Correlated Weights in Infinite Limits of Deep Convolutional Neural Networks

Adrià Garriga-Alonso
Mark van der Wilk

1Department of Engineering, University of Cambridge, UK
2Department of Computer Science, Imperial College London, UK

Abstract

Infinite width limits of deep neural networks often have tractable forms. They have been used to analyse the behaviour of finite networks, as well as being useful methods in their own right. When investigating infinitely wide convolutional neural networks (CNNs), it was observed that the correlations arising from spatial weight sharing disappear in the infinite limit. This is undesirable, as spatial correlation is the main motivation behind CNNs. We show that the loss of this property is not a consequence of the infinite limit, but rather of choosing an independent weight prior. Correlating the weights maintains the correlations in the activations. Varying the amount of correlation interpolates between independent-weight limits and mean-pooling. Empirical evaluation of the infinitely wide network shows that optimal performance is achieved between the extremes, indicating that correlations can be useful.

1 INTRODUCTION

Analysing infinitely wide limits of neural networks has long been used to provide insight into the properties of neural networks. [Neal, 1996] first noted such a relationship, through showing that infinitely wide Bayesian neural networks converge in distribution to Gaussian processes (GPs). The success of GPs raised the question of whether such a comparatively simple model could replace a complex neural network. [MacKay, 1998] noted that taking the infinite limit resulted in a fixed feature representation, a key desirable property of neural networks. Since this property is lost due to the infinite limit, MacKay inquired: “have we thrown the baby out with the bath water?”

In this work, we follow the recent interest in infinitely wide convolutional neural networks [Garriga-Alonso et al., 2019, Novak et al., 2019], to investigate another property that is lost when taking the infinite limit: correlation in the activations of patches in different parts of the image. Given that convolutions were developed to introduce these correlations, and that they improve performance [Arora et al., 2019], it seems undesirable that they are lost when more filters are added. Currently, the only way of reintroducing spatial correlations is to change the model architecture by introducing mean-pooling [Novak et al., 2019]. This raises two questions:

1) Is the loss of patchwise correlations a necessary consequence of the infinite limit?
2) Is an architectural change the only way of reintroducing patchwise correlations?

We show that the answer to both these questions is “no”. Correlations between patches can also be maintained in the limit without pooling by introducing correlations between the weights in the prior. The amount of correlation can be controlled, which allows us to interpolate between the existing approaches of full independence and mean-pooling. Our approach allows the discrete architectural choice of mean-pooling to be replaced with a more flexible continuous amount of correlation.

We empirically show that modest performance improvements can be obtained by replacing mean-pooling at the final layer with an intermediate amount of correlation. In addition, we show that in layers before the final one, the discrete architectural choice of mean-pooling can be replaced by an intermediate amount of correlation, without degrading performance. Avoiding discrete design decisions makes architecture search easier, by allowing continuous optimisation. We speculate that these results from infinite networks could be useful for adapting priors or initialisations in finite networks, leading to better performance, or easier design.

Overall, our work illustrates that non-standard choices in the weight prior can significantly influence properties in the infinite limit, and that good choices can lead to improved
performance. We hope that this work inspires investigation into correlated weights in finite neural networks, as well as more non-standard priors or initialisations.

2 SPATIAL CORRELATIONS IN SINGLE HIDDEN LAYER NETWORKS

To begin, we will analyse the infinite limit of a single hidden layer convolutional neural network (CNN). This illustrates the choices that lead to the disappearance of spatial correlation in the activations. We extend [Garriga-Alonso et al. 2019] and [Novak et al. 2019] by considering weight priors with correlations. By adjusting the correlation, we can interpolate between existing independent weight limits and mean-pooling, which previously had to be introduced as a discrete architectural choice. We also discuss how existing convolutional Gaussian processes [van der Wilk et al., 2017, Dutordoir et al., 2020] can be obtained from limits of correlated weight priors.

Consider a CNN with \( L = 2 \) layers. Figure 1 provides a graphical representation of the notation. The input \( X \) is a real-valued tensor of shape \( C^{(0)} \times F^{(0)} \), where \( C^{(0)} \in \mathbb{N} \) is the number of channels and \( F^{(0)} \in \mathbb{N}^D \) the spatial size of the input. Superscripts denote the layer index. For images, usually \( C^{(0)} = 3 \) (one per colour), and the number of spatial input dimensions is \( D = 2 \), so \( F^{(0)} = (F_{h}^{(0)}, F_{w}^{(0)}) \).

The convolution operation at layer \( \ell \in [L] \) divides its input into patches of size \( P^{(\ell)} \leq F^{(\ell-1)} \). For a given spatial location of the next activation \( q \in [F^{(\ell)}]^{D} \) the patch function \( \tilde{q}_i(p) \triangleq (\tilde{q}_i(p_1), \ldots, \tilde{q}_D(p_D)) \), where

\[
\tilde{q}_d(p_d) = sq_d - h(p_d - [P_d/2]) .
\]

Using eq. [3] it is possible to verify that eq. [1] is the usual deep learning convolution (appendix A).

In a single hidden layer CNN, these activations are followed by a fully-connected layer with weights \( W^{(2)} \in \mathbb{R}^{C^{(1)} \times P^{(2)}} \), where \( P^{(2)} = F^{(1)} \). Our final output is again given by a summation over the activations

\[
f(X) = \sum_{j=1}^{C^{(1)}} \sum_{p=1}^{P^{(2)}} W^{(2)}_{j, p} A^{(1)}_{j, p}(X) = \sum_{p=1}^{P^{(1)}} Z^{(f)}_{p}(X) ,
\]

where \( Z^{(f)}_{p}(X) \) denotes the result before the summation over spatial locations \( p \).

We analyse the distribution on function outputs \( f(X) \) for some Gaussian prior \( p(W) \) on the weights of all layers \( W \). In all the cases we consider, we take the prior to be independent over layers and channels. Here we extend earlier work by allowing spatial correlation in the final layer’s weights (we will consider all layers later) through the covariance tensor \( \Sigma^{(\ell)} \in \mathbb{R}^{C^{(\ell)} \times P^{(\ell)}} \). This gives the prior

\[
p(W^{(1)}) = \prod_{i=1}^{C^{(0)}} \prod_{j=1}^{P^{(1)}} \mathcal{N}
\left(W^{(1)}_{i, j} ; 0, I\right) ,
\]

\[
p(W^{(2)}) = \prod_{i=1}^{C^{(1)}} \mathcal{N}
\left(W^{(2)}_{i} ; 0, \frac{1}{C^{(1)}} \Sigma^{(2)}\right) .
\]

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\[1\] For some number \( P \in \mathbb{N} \), the expression \([P]\) is the set \( \{1, \ldots, P\} \). For a tuple \( P \in \mathbb{N}^D \), \([P]\) = \([P_1] \times \cdots \times [P_D] \).
with independence between different layers’ weights. Here, a tensor-valued covariance \( \Sigma^{(2)} \) expresses arbitrary covariance over the spatial dimensions of the tensor \( W^{(2)} \):

\[
\mathbb{C} \left[ W^{(2)}_{i,p}, W^{(2)}_{i',p'} \right] = \Sigma^{(2)}_{p,p'}/C^{(\ell-1)}.
\]

Since \( W^{(1)}, W^{(2)} \) are i.i.d. over channels \( i \in C^{(1)} \), the random variables \( \sum_{p=1}^{G^{(1)}} W^{(2)}_{i,p} A^{(1)}_{i,p}(X) \) are identically distributed and independent for each \( i \in [C^{(1)}] \). This allows us to apply the central limit theorem (CLT) to their sum \( f(X) \), showing that \( f(X) \) converges in distribution to a Gaussian process as \( C^{(1)} \rightarrow \infty \) [Neal 1996].

