DENOISING AUTOENCODER WITH MODULATED LATERAL CONNECTIONS LEARNS INVARIANT REPRESENTATIONS OF NATURAL IMAGES

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ABSTRACT

Suitable lateral connections between encoder and decoder are shown to allow higher layers of a denoising autoencoder (dAE) to focus on invariant representations. In regular autoencoders, detailed information needs to be carried through the highest layers but lateral connections from encoder to decoder relieve this pressure. It is shown that abstract invariant features can be translated to detailed reconstructions when invariant features are allowed to modulate the strength of the lateral connection. Three dAE structures with modulated and additive lateral connections, and without lateral connections were compared in experiments using real-world images. The experiments verify that adding modulated lateral connections to the model 1) improves the accuracy of the probability model for inputs, as measured by denoising performance; 2) results in representations whose degree of invariance grows faster towards the higher layers; and 3) supports the formation of diverse invariant poolings.

1 INTRODUCTION

Denoising autoencoders (dAE; Vincent et al., 2008) provide an easily accessible method for unsupervised learning of representations since training can be based on simple back-propagation and a quadratic error function. An autoencoder is built from two mappings: an encoder that maps corrupted input data to features, and a decoder that maps the features back to denoised data as output. Thus, in its basic form, autoencoders need to store all the details about the input in its representation.

Deep learning has used unsupervised pretraining (see Bengio [2013] for a review) but recently purely supervised learning has become the dominant approach at least in cases where a large number of labeled data is available (e.g., Ciresan et al. [2010], Krizhevsky et al. [2012]).

One difficulty with combining autoencoders with supervised learning is that autoencoders try to retain all the information whereas supervised learning typically loses some. For instance, in classification of images, spatial pooling of activations throws away some of the location details while retaining identity details. In that sense, the unsupervised and supervised training are pulling the model in very different directions.

From a theoretical perspective, it is clear that unsupervised learning must be helpful at least in a semi-supervised setting. Indeed, Kingma et al. [2014] obtained very promising results with variational autoencoders. This raises hopes that the same could be achieved with simpler dAEs.

Recently, Valpola (2015) proposed a variant of the denoising autoencoder that can lose information. The novelty is in lateral connections that allow higher levels of an autoencoder to focus on invariant abstract features and in layer-wise cost function terms that allow the network to learn deep
Figure 1: Examples of two-hidden-layer models: (a) denoising autoencoder and (b) Ladder network with lateral connections. Illustration of ratio, $\alpha$, of $h^{(2)}$ size to $h^{(1)}$ size (right) with hidden layers of sizes 2 and 8. Ratio of $\alpha = 1.0$ corresponds to hidden layers of equal size (a and b).

Valpola (2015) hypothesized that modulated lateral connections support the development of invariant features and provided initial results with artificial data to back up the idea. As seen in Figure 1, information can flow from the input to the output through alternative routes, and the details no longer need to be stored in the abstract representation. This is a step closer to being compatible with supervised learning which can select which types of invariances and abstractions are relevant for the task at hand.

In this paper, we focus on investigating the effects of lateral connections. We extend earlier results with experiments using natural image data and make comparisons with regular denoising autoencoders without lateral connections in Section 2. We show the following:

- The proposed structure attains a better model of the data as measured by ability to denoise. There are good reasons to believe that this indicates that the network has captured a more accurate probabilistic model of the data since denoising is one way of representing distributions (Bengio et al., 2013).
- Including the modulated lateral connections changes the optimal balance between the sizes of layers from balanced to bottom heavy.
- The degree of invariance of the representations grows towards the higher levels in all tested models but much faster with modulated lateral connections. In particular, the higher levels of the model seem to focus entirely on invariant representations whereas the higher levels of the regular autoencoder have a few invariant features mixed with a large number of details.
- Modulated lateral connections guide the layer above them to learn various types of poolings. The pooled neurons participate in several qualitatively different poolings that are each selective and invariant to different aspects of the input.

1.1 Invariant features through pooling

There are typically many sources of variation which are irrelevant for classification. For example, in object recognition from images, these sources could include position, orientation and scale of the recognized object and illumination conditions. In order to correctly classify new samples, these sources of variation are disregarded while retaining information needed for discriminating between different classes. In other words, classification needs to be invariant to the irrelevant transformations.

