Distance-Based Regularisation of Deep Networks for Fine-Tuning

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Abstract
We investigate approaches to regularisation during fine-tuning of deep neural networks. First we provide a neural network generalisation bound based on Rademacher complexity that uses the distance the weights have moved from their initial values. This bound has no direct dependence on the number of weights and compares favourably to other bounds when applied to convolutional networks. Our bound is highly relevant for fine-tuning, because providing a network with a good initialisation based on transfer learning means that learning can modify the weights less, and hence achieve tighter generalisation. Inspired by this, we develop a simple yet effective fine-tuning algorithm that constrains the hypothesis class to a small sphere centred on the initial pre-trained weights, thus obtaining provably better generalisation performance than conventional transfer learning. Empirical evaluation shows that our algorithm works well, corroborating our theoretical results. It outperforms both state of the art fine-tuning competitors, and penalty-based alternatives that we show do not directly constrain the radius of the search space.

1. Introduction
The ImageNet Large Scale Visual Recognition Challenges have resulted in a number of neural network architectures optimised for high accuracy when trained on large datasets of labelled examples (He et al., 2016; Tan & Le, 2019; Russakovsky et al., 2015). Although these models have been shown to achieve excellent performance in these benchmarks, in many real-world scenarios such volumes of data are not available, and one must resort to fine-tuning an existing model: taking the weights from a model trained on a large dataset, and using these to initialise the weights for a model that will be trained on a small dataset. The assumption being that the weights from the pre-trained model provide a better initialisation than randomly generated weights. Approaches for fine-tuning are typically ad hoc, requiring one to experiment with many problem-dependent tricks, and often a process that will work for one problem will not work for another. Transforming fine-tuning from an art into a well principled procedure is therefore an attractive prospect. This paper investigates, from both a theoretical and empirical point of view, the impact of different regularisation strategies when fine-tuning a pre-trained network for a new task.

Previous approaches to regularising the fine-tuning process have focused on augmenting the standard cross entropy loss with additional terms that indirectly or directly penalise the distance the fine-tuned weights move from the pre-trained values. While the intuition behind this seems sensible—the closer the fine-tuned weights are to the pre-trained weights, the less information is forgotten about the source dataset—it is not obvious how this idea should be translated into an effective algorithm. One should expect that the choice of distance metric is quite important, but existing methods exclusively make use of Euclidean distance (Li et al., 2019; 2018) without any theoretical or empirical justification regarding why that metric was chosen. These methods achieve only a small improvement in performance over standard fine-tuning, and it is reasonable to expect that using a metric more suited to the weight space of neural networks would lead to greater performance. Moreover, while the use of penalty terms to regularise neural networks is well established, the impact of using penalties vs constraints as regularisers has not been well studied in the context of deep learning.

In order to study the generalisation error of fine-tuned models, we derive new bounds on the empirical Rademacher complexity of neural networks based on the distance the trained weights move from their initial values. In contrast to existing theory (e.g., Neyshabur et al. (2018); Bartlett et al. (2017); Long & Sedghi (2019)), we do not resort to covering numbers or make use of distributions over models to make these arguments. By deriving two bounds utilising different distance metrics, but proved with the same techniques, we are able to conduct a controlled theoretical comparison of which metric one should use as the basis for a fine-tuning regularisation scheme. Our findings show that a metric...
based on the maximum absolute row sum (MARS) matrix norm is a more suitable measure of distance in the parameter space of convolutional neural networks than Euclidean distance. Additionally, we challenge the notion that using a penalty term to encourage the fine-tuned weights to lie near the pre-trained values is the best way restrict the effective hypothesis class. We instead demonstrate that using projected stochastic subgradient methods to constrain the distance the weights in each layer can move from the initial settings can lead to improved performance.

Several regularisation methods are proposed, with the aim of both corroborating the theoretical analysis with empirical evidence, and improving the performance of fine-tuned networks. One of these approaches is a penalty-based method that regularises the distance from initialisation according to the MARS-based distance metric. The other two techniques make use of efficient projection functions to enforce constraints on the Euclidean and MARS distance between the pre-trained and fine-tuned weights throughout training. The experimental results demonstrate that projected subgradient methods result in improved performance over using penalty terms, and that the widely used Euclidean metric is typically not the best choice of metric to measure distances in network parameter space.

2. Related Work

The idea of developing an algorithm to restrict the distance of weights from some unbiased set of reference weights has been explored in various forms to improve the performance of fine-tuned networks. Li et al. (2018) presented the $\ell^2$-SP regulariser, which consists of adding a term to the objective function that penalises the squared $\ell^2$ distance of the trained weights from the initial weights. This is based on an idea initially made use of when performing domain adaptation, where it was applied to linear support vector machines (Yang et al., 2007). The work of Li et al. (2019) follows the intuition that the features produced by the fine-tuned network should not differ too much from the pre-trained features. They also use Euclidean distance, but to measure distance between feature vectors rather than weights. The idea is extended to incorporate an attention mechanism that weights the importance of each channel. The method is implemented by adding a penalty term to the standard objective function.

Many recent meta-learning algorithms also make use of idea that keeping fine-tuned weights close to their initial values is desirable. However, these approaches typically focus on developing methods for learning the initial weights, rather than working with pre-specified initial weights. The model-agnostic meta-learning approach (Finn et al., 2017) does this by simulating few-shot learning tasks during the meta-learning phase in order to find a good set of initial weights for a neural network. Once the learned algorithm is deployed, it adapts to new few-shot learning tasks by fine-tuning the initial weights for a small number of iterations. Denevi et al. (2018) proposes a modified penalty term for ridge regression where, instead of penalising the distance of the parameters from zero, they are regularised towards a bias vector. This bias vector is learned during the course of solving least squares problems on a collection of related tasks. Denevi et al. (2019) extend this approach to a fully online setting and a more general family of linear models.

Approaches to constraining the distance weights have moved from the origin have also been explored for various choices of distance metric. Sedghi et al. (2019) provide a method for projecting the weights of convolutional layers such that the spectral norm of the linear transform they implement is bounded from above by some user-selected hyperparameter. Although their projection function is faster than the naïve approach of directly constructing the linear transform and applying the power method, it still takes on the order of seconds to compute, limiting its practicality. Gouk et al. (2018) present heuristic projection functions that constrain various norms of convolutional layers, but do not show that these projections satisfy the properties required for stochastic subgradient methods to converge towards stationary points. Gouk et al. (2018) also observe that enforcing spectral norm constraints with projections results in better performance than adding a spectral norm penalty term to the loss, which is congruent with the results we observe in Section 5.

Previous work investigating the generalisation performance of neural network based on the distance the weights have travelled from their initial values has done so with the aim of explaining why existing methods for training models work well. Bartlett et al. (2017) present a bound derived via covering numbers that shows the generalisation performance of fully connected networks is controlled by the distance the trained weights are from the initial weights. Their bound makes use of a metric that scales with the number of units in the network, which means if the result is extended to a class of simple convolutional networks then the generalisation performance will scale with the resolution of the feature maps. A similar bound can also be proved through the use of PAC-Bayesian analysis (Neyshabur et al., 2018). One can make use of different metrics and techniques for applying covering numbers to bounding generalisation that do not have the same implicit dependence on the number of units, but they instead depend directly on the number of weights in the network (Long & Sedghi, 2019).

