Representation Transfer by Optimal Transport

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Abstract

Deep learning currently provides the best representations of complex objects for a wide variety of tasks. However, learning these representations is an expensive process that requires very large training samples and significant computing resources. Thankfully, sharing these representations is a common practice, enabling to solve new tasks with relatively little training data and few computing resources; the transfer of representations is nowadays an essential ingredient in numerous real-world applications of deep learning. Transferring representations commonly relies on the parameterized form of the features making up the representation, as encoded by the computational graph of these features. In this paper, we propose to use a novel non-parametric metric between representations. It is based on a functional view of features, and takes into account certain invariances of representations, such as the permutation of their features, by relying on optimal transport. This distance is used as a regularization term promoting similarity between two representations. We show the relevance of this approach in two representation transfer settings, where the representation of a trained reference model is transferred to another one, for solving a new related task (inductive transfer learning), or for distilling knowledge to a simpler model (model compression).

1 Introduction

Deep learning requires numerous training samples and significant computing resources for learning good representations of input data; computation resources may also be too limited for evaluation in real-time applications. This computational burden, however, can be alleviated by the transfer of representations with transfer learning, or by compressing the representations of large models to smaller ones. This type of representation transfer relies on learning protocols that incorporate an implicit or explicit inductive bias towards the initial representation; regularization is a typical scheme for explicitly encouraging such biases. For example, in the situation of fine-tuning from pre-trained weights, the \(-SP\) parameter regularizers [Li et al., 2018] constrain the parameters to remain in the vicinity of the initial values, in order to preserve the knowledge encoded in these parameters.

However, although a neural network is fully described by its parametric function form, regularizing in parameter space is problematic, since the relationship between the parameters of a network and the function implemented by that network does not lend itself easily to analysis. As a result, there is no relevant measure of the differences between two deep networks that is based on the parametric expression of their function. In this paper, we devise regularizers penalizing the deviations between the input representations made by two models, one of them being a reference for the trainable one.

A representation is the encoding from inputs to the features computed at a given layer, that is, the neuron outputs of that layer. Computing relevant similarities between representations thus amounts

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to comparing these mappings. However, such a comparison should be invariant of the ordering of neurons, which is irrelevant regarding representations.

We propose to compare representations through Optimal Transport (OT). OT measures the difference between two sets of elements (neurons in our case), with the crucial property of being invariant to the ordering of these elements, reflecting the property of neural networks to be invariant to permutations of neurons within a layer. We thus propose to transfer representations by encouraging small deviations from a reference representation through an OT-based regularizer.

Our regularization framework suits all the training problems aiming at retaining some knowledge from past or concurrent experiences. It may thus be applied to all the protocols considering training on a series of related distributions, such as domain adaptation or multi-task learning. We validate the effectiveness of the OT-based regularizer in the transfer learning and model compression settings and provide some analyses on the transport effect.

2 A Representation Regularizer

A representation is the encoding of data at a given layer, which results from all the computations performed upstream in the network. The parametric form of this computation being hardly amenable to analyses, we rely on the activations of neurons for comparing representations.

2.1 Rationale

Distance Between Neurons We view each neuron as a measurable and bounded elementary function whose domain is the network input space and codomain is the output space of this neuron, that is, \(a \in L^p, a : \mathbb{R}^m \rightarrow \mathbb{R}\). The similarity of two neurons \(a\) and \(b\) can then be measured by the similarity of their activations, using the \(L^p\)-norm:

\[
\|a - b\|_p^p = \int |a(x) - b(x)|^p d\mu_x = \mathbb{E}_{x \sim \mu_x} [\|a(x) - b(x)\|^p],
\]

where \(\mu_x\), the distribution of the inputs \(x\) is used as the measure. In the remainder we choose \(p = 2\).

This expectation is a natural distance between neurons viewed as elementary functions. In practice, evaluating the full integral is in general intractable. Instead, the empirical distribution, or a variant thereof, such as the empirical distribution produced by some data augmentation scheme, can be used to compute a proxy for this distance.

