More Is More - Narrowing the Generalization Gap by Adding Classification Heads

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Abstract

Overfit is a fundamental problem in machine learning in general, and in deep learning in particular. In order to reduce overfit and improve generalization in the classification of images, some employ invariance to a group of transformations, such as rotations and reflections. However, since not all objects exhibit necessarily the same invariance, it seems desirable to allow the network to learn the useful level of invariance from the data. To this end, motivated by self-supervision, we introduce an architecture enhancement for existing neural network models based on input transformations, termed 'TransNet', together with a training algorithm suitable for it. Our model can be employed during training time only and then pruned for prediction, resulting in an equivalent architecture to the base model. Thus pruned, we show that our model improves performance on various data-sets while exhibiting improved generalization, which is achieved in turn by enforcing soft invariance on the convolutional kernels of the last layer in the base model. Theoretical analysis is provided to support the proposed method.

1. Introduction

Deep neural network models currently define the state of the art in many computer vision tasks, as well as speech recognition and other areas. These expressive models are able to model complicated input-output relations. At the same time, models of such large capacity are often prone to overfit, i.e. performing significantly better on the training set as compared to the test set. This phenomenon is also called the generalization gap.

We propose a method to narrow this generalization gap. Our model, which is called TransNet, is defined by a set of input transformations. It augments an existing Convolutional Neural Network (CNN) architecture by allocating a specific head - a fully-connected layer which receives as input the penultimate layer of the base CNN - for each input transformation (see Fig. 1). The transformations associated with the model’s heads are not restricted a priori.

The idea behind the proposed architecture is that each head can specialize in a different yet related classification task. We note that any CNN model can be viewed as a special case of the TransNet model, consisting of a single head associated with the identity transformation. The overall task is typically harder when training TransNet, as compared to the base CNN architecture. Yet by training multiple heads, which share the convolutional backbone, we hope to reduce the model’s overfit by providing a form of regularization.

In Section 3 we define the basic model and the training algorithm designed to train it (see Alg. 1). We then discuss the type of transformations that can be useful when learning to classify images. We also discuss the model’s variations: (i) pruned version that employs multiple heads during training and then keeps only the head associated with the identity transformation for prediction; (ii) the full version where all heads are used in both training and prediction.

Theoretical investigation of this model is provided in Section 4, using the dihedral group of transformations ($D_4$) that includes rotations by 90° and reflections. We first prove...
that under certain mild assumptions, instead of applying each dihedral transformation to the input, one can compile it into the CNN model’s weights by applying the inverse transformation to the convolutional kernels. In order to obtain intuition about the inductive bias of the model’s training algorithm in complex realistic frameworks, we analyze the model’s inductive bias using a simplified framework.

In Section 5 we describe our empirical results. We first introduce a novel invariance score (IS), designed to measure the model’s kernel invariance under a given group of transformations. IS effectively measures the inductive bias imposed on the model’s weights by the training algorithm. To achieve a fair comparison, we compare a regular CNN model traditionally trained, to the same model trained like a TransNet model as follows: heads are added to the base model, it is trained as a TransNet model, and then the extra heads are pruned. We then show that training as TransNet improves test accuracy as compared to the base model. This improvement was achieved while keeping the optimized hyper-parameters of the base CNN model, suggesting that further improvement by fine tuning may be possible. We demonstrate the increased invariance of the model’s kernels when trained with TransNet.

Our Contribution
- Introduce TransNet - a model inspired by self-supervision for supervised learning that imposes partial invariance to a group of transformations.
- Introduce an invariance score (IS) for CNN convolutional kernels.
- Theoretical investigation of the inductive bias implied by the TransNet training algorithm.
- Demonstrate empirically how both the full and pruned versions of TransNet improve accuracy.

2. Related Work

Overfit. A fundamental and long-standing issue in machine learning, overfit occurs when a learning algorithm minimizes the train loss, but generalizes poorly to the unseen test set. Many methods were developed to mitigate this problem, including early stopping - when training is halted as soon as the loss over a validation set starts to increase, and regularization - when a penalty term is added to the optimization loss. Other related ideas, which achieve similar goals, include dropout [27], batch normalization [14], transfer learning [25, 29], and data augmentation [3, 33].

