On the Power of Shallow Learning

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Abstract

A deluge of recent work has explored equivalences between wide neural networks and kernel methods. A central theme is that one can analytically find the kernel corresponding to a given wide network architecture, but despite major implications for architecture design, no work to date has asked the converse question: given a kernel, can one find a network that realizes it? We affirmatively answer this question for fully-connected architectures, completely characterizing the space of achievable kernels. Furthermore, we give a surprising constructive proof that any kernel of any wide, deep, fully-connected net can also be achieved with a network with just one hidden layer and a specially-designed pointwise activation function. We experimentally verify our construction and demonstrate that, by just choosing the activation function, we can design a wide shallow network that mimics the generalization performance of any wide, deep, fully-connected network.

1 Introduction

Many recent advances in our understanding of deep learning have stemmed from the study of infinitely-wide neural networks. The key insight is that functions computed by infinitely-wide neural networks are equivalent to Gaussian processes specified by two kernel functions: the neural network-Gaussian process (NNGP) kernel describes random initialization and a network’s Bayesian priors [1], while the neural tangent kernel (NTK) describes training via gradient descent [2,3]. These kernels, which take fairly simple analytical forms, have been derived for fully-connected networks (FCNs) [1,3], convolutional neural networks (CNNs) [4–6], and more [7,8], leading to both theoretical insights into deep networks [9–13] and improvements on state-of-the-art kernel methods [14–16].

Despite this progress, however, there are many major open problems, from characterizing the advantages of depth to performing principled architecture design, which neural network-Gaussian process equivalences still have great potential to illuminate. To attack these problems and improve understanding of deep learning, we frame three fundamental, unexplored questions about neural network kernels:

1. What subset of all conceivable kernels can actually be realized as wide neural networks of particular types?
2. Can deeper wide networks achieve a richer set of kernels than shallower wide networks?
3. Can we reverse-engineer networks to have desired kernels?

An answer to the first question would shed light on the flexibility and power of deep architectures. For the second question, a positive answer might provide clear theoretical motivation for using networks

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Code available at https://github.com/james-simon/shallow-learning

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of great depth, while a negative answer would have many counterintuitive implications. As for the third, the ability to map from kernels back to network architectures might allow us to design high-performing architectures and activation functions \textit{from first principles} and provide justification for existing architectures.

\textit{Here we answer all three questions for fully-connected networks, giving a surprising negative answer to the second question and, just as important, a positive answer to the third.}

1.1 Summary of Contributions

We begin by pointing out a simple constraint that any FCN architecture’s NNGP and NTK kernels must satisfy (Proposition 1). We then show that, for a polynomial activation function, the recursion relation specifying the NNGP kernel reduces to a simple form which we then solve to find a polynomial activation function approximating a desired recursion relation. We use this fact to prove that the choice of activation function gives enough freedom to saturate Proposition 1’s constraint (Proposition 2). Finally, combining these results, we prove that the NNGP and NTK kernels of any deep FCN can be realized in a shallow FCN (Theorem 1). These results assume data normalized to lie on a hypersphere.

We then conduct several experiments to verify our results. First, we show that we can in fact engineer shallow networks to achieve a variety of deep network and synthetic kernels, even for finite networks and fairly low approximation orders. Second, we demonstrate that, by mimicking the kernel of a high-performing wide deep network, we can achieve its performance in a wide shallow network. Finally, we demonstrate that, by optimizing the network kernel as a hyperparameter, we can find kernels that match or surpass the performance of the best ReLU kernels without any a priori knowledge of how they should look, suggesting an interesting new approach to network architecture design.

1.2 Related work

In addition to the previous studies cited above, there are several pre-NNGP results which are worth noting as background. First, the classic Universal Approximation Theorem [17] states that a wide shallow network can approximate any function, but it claims nothing about how shallow networks learn or generalize. By contrast, the present work shows that a wide shallow FCN can approximate any wide deep FCN’s two \textit{kernels}, which describe its Bayesian priors, its training, and ultimately its generalization behavior.

Rahimi and Recht (2007) [18] studied models with random features, showing that models with many random features drawn from the right distribution can approximate arbitrary desired kernels. Besides the use of the NNGP and NTK, the chief distinction between this and the present work is that, while Ref. [18] uses rather complex feature distributions, we work entirely within the standard framework of FCNs, achieving desired kernels just by choosing an activation function. We also consider networks of arbitrary depth, while random feature models are typically shallow.

Amit and Daniely (2016) [19] study kernels of finite-width networks, noting positive-semidefiniteness constraints similar to our Proposition 1.