The covariance between the final-layer activations for two inputs \( X, X' \) becomes

\[
\mathbb{C}_W \left[ Z^{(f)}_{p}(X), Z^{(f)}_{p'}(X') \right] = \mathbb{E}_W \left[ \sum_{j=1}^{C^{(1)}} \sum_{j'=1}^{C^{(1)}} \mathbb{E}_{W^{(1)}} \left[ A^{(1)}_{j,p}(X) A^{(1)}_{j',p'}(X') \right] \mathbb{E}_{W^{(2)}} \left[ W^{(2)}_{j,p} W^{(2)}_{j',p'} \right] \right],
\]

use independences to split the expectations, and substitute the weight covariance,

\[
\mathbb{C}_W \left[ Z^{(f)}_{p}(X), Z^{(f)}_{p'}(X') \right] = \sum_{j=1}^{C^{(1)}} \sum_{j'=1}^{C^{(1)}} \mathbb{E}_{W^{(1)}} \left[ A^{(1)}_{j,p}(X) A^{(1)}_{j',p'}(X') \right] \mathbb{E}_{W^{(2)}} \left[ W^{(2)}_{j,p} W^{(2)}_{j',p'} \right] \delta_{j,j'},
\]

eliminate one of the sums over \( j \) using \( \delta_{j,j'} \), and rearrange

\[
= \mathbb{E}_{W^{(1)}} \left[ \frac{1}{C^{(1)}} \sum_{j=1}^{C^{(1)}} A^{(1)}_{j,p}(X) A^{(1)}_{j,p'}(X') \right] \mathbb{E}_{W^{(2)}} \left[ W^{(2)}_{j,p} W^{(2)}_{j,p'} \right] \delta_{j,j'},
\]

\[
= V^{(1)}_{p,p'}(X, X') \Sigma^{(2)}_{p,p'}.
\]

The limit of the sum of the final expectation over \( W^{(1)} \) can be found in closed form for many activations (see section 3.2) and is denoted \( V^{(1)}_{p,p'}(X, X') \). Note in eq. 4 that the activations for some location \( p \in [F^{(1)}] \) only depend on the input patch at \( p \), that is, on the elements of \( X \) that are in the image \( \text{im}(\tilde{p}) \) of the patch function \( \tilde{p}(\cdot) \).

Thus, the kernel acts locally on patches: \( V^{(1)}_{p,p'}(X, X') = k^{(1)}(X_{\cdot, \text{im}(\tilde{p})}, X'_{\cdot, \text{im}(\tilde{p})}) \).

We find the final kernel for the GP by taking the covariance between function values \( f(X) \) and \( f(X') \) and performing the final sum in eq. 4

\[
K(X, X') = \mathbb{C} \left[ f(X), f(X') \right] = \sum_{p,p'} k^{(1)}(X_{\cdot, \text{im}(\tilde{p})}, X'_{\cdot, \text{im}(\tilde{p})}) \Sigma^{(2)}_{p,p'}. \tag{8}
\]

We can now see how different choices for \( \Sigma^{(2)} \) give different forms of spatial correlation.

**Independence.** Garriga-Alonso et al. [2019] and Novak et al. [2019] consider \( \Sigma^{(2)}_{p,p'} = \delta_{p,p'} \psi^2 \), i.e. the case where all weights are independent. The resulting kernel simply sums components over patches, which implies an additive model [Stone 1985], where a different function is applied to each patch, after which they are all summed together: \( f(X) = \sum_{p} f_p(X_{\cdot \text{im}(\tilde{p})}) \). This structure has commonly been applied to improve GP performance in high-dimensional settings [e.g. Duvenaud et al. 2011, Durrande et al. 2012]. Novak et al. [2019] point out that the same kernel can be obtained by taking an infinite limit of a locally connected network (LCN) [LeCun 1989] where connectivity is the same as in a CNN, but without weight sharing, indicating that a key desirable feature of CNNs is lost.

**Mean-pooling.** By taking \( \Sigma^{(2)}_{p,p'} = 1/|F^{(2)}|^2 \) we make the weights fully correlated over all locations leading to identical weights for all \( p \), i.e. \( W^{(2)}_{i,p} = W^{(2)}_{i,p'} \). This is equivalent to taking the mean response over all spatial locations (see eq. 4), or global average pooling. As Novak et al. [2019] discuss, this reintroduces the spatial correlation that is the intended result of weight sharing. The “translation invariant” convolutional GP of van der Wilk et al. [2017] can be obtained by this single-layer limit using Gaussian activation functions [van der Wilk 2019]. Since this mean-pooling was shown to be too restrictive in this single-layer case, Van der Wilk et al. [2017] considered pooling with constant weights \( \alpha_p \) (i.e. without a prior on them). In this framework, this is equivalent to placing a rank 1 prior on the final-layer weights by taking \( \Sigma^{(2)}_{p,p'} = \alpha_p \delta_{p,p'} \). This maintains the spatial correlations, but requires the \( \alpha_p \) parameters to be learned by maximum marginal likelihood (ML-II, empirical Bayes).

**Spatially correlated weights.** In the pooling examples above, the spatial covariance of weights is taken to be a rank-1 matrix. We can add more flexibility to the model by varying the strength of correlation between weights based on their distance in the image. We consider an exponential decay depending on the distance between two patches: \( \Sigma^{(2)}_{p,p'} = \exp(-d(p, p')/l) \). We recover full independence by taking \( l \rightarrow 0 \), and mean-pooling with \( l \rightarrow \infty \). Intermediate values of \( l \) allow the rigid assumption of complete weight sharing to be relaxed, while still retaining spatial correlations between similar patches. This construction gives the same kernel as investigated by Mairal et al. [2014] and Dutordoir et al. [2020], who named this property “translation insensitivity”, as opposed to the stricter invariance that mean-pooling gives. The additional flexibility improved performance without needing to add many parameters that are learned in a non-Bayesian fashion.

Our construction shows that spatial correlation can be retained in infinite limits without needing to resort to architec-

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\[F \in \mathbb{N}^D, \text{its number of elements is } |F| \triangleq \prod_{d=1}^{D} F_d.\]
tural changes. A simple change to the prior on the weights is all that is needed. This property is retained in wide limits of deep networks, which we investigate next.

3 SPATIAL CORRELATIONS IN DEEP NETWORKS

Here, we provide an informal extension of the previous section’s results to deep networks. In deep networks, correlated weights also retain spatial correlation in the activations. Appendix B provides a formal justification for this section, using the framework by Yang [2019].

The procedure for computing the kernel has a recursive form similar to existing analyses [Garriga-Alonso et al., 2019] [Novak et al., 2019]. Negligible additional computation is needed to consider arbitrary correlations, compared to only considering mean-pooling [Novak et al., 2019] [Arora et al., 2019]. The main bottleneck is the need for computing covariances for all pairs of patches in the image, as in eq. 8. For a D-dimensional convolutional layer, the corresponding kernel computation is a convolution of the activations’ second moment with the 2D-dimensional covariance tensor of the weights.

