Finite Versus Infinite Neural Networks: an Empirical Study

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Abstract

We perform a careful, thorough, and large scale empirical study of the correspondence between wide neural networks and kernel methods. By doing so, we resolve a variety of open questions related to the study of infinitely wide neural networks. Our experimental results include: kernel methods outperform fully-connected finite-width networks, but underperform convolutional finite width networks; neural network Gaussian process (NNGP) kernels frequently outperform neural tangent (NT) kernels; centered and ensembled finite networks have reduced posterior variance and behave more similarly to infinite networks; weight decay and the use of a large learning rate break the correspondence between finite and infinite networks; the NTK parameterization outperforms the standard parameterization for finite width networks; diagonal regularization of kernels acts similarly to early stopping; floating point precision limits kernel performance beyond a critical dataset size; regularized ZCA whitening improves accuracy; finite network performance depends non-monotonically on width in ways not captured by double descent phenomena; equivariance of CNNs is only beneficial for narrow networks far from the kernel regime. Our experiments additionally motivate an improved layer-wise scaling for weight decay which improves generalization in finite-width networks. Finally, we develop improved best practices for using NNGP and NT kernels for prediction, including a novel ensembling technique. Using these best practices we achieve state-of-the-art results on CIFAR-10 classification for kernels corresponding to each architecture class we consider.

1 Introduction

A broad class of both Bayesian [1–17] and gradient descent trained [13–16, 18–29] neural networks converge to Gaussian Processes (GPs) or closely-related kernel methods as their intermediate layers are made infinitely wide. The predictions of these infinite width networks are described by the Neural Network Gaussian Process (NNGP) [4, 5] kernel for Bayesian networks, and by the Neural Tangent Kernel (NTK) [18] and weight space linearization [24, 25] for gradient descent trained networks.

This correspondence has been key to recent breakthroughs in our understanding of neural networks [30–39] It has also enabled practical advances in kernel methods [8, 9, 15, 16, 26, 40–42], Bayesian deep learning [43–45], active learning [46], and semi-supervised learning [17]. The NNGP, NTK, and related large width limits [10, 30, 47–59] are unique in giving an exact theoretical description of large scale neural networks. Because of this, we believe they will continue to play a transformative role in deep learning theory.

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Finite gradient descent (GD)  |  Infinite GD  |  Infinite Bayesian

Figure 1: CIFAR-10 test accuracy for finite and infinite networks and their variations. Starting from the finite width base network of given architecture class described in §2, performance changes from centering (+C), large learning rate (+LR), allowing underfitting by early stopping (+U), input preprocessing with ZCA regularization (+ZCA), multiple initialization ensembling (+Ens), and some combinations are shown, for Standard and NTK parameterizations. The performance of the linearized (1ln) base network is also shown. See Table S1 for precise values for each of these experiments, as well as for additional experimental conditions not shown here.

Infinite networks are a newly active field, and foundational empirical questions remain unanswered. In this work, we perform an extensive and in-depth empirical study of finite and infinite width neural networks. In so doing, we provide quantitative answers to questions about the factors of variation that drive performance in finite networks and kernel methods, uncover surprising new behaviors, and develop best practices that improve the performance of both finite and infinite width networks. We believe our results will both ground and motivate future work in wide networks.

2 Experiment design

To systematically develop a phenomenology of infinite and finite neural networks, we first establish base cases for each architecture where infinite-width kernel methods, linearized weight-space networks, and nonlinear gradient descent based training can be directly compared. In the finite-width settings, the base case uses mini-batch gradient descent at a constant small learning rate [24] with MSE loss (implementation details in §H). In the kernel-learning setting we compute the NNGP and NTK for the entire dataset and do exact inference as described in [60, page 16]. Once this one-to-one comparison has been established, we augment the base setting with a wide range of interventions. We discuss each of these interventions in detail below. Some interventions will approximately preserve the correspondence (for example, data augmentation), while others explicitly break the correspondence in a way that has been hypothesized in the literature to affect performance (for example, large learning rates [39]). We additionally explore linearizing the base model around its initialization, in which case its training dynamics become exactly described by a constant kernel. This differs from the kernel setting described above due to finite width effects.

We use MSE loss to allow for easier comparison to kernel methods, whose predictions can be evaluated in closed form for MSE. See Table S2 and Figure S3 for a comparison of MSE to softmax-cross-entropy loss. Softmax-cross-entropy provides a consistent small benefit over MSE, and will be interesting to consider in future work.

Architectures we work with are built from either Fully-Connected (FCN) or Convolutional (CNN) layers. In all cases we use ReLU nonlinearities. Except if otherwise stated, we consider FCNs with 3-layers and CNNs with 8-layers. For convolutional networks we must collapse the spatial dimensions of image-shaped data before the final readout layer. To do this we either: flatten the image into a one-dimensional vector (VEC) or apply global average pooling to the spatial dimensions (GAP). Finally, we compare two ways of parameterizing the weights and biases of the network: the standard parameterization (STD), which is used in work on finite-width networks, and the NTK parameterization (NTK) which has been used in most infinite-width studies to date (see [27] for the
standard parameterization at infinite width).

Except where noted, for all kernel experiments we optimize over diagonal kernel regularization independently for each experiment. For finite width networks, except where noted we use a small learning rate corresponding to the base case. See §C.1 for details.

The experiments described in this paper are often very compute intensive. For example, to compute the NTK or NNGP for the entirety of CIFAR-10 for CNN-GAP architectures one must explicitly evaluate the entries in a $6 \times 10^7$-by-$6 \times 10^7$ kernel matrix. Typically this takes around 1200 GPU hours with double precision, and so we implement our experiments via massively distributed compute infrastructure based on beam [61]. All experiments use the Neural Tangents library [15], built on top of JAX [62].

To be as systematic as possible while also tractable given this large computational requirement, we evaluated every intervention for every architecture and focused on a single dataset, CIFAR-10 [63]. However, to ensure robustness of our results across dataset, we evaluate several key claims on CIFAR-100 and Fashion-MNIST [64].

### 3 Observed empirical phenomena

#### 3.1 NNGP/NTK can outperform finite networks

A common assumption in the study of infinite networks is that they underperform the corresponding finite network in the large data regime. We carefully examine this assumption, by comparing kernel methods against the base case of a finite width architecture trained with small learning rate and no regularization (§2), and then individually examining the effects of common training practices which break (large LR, L2 regularization) or improve (ensembling) the infinite width correspondence to kernel methods. The results of these experiments are summarized in Figure 1 and Table S1.

