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Abstract

Neural networks trained to minimize the logistic (a.k.a. cross-entropy) loss with gradient-based methods are observed to perform well in many supervised classification tasks. Towards understanding this phenomenon, we analyze the training and generalization behavior of infinitely wide two-layer neural networks with homogeneous activations. We show that the limits of the gradient flow on exponentially tailed losses can be fully characterized as a max-margin classifier in a certain non-Hilbertian space of functions. In presence of hidden low-dimensional structures, the resulting margin is independent of the ambiant dimension, which leads to strong generalization bounds. In contrast, training only the output layer implicitly solves a kernel support vector machine, which a priori does not enjoy such an adaptivity. Our analysis of training is non-quantitative in terms of running time but we prove computational guarantees in simplified settings by showing equivalences with online mirror descent. Finally, numerical experiments suggest that our analysis describes well the practical behavior of two-layer neural networks with ReLU activation and confirm the statistical benefits of this implicit bias.

1 Introduction

Artificial neural networks are successfully used in a variety of difficult supervised classification tasks, but the mechanisms behind their performance remain unclear. The situation is particularly intriguing when the number of parameters of these models exceeds by far the number of input data points and they are trained with gradient-based methods until zero training error, without any explicit regularization. In this case, the training algorithm induces an *implicit bias*: among the many classifiers which overfit on the training set, it selects a specific one which often turns out to perform well on the test set. In this paper, we study the implicit bias of wide neural networks with two layers (i.e., with a single hidden-layer) trained with gradient descent on the logistic loss, or any loss with an exponential tail. Our analysis lies at the intersection of two lines of research that study (i) the implicit bias of gradient methods, and (ii) the training dynamics of wide neural networks.

Implicit bias of gradient methods. Soudry et al. (2018) show that for linearly separable data, training a linear classifier with gradient descent on the logistic loss, or any loss with an exponential tail, implicitly leads to a max-margin linear classifier for the ℓ_2 norm. This result together with results in the boosting literature (Telgarsky, 2013) have led to a fruitful line of research. Fine analyses of convergence rates have been carried out by Nacson et al.

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(2019b); Ji and Telgarsky (2019b, 2018), and extensions to other gradient-based algorithms and to factored parameterizations are considered by Gunasekar et al. (2018a). Linear neural networks have been studied by Gunasekar et al. (2018b); Ji and Telgarsky (2019a); Nacson et al. (2019a), and some properties in general non-convex cases are given by Xu et al. (2018). Closer to the present paper, Lyu and Li (2019) show that for homogeneous neural networks the training trajectory converges in direction to a critical point of some nonconvex max-margin problem. In the present work, we improve this result for the two-layer case: we fully characterize the learnt classifier as the solution of a *convex* max-margin problem. Importantly, this characterization is precise enough to enable a statistical analysis (see Section 6).

Dynamics of infinitely wide neural networks. This fine characterization is made possible by looking at the infinite width limit of two-layer neural networks. This strategy has been used in several works to obtain insights on their statistical properties (Bengio et al., 2006; Bach, 2017a) or training behavior (Nitanda and Suzuki, 2017; Rotskoff and Vanden-Eijnden, 2018; Chizat and Bach, 2018; Mei et al., 2018; Sirignano and Spiliopoulos, 2019), which can be described by a Wasserstein gradient flow (Ambrosio et al., 2008). In particular, Chizat and Bach (2018) show that if the loss is convex, if the initialization is "diverse enough", and if the gradient flow of the objective converges, then its limit is a global minimizer. This result does not apply in our context because our gradient flow diverges, which turns out to be beneficial for the analysis of the implicit bias that we propose.

A general drawback of those *mean-field* analyses is that they are mostly non-quantitative, both in terms of number of neurons and number of iterations. While some works have shown quantitative results by modifying the dynamics (Mei et al., 2019; Wei et al., 2019; Chizat, 2019), we do not take this path in order to stay close to the way neural networks are used in practice and because our numerical experiments suggest that those modifications are not necessary to obtain a good practical behavior. Finally, we stress that our analysis does not take place in the *lazy training* regime (Chizat et al., 2019) which consists of training dynamics that can be analyzed in a perturbative regime around the initialization (see, e.g., Li and Liang, 2018; Jacot et al., 2018; Du et al., 2019). Lazy training is another kind of implicit bias that amounts to training a linear model and does not lead to adaptivity results as those shown in Section 6 (see Figure 3 for an illustration in our context).

1.1 Organization and contributions

After preliminaries on infinitely wide two-layer neural networks in Section 2, we make the following contributions :

- In Section 3, we show that for a class of two-layer neural networks and for losses with an exponential tail, the classifier learnt by the (non-convex) gradient flow is a max-margin classifier for a certain functional norm known as the variation norm.
- When fixing the "directions" of the neurons (Section 4), or when only training the output layer (Section 5), we show that the dynamics implicitly performs *online mirror ascent* on a sequence of smooth-margin objectives and thus naturally maximizes the margin. This leads to convergence guarantees in $O(\log(t)/\sqrt{t})$ in situations where no rate was previously known.
- In Section 6, we lower bound the margins of those classifiers and prove generalization bounds for classification that are independent of the input dimension in presence of hidden linear structures.

- We perform numerical experiments in Section 7 for two-layer ReLU neural networks. We confirm the statistical efficiency of the implicit bias in a high-dimensional setting and observe, in a specifically designed setting, that full training outperforms training only the output layer.

In summary, we show that training two-layer ReLU-like neural networks implicitly solves a problem with strong statistical benefits. We stress however that the runtime of the algorithm is still unknown, in particular we are not able to give a polynomial time or memory complexity.

1.2 Notation

We denote by $\mathcal{M}(\mathbb{R}^p)$ (resp. $\mathcal{M}_+(\mathbb{R}^p)$) the set of signed (resp. nonnegative) Borel measures on $\mathbb{R}^p$ with finite mass and by $\mathcal{P}(\mathbb{R}^p)$ (resp. $\mathcal{P}_2(\mathbb{R}^p)$) the set of probability measures (resp. with finite second moment, endowed with the Wasserstein distance). For readability, we reserve the notations ν and θ (resp. μ and w) for a measure and a point on the sphere $\mathbb{S}^{p-1}$ (resp. on $\mathbb{R}^p$). The set $\Delta^{m-1} = \{p \in \mathbb{R}_+^m \,;\, \mathbf{1}^\top p = 1\}$ is the simplex in $\mathbb{R}^m$.

2 Preliminaries on infinitely wide two-layer networks

2.1 2-homogeneous neural networks

We consider a binary classification problem with a training set $(x_i, y_i)_{i\in[n]}$ of n pairs of observations with $x_i \in \mathbb{R}^d$ and $y_i \in \{-1, +1\}$ and prediction functions of the form

$$h_m(\mathbf{w}, x) = \frac{1}{m}\sum_{j=1}^{m} \phi(w_j, x), \tag{1}$$

where $m \in \mathbb{N}_*$ is the number of units and $\mathbf{w} = (w_j)_{j\in[m]} \in (\mathbb{R}^p)^m$ are the trainable parameters. This setting covers two-layer neural networks where m is the size of the hidden layer. In this paper, we are interested in the over-parameterized regime where m is large, and the prefactor $1/m$ is needed to obtain a non-degenerate limit. We refer to ϕ as a *feature function*, and we focus on the case where ϕ is 2-*homogeneous* and *balanced*:

(A1) The function ϕ is (positively) 2-*homogeneous* in its first variable, i.e., $\phi(rw, x) = r^2\phi(w, x)$ for all $(r, w, x) \in \mathbb{R}_+ \times \mathbb{R}^p \times \mathbb{R}^d$ and it is *balanced*, which means that there is a map $T : \mathbb{S}^{p-1} \to \mathbb{S}^{p-1}$ such that for all $\theta \in \mathbb{S}^{p-1}$, $\phi(T(\theta), \cdot) = -\phi(\theta, \cdot)$.

Here are examples of models which satisfy (A1):

- *ReLU networks.* A two-layer neural network with the rectified linear unit (ReLU) activation function is obtained by setting $\phi(w, x) = a(b + c^\top x)_+$ where $w = (a, b, c) \in \mathbb{R}^{1+1+d}$. This is the motivating example of this article. It satisfies all forthcoming assumptions except differentiability.

- *S-ReLU networks.* With the function $\phi(w, x) = \epsilon \cdot (b + c^\top x)_+^2$ where $w = (b, c) \in \mathbb{R}^{1+d} \sqcup \mathbb{R}^{d+1}$ (two copies of $\mathbb{R}^{d+1}$) and where $\epsilon \in \{-1, +1\}$ depends on which copy w belongs to, we recover the same hypothesis class than two-layer neural networks with squared ReLU activation. This function is differentiable and rigorously covered by all theorems[1].

[1] Our arguments can indeed be applied to situations where the parameter space can be factored as $\mathbb{R}_+ \times \Theta$ where Θ is a compact Riemannian manifold without boundary, see Chizat (2019). For clarity, we limit ourselves to a parameter space $\mathbb{R}^p$ (which corresponds to $\Theta = \mathbb{S}^{p-1}$) while for S-ReLU, this would correspond to $\Theta = \mathbb{S}^{p-1} \sqcup \mathbb{S}^{p-1}$.

2.2 Parameterizing with a measure

The particular structure of two-layer neural networks allows for an alternative description of the predictor function. Letting $\mathcal{P}_2(\mathbb{R}^p)$ be the set of probability measures on $\mathbb{R}^p$ with finite second moments, we define for $\mu \in \mathcal{P}_2(\mathbb{R}^p)$,

$$h(\mu, x) = \int_{\mathbb{R}^p} \phi(w, x) \, \mathrm{d}\mu(w). \tag{2}$$

Finite width networks as in Eq. (1) are recovered when μ is a discrete measure with m atoms.

The representation in Eq. (2) can be reduced to the so-called *convex neural networks* (Bengio et al., 2006), which are parameterized by an unnormalized measure, as follows. We define the 2-homogenous projection operator, $\Pi_2 : \mathcal{P}_2(\mathbb{R}^p) \to \mathcal{M}_+(\mathbb{S}^{p-1})$ characterized by the property that, for any $\varphi \in \mathcal{C}(\mathbb{S}^{p-1})$, it holds

$$\int_{\mathbb{S}^{p-1}} \varphi(\theta) \, \mathrm{d}[\Pi_2(\mu)](\theta) = \int_{\mathbb{R}^p} \|w\|^2 \varphi(w/\|w\|) \, \mathrm{d}\mu(w), \tag{3}$$

where the last integrand is extended by continuity at $w = 0$. This operator projects the mass of μ on the unit sphere after re-weighting it by the squared distance to the origin. Seing $\Pi_2(\mu)$ as a measure on $\mathbb{R}^p$ supported on the sphere, it holds by construction $h(\mu, \cdot) = h(\Pi_2(\mu), \cdot)$ for all $\mu \in \mathcal{P}_2(\mathbb{R}^p)$. Note that the restriction to *nonnegative* measures, which is not present in convex neural networks, does not change the expressivity of the model thanks to the assumption that ϕ is balanced in (A1).

2.3 Max-margins and functional norms

Given the training set $(x_i, y_i)_{i \in [n]}$, the margin of a predictor $f : \mathbb{R}^d \to \mathbb{R}$ is given by

$$\min_{i \in [n]} y_i f(x_i).$$

When the margin is strictly positive, the predictor makes no error on the training set and its value is typically seen as the worst confidence of the predictor. Max-margin predictors are predictors that maximize the margin over a certain set of functions. When this set of functions is given by a unit ball for a certain norm $\|\cdot\|$, they solve

$$\max_{\|f\| \leq 1} \min_{i \in [n]} y_i f(x_i).$$

In this paper we deal with two notions of norms, that in turn define two types of max-margin classifiers. We refer to Bach (2017a) for a more detailed presentation.