The setup for the case of a deep neural network follows that of section [2] but with the number of layers \( L > 2 \). The outputs of the network are simply the pre-non-linearity activations of the \( L \)-th layer, \( Z^{(L)}(X) \). If we need several outputs, for example in \( K \)-class classification, we may set \( C^{(L)} = K \). If the output of the network should not be spatially extended, we set the spatial size to \( F^{(L)} = 1 \). This can be achieved by making the weights \( W^{(L)} \) (and their corresponding convolutional patch) have the same size as \( F^{(L−1)} \) (see fig. 1).

As pointed out by [Matthews et al., 2018], a straightforward application of the central limit theorem is not possible for deep networks. Fortunately, [Yang, 2019] developed a general framework for expressing neural network architectures and finding their corresponding Gaussian process infinite limits. The resulting kernel is given by the recursion that can be derived from a more informal argument which takes the infinite width limit in a sequential layer-by-layer fashion, as was used in [Garriga-Alonso et al., 2019]. We follow this informal derivation, as this more naturally illustrates the procedure for computing the kernel. A formal justification can be found in appendix B.

3.1 RECURSIVE COMPUTATION OF THE KERNEL

In our weight prior, we correlate weights within a convolutional filter. The weights remain independent over layers and channels. For each \( \ell \in [L] \),

\[
p(W^{(\ell)}) = \prod_{i=1}^{C^{(\ell)}} \prod_{j=1}^{C^{(\ell−1)}} \mathcal{N}(W_{i,j}; 0, \frac{1}{C^{(\ell−1)}}\Sigma^{(\ell)}).
\] (9)

As in section 2, \( W^{(\ell)} \in \mathbb{R}^{C^{(\ell)} \times C^{(\ell−1)} \times F^{(\ell)}} \), and the covariance tensor \( \Sigma^{(\ell)} \in \mathbb{R}^{F^{(\ell)} \times F^{(\ell)}} \) is positive semi-definite. Our derivation is general for any weight covariance, so layers with correlated weights can be interspersed with the usual layers.

A Gaussian process is determined by the mean and covariance of function values for pairs of inputs \( X, X' \). The mean is zero. Using the recursion in eq. 1 we can find the covariance between any two pre-non-linearity activations from a pair of inputs \( X, X' \) and the covariance of the previous layer. For \( i, i' \in [C^{(\ell)}] \) and \( q, q' \in [F^{(\ell)}] \),

\[
\mathbb{E}_{W} \left[ Z_{i,q}^{(\ell)}(X), Z_{i',q'}^{(\ell)}(X') \right] = \sum_{j,j', p,p'} \mathbb{E}_{W} \left[ W_{i,j,p}^{(\ell−1)} A_{j,q(p)}^{(\ell−1)}(X) W_{i',j',p'}^{(\ell−1)} A_{j',q'(p')}^{(\ell−1)}(X') \right],
\]

substituting the expression for the weight covariance,

\[
\delta_{i,i'} \sum_{p,p'} \sum_{j,j'} \mathbb{E}_{W} \left[ \frac{1}{C^{(\ell−1)}} \sum_{j=1}^{C^{(\ell−1)}} A_{j,q(p)}^{(\ell−1)}(X) A_{j',q'(p')}^{(\ell−1)}(X') \right] = \delta_{i,i'} K_{q,q'}^{(\ell)}(X, X').
\] (10)

We can see that the covariance of activations in different channels \( i \neq i' \) is zero. Otherwise, to calculate \( K^{(\ell)}(X, X') \), we need to calculate the expectation over \( W \), which we term \( V^{(\ell−1)}(X, X') \). The resulting kernel expression is

\[
K_{q,q'}^{(\ell)}(X, X') = \sum_{p=1}^{P^{(\ell)}} \sum_{p'=1}^{P^{(\ell)}} \mathbb{E}_{W} \left[ V_{q,q'}^{(\ell−1)}(X, X') \right],
\] (11)

which, because the concatenation of patch functions is a patch function (remark \( X, 3 \)), is equivalent to a 2D-dimensional convolution. This kernel does not correspond to a locally-connected network, because it uses off-diagonal elements of the previous layer’s kernel.

3.2 EXPECTATION OF THE NONLINEARITIES

For \( \ell = 0 \), the activations in the previous layer are the image inputs, i.e. \( A^{(0)}(X) = X \) (eq. 2), making \( V_{q,q'}^{(0)}(X, X') \) an inner product between image patches.

For \( \ell \geq 1 \), the expression inside the expectation in eq. 10 is a random variable, an average over \( j \in [C^{(\ell−1)}] \). From
We see that all its terms have the same expectation, i.e.

\[
V_{p,p'}^{(t)}(\mathbf{X}, \mathbf{X}') = \mathbb{E}_W \left[ \frac{1}{C^{(t)}} \sum_{j=1}^{C^{(t)}} A_{j,p}(\mathbf{X}) A_{j,p'}(\mathbf{X}') \right]
\]

\[
= \mathbb{E}_{Z^{(t)}(\mathbf{X}), Z^{(t)}(\mathbf{X}')} \left[ \phi \left( Z_{1,p}^{(t)}(\mathbf{X}) \right) \phi \left( Z_{1,p'}^{(t)}(\mathbf{X}') \right) \right]. \quad (12)
\]

For the purposes of eq.\,(12), in the infinite width limit, the pre-nonlinearities \(Z^{(t)}(\mathbf{X}), Z^{(t)}(\mathbf{X}')\) converge in distribution to a joint Gaussian (theorem B.7). Accordingly, the value of the expectation above depends only on the entries of their \(2 \times 2\) covariance matrix and the form of \(\phi\). Here we represent this dependence through the function \(F_\phi(\Sigma_x, \Sigma_y, \Sigma_{xy})\),

\[
V_{p,p'}^{(t)}(\mathbf{X}, \mathbf{X}') = F_\phi(\mathbf{X}, \mathbf{X}') = \left[ \phi \left( Z_{1,p}^{(t)}(\mathbf{X}) \right) \phi \left( Z_{1,p'}^{(t)}(\mathbf{X}') \right) \right]. \quad (13)
\]

Combining eq.\,(11) and the input inner product provides us with a recursive procedure to compute the covariances all the way up to the final layer.

For the balanced ReLU nonlinearity \(\phi(x) = \sqrt{2} \max(0, x)\), which we use in all the experiments in this paper, we can use the expression by Cho and Saul [2009]:

\[
F_\phi(\Sigma_x, \Sigma_y, \Sigma_{xy}) = \frac{1}{\pi} \sqrt{\frac{\Sigma_x \Sigma_y - \Sigma_{xy}^2}{\Sigma_x \Sigma_y}} + \left(1 - \frac{1}{\pi} \cos^{-1} \left( \frac{\Sigma_{xy}^2}{\Sigma_x \Sigma_y} \right) \right) \Sigma_{xy}. \quad (14)
\]

This expression implies that \(V_{p,p}^{(t)}(\mathbf{X}, \mathbf{X}) = K_{p,p}^{(t)}(\mathbf{X}, \mathbf{X})\), for all \(\mathbf{X}\) and \(p\) [Lee et al., 2018, Matthews et al., 2018].

### 3.3 Computational Complexity, Diagonal Propagation

To handle the covariance tensor for \(K^{(t)}(\mathbf{X}, \mathbf{X}')\), we need to compute and represent \(|F^{(t)}|^2\) entries. This can be considerably more expensive than the forward pass of the corresponding CNN, where the activations have size \(|F^{(t)}|\).

In special cases, the computation or memory costs can be reduced, compared to the 2D-dimensional convolution in eq.\,(11) which is a generalisation of previous algorithms. These cases do not include layers with mean-pooling, for which our algorithm is equally expensive to previous ones [Arora et al., 2019].