First focusing on base finite networks, we observe that infinite FCN and CNN-VEC outperform their respective finite networks. On the other hand, infinite CNN-GAP networks perform worse than their finite-width counterparts in the base case, consistent with observations in Arora et al. [26]. We emphasize that architecture plays a key role in relative performance. For example, infinite-FCNs outperform finite-width networks even when combined with various tricks such as high learning rate, L2, and underfitting. Here the performance becomes similar only after ensembling (§3.3).

One interesting observation is that ZCA regularization preprocessing (§3.10) can provide significant improvements to the CNN-GAP kernel, closing the gap to within 1-2%.

#### 3.2 NNGP typically outperforms NTK

Recent evaluations of infinite width networks have put significant emphasis on the NTK, without explicit comparison against the respective NNGP models [26, 29, 40, 41]. Combined with the view of NNGPs as “weakly-trained” [24, 26] (i.e. having only the last layer learned), one might expect NTK to be a more effective model class than NNGP. On the contrary, we usually observe that NNGP inference achieves better performance. This can be seen in Table S1 where SOTA performance among fixed kernels is attained with the NNGP across all architectures. In Figure 2 we show that this trend persists across CIFAR-10, CIFAR-100, and Fashion-MNIST (see Figure S5 for similar trends on UCI regression tasks). In addition to producing stronger models, NNGP kernels require about half the memory and compute as the corresponding NTK, and some of the most performant kernels do not have an associated NTK at all [42]. Together these results suggest that when approaching a new problem where the goal is to maximize performance, practitioners should start with the NNGP.

We emphasize that both tuning of the diagonal regularizer (Figure 5) and sufficient numerical precision (§3.7, Figure S1) were crucial to achieving an accurate comparison of these kernels.

#### 3.3 Centering and ensembling finite networks both lead to kernel-like performance

For overparameterized neural networks, some randomness from the initial parameters persists throughout training and the resulting learned functions are themselves random. This excess variance in the network’s predictions generically increases the total test error through the variance term of the bias-variance decomposition. For infinite-width kernel systems this variance is eliminated by using
validation accuracy with STD parameterization (§3.10), while regularization (Figure 5) is independently tuned for each.

Figure 2: NNGP often outperforms NTK in image classification tasks when diagonal regularization is carefully tuned. The performance of the NNGP and NT kernels are plotted against each other for a variety of data pre-processing configurations (§3.10), while regularization (Figure 5) is independently tuned for each.

Figure 3: Centering can accelerate training and improve performance. Validation accuracy throughout training for several finite width architectures. See Figure S6 for training accuracy.

the mean predictor. For finite-width models, the variance can be large, and test performance can be significantly improved by ensembling a collection of models. In Figure 4, we examine the effect of ensembling. For FCN networks, ensembling closes the gap with kernel methods, suggesting that FCN NNs underperform FCN kernels primarily due to variance. For CNN models, ensembling also improves test performance, and ensembled CNN–GAP models significantly outperform the best kernel methods.

Prediction variance can also be reduced by centering the model, i.e. subtracting the model’s initial predictions: \( \hat{f}_{\text{centered}}(t) = f(\theta(t)) - f(\theta(0)) \). A similar variance reduction technique has been studied in [25, 65–67]. In Figure 3, we observe that centering significantly speeds up training and improves generalization for FCN and CNN–VEC models, but has little-to-no effect on CNN–GAP architectures. We observe that the scale posterior variance of CNN–GAP, in the infinite-width kernel, is small relative to the prior variance given more data, consistent with centering and ensembles having small effect.

3.4 Large LRs and L2 regularization drive differences between finite networks and kernels

In practice, L2 regularization (a.k.a. weight decay) or larger learning rates can break the correspondence between kernel methods and finite width neural network training even at large widths.

Lee et al. [24] derives a critical learning rate \( \eta_{\text{critical}} \) such that wide network training dynamics are equivalent to linearized training for \( \eta < \eta_{\text{critical}} \). Lewkowycz et al. [39] argues that even at large width a learning rate \( \eta \in (\eta_{\text{critical}}, c \cdot \eta_{\text{critical}}) \) for a constant \( c > 1 \) forces the network to move away from its initial high curvature minimum and converge to a lower curvature minimum, while Li et al. [68] argues that large initial learning rates enable networks to learn ‘hard-to-generalize’ patterns.

In Figure 1 (and Table S1), we observe that the effectiveness of a large learning rate (LR) is highly sensitive to both architecture and parameterization: LR improves performance of FCN and CNN–GAP by about 1% for STD parameterization and about 2% for NTK parameterization. In stark contrast, it has little effect on CNN–VEC with NTK parameterization and surprisingly, a huge performance boost on CNN–VEC with STD parameterization (+5%).

L2 regularization (Equation S1) regularizes the squared distance between the parameters and the

Figure 4: Ensembling base networks enables them to match the performance of kernel methods, and exceed kernel performance for nonlinear CNNs. See Figure S7 for test MSE.
Figure 5: Layerwise scaling motivated by NTK makes L2 regularization more helpful in standard parameterization networks. See §3.5 for introduction of the improved regularizer, Figure S9 for further analysis on L2 regularization to initial weights, and Figure S8 for effects on varying widths.

Figure 6: Finite width networks generally perform better with increasing width, but CNN-VEC shows surprising non-monotonic behavior. L2: non-zero weight decay allowed during training. LR: large learning rate allowed. Dashed lines are allowing underfitting (U). See Figure S10 for plots for the standard parameterization, and §3.11 for discussion of CNN-VEC results.

L2 regularization consistently improves (+1-2%) performance for all architectures and parameterizations. Even with a well-tuned L2 regularization, finite width CNN-VEC and FCN still underperform NNGP/NTK. Combining L2 with early stopping produces a dramatic additional 10% - 15% performance boost for finite width CNN-VEC, outperforming NNGP/NTK. Finally, we note that L2+LR together provide a superlinear performance gain for all cases except FCN and CNN-GAP with NTK-parameterization. Understanding the nonlinear interactions between L2, LR, and early stopping on finite width networks is an important research question (e.g. see [39, 70] for LR/L2 effect on the training dynamics).

3.5 Improving L2 regularization for networks using the standard parameterization

We find that L2 regularization provides dramatically more benefit (by up to 6%) to finite width networks with the NTK parameterization than to those that use the standard parameterization (see Table S1). There is a bijective mapping between weights in networks with the two parameterizations, which preserves the function computed by both networks: \( W_{\text{STD}}^l = W_{\text{NTK}}^l / \sqrt{\pi} \), where \( W^l \) is the \( l \)th layer weight matrix, and \( n^l \) is the width of the preceding activation vector. Motivated by the improved performance of the L2 regularizer in the NTK parameterization, we use this mapping to construct a regularizer for standard parameterization networks that produces the same penalty as vanilla L2 regularization would produce on the equivalent NTK-parameterized network. This modified regularizer is \( R^l_{\text{Layerwise}} = \frac{1}{2} \sum_l n^l \| W_{\text{STD}}^l \|^2 \). This can be thought of as a layer-wise regularization constant \( \lambda^l = \lambda n^l \). The improved performance of this regularizer is illustrated in Figure 5.