A simple but naive way to achieve such invariance would be to list all the possible realizations of objects under various transformations, but this is not usually practical due to the vast amounts of possible realizations. Also, this does not offer any generalization to new objects.

A useful solution is to split the generation of invariance into more manageable parts by representing the inputs in terms of features which are each invariant to some types of transformations. Since different kinds of objects can be represented by the same set of features, this approach makes it possible to generalize the invariances to new, unseen objects.

So rather than listing all the possible realizations of individual objects, we can list possible realizations of their constituent features. Invariance is achieved by retaining only the information about
whether any of the possible realizations is present and discarding information about which one exactly. Such an operation is known as pooling and there are various ways of implementing it. In the case of binary inputs, OR operation is a natural choice. There are many ways to generalize this to continuous variables, including maximum operation (Riesenhuber & Poggio, 1999) or summation followed by a concave function (Fukushima, 1979).

While pooling achieves invariance to irrelevant transformations, the features also need to be discriminative along relevant dimensions. This selectivity is often achieved by coincidence detection, i.e. by detecting the simultaneous presence of multiple input features. In the binary case, it can be implemented by an AND operation. In the continuous case, possibilities include extensions of the AND operation, such as product or summation followed by a convex function, but also lateral inhibition (i.e., competition) among a set of feature detectors. All of these operations typically produce sparse coding where the output features are sensitive to specific combinations of input features. Since this type of coding tends to increase the number of features, it is also known as feature expansion.

The idea of alternating pooling and feature expansion dates at least back to Hubel & Wiesel (1962) who found that the early stages of visual processing in the cat cerebral cortex have alternating steps of feature expansion, implemented by lateral competition among so called simple cells, and invariance-generating poolings by so called complex cells. In such hierarchies of alternating steps, the degree of invariance grows towards the higher levels. Cortical processing also includes various normalizations, a feature which has also been included in some models (e.g., Fukushima, 1979).

There are various ways of finding poolings that generate invariances (from specialized to general):

1. Invariance by design. For instance, invariance to translation and small deformations is achieved by pooling shifted versions of a feature (Fukushima, 1979). Similar pooling operations are now popular in convolutional neural networks (see, e.g., Schmidhuber, 2015).

2. Invariance to hand-crafted transformations. The transformations are applied to input samples (e.g., image patches can be shifted, rotated, scaled or skewed, and colors or contrast can be modified) and pooling is then learned by requiring the output to stay constant over the transformation. This category includes supervised learning from inputs deformed by various transformations.

3. Invariance to transformations over time. Relies on nature to provide transformations as sequences during which the underlying feature (e.g., identity of object) changes slower than the transformation (e.g., Foldiákov, 1991).

4. Invariance by exploiting higher-order correlations within individual samples. This is how supervised learning can find poolings: target labels correlate nonlinearly with inputs. There are also unsupervised methods that can do the same. For example, subspace ICA can find complex-cell like poolings for natural images (Hyvärinen & Hoyer, 2000).

We focus on the last type: exploiting higher-order correlations. Very few assumptions are made so the method is very general but it is also possible to combine this approach with supervised learning or any of the more specialized ways of generating invariances.

1.2 Denoising Autoencoders

Autoencoder networks have a natural propensity to conserve information and are therefore well suited for feature expansion. Autoencoder networks consist of two parameterized functions, encoding $f$ and decoding $g$. Function $f$ maps from input space $x$ to feature space $h$, and $g$ in turn maps back to input space producing a reconstruction, $\hat{x}$, of the original input, when the training criterion is to minimize the reconstruction error. This enables learning of features in an unsupervised manner.

Denoising autoencoder (Vincent et al., 2008) is a variant of the traditional autoencoder, where the input $x$ is corrupted with noise and the objective of the network is to reconstruct the original uncorrupted input $x$ from the corrupted $\tilde{x}$. Bengio et al. (2013) show that denoising autoencoders implicitly estimate the data distribution as the asymptotic distribution of the Markov chain that alternates between corruption and denoising. This interpretation provides a solid probabilistic foundation for them. Consequently, the denoising teaching criterion enables learning of over-complete representations, a property which is crucial for adding lateral connections to an autoencoder.
As with normal feedforward networks, there are various options for choosing the cost function but, in the case of continuous input variables, a simple choice is
\[
C = \|\hat{x} - x\|^2 = \|g(f(\hat{x})) - x\|^2.
\] (1)

Denoising autoencoders can be used to build deep architectures either by stacking several on top of each other and training them in a greedy layer-wise manner (e.g., [Bengio et al., 2007]) or by chaining several encoding and decoding functions and training all layers simultaneously. For \(L\) layers and encoding functions \(f^{(l)}\), the encoding path would compose as \(f = f^{(L)} \circ f^{(L-1)} \circ \ldots \circ f^{(1)}\).