Variation norm. Given a feature function ϕ satisfying Assumption (A1), we consider the space $\mathcal{F}_1$ of functions that can be written as

$$f(x) = \int_{\mathbb{S}^{p-1}} \phi(\theta, x) \, \mathrm{d}\nu(\theta), \tag{4}$$

where $\nu \in \mathcal{M}_+(\mathbb{S}^{p-1})$ has finite mass (note that we could equivalently allow for signed measures thanks to the assumption that ϕ is balanced). The infimum of $\nu(\mathbb{S}^{p-1})$ over all such decompositions defines a norm $\|f\|_{\mathcal{F}_1}$, sometimes called the *variation norm* on $\mathcal{F}_1$ (Kurková and Sanguineti, 2001). The $\mathcal{F}_1$-max-margin of the training set is denoted γ_1 and given by

$$\gamma_1 \coloneqq \max_{\|f\|_{\mathcal{F}_1} \leq 1} \min_{i \in [n]} y_i f(x_i) = \max_{\substack{\nu \in \mathcal{M}_+(\mathbb{S}^{p-1}) \\ \nu(\mathbb{S}^{p-1}) \leq 1}} \min_{i \in [n]} y_i \int_{\mathbb{S}^{p-1}} \phi(\theta, x) \, \mathrm{d}\nu(\theta). \tag{5}$$

For ReLU networks, the variation norm defined above does not *a priori* coincide with the variation norm as defined by Bengio et al. (2006) and Bach (2017a). Indeed, in those references, the feature function is instead $\tilde{\phi}(\tilde{\theta}, x) = (a \cdot x + b)_+$ where $\tilde{\theta} = (a, b) \in \mathbb{R}^d \times \mathbb{R}$. Still, we show in Appendix B that in fact using ϕ or $\tilde{\phi}$ leads to norms which are equal up to a factor 2. The space $\mathcal{F}_1$ is described for ReLU networks in Savarese et al. (2019) for the univariate case and Ongie et al. (2019) for the multivariate case.

RKHS norm. Considering more specifically a two-layer neural network with activation function $\sigma : \mathbb{R} \to \mathbb{R}$, we can define another norm and function space, which leads to a reproducible kernel Hilbert space (RKHS). Let $\tau \in \mathcal{P}(\mathbb{S}^{p-1})$ be the uniform measure on the sphere $\mathbb{S}^{p-1}$ where $p = d + 1$ and define $\mathcal{F}_2$ as the space of functions of the form

$$f(x) = \int_{\mathbb{S}^{p-1}} \sigma(b + c^\top x) g(b, c) \, \mathrm{d}\tau(b, c),$$

for some square-integrable function $g \in L^2(\tau)$. The infimum of $\|g\|_{L^2(\tau)} = \left(\int |g(b,c)|^2 \, \mathrm{d}\tau(b,c)\right)^{\frac{1}{2}}$ over such decompositions defines a norm $\|f\|_{\mathcal{F}_2}$. It is shown by Bach (2017a) that $\mathcal{F}_2$ is a RKHS. The $\mathcal{F}_2$-max-margin of the training set is denoted γ_2 and given by

$$\gamma_2 := \max_{\|f\|_{\mathcal{F}_2} \leq 1} \min_{i \in [n]} y_i f(x_i) = \max_{\|g\|_{L^2(\tau)} \leq 1} \min_{i \in [n]} y_i \int_{\mathbb{S}^{p-1}} \sigma(b + c^\top x) g(b, c) \, \mathrm{d}\tau(b, c). \tag{6}$$

This is an unregularized kernel support vector machine problem.

Statistical and computational properties. In Section 6, we will show that the margin γ_1 can be large even in high dimension when the data set has hidden low dimensional structure, while the same is not known for γ_2. This leads to strong generalization guarantees for the $\mathcal{F}_1$-max-margin classifier. While $\mathcal{F}_2$-max-margin classifiers can be found with convex optimization techniques, it is not clear a priori how to efficiently find $\mathcal{F}_1$-max-margin classifiers. In this paper, we show that training an over-parameterized two-layer neural network precisely does that: it solves the $\mathcal{F}_1$-max-margin problem, as proved in the next section. In contrast, training only the output layer solves the $\mathcal{F}_2$-max-margin problem (Section 5).

2.4 Training dynamics in the infinite width limit

Assumptions. Given a loss function $\ell : \mathbb{R} \to \mathbb{R}_+$, we define the empirical risk associated to a predictor $h_m(\mathbf{w}, \cdot)$ of the form Eq. (1) as $\frac{1}{n} \sum_{i=1}^n \ell(-y_i h_m(\mathbf{w}, x_i))$. Our analysis of the training dynamics relies on the following assumptions for the loss:

(A2) The loss ℓ is differentiable with a locally Lipschitz-continuous gradient. It has an *exponential tail* in the sense that $\ell(u) \sim \ell'(u) \sim \exp(u)$ as $u \to -\infty$, and it is strictly increasing with $\ell'(u) \geq C > 0$ for $u \geq 0$.

The main examples are the logistic loss $\ell(u) = \log(1 + \exp(u))$ and exponential loss $\ell(u) = \exp(u)$. Note that for our main result Theorem 3.1, we do not need to assume convexity of the loss since only its tail behavior matters. We make the following assumptions on the feature function, in addition to (A1).

(A3) The family $(\phi(\cdot, x_i))_{i \in [n]}$ is free and for $i \in [n]$, the function $\phi(\cdot, x_i)$ is differentiable with a Lipschitz-continuous gradient and subanalytic.

Let us comment these assumptions. Requiring that the family is free is equivalent to requiring that arbitrary labels can be fitted on the training input $(x_i)_{i\in[n]}$ within our hypothesis class $\{x \mapsto \int \phi(\theta, x)\, \mathrm{d}\nu(\theta)\ ;\ \nu \in \mathcal{M}_+(\mathbb{S}^{p-1})\}$. This assumption is satisfied by ReLU and S-ReLU networks (Bach, 2017a) as soon as $x_i \neq x_{i'}$, $\forall i \neq i'$. The differentiability assumption is the most undesirable one because it excludes ReLU networks (but not S-ReLU networks). Although the training dynamic could potentially be defined without this assumption (Lyu and Li, 2019), the proof of Theorem 3.1 relies on it. Finally, subanalyticity is a mild assumption required in a technical proof step that invokes Sard's lemma. Functions defined by piecewise polynomials are subanalytic and thus both ReLU and S-ReLU networks satisfy it, see Bolte et al. (2006) for a definition.

Gradient flow of the smooth-margin objective. In order to obtain simpler proofs we consider maximizing minus the logarithm of the empirical risk, instead of the empirical risk itself. This allows to directly interpret the training dynamics as maximizing a *smooth-margin* and leads to the same continuous time dynamics up to time reparameterization. We define the function $S : \mathbb{R}^n \to \mathbb{R}$ as

$$S(u) = -\log\left(\frac{1}{n}\sum_{i=1}^{n} \ell(-u_i)\right). \tag{7}$$

When ℓ is the exponential, this function is known as the soft-min or the free energy and is concave (Mézard and Montanari, 2009). Notice however that for now we do not assume that ℓ is the exponential but only (A2), in order to cover the case of the logistic function.

With a model of the form Eq. (1), this leads to an objective function $F_m : (\mathbb{R}^p)^m \to \mathbb{R}$ on the vector of parameters $\mathbf{w} = (w_j)_{j\in[m]}$ defined as $F_m(\mathbf{w}) = S(\hat{h}_m(\mathbf{w}))$, where we have denoted $\hat{h}_m(\mathbf{w}) = (y_i\, h_m(\mathbf{w}, x_i))_{i\in[n]}$. We consider a (potentially random) initialization $\mathbf{w}(0) \in (\mathbb{R}^p)^m$ and the gradient flow of this objective function, which is a differentiable path $(\mathbf{w}(t))_{t\geq 0}$ starting from $\mathbf{w}(0)$ and such that for all $t \geq 0$,

$$\frac{d}{dt}\mathbf{w}(t) = m\nabla F_m(\mathbf{w}(t)). \tag{8}$$

Up to the gradient sign, this gradient flow is an approximation of gradient descent (Gautschi, 1997; Scieur et al., 2017) and stochastic gradient descent (SGD) (Kushner and Yin, 2003, Thm. 2.1) with small step sizes.[2] Classical results guarantee that under Assumption (A2), this gradient flow is uniquely well defined.

Wasserstein gradient flow. Taking the point of view presented in Section 2.2, we may interpret the training dynamics as a path $\mu_{t,m} = \frac{1}{m}\sum_{j=1}^{m} \delta_{w_j(t)}$ in $\mathcal{P}_2(\mathbb{R}^p)$. As we now explain, it turns out that this dynamics is a gradient flow for a function defined on $\mathcal{P}_2(\mathbb{R}^p)$, which allows to seamlessly take the limit $m \to \infty$. Let F be the functional on $\mathcal{P}_2(\mathbb{R}^p)$ be defined as

$$F(\mu) = S(\hat{h}(\mu)),$$

where similarly as above we define $\hat{h} : \mathcal{P}_2(\mathbb{R}^p) \to \mathbb{R}^n$ as $\hat{h}(\mu) = (y_i\, h(\mu, x_i))_{i\in[n]}$, and let F'_μ be its Fréchet derivative at μ, which is represented by the function $F'_\mu(w) = \sum_{i=1}^{n} y_i \phi(w, x_i) \nabla_i S(\hat{h}(\mu))$. Let us give a definition of Wasserstein gradient flow (tailored to our smooth setting), which will be connected to the training dynamics of Eq. (8) in Theorem 2.2.

[2] Although Theorem 3.1 below could be extended to discrete time analysis, this would be of little interest since the result is so far purely qualitative. In simpler settings, we study discrete time dynamics in Sections 4 and 5.

Definition 2.1 (Wasserstein gradient flow). *A Wasserstein gradient flow for the functional F is a path $(\mu_t)_{t\geq 0}$ such that there exists a flow $X : \mathbb{R}_+ \times \mathbb{R}^p \to \mathbb{R}^p$ satisfying $\mu_t = (X_t)_{\#}\mu_0$ (where $X_t(\cdot) = X(t, \cdot)$), $X(0, \cdot) = X_0 = \mathrm{id}_{\mathbb{R}^p}$ and for all $(t, w) \in \mathbb{R}_+ \times \mathbb{R}^p$,*

$$\frac{d}{dt}X(t, w) = \nabla F'_{\mu_t}(X(t, w)). \tag{9}$$

It can be directly checked that when μ_0 is discrete, we recover the training dynamics defined in Eq. (8). In this case, $X(t, w_j(0))$ represents the position (in parameter space) at time t of the hidden unit initialized with parameters $w_j(0)$. The following theorem shows that Wasserstein gradient flows characterize the training dynamics of infinitely wide two-layer neural networks. It is an application of Chizat and Bach (2018, Thm. 2.6), see details in Appendix C (hereafter, by convergence in $\mathcal{P}_2$, we mean convergence in the 2-Wasserstein distance, which is equivalent to weak convergence and convergence of the second-order moments (Ambrosio et al., 2008)).