Lastly, Ba and Caruana (2014) [20] showed that training shallow networks to mimic deep networks in a student-teacher fashion can give shallow networks with deep-network performance on certain problems.

2 Theoretical Results

2.1 Notation

Consider a fully-connected network (FCN) with input dimension \( n^0 \), a total of \( L-1 \) hidden layers with widths \( n^1, ..., n^{L-1} \), and output dimension \( n^L \). For each \( x \in \mathbb{R}^{n^0} \), we denote the pre- and post-activations at layer \( l \) as \( z^l(x) \) and \( x^l(x) \), respectively, with \( z^L(x) \) being the output of the network. The feedforward operation is given by
When a randomly-initialized network is evaluated on two different inputs $x_1, x_2$, the corresponding preactivations and network outputs will have correlations depending on the inputs. In the infinite-width limit (i.e. as \( n^l \to \infty \)), we can completely describe these correlations with the NNGP kernel, so called because it is the kernel of the neural network’s equivalent Gaussian process [3]. We write the kernel function at layer \( l \) as \( K^l(x_1, x_2) \equiv \mathbb{E}[z^l_1(x_1)z^l_2(x_2)] \), where the expectation is over the model parameters and the subscript \( i \) denotes an arbitrary element of the preactivation vector. Note that correlations between different indices are zero (i.e. \( \mathbb{E}[z^l_i(x_1)z^l_j(x_2)] = 0 \) if \( i \neq j \)).

The training of infinitely-wide FCNs via gradient descent with mean-squared-error loss is described by a second kernel function called the neural tangent kernel or NTK [2], defined as \( \Theta(x_1, x_2) \equiv (\nabla_\theta z^l_1(x_1))^T \nabla_\theta z^l_2(x_2) \), where \( \theta \) denotes the vector of all trainable network parameters and the subscript \( i \) denotes an arbitrary element of the output vector. We choose to define \( \Theta \) in terms of an arbitrary index \( i \) because, like the NNGP kernel, the NTK kernel for FCNs is independent of index, and cross-terms between different indices are zero. In the infinite-width limit, this kernel function remains constant throughout training.

In this paper, we largely confine our analysis to the NNGP kernel, but here we mention two facts about the NTK that will let us draw conclusions later. First, like all kernel functions, the NTK is a function that corresponds to real FCN architectures and show that each of them can be realized as the NNGP kernel of a shallow FCN. We simplify the problem by introducing the following normalization assumptions on the data:

**Assumption 1.** Every data vector \( x_i \) satisfies \( |x_i| = \sqrt{n^0} \).

While this assumption is not satisfied by most datasets, we expect that enforcing it and discarding a single degree of freedom will not greatly harm learning in most high-dimensional problems. Most
images, for example, can be brightened or darkened significantly while remaining recognizable. This assumption is also made in Ref. [19].

For a FCN, \( K^l(x_1, x_2) \) and \( \Theta(x_1, x_2) \) depend only on \( \frac{|x_1|^2}{n^0}, \frac{|x_2|^2}{n^0}, \) and \( \frac{x_1 \cdot x_2}{n^0} \), reflecting the fact that a FCN is statistically invariant to rotations of its input space. Under Assumption 1, the first two of these are always 1, and we can simply write \( K^l(x_1, x_2) = K^l(\frac{x_1}{n^0}, \frac{x_2}{n^0}) = K^l(\xi_1), \) and \( \Theta(x_1, x_2) = \Theta(\frac{x_1}{n^0}, \frac{x_2}{n^0}) = \Theta(\xi_1) \), where we have introduced the shorthand \( \xi_1 = \frac{x_1 \cdot x_2}{n^0} \in [-1, 1] \). We can also simplify Equation 2 to

\[
K^l(\xi_1) = f_{\phi, \sigma_w, \sigma_b}(K^{l-1}(1), K^{l-1}(\xi_1)),
\]

where

\[
f_{\phi, \sigma_w, \sigma_b}(K(1), K(\xi)) \equiv F_{\phi, \sigma_w, \sigma_b}(K(1), K(1), K(\xi)).
\]

We develop our main results as follows. Proposition 1 describes constraints on the achievable kernel functions, Proposition 2 characterizes the set of achievable recursion relations, and Theorem 1 combines these results to show that, for normalized data, a single-hidden-layer infinitely-wide FCN with the proper choice of \( \phi \) can achieve any possible kernel that can be achieved by a deep, infinitely-wide FCN.