Self-Supervised Learning. A family of learning algorithms that train a model using self generated labels (e.g. the orientation of an image), in order to exploit unlabeled data as well as extract more information from labeled data. Self training algorithms are used for representation learning, by training a deep network to solve pretext tasks where labels can be produced directly from the data. Such tasks include colorization [32, 16], placing image patches in the right place [22, 7], inpainting [23] and orientation prediction [10]. Typically, self-supervision is used in unsupervised learning [8], to impose some structure on the data, or in semi-supervised learning [31, 12]. Our work is motivated by RotNet, an orientation prediction method suggested by [10]. It differs from [31, 12], as we allocate a specific classification head for each input transformation rather than predicting the self-supervised label with a separate head.

Equivariant CNNs. Many computer vision algorithms are designed to exhibit some form of invariance to a transformation of the input, including geometric transformations [20], transformations of time [28], or changes in pose and illumination [24]. Equivariance is a more relaxed property, exploited for example by CNN models when translation is concerned. Work on CNN models that enforces strict equivariance includes [26, 9, 1, 21, 2, 5]. Like these methods, our method seeks to achieve invariance by employing weight sharing of the convolution layers between multiple heads. But unlike these methods, the invariance constraint is soft. Soft equivariance is also seen in works like [6], which employs a convolutional layer that simultaneously feeds rotated and flipped versions of the original image to a CNN model, or [30] that appends rotation and reflection versions of each convolutional kernel.

3. TransNet

Notations and definitions Let $X = \{(x_i, y_i)\}_{i=1}^n$ denote the training data, where $x_i \in \mathbb{R}^d$ denotes the i-th data point and $y_i \in [K]$ its corresponding label. Let $D$ denote the data distribution from which the samples are drawn. Let $\mathcal{H}$ denote the set of hypotheses, where $h_\theta \in \mathcal{H}$ is defined by its parameters $\theta$ (often we use $h = h_\theta$ to simplify notations). Let $\ell(h, x, y)$ denote the loss of hypothesis $h$ when given sample $(x, y)$. The overall loss is:

$$\mathcal{L}(h, X) = \mathbb{E}_{(x, y) \sim D}[\ell(h, x, y)]$$

Our objective is to find the optimal hypothesis:

$$h^* := \arg \min_{h \in \mathcal{H}} \mathcal{L}(h, X)$$

For simplicity, whenever the underlying distribution of a random variable isn’t explicitly defined we use the uniform distribution, e.g. $\mathbb{E}_{a \in A}[a] = 1/|A| \sum_{a \in A} a$.

3.1. Model architecture

The TransNet architecture is defined by a set of input transformations $T = \{t_j\}_{j=1}^m$, where each transformation
The transformation $t \in \mathbb{T}$ operates on the inputs $(t : \mathbb{R}^d \to \mathbb{R}^d)$ and is associated with a corresponding model’s head. Thus each transformation operates on datapoint $x$ as $t(x)$, and the transformed data-set is defined as:

$$t(X) := \{(t(x_i), y_i)\}_{i=1}^n$$  (3)

Given an existing NN model $h$, henceforth called the base model, we can split it to two components: all the layers except for the last one denoted $f$, and the last layer $g$ assumed to be a fully-connected layer. Thus $h = g \circ f$. Next, we enhance model $h$ by replacing $g$ with $|\mathbb{T}| = m$ heads, where each head is an independent fully connected layer associated with a specific transformation $t \in \mathbb{T}$. Formally, each head is defined by $h_t = g_t \circ f$, and it operates on the corresponding transformed input as $h_t(t(x))$.

The full model, with its $m$ heads, is denoted by $h_{\mathbb{T}} := \{h_t\}_{t \in \mathbb{T}}$, and operates on the input as follows:

$$h_{\mathbb{T}}(x) := \mathbb{E}_{t \in \mathbb{T}}[h_t(t(x))]$$

The corresponding loss of the full model is defined as:

$$L_T(h_{\mathbb{T}}, X) := \mathbb{E}_{t \in \mathbb{T}}[L(h_t, t(X))]$$  (4)

Note that the resulting model (see Fig. 1) essentially represents $m$ models, which share via $f$ all the weights up to the last fully-connected layer. Each of these models can be used separately, as we do later on.