Neyshabur et al. (2019) investigate the performance of two layer neural networks with ReLU activation functions, demonstrating that as the size of the hidden layer increases, the Frobenius distance (i.e., the Frobenius norm of the dif-
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The distance between initial and trained weight matrices shrinks. Inspired by this observation, they show that one can construct a bound on the Rademacher complexity of this class by using Euclidean distance between the initial weights and trained weights of each individual unit. Although they bound the Rademacher complexity directly, they still incur an explicit dependence on the size of the hidden layer, and their analysis is restricted to fully connected networks with only a single hidden layer.

In contrast to these previous studies, our focus is on designing an algorithm that will improve the performance of fine-tuned networks, rather than explain the performance of the standards methods that are already widespread. Therefore, we do not aim to infer what properties of existing methods enable networks to generalise well—we instead derive such properties and then develop algorithms that enforce them. Moreover, we put a particular emphasis on choosing a metric that is suitable for contemporary convolutional networks, and thus will not scale with the size of the feature maps, while also being easy to implement efficiently.

3. Distance-Based Rademacher Bounds

Throughout this section we will analyse a loss class consisting of feed-forward neural networks where both the norm of the weight matrix of each layer and the distance of the fine-tuned weights from the pre-trained weights are bounded from above. Formally, we define

\[ F_* = \{ f(y, V(\phi_L \circ \ldots \circ \phi_1)(\vec{x})) | \phi_j(x) = \varphi(W_j \vec{x}), \| V \|_* \leq B_V^*, \| W_j \|_* \leq B_j^*, \| W^0_j \|_* \leq B^*_j, \| W_j - W^0_j \|_* \leq D^*_j \}, \]

where \( j \) goes from 1 to \( L \), \( l \) is a \( \rho \)-Lipschitz loss function, \( \varphi \) is a 1-Lipschitz activation function applied element-wise, \( V \) is the new classification layer trained from scratch, and \( W^0_j \) is the pre-trained weight matrix for layer \( j \). We have used \( * \) as a placeholder for the norm used to measure the magnitude of weight matrices and the distance from the pre-trained weights. The primary focus is on using the MARS norm,

\[ \| W \|_\infty = \max_j \sum_{i=1}^{|W|} |W_{j,i}|, \]

to prove a bound on the empirical Rademacher complexity of \( F_* \). Using a standard result from statistical learning theory, one can make use of the empirical Rademacher complexity of \( F_* \) (denoted by \( \hat{R}(F_*)) \) to bound the generalisation error of models contained within the class.

**Theorem 1** (Ben-David (2014, p. 378)). For all \( f \in F \), the following holds with probability at least \( 1 - \delta \):

\[ \mathbb{E}_{\vec{x}, \vec{y}} \left( f(y, \vec{x}) \right) \leq \frac{1}{m} \sum_{i=1}^m f(y_i, \vec{x}_i) + 2\hat{R}(F) + O\left( \frac{\log(2/\delta)}{m} \right), \]

where \( (\vec{x}_i, y_i) \) are independent and identically distributed.

Our main theoretical result, presented below, is based on modifying the “peeling”-style arguments typically used to directly prove bounds on the Rademacher complexity of neural network hypothesis classes (for examples, see Neyshabur et al. (2015); Golowich et al. (2018)). Our modification of the argument allows us to rephrase the resulting theorem in terms of the distance the parameters can move from their initialisation during training.

**Theorem 2.** The empirical Rademacher complexity of \( F_\infty \) is bounded by

\[ \mathbb{E}(f) \leq \frac{\sqrt{2\log(2L)}c\rho C_\infty B_\infty}{\sqrt{m}} \sum_{j=1}^L \frac{D_\infty^j}{B_\infty^j} \prod_{j=1}^L 2B_\infty^j, \]

where \( m \) is the number of training examples, \( c \) is the number of classes, \( \vec{x}_i \in \mathbb{R}^d \), and \( \| \vec{x}_i \|_\infty \leq C_\infty \).

The proof for Theorem 2 is in Appendix A in the supplemental material. The two main terms in this theorem are (i) the product of bounds on the layer norms; and (ii) the summation, which is a bound on the distance the fine-tuned weights can be from the pre-trained weights. The first of these is primarily dependent on the weights obtained via pre-training, whereas (ii) can be controlled during the fine-tuning process. Moreover, one would expect that if better initial weights are selected via pre-training, then the distance the final weights will be from the initial values will be smaller, thus leading to better generalisation. This is the motivation behind the regularisers we develop in Section 4.

An analogous bound is also derived for the Frobenius norm (i.e., \( F_F \)) to facilitate a theoretical comparison between the proposed regularisation method and \( \ell^2 \)-SP, an existing approach that relies on penalising Euclidean distance between the pre-trained and fine-tuned parameters. In order to avoid a direct dependence on the number of parameters (as accomplished in Theorem 2) it was necessary to restrict \( F_F \) to use only ReLU activation functions.

**Theorem 3.** When \( F_F \) is restricted such that \( \varphi \) is the ReLU activation function, the following holds

\[ \mathbb{E}(f) \leq \frac{\sqrt{2c} \rho C_F B_F}{\sqrt{m}} \sum_{j=1}^L \frac{D_F^j}{B_F^j} \prod_{j=1}^L 2B_F^j, \]

where \( m \) is the number of training examples, \( c \) is the number of classes, and \( \| \vec{x}_i \|_2 \leq C_2 \).

The proof is given in Appendix B of the supplementary.

Theorem 3 exhibits a milder dependence on the number of classes than Theorem 2, and also does not have the same dependence on the dimensionality of the input. However,
the more interesting relationship is how the norms in each of the theorems scale with network architecture. In particular, consider the structure of each $W_i$ when the $i$th layer is a convolutional layer. In this case $W_i$ will be a doubly block circular matrix, and the size of the matrix will depend on the number input channels, output channels, and their resolution. Although the number of non-zero elements in each row will be independent of the number of output channels and the resolution of the feature maps, the number of rows will not. In the case of the MARS norm, this means the corresponding bound will be affected only by the number of input channels to a layer, in addition to the kernel size. In contrast, the Frobenius norm of $W_i$ will increase with the resolution and number of output feature maps. This suggests that the MARS norm could be a more appropriate choice for controlling the capacity of convolutional neural networks. We include a more detailed comparison with other bounds in Appendix C of the supplement.