Representation as a Neuronal Ensemble We view neurons as functions, which can be summarized by a vector for practical reasons, but instead of considering representations as the space spanned by these functions (or vectors) at a given layer, we adopt another viewpoint, where a layer is a subset of the neurons of the network. The similarity between two subsets of neurons will be assessed by an optimal transport functional, which allows for different subset sizes, is invariant of the permutations of neurons, and is usually robust to outliers and noise [Peyré & Cuturi, 2018].

Optimal Transport of Neurons In contrast to most uses of optimal transport (OT) in machine learning, the measures defining optimal transport are not interpreted here as probability distributions. As a quick reminder, OT considers two discrete measures: \(\sum_{i=1}^n \mu_i \delta_{u_i}\) and \(\sum_{i=1}^n \nu_i \delta_{v_i}\), with \(\sum_{i=1}^n \mu_i = \sum_{i=1}^n \nu_i = 1\), and \(\delta_u\) is the Dirac measure at \(\{u\}\). Then, with a defined cost matrix \(M \in \mathbb{R}^{n \times m}\), Kantorovich’s optimal transport problem reads:

\[
\min_{P \in \Pi(\mu, \nu)} \langle P, M \rangle_F,
\]

where \(\langle \cdot, \cdot \rangle_F\) is the Frobenius product, and \(\Pi(\mu, \nu) = \{ P \in \mathbb{R}^{n \times m} : P \|_m = \mu \text{ and } P^T \|_n = \nu\}\) is the set of all admissible couplings between the two measures (\(\|_m\) is a vector of ones of size \(m\)).

We note readily that, when \(n = m\), (scaled) permutations are among the admissible couplings.

The OT problem is a well known linear program with a computational complexity of \(O(n^3 \log(n))\). Cuturi [2013] promoted a fast approximate solution to the OT problem based on the iterative Sinkhorn-Knopp algorithm, which results in a reduced complexity and can be parallelized. The algorithm performs some smoothing that may be detrimental in our setting, e.g., regarding permutations. So we use a solver relying on a proximal point algorithm IPOT [Xie et al., 2019], still based on fast Sinkhorn iterations, but converging to the exact solution of Problem 1.
where \( \hat{T} \) with fine-tuning, \( d_T \)

A

where the optimal transport plan \( \Omega \)

P

\( \text{Structural Risk Minimization} \) Our representation regularizer fits in the structural risk minimization framework by following the general formulation where a regularization functional is added to the empirical risk during learning:

\[
\min_{w} \mathbb{E}_{\mathbf{x}, \mathbf{y} \sim \hat{\mu}_{xy}} \left[ \ell(f(\mathbf{x}; w), \mathbf{y}) + \alpha \Omega(T(\mathbf{x}), \mathbf{A}(\mathbf{x}; w)) \right],
\]

where \( \hat{\mu}_{xy} \) is the empirical joint distribution of data, \( f \) is the neural network with parameters \( w \), \( \ell \) is the loss function measuring the discrepancy between the network output and the ground truth \( \mathbf{y} \), \( \Omega \) is the regularizer, and \( \alpha \) is the regularization parameter that controls the regularization strength. The regularizer proposed here takes as arguments two representations: a fixed reference representation \( T(\mathbf{x}) \), obtained from a previously trained model, and the current representation \( \mathbf{A}(\mathbf{x}; w) \), which depends on the trainable parameters \( w \) (more precisely on upstream parameters). The arguments of \( T \) and \( \mathbf{A} \) will be omitted in the following for brevity. When the learning objective (2) is optimized by an iterative learning procedure relying on mini-batches, both the loss and the regularizer are computed on the current mini-batch, resulting in a Monte Carlo estimate of the empirical risk.

