Implicit Regularization in Deep Learning: A View from Function Space

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Abstract

We approach the problem of implicit regularization in deep learning from a geometrical viewpoint. We highlight a possible regularization effect induced by a dynamical alignment of the neural tangent features introduced by Jacot et al., along a small number of task-relevant directions. By extrapolating a new analysis of Rademacher complexity bounds in linear models, we propose and study a new heuristic complexity measure for neural networks which captures this phenomenon, in terms of sequences of tangent kernel classes along in the learning trajectories.

1 Introduction

Deep learning poses a challenge to learning theory: despite their enormous capacity, neural networks often generalize well on real data, even without explicit regularization (Neyshabur et al., 2015; Zhang et al., 2017; Hoffer et al., 2017). This seems at odds with the usual understanding of the bias-variance tradeoff (Geman et al., 1992; Neal et al., 2018; Belkin et al., 2019). In learning theory, this tradeoff is quantified by some suitable notion of model complexity showing up in generalization bounds, such as the Rademacher complexity (Bartlett & Mendelson, 2002).

Solving this apparent paradox requires understanding the role played by optimization (Neyshabur et al., 2015, 2017). As we understand well in the case of linear models (e.g. Gunasekar et al. (2018)), the choice of optimizer induces some type of inductive bias, which can act as implicit regularizer. The challenge is to get insights on such bias in a context where the training dynamics is largely intractable.

In this paper, we approach this problem from a geometrical viewpoint. We take inspiration from linear models: in this context, the interplay between capacity and the geometry of the feature space has been acknowledged for a long time (Schölkopf et al., 1999a). We examine the geometry of the neural tangent features (Jacot et al., 2018) along the optimization paths. The geometry directly impacts optimization, speeding up (resp. slowing down) learning in directions of large (resp. small) eigenvalues. We could expect good performance if training drives the network to regions where the geometry is well-aligned with the task. The intuition is that such a dynamical alignment acts as implicit regularizer, allowing the model to modulate its capacity and adapt it to the data.

Contributions. We take the following few steps in clarifying and formalizing the above intuition:

1. We revisit norm-based capacity measures for linear models (Section 3.2). We illustrate how meaningful norms critically depend on feature geometry, addressing issues raised in Zhang et al. (2017); Belkin et al. (2018); Muthukumar et al. (2020). We explain in particular why capacity measures based on the $\ell^2$ norm are uninformative when the features are highly anisotropic.

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As a step towards the non-linear case, we introduce the notion of classes of learning flows and provide bounds for their Rademacher complexity. We illustrate on a simple setting how an adaptive geometry, obtained by optimizing these bounds, can act as implicit regularizer (Section 3.3).

2. In the case of neural networks, we give various empirical insights on how neural tangent features and kernels (Jacot et al., 2018) adapt to the task during training, for various architectures on MNIST and CIFAR10 (Section 4). Our observations include (i) Non-isotropic increase of the spectrum (ii) Increasing similarity with the class labels as measured by centered kernel alignment (iii) Hierarchical alignment in the presence of noise or difficult examples.

3. We propose and empirically study a new type of complexity measures for neural networks in terms of sequences of (tangent) kernel classes along the learning trajectories.

2 Related Work

**Capacity and Geometry.** In the context of linear models, analysis of the relation between capacity and feature geometry can be traced back to early work on kernel methods (Schölkopf et al. (1999a)), leading to data-dependent error bounds in terms of the eigenvalues of the kernel Gram matrix (Schölkopf et al. (1999b)). Recent analysis of the minimum norm interpolators in overparametrized linear regression emphasized the impact of feature geometry – through the spectrum of the data covariance – on generalization performance (Bartlett et al., 2019; Muthukumar et al., 2019).

Specifically, these works highlight the key role of feature anisotropy. Intuitively, while overparametrization allows a harmless overfitting of the noise across a large number of features, the low norm bias favours the dominant features to fit structured signal (Muthukumar et al., 2019). Of course, for this to work, the features need to be well adapted to the task, e.g. the few dominant ones are highly correlated with the signal (Braun, 2005). Our working hypothesis in this paper is that the performance of neural networks is tied in part to their ability to learn (tangent) features satisfying these conditions.

**Generalization Measures.** There has been a large body of work on generalization measures for neural networks (see Jiang et al. (2020) and references therein), some of which theoretically motivated by norm or margin based bounds (e.g Neyshabur et al. (2019); Bartlett et al. (2017)). Liang et al. (2019) proposed using the Fisher-Rao norm to measure capacity in a geometrical invariant manner. Our approach aims at taking into account the geometry along the whole optimization trajectories. Closely related perspectives in the recent literature are the notion of stiffness (Fort et al., 2019) and coherent gradients (Chatterjee, 2020), tied to the structure of tangent kernels for the loss class.

**Spectral Bias and Tangent Kernels.** A recent line of work on the so-called spectral bias (Rahaman et al., 2019; Xu et al., 2019), relying on Fourier analysis, suggested that neural networks prioritize learning the lowest complexity components of the data during training. In linearized regimes where the training dynamics can be described by a fixed kernel (Jacot et al., 2018; Du et al., 2019; Chizat & Bach, 2018), this can be understood in terms of the standard learning bias along the kernel principal components in linear regression (Arora et al., 2019; Basri et al., 2019; Cao et al., 2019). Several other works (Bietti & Mairal, 2019; Basri et al., 2019; Yang & Salman, 2019) investigated implicit bias of neural networks through a spectral analysis in such regimes. In this paper, we highlight and discuss non-linear effects, in the feature learning regime where the tangent kernel evolves during training (Geiger et al., 2019; Woodworth et al., 2020).

Closest to our work, Kopitkov & Indelman (2019); Oymak et al. (2019) find empirical evidence of the alignment throughout training of the top eigenspaces of the neural tangent kernel or the network Jacobian with the label vectors. We obtain similar insights in Section 4.2, using centered kernel alignment (Cortes et al., 2012) as similarity index.

3 Insights from Linear Models

Implicit biases of gradient descent are relatively well understood in linear models (e.g Gunasekar et al. (2018)). For example when using square loss, it is well-known that gradient descent (initialized in the span of the data) converges to minimum $\ell^2$ norm (resp. RKHS norm) solutions in parameter space (resp. function space). Yet, as pointed out by Belkin et al. (2018); Muthukumar et al. (2020), measuring capacity in terms of such norms is not coherently linked with generalization in practice.

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We shed light on this issue by highlighting the critical dependence of meaningful norm-based capacity on the geometry of the features. We refer to Appendix A for proofs and technical details.

### 3.1 Setup

We consider a family \( \mathcal{F} \) of scalar functions \( f_w(x) = \langle w, \Phi(x) \rangle \) linearly parametrized by \( w \in \mathbb{R}^P \), where \( \Phi \) is a fixed mapping of the input space \( X \) into \( \mathbb{R}^P \). Given a training set \( S \) of size \( n \), we denote by \( \Phi = [\Phi(x_1), \cdots, \Phi(x_n)]^\top \) the \( n \times P \) feature matrix and by \( y = [y_1, \cdots, y_n]^\top \) the label vector. We are interested in the ‘overparametrized’ regime: we assume \( P \geq n \). We write the SVD of the feature matrix as \( \Phi = \sum_{j=1}^n \sqrt{\lambda_j} u_j v_j^\top \), where \( \lambda_1 \geq \cdots \geq \lambda_n \) are ranked in nonincreasing order. We will consider the minimum \( \ell^2 \) norm interpolators \citep{hastie2009elements},

\[
w^* = \Phi^\top K^{-1} y = \sum_{j=1}^n \frac{u_j^\top y}{\sqrt{\lambda_j}}
\]

We will refer to standard generalization bounds based on the Rademacher complexity \citep{bartlett2002rademacher}. Given a training set \( S \) of size \( n \), the (empirical) Rademacher complexity measures how well the family of functions \( \mathcal{F} \) correlates with random noise on \( S \):

\[
\hat{R}_S(F) = \mathbb{E}_{\sigma \in \{\pm 1\}^n} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \sigma_i f(x_i) \right],
\]

where the expectation is over \( n \) i.i.d uniform random variables \( \sigma_1, \cdots, \sigma_n \in \{\pm 1\} \). In Appendix A.2 we provide instances of margin-bounds based on Rademacher complexity, relevant for classification tasks \citep{Mohri2012}. The Rademacher complexity depends on the size (capacity) of the function class \( \mathcal{F} \). Suitable constraints on the capacity, obtained e.g. by taking into account the implicit biases of a given algorithm, can reduce the Rademacher complexity and lead to sharper bounds.