4. Fine-Tuning with Distance Regularisation

The analysis presented in Section 3 suggests that the weights in fine-tuned models should be close to the pre-trained weights in order to achieve good generalisation performance. More specifically, the learning process should search only within a set of weights within a predefined distance from the pre-trained weights. We discuss two strategies for accomplishing this: using projected subgradient methods to enforce a hard constraint, and augmenting the standard cross entropy objective with a term that penalises the distance between the pre-trained and fine-tuned weights. The method based on projection functions is attractive because it guarantees that the constraints will be fulfilled even if one uses a heuristic optimisation method to train the network parameters. However, the penalty-based approaches are more common in the literature, and convenient from an implementation point of view due to the ubiquity of automatic differentiation. Nevertheless, in contrast to the projection-based methods, the techniques that use penalties have weaker guarantees on whether a constraint is actually being enforced.

4.1. Optimising with Projections

One way to enforce constraints on the weights of neural networks during training is to use a variant of the projected stochasitic subgradient method. This is similar to typical stochastic subgradient methods used when training neural networks, but has the additional step of applying a projection operation after each weight update to ensure that the new weights lie inside the set of feasible parameters that satisfy the constraints. In the case of classic subgradient descent, in order to guarantee convergence towards a stationary point the projection function must perform a Euclidean projection,

$$\pi(\hat{W}) = \arg \min_W \frac{1}{2}\|W - \hat{W}\|^2_F$$

subject to $g(W) \leq 0$, where $\hat{W}$ are the newly updated parameters that may violate the constraint, $W$ are the projected parameters, and $g(\cdot)$ is a convex function specifying the constraint. Although the Euclidean projection is required for the classic projected subgradient method, other optimisation algorithms may require the projection to be performed with respect to a different metric. Looking at different optimisers as instantiations of mirror descent with different Bregman divergences is one way to determine the type of projection that should be performed. Unfortunately some of the most common optimisers used in deep learning, such as Adam (Kingma & Ba, 2015), are not guaranteed to converge even when there are no constraints on the parameters being optimised (Reddi et al., 2018). This is makes extending it to perform constrained optimisation a purely heuristic endeavour, further compounded by the fact that it is also not clear which metric the projection should be performed with respect to. As such, the projections used in our approaches are performed with respect to the norm that is most convenient from an efficiency point of view.

Rather than attempting to constrain the distance between the all pre-trained and fine-tuned weights in the network using a single projection, constraints are applied on a layer-wise basis. This makes optimisation more manageable and also allows practitioners to favour fine-tuning certain parts of the network—e.g., if one is fine-tuning a network pre-trained on photos to perform a task on paintings where the same underlying classes are present, one might wish to allocate more fine-tuning capacity to earlier layers in the network. The types of constraints that we wish to enforce take the form

$$\|W_j - W_j^{(0)}\|_s \leq \gamma_j,$$

where $\gamma_j$ is a hyperparameter that corresponds to the maximum allowable distance between the pre-trained weights and the fine-tuned weights for layer $j$. With a minor rearrangement, this yields a constraint specification in the form required for Equation 1,

$$g_j(W_j^{(0)}, W_j, \gamma_j) = \|W_j - W_j^{(0)}\|_s - \gamma_j,$$

where we have made the dependence on the pre-trained weights and the hyperparameter explicit. The resulting optimisation problem is

$$\min_{W_1:L, V} \sum_{i=1}^m l(y_i, V(\phi_L \circ \ldots \circ \phi_1)(\tilde{x}_i))$$

subject to $\|V\|_s \leq \gamma_V$

$$\|W_j - W_j^{(0)}\|_s \leq \gamma_j \ \forall j \in \{1 \ldots L\}.$$

The remainder of this section presents derivations for the projection functions, $\pi_F$ and $\pi_{\infty}$, corresponding to this constraint specification when it is instantiated with
Algorithm 1 A projected stochastic subgradient method for enforcing a distance constraint on each layer of a fine-tuned neural network, where $f_i$ is the objective function evaluated on a batch of data indexed by $t$. update($\cdot$) is a weight update rule such as Adam, and $\pi$ is a projection function.

**Inputs:** $W^{(0)}_{1:L}, V^{(0)}$, and $\gamma_i$

$t \leftarrow 0$

**while** $(W^{(t)}_{1:L}, V)$ not converged **do**

$t \leftarrow t + 1$

$\hat{V}^{(t)} \leftarrow \text{update}(V^{(t-1)}, \nabla_f(W^{(t-1)}_{1:L}, V^{(t-1)}))$

$V^{(t)} \leftarrow \pi(0, \hat{V}^{(t)}, \gamma_V)$

$\hat{W}^{(t)}_{1:L} \leftarrow \text{update}(W^{(t-1)}_{1:L}, \nabla W_{1:L} f_i(W^{(t-1)}_{1:L}, V^{(t-1)}))$

for $j = 1 \text{ to } L$ **do**

$W_j^{(t)} \leftarrow \pi(W_j^{(0)}, \hat{W}_j^{(t)}, \gamma_j)$

end for

end while

the Frobenius norm and the MARS norm, respectively. Algorithm 1 illustrates how these projections are integrated to the neural network fine-tuning procedure when using a variant of the stochastic subgradient method. We refer to the Frobenius norm instantiation as $\ell^2$-PGM and the MARS norm version as MARS-PGM, where the PGM indicates the use of projection gradient methods.

4.1.1. Constraining Frobenius Distance

When using the Frobenius distance, Equation 1 can be rewritten as

$$
\pi_F(W^{(0)}, \hat{W}, \gamma) = \arg \min_W \frac{1}{2} \|W - \hat{W}\|_F^2,
$$

s.t. $\|W - W^{(0)}\|_F - \gamma \leq 0$.

To simplify the problem, we can instead work on a translated version of the same parameter space where $W^{(0)}$ is the origin. Setting $\hat{T} = \hat{W} - W^{(0)}$ and $T = W - W^{(0)}$, the problem becomes

$$
\pi_2(\hat{T}, \gamma) = \arg \min_T \frac{1}{2} \|T - \hat{T}\|_F^2,
$$

s.t. $\|T\|_F - \gamma \leq 0$,

which is the Euclidean projection onto the $\ell^2$ ball with radius $\gamma$, and has the known closed form solution

$$
\pi_2(\hat{T}, \gamma) = \frac{1}{\max(1, \|\hat{T}\|_F)} \hat{T}.
$$

Expanding the definition of $\hat{T}$ and translating back into the correct parameter space yields the Frobenius distance projection function,

$$
\pi_F(W^{(0)}, \hat{W}, \gamma)
= W^{(0)} + \frac{1}{\max(1, \|W - W^{(0)}\|_F)} (\hat{W} - W^{(0)}),
\tag{3}
$$