**Proposition 1.** Any \( K^l(\cdot) \) or \( \Theta(\cdot) \) describing an infinitely wide FCN on normalized data must have the form of a Taylor series with all nonnegative coefficients.

**Proof.** This proposition essentially follows from the constraint that the NNGP and NTK kernels are positive semi-definite (PSD). As a reminder of what this condition means for bivariate functions, we say a function \( O : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) is PSD on a domain \( \mathcal{X} \) if and only if \( \int_\mathcal{X} \int_\mathcal{X} O(x_1, x_2)g(x_1)g(x_2)d\mu(x_1)d\mu(x_2) \geq 0 \) for all functions \( g : \mathcal{X} \to \mathbb{R} \). This ensures that, when evaluated for a set of points from \( \mathcal{X} \), the NNGP and NTK always give kernels that are PSD matrices. Because we have assumed normalized data, the domain \( \mathcal{X} \) for our problem is the hypersphere \( \sqrt{n^0} \cdot S_{n^0-1} \) (that is, all \( x \in \mathbb{R}^{n^0} \) such that \( |x| = n^0 \)). As previously discussed, the rotation invariance of FCNs implies that their NNGP and NTK kernels can then only depend on \( \xi_1 = \frac{x_1 \cdot x_2}{n^0} \).

The set of PSD rotation-invariant functions on hyperspheres was fully characterized by Schoenberg in 1942 [21]. This set depends on the dimension of the hypersphere, with higher-dimensional hyperspheres having a more constrained set of PSD functions. In particular, if a function \( K : [-1, 1] \to \mathbb{R} \) is PSD on \( S_a \), it is also PSD on any \( S_b \) with \( b < a \). The strongest constraints thus apply to \( S_{n^0} \), and they happen to be very simple: every positive-definite function on \( S_{n^0} \) takes the form

\[
K(\xi) = \sum_{i=0}^{\infty} a_i \xi^i, \quad \text{where} \quad a_i \geq 0 \quad \text{for all} \quad i.
\]

We do not take \( n^0 \to \infty \) in the infinite-width limit, but we can nonetheless show that \( K^l \) and \( \Theta \) must take the form of Equation 1 even for finite \( n^0 \). The key observation is that, while the forms of \( K^l \) and \( \Theta \) depend on many hyperparameters, they are independent of \( n^0 \), and thus if a particular choice of hyperparameters gives a particular kernel for some finite \( n^0 \), that same choice would yield the same kernel for arbitrarily large \( n^0 \). Therefore, any achievable \( K^l \) and \( \Theta \) for any \( n^0 \) must be PSD on \( S_{n^0} \), and thus must take the form of Equation 1. This proves the desired proposition.

\[\square\]

**Proposition 2.** There exists a choice of \( \phi \) such that the NNGP kernel recursion relation \( f_{\phi, 1, 0}(K(1), \cdot) \), where \( K(1) > 0 \) is specified, is any desired univariate function that has all nonnegative coefficients when expanded as a Taylor series.

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1This is true of both \( K^l \) and \( \Theta \) because the base cases of their recursive definitions depend only on these quantities.
We choose $\phi$. We can compute the expectation values in Equation (5) with Isserlis’ (a.k.a. Wick’s) theorem:

$$E_{z_1, z_2 \sim \mathcal{N}(0, \Sigma)} \left[ \phi(z_1) \phi(z_2) \right], \quad \Sigma = \begin{bmatrix} K(1), K(\xi) \\ K(\xi), K(1) \end{bmatrix}.$$ 

We choose $\phi(z) = \sum_{\alpha=0}^{\infty} \frac{c_\alpha z^{\alpha}}{\alpha!}$, where $c_\alpha \in \mathbb{R}$, as the form of $\phi$. Plugging this Taylor series into the above gives

$$f_{\phi, \sigma_w, \sigma_b} (K(1), K(\xi)) = \sigma_w^2 + \sigma_w^2 \sum_{\alpha=0}^{\infty} \sum_{\beta=0}^{\infty} \frac{c_\alpha c_\beta}{\alpha! \beta!} E_{z_1, z_2 \sim \mathcal{N}(0, \Sigma)} \left[ z_1^\alpha z_2^\beta \right]. \tag{5}$$