### 3.2. Training algorithm

Our method uses SGD with a few modifications to minimize the transformation loss (4), as detailed in Alg. 1. Relying on the fact that each batch is sampled i.i.d. from $\mathcal{D}$, we can prove (see Lemma 1) the desirable property that the sampled loss $L_T(h_{\mathbb{T}}, \mathbb{B})$ is an unbiased estimator for the transformation loss $L_T(h_{\mathbb{T}}, X)$. This justifies the use of Alg. 1 to optimize the transformation loss.

**Lemma 1.** Given batch $\mathbb{B}$, the sampled transformation loss $L_T(h_{\mathbb{T}}, \mathbb{B})$ is an unbiased estimator for the transformation loss $L_T(h_{\mathbb{T}}, X)$.

**Proof.**

$$
\mathbb{E}_{\mathbb{B} \sim \mathcal{D}^b}[L_T(h_{\mathbb{T}}, \mathbb{B})] \\
= \mathbb{E}_{\mathbb{B} \sim \mathcal{D}^b}[\mathbb{E}_{t \in \mathbb{T}}[L(h_t, t(\mathbb{B}))]] \\
= \mathbb{E}_{t \in \mathbb{T}}[\mathbb{E}_{\mathbb{B} \sim \mathcal{D}^b}[L(h_t, t(\mathbb{B}))]] \quad (\mathbb{B} \sim \mathcal{D}^b) \\
= \mathbb{E}_{t \in \mathbb{T}}[L(h_t, t(X))] \\
= L_T(h_{\mathbb{T}}, X)
$$

### 3.3. Transformations

**Which transformations should we use?** Given a specific data-set, we distinguish between transformations that occur naturally in the data-set versus such transformations that do not. For example, horizontal flip can naturally occur in the CIFAR-10 data-set, but not in the MNIST data-set. TransNet can only benefit from transformations that do not occur naturally in the target data-set, in order for each head to learn a well defined and non-overlapping classification task. Transformations that occur naturally in the data-set are often used for data augmentation, as by definition they do not change the data domain.

**Dihedral group $D_4$.** As mentioned earlier, the TransNet model is defined by a set of input transformations $\mathbb{T}$. We constrain $\mathbb{T}$ to be a subset of the dihedral group $D_4$, which includes reflections and rotations by multiplications of $90^\circ$. We denote a horizontal reflection by $r$, and a counter-clockwise $90^\circ$ rotation by $r^i$. Using these two elements we can express all the $D_4$ group elements as $\{r^i, m \circ r^i \mid i \in 0, 1, 2, 3\}$. These transformations were chosen because, as mentioned in [10], their application is relatively efficient and does not leave artifacts in the image (unlike scaling or change of aspect ratio).

Note that these transformations can be applied to any 3D tensor while operating on the height and width dimensions, including an input image as well as the model’s kernels. When applying a transformation $t$ to the model’s weights $\theta$, denoted $t(\theta)$, the notation implies that $t$ operates on the model’s kernels separately, not affecting other layers such as the fully-connected ones (see Fig. 2).
3.4. Model variations

Once trained, the full TransNet model can be viewed as an ensemble of $m$ shared classifiers. Its time complexity is linear with the number of heads, almost equivalent to an ensemble of the base CNN model, since the time needed to apply each one of the $D_4$ transformations to the input is negligible as compared to the time needed for the model to process the input. Differently, the space complexity is almost equivalent to the space complexity of only one base CNN model\(^1\).

We note that one can prune each one of the model’s heads, thus leaving a smaller ensemble of up to $m$ classifiers. A useful reduction prunes all the model’s heads except one, typically the one corresponding to the identity transformation, which yields a regular CNN that is equivalent in terms of time and space complexity to the base architecture used to build the TransNet model. Having done so, we can evaluate the effect of the TransNet architecture’s and its training algorithm’s inductive bias solely on the training procedure, by comparing the pruned TransNet to the base CNN model (see Section 5).

4. Theoretical Analysis

In this section we analyze theoretically the TransNet model. We consider the following basic CNN architecture:

$$h_{\theta} = g \circ l_{inv} \circ \prod_{i=1}^{k} c_i$$

where $g$ denotes a fully-connected layer, $l_{inv}$ denotes an invariant layer under the $D_4$ transformations group (e.g., a global average pooling layer - GAP), and $\{c_i\}_{i \in [k]}$ denote convolutional layers\(^2\). The TransNet model extends the basic model by appending additional heads:

$$h_{\tau, \theta} = \{g_t \circ l_{inv} \circ \prod_{i=1}^{k} c_i\}_{t \in \mathbb{T}}$$ (7)

We denote the parameters of a fully-connected or a convolutional layer by subscripts of $w$ (weight) and $b$ (bias), e.g., $g(x) = w \cdot x + b$.