2.2 OT Regularizer

The OT regularizer is computed at each iteration of the optimization algorithm, using the \( n \) examples of the current mini-batch to characterize neurons. Then, \( \mathbf{A}^{(i)}(t) \in \mathbb{R}^{d \times n} \) denotes the representation of these examples, as provided by the current activations of the \( d \) neurons of the penultimate layer at iteration \( t \); \( T \in \mathbb{R}^{d \times n} \) denotes the representation of the same examples on the fixed reference model, as computed by the activations of the \( d' \) neurons of its penultimate layer. For transfer learning with fine-tuning, \( d' = d \) and more specifically \( T = \mathbf{A}^{(0)} \); for model compression, we usually have \( d < d' \) since the student network is smaller than the teacher network. The cost matrix is then defined as:

\[
M^{(i)}_{ij} = \| \mathbf{A}^{(i)}(t) - T_j \|_2,
\]

where \( \mathbf{A}^{(i)}(t) \) are the activations on the mini-batch of neuron \( i \) of the trained model and \( T_j \) are the activations of neuron \( j \) of the fixed model.

Computing the cost on a mini-batch introduces random fluctuations on \( M^{(i)} \), which impact the optimal transport plan \( \mathbf{P}^{(i)} \). Both can be considered as stochastic estimations of the “exact” cost matrix and transport plan, computed from the whole training sample, at iteration \( t \). The situation differs from subsampling [see, e.g., Sommerfeld et al. 2019], since here the cost matrix is also approximated. As a result, the expectation of the estimated cost matrix is a smoothed version of the exact matrix that is computed from the entire training sample, resulting in a form of regularization of the exact optimal transport problem.

The OT representation regularizer is the optimal transport cost:

\[
\Omega_P = \langle \mathbf{P}^{(i)}, M^{(i)} \rangle_F = \min_{\mathbf{P} \in \Pi(\hat{\mu}, \nu)} \langle \mathbf{P}, M^{(i)} \rangle_F,
\]

where the optimal transport plan \( \mathbf{P}^{(i)} \) is obtained by the IPOT algorithm [Xie et al. 2019].

2.3 Learning

The overview of our proposed method is shown in Figure 1. During learning, a conceptually simple solution would be to compute the gradients of \( \Omega_P \) through the Sinkhorn-Knopp iterations. For nu-
merical stability and speed, we instead apply the envelop theorem [Afriat, 1971, Bonnans & Shapiro, 1998], which states here that the gradient of $\Omega$ with respect to $M^{(t)}$ can be calculated at the optimum transport plan $P^{(t)}$, as if $P^{(t)}$ did not depend on $M^{(t)}$.

A caveat is required since, relying on an iterative algorithm, we cannot guarantee that we reached an exact solution $P^{(t)}$. In another context, [Bach et al., 2004] provided guarantees on the approximate optimal solutions reached by similar optimization schemes. However, adapting these tools to the problem at hand is still an open issue. For completeness, we add that standard computation tricks are required for the numerical stability of gradients through $M_{ij}^{(t)}$ at $M_{ij}^{(t)} = 0$.

3 Related Works

Representation Transfer   Regularizing representations with respect to data distribution is very common in general transfer learning settings. In domain adaptation, [Tzeng et al., 2014, Long et al., 2015] aimed at finding a domain-invariant representations by penalizing the maximum mean discrepancy (MMD) between representations of source and target data. [Tzeng et al., 2015] and [Li & Hoiem, 2017] proposed to record the source knowledge using soft labels of target examples and preserve these soft labels for domain adaptation and lifelong learning respectively. [Courty et al., 2017] formalized domain adaptation as an optimal transport problem by adding a group-sparsity regularizer on the transport plan, and solved it with Sinkhorn algorithm [Cuturi, 2013]. More recently, [Li et al., 2019] proposed to align the feature maps between the pre-trained model and the fine-tuning one using a weighted Euclidean distance, with the weight being obtained by each neuron’s importance, for better transferring the knowledge from the source to the target. As for model compression and knowledge transfer, where the knowledge accumulated by a large teacher model has to be passed on to a small student model, knowledge distillation [Hinton et al., 2015] aligned the outputs of the teacher and student models, without considering the intermediate representations. Many works then focused on the representation transfer from the teacher model to the student model, e.g., by directly regressing the student representations from the student model on the teacher’s [Romero et al., 2014, Yim et al., 2017], using a variational approximation of the mutual information for pairing the teacher and student representations [Ahn et al., 2019], or considering the dissimilarities between the representations of the examples of (large) mini-batches, thereby providing invariance with respect to isometries [Tung & Mori, 2019, Park et al., 2019].