4.1.2. Constraining MARS Distance

The constraint on the MARS distance can be equivalently expressed as a collection of constraints on the $\ell^1$ distance of each row in the weight matrix from the corresponding row in the pre-trained weight matrix. That is,

$$
\|W - W^{(0)}\|_\infty \leq \gamma \iff \|\tilde{w}_i - \tilde{w}_i^{(0)}\|_1 \leq \gamma \quad \forall i,
$$

where $\tilde{w}_i$ is the $i$th row of $W$. One can then make use of the same translation trick used to derive the Frobenius distance projection function to change the $\ell^1$ distance constraints to $\ell^1$ norm constraints,

$$
\pi_1(\hat{t}_i, \gamma) = \arg \min_{\hat{t}_i} \frac{1}{2} \|\hat{t}_i - \tilde{t}_i\|_2^2
$$

s.t. $\|\tilde{t}_i\|_1 - \gamma \leq 0$,

where $\hat{t} = \tilde{w}_i - \tilde{w}_i^{(0)}$. The problem in Equation 4 is a Euclidean projection onto the $\ell^1$ ball with radius $\gamma$, for which there is no known closed form solution. There exist algorithms to find the $\ell^1$ projection in time linearly proportional to the dimensionality of the vector (Duchi et al., 2008), but they are not amenable to implementation on graphics processing units due to the sequential nature of the computations involved. Instead, we apply a projection that minimises the $\ell^1$ distance between the original point and its projection, subject to the projected point lying inside the $\ell^1$ ball with radius $\gamma$,

$$
\pi_1(\hat{t}_i, \gamma) = \frac{1}{\max(1, \|\hat{t}_i\|_1)} \hat{t}_i.
$$

This projection, while not providing the closest feasible point measured in Euclidean distance, still provides a point that satisfies the constraints, but is trivial to implement efficiently. Finally, the projection function for the entire weight matrix is given by applying $\pi_1$ row-wise, and translating back into the correct parameter space,

$$
\pi_\infty(W^{(0)}, \hat{W}, \gamma) = \begin{bmatrix}
\pi_1(\hat{w}_1^{\prime} - \tilde{w}_1^{(0)}, \gamma) + \tilde{w}_1^{(0)} \\
\vdots \\
\pi_1(\hat{w}_n^{\prime} - \tilde{w}_n^{(0)}, \gamma) + \tilde{w}_n^{(0)}
\end{bmatrix},
$$

where $\hat{W}$ contains $n$ rows.

4.2. Penalty Methods

One popular approach in the literature to encourage a model to not move too far from a set of initial weights is to augment the loss function with a penalty term. In our case, this would involve taking the standard objective for the problem at hand (e.g., cross entropy or the hinge loss), and adding
penalty terms corresponding to each layer,
\[
\min_{W_{1:L}, \lambda V} \sum_{i=1}^{m} l(y_i, V(\phi_L \circ \ldots \circ \phi_1)(x_i)) + \lambda V ||V||_s + \sum_{j=1}^{L} \lambda_j ||W_j - W_j^{(0)}||_s,
\]
where \( \lambda V \) and \( \lambda_j \) are hyperparameters used to balance the regularisation terms with the main loss function. Due to the subdifferentiability of the two norms considered in this paper, instantiations of Equation 5 can be trained via automatic differentiation and a variant of the stochastic subgradient method. In the case of the Frobenius norm, we actually penalise the squared Frobenius norm, which recovers the \( \ell^2 -SP \) approach of Li et al. (2018). We refer to the instantiation that penalises the MARS distance as MARS-SP.

The usual motivation for using a penalty term to enforce a norm constraint is based on the equivalence of constraints and penalties in the case of linear models with convex loss functions (Oneto et al., 2016). This equivalence tells us that for each choice of penalty hyperparameter, \( \lambda \), there is a corresponding setting for a constraint hyperparameter, \( \gamma \), such that the penalty-based approach and the projection-based optimiser will search the same hypothesis space. Although our case is quite different from the setting of Oneto et al. (2016), since we make use of nonlinear models and apply multiple norm constraints, it is still common to apply penalties to neural networks when one wishes to encourage some sort of structure in the weights of a model. The technique used to prove the equivalence in the linear case is based on reinterpreting the penalised loss function as the Lagrangian of the constrained problem. The Karush–Kuhn–Tucker theorem states that stationary points of the Lagrangian are local optimisers of the constrained problem. The problem with applying this in a deep learning context is that convergence is almost always measured in terms of predictive performance, rather than change in the parameters being optimised. As a consequence, it is rare that the fine-tuned weights will be a stationary point of the Lagrangian and the constraints implied by the values chosen for the penalty hyperparameter may not be enforced. In this case, the model resulting from the training process is not guaranteed to come from the pre-specified hypothesis class. In contrast, the projection-based methods are guaranteed to provide a model from the chosen hypothesis class even if a stationary point is not found.

5. Experiments

This section provides an empirical investigation into the predictive performance of the proposed methods relative to existing approaches for regularising fine-tuning, and also conducts experiments to demonstrate which properties of the novel algorithms are responsible for the change in performance. Several image datasets are used throughout this section: aircraft (Maji et al., 2013), butterfly (Chen et al., 2018), flowers (Nilsback & Zisserman, 2008), pets (Parkhi et al., 2012), and the PubFig collection of face images (Pinto et al., 2011). Basic statistics for each of the datasets are given in Table 1. Two network architectures are used: ResNet-101 (He et al., 2016), which is representative of a typical large neural network, and EfficientNetB0 (Tan & Le, 2019), a leading architecture intended for use on mobile devices. The Adam optimiser is used for all experiments (Kingma & Ba, 2015).

5.1. Predictive Performance

The first set of experiments is a performance comparison of the proposed methods and existing regularisation approaches for fine-tuning. The baselines considered are standard fine-tuning with no specialised regularisation, \( \ell^2 -SP \) (Li et al., 2018), and DELTA (Li et al., 2019). All regularisation hyperparameters are tuned using the HyperOpt package developed by Bergstra et al. (2015), which uses a tree of Parzen estimators to generate promising combinations of hyperparameters based on previously observed losses. To remain comparable with \( \ell^2 -SP \) and DELTA, we make use of only two hyperparameters for each of the methods proposed in Section 4: the hyperparameter corresponding to the layer trained from scratch (\( \lambda V \) and \( \gamma V \) for the penalty and constraint methods, respectively), and a single hyperparameter applied to all layers being fine-tuned (\( \lambda_j \) and \( \gamma_j \)). This also makes the hyperparameter optimisation process reliable, as the number of hyperparameters that must be tuned is not proportional to the number of layers being fine-tuned. HyperOpt is given 20 search iterations and hyperparameter combination with the best validation loss is selected. Once hyperparameters are obtained, each network architecture and regulariser combination is fine-tuned on both the training and validation folds of each dataset. The fine-tuning process is repeated five times with different random seeds to measure the robustness of each method to the composition of minibatches and initialisation of the final linear layer, which is trained from scratch. Test set accuracy is reported for the ResNet-101 and EfficientNetB0

| Dataset      | Train | Validation | Test  | Classes |
|--------------|-------|------------|-------|---------|
| Aircraft     | 3,334 | 3,333      | 3,333 | 100     |
| Butterfly    | 5,135 | 5,135      | 15,099| 200     |
| Flowers      | 1,020 | 1,020      | 6,149 | 102     |
| Pets         | 2,000 | 2,000      | 3,390 | 37      |
| PubFig       | 10,518| 1,660      | 1,660 | 83      |

Table 1. Statistics for the datasets used throughout the experiments. The Train, Validation, and Test columns contain the number of instances in each of the corresponding subsets.
architectures in Tables 2 and 3, respectively.