If weights are independent, only the diagonal of \(\Sigma^{(t)}\) has nonzero entries, so \(\Sigma_{p,p'}^{(t)} = \delta_{p,p'} \Sigma_{p,p'}^{(t)}\). One of the sums in the eq.\,(11) can then be removed,

\[
K_{q,q'}^{(t)}(\mathbf{X}, \mathbf{X}') = \sum_{p=1}^{P^{(t-1)}} \Sigma_{p,p}^{(t)} V_{q(p),q'(p)}^{(t-1)}(\mathbf{X}, \mathbf{X}'). \quad (15)
\]

The patch functions that access \(V^{(t-1)}(\mathbf{X}, \mathbf{X}')\) are still different (\(q(p)\) and \(q'(p)\)), but their argument \(p\) is the same.

Patch functions (definition 2) subtract their argument multiplied by the dilation. Consequently, the difference of two patch functions with the same argument is constant: \(q(p) - q'(p) = s \cdot (q - q')\). This means that the terms of the sum are on the same diagonal. Thus, to calculate the covariance for a given location pair \(q, q'\), we need to do a single sum over a diagonal of the second moment tensors \(V^{(t-1)}(\mathbf{X}, \mathbf{X}')\) and \(\Sigma^{(t)}\).

This results in exact same algorithm as [Arora et al., 2019], which convolves over the diagonals, for layers with independent weights. Its memory cost is still \(O(|F^{(t)}|^2)\), but the computational cost is reduced to \(O(|F^{(t)}|^2 |P^{(t)}|^2)\) compared to \(O(|F^{(t)}|^2 |P^{(t)}|^2)\) for non-diagonal covariance.

**Diagonal propagation with independent weights.** Exactly which diagonal of \(V^{(t-1)}(\mathbf{X}, \mathbf{X}')\) do we need to sum over? Clearly, it is the one indexed by \(s \cdot (q - q')\), i.e. the one that contains the position \((sq, sq')\). Thus, the number of diagonals of \(V^{(t-1)}(\mathbf{X}, \mathbf{X}')\) that we will need to access is exactly the number of possible values that \(q - q'\) can take. That number is determined by the size \(F^{(t)}\) of layer \(t\), but is completely unrelated to the size \(F^{(t-1)}\) of layer \(t - 1\).

Fix some layer \(t \in [L]\). We can iterate this argument from layer \(t\) to layer \(1\) to show that, for all \(m \leq t\), the number of diagonals of \(K^{(m)}(\mathbf{X}, \mathbf{X}')\) that one needs to calculate depends only on \(F^{(t)}\). This can yield significant computational savings when the stride is \(s \geq 2\) for one or more layers.

**Last layer not spatially extended.** When the last layer is not spatially extended, its size is \(F^{(L)} = 1\), so it only has one diagonal. If all the weights of the CNN are independent, this implies that we only need to calculate one diagonal of the covariance for every layer. That is:

\[
K_{q,q'}^{(t)}(\mathbf{X}, \mathbf{X}') = \sum_{p=1}^{P^{(t-1)}} \Sigma_{p,p}^{(t)} V_{q(p),q'(p)}^{(t-1)}(\mathbf{X}, \mathbf{X}'). \quad (16)
\]

With this simplification, the convolutions required to calculate the kernel are \(D\)-dimensional, bringing the memory cost to \(O(|F^{(t)}|)\) and computational cost to \(O(|F^{(t)}||P^{(t)}|)\), same as the finite CNN [Garriga-Alonso et al., 2019]. The resulting kernel is equivalent to that of a locally connected network.

### 3.4 Implementation

We extend the neural-tangents [Novak et al., 2020] library with a convolution layer and a fully connected layer, that admit a 4-dimensional covariance tensor for the weights. This allows interoperation with existing layers.
Since 4d convolutions are uncommon in deep learning, our implementation uses a sum over $P_h^{(l)}$ 3-d convolutions, where $P_h^{(l)} = 3$ is the spatial height of the convolutional filter. While this enables GPU acceleration, computing the kernel is a costly operation. Reproducing our results takes around 10 days using an nVidia RTX 2070 GPU. Access to computational resources limited our experiments to subsets of data on CIFAR-10.

4 EXPERIMENTS

By considering different amounts of correlation, we can interpolate between existing architectures that use independent weights or full mean-pooling. We consider two possible benefits of using this larger, continuously parameterised space of models:

1) Decreased reliance on discrete architectural choices like mean-pooling.

2) Improved performance by finding a better model in the expanded search space.

Discrete choices pose a challenge for architecture search, as a separate network needs to be trained to evaluate the effect of each choice, which is computationally expensive. Continuous choices are preferable, as gradients can often be used to adjust many choices simultaneously. We investigate whether the discrete choice of mean-pooling can instead be replaced by a suitable selection of the continuous correlation parameter in a larger convolutional filter. While searching in this larger space of kernels, we also hope to observe improved performance. We investigate these two questions by performing parameter search in the next two sections.

4.2 CORRELATED WEIGHTS IN THE LAST LAYER

In the next two experiments we investigate the cross-validation performance on subsets of CIFAR-10 for a sweep of correlation parameters on two different neural network architectures. We consider two architectures used in the neural network kernel literature, the CNN-GP [Novak et al., 2019 Arora et al., 2019] with 14 layers, and the Myrtle network [Shankar et al., 2020] with 10 layers. The CNNGP-14 architecture (((conv,relu) $\times$ 14, pool)) has a $32 \times 32$ sized layer at the end, which is usually transformed into the $1 \times 1$ output using global average pooling. The Myrtle10 architecture (((conv,relu) $\times$ 2, pool$_{2x2}$) $\times$ 3, pool)) has a $8 \times 8$ pooling layer at the end.

Figure shows how the 4-fold cross-validation accuracy on the training sets varies with the lengthscale $\lambda$ of the Matérn-3/2 kernel with lengthscale $\lambda$:

$$
\Sigma_{p,p'}^{(L)} = \left(1 + \frac{\sqrt{3}|p-p'|_2}{\lambda}\right) \exp\left(-\frac{\sqrt{3}|p-p'|_2}{\lambda}\right).
$$

where we see the patch locations $p, p'$ as vectors. The “extremes” of independent weights and mean pooling are represented by $\Sigma_{p,p'}^{(L)} = \delta_{p,p'}$ and $\Sigma_{p,p'}^{(L)} = 1$, respectively.

Figure 2 shows how the 4-fold cross-validation accuracy on the training sets varies with the lengthscale $\lambda$ of the Matérn-3/2 kernel, which controls the “amount” of spatial correlation in the weights of the last layer. For each data point in each line, we split the data set into 4 folds, and we calculate the test accuracy on 1 fold using the other 3 as training set, for each value of $\sigma$ that we try. We take the maximum accuracy over $\sigma$.

We investigate how the effect above varies with data set size. The results in fig. 4 show that particularly for the CNNGP-14 architecture, correlated weights in the final layer lead to a modest but consistent improvement in performance, with the effect becoming larger with increasing dataset size. We can also see the optimal lengthscale $\lambda$ converging to a similar value for both architectures, of about $\lambda \approx 17$, which is evidence that the improvement holds for larger data sets. The optimal lengthscale is the same for both networks, so we speculate it may be a property of the CIFAR10 data set.