Transport of Examples vs Transport of Features   Many works considered samples from the data distribution as in most usages of optimal transport in machine learning [Arjovsky et al., 2017, Genevay et al., 2018, Courty et al., 2017]. We emphasize that our regularizer considers the transportation of features/neurons, which seems more appealing for coping with the permutations of neurons during the transfer process, and is radically different from the transportation of examples. In our case, the number of neurons $d$ is thus the effective number of samples and the batch size $n$ is the length of each neuron.

Other Transport of Features   Few works have considered transporting neurons. [Huang & Wang, 2017] distilled the learned knowledge to a smaller student model by regularizing feature maps. Given one image, they proposed to minimize the MMD between two sets of feature maps, in order to transfer the activated regions to the student model. This approach differs from ours in that it focuses on the selected/activated regions of a neuron to guide the student model to preserve the region similarities, whereas we focus on knowledge preservation while being invariant to permutations, so as to account for neuron swapping during transfer. [Singh & Jaggi, 2019] also consider matching neurons from several trained networks with optimal transport. Although they handle permutations as we do, their work differs from ours in the following aspects: we are considering a dynamic transfer process where the OT-based regularizer is updated during the transfer process, directly impacting learning, whereas their use of optimal transport mainly consists in finding a static barycenter for averaging weights of two learned models, in order to combine meaningfully those models into a single one, then possibly allowing fine-tuning, but without updating transport in the meantime.

Neurons as Vectors of Activations   We view neurons as functions and summarize them as vectors of activations for practical reasons, and a representation is viewed as the set of neurons. This approach of modeling neurons and representations has also been applied elsewhere, yet mainly for
analyzing the representations of neural networks. Li et al. [2015] used the statistics of the activations on each neuron to measure the similarity between neurons, and found the permuted neurons between independently trained networks with bipartite matching. [Raghu et al. [2017] proposed to combine singular value decomposition and canonical correlation analysis (CCA) to analyze the similarity between representations learned from independently trained networks. This modeling is also found in Wang et al. [2018], Morcos et al. [2018], Kornblith et al. [2019]. While those works start from the same modeling, they basically consider a representation as the space spanned by the neuron vectors, which differs from ours: we directly assess the transport cost or dissimilarity between sets of neurons, by optimal transport, instead of comparing two spaces spanned by neurons. Another major difference is that the OT regularizer proposed in this paper is optimized together with the main loss function during training for a better representation transfer, whereas all the above works analyze the learned representations by measuring the similarity between representations of trained networks.

4 Experiments

This section provides experimental results assessing the relevance of the OT-based regularizer in transfer learning and in model compression. Some ablation studies will rely on the degraded regularizers presented below. Regarding run-times, solving the OT problem results in additional computations. In our implementation, with mini-batches of 64 examples, our OT-based regularizer is 2.7 more time consuming than when using a standard parameter regularizer. Using the IPOT algorithm is 1.6 faster than solving directly the linear program for computing the optimal transport Problem (4).

4.1 Two Degraded Representation Regularizers

Identity Mapping (No Transport) When $d' = d$, a simple and usual transport plan is to consider that there is no transport, that is, there is no neuron switching between the two representations. This amounts to replace the learned transport plan $\mathbf{P}^{(t)}$ by the fixed $d \times d$ scaled identity matrix:

$$\Omega_I = \frac{1}{d} \mathbf{I}_d, \mathbf{M}^{(t)}_F.$$ (5)

This regularizer resembles the $L^2$-SP regularizer, in the sense that the role of each neuron in the two representations is assumed to be identical. Replacing $\Omega_P$ by this regularizer in the experiments shows the value of allowing learned transport plans.