Theorem 2.2 (Infinite width limit of training). *Under Assumptions* (A1-3)*, assume that the sequence $(w_j(0))_{j\in\mathbb{N}_*}$ is such that $\mu_{0,m}$ converges in $\mathcal{P}_2(\mathbb{R}^p)$ to μ_0. Then $\mu_{t,m}$ converges in $\mathcal{P}_2(\mathbb{R}^p)$ to the unique Wasserstein gradient flow of F starting from μ_0. The convergence is uniform on bounded time intervals.*

This limit can be made quantitative using the geodesic convexity estimates of Chizat and Bach (2018), and the general stability results of Ambrosio et al. (2008, Thm. 11.2.1) but with an exponential dependency in time. In the different setting of the square loss, error estimates for SGD have been derived by Mei et al. (2018, 2019). This limit dynamics covers, but is not limited to, the lazy training dynamics studied by Li and Liang (2018); Jacot et al. (2018); Du et al. (2019) which, in our present context, corresponds to a short time analysis when the initialization has a large variance (see Figure 3 in Section 7).

3 Main result: implicit bias of gradient flow

We are in position to state the main theorem of this paper, which characterizes the implicit bias of training infinitely wide two-layer neural networks with a loss with an exponential tail.

Theorem 3.1 (Implicit bias). *Under* (A1-3)*, assume that $\Pi_2(\mu_0)$ has full support on $\mathbb{S}^{p-1}$. If $\nabla S(h(\mu_t))$ converges and $\bar{\nu}_t = \Pi_2(\mu_t)/([\Pi_2(\mu_t)](\mathbb{S}^{p-1}))$ converges weakly, then the limit $\bar{\nu}_\infty$ is a maximizer for the $\mathcal{F}_1$-max-margin problem in Eq. (5).*

We can make the following observations:

- The strength of this result is that the limit $\bar{\nu}_\infty$ of a *non-convex* dynamics is a *global* minimizer of Eq. (5). Its proof relies, among other things, on a compatibility between the optimality conditions and the dynamics of neurons' directions, which is very specific to the 2-homogeneous case. Indeed, the optimality conditions for Eq. (5) involve a Lagrange multiplier $\psi \in \mathcal{C}^1(\mathbb{S}^{p-1})$ such that any optimizer $\nu^* \in \mathcal{M}_+(\mathbb{S}^{p-1})$ is concentrated on $\arg\max \psi$. Asymptotically, the velocity of the neurons' directions is proportional to $\nabla\psi$, which vanishes when ν^* is concentrated on $\arg\max \psi$, hence the compatibility.

- Both $p(t)$ and $\bar{\nu}_t$ leave in compact spaces so the assumption that they converge is not unreasonable. However, it is an open question to actually prove that it converges in this setting. Note that we are in a situation where the global convergence result from Chizat and Bach (2018) (which has a similar assumption regarding the existence of a limit) does not apply because here the unnormalized measure ν_t does *not* converge.

- Unlike in the convex case (Soudry et al., 2018), the dynamics does not completely forget where it started from, as bad initialization may lead to convergence to a point which is not a global minimizer. One could for instance think of a gradient flow initialized with a Dirac measure: it converges to a Dirac measure, which is generally not a minimizer.

Combining Theorem 3.1 with Theorem 2.2 gives the following asymptotic property about the training of finite width neural networks.

Corollary 3.2. *Under the assumptions of Theorem 3.1, assume that the sequence $(w_j(0))_{j\in\mathbb{N}_*}$ is such that $\mu_{0,m}$ converges in $\mathcal{P}_2(\mathbb{R}^p)$ to μ_0. Then, denoting $\bar{\nu}_{m,t} = \Pi_2(\mu_{m,t})/[\Pi_2(\mu_{m,t})](\mathbb{S}^{p-1})$, it holds*

$$\lim_{m,t\to\infty} \left(\min_{i\in[n]} y_i \int \phi(\theta, x_i) \, \mathrm{d}\bar{\nu}_{m,t} \right) = \gamma_1.$$

Typically, the sequence of initial neurons parameters $(w_j(0))_{j\in\mathbb{N}_*}$ are samples from a measure μ_0 that satisfies the support condition of Theorem 3.1, such as a Gaussian distribution. Note that limits in t and m can be interchanged so the convergence is not conditioned on a particular scaling.

Following Bach (2017a), convex optimization algorithms on the space of measures, such as conditional gradient algorithms, could be used to solve Eq. (5). These algorithms incrementally build the optimal measure by combining Dirac measures, but in order to find the location of these Dirac measures, they require access to oracles which cannot be computed easily. Our gradient-based algorithm instead starts with a large number of these Dirac measures and optimize directly their locations, which is a non-convex optimization problem.

4 Insights on the convergence rate and choice of step-size

While making Corollary 3.2 quantitative in terms of number of neurons and the number of iterations is left as an open question, it is important to gain hints about what are good choices of step-size and initialization. In this section, we look at a simplified dynamics where the direction of each parameter $w_j(t)$ is fixed after initialization and only its magnitude evolves. It can be seen that the proof of Theorem 3.1 still applies but in fact a complete discrete-time analysis is possible in this case, using tools from convex analysis.

We thus consider a model of the form of Eq. (1) but with $w_j(t)$ written as $r_j(t)\theta_j$, where $r_j(t) \in \mathbb{R}_+$ is trained and $\theta_j \in \mathbb{S}^{p-1}$ is fixed at initialization. Plugging this model into the soft-min loss (7) yields an objective function $F_m : \mathbb{R}_+^m \to \mathbb{R}$ defined as

$$F_m(r) = -\log\left(\frac{1}{n} \sum_{i=1}^{n} \exp\left(-\frac{1}{m} \sum_{j=1}^{m} z_{i,j} r_j^2 \right) \right),$$

where $z_{i,j} = y_i \phi(\theta_j, x_i)$ are the signed fixed features. We focus on the exponential loss $\ell = \exp$ in this section (and the next one) for simplicity. We study the gradient ascent dynamics with initialization $r(0) \in \mathbb{R}_+^m$ and sequence of step-sizes $(\eta(t))_{t\in\mathbb{N}}$,

$$r(t+1) = r(t) + \eta(t) m \nabla F_m(r(t)).$$

This dynamics is studied by Gunasekar et al. (2018a) where it is shown to converge to a max ℓ_1-margin classifier under certain conditions. In the next proposition, we prove a convergence rate, by exploiting an analogy with online mirror ascent.

Proposition 4.1. *Let $a_j(t) = r_j(t)^2/m$ for $j \in [m]$, $\beta(t) = \|a(t)\|_1$ and $\bar{a}(t) = a(t)/\beta(t)$. For the step-sizes $\eta(t) = 1/(16\|z\|_\infty \sqrt{t+1})$ and a uniform initialization $z(0) \propto \mathbf{1}$, it holds*

$$\max_{0\le s\le t-1} \min_{i\in[n]} z_i^\top \bar{a}(s) \ge \gamma_1^{(m)} - \frac{\|z\|_\infty}{\sqrt{t}} (8\log(m) + \log(t) + 1) - \frac{4B\log n}{\sqrt{t}}.$$

where $\gamma_1^{(m)} := \max_{a \in \Delta^{m-1}} \min_{i \in [n]} z_i^\top a$ *and* $B := \sum_{s=0}^\infty \frac{1}{\beta(s)\sqrt{s+1}} < \infty$ *when* $\gamma_1^{(m)} > 0$.

This proposition shows convergence of the best iterate to maximizers at an asymptotic rate in $O(\log(t)/\sqrt{t})$. In the proof of Lemma E.2, it can be seen that our bound on B depends on $\gamma_1^{(m)}$ and grows to ∞ as $\gamma_1^{(m)}$ goes to zero.

Proof idea. To prove Proposition 4.1, we consider the family of *smooth-margin* functions

$$G_\beta(a) = -\frac{1}{\beta} \log \left(\frac{1}{n} \sum_{i=1}^n \exp \left(-\beta \sum_{j=1}^m z_{i,j} a_j \right) \right),$$

and we show that $\bar{a}(t)$ approximately follows *online mirror ascent* for the sequence of concave functions $G_{\beta(t)}$ in the simplex Δ^{m-1} with step-sizes $\eta(t)$. It then only remains to apply classical bounds for mirror descent and use the fact that $|\min_{i \in [n]} z_i^\top a - G_\beta(a)| \leq \log(n)/\beta$. This algorithm thus implicitly perform online optimization on the regularization path. It is also analogous to smoothing techniques in non-smooth optimization (Nesterov, 2005).

Continuous limit. Using the notations from Section 2, the dynamics $\sum_{j=1}^m \bar{a}_j(t) \delta_{\theta_j}$ solves

$$\gamma_1^{(m)} := \max_{\substack{\nu \in \mathcal{M}_+(\mathbb{S}^{p-1}) \\ \nu(\mathbb{S}^{p-1}) \leq 1}} \min_{i \in [n]} y_i \int_{\mathbb{S}^{p-1}} \phi(\theta, x_i) \, \mathrm{d}\nu(\theta) \quad \text{subject to} \quad \nu \text{ supported on } \{\theta_j\}_{j \in [m]}.$$

When $\frac{1}{m} \sum_{j=1}^m \delta_{\theta_j}$ converges to the uniform measure on the sphere, we thus recover the same implicit bias as in Theorem 3.1 and $\gamma_1^{(m)} \to \gamma_1$ (note that the logarithmic dependency in m in Proposition 4.1 is not an obstruction and could be removed with a slightly finer analysis as done by Chizat (2019)). While functions in $\mathcal{F}_1$ may be well-approximated with a small number of neurons (Bach, 2017a), this is not anymore true if the positions $\{\theta_j\}_{j \in [m]}$ of those neurons are fixed a priori (see Barron (1993) for exponential lower bounds in a similar setting). In Theorem 3.1, positions are allowed to vary during training: this is what makes its setting more challenging but also much more relevant.

5 Training only the output layer

For two-layer neural networks, it is instructive to compare the implicit bias of training both layers (as in Section 3) versus that of training only the output layer, the input layer being initialized randomly and fixed. Plugging this model into the soft-min loss yields an objective function $F : \mathbb{R}^m \to \mathbb{R}$ defined as

$$F(r) = -\log \left(\frac{1}{n} \sum_{i=1}^n \exp \left(-\frac{1}{m} \sum_{j=1}^m z_{i,j} r_j \right) \right),$$

where $z_{i,j} = y_i \sigma(b_j + x_i^\top c_j)$ is the signed output of neuron j for the training point i and $\sigma : \mathbb{R} \to \mathbb{R}$ is the non-linearity, e.g., $\sigma(u) = \max\{0, u\}$ for ReLU networks. We study the gradient ascent dynamics with initialization $r(0) \in \mathbb{R}^m$ and sequence of step-sizes $(\eta(t))_{t \in \mathbb{N}}$:

$$r(t+t) = r(t) + \eta(t) m \nabla F(r(t)).$$

Soudry et al. (2018) show that for a step-size of order $1/\sqrt{t}$, this dynamics converges in $O(\log(t)/\sqrt{t})$ to a max ℓ_2-margin classifier. In the following proposition, we show that it converges in $O(1/\sqrt{t})$ for much larger step-sizes, with a different proof technique. The fact that the algorithm converges at essentially the same speed for very different step-sizes shows an advantageous self-regularizing property.