Data partitioning. The largest data set size in each part of the plot was run only once because of computational con-
Figure 2: Cross-validation accuracy of the CNNGP-14 and Myrtle10 networks on subsets of CIFAR10, with varying lengthscale of the Matérn-$3/2$ kernel that determines the weight correlation in the last layer. With larger data set sizes $N$, the improvement is larger, and the optimal lengthscale $\lambda$ converges to a similar value ($\lambda \approx 17$). For all data sets except the largest, the values are averaged over several runs, and the thin lines represent the $\pm 2\sigma_n$, the estimated standard deviation of the mean. We can improve the performance of the classifier by choosing an intermediate $\lambda$.

Figure 3: Correlated weights in intermediate layers. We replace pooling layers in the Myrtle10 architecture with larger convolutional filters with correlated weights. The lengthscale, and thus the amount of correlation, is varied along the x-axis. By adding correlations to a convolutional layer, we can recover (but not, in this case, exceed) the performance of the hand-selected architecture with mean-pooling.
strains. We transform one data set of size \( N \) into two data sets of size \( N/2 \) by taking block diagonals of the stored kernel matrix, so we have more runs for the smallest sizes. This is an unbiased Monte Carlo estimate of the true accuracy under the data distribution, since the individual data points are uniformly distributed (but not independent, since they are sampled without replacement). It also has less variance than independent data sets, because the data sets taken are anti-correlated; they have no points in common. Accordingly, the error bars in figs. 2 and 3 are an estimate of the standard error: the square root of an upwards-biased estimator of the variance of the mean.

**Implementation.** We use the neural-tangents [Novak et al. 2020] library to calculate the spatial kernel at the previous-to-last layer, \( K^{(L-1)}(X, X') \), once. Since only the lengthscale of the last layer changes, we can cheaply obtain the final layer kernel matrix \( K^{(L)}_{XX} \) for all lengthscales.

### 4.3 CORRELATED WEIGHTS IN INTERMEDIATE LAYERS

We take the same approach to the experiment in fig. 3. To investigate whether correlated weights can replace mean-pooling, we replace the \( 2 \times 2 \) intermediate mean-pooling layer, together with the next \( 3 \times 3 \) convolution layer, in the Myrtle10 architecture with correlated weights. We change them to a \( 6 \times 6 \) weight-correlated convolution. We vary the lengthscale for the covariance of all the newly correlated layers, setting them to the same value.

We observe that for independent weights (lengthscale is 0) the performance of the network is significantly below the optimum. Correlating the weights improves performance, although after adding small amounts of correlation, performance stays roughly constant. This indicates that for intermediate layers mean-pooling is not a sub-optimal choice, as it is for the last layer. However, the amount of correlation is a continuous parameter, which could lead to avoiding this discrete choice in model architecture.

**Implementation.** In this experiment, the lengthscales vary across the whole network, so we need to calculate \( K^{(L-1)}(X, X') \) every time. For a given data set size, this makes each point in fig. 3 considerably more expensive. For each data point, we optimise over the lengthscale of the last layer like in fig. 2 picking the one with highest cross-validation accuracy.

### 5 RELATED WORK

Infinitely wide limits of neural networks are currently an important tool for creating approximations and analyses. Here we provide a background on the different infinite limits that have been developed, together with a brief overview of where they have been applied.

Interest in infinite limits first started with research into properties of Bayesian priors on the weights of neural networks. Neal [1996] noted that prior function draws from a single hidden layer neural network with appropriate Gaussian priors on the weights tended to a Gaussian process as the width grew to infinity. The simplicity of performing Bayesian inference in Gaussian process models led to their widespread adoption soon after Williams and Rasmussen [1996] Rasmussen and Williams [2006]. Over the years, the wide limits of networks with different weight priors and activation functions have been analysed, leading to various kernels which specify the properties of the limiting Gaussian processes [Williams [1997] Cho and Saul [2009].

With the increasing prominence of deep learning, recursive kernels were introduced in an attempt to obtain similar properties. Cho and Saul [2009]. Mairal et al. [2014] investigated such methods for fully-connected and convolutional architectures respectively. Despite similarities between recursive kernels and neural networks, the derivation did not provide clear relationships, or any equivalence in a limit. Hazan and Jaakkola [2015] took initial steps to showing the wide limit equivalence of a neural network beyond the single layer case. Recently, Matthews et al. [2018], Lee et al. [2018] simultaneously provided general results for the convergence of the prior of deep fully-connected networks to a GP. A different class of limiting kernels, the Neural Tangent Kernel (NTK), originated from analysis of the function implied by a neural network during optimisation [Jacot et al., 2018], rather than the prior implied by the weight initialisation. Just like the Bayesian prior limit, this kernel sheds light on certain properties of neural networks, as well as providing a method with predictive capabilities of its own. The two approaches end up with subtly different kernels, which both can be computed as a recursive kernel. Both such infinite limits have recently been used for predicting and analysing training properties of finite neural networks [Poole et al., 2016; Schoenholz et al. [2017]; Hayou et al., 2019], as well as for (Bayesian) training of infinitely wide networks.

With the general tools in place, Garriga-Alonso et al. [2019], Novak et al. [2019] derived limits of the prior of convolutional neural networks with infinite filters. These two papers directly motivated this work by noting that spatial correlations disappeared in the infinite limit. Spatial mean pooling at the last layer was suggested as one way to recover correlations, with Novak et al. [2019] providing initial evidence of its importance. Due to computational constraints, they were limited to using a Monte Carlo approximation to the limiting kernel, while Arora et al. [2019] performed the computation

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The derivation of the limiting kernel differs between the two papers, with the results being consistent. Matthews et al. [2018] carefully take limits of realisable networks, while Lee et al. [2018] take the infinite limit of each layer sequentially.
with the exact NTK. Very recent preprints provide follow-on work that pushes the performance of limit kernels [Shankar et al., 2020] and demonstrated the utility of limit kernels for small data tasks [Arora et al., 2020]. Extending on the results for convolutional architectures, Yang [2019] showed how infinite limits could be derived for a much wider range of network architectures.

In the kernel and Gaussian process community, kernels with convolutional structure have also been proposed. Notably, these retained spatial correlation in either a fixed [van der Wilk et al., 2017] or adjustable [Mairal et al., 2014] way. While these methods were not derived using an infinite limit, Van der Wilk [2019] provided an initial construction from an infinitely wide neural network limit. Inspired by these results, we propose limits of deep convolutional neural networks which retain spatial correlation in a similar way.

6 CONCLUSION

The disappearance of spatial correlations in infinitely wide limits of deep convolutional neural networks could be seen as another example of how Gaussian processes lose favourable properties of neural networks. While other work sought to remedy this problem by changing the architecture (mean-pooling), we showed that changing the weight prior could achieve the same effect. Our work has three main consequences:

1. Weight correlation shows that locally connected models (without spatial correlation) and mean-pooling architectures (with spatial correlation) actually exist at ends of a spectrum. This unifies the two views in the neural network domain. We also unify two known convolutional architectures that were introduced from the Gaussian process community.

2. We show empirically that performance improvements can be gained by using weight correlations between the extremes of locally connected networks or mean-pooling. We also show that mean-pooling in intermediate layers can be replaced by weight correlation in infinitely wide architectures.

3. Using weight correlation may provide advantages during hyperparameter tuning. Discrete architectural choices need to be searched through simple evaluation, while continuous parameters can use gradient-based optimisation. While we have not taken advantage of this in our current work, this may be a fruitful direction for future research.

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A PATCH FUNCTIONS AND DISCRETE CONVOLUTIONS

Usually, convolutions are defined explicitly by subtracting the indices of one input tensor from the other one, and not using patch functions. To make this paper clearer, it is convenient to abstract the details of a convolution, so we introduced the patch function.