We can compute the expectation values in Equation (5) with Isserlis’ (a.k.a. Wick’s) theorem:

$$E_{z_1, z_2 \sim \mathcal{N}(0, \Sigma)} \left[ z_1^\alpha z_2^\beta \right] = \sum_{\gamma=0}^{\min(\alpha, \beta)} \frac{K(\xi)^\gamma K(1)^{\alpha+\beta-2\gamma}}{\gamma! (\alpha-\gamma)! (\beta-\gamma)!} \cdot 1[\alpha = \beta = \gamma \mod 2], \tag{6}$$

where $n!!$ is the double factorial of $n$ with $0!! = 1$. Combining Equations (5) and (6) yields

$$f_{\phi, \sigma_w, \sigma_b} (K(1), K(\xi)) = \sigma_w^2 + \sigma_w^2 \sum_{\alpha=0}^{\infty} \sum_{\beta=0}^{\infty} \frac{c_\alpha c_\beta}{\alpha! \beta!} \frac{K(\xi)^\gamma K(1)^{\alpha+\beta-2\gamma}}{\gamma! (\alpha-\gamma)! (\beta-\gamma)!} \cdot 1[\alpha = \beta = \gamma \mod 2].$$

Now we choose $\sigma_w = 1$ and $\sigma_b = 0$ (i.e. there are no biases) and write $f_{\phi, 1, 0}$ in the form of a Taylor series, getting

$$f_{\phi, 1, 0} (K(1), K(\xi)) = \sum_{\gamma=0}^{\infty} \frac{a_{\gamma} K(\xi)^\gamma}{\gamma!}, \tag{7}$$

with positive coefficients given by

$$a_{\gamma} = \left[ \sum_{\alpha=\gamma}^{\infty} \frac{c_\alpha K(1)^{\frac{\alpha-\gamma}{2}}}{(\alpha-\gamma)!} \cdot 1[\alpha = \gamma \mod 2] \right]^2 = \left[ \sum_{\alpha=0}^{\infty} M_{\gamma, \alpha} c_\alpha \right]^2,$$

where we have defined the matrix $M_{\gamma, \alpha} \equiv \frac{K(1)^{\frac{\alpha-\gamma}{2}}}{(\alpha-\gamma)!} \cdot 1[\gamma \leq \alpha] \cdot 1[\gamma = \alpha \mod 2]$. Conveniely, this matrix is upper-triangular with nonzero elements on the diagonal, so it is invertible. In fact, its inverse can be written explicitly as

$$M_{\gamma, \alpha}^{-1} \equiv \frac{(-K(1))^{(\alpha-\gamma)/2}}{(\alpha-\gamma)!} \cdot 1[\gamma \leq \alpha] \cdot 1[\gamma = \alpha \mod 2]. \tag{8}$$

This matrix inverse allows us to choose $\{c_\alpha\}_\alpha$ to achieve any desired $\{a_{\gamma}\}_\gamma$ satisfying $a_{\gamma} \geq 0$. First, we simply define $b_\gamma = \pm \sqrt{\frac{\gamma}{\alpha}}$ (where we have the freedom to choose either root), and then set $c_\alpha = \sum_{\gamma=0}^{\infty} M_{\gamma, \alpha}^{-1} b_\gamma$. The function $\phi$ whose Taylor series coefficients are the resulting $\{c_\alpha\}_\alpha$ then gives the $f_{\phi, 1, 0}(K(1), \cdot)$ whose coefficients are the target $\{a_{\gamma}\}_\gamma$. This construction completes the proof.
As a final note, some might find it intriguing that, since the constraint that $a_\gamma \geq 0$ stemmed from the need to take a square root, an extension of neural networks to the complex numbers would allow us to achieve any $f_{\phi,1,0}$ equivalent to its Taylor series.

**Theorem 1** (Arbitrary kernels with shallow networks). Any NNGP or NTK kernel function corresponding to any deep, infinitely-wide FCN on normalized data can be achieved as the NNGP or NTK kernel of a single-hidden-layer FCN.

**Proof.** As discussed above, for any $(L-1)$-hidden-layer FCN architecture on normalized data, the NNGP and NTK kernels must take the form $K^L(x_1, x_2) = K^L(\xi_{12})$ and $\Theta(x_1, x_2) = \Theta(\xi_{12})$, respectively. By Proposition 1, $K^L(\cdot)$ and $\Theta(\cdot)$ must have all nonnegative coefficients when expanded as a Taylor series. To construct a single-hidden-layer network with either the NNGP or NTK kernel of a deep FCN of our choice, we first choose $\sigma_w = 1$ and $\sigma_b = 0$, so that $K^1(\xi_{12}) = \xi_{12}$, and then note that $K^2(\xi_{12}) = f_{\phi,1,0}(1, \xi_{12})$. Using the construction of Proposition 2, we can then choose $\phi$ so $K^2$ is the target NNGP or NTK kernel. If the target is an NNGP kernel, we have achieved our goal. Alternatively, if it is an NTK kernel, we freeze the first layer and only train the readout layer, giving $\Theta = K^2$.