Following \cite{belkin2018towards, muthukumar2020}, we center our discussion on interpolated classifiers. The results of \cite{muthukumar2020} suggest that with sufficient overparametrization, all training points are support vectors, bridging hard margin SVM with minimum norm interpolation.

### 3.2 Which Norm for Measuring Capacity?

A standard approach is to measure capacity in terms of the \( \ell^2 \) norm the weight vector. Considering

\[
\mathcal{F}_M = \{ f_w : x \mapsto \langle w, \Phi(x) \rangle \mid \|w\|_2 \leq M \},
\]

the Rademacher complexity of \( \mathcal{F}_M \) can be bounded as \cite[Lemma 22]{bartlett2002rademacher}:

\[
\hat{R}_S(\mathcal{F}_M) \leq (M/n)\|\Phi\|_F
\]

where \( \|\Phi\|_F \) is the Frobenius norm of the feature matrix.\footnote{Note that \( \|\Phi\|_F = \sqrt{\text{Tr} K} \) where \( K = \Phi \Phi^\top \) is the kernel matrix.}

Is the \( \ell^2 \) norm a good measure, even for algorithms biased towards low \( \ell^2 \) norm solutions? If the distribution of solutions \( w_v \), where \( \Sigma \sim \rho^2 \), is reasonably isotropic, taking the smallest \( \ell^2 \) ball containing them (with high probability) gives an accurate description of the class of trained models. However for very anisotropic distributions such as thin shells, the solutions do not fill any such ball so describing trained models in terms of \( \ell^2 \) balls is wasteful \citep{Scholkopf2019}. For the minimum \( \ell^2 \) norm interpolators (1), the solution distribution typically inherits the anisotropy of the features. For example, if \( y_i = \bar{y}(x_i) + \varepsilon_i \) where \( \varepsilon_i \sim \mathcal{N}(0, \sigma^2) \), the covariance of the solutions with respect to noise is \( \text{cov}_x(w^*, w^*) = \sum_j \frac{\sigma^2}{\lambda_j} v_j v_j^\top \), which scales as \( 1/\lambda_j \) along \( v_j \).

To visualize this on a simple setting, consider \( P \) random Fourier features \citep{rahimi2007random}, fit on 1D data \( x \) modelled by \( N \) equally spaced points in \([-a, a]\). In this setting, the (true) feature map is represented by a \( N \times P \) matrix with SVD \( \Phi = \sum_j \sqrt{\lambda_j} \psi_j \varphi_j^\top \). The labels are given by \( y(x) = \text{sign}(\psi_1(x)) \). To highlight the effect of feature anisotropy, we further rescale the singular values as \( \lambda_j' = 1 + \varepsilon (j - 1) \) so as to interpolate between whitened features \((c=0)\) and the original ones \((c=1)\). We set \( P = N = 1000 \). Fig 1 (left) shows 2D projections in the plane \((\varphi_1, \varphi_{10})\) of...
We emphasize that this issue is about the choice of norm and not about complexity-based bounds per se. In fact, note that anisotropies can in principle be compensated by a suitable linear reparametrization \( w \mapsto A^T w, \Phi \mapsto A^{-1} \Phi \). Any such \( A \) can be viewed as defining a new norm \( \| w \|_A := \sqrt{w^T g_A w} \) induced by the metric \( g_A = A A^T \). The following classes

\[
\mathcal{F}^A_{M_A} = \{ f_w : \mathbf{x} \mapsto \langle \mathbf{w}, \Phi(\mathbf{x}) \rangle \mid \| \mathbf{w} \|_A \leq M_A \},
\]

define a much richer set of complexity classes than (3), represented by ellipsoids of all shapes in parameter space. A direct extension of the standard result (4) yields

\[
\mathcal{R}_S(\mathcal{F}^A_{M_A}) \leq (M_A / n) \| A^{-1} \Phi^T \|_F
\]

in terms of the Frobenius norm of the rescaled feature matrix. More meaningful norms than the \( \ell^2 \) norm can be found by optimizing the bound (6) with \( M_A = \| w^* \|_A \), over a given class of reparametrization matrices \( A \). We give an example of this in the following Proposition.

**Proposition 1.** Consider the class of reparametrization matrices \( A_\nu = \sum_{j=1}^n \sqrt{\nu_j} v_j v_j^T + 1_{\mathsf{span}\{v_1, \ldots, v_n\}^\perp} \), which act as mere rescaling \( \lambda_j \rightarrow \lambda_j / \nu_j \) of the singular values of the feature matrix. Any minimizer of (6) for the minimum \( \ell^2 \)-norm interpolator takes the form

\[
\nu_j^* = \kappa \frac{\sqrt{\lambda_j}}{|v_j^* w^*|} = \kappa \frac{\lambda_j}{|u_j^* y|}
\]

where \( \kappa > 0 \) is a constant independent of \( j \).

Note that in the context of Proposition 1, the optimal norm \( \| \cdot \|_{A_\nu} \) depends both on the feature geometry – through the singular values – and on the task – through the labels –. As shown in Fig 1 (right, red plot), in the random Fourier feature setting, the corresponding bound has a much nicer behaviour than the standard bound (4) based on the \( \ell^2 \) norm.

### 3.3 Feature Alignment as Implicit Regularization

As a step towards the non-linear case, we illustrate on a simple setting how an adaptive feature geometry along optimization trajectories can act as an implicit regularizer. In such a setting, the idea is to learn a rescaling metric at each iteration of our algorithm, using a local version of the bounds (6).

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4We also have \( \| A^{-1} \Phi^T \|_F = \sqrt{\text{Tr} K_A} \) where \( K_A = \Phi g_A^{-1} \Phi^T \) is the rescaled kernel matrix.
SuperNat update ($\tilde{A}_0 = I, \Phi_0 = \Phi, K_0 = K$):

1. Perform gradient step $\tilde{w}_{t+1} \leftarrow w_t + \delta w_{\text{GD}}$
2. Find minimizer $\tilde{A}_{t+1}$ of $\|\delta w_{\text{GD}}\|_{\tilde{A}_t^{-1}} \Phi_t^T$.
3. Reparametrize:

\[ w_{t+1} \leftarrow \tilde{A}_{t+1}^T \tilde{w}_{t+1}, \Phi_{t+1} \leftarrow \tilde{A}_{t+1}^{-1} \Phi_t \]

Figure 2: (left) SuperNat algorithm and (right) validation curves obtained with standard and SuperNat gradient descent, on the noisy linear regression problem. At each iteration, SuperNat identifies dominant features and stretches the kernel along them, thereby slowing down and eventually freezing the learning dynamics in the noise direction. This naturally yields better generalization than standard gradient descent on this problem.

### 3.3.1 Complexity of Learning Flows

Since we are interested in functions $f_w$ that result from an iterative algorithm, we can assume they are written as $f_w = f_0 + \sum \delta f_w$, in terms of a sequence of updates $\delta f_w(x) = (\delta w_t, \Phi(x))$. In what follows we set $f_0 = 0$ to keep the notation simple. Instead of considering classes of functions with direct constraints on the parameter as in (3) or (5), we consider functions resulting from a learning flow with local constraints on the parameter updates:

\[ \mathcal{F}_m^A = \{ f_w : x \mapsto \sum \delta w_t, \Phi(x) \} \}

The result (6) extends as follows.

