randomly initialized $M_F$. The details of hyperparameters for knowledge distillation are described in Appendix D.5.

The results for retraining and knowledge distillation are reported in Table 4, further results can be found in Table 14. The first row shows the best performance for all combinations of hyperparameters. The second row is the mean of the best accuracies obtained at different temperatures. Using the fused model as an initialization achieves the best performance among different choices of initializations. It showcases the application of CLAFusion as an efficient initialization for knowledge distillation. If averaging over different temperatures, retraining the fused model (90.96) works better than vanilla distilling from the teacher model into the original student architecture (88.41, 90.73). Even the best accuracy of vanilla distillation (90.98) is slightly higher than that of retraining the fused model but comes with the cost of hyperparameter tuning. It further strengthens the claim that CLAFusion in combination with finetuning can act as a model compression method.

### 5 Conclusion

In the paper, we have presented a framework for model fusion. Our CLAFusion extends layer-wise model fusion methods to the setting of heterogeneous neural networks by solving a cross-layer alignment problem, followed by a layer balancing step. CLAFusion has been successfully applied in the setting of heterogeneous data as a skill transfer method. In addition, finetuning the fused network from CLAFusion achieves a better accuracy for RESNET trained on the CIFAR10 dataset. Furthermore, it shows potential applications for model compression and knowledge distillation.
Supplement to “Model Fusion of Heterogeneous Neural Networks via Cross-Layer Alignment”

In this supplement, we first present additional materials including the algorithm to solve CLA problem, discussion on layer representation, and some thoughts on the application of CLAFusion to multiple models scenario in Appendix A. The common settings, used assets, and computational resources are described in Appendix B. Next, we study the importance of constraints on the first and last layers as well as the efficiency of CLA in Appendix C. Finally, we provide additional results of our experiments and their detailed settings for fusing along with finetuning in Appendix D.

A Additional materials

Cross-layer alignment algorithm. We begin by introducing Algorithm 1 which is based on dynamic programming to solve the CLA problem. Given the cost matrix between layer representations of two networks, we want to find the optimal alignment from the shallower network (model B) to the deeper network (model A). The optimal alignment is a strictly increasing mapping that minimizes the total assignment cost. We denote $S(i, j)$ as the optimal assignment cost from the first $i$ layers of model B to the first $j$ layers of model A. We initialize $n \times m$ entities in matrix $S$ to be 0. Due to the strictly increasing property, when $i = j$, the optimal alignment is trivial. Assume that we have already found all optimal assignment costs before $S(i, j)(i <= j)$. There are two situations. If layer $j$ of model A is mapped to one layer in model B. Because the optimal alignment is an increasing mapping, layer $j$ of model A must be assigned to layer $i$ of model B. Otherwise, we can find another mapping that has a smaller assignment cost. The optimal assignment cost in this situation is $S(i - 1, j - 1) + C_{j,i}$. In the second situation, layer $j$ of model A is not mapped to any layers of model B. Thus, the optimal assignment cost is $S(i, j - 1)$. Considering all scenarios, the optimal assignment cost is the lower cost between $S(i - 1, j - 1) + C_{j,i}$ and $S(i, j - 1)$. After finding the optimal assignment cost $S(n, m)$ we can backtrack in the reverse direction to get the optimal CLA mapping. Note that we have two constraints on the first and last hidden layers. Therefore, $a(1) \leftarrow 1; a(n) \leftarrow m$.

Layer representation. An important process of computing the cost matrix is to design an appropriate representation for the hidden layer. We list three possible layer representations for hidden layers of two models. The first representation is the number of neurons in each layer. This encourages two layers that have a similar number of neurons to match with each other. The second choice is the activation matrix which is widely used for cross-layer comparison. We can also use the pre-activation matrix instead of the activation matrix. The third alternative is the weight matrix of the pre-trained model. The choice of the cost function (layer dissimilarity) also plays an important role in the CLA problem. For the first representation, either the Euclidean distance or its squared version is sufficient. To measure the discrepancy between two activation matrices we choose the dissimilarity index based on CKA while another option is the Wasserstein distance. Finally, the cosine distance, Kullback–Leibler divergence, and Wasserstein distance can be used in the weight matrix representation.