3.6 Performance can be non-monotonic in width beyond double descent

Deep learning practitioners have repeatedly found that increasing the number of parameters in their models leads to improved performance [9, 71–76]. While this behavior is consistent with a Bayesian perspective on generalization [77–79], it seems at odds with classic generalization theory which primarily considers worst-case overfitting [80–86]. This has led to a great deal of work on the interplay of overparameterization and generalization [87–96]. Of particular interest has been the phenomenon of double descent, in which performance increases overall with parameter account, but
Figure 7: **Diagonal kernel regularization acts similarly to early stopping.** Solid lines correspond to NTK inference with varying diagonal regularization $\varepsilon$. Dashed lines correspond to predictions after gradient descent evolution to time $t = \eta t$ (with $\eta = m/\text{tr}(K)$). Line color indicates varying training set size $m$. Performing early stopping at time $t$ corresponds closely to regularizing with coefficient $\varepsilon = Km/\eta t$, where $K = 10$ denotes number of output classes.

Figure 8: **Tail eigenvalues of infinite network kernels show power-law decay.** The red dashed line shows the predicted scale of noise in the eigenvalues due to floating point precision, for kernel matrices of increasing width. Eigenvalues for CNN-GAP architectures decay fast, and may be overwhelmed by float32 quantization noise for dataset sizes of $O(10^4)$. For float64, quantization noise is not predicted to become significant until a dataset size of $O(10^{10})$ (Figure S1). The key insight is that kernels with fast eigenvalue decay suffer from floating point noise. Empirically, the tail eigenvalue of the NNGP/NTK follows a power law (see Figure 8) and measuring 

3 Similar behavior was observed in [100].  

3.7 Diagonal regularization of kernels behaves like early stopping

When performing kernel inference, it is common to add a diagonal regularizer to the training kernel matrix, $K_{\text{reg}} = K + \varepsilon \frac{m}{\text{tr}(K)} I$. For linear regression, Ali et al. [101] proved that the inverse of a kernel regularizer is related to early stopping time under gradient flow. With kernels, gradient flow dynamics correspond directly to training of a wide neural network [18, 24].

We experimentally explore the relationship between early stopping, kernel regularization, and generalization in Figure 7. We observe a close relationship between regularization and early stopping, and find that in most cases the best validation performance occurs with early stopping and non-zero $\varepsilon$. While Ali et al. [101] do not consider a $\frac{m}{\text{tr}(K)}$ scaling on the kernel regularizer, we found it useful since experiments become invariant under scale of $K$.

3.8 Floating point precision determines critical dataset size for failure of kernel methods

We observe empirically that kernels become sensitive to float32 vs. float64 numerical precision at a critical dataset size. For instance, GAP models suffer float32 numerical precision errors at a dataset size of $\sim 10^4$. This phenomena can be understood with a simple random noise model (see §D for details). The key insight is that kernels with fast eigenvalue decay suffer from floating point noise. Empirically, the tail eigenvalue of the NNGP/NTK follows a power law (see Figure 8) and measuring
Figure 9: **Regularized ZCA whitening improves image classification performance for both finite and infinite width networks.** All plots show performance as a function of ZCA regularization strength. (a) ZCA whitening of inputs to kernel methods on CIFAR-10, Fashion-MNIST, and CIFAR-100. (b) ZCA whitening of inputs to finite width networks (training curves in Figure S11).

ther decay trend provides good indication of critical dataset size

\[ m^* \gtrsim \left( \frac{C}{\sqrt{2\sigma_n}} \right)^{\frac{2}{\alpha - 1}} \] if \( \alpha > \frac{1}{2} \) (\( \infty \) otherwise), \hspace{1cm} (1)

where \( \sigma_n \) is the typical noise scale, e.g. \( \texttt{float32} \) epsilon, and the kernel eigenvalue decay is modeled as \( \lambda_i \sim C i^{-\alpha} \) as \( i \) increases. Beyond this critical dataset size, the smallest eigenvalues in the kernel become dominated by floating point noise.

### 3.9 Linearized CNN-GAP models perform poorly due to poor conditioning

We observe that the linearized CNN-GAP converges extremely slowly on the training set (Figure S6), leading to poor validation performance (Figure 3). Even after training for more than 10M steps with varying L2 regularization strengths and LRs, the best training accuracy was below 90%, and test accuracy \( \sim 70\% \) – worse than both the corresponding infinite and nonlinear finite width networks.

This is caused by poor conditioning of pooling networks. Xiao et al. [33] (Table 1) show that the conditioning at initialization of a CNN-GAP network is worse than that of FCN or CNN-VEC networks by a factor of the number of pixels (1024 for CIFAR-10). This poor conditioning of the kernel eigenspectrum can be seen in Figure 8. For linearized networks, in addition to slowing training by a factor of 1024, this leads to numerical instability when using \( \texttt{float32} \).

### 3.10 Regularized ZCA whitening improves accuracy

ZCA whitening [102] (see Figure S2 for an illustration) is a data preprocessing technique that was once common [103, 104], but has fallen out of favor. However it was recently shown to dramatically improve accuracy in some kernel methods by Shankar et al. [42], in combination with a small regularization parameter in the denominator (see §F). We investigate the utility of ZCA whitening as a preprocessing step for both finite and infinite width neural networks. We observe that while pure ZCA whitening is detrimental for both kernels and finite networks (consistent with predictions in [105]), with tuning of the regularization parameter it provides performance benefits for both kernel methods and finite network training (Figure 9).

### 3.11 Equivariance is only beneficial for narrow networks far from the kernel regime

Due to weight sharing between spatial locations, outputs of a convolutional layer are translation-equivariant (up to edge effects), i.e. if an input image is translated, the activations are translated in the same spatial direction. However, the vast majority of contemporary CNNs utilize weight sharing in conjunction with pooling layers, making the network outputs approximately translation-invariant (CNN-GAP). The impact of equivariance alone (CNN-VEC) on generalization is not well understood – it is a property of internal representations only, and does not translate into meaningful statements about the classifier outputs. Moreover, in the infinite-width limit it is guaranteed to have no impact.
We performed an in-depth investigation of the phenomenology of finite and infinite width neural networks through a series of controlled interventions. We quantified phenomena having to do with generalization, architecture dependence, deviations between infinite and finite networks, numerical stability, data augmentation, data preprocessing, ensembling, network topology, and failure modes of linearization. We further developed best practices that improve performance for both finite and infinite networks. We believe our experiments provide firm empirical ground for future studies.