Uniform Transport We consider another simple fixed transport plan: the uniform joint law between the two sets of neurons, which was shown to be the limiting solution for the entropy regularized OT problem as the regularization parameter goes to infinity [Peyré & Cuturi, 2018, Proposition 4.1]:

$$\Omega_U = \langle \frac{1}{d} \mathbf{I}_{d \times d'}, \mathbf{M}^{(t)}_F \rangle_F,$$ (6)

where $\mathbf{I}_{d \times d'}$ is a $d \times d'$ matrix of ones. This regularizer encourages the matching of means and variance reduction. Contrary to the identity mapping, it does not assume a specific role to each neuron. It globally encourages all neurons of the learned representation to approach the mean of the reference representation. Replacing $\Omega_P$ by this regularizer in the experiments shows the value of looking for a coherent matching between individual neurons, instead of considering the matching of simple properties between the two populations of neurons.

4.2 Transfer Learning

For transfer learning, we consider a series of target image classification problems (Aircraft100, Birds200, Cars196, Dogs120 and Foods101), using ImageNet [Deng et al., 2009] as the source task. We use ResNet [He et al., 2016a] as the backbone network because of its important use in transfer learning. We follow standard experimental protocols for comparing regularization schemes during fine-tuning; experimental details are deferred to Appendix A. The baselines consist in applying no regularization during fine-tuning, applying the standard $L^2$ norm regularizer, also known as weight-decay, denoted $\Omega_{L^2}$, penalizing the $L^2$ distance from the pre-trained model, $\Omega_{L^2-SP}$ [Li et al., 2018], where -SP refers to the starting point of the optimization process.
We chose ResNet-1001 [He et al., 2016b] and WRN-28-10 [Zagoruyko & Komodakis, 2016] as teacher networks, and ResNet-56 and a slim version of ResNet-56 as student networks. ResNet-56-Slim is identical to ResNet-56 except that it has half as many channels at each layer. The temperature used in knowledge distillation is selected from {4, 5, 10}. All regularization hyperparameters

| Aircraft100 | Birds200 | Cars196 | Dogs120 | Foods101 | mean |
|------------|---------|---------|---------|----------|------|
| none       | 83.95±0.37 | 80.64±0.30 | 90.21±0.12 | 69.53±0.29 | 86.85±0.09 | 82.18 |
| $\Omega_{L^2}$ | 83.64±0.40 | 80.57±0.36 | 90.51±0.19 | 69.79±0.29 | 86.86±0.09 | 82.27 |
| $\Omega_{L^2-SP}$ | 83.94±0.39 | 81.10±0.24 | 90.75±0.12 | 77.05±0.19 | 87.15±0.14 | 83.99 |
| $\Omega_f$ | 83.44±0.45 | 82.25±0.19 | 90.40±0.20 | 77.15±0.17 | 86.88±0.07 | 84.02 |
| $\Omega_U$ | 84.74±0.52 | 81.53±0.27 | 91.49±0.14 | 71.40±0.28 | 86.90±0.10 | 83.21 |
| $\Omega_P$ (ours) | 85.19±0.36 | 82.37±0.24 | 91.29±0.13 | 77.43±0.13 | 87.06±0.06 | 84.67 |

Table 1: Average classification accuracy (in %) on transfer learning for no-regularized, $L^2$, $L^2$-SP and $\Omega_P$ regularized fine-tuning. The last column reports the average accuracy on all tasks.

There are 33 three-layer residual units in ResNet-101; our OT regularizer is applied to the higher level representation, that is, the penultimate layer. We also penalize an additional layer to preserve intermediate presentations; penalizing the activations of the 19th residual unit performs best among \{9th, 19th, 29th\}. All regularization hyper-parameters are selected by cross-validation from a range of five logarithmically spaced values from $10^{-4}$ to 1.