Definition A.1 (Discrete convolution). Let $D \in \mathbb{N}$ be a number of spatial dimensions, the tensor-valued weights $W \in \mathbb{R}^{F}$, input $X \in \mathbb{R}^{F}$, and output $Y \in \mathbb{R}^{F'}$. The tensor sizes $P$ (patch size) and $F, F'$ (feature sizes) are each a $D$-tuple, $P, F, F' \in \mathbb{N}^D$. We say that $Y$ is the result of the convolution operation $Y = W \ast X$, if

$$Y_{q_1,\ldots,q_D} = \sum_{p_1=1}^{P_1} \cdots \sum_{p_D=1}^{P_D} W_{p_1,\ldots,p_D} X_{\tilde{q}_1(p_1),\ldots,\tilde{q}_D(p_D)}.$$ (19)

Here, $\tilde{q}_d(\cdot) : [P_d] \rightarrow [F'_d]$ are the patch functions for a given output location $q$. Using $D$-tuples $p, q$ as indices, we may also write

$$Y_q = \sum_{p=1}^{P} W_p X_{\tilde{q}(p)}.$$ (20)

Counting from 1 to $P$ is done in such a way that $p$ takes all the values in $[P]$.  

Definition A.2 (Patch function). For each dimension $d \in [D]$, layer $\ell \in [L]$, fix a stride $s \in \mathbb{N}$, and dilation $h \in \mathbb{N}$. For output position $q$, the patch function of the $d$th dimension $\tilde{q}_d(\cdot) : [P_d] \rightarrow [F'_d]$ is

$$\tilde{q}_d(p_d) = sq_d - h \left( p_d - \left\lfloor \frac{P_d}{2} \right\rfloor \right).$$ (21)

For a $D$-tuple index $p$, we may compactly write $\tilde{q}(p) \equiv (\tilde{q}_1(p_1),\ldots,\tilde{q}_D(p_D))$.

It is possible to verify that definition A.2 overall yields the usual definition of a convolution in deep learning [Goodfellow et al., 2016, Section 9.1].

Remark A.3. The concatenation of two patch functions $\tilde{q}(\cdot), \tilde{q}'(\cdot)$ is also a patch function, with argument in $[P]^2$. That is, for $[p, p'] = s \in \mathbb{N}^{P \times P}$ and $[q, q'] = r$,

$$\begin{align*}
(q(p), q'(p')) &= (\tilde{q}_1(p_1),\ldots,\tilde{q}_D(p_D), \tilde{q}'_1(p'_1),\ldots,\tilde{q}'_D(p'_D)) \\
&= \tilde{r}(s).
\end{align*}$$ (22)

B PROOF THAT A CNN WITH CORRELATIONS IN THE WEIGHTS CONVERGES TO A GP

In this section, we formally prove that a CNN with correlated weights converges in distribution to a Gaussian process in the limit of infinite width. Using the NETSOR programming language due to Yang [2019], most of the work in the proof is done by one step: describe a CNN with correlated weights in NETSOR.

For the reader’s convenience, we informally recall the NETSOR programming language [Yang, 2019] and key properties of its programs (theorem B.7 and corollary B.8). The outline of our presentation here also closely follows Yang [2019]. Readers familiar with NETSOR should skip to appendix B.3 where we show the program that proves theorem B.10.

B.1 DEFINITION OF A NETSOR PROGRAM

A NETSOR program expresses numerical computations, such as those used to define the output of a neural network. Each line of a NETSOR program is simply the definition of a new variable, in terms of previously defined variables.

There are three types of variables: $G(n)$-vars, $A(n_1, n_2)$-vars, and $H(n)$-vars (henceforth called “NETSOR variables”). Each of these have one or two parameters, which are the widths we will take to infinity. For a given index in $[n]$ (or $[n_1] \times [n_2]$), each NETSOR variable is a random scalar. To represent vectors that do not grow to infinity, we need to use collections of $P$ NETSOR variables.

G-vars, A-vars and H-vars are all random when the program is run. To accommodate non-random variables that may change (like the input $X$ to a neural network (NN)) we must define a different NETSOR program, defining $X$ either as a constant or a G-var with variance zero.

What follows is an explanation of the three kinds of NETSOR variables, and example uses of them. The program indicates the type of a variable using “var : Type”.

G-vars (Gaussian-vars) are $n$-wise approximately independent and identically distributed (i.i.d) and Gaussian. By “$n$-wise (approximately) independent” we mean that there can be correlations between G-vars, but only within a single index $i \in 1,\ldots,n$. G-vars will converge in distribution to an $n$-wise independent, identically distributed Gaussian in the limit of $n \rightarrow \infty$, if all widths are $n$. They are used, for example, to define the biases of a fully connected neural network (FCNN).

A-vars represent matrices, like the weight matrices of a dense neural network. Their entries are always i.i.d. Gaussian with with zero mean, even for finite instantiations of the program (finite $n$). There are no correlations between different A-vars, or elements of the same A-var. They may be used to define the weight matrices of a FCNN.

H-vars represent variables that become $n$-wise i.i.d. (not necessarily Gaussian) in the infinite limit. G is a subtype of H, so all G-vars are also H-vars. Post-nonlinearity activations are H-vars.
O-vars (Output-vars) are used to define the output of the NETSOR program. A O(n)-var behaves like you would expect a hypothetical A(n, 1)-var to behave: its elements are i.i.d. Gaussian with mean zero, and it is independent of all other variables in the program.

Yang [2019] does not define O-vars, instead choosing to consider them part of the G-vars, since they both converge to i.i.d. Gaussians.

Definition B.1 (Netsor program). A NETSOR program consists of:

Input: A set that may contain G-vars, A-vars, and O-vars.

Body: Each line of the program defines a new variable in terms of existing ones. New variables may be defined using the following rules:

- MatMul: \( A(n_1, n_2) \times H(n_2) \rightarrow G(n_1) \). Given an \( A(n_1, n_2) \)-var (i.i.d. Gaussian matrix) and an \( H(n_2) \)-var (i.i.d. vector), their multiplication is a \( G(n_1) \)-var (that is, it converges to a Gaussian vector in the limit \( n_2 \rightarrow \infty \)).

- LinComb: Given constants \( a_1, \ldots, a_K \), and G-vars \( x_1, \ldots, x_K \) of type \( G(n_1) \), their linear combination \( \sum_{k=1}^K a_k x_k \) is a G-var.

- Nonlin: applying an elementwise nonlinear function \( \phi : \mathbb{R}^K \rightarrow \mathbb{R} \), we map several G-vars \( x_1, \ldots, x_K \) to one H-var.

Output: A tuple of scalars \((o_1^T x_1, \ldots, o_K^T x_K) / \sqrt{n_K}\). The variables \( o_k : O(n_k) \) are O-vars. They may be the case that \( o_j = o_k \) for different \( j, k \) (that is, the list \([v_1, \ldots, v_K]\) has repeated entries). Each \( x_k : H(n_k) \) is a H-var.

Outside of these rules, NETSOR does not have conditionals or loops.

In practice, we may use loops and conditionals to write a NETSOR program, so long as they do not access the values of NETSOR variables. Conceptually, these behave like a LISP-style “macro” that generates a NETSOR program.

B.2 THE OUTPUT OF A NETSOR PROGRAM CONVERGES TO A GAUSSIAN PROCESS

For simplicity, we assume that the width of all the NETSOR variables is \( n \). Yang [2019] also considers the case where each \( n_k \) is different. First, the necessary assumptions.