The normalized Gaussian Myrtle kernel used in Shankar et al. [42] does not have a corresponding finite-width CNN-VEC architecture. Thus, while CNN-VEC+L2+narrow benefits from equivariance, it falls off much slower. Translation-invariant CNN-GAP remains, as expected, the most robust. Details in §3.11, §C.1.

4 Discussion

We performed an in-depth investigation of the phenomenology of finite and infinite width neural networks through a series of controlled interventions. We quantified phenomena having to do with generalization, architecture dependence, deviations between infinite and finite networks, numerical stability, data augmentation, data preprocessing, ensembling, network topology, and failure modes of linearization. We further developed best practices that improve performance for both finite and infinite networks. We believe our experiments provide firm empirical ground for future studies.

**Figure 10:** **Equivariance is only leveraged in a CNN model outside of the kernel regime.** If a CNN model is able to utilize equivariance effectively, we expect it to be more robust to crops and translations than an FCN. Surprisingly, performance of a wide CNN-VEC degrades with the magnitude of the input perturbation as fast as that of an FCN, indicating that equivariance is not exploited. In contrast, performance of a narrow model with weight decay (CNN-VEC+L2+narrow) falls off much slower. Translation-invariant CNN-GAP remains, as expected, the most robust. Details in §3.11, §C.1.
Table 1: CIFAR-10 test accuracy for kernels of the corresponding architecture type

| Architecture | Method | NTK | NNGP |
|--------------|--------|-----|------|
| FC           | Novak et al. [9] | -   | 59.7 |
|              | ZCA Reg (this work) | 59.7 | 59.7 |
|              | DA Ensemble (this work) | **61.5** | **62.4** |
| CNN-VEC      | Novak et al. [9]  | -   | 67.1 |
|              | Li et al. [40]    | 66.6 | 66.8 |
|              | ZCA Reg (this work) | 69.8 | 69.4 |
|              | Flip Augmentation, Li et al. [40] | 69.9 | 70.5 |
|              | DA Ensemble (this work) | **70.5** | **73.2** |
| CNN-GAP      | Arora et al. [26], Li et al. [40] | 77.6 | 78.5 |
|              | ZCA Reg (this work) | 83.2 | 83.5 |
|              | Flip Augmentation, Li et al. [40] | 79.7 | 80.0 |
|              | DA Ensemble (this work) | **83.7 (32 ens)** | **84.8 (32 ens)** |
| Myrtle       | Myrtle ZCA and Flip Augmentation, Shankar et al. [42] | -   | **89.8** |

Broader Impact

Developing theoretical understanding of neural networks is crucial both for understanding their biases, and predicting when and how they will fail. Understanding biases in models is of critical importance if we hope to prevent them from perpetuating and exaggerating existing racial, gender, and other social biases [112–115]. Understanding model failure has a direct impact on human safety, as neural networks increasingly do things like drive cars and control the electrical grid [116–118].

We believe that wide neural networks are currently the most promising direction for the development of neural network theory. We further believe that the experiments we present in this paper will provide empirical underpinnings that allow better theory to be developed. We thus believe that this paper will in a small way aid the engineering of safer and more just machine learning models.

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A Glossary

We use the following abbreviations in this work:

- L2: L2 regularization a.k.a. weight decay;
- LR: using large learning rate;
- U: allowing underfitting;
- DA: using data augmentation;
- C: centering the network so that the logits are always zero at initialization;
- Ens: neural network ensembling logits over multiple initialization;
- ZCA: zero-phase component analysis regularization preprocessing;
- FCN: fully-connected neural network.;
- CNN-VEC: convolutional neural network with a vectorized readout layer;
- CNN-GAP: convolutional neural network with a global average pooling readout layer;
- NNGP: neural network Gaussian process;
- NTK: neural tangent kernel.

B Main table

Table S1: CIFAR-10 classification accuracy for nonlinear and linearized finite neural networks, as well as for NTK and NNGP kernel methods. Starting from Base network of given architecture class described in §2, performance change of centering (+C), large learning rate (+LR), allowing underfitting by early stopping (+U), input preprocessing with ZCA regularization (+ZCA), multiple initialization ensembling (+Ens), and some combinations are shown, for Standard and NTK parameterization. See also Figure 1.

| Param    | Base | +C  | +LR | +L2 | +L2 +U | +L2 +LR +U | +L2 +LR +ZCA | +Ens +Ens +C +DA +L2 +LR +U | NTK +ZCA | +DA +ZCA | NNGP +ZCA | +DA +ZCA +C |
|----------|------|-----|-----|-----|--------|------------|---------------|--------------------------|---------|---------|----------|-------------|
| FCN      | STD  | 48.82 | 53.22 | 49.07 | 49.82 | 52.32 | 55.82 | 44.29 | 55.90 | 58.11 | 58.25 | 65.29 | 67.43 |
| NTK      | 46.16 | 51.74 | 48.14 | 54.27 | 55.11 | 54.44 | 44.86 | 54.44 | 58.14 | 58.31 | 61.87 | 69.35 |
| CNN-VEC  | STD  | 56.68 | 60.82 | 62.16 | 57.15 | 67.07 | 62.16 | 68.99 | 57.39 | 68.99 | 67.30 | 65.65 | 76.73 | 83.01 |
| NTK      | 60.73 | 58.09 | 60.73 | 61.30 | 75.85 | 76.93 | 77.47 | 61.35 | 77.47 | 71.32 | 67.23 | 83.92 | 85.63 |
| CNN-GAP  | STD  | 80.26 | 81.25 | 80.95 | 81.67 | 81.10 | 83.69 | 83.01 | 84.90 | 84.22 | 84.15 | 84.62 | 84.36 | 86.45 |
| NTK      | 80.61 | 81.73 | 82.44 | 81.17 | 81.17 | 82.44 | 82.43 | 83.75 | 83.92 | 85.22 | 85.75 | 84.07 | 86.68 |
| FCN      | STD  | 43.09 | 51.48 | 44.16 | 50.77 | 57.85 | 57.99 | 58.05 | 59.65 | 58.28 | 59.68 | 58.51 | 59.70 | 62.40 |
| NTK      | 48.61 | 52.12 | 51.77 | 51.77 | 58.04 | 58.16 | 58.16 | - | - | 61.54 | 58.61 | 59.70 | 62.40 |
| CNN-VEC  | STD  | 52.43 | 60.61 | 58.41 | 58.41 | 64.58 | 64.67 | 66.66 | 69.65 | 66.78 | 69.79 | 70.52 | 66.69 | 73.23 |
| NTK      | 55.88 | 58.94 | 58.52 | 58.50 | 65.45 | 65.54 | 65.54 | - | - | 69.44 | 69.44 | 73.23 |
| CNN-GAP  | STD  | >70.00* (Train accuracy 86.22 after 14M steps) | >68.59* (Train accuracy 79.90 after 14M steps) | >70.00* (Train accuracy 86.22 after 14M steps) | >68.59* (Train accuracy 79.90 after 14M steps) | 76.97 | 83.24 | 77.00 | 83.24 | 83.74 | 78.00 | 83.45 | 84.82 |

C Experimental details

For all experiments, we use Neural Tangents (NT) library [15] built on top of JAX [125]. First we describe experimental settings that is mostly common and then describe specific details and hyperparameters for each experiments.