2.4 An algorithm for designing $\phi$ to give a desired kernel

Importantly, our proof of the universality of shallow FCN kernels is constructive: given a desired kernel, it provides a method to engineer a corresponding $\phi$. We formalize this simple procedure in Algorithm 1.

**Algorithm 1:** Constructing $\phi(\cdot)$ to approximate a desired kernel $K(\cdot)$ with one hidden layer.

| Input | // Desired kernel function |
|-------|---------------------------|
| $K$   | // Approximation order     |
| $m$   | // Approximation order     |
| $\epsilon$ | // Kernel sample spacing |
| $M^{-1}$ | // The upper-triangular matrix of Eqn. 8 with $K(1)=1$ |
| psd_polyfit | // Fitting fn returning nonnegative Taylor series coeffs |

| Output | // Activation function |
|--------|-----------------------|
| $\phi$ |                       |

$r = \text{range}(\text{start}=-1, \text{end}=1, \text{step}=\epsilon)$

$k = K(r)$

$a = \text{psd.polyfit}(xs=r, ys=k, \text{order}=m)$

$b = a^{1/2}$ // Elementwise square root

$c = M^{-1}a$ // Only using the top-left $m \times m$ block of $M^{-1}$

$\phi(z) = \sum_{\alpha=0}^{m} \frac{c_\alpha}{\alpha!} z^\alpha$

2.5 Decomposing a desired kernel into many hidden layers

As per Equation (3), the kernel of a deep network is given by the composition of many PSD polynomial functions $f$, one for each layer. This means that realizing a desired FCN kernel with many hidden layers that can potentially have different activation functions essentially involves decomposing it into many composed PSD functions, as $K(\cdot) = f^{L-1}(f^{L-2}(\ldots f^1(\xi)) \ldots)$. There are usually many possible decompositions, but for certain choices of kernel function, it is required that all but one of the $f^i$ have only a linear term, corresponding to linear activations. An example is $K(\xi) = \xi^a + \xi$ with $a > 1$; no FCN with more than one layer of nonlinearities can achieve this kernel. This implies, surprisingly, that there are kernels that can only be achieved with FCNs that are effectively shallow!
3 Experiments

3.1 Approximating arbitrary kernels with shallow nets

Our first set of experiments demonstrates that any achievable FCN kernel can be realized as the NNGP kernel of a single-hidden-layer FCN with an appropriately engineered activation function. Our first step is to collect several target kernel functions. We choose the NNGP and NTK kernels of two 4-hidden-layer FCN architectures, one with \( \phi = \text{ReLU}, \sigma_w = 1.5, \sigma_b = 0.1 \) and one with \( \phi = \text{Erf}, \sigma_w = 1.5, \sigma_b = 0.3 \) (we choose these \( \sigma_w, \sigma_b \) in all experiments using these nonlinearities). Both ReLU- and Erf-nets have known analytical kernel recursion relations (see Appendix C of Ref. [3]). We use the Neural Tangents library [22] to compute the NNGP and NTK kernels in all our experiments. To get \( K(\xi) \) for a particular value of \( \xi \), we construct \( x_1, x_2 \) such that \( x_1 \cdot x_2 = \xi \) and compute \( K(x_1, x_2) \) with Neural Tangents. In addition to these deep-FCN kernels, we also include several target kernels with simple analytical forms, all of which have all nonnegative Taylor series as required.

For each desired kernel, we compute a shallow network activation function using Algorithm 1 with \( m = 7 \) and \( \epsilon \approx 0.0025 \). We find that low-order polynomial approximation would often have large errors at \( \xi = \pm 1 \) (especially for kernels like the ReLU NTK which approach infinite slope at these endpoints), so we use a polyfit function that assigns 10% of the weight to the MSE error at \( \xi = \pm 1 \) and 80% to the remaining points. We use these engineered activation functions in single-hidden-layer networks with \( \sigma_w = 1, \sigma_b = 0 \).

In order to verify that our shallow architectures have the desired kernels, we numerically compute their NNGP kernel functions with Neural Tangents. We also empirically measure the NNGP kernel for finite nets with width 10000 and output dimension 100; each kernel measurement is the empirical correlation of the network output evaluated on two appropriate inputs, averaged across all output nodes and over 10000 random initializations.