Proposition 5.1. *Let* $a(t) = r(t)/m$, $\beta(t) = \max\{1, \max_{0\le s\le t}\sqrt{m}\|a(t)\|_2\}$ *and* $\bar{a}(t) = a(t)/\beta(t)$. *Assume that* $\gamma_2^{(m)} := \max_{\sqrt{m}\|a\|_2\le 1}\min_{i\in[n]} z_i^\top a > 0$. *For the step-sizes* $\eta(t) = \beta(t)\sqrt{2}/(\|z\|_\infty\sqrt{t+1})$ *and initialization* $r(0) = 0$, *it holds*

$$\max_{0\le s\le t-1}\min_{i\in[n]} z_i^\top \bar{a}(s) \ge \gamma_2^{(m)} - \frac{\|z\|_\infty}{\sqrt{t}}\left(2\sqrt{2} + \frac{\sqrt{3}\log n}{\gamma_2^{(m)}}\right).$$

Proof idea. Similarly than in the proof of Proposition 4.1, we show that $\bar{a}(t)$ follows an *online projected gradient ascent* for the sequence of functions $G_{\beta(t)}$ in the ball $\{a \in \mathbb{R}^m \ ; \ \|a\|_2 \le 1/\sqrt{m}\}$ and with step-sizes $\eta(t)/(m\beta(t))$. From there, we use standard optimization results and prove that $\beta(t) \to \infty$ to conclude. Note that a different reduction to mirror descent for this dynamics was also exhibited by Ji and Telgarsky (2019b) and used to derive tight convergence rates but with a much smaller step-size than in Proposition 5.1 and with a different Bregman divergence.

Random features for kernel max-margin classifier. Using the notations from Section 2, the dynamics $(r_j)_{j\in[m]}$ converges to a solution to

$$\gamma_2^{(m)} = \max_{g\in L^2(\tau_m)}\min_{i\in[n]} y_i \int g(b,c)\sigma(b + x_i^\top c)\,\mathrm{d}\tau_m(b,c) \quad \text{subject to} \quad \|g\|_{L^2(d\tau_m)} \le 1,$$

where $\tau_m = \frac{1}{m}\sum_{j=1}^m \delta_{(b_j,c_j)}$. Typically, the input layer parameters are sampled from a distribution $\tau \in \mathbb{R}^{1+d}$, which corresponds to a random feature approximation for the $\mathcal{F}_2$-max-margin problem of Eq. (6) and we have $\gamma_2^{(m)} \to \gamma_2$. In stark contrast to the space $\mathcal{F}_1$, functions in $\mathcal{F}_2$ can be well approximated with a few number of random features even in high dimension. See Rahimi and Recht (2008); Bach (2017b) for a analysis of the number of features needed for an approximation with error ε, typically of order $1/\varepsilon^2$.

6 Dimension independent generalization bounds

In this section, we give arguments showing the favorable statistical properties of the bias exhibited in Theorem 3.1 for ReLU networks. We propose to measure the complexity of the dataset $S_n = (x_i, y_i)_{i=1}^n$ with the following *projected interclass distance* defined, for $r \in [d]$, as

$$\Delta_r(S_n) := \sup_P \left\{ \inf_{y_i\neq y_{i'}} \|P(x_i) - P(x_{i'})\|_2 \ ; \ P \text{ is a rank-}r \text{ projection} \right\}. \tag{10}$$

For each dimension r, it looks for the r-dimensional subspace which maximizes the distance between the two classes. Interclass distance often appears in the statistical analysis of classification problems (see, e.g., Li and Liang, 2018) often complemented with "clustered data" assumptions. Our definition is designed to capture the fact that if $\Delta_r \approx \Delta_d$ for $r \ll d$, then there is a hidden structure which can be exploited for statistical efficiency. We first lower-bound the margins γ_1 and γ_2 on the training data S_n using this quantity.

Lemma 6.1. *Assume that* $\|x_i\|_2 \le R$ *for* $i \in [n]$. *For any* $\epsilon \in (0,1)$ *and* $r \in [d]$, *there exists* $C(r), C_\epsilon(r) > 0$ *such that*

$$\gamma_2 \ge \min\left\{C(d), C_\epsilon(d)\left(\frac{\Delta_d(S_n)}{R}\right)^{\frac{d+3}{2-\epsilon}}\right\} \quad \textit{and} \quad \gamma_1 \ge \min_{r\in[d]}\min\left\{C(r), C_\epsilon(r)\left(\frac{\Delta_r(S_n)}{R}\right)^{\frac{r+3}{2-\epsilon}}\right\}.$$

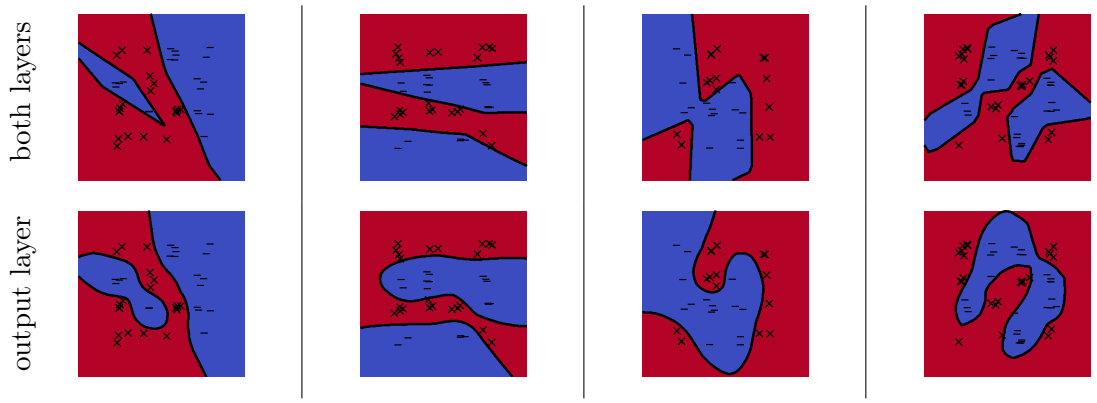


Figure 1: Comparison of the implicit bias of training (top) both layers versus (bottom) the output layer for ReLU networks with $d = 2$ and for 4 different random training sets.

We then apply margin-based generalization bounds (Koltchinskii and Panchenko, 2002) and bounds on the Rademacher complexity of the unit ball in $\mathcal{F}_1$ to get dimension independent guarantees.

Theorem 6.2 (Generalization bound)**.** *For any $\epsilon \in (0,1)$ and $r \in [d]$, there exist $C(r), C_\epsilon(r) > 0$ such that the following holds. If $(x,y) \sim \mathbb{P}$ is such that for some $R > 0$ and $0 < \Delta_r(\mathbb{P}) \leq C(r)$, it holds $\Delta_r(S_n) \leq \Delta_r(\mathbb{P})$ and $\|x\|_2 \leq R$ almost surely, then it holds with probability at least $1-\delta$ over the choice of i.i.d. samples $S_n = (x_i, y_i)_{i=1}^n$, for f the $\mathcal{F}_1$-max-margin classifier on S_n,*

$$\mathbb{P}[yf(x) < 0] \leq \frac{C_\epsilon(r)}{\sqrt{n}} \left(\frac{R}{\Delta_r(\mathbb{P})} \right)^{\frac{r+3}{2-\epsilon}} + \sqrt{\frac{\log(B)}{n}} + \sqrt{\frac{\log(1/\delta)}{2n}}.$$

where $B = \log_2(4(R+1)C_2(r)) + (r+2)\log_2(R/\Delta_r(\mathbb{P}))$. The same bound applies to the $\mathcal{F}_2$-max-margin classifier for $r = d$.

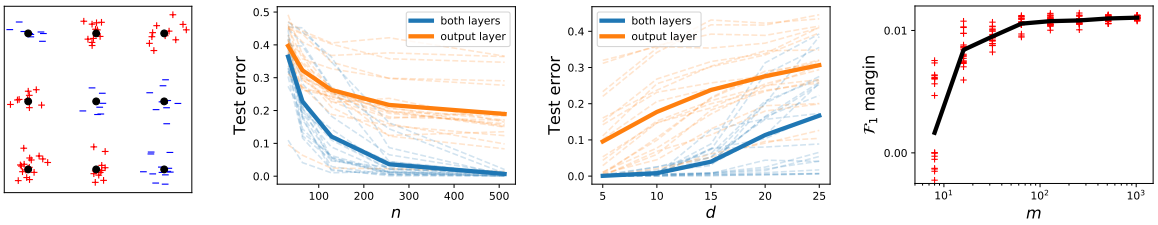
The strength of this generalization bound is that d does not appear in the exponent of the first term for the $\mathcal{F}_1$-max-margin classifier. Related generalization bounds are given by Wei et al. (2019), where a factor d improvement for the $\mathcal{F}_1$ versus $\mathcal{F}_2$-max-margin classifier is shown on a specific example. Also Montanari et al. (2019) prove high-dimensional generalization bounds for linear max-margin classifiers.

7 Numerical experiments

In this section, we consider a large ReLU network with $m = 1000$ hidden units, and compare the implicit bias and statistical performances of training both layers – which leads to a max margin classifier in $\mathcal{F}_1$ – versus the output layer – which leads to max margin classifier in $\mathcal{F}_2$. All the experiments are reproducible with the Julia code that can be found online[3].

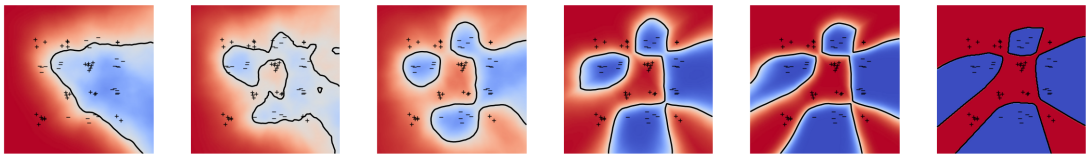
Setting. Our data distribution is supported on $[-1/2, 1/2]^d$ and is generated as follows. In dimension $d = 2$, the distribution of input variables is a mixture of k^2 uniform distributions on disks of radius $1/(3k-1)$ on a uniform 2-dimensional grid with step $3/(3k-1)$, see Figure 2(a) for an illustration with $k = 3$. In dimension larger than 2, all other coordinates follow a uniform distribution on $[-1/2, 1/2]$. Each cluster is then randomly assigned a class in $\{-1, +1\}$. For such distributions, the parameters appearing in Theorem 6.2 satisfy $\Delta(2) \geq 1/(3k-1)$ and $R \leq \sqrt{d}$.

[3] https://github.com/lchizat/2020-implicit-bias-wide-2NN



(a) Distribution (b) Test error vs. n (c) Test error vs. d (d) Margin vs. m

Figure 2: (a) Projection of the data distribution on the two first dimensions, (b) test error as a function of n (with $d = 15$, $k = 3$), (c) test error as a function of d (with $n = 256$, $k = 3$) (d) $\mathcal{F}_1$-margin at convergence as a function of m when training both layers ($n = 256$, $d = 15$, $k = 3$).



(a) $t = 100$ (b) $t = 500$ (c) $t = 5000$ (d) $t = 35000$ (e) $t = 65000$ (f) $t = 300000$

Figure 3: Dynamics of the classifier while training both layers. Since the initialization has a large variance and the initial step-size is small, the classifier first approaches the max-margin classifier for the *tangent kernel* (Jacot et al., 2018) (snapshot 3). It eventually converges to the $\mathcal{F}_1$-max-margin (snapshot 6).

Low dimensional illustrations. Figure 1 illustrates the differences in the implicit biases when $d = 2$. It represents a sampled training set and the resulting decision boundary between the two classes for 4 examples. We can see that the max-margin classifier in $\mathcal{F}_1$ is non-smooth and piecewise affine. This is explained by the fact that the mass constraint in Eq.(5) favors sparse solutions. In contrast, the max-margin classifier in $\mathcal{F}_2$ has a smooth decision boundary, which is a classical property of learning in a RKHS.