The most salient trend is that the projection-based methods exhibit a significant increase in accuracy over their penalty counterparts that use the same distance metric. This suggests that, in the case of fine-tuning, using a projection to enforce a constraint on the weights throughout the training process is a better regularisation strategy than adding a term to the objective function that penalises the deviations of weights from their pre-trained values. Additionally, looking further at the relative performance of the two projection-based regularisers, we can see that the MARS distance variant is more often a better choice than the Frobenius distance. This observation further supports the conclusions of the comparison of the bounds in Section 3.

### 5.2. Convergence of Penalty Methods

Section 4.2 discusses some of the potential issues with using penalty terms to enforce constraints on the parameters on neural networks. In particular, it is hypothesised that the weights produced by the fine-tuning process may not actually lie at an extreme point of the loss surface. We explore this further by examining the Euclidean norm of the gradient of the training loss with respect to the parameters—a quantity that should be zero if the parameters are at a stationary point. Figure 1 shows plots of the gradient norms, as well as the training and testing accuracy, over the course of training ResNet101 and EfficientNetB0 networks on the pets dataset while applying the MARS-SP regulariser. From these plots we can see that the training and testing accuracy converges in the expected manner, but the gradient norms remain almost constant throughout the entire training process. This corroborates our hypothesis that users who stop based on train or validation accuracy are likely not to be at an extrema of the loss, and hence not benefit from any enforced constraints.

### 5.3. Distance from Initialisation

To further investigate the relationship between the penalty and projection strategies for regularisation, we analyse the distances between the pre-trained and fine-tuned weights at a per-layer basis. Figure 2 provides histograms indicating the distributions of per-layer MARS distances for the models without any regularisation, regularised with MARS-SP, trained with the MARS-PGM, and also DELTA. All networks were trained on the Pets dataset with the same hyperparameters used by the models examined in Section 5.1. We observe three trends from these plots. Firstly, both the penalty and projection methods reduce the MARS distance between the pre-trained and fine-tuned weights to a similar extent. Second, a significant number of the constraints enforced by the penalty method are activated—i.e., many of the weight matrices lie on the boundary of the feasible set. In contrast, the penalty-based regulariser does not enforce similarly activated constraints. Finally, the results demonstrate that the DELTA method of Li et al. (2019) does not operate by implicitly regularising the same quantity, as its MARS distance histogram is longer tailed than the others.

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### Table 2

Results obtained with different regularisation approaches when fine-tuning a ResNet-101 pre-trained on the ILSVRC-2012 subset of ImageNet. We report the mean ± std. dev. of accuracy measured across five different random seeds.

| Regularisation | Aircraft | Butterfly | Flowers | Pets   | PubFig |
|----------------|----------|-----------|---------|--------|--------|
| None           | 51.81±0.87| 70.02±0.16| 76.68±1.07| 84.19±0.34| 75.36±0.67 |
| DELTA (Li et al., 2019) | 60.38±1.26| 77.91±0.24| 86.57±0.27| 88.11±0.52| 82.23±2.48 |
| $\ell^2$-SP (Li et al., 2018) | 60.16±1.33| 76.56±0.19| 83.11±0.27| 86.23±0.41| 83.79±3.69 |
| MARS-SP        | 58.52±1.23| 69.54±0.36| 75.90±1.04| 84.22±0.45| 79.17±0.73 |
| $\ell^2$-PGM   | 69.61±0.15| 77.97±0.13| 86.91±0.66| 90.47±0.33| 84.14±0.81 |
| MARS-PGM       | 63.67±1.37| 79.50±0.36| 87.42±0.41| 88.42±0.32| 88.75±0.28 |

### Table 3

Results obtained with different regularisation approaches when fine-tuning an EfficientNetB0 pre-trained on the ILSVRC-2012 subset of ImageNet. We report the mean ± std. dev. of accuracy measured across five different random seeds.

| Regularisation | Aircraft | Butterfly | Flowers | Pets   | PubFig |
|----------------|----------|-----------|---------|--------|--------|
| None           | 54.58±0.65| 69.43±0.47| 77.43±0.14| 84.87±0.19| 75.51±0.83 |
| DELTA (Li et al., 2019) | 70.61±0.18| 79.61±0.21| 84.60±0.23| 89.27±0.22| 88.62±0.54 |
| $\ell^2$-SP (Li et al., 2018) | 69.26±0.26| 78.88±0.27| 86.61±0.48| 89.79±0.28| 84.04±0.98 |
| MARS-SP        | 66.96±0.49| 72.01±0.20| 77.79±0.48| 89.24±0.40| 85.33±0.59 |
| $\ell^2$-PGM   | 70.87±0.33| 81.81±0.22| 86.95±0.17| 89.33±0.19| 88.45±0.36 |
| MARS-PGM       | 75.22±0.34| 80.19±0.16| 90.36±0.15| 91.38±0.24| 87.93±0.43 |
Figure 1. Plots demonstrating the convergence properties of MARS-SP when applied to ResNet101 and EfficientNetB0 when fine-tuned on the pets dataset. Subfigures (a) and (c) demonstrate that the norms of the gradient do not necessarily become zero, even when the accuracies in subfigures (b) and (d) have converged.

Figure 2. Histograms of MARS distances between pre-trained and fine-tuned weights for the specified regularisation strategies. MARS-PGM successfully constrains weight distances to be less than $\gamma_j$, indicated by the dashed line. All histograms correspond to ResNet101 (top) and EfficientNetB0 (bottom) models trained on the pets dataset.

6. Conclusion

This paper investigates different regularisation methods for fine-tuning deep learning networks. To facilitate this, we provide two new bounds on the generalisation performance of neural networks based on the distance of the final weights from their initial values. The discussion comparing these bounds suggests that the MARS distance is a more appropriate metric in the parameter space of convolutional networks than Frobenius distance. Additionally, several new algorithms are presented that enable an experimental comparison between different regularisation strategies. The empirical results corroborate our theoretical investigation, demonstrating that constraining MARS distance is more effective than constraining Euclidean distance. Crucially, we also show that, in line with our theoretical results, enforcing a hard constraint throughout the entire training process on the distances the parameters can move is far more effective than the widely used strategy of adding a penalty term to the objective function. Implementations of the methods used in this paper are available online.¹

¹https://github.com/henrygouk/mars-finetuning
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References

Bartlett, P. L., Foster, D. J., and Telgarsky, M. J. Spectrally-normalized margin bounds for neural networks. In Advances in Neural Information Processing Systems 30, pp. 6240–6249, 2017.

Ben-David, S. Understanding Machine Learning: From Theory to Algorithms. Cambridge University Press, 2014.

Bergstra, J., Komer, B., Eliasmith, C., Yamins, D., and Cox, D. D. Hyperopt: A Python library for model selection and hyperparameter optimization. Computational Science & Discovery, 8(1):014008, July 2015.