CLAFusion for multiple neural networks. The cross-layer alignment problem for multiple neural networks is a non-trivial task. It can be formulated as a multi-index assignment problem [33, 15]. In addition, it has some connections to the multi-marginal optimal partial optimal transport [9, 18]. It is an interesting direction for future work. Nevertheless, there are two naive approaches to extend
Algorithm 1 Cross-layer alignment algorithm

| Algorithm 1 Cross-layer alignment algorithm |
|--------------------------------------------|
| **Input:** $C = [C_{i,j}]_{i,j}$           |
| $S(i, i) ← \sum_{l=1}^{n} C_{l,l}, i \in [n]$ |
| $S(0, j) ← 0, j \in [m]$                   |
| $S(i, 0) ← 0, i \in [n]$                   |
| **for** $i = 1$ **to** $n$ **do**           |
|     **for** $j = i + 1$ **to** $m$ **do**   |
|     $S(i, j) ← \min \{S(i, j - 1), S(i - 1, j - 1) + C_{j,i}\}$ |
|     **end for**                             |
| **end for**                                |
| $a(1) ← 1; a(n) ← m; i ← n - 1; j ← m - 1$ |
| **while** $i \geq 2$ **do**                |
|     **while** $j \geq i + 1$ and $S(i, j) = S(i, j - 1)$ **do** |
|     $j ← j - 1$                            |
|     **end while**                          |
|     $a(i) = j; i ← i - 1; j ← j - 1$      |
| **end while**                              |
| **Output:** $a$                            |

CLAFusion to the case of multiple networks. Consider $K$ pre-trained models $\{M_i\}_{k=1}^{K}$. In the first approach, we can apply CLAFusion for two models iteratively $K - 1$ times to fuse $K$ models. In each iteration, we fuse a pair of models and replace them with their fused model, thus the number of models reduces by 1. The second approach is similar to what they did in OTFusion [31]. Starting with an estimation of the fused model $M_F$. We apply the first and second parts of CLAFusion $K$ times to align $K$ pre-trained models with respect to the fused model. Finally, we average the weights of those aligned networks to produce the final weights for the fused model. The choice of $M_F$ plays an important role in this approach. However, it is unclear how it is chosen in OTFusion.

**B Experiment settings**

The layer-wise model fusion is computed using the activation-based alignment strategy of OTFusion in which the pre-activation matrix instead of the activation matrix is used for the neuron measure. Because we empirically found that the pre-activation matrix often produced a more favorable performance of the fused model. The hyperparameters for pre-trained models are summarized in Table 5. Without any further specification, the random seed for training or retraining is set to its default value. The accuracy of pre-trained MLP is the accuracy of the last epoch. While the accuracies of VGG and RESNET are reported as the best performing checkpoint. For all finetuning experiments, we always chose the best record among all epochs.

**Open source code.** We adapt the official implementation of OTFusion\(^1\) [31] in our implementation. For computing the optimal transport, we use Python Optimal Transport (POT) library\(^2\) [10]. For

\(^1\)https://github.com/sidak/otfusion
\(^2\)https://github.com/PythonOT/POT
model transfer, the source code of the original paper\textsuperscript{3} \cite{37} is utilized.

**Computational resources.** All training are done on 1 Tesla V100 GPU.

### C Ablation studies

**Settings.** We compare the performance of different combinations of layer representation and layer balancing method in our framework. To prove the efficiency of the CLA step, we compare the result of fusing two models using different mappings. We also consider removing the constraint on the first and last hidden layers. We train two pairs of MLP in 5 different seeds. In both two pairs, model A has 5 hidden layers of size 400, 200, 100, 50, 25. Model B has 2 hidden layers of size 400, 100 in the first pair while it has 3 hidden layers of size 400, 200, 100 in the second pair.

**Results of the optimal mappings.** The cross-layer mappings obtained using Algorithm 1 with different combinations are given in Table 6. We observe that changing the random seed barely affects the result of CLA in this setting. When keeping both first and last layer constraints, all three combinations yield the same mappings in both pairs. For the second pair, all three combinations share the same mappings in 4 out of 5 seeds even if none of the two constraints are placed (When the random seed is 2, the optimal mapping for pre-activation matrix $+ 1$ - linear CKA is $[1, 2, 5]$ instead of $[1, 2, 3]$). On the other hand, removing both constraints in the first pair makes each combination have a different mapping.