4.1. Transformation compilation

Transformations in the dihedral $D_4$ group satisfy another important property, expressed by the following proposition:

**Proposition 1.** Let $h_{\theta}$ denote a CNN model where the last convolutional layer is followed by an invariant layer under the $D_4$ group. Then any transformation $t \in D_4$ applied to the input image can be compiled into the model’s weights $\theta$ as follows:

$$\forall t \in D_4 \forall x \in \mathbb{X} : h_{\theta}(t(x)) = h_{e^{-t}(\theta)}(x)$$ (8)

**Proof.** By induction on $k$ we can show that:

$$\prod_{i=1}^{k} c_i \circ t(x) = t \circ \prod_{i=1}^{k} t^{-1}(c_i)(x)$$ (9)

(see Fig. 2). Plugging (9) into (6), we get:

$$h_{\theta}(t(x)) = g \circ l_{inv} \circ \prod_{i=1}^{k} c_i \circ t(x)$$

$$= g \circ l_{inv} \circ t \circ \prod_{i=1}^{k} t^{-1}(c_i)(x)$$

$$= g \circ l_{inv} \circ \prod_{i=1}^{k} t^{-1}(c_i)(x) \quad (l_{inv} \circ t = l_{inv})$$

$$= h_{e^{-t}(\theta)}(x)$$

\[\square\]

**Implication.** The ResNet model [11] used in our experiments satisfies the pre-condition in the proposition stated above, since it contains a GAP layer [19] after the last convolutional layer, and GAP is invariant under $D_4$.

4.2. Single vs. multiple headed model

In order to acquire intuition regarding the inductive bias implied by training algorithm Alg. 1, we consider two cases, a single and a double headed model, trained with the same training algorithm. A single headed model is a special case of the full multi-headed model, where all the heads share weights $h_t(t(x)) = h(t(x))$ for all $t$, and the loss in line 5 of Alg. 1 becomes $\mathcal{L}(h, \mathbb{B}) = \frac{1}{b} \sum_{k=1}^{b} \ell(h(t(x_k), y_k)$.

\[1\] Each additional head adds 102K ($\sim$0.45\%) and 513K ($\sim$0.90\%) extra parameters to the basic ResNet18 model when training CIFAR-100 and ImageNet-200 respectively.

\[2\] While each convolutional layer may be followed by ReLU and Batch Normalization [14] layers, this doesn’t change the analysis so we obviate the extra notation.
As it’s hard to analyze non-convex deep neural networks, we focus on a simplified framework and consider a convex optimization problem where the loss function is convex w.r.t. the model’s parameters $\theta$. We also assume that the model’s transformations in $\mathbb{T}$ form a group $^3$.

**Single Headed model Analysis.** In this simplified case, we can prove the following strict proposition:

**Proposition 2.** Let $h_\theta$ denote a CNN model satisfying the pre-condition of Prop. 1, and $\mathbb{T} \subset D_4$ a transformations group. Then the optimal transformation loss $L_{\mathbb{T}}$ (see Eq. 4) is obtained by invariant model’s weights under the transformations $\mathbb{T}$. Formally:

$$\exists \theta : (\forall t \in \mathbb{T} : \theta = t(\theta_0)) \wedge (\theta_0 \in \arg \min_{\theta} L_{\mathbb{T}}(\theta, X))$$

**Proof.** To simplify the notations, henceforth we let $\theta$ denote the model $h_\theta$.

$$L_{\mathbb{T}}(\theta, X) = \mathbb{E}_{t \in \mathbb{T}}[L(\theta, t(X))] = \mathbb{E}_{t \in \mathbb{T}}[\mathbb{E}(x, y) \sim \mathcal{D}[l(t^{-1}(\theta), x, y))] \quad \text{(by Prop. 1)}$$

$$\geq \mathbb{E}(x, y) \sim \mathcal{D}[\mathbb{E}_{t \in \mathbb{T}}[L(t^{-1}(\theta), x, y))] \quad \text{(Jensen’s inequality)}$$