Chen, T., Wu, W., Gao, Y., Dong, L., Luo, X., and Lin, L. Fine-grained representation learning and recognition by exploiting hierarchical semantic embedding. In Proceedings of the 26th ACM International Conference on Multimedia, pp. 2023–2031, 2018.

Denevi, G., Ciliberto, C., Stamos, D., and Pontil, M. Learning to learn around a common mean. In Advances in Neural Information Processing Systems 31, pp. 10169–10179, 2018.

Denevi, G., Ciliberto, C., Grazzi, R., and Pontil, M. Learning-to-learn stochastic gradient descent with biased regularization. In Proceedings of the 36th International Conference on Machine Learning, pp. 1566–1575, 2019.

Duchi, J., Shalev-Shwartz, S., Singer, Y., and Chandra, T. Efficient projections onto the 1 1-ball for learning in high dimensions. In Proceedings of the 25th International Conference on Machine Learning, pp. 272–279, 2008.

Finn, C., Abbeel, P., and Levine, S. Model-agnostic meta-learning for fast adaptation of deep networks. In Proceedings of the 34th International Conference on Machine Learning, pp. 1126–1135, 2017.

Golowich, N., Rakhlin, A., and Shamir, O. Size-Independent Sample Complexity of Neural Networks. In Conference On Learning Theory, pp. 297–299, July 2018.

Gouk, H., Frank, E., Pfahringer, B., and Cree, M. Regularisation of Neural Networks by Enforcing Lipschitz Continuity. arXiv preprint arXiv:1804.04368, 2018.

He, K., Zhang, X., Ren, S., and Sun, J. Deep residual learning for image recognition. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp. 770–778, 2016.

Kingma, D. and Ba, J. Adam: A method for stochastic optimization. In International Conference on Learning Representations, 2015.

Ledoux, M. and Talagrand, M. Probability in Banach Spaces Isoperimetry and Processes. Springer, 1991.

Li, X., Grandvalet, Y., and Davoine, F. Explicit inductive bias for transfer learning with convolutional networks. In Proceedings of the 35th International Conference on Machine Learning, 2018.

Li, X., Xiong, H., Wang, H., Rao, Y., Liu, L., and Huan, J. DELTA: DEep Learning Transfer using Feature Map with Attention for Convolutional Networks. In International Conference on Learning Representations, 2019.

Long, P. M. and Sedghi, H. Size-free generalization bounds for convolutional neural networks. arXiv preprint arXiv:1905.12600, 2019.

Maji, S., Kannala, J., Rahtu, E., Blaschko, M., Vedaldi, A., Maji, S., Rahtu, E., Kannala, J., Blaschko, M., and Vedaldi, A. Fine-grained visual classification of aircraft. Technical report, 2013.

Maurer, A. A vector-contraction inequality for rademacher complexities. In International Conference on Algorithmic Learning Theory, pp. 3–17. Springer, 2016.

Neyshabur, B., Tomioka, R., and Srebro, N. Norm-based capacity control in neural networks. In Conference on Learning Theory, 2015.

Neyshabur, B., Bhojanapalli, S., and Srebro, N. A PAC-Bayesian Approach to Spectrally-Normalized Margin Bounds for Neural Networks. In International Conference on Learning Representations, February 2018.

Neyshabur, B., Li, Z., Bhojanapalli, S., LeCun, Y., and Srebro, N. Towards understanding the role of over-parametrization in generalization of neural networks. In International Conference on Learning Representations, 2019.

Nilsback, M.-E. and Zisserman, A. Automated flower classification over a large number of classes. In Proceedings of the 6th Indian Conference on Computer Vision, Graphics & Image Processing, pp. 722–729. IEEE, 2008.

Oneto, L., Ridella, S., and Anguita, D. Tikhonov, Ivanov and Morozov regularization for support vector machine learning. Machine Learning, 103(1):103–136, 2016.
Parkhi, O. M., Vedaldi, A., Zisserman, A., and Jawahar, C. Cats and dogs. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp. 3498–3505. IEEE, 2012.

Pinto, N., Stone, Z., Zickler, T., and Cox, D. Scaling up biologically-inspired computer vision: A case study in unconstrained face recognition on facebook. In *IEEE CVPR Workshops*, pp. 35–42. IEEE, 2011.

Reddi, S. J., Kale, S., and Kumar, S. On the convergence of Adam and beyond. In *International Conference on Learning Representations*, 2018.

Russakovsky, O., Deng, J., Su, H., Krause, J., Satheesh, S., Ma, S., Huang, Z., Karpathy, A., Khosla, A., Bernstein, M., Berg, A. C., and Fei-Fei, L. ImageNet Large Scale Visual Recognition Challenge. *International Journal of Computer Vision*, 115(3):211–252, December 2015.

Sedghi, H., Gupta, V., and Long, P. M. The Singular Values of Convolutional Layers. In *International Conference on Learning Representations*, 2019.

Tan, M. and Le, Q. Efficientnet: Rethinking model scaling for convolutional neural networks. In *Proceedings of the 36th International Conference on Machine Learning*, pp. 6105–6114, 2019.

Yang, J., Yan, R., and Hauptmann, A. G. Adapting svm classifiers to data with shifted distributions. In *Proceedings of the 7th IEEE International Conference on Data Mining Workshops*, pp. 69–76. IEEE, 2007.
A. Proof of Theorem 2

We begin with a lemma that demonstrates how norm-constraining the weights in the final classification layer impacts generalisation.

Lemma 1. For $\mathcal{F}_\infty$ as defined in Section 3, the following inequality holds

$$\hat{R}(\mathcal{F}_\infty) \leq \frac{\sqrt{2}c\rho B V}{m} \rho \left[ \sup_{V,W} \left( \sum_{i=1}^{m} \sigma_i(\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i) \right) \right]$$

where $c$ is the number of classes.

Proof.

$$\hat{R}(\mathcal{F}_\infty)
= \frac{1}{m} \mathbb{E} \left[ \sup_{V,W} \left( \sum_{i=1}^{m} \sigma_i(y_i, V(\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i)) \right) \right]
\leq \frac{\rho \sqrt{2}}{m} \mathbb{E} \left[ \sup_{V,W} \left( \sum_{j=1}^{c} \sum_{i=1}^{m} \sigma_{i,j} \bar{v}_j \cdot (\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i) \right) \right]
= \frac{\rho \sqrt{2}}{m} \mathbb{E} \left[ \sup_{V,W} \left( \sum_{j=1}^{c} \bar{v}_j \cdot \sum_{i=1}^{m} \sigma_{i,j}(\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i) \right) \right]
\leq \frac{\rho \sqrt{2}}{m} \mathbb{E} \left[ \sup_{V,W} \left( \sum_{j=1}^{c} \bar{v}_j \cdot \sum_{i=1}^{m} \sigma_{i,j}(\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i) \right) \right]
\leq \frac{\rho \sqrt{2}}{m} \mathbb{E} \left[ \sup_{V,W} \left( \sum_{j=1}^{c} \bar{v}_j \cdot \sum_{i=1}^{m} \sigma_{i,j}(\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i) \right) \right]
\leq \frac{\rho \sqrt{2}}{m} \mathbb{E} \left[ \sup_{V,W} \left( \sum_{j=1}^{c} \bar{v}_j \cdot \sum_{i=1}^{m} \sigma_{i,j}(\phi_L \circ \ldots \circ \phi_1)(\bar{x}_i) \right) \right],$$

where (i) can be performed via applying the main result of Maurer (2016), (ii) is due to Hölder’s inequality, and (iii) follows from the definition of the $\| \cdot \|_\infty$ matrix norm.