We denote the intermediate feature vectors by \(h^{(l)}\) and corresponding decoded, denoised, vectors by \(\hat{h}^{(l)}\). Figure 1a depicts such a structure for \(L = 2\). Encoding functions are of the form
\[
h^{(l)} = f^{(l)}(h^{(l-1)}) = \phi(W_f^{(l)}h^{(l-1)} + b_f^{(l)}), \quad 1 \leq l \leq L,
\] (2)
starting from \(h^{(0)} = \hat{x}\). The corresponding decoding functions are
\[
\hat{h}^{(L)} = h^{(L)}
\]
(3)
\[
\hat{h}^{(l)} = g^{(l)}(\hat{h}^{(l+1)}) = \phi(W_g^{(l)}\hat{h}^{(l+1)} + b_g^{(l)}), \quad 1 \leq l \leq L-1,
\] (4)
\[
\hat{x} = g^{(0)}(\hat{h}^{(1)}) = W_g^{(0)}\hat{h}^{(1)} + b_g^{(0)}.
\] (5)

Function \(\phi\) is the activation function and typically left out from the lowest layer.

2 Experiments

The tendency of regular autoencoders to preserve information seems to be at odds with the development of invariant features which relies on poolings that selectively discard some types of information. Our goal here is to investigate the hypothesis that suitable lateral connections allow autoencoders to discard details from higher layers and only retain abstract invariant features because the decoding functions \(g^{(l)}\) can recover the discarded details from the encoder.

We compare three different denoising autoencoder structures: basic denoising autoencoder and two variants with lateral connections. We experimented with various model definitions prior to deciding the ones defined in Section 2.1 because there are multiple ways to merge lateral connections.

2.1 Models with Lateral Connections

We add lateral connections from \(h^{(l)}\) to \(\hat{h}^{(l)}\) as seen in Figure 1b. Autoencoders trained without noise would short-circuit the input and output with an identity mapping. Now that input contains noise, there is pressure to find meaningful higher-level representations that capture regularities and allow for denoising. Note that the encoding function \(f\) has the same form as before in Eq. 2.

2.1.1 Additive Lateral Connections

As the first version, we replace the decoding functions in Eq. 3-4 with
\[
\hat{h}^{(L)} = g^{(L)}(h^{(L)}) = h^{(L)} + b_a^{(L)} \odot \sigma(a^{(L)} \odot h^{(L)} + b_b^{(L)}),
\] (6)
\[
\hat{h}^{(l)} = g^{(l)}(h^{(l)}, \hat{h}^{(l+1)}) = (h^{(l)} + b_a^{(l)} \odot \sigma(a^{(l)} \odot h^{(l)} + b_b^{(l)}) + \phi(W_g^{(l)}\hat{h}^{(l+1)} + b_g^{(l)}),
\] (7)
where \(\odot\) is the element-wise (i.e., Hadamard) product, \(a^{(l)}\), \(b_a^{(l)}\), and \(b_b^{(l)}\) are learnable parameter vectors along with weights and biases, and \(\sigma\) is a sigmoid function to ensure that the modulation stays within reasonable bounds. Function \(g^{(0)}\) stays affine as in Eq. 5. The functional form of Eq. 6, with element-wise decoding, is motivated by element-wise denoising functions that are used in denoising source separation ([Särkelä & Valpola, 2005]) and corresponds to assuming the elements of \(h\) independent a priori.
2.1.2 Modulated lateral connections

Our hypothesis is that an autoencoder can learn invariances efficiently only if its decoder can make good use of them. Valpola (2015) proposed connecting the top-down mapping inside the sigmoid term of Eq. (7), a choice motivated by optimal denoising in hierarchical variance models.