**Theorem 1** (Complexity of Learning Flows). Given any sequences $A$ and $m$ of invertible matrices $A_t \in \mathbb{R}^{P \times P}$ and positive numbers $m_t > 0$, the Rademacher complexity of $\mathcal{F}_m^A$ is bounded as,

\[ \hat{R}_S(\mathcal{F}_m^A) \leq \sum_i (m_t/n) \| A_t^{-1} \Phi_t^T \| \]

Equ. 9 provides us with bounds written in terms of local contributions at each iteration $t$. We recover the bound (6) by choosing a constant matrix $A_t = A$, and $m$ such that $\sum m_t \leq M$: indeed in this case $\mathcal{F}_m^A \subset \mathcal{F}_M^A$ by the triangular inequality, and hence $\hat{R}_S(\mathcal{F}_m^A) \leq \hat{R}_S(\mathcal{F}_M^A)$.

Note that the same result can be formulated in terms of the evolving feature map $\Phi_t = A_t^{-1} \Phi$. The function class (8) can equivalently be written as $\mathcal{F}_m^A = \mathcal{F}_m^\Phi$ where $\Phi = \{ \Phi_t \}$ and

\[ \mathcal{F}_m^\Phi = \{ f_w : x \mapsto \sum_i (\delta w_t, \Phi_t(x)) \} \}

In this formulation, the result (9) reads:

\[ \hat{R}_S(\mathcal{F}_m^\Phi) \leq \sum_i (m_t/n) \| \Phi_t \| \]

### 3.3.2 SuperNatural Gradient

To obtain learning flows with low complexity, Thm. 1 suggests to include, at each iteration $t$, a reparametrization step with a suitable matrix $A_t$ giving a low contribution to the bound (9). Applied to gradient descent (GD), this leads to a new update rule sketched as in Fig 2 (left), where the optimization in Step 2 is over a given class of reparametrization matrices.

**Proposition 2.** At each iteration $t$, consider the class of matrices $A_t$ as in Proposition 1. Any minimizer in Step 2 in Fig 2, where $\delta w_{\text{GD}} = -\eta \nabla_{w_L}$ is a GD updates w.r.t a loss $L$, takes the form

\[ \nu^{\text{st}}_j \leftarrow \frac{1}{|w_j^{\text{st}} |} \nabla_{\nu_j^{\text{st}} |} \]

where $\nabla_{\nu_j^{\text{st}}}$ denotes the gradient w.r.t $f_w := [f_w(x_1), \cdots f_w(x_n)]$, for some constant $\kappa > 0$.

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3In order to not assume a specific upper bound on the number of iterations, we can think of the updates from an iterative algorithm as an infinite sequence $\{\delta w_0, \cdots \delta w_t, \cdots \}$ such that for some $T$, $\delta w_t = 0$ for all $t > T$. 
The successive reparametrizations yield a varying feature map \( \Phi_t = A_t^{-1} \Phi \) where \( A_t = \tilde{A}_0 \cdots \tilde{A}_t \). In the original representation \( \Phi \), SuperNat amounts to performing natural gradient descent with respect to the local metric \( g_{A_t} = A_t A_t^\top \). In the context of Proposition 2, this yields the following update rule, up to isotropic rescaling, for the singular values of the feature matrix \( \Phi_t \):

\[
\lambda_j(t+1) = |u_j^\top \nabla f, L| \lambda_j(t)
\]

In this illustrative setting, we see how the feature (or kernel) adapts to the task, by stretching (resp. contracting) its geometry in directions \( u_j \) along which the residual \( \nabla f, L \) has large (resp. small) components. Intuitively, if a large component \( |u_j^\top \nabla f, L| \) corresponds to signal and a small one \( |u_k^\top \nabla f, L| \) corresponds to noise, then the ratio \( \lambda_j / \lambda_k \) of singular values gets rescaled by the signal-to-noise ratio, thereby increasing the alignment of the learned feature matrix to the signal.

Fig 2 (right) shows results for the following regression setup. We consider Gaussian features \( \Phi = [\varphi, \varphi_{\text{noise}}] \in \mathbb{R}^{d+1} \) where \( \varphi \sim \mathcal{N}(0, 1) \) and \( \varphi_{\text{noise}} \sim \mathcal{N}(0, \frac{1}{d} I_d) \). Given \( n \) training features, we assume the label vector takes the form \( y = \varphi + P_{\text{noise}}(\epsilon) \), where Gaussian noise \( \epsilon \sim \mathcal{N}(0, \sigma^2 I_n) \) is projected onto the noise features through \( P_{\text{noise}} = \varphi_{\text{noise}} \varphi_{\text{noise}}^\top \). The model is trained by gradient descent of mean square loss and its SuperNat variant, where Step 2 uses the analytical solution of Proposition 2. We set \( d = 10 \), \( \sigma^2 = 0.1 \) and use \( n = 50 \) training points. At each iteration, SuperNat identifies dominant features (here \( \varphi \)) and stretches the metric along them, thereby slowing down and eventually freezing the dynamics in the orthogonal (noise) directions.

## 4 Feature Alignment in Neural Networks

We now extend the discussion to the case of non-linear models such as neural networks. Following the line of Jacot et al. (2018), the idea is to look at the function updates at first order in their Taylor expansion w.r.t. the parameters,

\[
\delta f_{\omega_t}(x) = \langle \delta \omega, \Phi_{\omega_t}(x) \rangle + O(\|\delta \omega\|^2),
\]

written in terms of the so-called **tangent features**:\(^6\)

\[
\Phi_{\omega}(x) := \nabla_\omega f_{\omega}(x)
\]

In Section 4.1, we introduce tangent features from a geometrical point of view (we refer to Appendix B for more formal detail). Section 4.2 presents empirical results on how the tangent features evolve during training for classical architectures trained on real datasets, highlighting an alignment dynamics akin to the one enforced by SuperNat in Section 3.3. Finally in Section 4.3, by an extrapolation of Equ 11, we propose a new complexity measure for neural networks, expressed in terms of (tangent) kernel classes along the learning trajectories, and show that it correlates with performance.

### 4.1 Tangent Features and Geometry

We restrict the discussion to scalar functions \( f_{\omega} \in \mathcal{F} \) to keep Notation light. The extension to vector-valued functions, relevant for multiclass classification setting, is straightforward and presented in Appendix B, along with more details of the construction.

#### Tangent Features

For a given value \( \omega \in \mathbb{R}^P \) of the parameter, we define the **tangent features** \( \Phi_\omega(x) \) as in (15). The tangent features define an (uncentered) covariance matrix and a kernel:

\[
g_\omega = \mathbb{E}_{x \sim \rho} \left[ \Phi_\omega(x) \Phi_\omega(x)^\top \right], \quad k_\omega(x, \bar{x}) = \langle \Phi_\omega(x), \Phi_\omega(\bar{x}) \rangle
\]

where the expectation is over the input data distribution \( \rho \). The covariance acts as a **metric tensor** on the parameter space: assuming \( \mathcal{F} \subset L^2(\rho) \), this is the metric induced by pullback of the \( L^2 \) scalar product \( \langle f, g \rangle_\rho = \mathbb{E}_{x \sim \rho}[f(x)g(x)] \) on the function space. This can be seen by spelling out the line element \( ds^2 := \|df_\omega\|_{\rho}^2 \)

\[
\|df_\omega\|_{\rho}^2 = \sum_{p, q=1}^{P} \left( \frac{\partial f_\omega}{\partial w_p} dw_p, \frac{\partial f_\omega}{\partial w_q} dw_q \right)_{\rho} = \sum_{p, q=1}^{P} \left( g_\omega \right)_{pq} dw_p dw_q
\]

\(^6\)Formally, assuming \( \omega \rightarrow f_\omega \) is a smooth mapping from a parameter space \( \mathcal{W} \simeq \mathbb{R}^P \) to \( \mathcal{F} \), the tangent feature map is the differential \( df_\omega : \mathcal{X} \rightarrow T_\omega \mathcal{W} \simeq \mathbb{R}^P \) mapping inputs to the (co)tangent space at \( \omega \). For a linear model \( f_\omega(x) := \langle x, \Phi(x) \rangle \) we recover the global feature map \( \Phi \).
The kernel is **tangent kernel** (Jacot et al., 2018). Feature covariance and the tangent kernel share the same non-zero eigenvalue spectrum, which characterizes the local geometry of the model.