$$= \mathbb{E}(\bar{\theta}, X) \sim \mathcal{D}[\mathbb{E}_{t \in \mathbb{T}}[L(t^{-1}(\theta), x, y))] \quad \text{(by Prop. 1)}$$

$$= L(\bar{\theta}, X)$$

Above we use the fact that $\bar{\theta}$ is invariant under $\mathbb{T}$ since $\mathbb{T}$ is a group and thus $t_0 \mathbb{T} = \mathbb{T}$, hence:

$$t_0(\bar{\theta}) = t_0(\mathbb{E}_{t \in \mathbb{T}}[L(t(\theta))]) = \mathbb{E}_{t \in \mathbb{T}}[t_0 \circ t(\theta)] = \mathbb{E}_{t \in \mathbb{T}}[t(\theta)] = \bar{\theta} \quad \blacksquare$$

**Double headed model.** In light of Prop. 2 we now present a counter example, which shows that Prop. 2 isn’t true for the general TransNet model.

**Example 1.** Let $\mathbb{T} = \{t_1 = r^0, t_2 = m \circ r^2\} \subset D_4$ denote the transformations group consisting of the identity and the vertical reflection transformations. Let $h_{\mathbb{T}, \theta} = \{h_i = g_i \circ GAP \circ c_i\}_{i=1}^2$ denote a double headed TransNet model, which comprises a single convolutional layer (1 channel in and 2 channels out), followed by a GAP layer and then 2 fully-connected layers $\{g_i\}_{i=1}^2$, one for each head. Each $g_i$ outputs a vector of size 2. The data-set $X = \{(x_1, y_1), (x_2, y_2)\}$ consists of 2 examples:

$$x_1 = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, y_1 = 1, \quad x_2 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix}, y_2 = 2$$

Note that $x_2 = t_2(x_1)^4$.

Now, assume the model’s convolutional layer $c$ is composed of 2 invariant kernels under $\mathbb{T}$, and denote it by $c_{inv}$. Let $i \in 1, 2$, then:

$$h_i(x_2) = h_i(t_2(x_1)) = g_i \circ GAP \circ c_{inv} \circ t_2(x_1) = g_i \circ GAP \circ c_{inv}(x_1) = h_i(x_1)$$

In this case both heads predict the same output for both inputs with different labels, thus:

$$L(h_i, t_i(X)) > 0 \implies L(h_{\mathbb{T}, \theta}, X) > 0$$

In contrast, by setting $c_w = (x_1, x_2), c_b = (0, 0)$, which isn’t invariant under $\mathbb{T}$, as well as:

$$g_{1,w} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, g_{1,b} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, g_{2,w} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, g_{2,b} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

we obtain:

$$L(h_i, t_i(X)) = 0 \implies L(h_{\mathbb{T}, \theta}, X) = 0.$$  

We may conclude that the optimal model’s kernels aren’t invariant under $\mathbb{T}$, as opposed to the claim of Prop. 2.

**Discussion.** The intuition we derive from the analysis above is that the training algorithm (Alg. 1) implies an invariant inductive bias on the model’s kernels as proved in the single headed model, while not strictly enforcing invariance as shown by the counter example of the double headed model.

### 5. Experimental Results

**data-sets.** For evaluation we used the 5 image classification data-sets detailed in Table 1. These diverse data-sets allow us to evaluate our method across different image resolutions and number of predicted classes.

**Implementation Details.** We employed the ResNet18 [11] architecture for all the data-sets except for ImageNet-200, which was evaluated using the ResNet50 architecture (see Appendix A for more implementation details).

**Notations.**

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$^3\mathbb{T}$ being a group is a technical constraint needed for the analysis, not required by the algorithm.

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$^4$This example may seem rather artificial, but in fact this isn’t such a rare case. E.g., the airplane and the ship classes, both found in the CIFAR-10 data-set, that share similar blue background.
Next, we evaluate the full TransNet model, where all models are identical to the "base-CNN" model regardless of their ensembles, across all the data-sets listed in Table 1.

To denote an ensemble of the models above, we add a suffix of a number in parentheses, e.g. T2-CNN (3) is an ensemble of 3 T2-CNN models.

5.1. Models accuracy, comparative results

We now compare the accuracy of the "base-CNN", "PTm-CNN" and "Tm-CNN" models, where m = 2, 3, 4 denotes the number of heads of the TransNet model, and their ensembles, across all the data-sets listed in Table 1.