Our final proposed model includes the encoding functions in Eq. (2), the top connection $g^{(L)}$ in Eq. (6), bottom decoding function $g^{(0)}$ as in Eq. (5), but the middle decoding functions are defined as

$$g^{(l)}(h^{(l)}, \hat{h}^{(l+1)}) = (h^{(l)} + b^{(l)}_g) \odot \sigma (a^{(l)} \odot h^{(l)} + W^{(l)}_g \hat{h}^{(l+1)} + b^{(l)}_b), \quad 1 \leq l \leq L - 1. \quad (8)$$

In contrast to additive lateral connection in Eq. (7), the signal from the abstract layer $\hat{h}^{(l+1)}$ is used to modulate the lateral connection so that the top-down connection has moved from $\phi(\cdot)$ to $\sigma(\cdot)$, and the bias $b^{(l)}_g$ has dropped because it is redundant with the bias term $b^{(l)}_b$ in $\sigma(\cdot)$.

Modulated (also known as gated or three-way) connections have been used in autoencoders before but in a rather different context. Memisevic (2011) uses a weight tensor to connect two inputs to a feature. We connect the $i$th component of $h^{(l)}$ only to the $i$th component of $\hat{h}^{(l)}$, keeping the number of additional parameters small.

2.2 Training procedure

In order to compare the models, we optimized each model structure constraining to 1 million parameters and 1 million mini-batch updates to find the best denoising performance, that is, the lowest reconstruction cost $C$ in Eq. (1). The better the denoising performs the better the implicit probabilistic model is. The tasks is the same for all models, so the comparison is fair. With two-layer models ($L = 2$) the focus was to find the optimal size for layers, especially the ratio of $h^{(2)}$ size to $h^{(1)}$ size (see Fig. 1c for the definition of the ratio $\alpha$). All the models use rectified linear unit as the activation function $\phi(\cdot)$ and the noise was Gaussian with zero mean and standard deviation scaled to be 50% of that of the data.

In order to find the best possible baseline for comparison, we evaluated weight tying for autoencoder without lateral connections, that is, $W^{(l)}_g = W^{(l+1)}_f^T$, and noticed that tying weights resulted in faster convergence and thus better denoising performance than without weight tying. However, when combining both so that weights are tied in the beginning and untied for the latter half of the training, denoising performance improved slightly (by 1%), but did not affect the relative difference of various models. Since weight tying had only negligible impact on the results, but it complicates training and reproducibility, we designed the experiments so that all models use tied weights counting tied weights as separate parameters. Results of the denoising performance are described in Section 2.3.

We performed the analysis on natural images because the invariances and learned features are easy to visualize, we know beforehand that such invariances do exist, and because computer vision is an important application field in its own right. We used 16 × 16 patches from two image datasets: CIFAR-10 (Krizhevsky & Hinton, 2009) and natural images used by Olshausen & Field (1996). We refer to this dataset as O&F.

The training length was limited to 1 million mini-batch updates with mini-batch of size 50 and learning rate was adapted with ADADELTA (Zeiler, 2012). The best variants of each model were then trained longer, for 4 million updates, and further analyzed to determine invariance of the learned representations. This is described and reported in Section 2.4. Supplementary material provides more details about data preprocessing, division between training and validation sets, training procedure, hyperparameters used with ADADELTA, and how weights were initialized.

We also tried stacked layer-wise training by training each layer for 500,000 updates followed by fine-tuning phase of another 500,000 updates such that the total number of updates for each parameter equals to 1 million. We also tried a local cost function and noise source on each layer or using the global cost, but we did not find any such stacked training beneficial compared to the direct simultaneous training of all layers, which is what we report in this paper.

Available at [https://redwood.berkeley.edu/bruno/sparsenet/](https://redwood.berkeley.edu/bruno/sparsenet/)
2.3 Denoising performance

The results of denoising performance for models with one and two layers is presented in the Figure 2 which shows the lowest reconstruction cost on a validation dataset for both datasets. Each configuration was trained 5 times with different random initialization for confidence bounds calculated as corrected sample standard deviation of the lowest reconstruction cost.

The best performing No-lat model (autoencoder without lateral connections) is a one-layer model and is shown in dashed line. The best two-layer No-lat models in CIFAR-10 and O&F have ratios of $\alpha_{min} = 1.0$ and $\alpha_{min} = 1.4$, respectively. Since No-lat autoencoders need to push all the information through each layer, it is intuitive that very narrow bottlenecks are bad for the model, that is, large and small ratios perform poorly. A further study of why the optimal ratio is larger for O&F revealed that the lower layer can be smaller because the effective dimensionality in terms of principal components is lower for O&F compared to CIFAR-10. Second layer is not beneficial with No-lat model given the parameter number constraint.