Performance. In higher dimensions, we observe the superiority of training both layers by plotting the test error versus m or d on Figure 2(b) and 2(c). We ran 20 independent experiments and show with a thick line the average of the test error $\mathbb{P}(yf(x) < 0)$ after training. Note that R grows as $\sqrt{d}$ so the dependency in d observed in Figure 2(c) is not in contradiction with Theorem 6.2. Finally, Figure 2(d) illustrates Corollary 3.2 and shows the $\mathcal{F}_1$-margin after training both layers. For each m, we ran 30 experiments using fresh random samples from the same data distribution. As for the convergence speed of the training dynamics, numerical experiments are carried out in Lyu and Li (2019); Nacson et al. (2019b).

Two implicit biases in one dynamics. In Figure 3, we illustrate for $d = 2$ a case where *two* different kinds of implicit biases show up in a single dynamics (t is the number of iterations with a constant step-size). We initialize the ReLU network with a large variance ($\mathcal{N}(0, 40^2)$). The model is at first in the *lazy regime* (Chizat et al., 2019) and follows closely the dynamics of its linearization around initialization, which converges to the max-margin classifier for the *tangent kernel* (Jacot et al., 2018). It then converges to the $\mathcal{F}_1$-max-margin classifier as suggested by Theorem 3.1. Note that to observe this intermediate implicit bias, one needs an initial step-size inversely proportional to the scale of the initialization (Chizat et al., 2019).

8 Conclusion

We have shown that for wide two-layer ReLU-like neural networks, training both layers or only the output layer leads to very different implicit biases. When training both layers, the classifier converges to a max-margin classifier for a non-Hilbertian norm, which enjoys favorable statistical properties. Interestingly, this problem does not seem to be directly solvable with known convex methods in high dimension. Proving complexity guarantees for this non-convex gradient flow is an important open question for future work. In particular, even for infinite width, continuous time dynamics as in Theorem 3.1, it is still unknown whether a convergence rate can be given under reasonable conditions.

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A Organization of the appendix

- In Appendix B, we prove the equivalence between our definition of the variation norm in Section 2.3 with the one that is used in the literature on convex neural networks.
- In Appendix C, we give alternative formulae for our Wasserstein gradient flow and justify Theorem 2.2.
- In Appendix D, we prove our main theorem Theorem 3.1 and its corollary.
- In Appendix E, we prove Proposition 4.1 about the convergence rates when fixing the "positions" of the neurons.
- In Appendix F, we prove Proposition 5.1 about the convergence rate when only training the output layer.
- In Appendix G, we prove the bounds on the margin and generalization performance (Theorem 6.2).

B Equivalence of two variation norms

Let us introduce, for ReLU networks, the variation norm introduced in Section 2.3 and the different definition from the literature (Bengio et al., 2006; Bach, 2017a). We will show that they are equal up to a factor 2. We stress that the analogous equivalence would fail for the RKHS norms, i.e., such simple modification of the feature function could lead to different functional spaces.

Consider the feature functions $\phi(\theta, z) = c(a \cdot z)_+$ where $\theta = (a, c) \in \mathbb{S}^{p-1}$ and $z = (x, 1)$ (here we see $\mathbb{S}^{p-1}$ as a subset of $\mathbb{R}^{p-1} \times \mathbb{R}$) and $\tilde{\phi}(a, z) = (a \cdot z)_+$ where $a \in \mathbb{S}^{p-2}$. For a function $f : \mathbb{S}^{p-2} \to \mathbb{R}$, we consider two norms

$$\|f\|_{\mathcal{F}_1} = \inf \left\{ \nu(\mathbb{S}^{p-1}) \; ; \; f(z) = \int \phi(\theta, z) \, \mathrm{d}\nu(\theta), \; \nu \in \mathcal{M}_+(\mathbb{S}^{p-1}) \right\}$$

and

$$\|f\|_{\tilde{\mathcal{F}}_1} = \inf \left\{ |\tilde{\nu}|(\mathbb{S}^{p-2}) \; ; \; f(z) = \int \tilde{\phi}(a, z) \, \mathrm{d}\tilde{\nu}(a), \; \nu \in \mathcal{M}(\mathbb{S}^{p-2}) \right\},$$

and the associated functional spaces $\mathcal{F}_1$ and $\tilde{\mathcal{F}}_1$ where these two norms are finite. Classical weak compactness arguments guarantee that the infimum defining these two norms is attained.

Proposition B.1. *It holds $\mathcal{F}_1 = \tilde{\mathcal{F}}_1$ and for all $f \in \mathcal{F}_1$, it holds $\|f\|_{\mathcal{F}_1} = 2\|f\|_{\tilde{\mathcal{F}}_1}$. Moreover, any measure that reaches the infimum for $\|\cdot\|_{\mathcal{F}_1}$ is concentrated on the set*

$$\left\{ (a, c) \in \mathbb{R}^{p-1} \times \mathbb{R} \; ; \; \|a\| = |c| = 1/\sqrt{2} \right\}.$$

An interesting consequence of this result is that empirical risk minimization with the commonly used *weight decay* regularization and the total variation regularization used by Bach (2017a) (the path-norm) are equivalent.

Proof. We give a constructive proof where we explicitly build a minimizer for each norm given a minimizer for the other norm. Let us start with a measure $\nu \in \mathcal{M}_+(\mathbb{S}^{p-1})$ such that $f(x) = \int \phi(\theta, x) \, \mathrm{d}\mu(\theta)$. We define the linear operator $\Pi : \mathcal{M}_+(\mathbb{S}^{p-1}) \to \mathcal{M}(\mathbb{S}^{p-2})$ where $\Pi(\nu)$ is characterized by

$$\int \varphi \, \mathrm{d}\Pi(\nu) = \int c\|a\| \varphi(a/\|a\|) \, \mathrm{d}\nu((a, c)),$$

where, as usual, the integrand is extended by continuity at $a = 0$. By construction, it holds $\forall z \in \mathbb{R}^{p-2}$,

$$\int \tilde{\phi}(a, z) \, \mathrm{d}\Pi(\nu)(a) = \int c\|a\| \tilde{\phi}(a/\|a\|, z) \, \mathrm{d}\nu((a, c)) = \int \phi((a, c), z) \, \mathrm{d}\nu((a, c)) = f(z).$$

As for the total variation norm $\|\Pi(\nu)\| := |\Pi(\nu)|(\mathbb{S}^{p-2})$ of $\Pi(\nu)$, it can be bounded as follows. In the definition of $\Pi(\nu)$, we may restrict the integral over $\{c > 0\}$, which defines a measure $\Pi_+(\nu) \in \mathcal{M}_+(\mathbb{S}^{p-2})$. Similarly restricting the integral over $\{c < 0\}$ an taking the opposite gives another measure $\Pi_-(\nu) \in \mathcal{M}_+(\mathbb{S}^{p-2})$. It holds $\Pi(\nu) = \Pi_+(\nu) - \Pi_-(\nu)$ and thus $\|\Pi(\nu)\| \leq \|\Pi_+(\nu)\| + \|\Pi_-(\nu)\|$. Moreover, by integrating against $\varphi = 1$, it holds

$$\|\Pi_+(\nu)\| = \int 1 \, \mathrm{d}\Pi_+(\nu) = \int_{c>0} c\|a\| \, \mathrm{d}\nu((a, c)) \leq \frac{1}{2} \int_{c>0} \mathrm{d}\nu((a, c)),$$

since $c\|a\| \leq (\|a\|^2 + c^2)/2 = 1/2$ for $(a, c) \in \mathbb{S}^{p-1}$. Using a similar bound for $\|\Pi_-(\nu)\|$, we get that

$$\|\Pi(\nu)\| \leq \frac{1}{2} \int_{c>0} \mathrm{d}\nu((a, c)) + \frac{1}{2} \int_{c<0} \mathrm{d}\nu((a, c)) \leq \frac{1}{2}\nu(\mathbb{S}^{p-1}).$$

Finally, tracking the equality cases, it holds $\|\Pi(\nu)\| = \frac{1}{2}\nu(\mathbb{S}^{p-1})$ if and only if ν is concentrated on the set given in Proposition B.1, which is the intersection of the sphere with the set of points satisfying $2|c|\|a\| = \|a\|^2 + |c|^2$.

Conversely, let $\nu \in \mathcal{M}(\mathbb{S}^{p-2})$ and consider its Jordan decomposition $\nu = \nu_+ - \nu_-$ into two nonnegative measures, which is such that $\|\nu\| = \|\nu_+\| + \|\nu_-\|$. We define two maps $T^+, T^- : \mathbb{S}^{p-2} \to \mathbb{S}^{p-1}$ as $T^+(a) = (a, 1)/\sqrt{2}$ and $T^-(a) = (a, -1)/\sqrt{2}$. Now, define the linear map $T : \mathcal{M}(\mathbb{S}^{p-2}) \to \mathcal{M}_+(\mathcal{S}^{p-1})$ as

$$T(\nu) = 2(T^+_\# \nu_+ + T^-_\# \nu_-).$$

Clearly, since pushforwards preserve the mass of nonnegative measures, it holds $\|T(\nu)\| = 2(\|\nu_+\| + \|\nu_-\|) = 2\|\nu\|$. Moreover, using the definition of pushforward measures, we have

$$\begin{aligned}\int \phi(\theta, z) \, \mathrm{d}T(\nu)(\theta) &= 2 \int \phi((a, 1)/\sqrt{2}, z) \, \mathrm{d}\nu_+(a) + 2 \int \phi((a, -1)/\sqrt{2}, z) \, \mathrm{d}\nu_-(a) \\ &= \int \tilde{\phi}(a, z) \, \mathrm{d}\nu_+(a) - \int \tilde{\phi}(a, z) \, \mathrm{d}\nu_-(a) = \int \tilde{\phi}(a, z) \, \mathrm{d}\nu(a) = f(z).\end{aligned}$$

To sum up, for any feasible measure ν for the definition of $\|f\|_{\mathcal{F}_1}$, we have built a measure $\Pi(\nu)$ that is feasible for $\|f\|_{\tilde{\mathcal{F}}_1}$ with a norm divided by at most 2. Conversely, for any feasible measure ν for the definition of $\|f\|_{\tilde{\mathcal{F}}_1}$, we have built a measure $T(\nu)$ that is feasible for $\|f\|_{\mathcal{F}_1}$ with a norm multiplied exactly by 2. This concludes the proof. □

C Details on Wasserstein gradient flows

C.1 Alternative formulations of the Wasserstein gradient flow

- (Divergence form) It can be shown that a Wasserstein gradient flow as defined in Definition 2.1 satisfies, in the sense of distributions, the following partial differential equation (Ambrosio et al., 2008)

$$\partial_t \mu_t = -\mathrm{div}(\nabla F'_{\mu_t} \mu_t).$$

- (Projected representation) If we look at the projected trajectory $\nu_t = \Pi_2(\mu_t)$, it can be shown that it solves the following dynamic, which is known as Wasserstein-Fisher-Rao or Hellinger-Kantorovich gradient flow of the functional $J : \mathcal{M}_+(\mathbb{S}^{p-1})$ satisfying $J(\Pi_2(\mu)) = F(\mu)$. In equation,

$$\partial_t \nu_t = -\mathrm{div}(\nabla J'_{\nu_t} \nu_t) + 4 J'_{\nu_t} \nu_t, \tag{11}$$

  where $J'_\nu(\theta) = \sum_{i=1}^n \nabla_i S(\hat{h}(\nu)) y_i \phi(\theta, x_i)$ is defined on the sphere, see Chizat (2019). Note that there is also a Lagrangian representation for this projected dynamics (Maniglia, 2007) .