The following lemma uses the “peeling” method of Neyshabur et al. (2015) to bound the Rademacher complexity of a network based on the product of weight matrix norms.

Lemma 2. For $\mathcal{F}_\infty$ as defined in Section 3, the following inequality holds

$$\mathbb{E} \left[ \sup_{W_{1:k}} \left( \sum_{i=1}^{m} \sigma_i f_k(\bar{x}_i) \right) \right] \leq \sqrt{2m\log(2d)} C_\infty \prod_{j=1}^{k} 2B_j^\infty$$

where $f = \phi_k \circ \ldots \circ \phi_1$, $\bar{x}_i \in \mathbb{R}^d$, and $\| \bar{x}_i \|_\infty \leq C_\infty$. 

Proof.

\[
\begin{align*}
\mathbb{E} \left[ \sup_{W_{1:k}} \left\| \sum_{i=1}^{m} \sigma_i \varphi(W_k f_{k-1}(\vec{x}_i)) \right\|_\infty \right] \\
= \mathbb{E} \left[ \sup_{W_{1:k-1}, \vec{w}_k} \left\| \sum_{i=1}^{m} \sigma_i \varphi(\vec{w}_k \cdot f_{k-1}(\vec{x}_i)) \right\|_\infty \right] \\
\leq 2 \mathbb{E} \left[ \sup_{W_{1:k-1}, \vec{w}_k} \left\| \sum_{i=1}^{m} \sigma_i \vec{w}_k f_{k-1}(\vec{x}_i) \right\|_\infty \right] \\
\leq 2 \mathbb{E} \left[ \sup_{W_{1:k}} \left\| W_k \right\| \left\| \sum_{i=1}^{m} \sigma_i f_{k-1}(\vec{x}_i) \right\|_\infty \right] \\
= 2B_k^{\infty} \mathbb{E} \left[ \sup_{W_{1:k}} \left\| \sum_{i=1}^{m} \sigma_i f_{k-1}(\vec{x}_i) \right\|_\infty \right],
\end{align*}
\]

where (i) is due to the Lipschitz composition property of Rademacher complexities (Ledoux & Talagrand, 1991) and (ii) follows from Hölder’s inequality. Iterating this process for all layers of the network results in

\[
\mathbb{E} \left[ \sup_{W_{1:k}} \left\| \sum_{i=1}^{m} \sigma_i f_k(\vec{x}_i) \right\|_\infty \right] \leq \left( \prod_{j=1}^{k} 2B_j^{\infty} \right) \mathbb{E} \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^{m} \sigma_i \vec{x}_i \right\|_\infty \right].
\]

The expectation can be bounded via Massart’s inequality (Ben-David, 2014, p. 383) to conclude the proof. \qed

We now prove Theorem 2.

Proof. Lemma 1 tells us that

\[
\mathcal{R}(\mathcal{F}_\infty) \leq \frac{\sqrt{2cpB^\infty}}{m} \mathbb{E} \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^{m} \sigma_i (\phi_L \circ \ldots \circ \phi_1)(\vec{x}_i) \right\|_\infty \right],
\]

hence it suffices to show that

\[
\begin{align*}
\mathbb{E} \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^{m} \sigma_i f_L(\vec{x}_i) \right\|_\infty \right] \\
\leq \sqrt{2m \log(2d)C_\infty} \sum_{j=1}^{L} \frac{D_j^{\infty}}{2B_j} \prod_{j=1}^{L} 2B_j^{\infty},
\end{align*}
\]

where \( f_k = \phi_k \circ \ldots \circ \phi_1 \).

Expanding the first composition in \( f \) yields

\[
\begin{align*}
\mathbb{E} \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^{m} \sigma_i \varphi(W_L f_{L-1}(\vec{x}_i)) \right\|_\infty \right],
\end{align*}
\]
which can be bounded by

\[
\mathbb{E}_\sigma \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^m \sigma_i \varphi(W_{L-1}(\vec{x}_i)) \right\|_\infty \right] \\
= \mathbb{E}_\sigma \left[ \sup_{W_{1:L-1}, \vec{w}_L} \left\| \sum_{i=1}^m \sigma_i \varphi(\vec{w}_{L-1}(\vec{x}_i)) \right\|_\infty \right] \\
\overset{(i)}{\leq} 2 \mathbb{E}_\sigma \left[ \sup_{W_{1:L-1}, \vec{w}_L} \left\| \vec{w}_L \right\|_1 \left\| \sum_{i=1}^m \sigma_i f_{L-1}(\vec{x}_i) \right\|_\infty \right] \\
= 2 \mathbb{E}_\sigma \left[ \left\| W_L \right\|_\infty \left\| \sum_{i=1}^m \sigma_i f_{L-1}(\vec{x}_i) \right\|_\infty \right] \\
= 2 \mathbb{E}_\sigma \left[ \left\| W_{L} - W_{L}^0 + W_{L}^0 \right\|_\infty \left\| \sum_{i=1}^m \sigma_i f_{L-1}(\vec{x}_i) \right\|_\infty \right] \\
\overset{(ii)}{\leq} 2 \mathbb{E}_\sigma \left[ \left\| W_{L} - W_{L}^0 \right\|_\infty \left\| \sum_{i=1}^m \sigma_i f_{L-1}(\vec{x}_i) \right\|_\infty \right] \\
+ 2 \mathbb{E}_\sigma \left[ \left\| W_{L}^0 \right\|_\infty \left\| \sum_{i=1}^m \sigma_i f_{L-1}(\vec{x}_i) \right\|_\infty \right] \\
\overset{(iii)}{\leq} \sqrt{2m \log(2d)C} \frac{D_\infty}{B_L^\infty} \prod_{j=1}^L 2B_j^\infty
\]

where (i) follows from the Ledoux-Talagrand contraction property \cite{LedouxTalagrand1991}, (ii) is due to the triangle inequality, and (iii) is an application of lemma 2.

From here, one can take the second term of the right hand side of the final inequality and iteratively apply the same set of steps, from which the result follows. \hfill \box

\section{B. Proof of Theorem 3}

The proof of Theorem 3 follows the same structure as the proof for Theorem 2. For conciseness, some details are omitted due to their similarity with the previous proof. We begin with a lemma corresponding to Lemma 1.