Finite width neural networks We train finite width networks with Mean Squared Error (MSE) loss

$$\mathcal{L} = \frac{1}{2|\mathcal{D}|K} \sum_{(x_i, y_i) \in \mathcal{D}} \| f(x_i) - y_i \|^2,$$
where $K$ is the number of classes and $\| \cdot \|$ is the $L^2$ norm in $\mathbb{R}^K$. For the experiments with +L2, we add L2 regularization to the loss

$$ R_{L2} = \frac{\lambda}{2} \sum_i \|W_i\|^2, \quad (S1) $$

and tune $\lambda$ using grid-search optimizing for the validation accuracy.

We optimize the loss using mini-batch SGD with constant learning rate. We use batch-size of 100 for FCN and 40 for both CNN-VEC and CNN-GAP (see §H for further details on this choice). Learning rate is parameterized with learning rate factor $c$ with respect to the critical learning rate

$$ \eta = c \eta_{\text{critical}}. \quad (S2) $$

In practice, we compute empirical NTK $\hat{\Theta}(x, x') = \sum_j \partial_j f(x) \partial_j f(x')$ on 16 random points in the training set to estimate $\eta_{\text{critical}}$ [24] by maximum eigenvalue of $\hat{\Theta}(x, x)$. This is readily available in NT library [15] using nt.monte_carlo_kernel_fn and nt.predict.max_learning_rate. Base case considered without large learning rate indicates $c \leq 1$, and large learning rate (+LR) runs are allowing $c > 1$. Note that for linearized networks $\eta_{\text{critical}}$ is strict upper-bound for the learning rates and no $c > 1$ is allowed [24, 36, 39].

Training steps are chosen to be large enough, such that learning rate factor $c \leq 1$ can reach above 99% accuracy on 5k random subset of training data for 5 logarithmic spaced measurements. For different learning rates, physical time $t = \eta \times (\# \text{ of steps})$ roughly determines learning dynamics and small learning rate trials need larger number of steps. Achieving termination criteria was possible for all of the trials except for linearized CNN-GAP and data augmented training of FCN, CNN-VEC. In these cases, we report best achieved performance without fitting the training set.

**NNGP / NTK** For inference, except for data augmentation ensembles for which default zero regularization was chosen, we grid search over diagonal regularization in the range numpy.logspace(-7, 2, 14) and 0. Diagonal regularization is parameterized as

$$ \mathcal{K}_{\text{reg}} = \mathcal{K} + \frac{\epsilon_{\text{tr}}}{m} I $$

where $\mathcal{K}$ is either NNGP or NTK for the training set. We work with this parameterization since $\epsilon$ is invariant to scale of $\mathcal{K}$.

**Dataset** For all our experiments (unless specified) we use train/valid/test split of 45k/5k/10k for CIFAR-10/100 and 50k/10k/10k for Fashion-MNIST. For all our experiments, inputs are standardized with per channel mean and standard deviation. ZCA regularized whitening is applied as described in §F. Output is encoded as mean subtracted one-hot-encoding for the MSE loss, e.g. for a label in class $c$, $-0.1 \cdot 1 + c$. For the softmax-cross-entropy loss in §G, we use standard one-hot-encoded output.

For data augmentation, we use widely-used augmentation for CIFAR-10; horizontal flips with 50% probability and random crops by 4-pixels with zero-padding.

**Details of architecture choice:** We only consider ReLU activation (with the exception of Myrtle-kernel which use scaled Gaussian activation [42]) and choose critical initialization weight variance of $\sigma_w^2 = 2$ with small bias variance $\sigma_b^2 = 0.01$. For convolution layers, we exclusively consider $3 \times 3$ filters with stride 1 and SAME (zero) padding so that image size does not change under convolution operation.

### C.1 Hyperparameter configurations for all experiments

We used grid-search for tuning hyperparameters and use accuracy on validation set for deciding on hyperparameter configuration or measurement steps (for underfitting / early stopping). All reported numbers unless specified is test set performance.

**Figure 1, Table S1:** We grid-search over L2 regularization strength $\lambda \in \{0\} \cup \{10^{-k} | k \text{ from -9 to -3}\}$ and learning rate factor $c \in \{2^k | k \text{ from -2 to 5}\}$. For linearized networks same search space is used except that $c > 1$ configuration is infeasible and training diverges. For non-linear, centered runs $c \in \{2^k | k \text{ from 0 to 4}\}$ is used. Network ensembles uses base configuration with $\lambda = 0, c = 1$ with 64 different initialization seed. Kernel ensemble is over 50 predictors for FCN and CNN-VEC and 32 predictors for CNN-GAP. Finite networks trained with data-augmentation has different learning rate factor range of $c \in \{1, 4, 8\}$. 

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Figure 2: Each datapoint corresponds to either standard preprocessed or ZCA regularization preprocessed (as described in §3.10) with regularization strength was varied in \{10^{-k} | k \in [-6, -5, \ldots, 4, 5]\} for FCN and CNN-VEC, \{10^{-k} | k \in [-3, -2, \ldots, 2, 3]\} for CNN-GAP.

Figure 3, Figure 4, Figure S6, Figure S7: Learning rate factors are \(c = 1\) for non-linear networks and \(c = 0.5\) for linearized networks. While we show NTK parameterized runs, we also observe similar trends for STD parameterized networks. Shaded regions show range of minimum and maximum performance across 64 different seeds. Solid line indicates the mean performance.

Figure 5: While FCN is the base configuration, CNN-VEC is a narrow network with 64 channels per layer since moderate width benefits from L2 more for the NTK parameterization Figure S10. For CNN-GAP 128 channel networks is used. All networks with different L2 strategy are trained with +LR (\(c > 1\)).

Figure 6, Figure S8, Figure S10: \(\lambda \in \{0, 10^{-9}, 10^{-7}, 10^{-5}, 10^{-3}\}\) and \(c \in \{2^k | k \text{ from } -2 \text{ to } 5\}\).