**Not all Parameters are Equal.** To make this more concrete, let us pick \( n \) input samples and represent each function by its output sample vector \( f_w = [f_w(x_1), \ldots, f_w(x_n)]^T \) in \( \mathbb{R}^n \). The empirical versions of (16) can be written in terms of the \( n \times P \) Jacobian matrix \( \Phi_w = \nabla w f_w \) as \( G_w = \Phi_w^T \Phi_w \) and \( K_w = \Phi_w \Phi_w^T \), whose eigenvalue decompositions follow from the SVD \( \Phi_w = \sum_{j=1}^n \sqrt{\lambda_j} u_{wj} v_{wj}^T \).

Such a decomposition summarizes the predominant directions both in parameter and feature space, in the neighborhood of \( w \). For example, a perturbation \( \delta w_j \) in the direction of \( v_{wj} \) induces a variation \( \delta f_{wj} \) in the direction of \( u_{wj} \) such that \( \|\delta f_{wj}\| = \|\delta w_j\| \sqrt{\lambda_j} \). Varying the parameter in directions of very low eigenvalues has almost no effect on the function.

Empirical results (see e.g Fig 9 in Appendix B for a VGG11 network trained for a few epochs on CIFAR10) suggest a fast decay of the eigenvalue spectrum, leading to a large number of irrelevant features that the model is prioritizing during the learning process.

**Spectral Bias.** The following elementary result shows how, upon gradient descent w.r.t a loss \( L \), the function updates decompose in the basis of **principal components** of the tangent kernel:7

\[
\tilde{u}_{wj}(x) = \frac{1}{\sqrt{\lambda_j}} (v_{wj}, \Phi_w(x)), \quad j \in \{1 \cdots n\}
\]  

**Lemma 1.** The gradient descent function updates, in first order Taylor approximation, decompose as

\[
\delta f_{GD}(x) = \sum_{j=1}^n \delta f_j \tilde{u}_{wj}(x), \quad \delta f_j = -\eta \lambda_j u_{wj}^T \nabla_x L
\]  

This shows how the singular values act as a mode-specific rescaling \( \eta \lambda_{wj} \) of the learning rate. Intuitively, in such approximation, the principal components of the tangent kernel correspond to features that the model is prioritizing during the learning process.

In linearized regimes where the tangent kernel remains constant during training (Jacot et al., 2018; Du et al., 2019), this can be understood in terms of the standard learning bias along the principal components in linear regression (see Appendix C.2). Fig 3 shows the Fourier decomposition of the eigenvectors of the tangent kernel matrix for a randomly initialized MLP on 1D uniform data. We observe that eigenvectors with increasing index \( j \) indeed correspond to modes with increasing Fourier frequency, with a remarkable alignment with Fourier modes for the first half of the spectrum. We claim this explains the observations of Rahaman et al. (2019); Xu et al. (2019) from a purely linear standpoint.

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7These form an orthonormal family of function for the in-sample scalar product \( \langle f, g \rangle_{in} = \sum_{i=1}^n f(x_i) g(x_i) \). As follows from the SVD of \( \Phi_w \), the sample vector \( \tilde{u}_{wj} = [\tilde{u}_{wj}(x_1), \ldots, \tilde{u}_{wj}(x_n)]^T \) coincides with the \( j \)-th kernel eigenvector \( u_{wj} \). In the standard case of Mercer kernels (such as Gaussian kernels), the kernel principal components approximate the eigenfunctions of the kernel integral operator (e.g Bengio et al. (2004)).
By contrast, as an illustration of the effects of non-linearity, Fig. 4 (details in Appendix D.2) shows visualizations of principal components of the tangent kernel during training of a MLP on a simple binary classification task: \( y(x) = \pm 1 \) depending on whether \( x \sim \text{Unif}[-1, 1]^2 \) is in the centered disk of radius \( \sqrt{2/\pi} \). After a number of iterations, we observe high frequency modes corresponding to the class structure (e.g boundary circle) showing up in the top principal components of the learned kernel. The interpretation is that the tangent kernel stretches in the directions of the signal.

4.2 Empirical Study: Learning Tangent Features

We now investigate in more detail the evolution of tangent features and kernels during training. We run experiments on MNIST (LeCun et al., 2010) and CIFAR10 (Krizhevsky & Hinton, 2009) using standard MLPs, VGG (Simonyan & Zisserman, 2014) and Resnet (He et al., 2016) architectures. In the multiclass settings, tangent kernels on \( n \) samples carry additional class indices \( y \in \{1 \cdots c\} \) and are treated as \( nc \times nc \) matrices. We evaluate it on the test set using mini-batches of size \( n = 100 \).

Spectrum Evolution. We first investigate the evolution of the tangent kernel spectrum for a VGG19 on CIFAR 10, with and without label noise (Fig.5). We first observe a significant increase of the spectrum, early in training (within the first pass through the dataset): the maximum and average eigenvalues \( \lambda_{\text{max}} \) have gained more than 2 orders of magnitude by the time it reaches 100% accuracy. We also note that this evolution is highly anisotropic. We quantify this through the various trace ratios \( T_k = \sum_{j<k} \lambda_j / \sum_j \lambda_j \) as measures of the relative importance of the top \( k \) eigenvalues; and using a notion of effective rank based on spectral entropy (Roy & Vetterli, 2007) (see Appendix E).

We note an important decrease of the effective rank early in training, reaching a phase where only a few top eigenvalues account for most of the trace. This can be observed directly from the highlighted (in red) ratios \( T_{40}, T_{80} \) and \( T_{100} \), that become larger than the remaining eigenvalues. This denotes a stretch of the geometry along a few number of directions (with a relative contraction along the others). Interestingly, in the presence of high label noise, the effective rank remains low during the learning phase (increase of test accuracy) and rises when overfitting starts (decrease of test accuracy).

\[8\] We will report results on kernels obtained from centered features \( \Phi_w(x) \rightarrow \Phi(x) - \mathbb{E}_x \Phi(x) \). Similar plots for the uncentered tangent kernel are shown in Appendix D.3.
Alignment to class labels. We now include the evolution of the eigenvectors in our analysis. We investigate the similarity of the learned tangent features with the class label through centered kernel alignment (CKA) (Cristianini et al., 2002; Cortes et al., 2012; Kornblith et al., 2019). Given two kernel matrices $K$ and $K'$ in $\mathbb{R}^{n \times n}$ such that $\|K\|_F \neq 0$ and $\|K\|_F \neq 0$, the centered alignment between $K$ and $K'$ is defined as

$$\rho(K, K') = \frac{\text{Tr}[K_c K'_c]}{\|K_c\|_F \|K'_c\|_F} \in [0, 1]$$

(20)

where the $c$ index in $K_c$ denotes centering: $K_c = C K C$ where $C = I_n - \frac{1}{n} 1_n 1_n^T$ is the centering matrix. Similarity with the labels is measured through CKA with the rank-one kernel $K_y := yy^T$:

$$\text{CKA}(K, y) = \frac{y^T K_c y}{\|K_c\|_F \|y\|^2}$$

(21)

Intuitively, a kernel that has high CKA with $K_y$ has low (effective) rank and a low angle between $y$ and its few top eigenspaces. Maximizing the CKA between kernel and class labels has been used as a criterion for kernel selection in the literature on learning kernels (Cortes et al., 2012).
Hierarchical Alignment. A key aspect of the generalization question for deep networks concerns the articulation between learning and memorization, in the presence of noise (Zhang et al., 2017), difficult examples or minority groups (Sagawa et al., 2020). Motivated by this, we would like to probe the geometry and its evolution separately in the directions of both type of examples in such settings. To do so, our strategy is to measure partial CKA on examples from two subsets of the same size in the dataset – one with ‘easy’ examples, the other with ‘difficult’ ones. Our setup is to augment 10,000 MNIST training examples with 1000 difficult examples of 2 types: (i) examples with random labels and (ii) examples from the dataset KMNIST (Clanuwat et al., 2018). KMNIST images present similar features than MNIST digits (grayscale handwritten characters) but are arguably useless for solving the task of classifying digits since they represent Japanese characters.