\textbf{Lemma 3.} For $\mathcal{F}_F$ as defined in Section 3, the following inequality holds

\[
\hat{\mathcal{R}}(\mathcal{F}_F) \leq \frac{\sqrt{2c \rho B_L^F}}{m} \mathbb{E}_\sigma \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^m \sigma_i (\phi_L \circ \ldots \circ \phi_1)(\vec{x}_i) \right\|_2 \right]
\]

where $c$ is the number of classes.

\textit{Proof.} From the proof of Lemma 1 we have that

\[
\hat{\mathcal{R}}(\mathcal{F}_F) = \frac{\rho \sqrt{2}}{m} \mathbb{E}_\sigma \left[ \sum_{V,W_{1:L}} \sum_{j=1}^c \sigma_{V,j} \sum_{i=1}^m \sigma_{i,j} (\phi_L \circ \ldots \circ \phi_1)(\vec{x}_i) \right].
\]

Noting the summation over dot products is itself a dot product, this can be bounded by

\[
\hat{\mathcal{R}}(\mathcal{F}_F) = \frac{\rho \sqrt{2}}{m} \mathbb{E}_\sigma \left[ \sum_{V,W_{1:L}} \sqrt{c} \left\| V \right\|_F \left\| \sum_{i=1}^m \sigma_i (\phi_L \circ \ldots \circ \phi_1)(\vec{x}_i) \right\|_2 \right],
\]

from which the lemma follows. \hfill \box
Next, we provide a lemma demonstrating the peeling argument for Frobenius norm-bounded networks.

**Lemma 4.** For \( F \) as defined in Section 3, the following inequality holds

\[
\mathbb{E} \left[ \sup_{W_{1:k}} \left\| \sum_{i=1}^{m} \sigma_i f_k(\bar{x}_i) \right\|_2^2 \right] \leq \sqrt{m} C_2 \prod_{j=1}^{k} 2B_j^F
\]

where \( f = \phi_k \circ \cdots \circ \phi_1, \varphi \) is the ReLU activation function, and \( \|\bar{x}_i\|_2 \leq C_2 \).

**Proof.** Iterative applying Lemma 1 from Golowich et al. (2018) results in

\[
\mathbb{E} \left[ \sup_{W_{1:k}} \left\| \sum_{i=1}^{m} \sigma_i f_k(\bar{x}_i) \right\|_2^2 \right] \leq \mathbb{E} \left[ \left\| \sum_{i=1}^{m} \sigma_i \bar{x}_i \right\|_2^2 \right] \prod_{j=1}^{k} 2B_j^F,
\]

and the expectation can be further bounded by

\[
\mathbb{E} \left[ \left\| \sum_{i=1}^{m} \sigma_i \bar{x}_i \right\|_2^2 \right] = \mathbb{E} \left[ \sqrt{\sum_{i=1}^{m} \sigma_i \bar{x}_i} \right]^2 = \sqrt{m} C_2.
\]

Finally, we prove Theorem 3.

**Proof.** The proof for this theorem follows the same process as the proof for Theorem 2. Due to Lemma 3, it is enough to show

\[
\mathbb{E} \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^{m} \sigma_i f_L(\bar{x}_i) \right\|_2^2 \right] \leq \sqrt{m} C_2 \sum_{j=1}^{L} \frac{D_j^F}{2B_j} \prod_{j=1}^{L} 2B_j^F.
\]

The left hand side of the above inequality can be expressed as

\[
\mathbb{E} \left[ \sup_{W_{1:L}} \left\| \sum_{i=1}^{m} \sigma_i \varphi(W_L f_{L-1}(\bar{x}_i)) \right\|_2^2 \right],
\]

and due to Lemma 1 from Golowich et al. (2018) this can be bounded by

\[
\mathbb{E} \left[ \sup_{W_{1:L}} \|W_L\|_F \left\| \sum_{i=1}^{m} \sigma_i f_{L-1}(\bar{x}_i) \right\|_2^2 \right].
\]

Subtracting and adding the pre-trained weights gives

\[
\mathbb{E} \left[ \sup_{W_{1:L}} \|W_L - W_L^{(0)} + W_L^{(0)}\|_F \left\| \sum_{i=1}^{m} \sigma_i f_{L-1}(\bar{x}_i) \right\|_2^2 \right],
\]

after which the triangle inequality and Lemma 4 can be applied as in the proof for Theorem 2, from which the result follows by iteration.

**C. Comparison of Bounds**

This section provides a comparison of our bounds with previous work that investigates bounding the generalisation gap.\(^2\)

\[
G = \mathbb{E}_{\bar{x},y} \left[ f(y, \bar{x}) \right] - \frac{1}{m} \sum_{i=1}^{m} f(y_i, \bar{x}_i).
\]

\(^2\)To simplify the comparison, we omit the terms proportional to \( \sqrt{\ln(1/\delta)/m} \) that appear in all bounds. It should be noted that all bounds hold with probability \( 1 - \delta \).
In particular, we consider the main result of Bartlett et al. (2017),
\[
G \leq O\left(\frac{\ln(n)}{\sqrt{m}} \rho C_2 \left( \sum_{j=1}^{L} \left( \frac{D_j^{2,1}}{B_j^2} \right)^{2/3} \prod_{j=1}^{L} B_j^2 \right) \right),
\]
and using our notation the main result of Long & Sedghi (2019) is,
\[
G \leq O\left( \sqrt{n} m \rho C_2 \left( \sum_{j=1}^{L} D_j^2 \prod_{j=1}^{L} B_j^2 \right) \right).
\]
These bounds depend on slightly different quantities: we use \(n\) to represent the number of parameters in the network, \(B_j^2\) and \(D_j^2\) indicates upper bounds on the spectral norm and the the associated distance metric, and \(D_j^{2,1}\) corresponds to an upper bound on distance metric induced by the matrix \((2, 1)\)-norm, \(\|W\|_{2,1} = \sum_j \sqrt{\sum_i W_{j,i}^2}\).

In contrast to the aforementioned bounds, which were shown to be true via covering number arguments, the bounds presented in this paper are proved by directly bounding the empirical Rademacher complexity. As a consequence of these different proof techniques, the constants that appear in each bound are quite different. The covering number bound both have explicit dependences on the number of parameters in the network—with the bound of Long & Sedghi (2019) being much stronger than that of Bartlett et al. (2017). Our bound does not have this dependence, but it does incur an extra factor of two for every application of the Ledoux-Talagrand contraction inequality used in the peeling argument. This results in an explicit exponential dependence on the depth of the network. We note that recent work by Golowich et al. (2018) shows how the peeling method can be adapted to reduce this to a very mild dependence in some situations.

In addition to inspecting the constants in each bound, one can consider how the norms compare. The \((2, 1)\)-norm used in Equation 6 and the Frobenius norm used in Theorem 3 are both sensitive to the resolution of the intermediate feature maps in convolutional networks. In contrast, the spectral norms from Equation 7 and the MARS norm in Theorem 2 are independent of these feature map sizes. As such, the spectral norm bound and the MARS bound are more suited to explaining generalisation in convolutional networks.