Table 1 shows the results of fine-tuning on the five target datasets. We report the average accuracy and its standard deviation on five different runs. Since we use the same data and the same starting point, these runs only differ due to the randomness of stochastic gradient descent and to the random initialization of the parameters from the last layer. Our results confirm that the $L^2$-SP regularizer is a better choice than the standard weight decay or the absence of regularization. Our OT regularizer is always better, except on Foods101, where all methods are within 0.3%. Overall, the benefit of the OT regularizer over $L^2$-SP is about half that of $L^2$-SP over simple fine-tuning.

The identity mapping $\Omega_f$ behaves similarly to $L^2$-SP, suggesting that assuming fixed transport plans and asking representations to be alike produces similar effects than constraining the parameters. $\Omega_P$ is always better than the identity mapping: penalizing the deviations from the reference representation in terms of sets of neurons is beneficial.

The uniform transport $\Omega_U$ is sometimes quite effective, reaching the highest accuracy on Cars196, but sometimes completely unproductive, being very bad on Dogs120. On this dataset, the role of the neurons hardly changes during the $L^2$-SP fine-tuning (cf. Figure 2), and this is very badly handled by the sole preservation of the global mean of the initial representation. In comparison, $\Omega_P$ always yields best or close to the best performances: matching individual neurons is a more stable and advantageous strategy than matching populations of neurons.

### 4.3 Model Compression

Knowledge distillation aims at compressing a complex model or ensemble into a single smaller model [Hinton et al., 2015]. For this purpose, the training objective follows the general regularized form (2), where the regularization term uses the smoothed response of the large teacher model as the reference for the smaller student model:

$$\Omega_{KD} = KL(g^\tau(x), f^\tau(x; w)),$$

with $g_h^\tau(x) = \frac{\exp(h_k(x)/\tau)}{\sum_{k=1}^K \exp(h_k(x)/\tau)}$, (7)

where $KL(p, q)$ is the Kullback-Leibler divergence of $q$ from $p$, $g^\tau$ and $f^\tau$ are the smoothed responses of the teacher and student model respectively. The smoothed responses are computed from the vector of activations of the final softmax layer, denoted here $(h_1(x), \ldots, h_K(x))$ ($K$ is the number of classes). The so-called temperature $\tau$, which is usually set to 1, provides smoother responses when set higher, by spreading the non-saturated regions of the softmax, thereby putting stronger emphasis on the boundaries of the classes estimated by the teacher model. Though several alternatives have been developed, conventional knowledge distillation remains a solid baseline for assessing our representation regularizers [see, e.g., Tian et al., 2020, Ruffy & Chahal, 2019]. We compare here our representation regularizer to knowledge distillation on the CIFAR datasets.

We chose ResNet-1001 [He et al., 2016b] and WRN-28-10 [Zagoruyko & Komodakis, 2016] as teacher networks, and ResNet-56 and a slim version of ResNet-56 as student networks. ResNet-56-Slim is identical to ResNet-56 except that it has half as many channels at each layer. The temperature used in knowledge distillation is selected from {4, 5, 10}. All regularization hyperparameters
Table 2: Average classification accuracy (in %) on model compression on CIFAR-10 and CIFAR-100. Letters L, M, S, and W denote the large ResNet-1001, the medium ResNet-56, the small ResNet-56-Slim and the wide WRN-28-10 respectively. The line labeled “none” is for directly training the student model, without teacher.

|          | CIFAR10       |          | CIFAR100      |
|----------|---------------|----------|---------------|
|          | L → S | L → M | W → S | W → M | L → S | L → M | W → S | W → M |
| none     | 91.8±0.2 | 93.6±0.2 | 91.8±0.2 | 93.6±0.2 | 69.6±0.3 | 73.7±0.2 | 69.6±0.3 | 73.7±0.2 |
| $\Omega_I$ | 94.5±0.2 |         |         |         | 73.2±0.1 |         |         |         |
| $\Omega_E$ | 91.8±0.2 | 93.8±0.1 | 91.8±0.3 | 93.7±0.2 | 70.0±0.4 | 74.2±0.3 | 69.8±0.3 | 73.9±0.4 |
| $\Omega_{ED}$ | 92.4±0.1 | 94.0±0.2 | 92.3±0.3 | 94.1±0.1 | 71.0±0.1 | 74.8±0.2 | 70.7±0.2 | 75.6±0.2 |
| $\Omega_{EP}$ (ours) | 92.8±0.1 | 94.5±0.1 | 92.5±0.2 | 94.7±0.1 | 70.6±0.2 | 75.6±0.1 | 70.5±0.2 | 75.6±0.2 |