Mod (modulated lateral connections) model benefits from the second layer and works best when the ratio is small, namely $\alpha_{min} = 0.03$ and $\alpha_{min} = 0.12$ for CIFAR-10 and O&F, respectively. The second layer does not hurt or benefit Add (additive lateral connection) model significantly and its performance is between No-lat and Mod models. The results are also presented as numbers in Table 1 in supplementary material.
2.4 Resulting Invariant Features

Practically no prior information about poolings was incorporated in either the model structure or treatment of training data. This means that any invariances learned by the model must have been present in the higher-order correlations of the inputs, as explained in Section 1.1. It is well known that such invariances can be developed from natural images (e.g., Hyvärinen & Hoyer, 2000) but the question is, how well are the different model structures able to represent and learn these features.

To test this, we generated sets of rotated, scaled and translated images and measured how invariant the activations $h^{(l)}$ are for each type of transformation separately. As an example for translation, each set contained 16 translated images (from a $4 \times 4$ grid). For each set $s$ in a given transformation type, we calculated the mean activation $\langle h^{(l)}_i \rangle_s$ and compared their variances with the variance $\text{var}\{h^{(l)}_i\}$ over all samples:

$$
\gamma^{(l)}_i = \text{var}\{h^{(l)}_i\}_s / \text{var}\{h^{(l)}_i\}.
$$

From the definition it follows that $0 \leq \gamma^{(l)}_i \leq 1$. If the feature is completely invariant with respect to the transformation, $\gamma^{(l)}_i$ equals one. As the overall conclusions are similar to all tested transformations, the main text concentrates on the translation invariance. Results for other invariances are reported in supplementary material, Section 4.4. The average layer-wise invariance, $\gamma^{(l)} = \langle \gamma^{(l)}_i \rangle$, grows towards the higher layers in all models but much faster in the best Mod models than in other i.e. for CIFAR-10 the best Mod model has $\gamma^{(0)\ldots(2)} = (0.20, 0.31, 0.84)$, whereas for the best No-lat $\gamma^{(0)\ldots(2)} = (0.20, 0.23, 0.30)$. All $\gamma^{(l)}$ values are reported in Table 1 in supplementary material.

To further illustrate this, we plotted in Figure 3 the invariance measures $\gamma^{(2)}_i$ for the best variant of each model. In each plot, dots correspond to hidden neurons $h^{(2)}_i$ and the color reflects the average sign of the encoder connection to that neuron (blue for negative, red for positive). The horizontal axis is the significance of a neuron, a measure of how much the model uses that hidden neuron, which is defined and analyzed in supplementary material, Section 4.3.

There are two notable observations. First, all $h^{(2)}_i$ neurons of Mod model are highly invariant, whereas the other models have only few invariant neurons and the vast majority of neurons have very low invariance. For No-lat model, invariance seems to be even smaller for those neurons that the model uses more. Moreover, we tested that the second layer of Mod model stays highly invariant even if the layer size is increased (shown in Figure 7c in supplementary material). Second, invariant neurons tend to have far more and stronger negative than positive weights, especially so with Mod and No-lat models. Since the nonlinearity $\phi(x)$ on each layer was the rectified linear unit, a convex function which saturates on the negative side, negative tied weights mean that the network flipped these functions into $-\phi(-x)$, that is, concave functions that saturate on the positive side resembling OR operation. This interpretation is further discussed in supplementary material, Section 4.3.3.

2.5 Learned Poolings

The modulated Mod model used practically all of the second layer neurons for pooling. When studying the poolings, we found that typically every Layer 1 neuron participates in several qualitatively different poolings. As can be seen from the Figure 4 each Layer 1 neuron (shown on the left-most column) participates in different kinds of poolings each of which is sensitive to a particular set of features and invariant to other types. For example, Layer 1 neuron (c) is selective to orientation, frequency and color but it participates in three different Layer 2 poolings. The first one is selective to color but invariant to orientation. The second one is selective to orientation but invariant to color. The third one only responds to high frequency and orientation. More details of the analysis are available in supplementary material.

Various measures of invariance have been proposed (e.g., Goodfellow et al., 2009). Our invariance measure $\gamma$ is closely related to autocorrelation which has been used to measure invariance, e.g., by Dosovitskiy et al., 2014. The set of translated patches includes pairs with various translations and therefore our measure is a weighted average of the autocorrelation function. The wider the autocorrelation, the larger the measure $\gamma$.