Definition B.2 (Controlled function [Yang, 2019]). A function \( \phi : \mathbb{R}^K \rightarrow \mathbb{R} \) is controlled if it is measurable and

\[
|\phi(x)| \leq \exp\left(C\|x\|_2^{(2-c)} + c\right)
\]

for some \( C, c, \epsilon > 0 \), where \( \| \cdot \|_2 \) is the L2 norm.

If a function is controlled, it is L2 integrable with a Gaussian. That is, if the argument \( x \) of the function is Gaussian, the variance of \( \phi(x) \) is finite. This in turn ensures that the NN function has finite variance. All common nonlinearities (ReLU, tanh, SiLU, . . . ) are controlled. This is a very weak assumption; it is vanishingly unlikely that future nonlinearities will grow as fast as \( O(e^x) \).

Assumption B.3. All nonlinear functions \( \phi(\cdot) \) in the NETSOR program are controlled.

Assumption B.4 (Distribution of A-var inputs). Consider each \( A(n, n) \)-var in the program, \( W \). Each of its elements \( W_{i,j} \), where \( i, j \in [n] \), is sampled from the zero-mean, i.i.d. Gaussian, \( W_{i,j} \sim \mathcal{N}(0, \sigma_m^2 / n) \).

Assumption B.5 (Distribution of G-var inputs). Consider the input vector of all \( G(n) \)-vars for each channel \( i \in [n] \), that is, the vector \( x_i \triangleq [x_1 : x \; \text{is input \; G-var.}] \). It is drawn from a Gaussian, \( x_i \sim \mathcal{N}((\mu^m, \Sigma^m) \). The covariance \( \Sigma^m \) may be singular.

Assumption B.6 (Distribution of O-vars). Each \( O(n_k) \)-var \( v_k \) in the program is an independent Gaussian for each channel. Different O-vars may have different variances. That is, for each \( k \in [K] \), \( i \in [n] \), \( v_{i,k} \sim \mathcal{N}(0, \sigma_k^2 / n_K) \).

Theorem B.7 (NETSOR master theorem, Yang, 2019). Fix any NETSOR program satisfying assumptions B.3, B.4, B.5, B.6. If \( g^{(1)}, \ldots, g^{(M)} \) are all the G-vars in the entire program, then for any controlled \( \psi : \mathbb{R}^M \rightarrow \mathbb{R} \), as \( n \rightarrow \infty \),

\[
\frac{1}{n} \sum_{i=1}^n \psi(g_i^{(1)}, \ldots, g_i^{(M)}) \quad \xrightarrow{\text{a.s.}} \quad \mathbb{E}_{z \sim \mathcal{N}(m, K)} \left[ \psi(z^{(1)}, \ldots, z^{(M)}) \right].
\]

Here \( \text{a.s.} \) is almost sure convergence [Rosenthal, 2006 sec. 5.2]. The mean \( m \) and covariance \( K \) are calculated under the assumption that all the G-vars are jointly Gaussian, like in section 5.

Proof sketch. The proof is by induction on the number of G-vars included in the output, added in order of definition. The induction invariant is that, for some \( m < M \), eq. 23 holds; and that a subset of G-vars in \([m]\) which form a basis have a non-singular distribution. The detailed proof is in Yang [2019] Appendix H].

The following corollary is a consequence of the Master theorem (B.7) and the Central Limit Theorem.

Corollary B.8 (Corollary 5.5, abridged, Yang, 2019). Fix any NETSOR program which satisfies assumptions B.3 to B.6. For simplicity, fix the widths of all the variables to \( n \). The program outputs are \((o_1^T x_1, \ldots, o_K^T x_K)\), where each
\(x_k\) is an H-var, and each \(o_k\) is a O-var. Then, as \(n \to \infty\), the output tuple converges in distribution to a Gaussian \(\mathcal{N}(0, K)\). The covariance \(K\) is given by doing calculations like section 3, assuming that G-vars are jointly Gaussian.

### B.3 NETSOR PROGRAM AND GP BEHAVIOUR: CNN WITH CORRELATED WEIGHTS

NETSOR only has native support for matrix-vector multiplications and linear combinations with constants. How can we represent a convolution operation for convolutional neural network (CNN)? Consider the convolutional layer definition (eq. 4). Changing the sum order, we obtain

Thus, we may express a convolution with multiple filters as

\(Ru\)

expression of a Gaussian random variable with mean zero. Here we run into a problem. Equation 9 states that CNN is a sum of matrix-vector multiplications. This is the canonical way to represent convolutional filters in NETSOR [Yang et al. 2019] NETSOR program 4.

Here we run into a problem. Equation 9 states that CNN filters are spatially correlated, but assumption 4.4 states that A-vars have to be independent. To solve this, we will use the following well-known lemma, which is the \(R\)x expression of a Gaussian random variable with mean zero. The tensor \(R\) is a square root of the covariance.

**Lemma B.9.** Let \(\Sigma \in \mathbb{R}^{P^2}\) be an arbitrary real-valued covariance tensor. Then there exists another real-valued tensor \(\tilde{R} \in \mathbb{R}^{P^2}\) such that \(\Sigma_{a,q} = \sum_{p=1}^{P} R_{a,p} R_{q,p}\). Next, let \(u, w \in \mathbb{R}^P\) be real-valued tensors, such that \(w = Ru\). Suppose the elements of \(u\) are i.i.d. standard Gaussian variables, \(\{u_p\}_{p \in [P]} \sim \mathcal{N}(0, 1)\). Then, \(w\) has a multivariate Gaussian distribution with mean zero and covariance tensor \(\Sigma\).

**Proof.** Let \(K = |P|\), and \(\Sigma\) be \(K \times K\) matrices, obtained by flattening the dimensions of \(\Sigma\) respectively. Then \(\Sigma\) is a real-valued covariance matrix, so it is positive semi-definite and a square matrix \(\tilde{R}\) s.t. \(\tilde{R}R^T = \Sigma\) always exists. Un-flattening \(\tilde{R}\) we obtain \(R\). The variable \(w\) is Gaussian because it is a linear transformation of the Gaussian \(u\). Calculating the second moment of \(w\) finishes the proof.

Thus, to express convolution in NETSOR with correlated weights \(w\), we can use the following strategy. First, express several convolutions with uncorrelated weights \(u\), using eq. 25. Then, combine the output of the convolutions using LinComb and coefficients of the tensor \(R\).

Given a collection of A-vars \(\{\tilde{F}_{i}^{(t)}\}_{p \in [P]}\), we can express the convolutional weights \(W^{(t)}\) which have covariance \(\Sigma^{(t)} = R^{(t)}(R^{(t)})^T\) as

\[
W_{i::p}^{(t)} = \sum_{s=1}^{P} R_{p,s}^{(t)} U_{i::s}^{(t)}.
\]

Substituting this into eq. 25, we obtain

\[
Z_{i::q}^{(t)}(X) = \sum_{p=1}^{P} \sum_{s=1}^{P} R_{p,s}^{(t)} U_{i::s}^{(t)} A_{::q(p)}^{(t-1)}(X).
\]

To express this computation with NETSOR rules we may write

**MatMul:** \(H_{i,s,p}^{(t)}(X) \triangleq U_{i,s}^{(t)} A_{::q(p)}^{(t-1)}(X)\)

for \(s \in [P^{(t)}], p \in [F^{(t-1)}],\)

**LinComb:** \(Z_{i::q}^{(t)}(X) \triangleq \sum_{p=1}^{P} \sum_{s=1}^{P} R_{p,s}^{(t)} H_{i,s,q(p)}^{(t)}(X)\)

for \(q \in [F^{(t)}].\)

Algorithm \[ uses this construction for every layer to express an \(L\)-layer CNN with correlated weights, applied to an input data set \(X : [X_1, \ldots, X_M]\).