Table 2 summarizes the results. For CIFAR-10, our representation regularizer consistently improves upon knowledge distillation, with improvements that are of the same order of magnitude as the improvement brought by knowledge distillation itself upon the standard learning of the student network, without teacher. For CIFAR-100, the results are less decisive: representation transfer tends to perform slightly better for the medium-sized student network whereas knowledge distillation is slightly better for the slim student network. Knowledge distillation looks at representations through the lens of smoothed estimations of probabilities. This view is highly relevant for classification purposes, but provides a very rough summary when the representation space is large relative to the number of classes. In these situations, represented here by all scenarios for CIFAR10 and by the widest student networks for CIFAR100, a more exhaustive transfer of representations is more advantageous. Note that OT regularization can also be readily applied to other learning problems such as regression or ranking.

The identity mapping $\Omega_I$ is only applicable for representation spaces of same dimension. The strategy is effective on CIFAR10, but fails on CIFAR100, probably due to optimization problems arising from the constraints pertaining to the fixed matching between neurons.

Overall, the uniform transport $\Omega_U$ has little value, with only slight improvements compared to learning the student model from scratch. Here, the mean of the initial representation is too vague an indication to guide learning.

5 Analyses of Transport Solutions

Is Transport Necessary to Compare Representations? Our first analysis aims to quantify the importance of neuron permutations in a standard fine-tuning process used for transfer learning. To measure this importance, we rely on optimal transport, but now used as a tool for post hoc analysis, whereas fine-tuning uses the $L^2$-SP regularization that implicitly assumes that neurons maintain their original role throughout learning. The change of the role of neurons before and after fine-tuning is measured by the trace of the transport plan computed from the representations of the pre-trained model and the fine-tuned model; OT being used here as an analysis tool, the cost matrix is computed on a large representative dataset (3,000 validation examples).
Figure 2 shows the trace of the transport plans versus the layer depth. The trace of the transport plan at a given layer is one if the activation of its neurons after fine-tuning remains more similar to their initial activation than to any other one. More generally, it can be interpreted as the ratio of fine-tuned neurons matching their initial activation. As expected, the trend is non-increasing with depth: the role of a neuron is more likely to change if the role of its ancestors in the computation graph change. Among the five target datasets, Dogs120 is the only one where these roles remain unchanged throughout the network. This is because the training set of Dogs120 is a subset of ImageNet, with classes also belonging to ImageNet. The dataset Birds200 has also some overlap with ImageNet, but the classification of bird species of Birds200 is more fine-grained; the representation of Birds200 after transfer learning is slightly changed. As for Foods101, Cars196 and Aircraft100, neurons all along the network have permutated to some extent after transfer learning.

This analysis shows that, though $L^2$-SP implicitly assumes a perfect matching between the initial and the fine-tuned representation features during fine-tuning, neurons may swap around, possibly in large proportions. This should be appropriately accounted for by the regularizer, as shown by the performances with the identity mapping $\Omega_I$ (5), that are very similar to the ones of $L^2$-SP.

**Effective Transport.** Our OT-based regularizer computes an estimation of the permutations among neurons. Figure 3 displays the evolution of $\text{tr}(P(t))$ on the penultimate layer during fine-tuning with $\Omega_P$. The trace of this optimal transport plan is a noisy estimate of the proportion of neuron permutations in that layer since it is based only on the examples in the current mini-batch. The computed optimal transport plan is very different from the identity mapping for all datasets except Dogs120. These traces demonstrate that the identity is not always the optimal choice for regularizing the neurons during transfer learning, in order to preserve the representation, and the choice from the optimal transport may be a better option for addressing this problem. Figure 3 also shows that optimal transport does not behave similarly on all datasets, but the optimal transport regularizer able to find a distinct transform to each of the five target datasets and obtain better results than identity mapping or uniform transport.