**The effectiveness of the optimal mapping.** We fuse each pair of MLPs for all 10 possible mappings between two models A and B. For the layer balancing method, we try both adding layers and merging layers (the sign of sum estimation). The average performance of pre-trained models and the fused model across 5 random seeds are summarized in Table 7. In three out of four scenarios, the best accuracy of the fused model is achieved when imposing both the first and last layer constraints. Removing the last layer constraint decreases the performance of the fused model. When removing the first layer constraint, the accuracy drops even more significantly. Because an input image may

\begin{table}[h]
\centering
\caption{Training details}
\begin{tabular}{lccc}
\hline
 & MLP & VGG & RESNET \\
\hline
Number of epochs & 10 & 300 & 300 \\
Training batch size & 64 & 128 & 256 \\
Test batch size & 1000 & 1000 & 1000 \\
Optimizer & SGD & SGD & SGD \\
Initial LR & 0.01 & 0.05 & 0.1 \\
Momentum & 0.5 & 0.9 & 0.9 \\
Weight decay & 0.0005 & 0.0001 & 0.0001 \\
LR decay factor & 2 & 10 & 10 \\
LR decay epochs & 30,60,\ldots,270 & 150,250 & \\
Default seed & 0 & 42 & 42 \\
5 seeds & 0,1,2,3,4 & 40,41,42,43,44 & 40,41,42,43,44 \\
\hline
\end{tabular}
\end{table}

\textsuperscript{3}https://anonymous.4open.science/r/6ab184dc-3c64-4fdd-ba6d-1e5097623dfd/a_hetero_model_transfer.py
Table 6: The optimal CLA for different combinations of layer representation and cost function

| Pair | Layer representation | Cost function | Both | Last layer constraint | First layer constraint | None |
|------|-----------------------|---------------|------|-----------------------|------------------------|------|
| 1    | Number of neurons     | squared Euclidean | [1, 5] | [1, 5]                | [1, 3]                 | [1, 3] |
|      | Pre-activation matrix | 1 - linear CKA | [1, 5] | [1, 5]                | [1, 2]                 | [1, 2] |
|      | Pre-activation matrix | Wasserstein distance | [1, 5] | [2, 5]                | [1, 3]                 | [2, 3] |
| 2    | Number of neurons     | squared Euclidean | [1, 2, 5] | [1, 2, 5]           | [1, 2, 3]             | [1, 2, 3] |
|      | Pre-activation matrix | 1 - linear CKA | [1, 2, 5] | [1, 2, 5]           | [1, 2, 3]             | [1, 2, 3] |
|      | Pre-activation matrix | Wasserstein distance | [1, 2, 5] | [1, 2, 5]           | [1, 2, 3]             | [1, 2, 3] |

Table 7: Performance comparison between different combinations of mapping and balancing method

| Pair | Mapping | $M_A$ | $M_B$ | $M_F$ |
|------|---------|-------|-------|-------|
|      | Add | Merge |       |       |
| 1    | [1, 2] | 91.91 |       | 95.11 |
|      | [1, 3] | 91.95 | 94.20 |       |
|      | [1, 4] | 92.26 | 93.30 |       |
|      | [1, 5] | 92.38 | 93.30 |       |
|      | [2, 3] | 96.95 | 97.59 |       |
|      | [2, 4] | 96.95 | 97.59 |       |
|      | [2, 5] | 96.95 | 97.59 |       |
|      | [3, 4] | 96.95 | 97.59 |       |
|      | [3, 5] | 96.95 | 97.59 |       |
|      | [4, 5] | 96.95 | 97.59 |       |
| 2    | [1, 2, 3] | 92.33 | 93.90 |       |
|      | [1, 2, 4] | 92.48 | 93.41 |       |
|      | [1, 2, 5] | 92.49 | 94.00 |       |
|      | [1, 3, 4] | 90.69 | 92.21 |       |
|      | [1, 3, 5] | 96.95 | 97.75 |       |
|      | [1, 4, 5] | 96.95 | 97.75 |       |
|      | [2, 3, 4] | 96.95 | 97.75 |       |
|      | [2, 3, 5] | 96.95 | 97.75 |       |
|      | [2, 4, 5] | 96.95 | 97.75 |       |
|      | [3, 4, 5] | 96.95 | 97.75 |       |

consist of negative cell values due to normalization, adding a new layer as the first hidden layer
does not maintain the accuracy of the shallower model. Therefore, it is necessary to match the
first and last hidden layers of the two models. In addition, the mappings obtained from the CLA
step generally result in higher accuracy than other mappings, proving the efficiency of the CLA.
Comparing between layer balancing methods, the merging layers method runs slower but leads to a
higher accuracy than the adding layers in both pairs.
### D Additional experiment results

#### D.1 Skill transfer

**Settings.** We train a MLP with 3 hidden layers of size 400,200,100 for model A and a MLP with 4 hidden layers of size 400,200,100,50 for model B. The pre-activation matrix is obtained by running inference for 400 samples. We use the number of neurons as layer representation and adding layers as the balancing method. Here we assume that the training data cannot be shared due to privacy constraints, thus only the training data of model A are used for computing the activations. The weight proportion of model B, which is referred to as $w_B$, is swept over 11 different values: $w_B = \{0.0, 0.1, \ldots, 1.0\}$.