Figure 7: We use 640 subset of validation set for evaluation. CNN-GAP is a variation of the base model with 3 convolution layers with \(\sigma_\delta^2 = 0.1\) while FCN and CNN-VEC is the base model. Training evolution is computed using analytic time-evolution described in Lee et al. [24] and implemented in NT library via \texttt{nt.predict.gradient_descent_mse} with 0 diagonal regularization.

Figure 8: Kernel experiments details are same as in Figure 2. Finite networks are base configuration with \(c = 1\) and \(\lambda = 0\).

Figure 10: Evaluated networks uses NTK parameterization with \(c = 1\). CNN-VEC+L2+narrow uses 128 channels instead of 512 of the base CNN-VEC and CNN-GAP networks, and trained with L2 regularization strength \(\lambda = 10^{-7}\). Crop transformation uses zero-padding while Translate transformation uses circular boundary condition after shifting images. Each transformation is applied to the test set inputs where shift direction is chosen randomly. Each points correspond to average accuracy over 20 random seeds. FCN had 2048 hidden units.

Figure 11, Table 1: For all data augmentation ensembles, first instance is taken to be from non-augmented training set. Further details on kernel ensemble is described in §E. For all kernels, inputs are preprocessed with optimal ZCA regularization observed in Figure 9 (10 for FCN, 1 for CNN-VEC, CNN-GAP and Myrtle.). We ensemble over 50 different augmented draws for FCN and CNN-VEC, whereas for CNN-GAP, we ensemble over 32 draws of augmented training set.

Figure S3, Table S2: Details for MSE trials are same as Figure 1 and Table S1. Trials with softmax-cross-entropy loss was tuned with same hyperparameter range as MSE except that learning rate factor range was \(c \in \{1, 4, 8\}\).

Figure S4: We present result with NTK parameterized networks with \(\lambda = 0\). FCN network is width 1024 with \(\eta = 10.0\) for MSE loss and \(\eta = 2.0\) for softmax-cross-entropy loss. CNN-GAP uses 256 channels with \(\eta = 5.0\) for MSE loss and \(\eta = 0.2\) for softmax-cross-entropy loss. Random seed was fixed to be the same across all runs for comparison.

Figure S9: NTK parameterization with \(c = 4\) was used for both L2 to zero or initialization. Random seed was fixed to be the same across all runs for comparison.

D Noise model

In this section, we provide details on noise model discussed in §3.8. Consider a random \(m \times m\) Hermitian matrix \(\tilde{N}\) with entries order of \(\sigma_n\) which is considered as noise perturbation to the kernel matrix \(\tilde{K} = K + \tilde{N}\). (S3)

Eigenvalues of this random matrix \(\tilde{N}\) follow Wigner’s semi-circle law, and the smallest eigenvalue is given by \(\lambda_{\min}(\tilde{N}) \approx -\sqrt{2m} \sigma_n\). When the smallest eigenvalue of \(K\) is smaller (in order) than \(|\lambda_{\min}(\tilde{N})|\), one needs to add diagonal regularizer larger than the order of \(|\lambda_{\min}(\tilde{N})|\) to ensure positive definiteness. For estimates, let us use machine precision\(^1\) \(\epsilon_{32} \approx 10^{-7}\) and \(\epsilon_{64} \approx 2 \times 10^{-16}\) which we use as proxy values for \(\sigma_n\). Note that noise scale is relative to elements in \(K\) which is assume to be \(O(1)\). Naively scaling \(K\) by multiplicative constant will also scale \(\sigma_n\).

\(^1\)np.finfo(np.float32).eps, np.finfo(np.float64).eps
Empirically one can model tail $i$th eigenvalues of infinite width kernel matrix of size $m \times m$ as
\[
\lambda_i \approx C m^{\frac{i}{\alpha}}. \tag{S4}
\]
Note that we are considering $O(1)$ entries for $K$ and typical eigenvalues scale linearly with dataset size $m$. For a given dataset size, the power law observed is $\alpha$ and $C$ is dataset-size independent constant. Thus the smallest eigenvalue is order $\lambda_{\text{min}}(K) \sim C m^{1-\alpha}$.

In the noise model, we can apply Weyl’s inequality which says
\[
\lambda_{\text{min}}(K) - \sqrt{2m} \sigma_n \leq \lambda_{\text{min}}(\hat{K}) \leq \lambda_{\text{min}}(K) + \sqrt{2m} \sigma_n . \tag{S5}
\]
Consider the worst-case where negative eigenvalue noise affecting the kernel’s smallest eigenvalue. In that case perturbed matrices minimum eigenvalue could become negative, breaking positive semi-definiteness (PSD) of the kernel.

This model allows to predict critical dataset size ($m^*$) over which PSD can be broken under specified noise scale and kernel eigenvalue decay. With condition that perturbed smallest eigenvalue becomes negative
\[
C m^{1-\alpha} \lesssim \sqrt{2m} \sigma_n , \tag{S6}
\]
we obtain
\[
m^* \gtrsim \begin{cases} 
\left( \frac{C}{\sqrt{2} \sigma_n} \right)^{\frac{2}{\alpha-1}} & \text{if } \alpha > \frac{1}{2} \\
\infty & \text{else}
\end{cases} \tag{S7}
\]
When PSD is broken, one way to preserve PSD is to add diagonal regularizer ($\S3.7$). For CIFAR-10 with $m = 50k$, typical negative eigenvalue from float32 noise is around $4 \times 10^{-5}$ and $7 \times 10^{-14}$ with float64 noise scale, considering $\sqrt{2m} \sigma_n$. Note that Arora et al. [26] regularized kernel with regularization strength $5 \times 10^{-5}$ which is on par with typical negative eigenvalue introduced due to float32 noise. Of course, this only applies if kernel eigenvalue decay is sufficiently fast that full dataset size is above $m^*$.

We observe that FCN and CNN-VEC kernels with small $\alpha$ would not suffer from increasing dataset-size under float32 precision. On the other-hand, worse conditioning of CNN-GAP not only affects the training time ($\S3.9$) but also required precision. One could add sufficiently large diagonal regularization to mitigate effect from the noise at the expense of losing information and generalization strength included in eigen-directions with small eigenvalues.