The results are shown in Fig. 7. As training progresses, the CKA on the easy examples increases faster (and to a higher value); in the case of the (structured) difficult examples from KMNIST, we observe an increase of the CKA later in training. This demonstrates a hierarchy in the adaptation of the kernel, measured by the ratio between both alignments. This may favor a sequentialization of the learning due to the non-linearity of the dynamics, a phenomenon analogous to one pointed out in the context of deep linear networks (Saxe et al., 2014; Lampinen et al., 2018; Gidel et al., 2019).

4.3 A New Complexity Measure

Equ. (11) provides a bound of the Rademacher complexity for the function classes (8) specified by a fixed sequence of adaptive kernels (see Appendix A.4 for a generalization to the multiclass setting). By extrapolation to the case of non-deterministic sequences of kernels, we propose using

\[
C(f_w) = \sum_t \| \delta w_t \|_2 \| \Phi_t \|_F
\]

where \( \Phi_t \) is the tangent feature matrix\(^9\) at training iteration \( t \), as a heuristic measure of complexity for neural networks. Fig. 8 shows its behaviour for 1 hidden layer networks trained to convergence of the margin loss, with (left) fixed architecture and varying level of corruption in the labels and (right) varying hidden layer size up to 4 millions parameters, against other capacity measures proposed in the recent literature. We observe that it correctly reflects the shape of the generalization gap.

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\(^9\)In terms of tangent kernels, \( \| \Phi_t \|_F = \sqrt{\text{Tr} K_t} \) where \( K_t \) is the tangent kernel matrix.
Figure 8: Complexity measures for a one hidden layer MLP, trained on MNIST classification until ramp loss reaches 0. Left: as we increase the hidden layer size. Right: for a fixed hidden layer of 256 units as we increase label corruption. Our proposed complexity measure and the one proposed by Neyshabur et al. 2018 are the only ones to correctly reflect the shape of the generalization gap. Note that our measure is general and can in principle be applied to any kind of architecture, whereas Neyshabur et al’s is specific to a one-hidden layer MLP.

5 Conclusion

The results of this paper open several avenues for further investigation. The type of complexity measure we propose suggests a new principled way to choose the geometry in which to perform gradient descent (Srebro et al., 2011; Neyshabur et al., 2017). Whether a procedure such as SuperNat, which optimizes a preconditioning matrix so as to minimize a generalization bound\[^{10}\], can produce meaningful practical results for neural networks, remains to be seen.

The alignment effect highlighted here might enhance learning from a small number of highly predictive, task-dependent features. While this feature selection ability might explain in part the performance of neural networks on simple supervised tasks, it may also might underpin their notorious sensitivity to spurious correlations (Sagawa et al., 2020) and weakness to generalize out-of-distribution (Geirhos et al., 2020). Resolving this tension is a fascinating challenge.

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\[^{10}\]See the recent work by Vaswani et al. (2020) for further empirical investigations of this problem in the context of linear models.
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A Complexity Bounds

A.1 Rademacher Complexity

Given a family $\mathcal{G} \subset \mathbb{R}^Z$ of real-valued functions on a probability space $(Z, \rho)$, the empirical Rademacher complexity of $\mathcal{G}$ with respect to a sample $S = \{z_1, \cdots, z_n\} \sim \rho^n$ is defined as (Mohri et al., 2012):

$$\hat{R}_S(\mathcal{G}) = \mathbb{E}_{\sigma \in \{\pm 1\}^n} \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i g(z_i) \right],$$

(23)

where the expectation is over $n$ i.i.d uniform random variables $\sigma_1, \cdots, \sigma_n \in \{\pm 1\}$. For any $n \geq 1$, the Rademacher complexity with respect to samples of size $n$ is then $R_n(\mathcal{G}) = \mathbb{E}_{S \sim \rho^n} \hat{R}_S(\mathcal{G})$.

A.2 Generalization Bounds

Generalization bounds based on Rademacher complexity are standard (Bartlett et al., 2017; Mohri et al., 2012). We give here one instance of such a bound, relevant for classification task.

Setup. We consider a family $\mathcal{F}$ of functions $f_w : X \rightarrow \mathbb{R}^c$ that output a score or probability $f_w(x)[y]$ for each class $y \in \{1, \cdots, c\}$ (we take $c = 1$ for binary classification). The task is to find a predictor $f_w \in \mathcal{F}$ with small expected classification error, which can be expressed e.g. as

$$L_0(f_w) = \mathbb{P}_{(x,y) \sim \rho} \{ \mu(f_w(x), y) < 0 \}$$

(24)

where $\mu(f(x), y)$ denotes the margin,

$$\mu(f(x), y) = \begin{cases} f(x) & \text{binary case} \\ f(x)[y] - \max_{y' \neq y} f(x)[y'] & \text{multiclass case} \end{cases}$$

(25)

Margin Bound. We consider the margin loss,

$$\ell_{\gamma}(f_w(x), y)) = \phi_{\gamma}(\mu(f_w(x), y))$$

(26)

where $\gamma > 0$, and $\phi_{\gamma}$ is the ramp function: $\phi_{\gamma}(u) = 1$ if $u \leq 0$, $\phi(u) = 0$ if $u > \gamma$ and $\phi(u) = 1 - u/\gamma$ otherwise. We have the following bound for the expected error (24). With probability at least $1 - \delta$ over the draw $S = \{z_i = (x_i, y_i)\}_{i=1}^{n}$ of size $n$, the following holds for all $f_w \in \mathcal{F}$ (Mohri et al., 2012, Theorems 4.4 and 8.1):

$$L_0(f_w) \leq \hat{L}_\gamma(f_w) + 2\hat{R}_S(\ell_{\gamma}(\cdot, \cdot)) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2n}}$$

(27)

where $\hat{L}_\gamma(f_w) = \frac{1}{n} \sum_{i=1}^{n} \ell_{\gamma}(f_w(x_i), y_i)$ is the empirical margin error and $\ell_{\gamma}(\cdot, \cdot)$ is the loss class,

$$\ell_{\gamma}(\mathcal{F}, \cdot) = \{(x, y) \mapsto \ell_{\gamma}(f_w(x), y) \mid f_w \in \mathcal{F}\}$$

(28)

For binary classifiers, because $\phi_{\gamma}$ is $1/\gamma$-Lipschitz, we have in addition

$$R_S(\ell_{\gamma}(\cdot, \cdot)) \leq \frac{1}{\gamma}R_S(\mathcal{F})$$

(29)

by Talagrand’s contraction lemma (Ledoux & Talagrand, 2013) (see e.g. Mohri et al. (2012, lemma 4.2) for a detailed proof).

A.3 Complexity Bounds: Proofs

We first derive standard bounds for the linear families (5) of scalar functions ($c = 1$):

$$\mathcal{F}_{M_A}^A = \{ f_w : x \mapsto \langle w, \Phi(x) \rangle \mid \|w\| \leq M_A \}$$

(30)

Theorem 2. The empirical Rademacher complexity of $\mathcal{F}_{M_A}^A$ is bounded as,

$$\hat{R}_S(\mathcal{F}_{M_A}^A) \leq (M_A/n) \sqrt{\text{Tr}K_A}$$

(31)

where $(K_A)_{ij} = k_A(x_i, x_j)$ is the kernel matrix associated to the rescaled features $A^{-1}\Phi$. 