Our measure $\gamma$ can be fooled by copying the same invariant feature to many hidden neurons but we verified that this is not happening here: slow feature analysis is robust against such redundancy but yields qualitatively the same results for the tested networks.

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Figure 4: Various pooling groups a neuron. Each set (a)-(d) represents three relevant pooling groups the selected neuron \( h^{(1)}_a \ldots h^{(1)}_d \), depicted in the first column, belongs to. Each row represents an \( h^{(2)} \) pooling neuron by showing the 20 most relevant \( h^{(1)} \) neurons associated with it. Poolings were found by selecting a few Layer 1 neurons and following their strongest links to Layer 2 to identify the poolings in which they participate. Consecutively, the Layer 1 neurons corresponding to each pooling group were identified by walking back the strongest links from each Layer 2 neuron. Best viewed in color. The procedure of choosing features in the plot is also depicted in Figure 8 in supplementary material.

3 Discussion

The experiments showed that invariance in denoising autoencoders increased towards the higher layers but significantly so only if the decoder had a suitable structure where details could be combined with invariant features via multiplicative interactions. Lateral connections from encoder to decoder allowed the models to discard details from the higher levels but only if the details and invariant features were combined suitably.

The best models with modulated lateral connections were able to learn a large number of poolings in an unsupervised manner. We tested their invariance but nothing in the model biased learning in that direction and we observed invariance and selective discrimination of several different dimensions such as color, orientation and frequency.

In summary, these findings are fully in line with the earlier proposition that the unsupervised denoising autoencoder with modulated lateral connections can work in tandem with supervised learning because, as we have shown here for the first time, the higher layers of the model have the ability to focus on abstract representations and, unlike regular autoencoders, should therefore be able to discard details if supervised learning deems them irrelevant. It now becomes possible to combine autoencoders with the popular supervised learning pipelines which include in-built pooling operations (see, e.g., [Schmidhuber, 2015]).

There are multiple ways to extend the work, including 1) explicit bias towards invariances; 2) sparse structure such as convolutional networks, making much larger scale models and deeper hierarchies feasible; 3) dynamic models; and 4) semi-supervised learning.

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Table 1: Denoising performance and translation invariance measure of selected models. All models have exactly the same input layer and data so the average invariance is the same for all models, e.g. for CIFAR-10, \( \gamma^{(0)} = 0.20 \).

| Dataset | Model     | Layer sizes | Ratio \( \alpha \) | Min cost ± std | Invariance, \( \gamma^{(l)} \) |
|---------|-----------|-------------|--------------------|----------------|--------------------------------|
| CIFAR-10| Linear    | 256         | 0.00               | 0.20316 ± 0.00011 | NA               |
| CIFAR-10| No-lat    | 256-1948    | 0.00               | 0.16144 ± 0.00007 | 0.20, 0.29       |
| CIFAR-10| Add/Mod   | 256-1937    | 0.00               | 0.15793 ± 0.00007 | 0.20, 0.29       |
| CIFAR-10| No-lat    | 256-590-589 | 1.00               | 0.17595 ± 0.00034 | 0.20, 0.23, 0.30 |
| CIFAR-10| Add       | 256-839-336 | 0.40               | 0.15734 ± 0.00015 | 0.20, 0.27, 0.33 |
| CIFAR-10| Mod       | 256-1622-50 | 0.03               | 0.15086 ± 0.00022 | 0.20, 0.31, 0.84 |
| O&F     | Linear    | 256         | 0.00               | 0.14686 ± 0.00010 | NA               |
| O&F     | No-lat    | 256-1948    | 0.00               | 0.12290 ± 0.00008 | 0.16, 0.24       |
| O&F     | Add/Mod   | 256-1937    | 0.00               | 0.11891 ± 0.00006 | 0.16, 0.25       |
| O&F     | No-lat    | 256-512-718 | 1.40               | 0.12446 ± 0.00015 | 0.16, 0.19, 0.27 |
| O&F     | Add       | 256-1061-212| 0.20               | 0.11723 ± 0.00009 | 0.16, 0.25, 0.41 |
| O&F     | Mod       | 256-1395-100| 0.07               | 0.11234 ± 0.00005 | 0.16, 0.24, 0.95 |

4 SUPPLEMENTARY MATERIAL

4.1 PREPROCESSING OF DATA

Patches of size \( 16 \times 16 \) were sampled randomly and continuously during training. Separate test images were put aside for testing generalization performance: the last 10,000 samples for CIFAR-10 and the sixth image of O&F dataset. Continuous sampling allows generation of millions of data samples alleviating overfitting problems. O&F dataset was already (partially) whitened so no further preprocessing was applied to it. RGB color patches of CIFAR-10 were whitened and dimensionality was reduced to 256 with PCA to match the dimensionality of grayscale images of O&F. Despite dimensionality reduction, 90% of the variance was retained.