- (Renormalized dynamics) It can also be seen with a direct computation that the normalized dynamics $\bar{\nu}_t = \nu_t / \|\nu_t\|$ satisfies the following dynamics

$$\partial_t \bar{\nu}_t = -\mathrm{div}(\nabla J'_{\nu_t} \bar{\nu}_t) + 4 \left(J'_{\nu_t} - \int J'_{\nu_t} \, \mathrm{d}\bar{\nu}_t \right) \bar{\nu}_t. \tag{12}$$

  When the driving potential is $J'_{\bar{\nu}_t}$ (instead of J'_{ν_t}), this dynamics is known as the spherical Wasserstein-Fisher-Rao or spherical Hellinger Kantorovich gradient flow (Kondratyev and Vorotnikov, 2019) and was considered by Rotskoff et al. (2019) for neural networks training.

C.2 Proof of Theorem 2.2

We just need to prove that the assumptions of Chizat and Bach (2018, Theorem 2.6) are satisfied and justify that non-compactly supported initialization are also allowed.

Checking regularity assumptions. With the notations used by Chizat and Bach (2018, Assumptions 2.1), the Hilbert space $\mathcal{F}$ is $\mathbb{R}^n$, the domain "Ω" is $\mathbb{R}^p$, the risk "R" is the smooth-margin S, the function "Φ" is here $\Phi(\theta) = (y_i \phi(\theta, x_i))_{i \in [n]}$, there is no regularization, and the family of nested sets "Ω_r" are the closed balls of radius r in $\mathbb{R}^p$. We can directly check that

- under Assumption (A2), $S : \mathbb{R}^n \to \mathbb{R}$ is differentiable and its gradient given in coordinates by $\nabla_i S(u) = \ell'(-u_i)/(\sum_{i'} \ell(-u_{i'}))$ is Lipschitz continuous and bounded on sublevel sets;

- under Assumption (A3), the function Φ is differentiable with a locally Lipschitz continuous gradient. Moreover its gradient has at most a linear growth by 2-homogeneity (this verifies assumptions from Chizat and Bach (2018, Assumptions 2.1-(iii)-(c))).

Removing the compact support assumption. Chizat and Bach (2018, Theorem 2.6) only allow an initialization in some "Ω_r", which means here μ_0 should be compactly supported. However, when Φ is exactly 2-homogeneous, this condition can be relaxed (Chizat, 2019, Appendix C.1) because the dynamics is entirely characterized by its projection on the sphere (through Π_2). Indeed, for any $\mu \in \mathcal{P}_2(\mathbb{R}^p)$, there exists a compactly supported $\tilde{\mu} \in \mathcal{P}_2(\mathbb{R}^p)$ such that $\Pi_2(\mu) = \Pi_2(\tilde{\mu})$. Since we have existence and uniqueness for the Wasserstein gradient flow starting from $\tilde{\mu}$, we get existence and uniqueness from the Wasserstein gradient flow $(\mu_t)_t$ starting fom μ (since it is entirely determined by the velocity field $\nabla F'_{\mu_t}$ which is itself determined by the projection of the dynamics $\Pi_2(\mu_t)$. With similar arguments we can adapt the proof of Chizat and Bach (2018, Theorem 2.6) to any initialization $\mu \in \mathcal{P}_2(\mathbb{R}^p)$.

D Appendix to Section 3

D.1 Proof of the main theorem

Let us restate Theorem 3.1 and give its proof. We recall the notations $\nu_t := \Pi_2(\mu_t)$ and $\bar{\nu}_t := \nu_t/(\nu_t(\mathbb{S}^{p-1}))$.

Theorem D.1. *Under* (A1-3)*, assume that* $\Pi_2(\mu_0)$ *has full support on* $\mathbb{S}^{p-1}$*, that* $\nabla S(h(\mu_t))$ *converges and that* $\bar{\nu}_t$ *converges weakly towards* $\bar{\nu}_\infty$*. Then* $\bar{\nu}_\infty$ *is a maximizer of Eq.* (5)*.*

Proof. By Lemma D.5 the limit $p(\infty) \in \mathbb{R}^n$ of $p(t) := \nabla S(\hat{h}(\mu_t))$ is non-zero. This implies that J'_{ν_t} converges in $\mathcal{C}^1(\mathbb{S}^{p-1})$, to a function $J'_\infty : \theta \mapsto \sum_{i=1}^n p_i(\infty) y_i \phi(\theta, x_i)$ (defined on the sphere) which is non-zero because the family $(\phi(\cdot, x_1), \dots, \phi(\cdot, x_n))$ is free by (A3). Since ϕ is balanced by (A1), we get that $M := \max_{\theta \in \mathbb{S}^{p-1}} J'_\infty(\theta) > 0$. The rest of the proof is divided into 3 steps.

Step 1: mass grows unbounded. In a first step, we prove that $\nu_t(\mathbb{S}^{p-1}) \to \infty$. Assume that J'_∞ is not constant (the other case will be considered later), and let $v \in]0, M/8[$ be such that $m - v$ is a regular value of J'_∞, i.e., be such that $\|\nabla J'_\infty\|$ does not vanish on the $M - v$ level-set of J'_∞. Such a v is guaranteed to exist thanks to non-smooth versions of Morse-Sard's lemma (Bolte et al., 2006), and to our assumption that ϕ is subanalytic, which implies that J'_∞ also is subanalytic. Let $K_v = (J'_\infty)^{-1}([M - v, M]) \subset \mathbb{S}^{p-1}$ be the corresponding super-level set. By the regular value theorem, the boundary ∂K_v of K_v is a differentiable orientable compact submanifold of $\mathbb{S}^{p-1}$ and is orthogonal to $\nabla J'_\infty$. By construction, it holds for all $\theta \in K_v$, $J'_\infty(\theta) \geq M - v$ and, for some $u > 0$, by the regular value property, $\nabla J'_\infty(\theta) \cdot \vec{n}_\theta \geq u$ for all $\theta \in \partial K_v$ where $\vec{n}_\theta$ is the unit normal vector to ∂K_v at θ pointing inwards. Since J'_{ν_t} converges in $\mathcal{C}^1(\mathbb{S}^{p-1})$ towards J'_∞, there exists $t_0 > 0$ such that for all $t \geq t_0$, $\|J'_{\nu_t} - J'_\infty\|_{\mathcal{C}^1(\mathbb{S}^{p-1})} \leq \min\{v, u/2\}$ and thus

$$\forall \theta \in K_v, \quad J'_{\nu_t}(\theta) \geq m - 2v \qquad \text{and} \qquad \forall \theta \in \partial K_v, \quad \nabla J'_{\nu_t}(\theta) \cdot \vec{n}_\theta \geq u/2.$$

This second property guarantees that no mass leaves K_v due to the divergence term in Eq. (11) for $t \geq t_0$. Thus, taking into account the reaction/growth term in Eq. (11), it holds for $t \geq t_0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\nu_t(K_v) \geq 4 \int_{K_v} J'_{\nu_t} \,\mathrm{d}\nu_t \geq 4(M - 2v)\nu_t(K_v).$$

It follows by Grönwall's lemma that $\nu_t(K_v) \geq \exp(4(M - 2v)t)\nu_{t_0}(K_v)$ for $t \geq t_0$. One the other hand, ν_{t_0} has full support on $\mathbb{S}^{p-1}$ since it can be written as the pushforward of a rescaled version of ν_0 by a diffeomorphism, see Maniglia (2007, Eq. (1.3)) (this is the only place where the assumption on the support is needed). Thus $\nu_{t_0}(K_v) > 0$ and it follows that $\nu_t(\mathbb{S}^{p-1}) \to \infty$. To deal with the case where J'_∞ is constant equal to $M > 0$, we can directly take $K = \mathbb{S}^{p-1}$ to show that $\nu_t(\mathbb{S}^{p-1}) \to \infty$.

Step 2: complementary slackness (I). We now show that $\min_i \hat{h}_i \to \infty$. Using the property of gradient flows and previously established estimates, we have for $T > 0$,

$$F(\mu_T) - F(\mu_0) = \int_0^T \|\nabla F'_{\mu_t}\|^2 \,\mathrm{d}\mu_t \geq \int_{t_0}^T \int_{K_v} 4|J'_{\nu_t}|^2 \,\mathrm{d}\nu_t \,\mathrm{d}t \geq 4(M - 2v)^2 \int_{t_0}^T \nu_t(K_v) \,\mathrm{d}t \to \infty.$$

Thus $F(\mu_t) \to \infty$ which implies that for all $i \in [n]$, $\ell(-\hat{h}_i(\mu_t)) \to 0$ and thus $\hat{h}_i(\mu_t) \to \infty$. Applying Lemma D.6, it follows that $p_{i_0}(\infty) = 0$ for all $i_0 \in \arg\min_i \hat{h}_i(\nu_\infty)$.

Step 3: complementary slackness (II). We now show that $\bar{\nu}_\infty$ is concentrated on $(J'_\infty)^{-1}(M)$, where $\bar{\nu}_t = \nu_t/\|\nu_t\| \in \mathcal{P}(\mathbb{S}^{p-1})$ is the normalized path and $\bar{\nu}_\infty$ its limit. This is immediate if J'_∞ is constant. Otherwise, assuming that $M - 4v$ is also a regular value of J'_∞

and taking a potentially smaller u (which can always be achieved by perturbing v if needed), it holds for $t \geq t_0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\nu_t(\mathbb{S}^{p-1} \setminus K_{4v}) \leq 4 \int_{\mathbb{S}^{p-1}\setminus K_{4v}} J'_{\nu_t} \,\mathrm{d}\nu_t \leq 4(m-3v)\nu_t(K_{4v})$$

using the fact that no mass enters into $\mathbb{S}^{p-1} \setminus K_{4v}$ due to the divergence term in Eq. (11) for $t \geq t_0$. Comparing the rate of growth of the mass in K_v and in $\mathbb{S}^{p-1} \setminus K_{4v}$, we get that $\bar{\nu}_\infty(\mathbb{S}^{p-1} \setminus K_{4v}) \leq \lim_{t\to\infty} \bar{\nu}_t(\mathbb{S}^{p-1} \setminus K_{4v}) = 0$ since $\mathbb{S}^{p-1} \setminus K_{4v}$ is open and by the properties of weak convergence of measures (Portmanteau theorem). Since this holds for v arbitrarily close to 0, it follows that $\bar{\nu}_\infty$ is concentrated on $(J'_\infty)^{-1}(m)$.