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Proof. We use the notation of Section 3.2. For given Rademacher variables \( \sigma \in \{ \pm 1 \}^n \), we have,

\[
\sup_{f \in F^A_{M_A}} \sum_{i=1}^n \sigma_i f(x_i) = \sup_{\|w\|_A \leq M_A} \sum_{i=1}^n \sigma_i \langle w, \Phi(x_i) \rangle \\
= \sup_{\|w\|_2 \leq M_A} \sum_{i=1}^n \sigma_i \langle A^\top w, A^{-1} \Phi(x_i) \rangle \\
= \sup_{\|\tilde{w}\|_2 \leq M_A} \sum_{i=1}^n \sigma_i A^{-1} \Phi(x_i) \\
= M_A \left\| \sum_{i=1}^n \sigma_i A^{-1} \Phi(x_i) \right\|_2 \\
= M_A \sqrt{\sigma^\top K_A \sigma} \\
\tag{32}
\]

From (32) and the definition (23) we obtain:

\[
\hat{R}_S(F^A_{M_A}) = M_A n \mathbb{E}_{\sigma} \left[ \sqrt{\sigma^\top K_A \sigma} \right] \\
\leq M_A n \mathbb{E}_{\sigma} |\sigma^\top K_A \sigma| \\
\leq M_A n \sqrt{\text{Tr} K_A} \\
\tag{33}
\]

where we used Jensen’s inequality to pass \( \mathbb{E}_{\sigma} \) under the root, and the properties that \( \mathbb{E}[\sigma_i] = 0 \) and \( \sigma_i^2 = 1 \) for all \( i \). \( \Box \)

We now extend the result to the families (8) of learning flows:

\[
F^A_m = \{ f_w : x \mapsto \sum_i \langle \delta w_i, \Phi(x) \rangle | \| \delta w_i \|_{A_i} \leq m_i \} \\
\tag{34}
\]

Theorem 3 (Theorem 1 restated). The empirical Rademacher complexity of \( F^A_m \) is bounded as,

\[
\hat{R}_S(F^A_m) \leq \sum_i (m_i/n) \sqrt{\text{Tr} K_{A_i}} \\
\tag{35}
\]

where \( (K_{A_i})_{ij} = k_{A_i}(x_i, x_j) \) is the kernel matrix associated to the rescaled features \( A_i^{-1} \Phi \).

Proof. This is simple extension of the previous proof:

\[
\sup_{f \in F^A_m} \sum_{i=1}^n \sigma_i f(x_i) = \sup_{\|\delta w_i\|_{A_i} \leq m_i} \sum_{i=1}^n \sigma_i \sum_t \langle \delta w_t, \Phi(x_i) \rangle \\
= \sum_t \sup_{\|\delta w_t\|_2 \leq m_t} \langle \delta w_t, \sum_{i=1}^n \sigma_i A_t^{-1} \Phi(x_i) \rangle \\
= \sum_t m_t \sqrt{\sigma^\top K_{A_t} \sigma} \\
\tag{36}
\]

and we conclude as in (33). \( \Box \)

Finally, we note that the same result can be formulated in terms of an evolving feature map \( \Phi_t = A_t^{-1} \Phi \) with kernel \( k_t(x, \tilde{x}) = \langle \Phi_t(x), \Phi_t(\tilde{x}) \rangle \). In fact by reparametrization invariance, the function updates can also be written as \( \delta f_w(x) = \langle \delta w_t, \Phi_t(x) \rangle \) where \( \delta w_t = A_t^\top \delta w_t \). The function class (8) can equivalently be written as \( F^A_m = F^\Phi_m \) where \( \Phi \) denotes a fixed sequence of feature maps, \( \Phi = \{ \Phi_t \}_t \) and

\[
F^\Phi_m = \{ f_w : x \mapsto \sum_t \langle \delta w_t, \Phi_t(x) \rangle | \| \delta w_t \|_2 \leq m_t \} \\
\tag{37}
\]

In this formulation, Theorem 1 becomes:

Theorem 3bis. The empirical Rademacher complexity of \( F^\Phi_m \) is bounded as,

\[
\hat{R}_S(F^\Phi_m) \leq \sum_t (m_t/n) \sqrt{\text{Tr} K_t} \\
\tag{38}
\]

where \( (K_t)_{ij} = k_t(x_i, \tilde{x}_j) \) is the kernel matrix associated to the feature map \( \Phi_t \).
A.4 Bounds for Multiclass Classification

The generalization bound (27) is based on the margin loss class (28); the complexity measure studied in Section 4.3 (Fig 8) is based on loss class tangent kernels. In this section, we show how to bound $\hat{\mathcal{R}}_S(\ell, (\mathcal{F}, \cdot))$ in terms of tangent kernels for the original class $\mathcal{F}$ of functions $f_w : \mathcal{X} \to \mathbb{R}^c$ instead. Although the proof is adapted from standard techniques, to our knowledge Lemma 2 and Theorem 4 below are new results. In what follows, we denote by $\mu_\mathcal{F}$ the margin class,

$$\mu_\mathcal{F} = \{(x, y) \rightarrow \mu(f_w(x), y) | f_w \in \mathcal{F}\}$$

where $\mu(f_w(x), y)$ is the margin (25). We also define, for each $y \in \{1 \cdots c\}$,

$$\mathcal{F}_y = \{x \mapsto f_w(x)[y] | f_w \in \mathcal{F}\}, \quad \mu_{\mathcal{F}, y} = \{x \mapsto \mu(f_w(x), y) | f_w \in \mathcal{F}\}$$

**Lemma 2.** The following inequality holds:

$$\hat{\mathcal{R}}_S(\ell, (\mathcal{F}, \cdot)) \leq \frac{c}{\gamma} \sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mathcal{F}_y)$$

**Proof.** We first follow the first steps of the proof of Mohri et al. (2012, Theorem 8.1) to show that

$$\hat{\mathcal{R}}_S(\ell, (\mathcal{F}, \cdot)) \leq \frac{1}{\gamma} \sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mu_{\mathcal{F}, y})$$

We reproduce these steps here for completeness: first, it follows from the $1/\gamma$-Lipschitzness of the ramp loss $\phi_\gamma$ in (26) and Talagrand’s contraction lemma (Mohri et al., 2012, lemma 4.2) that

$$\hat{\mathcal{R}}_S(\ell, (\mathcal{F}, \cdot)) \leq \frac{1}{\gamma} \hat{\mathcal{R}}_S(\mu_\mathcal{F})$$

Next, we write

$$\hat{\mathcal{R}}_S(\mu_\mathcal{F}) := \frac{1}{n} \mathbb{E}_\sigma \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i \mu(f_w(x_i), y_i) \right]$$

$$=\frac{1}{n} \mathbb{E}_\sigma \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i \mu(f_w(x_i), y) \delta_{y, y_i} \right]$$

$$=\frac{1}{n} \sum_{y=1}^{n} \mathbb{E}_\sigma \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i \mu(f_w(x_i), y) \delta_{y, y_i} \right]$$

where $\delta_{y, y_i} = 1$ if $y = y_i$ and 0 otherwise; the second inequality follows from the sub-additivity of sup. Substituting $\delta_{y, y_i} = \frac{1}{2} (\epsilon_i + \frac{1}{2})$ where $\epsilon_i = 2\delta_{y, y_i} - 1 \in \{\pm 1\}$, we obtain

$$\hat{\mathcal{R}}_S(\mu_\mathcal{F}) \leq \frac{1}{2n} \sum_{y=1}^{n} \mathbb{E}_\sigma \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \epsilon_i \sigma_i \mu(f_w(x_i), y) \right] + \frac{1}{2n} \sum_{y=1}^{n} \mathbb{E}_\sigma \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i \mu(f_w(x_i), y) \right]$$

$$= \frac{1}{2n} \sum_{y=1}^{n} \mathbb{E}_\sigma \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i \mu(f_w(x_i), y) \right]$$