Models with the same space and time complexity. First, we evaluate the pruned TransNet model by comparing the "PTm-CNN" models with the "base-CNN" model, see Table 2. Essentially, we evaluate the effect of using the TransNet model only for training, as the final "PTm-CNN" models are identical to the "base-CNN" model regardless of m. We can clearly see the inductive bias implied by the training procedure. We also see that TransNet training improves the accuracy of the final "base-CNN" classifier across all the evaluated data-sets.

Models with similar space complexity, different time complexity. Next, we evaluate the full TransNet model by comparing the "Tm-CNN" models with the "base-CNN" model, see Table 3. Despite the fact that the full TransNet model processes the (transformed) input m times more as compared to the "base-CNN" model, its architecture is not significantly larger than the base-CNN’s. The full TransNet adds to the "base-CNN" a negligible number of parameters, in the form of its multiple heads. Clearly the full TransNet model improves the accuracy as compared to the "base-CNN" model, and also as compared to the pruned TransNet model. Thus, if the additional runtime complexity during test is not an issue, it is beneficial to employ the full TransNet model during test time.

Ensembles: models with similar time complexity, different space complexity. Here we evaluate ensembles of pruned TransNet models, and compare them to a single full TransNet model that can be seen as a space-efficient ensemble: full TransNet generates m predictions with only 1/m parameters, where m is the number of TransNet heads. Results are shown in Fig. 3. Clearly an ensemble of pruned TransNet models is superior to an ensemble of base CNN models, suggesting that the accuracy gain achieved by the pruned TransNet model doesn’t overlap with the accuracy gain achieved by using an ensemble of classifiers. Furthermore, we observe that the full TransNet model exhibits competitive accuracy results, with 2 and 3 heads, as compared to an ensemble of 2 or 3 base CNN models respectively. This is achieved while utilizing 1/2 and 1/3 as many parameters respectively.

### Table 1: The data-sets used in our experiments. The dimension of each example, a color image, is \( \text{dim} \times \text{dim} \times 3 \) pixels. ImageNet200 represents 200 classes from ImageNet (same classes as in [17]).

| Name          | Classes | Train/Test dim Samples | dim |
|---------------|---------|-------------------------|-----|
| CIFAR-10 [15] | 10      | 50K/10K                 | 32  |
| CIFAR-100 [15]| 100     | 50K/10K                 | 32  |
| ImageNette [13]| 10     | 10K/4K                  | 224 |
| ImageWoof [13]| 10      | 10K/4K                  | 224 |
| ImageNet-200  | 200     | 260K/10K                | 224 |

Figure 3: Model accuracy as a function of the number of instances (X-axis) processed during prediction. Each instance requires a complete run from input to output. An ensemble includes: m independent base CNN classifiers for "CNN"; m pruned TransNet trained with 2 heads for "PT2-CNN"; and one TransNet model with m heads, where m is the ensemble size, for "Tm-CNN".

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5In our experiments we chose the head associated with the identity transformation when evaluating a pruned TransNet. Note, however, that we could have chosen the best head in terms of accuracy, as it follows from Prop. 1 that its transformation can be compiled into the model’s weights.
**Accuracy vs. generalization.** In Fig. 3 we can see that 2 heads improve the model’s performance across all data-sets, 3 heads improve it on most of the data-sets, and 4 heads actually reduce performance on most data-sets. We hypothesize that too many heads impose too strict an inductive bias on the model’s kernels. Thus, although generalization is improved, test accuracy is reduced due to insufficient variance. Further analysis is presented in the next section.

5.2. Generalization

We’ve seen in Section 5.1 that the TransNet model, whether full or pruned, achieves better test accuracy as compared to the base CNN model. This occurs despite the fact that the transformation loss $\mathcal{L}_T(h_T, X)$ minimized by the TransNet model is more demanding than the loss $\mathcal{L}(h, X)$ minimized by the base CNN, and appears harder to optimize. This conjecture is justified by the following Lemma:

**Lemma 2.** Let $h_T$ denote a TransNet model that obtains transformation loss of $a := \mathcal{L}_T(h_T, X)$. Then there exists a reduction from $h_T$ to the base CNN model $h$ that obtains a loss of at most $a$, i.e. $\mathcal{L}(h, X) \leq a$.