Our results are shown in Figure 1. In all cases, the shallow net NNGP is quite close to the target kernel, and the empirical kernel has near-perfect agreement with the analytical kernel. We also plot the activation functions corresponding to each experiment; all are nonmonotonic and generally very different from popular activation functions. Note that, while prior works have usually plotted FCN kernels as a function of the angle \( \theta \) between samples [1, 15], here we plot them as functions of \( \xi \equiv \cos(\theta) \).

3.2 Achieving the performance of a deep net with a shallow net

Our next experiment shows that, by approximating the kernel of a desired wide deep FCN, we can engineer a wide shallow FCN that achieves equivalent performance. We evaluate the performance of various deep and shallow networks on the CIFAR-10 and CIFAR-100 datasets [23] with two modifications: the data is normalized to lie on a hypersphere (as per Assumption 1), and we only use the first 10k training points due to memory considerations.\(^2\) We use Neural Tangents with one GPU to perform Gaussian process inference on 10k test images for various kernels corresponding to deep and shallow FCNs. Formally, this is equivalent to taking the mean prediction of an infinite ensemble of infinitely-wide networks.

Our results are shown in Figure 2. We first test the performance of ReLU and Erf nets of various depths. We observe that ReLU nets generally perform better, and for both nonlinearities, the NTK kernels perform better at low depths, while the NNGP kernels are better at high depths. The best performance comes from the 15-hidden-layer ReLU NNGP kernel, so we engineer a shallow network with a degree-20 approximation to that kernel and observe that it achieves identical test accuracy on CIFAR-10, much higher than any of the standard single-hidden-layer kernels. We also explore how performance depends on the degree of the approximation, finding that test accuracy is close to its asymptotic value even for fairly low degrees.

\(^2\)We use CIFAR datasets because we found that, for easier problems such as MNIST and FMNIST, standard deep and shallow FCNs performed very similarly.
Figure 1: Any achievable deep FCN kernel can be realized as the NNGP kernel of a single-hidden-layer FCN with a polynomial activation function. (A-G) Various target kernels (blue curves), NNGP kernels of our corresponding shallow nets (red curves), and empirical kernels sampled using finite networks as described in the text (red dots). The target kernels were approximated with degree-7 polynomials, and that choice of order explains the discrepancies between the target and shallow-net kernels in (B) and (D). (H) The engineered activation functions used in (A-G), which are all polynomials of degree 4 to 7 (see Appendix A).

Figure 2: One can design an activation function for a shallow FCN so that it generalizes as well as any given deep FCN in the infinite-width limit. (A) Curves show CIFAR-10 test accuracy for GP inference using kernels corresponding to ReLU and Erf networks of different depths. The green dot indicates the performance of a single-hidden-layer network with an activation function engineered to mimic a depth-15 ReLU network’s NNGP kernel (purple circle), the deep kernel with highest test accuracy. As shown by the horizontal green dashed line, the engineered shallow net performs as well as the target. (B) Test accuracy as a function of the degree of the polynomial approximation to the target kernel. The degree-20 approximation was used to design the $\phi$ used in (A). The accuracies for all degrees $\geq 6$ are within 1% of degree 20. For the form of $\phi$ and similar experiments on CIFAR-100, see Appendix B.
Table 1: Optimized kernels perform marginally better than the best ReLU kernels on CIFAR-10. The first two columns show the performance of the best-depth NNGP and NTK ReLU kernels (corresponding to maxima in Figure 2A). The third column shows that random kernels perform poorly compared to the ReLU kernels, while the fourth shows that optimized kernels slightly outperform them. The very tight error bounds indicate that optimization finds essentially the same kernel every time.

|               | 15L ReLU (NNGP) | 6L ReLU (NTK) | Random Kernels | Opt. Random Kernels |
|---------------|-----------------|---------------|----------------|---------------------|
| Acc.          | 49.49           | 49.50         | 45.76 ± 2.97   | 49.73 ± 0.05        |
| MSE           | 0.3382          | 0.3404        | 0.3773 ± 0.0301| 0.3361 ± 0.00002    |

### 3.3 Optimizing kernels as hyperparameters

The ability to engineer networks with arbitrary kernels suggests a new approach to deep learning: first, choose or design an optimal kernel for the dataset at hand, then engineer a network with that desired kernel, and finally train it as per usual. This approach, which treats the kernel as a hyperparameter, has the potential to yield architectures better tuned for the dataset at hand.