Together with (43), this leads to (42).
Now, spelling out $\mu(f_w(x_i, y))$ gives

$$
\hat{\mathcal{R}}_S(\mu_{F, y}) = \frac{1}{n} E_{\sigma} \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i(f_w(x_i)[y] - \max_{y' \neq y} f_w(x_i)[y']) \right]
$$

$$
= \hat{\mathcal{R}}_S(\mathcal{F}_y) + \frac{1}{n} E_{\sigma} \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} (-\sigma_i) \max_{y' \neq y} f_w(x_i)[y'] \right]
$$

$$
= \hat{\mathcal{R}}_S(\mathcal{F}_y) + \frac{1}{n} E_{\sigma} \left[ \sup_{f_w \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i \max_{y \neq y'} f_w(x_i)[y'] \right]
$$

$$
\leq \hat{\mathcal{R}}_S(\mathcal{F}_y) + \hat{\mathcal{R}}_S(\mathcal{G}_y)
$$

(46)

where $\mathcal{G}_y = \{\max_{y'} f_{y'} : y' \neq y \} | f_{y'} \in \mathcal{F}_{y'}$. Now Mohri et al. (2012, lemma 8.1) show that $\hat{\mathcal{R}}_S(\mathcal{G}_y) \leq \sum_{y' \neq y} \hat{\mathcal{R}}_S(\mathcal{F}_{y'})$. This leads to

$$
\sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mu_{F, y}) \leq \sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mathcal{F}_y) + \sum_{y=1}^{c} \sum_{y' \neq y} \hat{\mathcal{R}}_S(\mathcal{F}_{y'})
$$

$$
= \sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mathcal{F}_y) + (c-1) \sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mathcal{F}_y)
$$

$$
= c \sum_{y=1}^{c} \hat{\mathcal{R}}_S(\mathcal{F}_y)
$$

(47)

Substituting in (42) finishes the proof. $\square$

In the linear case, this results leads to analogous theorems as in A.3 in the multiclass setting. For example, considering the linear families of functions $\mathcal{X} \rightarrow \mathbb{R}^c$,

$$
\mathcal{F}_{M_x}^A = \{x \mapsto f_w(x)[y] := \langle w, \Phi(x)[y] \rangle | \|w\|_A \leq M_A \}
$$

(48)

where $(x, y) \mapsto \Phi(x)[y]$ is some joint feature map, we have the following

**Theorem 4.** The emp. Rademacher complexity of the margin loss class $\ell_{\gamma}(\mathcal{F}_{M_x}^A, \cdot)$ is bounded as,

$$
\hat{\mathcal{R}}_S(\ell_{\gamma}(\mathcal{F}_{M_x}^A, \cdot)) \leq \frac{\gamma^{3/2} M_A}{\gamma n} \sqrt{\text{Tr} K_A}
$$

(49)

where $(K_A)^{yy'}_{ij}$ is the kernel $nc \times nc$ matrix associated to the rescaled features $A^{-1} \Phi(x)[y]$. 

**Proof.** Eq.41, and Theorem 4 applied to each linear family $\mathcal{F}_y$ of (scalar) functions leads to

$$
\hat{\mathcal{R}}_S(\ell_{\gamma}(\mathcal{F}_{M_x}^A, \cdot)) \leq \frac{c}{\gamma} \sum_{y=1}^{c} \frac{M_A}{n} \sqrt{\text{Tr} K_A^{yy'}}
$$

(50)

where $\text{Tr} K_A^{yy'} := \sum_{i=1}^{n} (K_A)^{yy'}_{ii}$ is computed w.r.t to the indices $i = 1, ..., n$ for fixed $y$. Passing the average $\frac{1}{c} \sum_{y=1}^{c}$ under the root using Jensen inequality, we conclude:

$$
\hat{\mathcal{R}}_S(\ell_{\gamma}(\mathcal{F}_{M_x}^A, \cdot)) \leq \frac{c}{\gamma n} \sqrt{\frac{1}{c} \sum_{y=1}^{c} \text{Tr} K_A^{yy'}}
$$

$$
= \frac{c^{3/2} M_A}{\gamma n} \sqrt{\text{Tr} K_A}
$$

(51)

$\square$
We assume that

We describe in more formal detail the notion of geometry we consider in the paper for parametric

induces the first order variation

with respect to the parameters

where

where the parameter space

(co)tangent space. Thus, in a given basis, the tangent feature map

This geometry has a dual description in function space in terms of

The parameter space

inherits a metric tensor

where

Given

input samples

, we represent the sample output scores

as a function mapping each pair

as flattened in

. The metric is represented by the matrix of gradient second moments:

This geometry has a dual description in function space in terms of kernels. The idea is to view the differential at each

as a map

. Assuming

, the metric is represented by the matrix of gradient second moments:

This notation, (55) and (58) yield the sample covariance

where

is the set of classes.

The parameter space

inherits a metric tensor

where

is some input data

. Assuming

, the metric is represented by the matrix of gradient second moments:

This geometry has a dual description in function space in terms of kernels. The idea is to view the differential at each

as a map

. Assuming

, the metric is represented by the matrix of gradient second moments:

This notation, (55) and (58) yield the sample covariance

where

is the set of classes.

The tangent feature map

is the set of classes.

The tangent feature map

is the set of classes.

The tangent feature map

is the set of classes.

The tangent feature map

is the set of classes.
Figure 9: Variations of $f_w$ (evaluated on a test set) when perturbing the parameters in the directions given by the right singular vectors of the Jacobian (first 50 directions) or in randomly sampled directions (last 50 directions) on a VGG11 network trained for 10 epochs on CIFAR10. We observe that perturbations in most directions have almost no effect, except in those aligned with the top singular vectors.

### C Spectral Bias

We spell out some more detail for the content of Section 4.1.

#### C.1 Proof of Lemma 1

We consider parameter updates $\delta w_{GD} := -\eta \nabla_w L$ for gradient descent w.r.t the loss $L$. Using the chain rule, we can also write,

$$\delta w_{GD} = -\eta \Phi_w^\top (\nabla f_w L)$$

**Theorem 5** (Lemma 1 restated). The gradient descent function updates in first order Taylor approximation, $\delta f_{GD}(x) := \langle \delta w_{GD}, \Phi_w(x) \rangle$, decompose as,

$$\delta f_{GD}(x) = \sum_{j=1}^n \delta f_j \tilde{u}_{w,j}(x), \quad \delta f_j = -\eta \lambda_{w,j} (u_{w,j}^\top \nabla f_w L)$$

in terms of the kernel principal components $\tilde{u}_{w,j}$ defined by (18).

**Proof.** This follows immediately from (61), the SVD of $\Phi_w$, and the definition (18):

$$\delta f_{GD}(x) = -\eta \langle (\nabla f_w L)^\top \Phi_w, \Phi_w(x) \rangle = \sum_{j=1}^n \delta f_j \tilde{u}_{w,j}(x)$$

\[63\]

\[\square\]

#### C.2 The case of linear regression

In this case $L = \frac{1}{2} \|f_w - y\|^2$ with $f_w = \langle w, \Phi(x) \rangle$ (setting of Section 3), we can make the ‘spectral bias’ more explicit. A straightforward consequence of (62) is that the linear system governing the training dynamics in function space decouple in the basis of kernel principal components.