**Results.** The results of skill transfer for 5 different random seeds are reported in Table 8. The best accuracy for each seed is written in bold font. The special list model A generally has higher accuracy than the generalist model B seeds because it has been trained on all 10 labels. In 4 out of 5 seeds, the fused model improves over both individual models when the weight proportion of model B is small ($w_B = \{0.1, 0.2\}$).

**Comparison between two layer balancing methods.** For comparison purposes, we further conduct the same procedure but replacing adding layers by merging layers (the sign of sum estimation). Similar to the previous experiment, the fused model attains the best performance when the weight proportion of model B is small ($w_B = \{0.1, 0.2\}$). Figure 5 illustrates the average performance of two layer balancing methods on the skill transfer task. When averaging over 5 random seeds, both methods perform best if $w_B = 0.1$. The best accuracy of merging layers (91.57) is slightly higher than that of adding layers (91.31) even though the accuracy of $M_B$ aligned drops from 87.58 to 82.10.

#### D.2 CLAFusion as an efficient initialization

**Settings.** We train a RESNET34 and a RESNET18 on the CIFAR10 dataset. We choose the pre-activation matrix of 200 samples as layer representation. The cost function is calculated by
subtracting the linear CKA from 1. After fusing two models, the output does not immediately show any performance improvement compared to the individual models. Therefore, we perform finetuning to improve the accuracy of the fused model as observed in previous model fusion works \cite{6, 31}. The finetuning hyperparameters, which is adopted from \cite{31, Section S3.1.3}, for RESNET models are reported in Table 9.

### Baselines.
We compare CLAFusion with NET2NET. We use NET2NET to generate a RESNET34 model \((M_B \text{ aligned})\) which preserve the performance of \(M_B\). Note that \(M_B \text{ aligned}\) has the same accuracy as the smaller model and the same architecture as the fused model. In this setting, both \(M_B \text{ aligned}\) and the fused model \((M_F)\) become RESNET34.

### Results.
Finetuning from the fused model always improves the accuracy of the pre-trained models as illustrated in Table 11. In comparison with other initializations, it yields the best performance in 4 out of 5 seeds. \(M_B \text{ aligned}\), which is the result of NET2NET \cite{5} operation, only performs better than finetuning from scratch and be comparable to that of HMT. Starting from the results of NET2NET and HMT are even worse than that from the smaller pre-trained model. (Note that \(M_B \rightarrow M_A\) divergences with \(LR = 0.1\) so its accuracy is 10, which equals to random guessing.)
Table 11: Finetuning RESNET across 5 different seeds

| SEED | \(M_A\) | \(M_B\) | ENSEMBLE \(M_F\) | FINETUNING \(M_A\) | \(M_B\) | \(M_F\) | \(M_B\) ALIGNED | RANDOM RESNET34 |
|------|--------|--------|----------------|-----------------|--------|--------|----------------|----------------|
| 40   | 93.42  | 93.21  | 94.10          | 67.83           | 93.50  | 93.47  | \textbf{93.60} | 93.25          | 91.95 |
| 41   | 93.37  | 92.90  | 93.81          | 63.16           | 93.61  | 93.26  | \textbf{93.73} | 93.43          | 91.93 |
| 42   | 93.31  | 93.05  | 93.94          | 68.44           | 93.61  | 93.36  | \textbf{93.77} | 93.19          | 92.25 |
| 43   | 93.39  | 92.78  | 93.71          | 66.60           | 93.50  | 93.30  | 93.47         | 93.20          | 91.76 |
| 44   | 93.06  | 92.65  | 93.49          | 61.86           | 93.37  | 93.05  | \textbf{93.41} | 93.01          | 92.12 |
| AVG  | 93.31  | 92.92  | 93.81          | 65.58           | 93.52  | 93.29  | \textbf{93.60} | 93.22          | 92.00 |