### E Data augmentation via kernel ensembling

We start considering general ensemble averaging of predictors. Consider a sequence of training sets $\{D_i\}$ each consisting of $m$ input-output pairs $\{(x_1, y_1), \ldots, (x_m, y_m)\}$ from a data-generating distribution. For a learning algorithm, which we use NNGP/NTK inference for this study, will give prediction $\mu(x^*, D_i)$ of unseen test point $x^*$. It is possible to obtain better predictor by averaging output of different predictors
\[
\tilde{\mu}(x^*) = \frac{1}{E} \sum_i \mu(x^*, D_i) , \tag{S8}
\]
where $E$ denotes the cardinality of $\{D_i\}$. This ensemble averaging is simple type of committee machine which has long history [128, 129]. While more sophisticated ensembling method exists (e.g. [130–135]), we strive for simplicity and considered naive averaging. One alternative we considered is generalizing average by
\[
\tilde{\mu}_w(x^*) = \frac{1}{E} \sum_i w_i \mu(x^*, D_i) , \tag{S9}
\]
were $w_i$ in general is set of weights satisfying $\sum_i w_i = 1$. We can utilize posterior variance $\sigma^2$ from NNGP or NTK with MSE loss via Inverse-variance weighting (IVW) where weights are given as
\[
w_i = \frac{\sigma_i^{-2}}{\sum_j \sigma_j^{-2}} . \tag{S10}
\]
Figure S1: The CNN-GAP architecture has poor kernel conditioning (a) Eigenvalue spectrum of infinite network kernels on 10k datapoints. Dashed lines are noise eigenvalue scale from float32 precision. Eigenvalue for CNN-GAP’s NNGP decays fast and negative eigenvalue may occur when dataset size is $O(10^4)$ in float32 but is well-behaved with higher precision. (b-c) Critical dataset size as function of eigenvalue decay exponent $\alpha$ or noise strength $\sigma_n$ given by Equation 1.

In simple bagging setting [131], we observe small improvements with IVW over naive averaging. This indicates posterior variance for different draw of $\{D_i\}$ was quite similar.

Application to data augmentation (DA) is simple as we consider process of generating $\{D_i\}$ from a (stochastic) data augmentation transformation $T$. We consider action of $T(x, y) = T(x, y)$ be stochastic (e.g. $T$ is a random crop operator) with probability $p$ augmentation transformation (which itself could be stochastic) and probability $(1-p)$ of $T = Id$. Considering $D_0$ as clean un-augmented training set, we can imagine dataset generating process $D_i \sim T(D_0)$, where we overloaded definition of $T$ on training-set to be data generating distribution.

For experiments in §3.12, we took $T$ to be standard augmentation strategy of horizontal flip and random crop by 4-pixels with augmentation fraction $p = 0.5$ (see Figure S12 for effect of augmentation fraction on kernel ensemble). In this framework, it is trivial to generalize the DA transformation to be quite general (e.g. learned augmentation strategy studied by Cubuk et al. [109, 110]).

### F ZCA whitening

Consider $m$ (flattened) $d$-dimensional training set inputs $X$ (a $d \times m$ matrix) with data covariance

$$\Sigma_X = \frac{1}{d}XX^T. \tag{S11}$$

The goal of whitening is to find a whitening transformation $W$, a $d \times d$ matrix, such that the features of transformed input

$$Y = WX \tag{S12}$$

are uncorrelated, e.g. $\Sigma_Y \equiv \frac{1}{d}YY^T = I$. Note that $\Sigma_X$ is constructed only from training set while $W$ is applied to both training set and test set inputs. Whitening transformation can be efficiently
Figure S2: Illustration of ZCA whitening. Whitening is a linear transformation of a dataset that removes correlations between feature dimensions, setting all non-zero eigenvalues of the covariance matrix to 1. ZCA whitening is a specific choice of the linear transformation that rescales the data in the directions given by the eigenvectors of the covariance matrix, but without additional rotations or flips. (a) A toy 2d dataset before and after ZCA whitening. Red arrows indicate the eigenvectors of the covariance matrix of the unwhitened data. (b) ZCA whitening of CIFAR-10 images preserves spatial and chromatic structure, while equalizing the variance across all feature directions. Figure reproduced with permission from Wadia et al. [105]. See also §3.10.

computed by eigen-decomposition\(^6\)

\[ \Sigma_X = U D U^T \] (S13)

where \( D \) is diagonal matrix with eigenvalues, and \( U \) contains eigenvector of \( \Sigma_X \) as its columns.

With this ZCA whitening transformation is obtained by following whitening matrix

\[ W_{\text{ZCA}} = U \sqrt{\left( D + \epsilon \frac{\text{tr}(D)}{d} I_d \right)^{-1}} U^T. \] (S14)

Here, we introduced trivial reparameterization of conventional regularizer such that regularization strength \( \epsilon \) is input scale invariant. It is easy to check \( \epsilon \to 0 \) corresponds to whitening with \( \Sigma_Y = I \). In §3.10, we study the benefit of taking non-zero regularization strength for both kernels and finite networks. We denote transformation with non-zero regularizer, ZCA regularization preprocessing. ZCA transformation preserves spatial and chromatic structure of original image as illustrated in Figure F. Therefore image inputs are reshaped to have the same shape as original image.

In practice, we standardize both training and test set per (RGB channel) features of the training set before and after the ZCA whitening. This ensures transformed inputs are mean zero and variance of order 1.

\section*{G MSE vs Softmax-cross-entropy loss training of neural networks}

Our focus was mainly on finite networks trained with MSE loss for simple comparison with kernel methods that gives closed form solution. Here we present comparison of MSE vs softmax-cross-entropy trained networks. See Table S2 and Figure S3.

\section*{H Comment on batch size}

Correspondence between NTK and gradient descent training is direct in the full batch gradient descent (GD) setup (see [136] for extensions to mini-batch SGD setting). Therefore base comparison between finite networks and kernels is the full batch setting. While it is possible to train our base models with GD, for full CIFAR-10 large empirical study becomes impractical. In practice, we use mini-batch SGD with batch-size 100 for FCN and 40 for CNNs.

We studied batch size effect of training dynamics in Figure S4 and found that for these batch-size choices does not affecting training dynamics compared to much larger batch size. Shallue et al. [137], McCandlish et al. [138] observed that universally for wide variety of deep learning models there are batch size beyond which one could gain training speed benefit in number of steps. We observe that maximal useful batch-size in workloads we study is quite small.