Step 4: conclusion. Since we have proved the two complementary slackness properties, by Proposition D.3, the pair $(\bar{\nu}_\infty, p(\infty))$ satisfies the optimality conditions, which concludes the proof. □

D.2 Proof of Corollary 3.2

Corollary D.2. *Under the assumptions of Theorem 3.1, assume that the sequence $(w_j(0))_{j\in\mathbb{N}_*}$ is such that $\mu_{0,m}$ converges in $\mathcal{P}_2(\mathbb{R}^p)$ to μ_0. Then, denoting $\bar{\nu}_{m,t} = \Pi_2(\mu_{m,t})/[\Pi_2(\mu_{m,t})](\mathbb{S}^{p-1})$, it holds*

$$\lim_{m,t\to\infty} \left(\min_{i\in[n]} y_i \int \phi(\theta, x_i) \,\mathrm{d}\bar{\nu}_{m,t} \right) = \gamma_1.$$

Proof. The fact that

$$\lim_{t\to\infty} \lim_{m\to\infty} \left(\min_{i\in[n]} y_i \int \phi(\theta, x_i) \,\mathrm{d}\bar{\nu}_{m,t}(\theta) \right) = \gamma_1$$

is obtained by combining Theorem 2.2 with Theorem 3.1 because $\int \phi(\theta, \cdot)\bar{\nu}_{m,t}$ depends continuously on $\mu_{t,m}$ in $\mathcal{P}_2(\mathbb{R}^p)$, so we only need to prove that limits can be interchanged. We detail the proof for $\ell = \exp$, noticing that we only use the asymptotic behavior of ℓ and ℓ' so it extends to any loss satisfying (A2). Intuitively, in order to prove the other limit, we need to show that if for some (t_0, m_0) the classifier is close to the max-margin classifier, then this remains true for (t, m_0), $t \geq t_0$. First, for $\beta = \|\nu_t\| > 0$, it holds at time t

$$\frac{d}{dt} S_\beta(\hat{h}(\bar{\nu}_t)) = \int \|\nabla J'_{\nu_t}\|^2 \,\mathrm{d}\bar{\nu}_t + 4 \left(\int |J'_{\nu_t}|^2 \,\mathrm{d}\bar{\nu}_t - \left(\int |J'_{\nu_t}| \,\mathrm{d}\bar{\nu}_t \right)^2 \right) \geq 0.$$

On the other hand, direct computations using the fact that $\nabla S(u) \in \Delta^{n-1}$ leads to

$$\partial_\beta S_\beta(u) = -\frac{1}{\beta^2} \sum_{i=1}^n \nabla_i S(u) \log(n \nabla_i S(u)) \geq -\frac{n}{\beta^2}.$$

Combining both gives the total derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} S_{\|\nu_t\|}(\hat{h}(\bar{\nu}_t)) \geq -n \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{\|\nu_t\|} \right) \qquad \Rightarrow \qquad S_{\|\nu_t\|}(\hat{h}(\bar{\nu}_t)) \geq S_{\|\nu_{t_0}\|}(\hat{h}(\bar{\nu}_{t_0})) - \frac{n}{\|\nu_{t_0}\|}.$$

From the first limit above, for any $\epsilon > 0$, there exists (t_0, m_0) such that for all $m \geq m_0$, $\min_{i\in[n]} y_i \int \phi(\theta, x_i) \,\mathrm{d}\bar{\nu}_{m,t_0}(\theta) \geq \gamma_1 - \epsilon/3$. We have shown in the proof of Theorem 3.1 that $\|\nu_t\| \to \infty$ so choosing t_0 and m_0 potentially larger if needed, since $\|\nu_{t,m}\| \to \|\nu_t\|$ it also holds $\|\nu_{t_0,m}\| \geq 3n/\epsilon$ for $m \geq m_0$. By the inequality above, we thus have for all $t \geq t_0$ and $m \geq m_0$

$$S_{\|\bar{\nu}_{t,m}\|}(\hat{h}(\bar{\nu}_{t,m})) \geq S_{\|\bar{\nu}_{t_0,m}\|}(\hat{h}(\bar{\nu}_{t_0,m})) - \epsilon/3.$$

Moreover, by Lemma D.4, we have $|S_{\|\nu_t\|}(u) - \min_i u| \leq \epsilon/3$ for $\|\nu_t\|$ large enough, uniformly for u in a compact set. Hence for all $m \geq m_0$,

$$\lim_{t\to\infty} S_{\|\nu_{t,m}\|}(\hat{h}(\bar{\nu}_{t,m})) \geq S_{\|\nu_{t_0,m}\|}(\hat{h}(\bar{\nu}_{t_0,m})) - \epsilon/3 \geq \gamma_1 - \epsilon.$$

It remains to show that $\liminf_{t\to\infty} \|\nu_{t,m}\|$ is lower bounded by an arbitrarily large constant for m large enough, so that we deduce from the above

$$\lim_{t\to\infty} \min_{i\in[n]} \hat{h}(\bar{\nu}_{t,m}) \geq \gamma_1 - 2\epsilon.$$

Since ϵ is arbitrary, it would follow that $\lim_{m\to\infty} \lim_{t\to\infty} \min_{i\in[n]} \hat{h}(\bar{\nu}_{\infty,t}) \geq \gamma_1$ which is our claim.

To see this, it is sufficient to notice that since $F(\nu_t)$ is increasing and $S(u) - \log(n) \leq \min_i u$, we have that $\min \hat{h}(\nu_{t,m})$ is lower bounded by some constant which can be made arbitrarily large by taking t, m large enough, and thus the same holds for $\|\bar{\nu}_{t,m}\|$. □

D.3 Additional Lemmata

Proposition D.3 (Optimality conditions)**.** *The maximization problem (5) admits global maximizers $\nu^\star \in \mathcal{M}_+(\mathbb{S}^{p-1})$. Moreover, a measure $\nu^\star \in \mathcal{M}_+(\mathbb{S}^{p-1})$ is a global minimizer of (5) if and only if $\nu^\star \in \mathcal{P}(\mathbb{S}^{p-1})$ and there exists $p^\star \in \Delta^{n-1})$ such that (i) $\operatorname{spt} \nu^\star \subset \arg\max_\theta \sum_i p_i y_i \phi(\theta, x_i)$ and (ii) $\operatorname{spt} p \subset \arg\min_i y_i \int \phi(\theta, x_i) \, \mathrm{d}\nu^\star(\theta)$.*

Proof. By minimax duality (Sion, 1958), we can rewrite Eq (5) as the minimax problem

$$\sup_{\nu\in\mathcal{P}(\Theta)} \inf_{p\in\Delta^{n-1}} \sum_{i=1}^n p_i y_i \int \phi(\theta, x_i) \, \mathrm{d}\nu(\theta) = \inf_{p\in\Delta^{n-1}} \sup_{\nu\in\mathcal{P}(\Theta)} \sum_{i=1}^n p_i y_i \int \phi(\theta, x_i) \, \mathrm{d}\nu(\theta)$$

and it admits (at least) a saddle point $(\nu^\star, p^\star)$. Moreover, the optimality conditions are necessary and sufficient for the right-hand side to equal the left-hand side. □

We now prove useful properties of the soft-min function

$$S_\beta(u) = -\frac{1}{\beta} \log\left(\frac{1}{n}\sum_{i=1}^n \ell(-\beta u_i)\right), \tag{13}$$

which is a soft-min function under assumption (A2), as shown in the next lemma.

Lemma D.4. *If $\ell(u) \sim \exp(u)$ as $u \to \infty$, and if $\bar{u} \in (\mathbb{R}_+^*)^n$, then*

$$\lim_{\beta\to\infty} S_\beta(\bar{u}) = \min_{i\in[n]} \bar{u}.$$

Proof. Let $m \coloneqq \min_{i\in[n]} \bar{u}_i$. We have $\exp\left(-\beta\left(S_\beta(\bar{u}) - m\right)\right) = \frac{1}{n}\sum_{i=1}^n \ell(-\beta\bar{u}_i)\exp(\beta m)$, where each term satisfies, in the large β regime,

$$\ell(-\beta\bar{u}_i)\exp(\beta m) \sim \exp(-\beta(\bar{u}_i - m)) \to \begin{cases} 1 & \text{if } i \in \arg\min_i \bar{u}_i, \\ 0 & \text{otherwise.} \end{cases}$$

As a consequence, $\exp\left(-\beta\left(S_\beta(\bar{u}) - m\right)\right) \to \frac{1}{n}\#\arg\min_i \bar{u}_i \in]0, 1[$. Thus, $S_\beta(\bar{u}) \to m$. □

The next lemma is a technical result used in the proof of Theorem 3.1.

Lemma D.5. *Under Assumption (A2), let $u(t)$ be a sequence such that $S(u(t))$ is lower bounded and $\nabla S(u(t))$ converges. Then $\lim_{t\to\infty} \nabla S(u(t)) \neq 0$.*

Proof. We analyze separately two cases, whether there is $i_0 \in [n]$ such that $u_{i_0}(t)$ is upper bounded or not. In the first case, we have

$$\nabla_{i_0} S(u(t)) = \frac{\ell'(-u_{i_0}(t))}{\sum_i \ell(-u_i(t))} = \frac{1}{n} \ell'(-u_{i_0}(t)) \exp(S(u(t)))$$

which is uniformly lower bounded by a positive constant under (A2) and due to the lower bound on $S(u(t))$ hence $\lim_{t\to\infty} \nabla S_{i_0}(u(t)) \neq 0$. In the other case, up to taking a subsequence (which does not change the limit), we can assume that $u_i(t) \to \infty$ for all $i \in [n]$. Then using the equivalent of ℓ and ℓ' at $-\infty$, we have that $\lim_{t\to\infty} \sum_{i\in[n]} \nabla S(u(t)) = 1$ which is sufficient to conclude. □

The next lemma is adapted from Gunasekar et al. (2018a, Lemma 8) and exploits the fact that the gradient of S is a soft-argmax. It allows to recover part of the optimality conditions in the proof of Theorem 3.1.

Lemma D.6 (Convergence of soft-argmin)**.** *Let $\beta : \mathbb{R}_+ \to \mathbb{R}_+$ and $\bar{u} : \mathbb{R}_+ \to \mathbb{R}^n$ be such that $\beta(t) \to \infty$ and $\bar{u}(t) \to \bar{u}(\infty) \in (\mathbb{R}_+^*)^n$ as $t \to \infty$. If $\ell(-u) \sim \ell'(-u) \sim \exp(-u)$ as $u \to \infty$, then for any $i_0 \notin \arg\min_i \bar{u}_i(\infty)$, as $t \to \infty$, it holds $\nabla_{i_0} S_{\beta(t)}(\bar{u}(t)) \to 0$.*

Proof. Consider any $\gamma \in \,]\min_i \bar{u}_i(\infty), \bar{u}_{i_0}(\infty)[$.

$$\nabla_{i_0} S_{\beta(t)}(\bar{u}(t)) = \frac{\ell'(-\beta \bar{u}_{i_0}(t))}{\sum_{i=1}^n \ell(-\beta \bar{u}_i(t))} = \frac{\ell'(-\beta \bar{u}_{i_0}(t)) \exp(\beta\gamma)}{\sum_{i=1}^n \ell(-\beta \bar{u}_i(t)) \exp(\beta\gamma)}$$

By the assumption on ℓ', the numerator is equivalent to $\exp(-\beta(\bar{u}_{i_0}(t) - \gamma))$ and goes to 0 as $t \to \infty$. Also, by the assumption on ℓ, each of the term in the denominator is equivalent to $\exp(-\beta(\bar{u}_i(t) - \gamma))$ which goes to ∞ for $i \in \arg\min_i \bar{u}_i(\infty)$, hence the conclusion. □

E Appendix for Section 4

Let us define

$$G_\beta(a) = -\frac{1}{\beta} \log\left(\frac{1}{n} \sum_{i=1}^n \exp\left(-\beta \sum_{j=1}^m z_{i,j} a_j \right) \right),$$

which satisfies

$$\min_{i\in[n]} z_i^\top a \leq G_\beta(a) \leq \min_{i\in[n]} z_i^\top a + \frac{\log n}{\beta}. \tag{14}$$

Let us recall Proposition 4.1 and prove it.