4.2 DETAILS OF THE TRAINING PROCEDURE

White additive Gaussian noise of \( \sigma_N = 0.5 \) was used for corrupting the inputs which were scaled to have standard deviation of \( \sigma = 1.0 \). During training, ADADELTA was used to adapt the learning rate with its momentum set to 0.99, and \( \epsilon = 10^{-8} \). All weight vectors were initialized from normal distribution to have a norm of 1.0, and orthogonalized. In order to improve the convergence speed of all models, we centered the hidden unit activations following Raiko et al. (2012): there is an auxiliary bias term \( \beta \) (Raiko et al., 2012, Eq. (2)), applied immediately after the nonlinearity, that centers the output to zero mean.

4.3 ANALYSIS OF MAPPINGS

We analyzed the mappings learned by different types of models in several ways and present here some of the most interesting findings.

First, it turned out that different models had very different proportions of invariant neurons on \( h^{(2)} \) (invariance measure \( \gamma \) is defined in Eq. (9)) and we wanted to understand better what was going on. Some key questions were how important roles different types of features had and how the invariances were formed. Second level invariances could be low-frequency features which are invariant already on the first layer (and thus not particularly interesting) or formed through pooling Layer 1 neurons.

The first question can be answered by looking at where the connections are coming from. The connections \( W_g^{(l)} \) are visualized in Figures 5a-5c. The neurons on each layer have been ordered with respect to invariance which increases from left to right. The connecting edges have been colored according to the sign of the connecting weight and the strength of each edge reflects the significance of the connection. Significance is defined as the proportion of variance that the higher-level neuron

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4 We did not use the other transformation \( \alpha \) since it would have required shortcut connections.
generates on the lower-level neurons. We initially tried visualizing simply the magnitudes of the weights but the problem is that when an input neuron has a low variance or the output neuron is saturated, a large weight magnitude does not indicate that the connection is important; it would not make much difference if such a connection were removed.

4.3.1 Significance Measure

When visualizing $W_g^{(l)}$, we first took the squares and scaled them by the input neuron’s variance $\text{var}\{h_i^{(l+1)}\}$. Assuming input neurons are independent, this quantity reflects the input variance each neuron $h_j^{(l)}$ receives. Depending on the saturation of the neuron, a smaller or greater proportion of this variance is transmitted to the actual output variance $\text{var}\{h_j^{(l)}\}$. We therefore scaled all the incoming variances for each $h_j^{(l)}$ such that their sum matches the output variance $\text{var}\{h_j^{(l)}\}$. We named this quantity the significance of the connection and it approximately measures where the output variance of each layer originates from. This significance is also depicted in Figure 3 where the x coordinate is the sum of output significances for each $h_i^{(2)}$.

4.3.2 Role of Negative Weights

It turned out that the invariant neurons tend to have far more and stronger negative than positive weights. We visualized this with color in Figure 5: blue signifies negative and red positive weights. In the images, the connections are translucent which means that equal number (and significance) of positive and negative weights results in purple color.

A striking feature of these plots is that the most invariant features tend to have all negative weights. Since the nonlinearity $\phi(x)$ on each layer was the rectified linear unit, a convex function which saturates on the negative side, negative tied weights mean that the network flipped these functions into $-\phi(-x)$, that is, concave functions that saturate on the positive side. It therefore looks like the network learned to add a layer of concave OR-like invariance-generating poolings on top of convex AND-like coincidence detectors. Forming convex AND using positive weights and concave OR using negative weights is demonstrated respectively as truth tables in Table 2 and Table 3, and the geometric form is illustrated in Figure 6a and Figure 6b.