6 Discussion and Conclusion

A feed-forward neural network learns a series of representations of the input at each layer, through the activations of the neurons of that layer. Each neuron can be fully described by its analytic parametric expression that is hardly amenable to an analysis: computing a relevant similarity between neurons from their parameters is difficult. We thus opt for a more direct functional view of neurons, for which relevant similarities are well-defined. Representations themselves are then formed by concatenating neurons. This concatenation is commonly carried out by considering that representations are vector spaces of neurons. Considering representations as being formed by a set of neurons provides analyses that are invariant to the order of neurons in a layer, which is desirable property since a neural network is invariant to that neuron permutations. This set representation avoids the problems encountered when considering neurons as ordered features defining a representation space. In particular, it avoids the use of factorial analysis [Raghu et al., 2017] to compare representations.

Based on this view, we proposed a novel regularizer operating on pairs of representations. This regularizer measures the difference between the sets of neurons in the two representations, using optimal transport. It is invariant to the ordering of neurons, and tolerant of non overlapping supports of features. Our regularizer performs well compared to state of the art on two different tasks, and we show the benefit of the transport effect by comparing to two degraded versions of the transport.

\footnote{The test set of Dogs120 was edited to suppress intersections with ImageNet training set (see A.1.1).}


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A Experimental Details

We describe here the experimental protocol implemented in the companion source code.

A.1 Transfer Learning

A.1.1 Datasets

ImageNet [Deng et al., 2009] is used as the source task for its large-scale representation of many categories, to ensure that the source knowledge is sufficiently rich. As for the target tasks, we have chosen several classification problems on data sets widely used for transfer learning: aircraft models [Maji et al., 2013], birds [Welinder et al., 2010], cars [Krause et al., 2013], dogs [Khosla et al., 2011] and foods [Martinel et al., 2018]. Each target dataset is split into training and test sets following the suggestion of their creators, except for Stanford Dogs 120, whose original test set is a subset of the ImageNet training set. Since the ImageNet training set is used as the source dataset, evaluation in Dogs120 should avoid using the same images, so we use a part of the ImageNet validation set, which contains only those 120 breeds of dogs, for evaluating the performance on Dogs120.

A.1.2 Pre-Processing and Post-Processing

We follow the data processing techniques in [He et al., 2016a]. The pre-processing of images involves image resizing and data augmentation. We keep the aspect ratio of images and resize the images with the shorter edge being 256. We adopt random blur, random mirror and random crop to \(224 \times 224\) for data augmentation during training. Regarding testing, we resize the image in the same ways as training, and then we average the scores of 10 cropped patches (the center patch, the four corner patches, and all their horizontal reflections) for getting the final decision.

A.1.3 Optimization

All optimisations start from a starting point where all layers are initialized with the parameters obtained on ImageNet, except the last layer, whose size is modified according the number of classes in the target task. The latter is initialized randomly.

The optimization solver is Stochastic Gradient Descent (SGD) with momentum 0.9. We run for 9000 iterations and divide the learning rate by 10 after 6000 iterations for all target tasks, except for Foods101 for which we run for 16000 iterations and divide the learning rate after 8000 and 12000 iterations. The batch size is 64. The learning rates are set by cross-validation from \{0.005, 0.01, 0.02, 0.04\}.

A.2 Model Compression

For both training and testing, we follow the protocol of [He et al., 2016a]. For all networks, we run stochastic gradient descent with momentum 0.9, for 160K iterations with batch size 64. The learning rate is set to 0.1 at the beginning of training and divided by 10 at 80K and 120K iterations. A standard weight decay with a small regularization parameter (10\(^{-4}\)) is applied for all trainings.