**Theorem B.10** (Correlated CNN behaves like a GP). Consider a countable set of input points \(\mathcal{X}\), and a fixed number of layers \(L\). Apply the L-layer convolutional neural network (eqs. 1 and 2) with correlated weights (eq. 9) to \(X\). Assume its nonlinearities are controlled (assumption B.3). For simplicity, fix all layers to have the same number of channels: \(C = C^{(1)} = \cdots = C^{(L)}\). Then, as the number of channels \(C \to \infty\), the activations \(Z^{(L)}(\mathcal{X})\) converge in distribution to a Gaussian process with mean function \(E\left[Z_i^{(L)}(\mathcal{X})\right] = m^{(L)}(\mathcal{X})\) and covariance function \(\mathbb{C}[Z_i^{(L)}(\mathcal{X}), Z_{i'}^{(L)}(\mathcal{X})] = \delta_{i,i'} R_{q,q}^{(L)}(\mathcal{X}, \mathcal{X})\) (section 3).

**Proof.** We need to show

1. that algorithm \[ including the postprocessing part, implements a correlated-weight CNN correctly,
2. that the full program converges weakly to a Gaussian process (GP) on \(\mathcal{X}\),
3. that the moments of this GP match the ones in section 3.
Algorithm 1 NETSOR description of an $L$-layer CNN with correlated weights, with input $\mathcal{X}$.

```
/* G-vars for layer 1 activations, for all spatial locations $p$ and input points $X_m$. */
Input: $Z_p^{(1)}(X_m) : G(C^{(1)})$
for $p \in [F^{(1)}]$ and $m = 1, \ldots, M$.
/* A-vars for the independent convolutional weights */
Input: $U^{(\ell)} : A(C^{(\ell)}, C^{(\ell - 1)})$
for $p \in [P^{(\ell)}]$ and $\ell = 2, \ldots, L - 1$.
/* O-vars for the output, for every patch location $s$ and channel $i$ */
Input: $o_{t,s} : O(C^{(L-1)})$
for $s \in [P^{(L)}]$ and $i = 1, \ldots, C^{(L)}$.

for $m = 1, \ldots, M$ (data points of $m$) do
  for $\ell = 2, \ldots, L - 1$ (layer $\ell$) do
    for $p = 1, \ldots, F^{(\ell - 1)}$ do
      Nonlin: $H(C^{(\ell - 1)})$
      $A^{(\ell - 1)}_{p.s}(X_m) \triangleq \phi(Z^{(\ell - 1)}_{p.s}(X_m))$
      for $s = 1, \ldots, P^{(\ell)}$ (patch location $s$) do
        MatMul: $G(C^{(\ell)})$
        $H^{(\ell)}_{s.p}(X_m) \triangleq U^{(\ell)}_{s.p} A^{(\ell - 1)}_{p.s}(X_m)$
      end
    end
    for $q = 1, \ldots, F^{(\ell)}$ (spatial location $q$) do
      LinComb: $C^{(\ell)}(X_q)$
      $Z^{(\ell)}_{p.q}(X_m) \triangleq \sum_p \sum_s P^{(\ell)}_s R^{(\ell)}_{s.p} H^{(\ell)}_{s.p}(X_m)$
    end
  end
end

for $p \in [F^{(L - 1)}]$ (spatial location $p$) do
  Nonlin: $H(C^{(L - 1)})$
  $A^{(L - 1)}_{p.s}(X_m) \triangleq \phi(Z^{(L - 1)}_{p.s}(X_m))$
end

/* One output for every spatial location $p$, patch location $s$, channel $i$ and data point $m$. */
Output: $(o_{t,s}^T A^{(L - 1)}_{p.s}(X_m))$: for $p \in [F^{(L)}]$, $s \in [P^{(L)}]$
$i \in [C^{(L)}]$ and $m \in [M]$.

Output postprocessing: correlate the outputs and add biases (not part of NETSOR)
for $m \in [M]$, $i \in [C^{(L)}]$ and $q \in [F^{(L)}]$ do
  $Z_{i,q}^{(L)}(X_m) \triangleq \sum_p P^{(L)}_s R^{(L)}_{p.s} (o_{t,s}^T A^{(L - 1)}_{q.p}(X_m))$
end
```

For the first claim, the key is the equivalence between a convolutional layer with correlated weights (eq. 1), and a spatial outer product followed by linear combination (eqs. 28 and 29). Keeping this in mind, we can verify by inspection that the steps of algorithm 1 including the output postprocessing, implement the recursive CNN equations (eqs. 1 and 2).

The second claim is somewhat more involved. Invoking the Kolmogorov extension theorem [Tak[2011] Thm. 2.4.3] we restrict our attention to finite subsets $\mathcal{X} \subseteq \mathcal{X}$, which are going to be compatible distributions if claim 3 is true. Since $X \in \mathcal{X}$ are tensors, we may use the Euclidean metric. We then show by theorem B.7 that the output tuple of the CNN NETSOR program converges weakly to a Euclidean metric. Each activation in the postprocessing is defined as a linear combination of a Gaussian random variable (RV) (the bias) and a RV that converges weakly to a Gaussian, and thus the resulting distribution on $\mathcal{X}$ converges weakly to a Gaussian too.

Finally, we have to show that the postprocessed output has the correct kernel. The output tuple and the activations have mean zero, which is correct. We thus compute the covariance of the output tuple in algorithm 1 for $X, X' \in \mathcal{X}$:

$$
C \left[ o_{t,s}^T A^{(L - 1)}_{p.s}(X), o_{t',s'}^T A^{(L - 1)}_{p'.s'}(X') \right] = \delta_{i,i'} \delta_{s,s'} V^{(L - 1)}_{p.p'}(X, X').
$$

(30)

The delta functions appear because the O-vars and their elements are all independent. Using this, we can calculate the covariance function of the activations

$$
C \left[ Z^{(L)}_{i,q}(X), Z^{(L)}_{i',q'}(X') \right] = \sum_{p,p'} \sum_{s,s'} P^{(L)}_{p,s} P^{(L)}_{p',s'} C \left[ o_{t,s}^T A^{(L - 1)}_{p,s}(X), o_{t',s'}^T A^{(L - 1)}_{p',s'}(X') \right].
$$

(31)

Substitute the value of the expectations and eliminate one of the sums due to $\delta_{s,s'}$.

$$
C \left[ Z^{(L)}_{i,q}(X), Z^{(L)}_{i',q}(X') \right] = \delta_{i,i'} \sum_{p,p'} \sum_{s=1}^{p^{(L)}_{p,s}} R^{(L)}_{p,s} R^{(L)}_{p',s'} V^{(L - 1)}_{q,q'}(X, X').
$$

(32)

Finally, noting that $\Sigma^{(L)}_{p,p'} = \sum_{s=1}^{p^{(L)}_{p,s}} R^{(L)}_{p,s} R^{(L)}_{p',s'}$ (lemma B.9), and using the definition of $K^{(L)}_{q,q'}(X, X')$ (eq. 11), we obtain the claim.

$$
\delta_{i,i'} K^{(L)}_{q,q'}(X, X').
$$

(33)