**Lemma 3.** Gradient descent yields the function iterates,

$$f_{w_t} = f_{w^*} + (id - \eta K)^t (f_{w_0} - f_{w^*})$$

where $id$ is the identity map and $K$ is the operator acting on functions as $(K f)(x) = \sum_{i=1}^n k(x, x_i) f(x_i)$ in terms of the kernel $k(x, \tilde{x}) = \langle \Phi(x), \Phi(\tilde{x}) \rangle$.

**Proof.** The updates (61) induce the functional updates $\delta f_{GD} = f_{w_{t+1}} - f_{w_t}$ given by

$$\delta f_{GD}(x) = -\eta \sum_{i=1}^n k(x, x_i) (f_{w_t}(x_i) - y_i)$$

Substituting $y_i = f_{w^*}(x_i)$ gives $f_{w_{t+1}} - f_{w^*} = (id - \eta K)(f_{w_t} - f_{w^*})$. Equ. 64 follows by induction. \[\square\]
Figure 10: Spectrum evolution of the softmax and margin loss tangent kernels during training of a VGG11 on CIFAR10 with 0% (left) and 80% label noise (right). The top 50 eigenvalues of the tangent kernel are plotted on the y axis, colored by their rank, as evaluated on a train (2nd and 4th rows) and test (3rd and 5th rows) batch.

**Lemma 4.** The operator $K$ has eigenvalues $\lambda_1, \cdots, \lambda_n$ with eigenfunctions $\tilde{u}_j(x)$ given by (18).

**Proof.** We can write $\tilde{u}_j(x) = \sum_{i=1}^{n} k(x, x_i) u_{ji}$ where $u_{ji} = [u_{j1} \cdots u_{jn}]^\top$ are the eigenvectors of $K$. Observe that $(K \tilde{u}_j)(x) = \sum_{i=1}^{n} k(x, x_i) (K u_{ji}) = \sum_{i=1}^{n} k(x, x_i) (\lambda_j u_{ji}) = \lambda_j \tilde{u}_j(x)$. Conversely, if $\lambda$ is an eigenvalue of $K$ with eigenfunction $\tilde{u}$, consider the vector $u = [\tilde{u}(x_1) \cdots \tilde{u}(x_n)]^\top$. Since $\lambda u_j = \tilde{u}(x_i) = (K \tilde{u})(x_i) = (K u)_i$, $u$ is an eigenvector of $K$ and $\lambda$ is one of the $\lambda_j$. \hfill $\square$

**Corollary 1** (Spectral Bias for Linear Regression). By initializing $w_0 = \Phi^\top \alpha_0$ in the span of the features, the function iterates in Eqn.64 uniquely decompose as $f_{w_0}(x) = \sum_{j=1}^{n} f_j \tilde{u}_j(x)$ with

$$f_j - \hat{f}_j^* = (1 - \eta \lambda_j)^{t} (f_{j0} - \hat{f}_j^*)$$

(66)

where $f_j^*$ are the coefficients of the (minimum norm) interpolating solution.

**D Additional experiments**

**D.1 Loss Tangent Kernels: Spectrum Evolution**

We show in Fig 10 the evolution of the tangent kernel\textsuperscript{11} spectrum (top 50 eigenvalues, normalized with the top one) during training of a VGG11 network on CIFAR10. We observe (i) a fast decay of the eigenvalue spectra (note the log scale), leading to a large number of irrelevant directions in parameter (and feature) space; (ii) a large scale separation between eigenvalues: both during the initial rapid expansion phase (not easily visible on those plots) where a few number of relevant features are selected, and in the ‘overfitting’ regime, where all but a few numbers of eigenvalues quickly decay to very low values.

**D.2 Synthetic Experiments**

To visualize the adaptation of the tangent kernel to the task during training, we perform the following synthetic experiment. We train a 6-layer deep 256-unit wide MLP on $n = 500$ points of the Disc dataset $(x, y)$ where $x \sim \text{Unif}[-1,1]^d$ and $y(x) = \pm 1$ depending on whether is within the disk of

\textsuperscript{11}The functions $f_w$ considered in this plot are the output of the softmax layer evaluated on the true classes.
Figure 11: Disk dataset. **Left:** Training set of $n = 500$ points $(x_i, y_i)$ where $x \sim \text{Unif}[-1, 1]^2$, $y_i = 1$ if $\|x_i\|_2 \leq r = \sqrt{2/\pi}$ and $-1$ otherwise. **Right:** Large test sample (2500 points forming a $50 \times 50$ grid) used to evaluate the tangent kernel.

Figure 12: Same as figure 6 but without centering the kernel. Evolution of the uncentered kernel alignment between the tangent kernel and the class label kernel $K_Y = YY^T$ measured on a held-out test set for different architectures: (left) 6 layers of 80 hidden units MLP on MNIST (middle) VGG19 on CIFAR10 (right) Resnet18 on CIFAR10. We observe an increase of the alignment to the target function.

D.3 Uncentered kernel experiments

We show in Fig 12 the evolution of the alignment to the *uncentered* kernel, in order to assess whether this effect is consistent when removing centering. The experimental details are the exact same as in section 4.2 and we also observe a similar increase of the alignment as training progresses.

D.4 Effect of depth on alignment

In order to study the influence of the architecture on the alignment effect, we measure the CKA for different networks and different initialization as we increase the depth. The results in Fig 13 suggest that the alignment effect is magnified as depth increases. We also observe that the ratio of the maximum alignment between easy and difficult examples is increased with depth, but stays high for a smaller number of iterations.

E CKA and Spectral entropy

We make explicit a couple of metrics used in Section 4.2.

**Centered kernel alignment (CKA).** We used CKA Cortes et al. (2012) to measure the similarity between tangent features and labels. Given two kernel matrices $K$ and $K'$ in $\mathbb{R}^{n \times n}$ such that
Figure 13: Effect of depth on alignment. 10,000 MNIST examples with 1000 random labels MNIST examples trained with learning rate=0.01, momentum=0.9 and batch size=100 for MLP with hidden layers size 60 and (in rows) varying depths (in columns) varying random initialization/minibatch sampling. As we increase the depth, the alignment starts increasing later in training and increases faster; and the ratio between easy and difficult alignments reaches a higher value.
\[ \|K\|_F \neq 0 \text{ and } \|K\|_{F'} \neq 0, \text{ the centered alignment between } K \text{ and } K' \text{ is defined as} \]
\[ \rho(K, K') = \frac{\text{Tr}[K_c K'_c]}{\|K_c\|_F \|K'_c\|_F} \in [0, 1] \tag{67} \]

where the \( c \) index in \( K_c \) denotes centering: \( K_c = C K C \) where \( C = I_n - \frac{1}{n} 1_n 1_n^T \) is the centering matrix. The normalization by the Frobenius norm makes CKA invariant under isotropic rescaling. Similarly with the labels is measured through CKA with the rank-one kernel \( K_y := yy^\top \). Since \( \|K_y\|_F = \|y\|^2 \), the normalized kernel \( K_y/\|K_y\|_F \) acts as a projector onto the the normalized label vector \( y/\|y\| \) in \( \mathbb{R}^n \).

**Effective rank.** We used a notion of effective rank based on spectral entropy (Roy & Vetterli, 2007). Given a kernel matrix \( K \) with (strictly) positive eigenvalues \( \lambda_1, \ldots, \lambda_n \), let
\[ \mu_j = \lambda_j/\text{Tr}K, \quad \text{Tr}K = \sum_{i=1}^n \lambda_i \tag{68} \]
be the trace-normalized eigenvalues. The effective rank is defined as (Roy & Vetterli, 2007):
\[ \text{erank} = \exp(H(\mu_1, \ldots, \mu_n)) \tag{69} \]
where \( H(\mu) \) is the Shannon entropy given by
\[ H(\mu_1, \ldots, \mu_n) = -\sum_{j=1}^n \mu_j \log(\mu_j) \tag{70} \]
This effective rank is a real number between 1 and \( n \), upper bounded by \( \text{rank}(K) \), which measures the 'uniformity' of the spectrum through the entropy.