4.4 Invariance

We also studied invariance of the second layer neurons for scaling and rotation transformations using the same invariance measure as defined in Section 2.4 for translation. We formed sets of 16 samples by scaling CIFAR-10 images with a zoom factors 0.6, 0.65, ..., 1.35 and rotating images $-32^\circ$, $-28^\circ$, ..., $28^\circ$ for scaling and rotation invariance experiments, respectively. The results are shown in Figure 7a and Figure 7b and are similar to the translation invariance in Figure 3.

Figure 7c illustrates the impact of increasing $\alpha$, i.e. increasing the size of the second layer. Notably all second layer neurons stay highly invariant even when the layer size is increased.
Figure 5: Neurons are ordered according to increasing translation invariance from left to right. Blue denotes negative and red positive weights in $W^{(l)}_g$. Strength of the connections depends on the significance of the connection (see text for details). Layer 2 neurons of this model are also visualized in Figure 5. Best viewed in color.
Table 2: Truth table for logical AND operation given three-element binary input vector $x$ and a single perceptron with ReLU activation function $\phi(\cdot)$.

$$\phi(z) = \phi(x^Tw + b) = \phi(x_0w_0 + x_1w_1 + x_2w_2 + b)$$

| $x_0$ | $x_1$ | $x_2$ | $w_1$ | $b$ | $z$ | $\phi(z)$ | AND |
|-------|-------|-------|-------|-----|-----|------------|-----|
| 0     | 0     | 0     | 1     | -2  | -2  | 0          | 0   |
| 0     | 0     | 1     | 1     | -2  | -1  | 0          | 0   |
| 0     | 1     | 0     | 1     | -2  | -1  | 0          | 0   |
| 0     | 1     | 1     | 1     | -2  | 0   | 0          | 0   |
| 1     | 0     | 0     | 1     | -2  | -1  | 0          | 0   |
| 1     | 0     | 1     | 1     | -2  | 0   | 0          | 0   |
| 1     | 1     | 0     | 1     | -2  | 0   | 0          | 0   |
| 1     | 1     | 1     | 1     | -2  | 1   | 1          | 1   |

Table 3: Truth table for logical OR operation given three-element binary input vector $x$ and a single perceptron with ReLU activation function $\phi(\cdot)$.

$$\phi(z) = \phi(x^Tw + b) = \phi(x_0w_0 + x_1w_1 + x_2w_2 + b)$$

| $x_0$ | $x_1$ | $x_2$ | $w_1$ | $b$ | $z$ | $\phi(z)$ | $1 - \phi(z)$ | NOR | OR |
|-------|-------|-------|-------|-----|-----|------------|----------------|-----|----|
| 0     | 0     | 0     | -1    | 1   | 1   | 1          | 0              | 1   | 0  |
| 0     | 0     | 1     | -1    | 1   | 0   | 0          | 1              | 0   | 1  |
| 0     | 1     | 0     | -1    | 1   | 0   | 0          | 1              | 0   | 1  |
| 0     | 1     | 1     | -1    | 1   | -1  | 0          | 1              | 0   | 1  |
| 1     | 0     | 0     | -1    | 1   | 0   | 0          | 1              | 0   | 1  |
| 1     | 0     | 1     | -1    | 1   | -1  | 0          | 1              | 0   | 1  |
| 1     | 1     | 0     | -1    | 1   | -1  | 0          | 1              | 0   | 1  |
| 1     | 1     | 1     | -1    | 1   | -2  | 0          | 1              | 0   | 1  |

Figure 6: Conceptual illustration of linear rectifier unit, $\phi(\cdot)$, performing logical AND and OR operations for three-element binary input $x, x_i \in \{0, 1\}$ after the affine transform $z = x^Tw + b = x_0w_0 + x_1w_1 + x_2w_2 + b$. AND operations has positive weights and convex form, whereas OR operation has negative weights and concave functional form.
Figure 7: Various invariance measures for neurons of $h^{(2)}$ as a function of significance for CIFAR-10. Color indicates the average sign of the connected weights from negative (blue) to positive (red). Best viewed in color. See Section 2.4 for more details.
Figure 8: Method for selecting pooling groups including a given $h^{(1)}$ neuron contains two phases. First, follow the strongest links up to the second layer to identify 3 pooling groups the first-layer neuron belongs to (left). Second, visualize each pooling group by identifying the Layer 1 neurons that have the strongest links back from each Layer 2 neuron (right). In this example, the first pooling group contains neurons marked with green, the second pooling group with red, and the third consist of purple neurons. Colors correspond to rows in Figure 4 and both phases were performed for each set (a)-(d).