**Proof.** $a = \mathcal{L}_T(h_T, X) = E_{t \in T}[\mathcal{L}(h_{\theta_t}, t(X))]$, so there must be a transformation $t \in T$ s.t. $\mathcal{L}(h_{\theta_t}, t(X)) \leq a$. Now, one can compile the transformation $t$ into $h_{\theta_t}$ (see Prop. 1) and get a base CNN: $h = h_{t^{-1}(\theta)}$ which obtains $\mathcal{L}(h, X) = \mathcal{L}(h_{t^{-1}(\theta)}, t(X)) = \mathcal{L}(h_{\theta_t}, t(X)) \leq a$. □

Why is it, then, that the TransNet model achieves overall better accuracy than the base CNN? The answer lies in its ability to achieve a better generalization.

In order to measure the generalization capability of a model w.r.t. a data-set, we use the ratio between the test-set and train-set loss, where a lower ratio indicates better generalization. As illustrated in Fig. 4, clearly the pruned TransNet models exhibit better generalization when compared to the base CNN model. Furthermore, the generalization improvement increases with the number of TransNet model heads, which are only used for training and then pruned. The observed narrowing of the generalization gap occurs because, although the TransNet model slightly increases the training loss, it more significantly decreases the test loss as compared to the base CNN.

**5.3. Kernel invariance**

What characterizes the beneficial inductive bias implied by the TransNet model and its training algorithm Alg. 1?
To answer this question, we investigate the emerging invariance of kernels in the convolutional layers of the learned network, w.r.t. the TransNet transformations set $T$.

We start by introducing the "Invariance Score" ($IS$), which measures how invariant a 3D tensor is w.r.t. a transformations group. Specifically, given a convolutional kernel denoted by $w$ (3D tensor) and a set of transformations group $T$, the $IS$ score is defined as follows:

$$IS(w, T) := \min_{u \in INV_T} \|w - u\|$$  \hspace{1cm} (11)$$

where $INV_T$ is the set of invariant kernels (same shape as $w$) under $T$, i.e. $INV_T := \{ u : u = t(u) \ \forall t \in T \}$.

**Lemma 3.** $\arg \min_{u \in INV_T} \|w - u\| = E_{t \in T}[t(w)]$

**Proof.** Let $u$ be an invariant tensor under $T$. Define $f(u) := \|w - u\|^2$. Note that $\arg \min_{u \in INV_T} \|w - u\| = \arg \min_{u \in INV_T} f(u)$.

$$f(u) = \|w - u\|^2$$

$$= E_{t \in T}[\|w - t(u)\|^2] \quad (u \text{ is invariant under } T)$$

$$= E_{t \in T}[\|t^{-1}(w) - u\|^2]$$

$$= E_{t \in T}[\|t(w) - u\|^2] \quad (T = T^{-1})$$

$$= E_{t \in T} \left[ \sum_{i=1}^{\text{size}(w)} (t(w)_i - u_i)^2 \right]$$

Where index $i$ runs over all the tensors’ elements. Finally, we differentiate $f$ to obtain its minimum:

$$\frac{\partial f}{\partial u_i} = E_{t \in T}[-2(t(w)_i - u_i)] = 0$$

$$\implies u_i = E_{t \in T}[t(w)_i] \implies u = E_{t \in T}[t(w)] \quad \Box$$

Lemma 3 gives a closed-form expression for the IS gauge:

$$IS(w, T) = \|w - E_{t \in T}[t(w)]\|$$  \hspace{1cm} (12)$$

Equipped with this gauge, we can inspect the invariance level of the model’s kernels w.r.t. a transformations group. Note that this measure allows us to compare the full TransNet model with the base CNN model, as both share the same convolution layers. Since the transformations of the TransNet model don’t necessarily form a group, we use the minimal group containing these transformations - the group of all rotations $\{r^i\}_{i=1}^4$.

In Fig. 5 we can see that the full TransNet model “T2-CNN” and the base CNN model demonstrate similar invariance level in all the convolutional layers but the last one. In Fig. 6, where the distribution of the IS score over the last layer of 4 different models is fully shown, we can more clearly see that the last convolutional layer of full TransNet models exhibits much higher invariance level as compared to the base CNN. This phenomenon is robust to the metric used in the IS definition, with similar results when using “Pearson Correlation” or “Cosine Similarity”.

The increased invariance in the last convolutional layer is monotonically increasing with the number of heads in the TransNet model, which is consistent with the generalization capability of these models (see Fig 4).