We test this strategy for FCNs on CIFAR-10 and CIFAR-100. We begin by defining a degree-20 polynomial kernel with random positive coefficients (which corresponds to a shallow FCN as shown in Section 2), then optimize those coefficients by the Broyden-Fletcher-Goldfarb-Shannon (BFGS) algorithm, a quasi-Newton method that uses an approximation of the inverse Hessian matrix to steer the parameter search, to minimize mean squared error (MSE) across four folds of the training set; this algorithm was chosen as it was found empirically to converge the fastest of those tried. We find that the optimized kernels perform as well as or marginally better than the best-depth ReLU NNGP and NTK kernels, as shown in Table 1, and far better than shallow ReLU kernels, as can be seen by comparing to Figures 2 and S1.

Surprisingly, we find that optimization with different random seeds consistently yields essentially the same optimized kernel, as shown in Figure S2. This suggests we consistently find the global minimum, meaning that (a) kernel optimization in this fashion can be amenable to simple gradient-based methods despite generally being nonconvex, and (b) the best ReLU kernels are surprisingly close to optimal. Experimental methods and detailed results are in Appendix C.

### 4 Discussion

In this work, we have characterized the full set of achievable FCN kernel functions and provided a simple algorithm to engineer a wide shallow network to have any achievable kernel, even those corresponding to deep FCNs. Our experiments validate our theory and show that a wide shallow network closely approximating a deep network’s kernel also closely approximates its generalization performance.

The universality of shallow FCN kernels is a surprise given the overwhelming belief that deep architectures are qualitatively more powerful than shallow architectures [24–31]. In particular, Ref. [25] showed that as depth increases, FCNs with tanh activations can exhibit chaotic behavior, reflected in their kernels, that shallow FCNs do not. Our results add a surprising twist to this result: shallow FCNs actually can have the “chaotic” priors of a deep FCN given a sufficiently complicated activation function! We conjecture that deeper nets in the chaotic phase require more complicated activation functions to approximate their kernels.

In future work, we will explore whether our performance results translate to finite-width networks. If finite shallow FCNs can indeed be engineered to perform as well as finite deep FCNs, perhaps by extending our calculations to incorporate finite-width corrections [32, 33], this would have fundamental implications for the design of deep learning systems; if they cannot, this suggests that the advantages of depth are due to finite-width effects, at least for FCNs.

Another important question this paper raises is whether similar results hold for CNNs. The fact that CNNs are more widely used and have many more hyperparameters than FCNs means that insights into their design will have correspondingly more practical value, even without a strict shallow-deep kernel equivalence as we have demonstrated here.
Reverse-engineering kernels could also prove useful in the design of activation functions, most of which have been found through trial and error or brute-force optimization \[^{34}\]. Though we suspect our high-order polynomial activation functions would generally give networks that are difficult to train, we expect that by choosing a different functional form for \( \phi \), such as a Fourier series or a piecewise-linear function, one could achieve a desired kernel without superlinear divergence in \( \phi \). One could also design activation functions achieving a desired kernel in realistic networks with more than one hidden layer. This line of inquiry could both help explain why ReLU-like activations perform well and help discover new alternatives.

Lastly, the ability to engineer networks with arbitrary desired priors could prove very useful for the design of network architectures, particularly if it can be extended beyond FCNs. The space of kernels is much simpler than the space of architectures, so it seems likely that first optimizing a kernel and then mapping it to a deep model could be easier and give better results than choosing a model directly. This approach could also allow one to build in prior knowledge about a data distribution in a principled way. For example, it is well known that the statistics of natural images closely follow powerlaw power spectra \[^{35}\], and one could imagine analytically crafting a convolutional kernel well-suited to these statistical laws, then translating it to a high-performing network with a clear theoretical motivation. This effort will be a central focus of our future work.

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Supplemental Material

A Polynomial Activation Functions Used in Figure 1

The following are the activation functions used to generate the shallow FCN kernels plotted in Figure 1:

\[ \phi_A(z) = 0.6941 - 0.0071z + 0.5839z^2 + 0.3241z^3 - 0.1169z^4 - 0.0506z^5 + 0.0085z^6 + 0.0026z^7 \]

\[ \phi_B(z) = 0.2037 - 0.6345z + 2.8019z^2 + 1.8711z^3 - 0.7304z^4 - 0.3742z^5 + 0.0487z^6 + 0.0178z^7 \]

\[ \phi_C(z) = 0.0931 - 0.1488z + 0.4315z^2 + 0.6013z^3 - 0.4183z^4 - 0.0736z^5 + 0.0076z^6 + 0.0035z^7 \]

\[ \phi_D(z) = -0.0304 - 1.0122z + 1.7028z^2 + 1.9182z^3 - 0.5676z^4 - 0.3588z^5 + 0.0378z^6 + 0.0171z^7 \]

\[ \phi_E(z) = 0.6123 + 1.0000z - 1.2247z^2 + 0.2041z^4 \]

\[ \phi_F(z) = 1.7320 + 1.3689z - 0.9126z^3 + 0.0913z^5 \]

\[ \phi_G(z) = 0.4528z + 0.2529z^3 - 0.0032z^5 + 0.0024z^7 \]

\[ \phi_H(z) = 0.3176 + 0.5431z^2 - 0.0132z^4 + 0.0119z^6 \]