\footnote{\textbf{For PSD matrices, it is numerically more reliable to obtain via SVD.}}
Figure S3: MSE trained networks are competitive while there is a clear benefit to using Cross-entropy loss

Table S2: Effects of MSE vs softmax-cross-entropy loss on base networks with various interventions

| Architecture | Type     | Param | Base   | +LR+U  | +L2+U  | +L2+LR+U | Best    |
|--------------|----------|-------|--------|--------|--------|----------|---------|
| FCN          | MSE      | STD   | 47.82  | 49.07  | 49.82  | 55.32    | 55.90   |
|              |          | NTK   | 46.16  | 49.17  | 54.27  | 55.44    | 55.44   |
| XENT         | STD      | 55.01 | 57.28  | 53.98  | 57.64  | 57.64    | 57.64   |
|              | NTK      | 53.39 | 56.59  | 56.31  | 58.99  | 58.99    | 58.99   |
| MSE+DA       | STD      | 65.29 | 66.11  | 65.28  | 67.43  | 67.43    | 67.43   |
|              | NTK      | 61.87 | 62.12  | 67.58  | 69.35  | 69.35    | 69.35   |
| XENT+DA      | STD      | 64.15 | 64.15  | 67.93  | 67.93  | 67.93    | 67.93   |
|              | NTK      | 62.88 | 62.88  | 67.90  | 67.90  | 67.90    | 67.90   |
| CNN-VEC      | MSE      | STD   | 56.68  | 63.51  | 67.07  | 68.99    | 68.99   |
|              |          | NTK   | 60.73  | 61.58  | 75.85  | 77.47    | 77.47   |
| XENT         | STD      | 64.31 | 65.30  | 64.57  | 66.95  | 66.95    | 66.95   |
|              | NTK      | 67.13 | 73.23  | 72.93  | 74.05  | 74.05    | 74.05   |
| MSE+DA       | STD      | 76.73 | 81.84  | 76.66  | 83.01  | 83.01    | 83.01   |
|              | NTK      | 83.92 | 84.76  | 84.87  | 85.63  | 85.63    | 85.63   |
| XENT+DA      | STD      | 81.84 | 83.86  | 81.78  | 84.37  | 84.37    | 84.37   |
|              | NTK      | 86.83 | 88.59  | 87.49  | 88.83  | 88.83    | 88.83   |
| CNN-GAP      | MSE      | STD   | 80.26  | 80.93  | 81.10  | 83.01    | 84.22   |
|              |          | NTK   | 80.61  | 82.44  | 81.17  | 82.43    | 83.92   |
| XENT         | STD      | 83.66 | 83.80  | 84.59  | 83.87  | 83.87    | 83.87   |
|              | NTK      | 83.87 | 84.40  | 84.51  | 84.51  | 84.51    | 84.51   |
| MSE+DA       | STD      | 84.36 | 83.88  | 84.89  | 86.45  | 86.45    | 86.45   |
|              | NTK      | 84.07 | 85.54  | 85.39  | 86.68  | 86.68    | 86.68   |
| XENT+DA      | STD      | 86.04 | 86.01  | 86.42  | 87.26  | 87.26    | 87.26   |
|              | NTK      | 86.87 | 87.31  | 86.39  | 88.26  | 88.26    | 88.26   |

I Additional tables and plots
Figure S4: Batch size does not affect training dynamics for moderately large batch size.
Table S3: CIFAR-10 classification mean squared error (MSE) for nonlinear and linearized finite neural networks, as well as for NTK and NNGP kernel methods. Starting from Base network of given architecture class described in §2, performance change of centering (+C), large learning rate (+LR), allowing underfitting (+U), input preprocessing with ZCA regularization (+ZCA), multiple initialization ensembling (+Ens), and some combinations are shown, for Standard and NTK parameterization. See also Table S1 and Figure 1 for accuracy comparison.

| Param | Base | +C | +LR | +L2 | +L2+U | +L2+LR | +L2+LR+U | +ZCA | Best w/o DA | +Ens | +Ens+C | +DA | +L2 | +LR | +U |
|-------|------|----|-----|-----|-------|--------|----------|------|-------------|-----|--------|-----|-----|-----|----|
| FCN   | STD  | 0.0443 | 0.0363 | 0.0386 | 0.0355 | 0.0337 | 0.0320 | 0.0343 | 0.0319 | 0.0301 | 0.0304 | 0.0267 | 0.0242 |
| NTK   | 0.0465 | 0.0371 | 0.0423 | 0.0338 | 0.0336 | 0.0308 | 0.0308 | 0.0484 | 0.0308 | 0.0300 | 0.0302 | 0.0281 | 0.0225 |
| CNN-VEC | STD  | 0.0381 | 0.0300 | 0.0340 | 0.0279 | 0.0340 | 0.0265 | 0.0383 | 0.0265 | 0.0278 | 0.0287 | 0.0228 | 0.0183 |
| NTK   | 0.0355 | 0.0353 | 0.0355 | 0.0231 | 0.0246 | 0.0227 | 0.0236 | 0.0227 | 0.0254 | 0.0278 | 0.0164 | 0.0143 |
| CNN-GAP | STD  | 0.0209 | 0.0201 | 0.0207 | 0.0201 | 0.0201 | 0.0179 | 0.0177 | 0.0190 | 0.0159 | 0.0172 | 0.0157 | 0.0185 | 0.0149 |
| NTK   | 0.0209 | 0.0201 | 0.0195 | 0.0205 | 0.0181 | 0.0175 | 0.0170 | 0.0194 | 0.0161 | 0.0163 | 0.0157 | 0.0186 | 0.0145 |

Figure S5: On UCI dataset NNGP often outperforms NTK on RMSE. We evaluate predictive performance of FC NNGP and NTK on UCI regression dataset in the standard 20-fold splits first utilized in [139, 140]. We plot average RMSE across the splits. Different scatter points are varying hyperparameter settings of (depth, weight variance, bias variance). In the tabular data setting, dominance of NNGP is not as prominent across varying dataset as in image classification domain.

Figure S6: Centering can accelerate training. Validation (top) and training (bottom) accuracy throughout training for several finite width architectures. See also §3.3 and Figure 3.
Figure S7: Ensembling base networks causes them to match kernel performance, or exceed it for nonlinear CNNs. See also §3.3 and Figure 4.

Figure S8: Performance of nonlinear and linearized networks as a function of L2 regularization for a variety of widths. Dashed lines are NTK parameterized networks while solid lines are networks with standard parameterization. We omit linearized CNN–GAP plots as they did not converge even with extensive compute budget. L2 regularization is more helpful in networks with an NTK parameterization than a standard parameterization.

Figure S9: L2 regularization to initial weights does not provide performance benefit. (a) Comparing training curves of L2 regularization to either 0 or initial weights. (b) Peak performance of after L2 regularization to either 0 or initial weights. Increasing L2 regularization to initial weights do not provide performance benefits, instead performance remains flat until model’s capacity deteriorates.

Figure S10: Finite width networks generally perform better with increasing width, but CNN–VEC shows surprising non-monotonic behavior. See also §3.6 and Figure 6 L2: non-zero weight decay allowed during training LR: large learning rate allowed. Dashed lines are allowing underfitting (U).
Figure S11: **ZCA regularization helps finite network training.** (upper) Standard parameterization, (lower) NTK parameterization. See also §3.10 and Figure 9.

Figure S12: **Data augmentation ensemble for infinite network kernels with varying augmentation fraction.** See also §3.12.