![Figure 5: CIFAR-100 results, plotting the distribution of the IS scores (mean and std) for the kernels in each layer of the different models. Invariance is measured w.r.t. the group of 90° rotations.](image)

![Figure 6: CIFAR-100 results, plotting the full distribution of the IS scores for the kernels in the last (17-th) layer of the different models. Invariance is measured w.r.t. the group of 90° rotations.](image)

5.4. Ablation Study

Our method consists of 2 main components - the TransNet architecture as well as the training algorithm Alg. 1. To evaluate the accuracy gain of each component we consider two variations:
nel’s invariance level, i.e. serving that each data-set achieves its own optimal kernel’s invariance on the one hand, while the multi-head architecture encourage the model to capture meaningful orientation information on the other hand.

6. Summary

We introduced a model inspired by self-supervision, which includes a base CNN model attached to multiple heads, each corresponding to a different transformation from a fixed set of transformations. The self-supervised aspect of the model is crucial, as the chosen transformations must not occur naturally in the data. When the model is pruned back to match the base CNN, it achieves better test accuracy and improved generalization, which is attributed to the increased invariance of the model’s kernels in the last layer. We observed that excess invariance, while improving generalization, eventually curtails the test accuracy.

We evaluated our model on various image data-sets, observing that each data-set achieves its own optimal kernel’s invariance level, i.e. there’s no optimal number of heads for all data-sets. Finally, we introduced an invariance score gauge (IS), which measures the level of invariance achieved by the model’s kernels. IS may be leveraged to determine the optimal invariance level, as well as potentially function as an independent regularization term.

Table 4: Accuracy of the ablation study models with the same space and time complexity, these 4 models enable us to evaluate the effect of the TransNet architecture as well as the TransNet algorithm separately. Mean and standard error for 3 repetitions are shown.

| MODEL      | CIFAR-10 | CIFAR-100 | ImageNette | ImageWoof | ImageNet-200 |
|------------|----------|-----------|------------|------------|--------------|
| base-CNN   | 95.57 ± 0.08 | 76.56 ± 0.16 | 92.97 ± 0.16 | 87.27 ± 0.15 | 84.39 ± 0.07 |
| Alg. only  | 93.85 ± 0.63 | 76.64 ± 0.69 | 92.60 ± 0.07 | 87.64 ± 0.30 | 80.58 ± 0.08 |
| Arch. only | 95.68 ± 0.05 | 76.98 ± 0.13 | 93.49 ± 0.03 | 87.40 ± 0.74 | 84.47 ± 0.13 |
| PT2-CNN    | 95.99 ± 0.07 | 79.33 ± 0.15 | 93.84 ± 0.14 | 88.09 ± 0.30 | 85.17 ± 0.10 |

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Appendix
A. Implementation details

We employed the ResNet [11] architecture, specifically the ResNet18 architecture for all the data-sets except for the ImageNet-200 which was evaluated using the ResNet50 architecture. It’s important to notice that we haven’t changed the hyper-parameters used by the regular CNN architecture which TransNet is based on. This may strengthen the results as one may fine tune these hyper-parameters to suit best the TransNet model.

We used a weight decay of 0.0001 and momentum of 0.9. The model was trained with a batch size of 64 for all the data-sets except for ImageNet-200 where we increased the batch size to 128. We trained the model for 300 epochs, starting with a learning rate of 0.1, divided by 10 at the 150 and 225 epochs, except for the ImageNet-200 model which was trained for 120 epochs, starting with a learning rate of 0.1, divided by 10 at the 40 and 80 epochs. We normalized the images as usual by subtracting the image’s mean and dividing by the image’s standard deviation (color-wise).

We employed a mild data augmentation scheme - horizontal flip with probability of 0.5. For the CIFAR data-sets we padded each dimension by 4 pixels and cropped randomly (uniform) a 32×32 patch from the enlarged image while for the ImageNet family data-sets we cropped randomly (uniform) a 224×224 patch from the original image.

In test time, we took the original image for the CIFAR data-sets and a center crop for the ImageNet family data-sets. The prediction of each model is the mean of the model’s output on the original image and a horizontally flipped version of it. Note that a horizontal flip occurs naturally in every data-set we use for evaluation and therefore isn’t associated with any of the TransNet model’s heads that we evaluate.

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