Table 12: The results of model transfer from \(M_B\) to \(M_A\) across 5 different seeds

| METHOD  | SEED | HMT | HMT + NAIVE AVG | HMT + OTFUSION | HMT + CLA + OTFUSION |
|---------|------|-----|----------------|----------------|---------------------|
| TRANSFER | 40   | 9.55| 37.80          | 20.17          | 60.72               |
|         | 41   | 10.13| 37.66         | 17.66          | 52.09               |
|         | 42   | 10.45| 43.44         | 19.25          | 55.94               |
|         | 43   | 12.44| 39.24         | 15.20          | 55.82               |
|         | 44   | 11.37| 29.33         | 19.30          | 51.55               |
| AVG     | 10.79| 37.49| 18.32         | 55.22          |

| FINETUNE | 40   | 93.29| 93.63          | 93.61          | 93.76               |
|          | 41   | 93.14| 93.28          | \textbf{93.69} | 93.69               |
|          | 42   | 92.48| 93.16          | \textbf{93.78} | 93.68               |
|          | 43   | 93.20| 93.27          | \textbf{93.80} | 93.62               |
|          | 44   | 92.93| 83.35          | 93.41          | \textbf{93.75}     |
| AVG     | 92.93| 91.34| 93.66          | \textbf{93.70} |

D.3 Applications to heterogeneous model transfer

**Settings.** We use the same pre-trained models, layer representation, layer dissimilarity, and finetuning hyperparameters as in Appendix D.2

**Competing methods.** The heterogeneous model transfer method in the original paper [37] is used. Model parameters of the pre-trained RESNET18 are transferred to the pre-trained RESNET34. The weights that are not transferred are set to the weights of the pre-trained RESNET34. In the second method, after transferring we apply naive ensembling to the transferred RESNET34 and the pre-trained RESNET34. Naive ensembling is replaced with OTFusion in the third method. Finally, the optimal mapping from the CLA problem is utilized instead of the longest chain when the layer-to-layer transfer is performed.

**Results.** Table 11 details the results of 4 different model transfer methods. Combining CLA and OTFusion with HMT always results in a great boost (at least 17.73) in the accuracy of the transferred model. After finetuning, it gives the best performance in 3 out of 5 random seeds.

D.4 Teacher-student fusion

**Settings.** Model A has VGG13 architecture with a double number of neurons at each layer while model B has VGG11 architecture with a half number of neurons at each layer (Following
The architecture in OTFusion, we did not alter the sizes of the first and last convolution layers.) After fusing the teacher and student models, we further retrain the fused model and compare it to the retraining result of the student model. The layer measure and the layer dissimilarity are identical to Appendix D.2. We adopt the best hyperparameters as reported in [31, Section S11] for retraining. All models are retrained for 120 epochs with an initial learning rate of 0.01. Other finetuning hyperparameters are reported in Table 10.

Results. Table 13 illustrates the finetuning result of teacher and student models across 5 different seeds. The fused model $M_F$ is the most productive initialization for student models in 4 out of 5 seeds. Retraining the fused model always yields higher accuracy than continuing training the student model.

Discussion. At first glance, our approach may resemble the NET2NET operations. Although both approaches increase the depth of the student network and use the deeper student as a good initialization, there are two major differences between ours and NET2NET. Firstly, we present a systematic way of finding the location to add the identity mappings for different types of network architectures while NET2NET is manually designed for a specific type of network. Secondly, we do not enlarge the width of the student network (equivalently, use only NET2DEEPNET operation) so that the student network remains more compact than the teacher network.
D.5 Knowledge distillation

Settings. We sweep over a set of hyperparameters to choose the best combination (temperature + loss-weight factor) that maximizes the accuracy of the student model. The sets of hyperparameters for distillation follows the setting in [31, Section S12]: temperature $T = \{20, 10, 8, 4, 1\}$ and loss-weight factor $\gamma = \{0.05, 0.1, 0.5, 0.7, 0.95, 0.99\}$. For a fair comparison, the hyperparameters for training student models are identical to finetune hyperparameters in Appendix D.4.

Results. The results of distilling the teacher model into the student model are given in Table 14. For each temperature, we report the best performance along with the corresponding loss-weight factor indicated in brackets. Knowledge distillation from the fused model leads to the best accuracy in 4 out of 5 temperatures. In addition, both its average and best performance are the highest among all initializations. Naive knowledge distillation into either random initialized student models yields a much lower accuracy. This suggests that CLAFusion can serve as an efficient initialization for knowledge distillation.

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