One point of interest is that even (odd) kernels correspond to even (odd) activation functions, as can be seen in \( \phi_G \) and \( \phi_H \). This comes directly from the form of \( M^{-1} \) (see Equation (8)), and less directly from the fact that an odd function integrated against a Gaussian is zero.

B Mimicking A Deep Kernel for CIFAR-100

Figure S1: One can design an activation function for a shallow FCN so that it generalizes as well as any given deep FCN in the infinite-width limit. This is the same experiment as in Figure 2, but using CIFAR-100. (A) Curves show CIFAR-100 test accuracy for GP inference using kernels corresponding to ReLU and Erf networks of different depths. The green dot indicates the performance of a single-hidden-layer network with an activation function engineered to mimic a depth-6 ReLU network’s NTK kernel (purple circle), the deep kernel with highest test accuracy. As shown by the horizontal green dashed line, the engineered shallow net performs far better than other wide shallow nets and almost as well as the target kernel. We believe the small discrepancy is due to approximation error from using a finite-order polynomial: ReLU NTK kernels’ slopes go to infinity at \( \xi = 1 \) and are thus hard to approximate (see Figure 1). (B) Test accuracy as a function of the degree of the polynomial approximation to the target kernel. The degree-20 approximation was used to design the \( \phi \) used in (A). The accuracies for all degrees \( \geq 8 \) are within 1% of degree 20.

The activation functions used in Figures 2 and S1 are as follows:
\[ \phi_{figS1}(z) = 2.342 - 0.1251z - 0.8903z^2 + 1.3029z^3 + 1.5253z^4 - 1.1161z^5 \\
- 0.8273z^6 + 0.3789z^7 + 0.2082z^8 - 0.06314z^9 - 0.02785z^{10} \\
+ 0.0057z^{11} + 0.0021z^{12} - 0.0003z^{13} \]

\[ \phi_{figS2}(z) = 2.342 - 0.1251z - 0.8903z^2 + 1.3029z^3 + 1.5253z^4 - 1.1161z^5 \\
- 0.8273z^6 + 0.3789z^7 + 0.2082z^8 - 0.06314z^9 - 0.02785z^{10} \\
+ 0.0057z^{11} + 0.0021z^{12} - 0.0003z^{13} \]

### C Optimizing Kernels as Hyperparameters

For the kernel optimization experiments of Section 3.3, we assume polynomial kernels of degree 20, whose coefficients we optimize to minimize MSE calculated from 4-fold cross validation on the training set. At initialization, we set all coefficients to random values in the range \([0, 1]\), then zero out a random 80% of coefficients to provide heterogeneity. We optimize with L-BFGS-B, a quasi-Newton approach that allows for the positivity constraints on the polynomial coefficients required by Equation (7).

In Fig. S2, we show the form of kernels before and after optimization. We normalize the kernels before plotting, first subtracting \(K(0) = 0\) and then dividing by \(K(1) = 1\); these performance of these 10 kernels before and after optimization are presented in Table 1. We also include the forms of the ReLU NNGP (depth 15) and ReLU NTK (depth 6), the best performing kernels on CIFAR-10, for comparison. Note that all optimized kernels are essentially the same. Variation in the optimized kernels near \(\xi = -1\) is expected, as it is very rare for two data points to have \(\xi \approx -1\) (i.e. to be near-perfectly antialigned), and so there is little to no optimization pressure on the value of \(K(-1)\).

In Fig. S2, we show the form of kernels before and after optimization. We normalize the kernels before plotting, first subtracting \(K(0)\) and then dividing by \(K(1)\). The second step is justified because Gaussian process is invariant to multiplication of the kernel by a constant, and we perform the first step because we observe that it has very little effect on kernel performance. Even though the random kernels initially have wildly varying forms (and performance, as can be seen in Table 1), after optimization the kernels all dramatically collapse to essentially the same curve, which we conjecture is effectively the global minimum for MSE. We note that optimization starting from polynomial approximations to the ReLU kernels also finds this same solution.