Proposition E.1. *Let $a_j(t) = r_j(t)^2/m$ for $j \in [m]$, $\beta(t) = \|a(t)\|_1$ and $\bar{a}(t) = a(t)/\beta(t)$. For the step-sizes $\eta(t) = 1/(16\|z\|_\infty \sqrt{t+1})$ and a uniform initialization $z(0) \propto \mathbf{1}$, it holds*

$$\max_{0\leq s\leq t-1} \min_i z_i^\top \bar{a}(s) \geq \gamma_1^{(m)} - \frac{\|z\|_\infty}{\sqrt{t}} (8\log(m) + \log(t) + 1) - \frac{4\log n}{\sqrt{t}} \sum_{s=0}^{t-1} \frac{1}{\beta(s)\sqrt{s+1}}. \tag{15}$$

where $\gamma_1^{(m)} := \max_{a\in\Delta^{m-1}} \min_{i\in[n]} z_i^\top a$ and the last sum is uniformly bounded in t as soon as $\gamma_1^{(m)} > 0$.

Proof. Let us first prove that the normalized dynamics $\bar{a}(t)$ satisfies the (perturbed) *online mirror ascent* recursion:

$$\begin{cases} b_j(t+1) = \bar{a}_j(t) \left(1 + 4\eta(t) \nabla_j G_{\beta(t)}(\bar{a}(t)) + 4\eta(t)^2 |\nabla_j G_{\beta(t)}(\bar{a}(t))|^2\right), \ \forall j \in [m] \\ \bar{a}(t+1) = b(t+1)/\|b(t+1)\|_1. \end{cases}$$

We mention that it is perturbed because for the plain *online mirror ascent*, the multiplicative term in the first line would be $\exp(4\eta(t)\nabla G_{\beta(t)}(\bar{a}(t))$, so we have second order corrections in $\eta(t)$. Since $\nabla_j F(r(t)) = (2/m) r_j(t) \nabla G_1(a(t))$, it follows

$$\begin{aligned} a_j(t+1) &= (r_j(t) + 2\eta(t) r_j(t) \nabla_j G_1(a(t)))^2 \\ &= r_j(t)^2 + 4\eta(t) r_j(t)^2 \nabla_j G_1(a(t)) + 4\eta(t)^2 r_j(t)^2 |\nabla_j G_1(a(t))|^2 \\ &= a_j(t) \left(1 + 4\eta(t) \nabla_j G_1(a(t)) + 4\eta(t)^2 |\nabla_j G_1(a(t)|^2\right) \end{aligned}$$

Now using the fact that $\nabla G_1(a) = \nabla G_{\|a\|_1}(a/\|a\|_1)$, it follows

$$\bar{a}_j(t+1) = \frac{\|a(t)\|_1}{\|a(t+1)\|_1} \bar{a}_j(t) \left(1 + 4\eta(t) \nabla_j G_{\beta(t)}(\bar{a}(t)) + 4\eta(t)^2 |\nabla_j G_{\beta(t)}(\bar{a}(t)|^2\right)$$

hence the iterations. Let us rewrite these iterations using the framework of Bregman divergences (see Bubeck (Chap. 4 2015) for details). For $a, b \in \mathbb{R}_+^m$, let $\phi(a) = \sum_{i=1}^m a_j \log(a_j) - a_j$, let $D(a,b) = \phi(a) - \phi(b) - \nabla\phi(b)^\top (a-b)$ and let $\Pi(a) = a/\|a\|_1 = \arg\min_{b \in \Delta^{m-1}} D(b,a)$ be the Bregman projection on the simplex for the divergence D. With $g(s) = \nabla G_{\beta(s)}(\bar{a}(s))$, we have

$$\begin{cases} \nabla\phi(b(t+1)) = \nabla\phi(\bar{a}(t)) + \eta(t) g(t) + \eta_t^2 e(t) \\ \qquad \bar{a}(t+1) = \Pi(b(t+1)). \end{cases}$$

which are the online mirror ascent updates, with a second-order error term $e(t)_j = \log(1 + 4\eta(s) g_j(t) + 4\eta(t)^2 g_j(t)^2) - 4\eta(t) g_j(t)$. Notice that $\forall t$, $\|g(t)\|_\infty \leq \|z\|_\infty$ so if we assume that $\eta(t) \leq 1/(16\|z\|_\infty)$ we have $\eta(t)\|g(t)\|_\infty \leq 1/16$. Using the inequality $|\log(1+u) - u| \leq u^2$ for $|u| \leq 1/2$, we get (applying it with $u_j = 4\eta(t) g_j(t) + 4\eta(t)^2 g_j(t)^2$)

$$\|e(s)\|_\infty \leq (4\eta(t)\|z\|_\infty + 4\eta(t)^2 \|z\|_\infty^2)^2 + 4\eta(t)^2 \|z\|_\infty^2 \leq 23\eta(t)^2 \|z\|_\infty^2$$

We now follow the usual proof of mirror ascent from Bubeck (2015, Thm. 4.2) (or Beck and Teboulle (2003) for the variable step-size case) and including this error term leads to, for all $\bar{a}^* \in \Delta^{m-1}$,

$$4\eta(t) g(t)^\top (\bar{a}^* - \bar{a}(t)) \leq D(\bar{a}^*, \bar{a}(t)) - D(\bar{a}^*, \bar{a}(t+1)) + 24\eta(t)^2 \|z\|_\infty^2.$$

We get a telescopic sum and using the concavity of each G_β,

$$S(t) := \sum_{s=0}^{t-1} \eta(s)(G_{\beta(s)}(\bar{a}^*) - G_{\beta(s)}(\bar{a}(s))) \leq \frac{1}{4} D(\bar{a}^*, \bar{a}(0)) + 6\|z\|_\infty^2 \sum_{s=0}^{t-1} \eta(s)^2.$$

With our choice of initialization, $D(\bar{a}^*, \bar{a}(0)) \leq \log(m)$. Let us choose $\eta(t) = \tau/\sqrt{t+1}$. Using the inequalities

$$\sum_{s=0}^{t-1} \frac{1}{\sqrt{s+1}} \geq \int_1^{t+1} \frac{ds}{\sqrt{s}} = 2\sqrt{t+1} - 2.$$

and

$$\sum_{s=0}^{t-1} \left(\frac{1}{\sqrt{s+1}}\right)^2 = \sum_{s=1}^{t} \frac{1}{s} \leq 1 + \int_{s=1}^{t} \frac{ds}{s} = 1 + \log(t).$$

It follows that for all $t \geq 1$,

$$S(t) := \frac{\sum_{s=0}^{t-1} \eta(s)(G_{\beta(s)}(\bar{a}^*) - G_{\beta(s)}(\bar{a}(s)))}{\sum_{s=0}^{t-1} \eta(s)} \leq \frac{\log(n)/4 + 6\tau^2 \|z\|_\infty^2 (1 + \log(t))}{2\tau(\sqrt{t+1} - 1)}.$$

In particular, with the choice $\tau = 1/(16\|z\|_\infty)$, we get

$$S(t) \leq \frac{\|z\|_\infty}{\sqrt{t+1}-1}\Big(2\log(m) + (1+\log(t))/4\Big) \leq \frac{\|z\|_\infty}{\sqrt{t}}(8\log(m)+\log(t)+1).$$

where we used $\sqrt{t}/4 \leq \sqrt{t+1}-1$ to simplify the expression. Finally, using inequality (14), we have

$$G_{\beta(s)}(\bar{a}^*) - G_{\beta(s)}(\bar{a}(s)) \geq \min_i z_i^\top \bar{a}^* - \min_i z_i^\top \bar{a}(s) - \frac{\log n}{\beta(s)}.$$

Taking the weighted sum gives

$$\begin{aligned}\gamma_1^{(m)} - \max_{0\leq s\leq t-1} \min_i z_i^\top \bar{a}(s) &\leq S(t) + \frac{\sum_{s=0}^{t-1}\eta(s)(\log n)/\beta(s)}{\sum_{s=0}^{t-1}\eta(s)} \\ &\leq \frac{\|z\|_\infty}{\sqrt{t}}(8\log(m)+\log(t)+1) + \frac{4\log n}{\sqrt{t}}\sum_{s=0}^{t-1}\frac{1}{\beta(s)\sqrt{s+1}}.\end{aligned}$$

The conclusion follows by Lemma E.2. □

In the next result, we show that the norm of the iterates grows to $+\infty$ and that $\sum_{s=0}^{t-1}\frac{1}{\beta(s)\sqrt{s+1}}$ is finite. For simplicity, we do not track the constants.

Lemma E.2. *Under the assumptions of Proposition 4.1, we have that $\beta(t) \to \infty$ and $\sum_{s=0}^{t-1}\frac{1}{\beta(s)\sqrt{s+1}}$ is bounded uniformly in t.*

Proof. For this result, we look at a different online mirror ascent dynamics. We consider $\alpha > 0$ (to be chosen appropriately later) and define $\tilde{\beta}(t) = \max\{1, \max_{0\leq s\leq t}\{\beta(s)/\alpha\}\}$ and the iterates $\tilde{a}(t) = a(t)/\tilde{\beta}(t)$. With the same arguments than in the proof of Proposition 5.1 (below), it can be seen that those iterates satisfy the recursion, with $g(t) = \nabla G_{\tilde{\beta}(t)}(\tilde{a}(t))$,

$$\begin{cases} b_j(t+1) = \tilde{a}_j(t)(1 + 4\eta(t)g_j(t) + 4\eta(t)^2 g_j(t)^2). \\ \tilde{a}(t+1) = b(t+1)/\|b(t+1)\|. \end{cases}$$

These are (perturbed) online mirror ascent iterates for the sequence of losses $G_{\tilde{\beta}(t)}$, step-sizes η_t on the set $\alpha B_+^1 = \{\tilde{a} \in \mathbb{R}_+^m \,;\, \sum_j \tilde{a}_j \leq \alpha\}$. Note that the entropy $\phi(s) = s\log s - s + 1$ is $1/\alpha$ strongly convex with respect to $\|\cdot\|_1$ on this set, and that $\|g\|_\infty$ is bounded uniformly in α. We have the usual mirror descent bound (Chap. 4 Bubeck, 2015) with $\bar{a}^*$ the ℓ_1-max-margin solution,

$$\eta(t)g(s)^\top(\alpha\bar{a}^* - \tilde{a}(t)) \leq H(\alpha\bar{a}^*, \tilde{a}(t+1)) - H(\alpha\bar{a}^*, \tilde{a}(t)) + \alpha C\eta(t)^2$$

where C only depend on $\|z\|_\infty$. By summing we get

$$\begin{aligned}S_\alpha(t) := \frac{\sum_{s=0}^{t-1}\eta(s)g(s)^\top(\alpha\bar{a}^* - \tilde{a}(s))}{\sum_{s=0}^{t-1}\eta(s)} &\leq \frac{H(\alpha\bar{a}^*, \tilde{a}(0)) + C\alpha\sum_{s=0}^{t-1}\eta(s)^2}{\sum_{s=0}^{t-1}\eta(s)} \\ &\lesssim \frac{\alpha\log(\alpha)+\log(t)}{\sqrt{t+1}-1}\end{aligned}$$

where we only track the dependency in t and α. On the other hand, using inequality (14),

$$\begin{aligned}S_\alpha(t) &\geq \frac{\sum_{s=0}^{t-1}\eta(s)(G_{\tilde{\beta}(s)}(\alpha\bar{a}^*) - G_{\tilde{\beta}(s)}(\tilde{a}(s)))}{\sum_{s=0}^{t-1}\eta(s)} \\ &\geq \alpha\gamma_1^{(m)} - \log(n)\Big(\frac{\sum_{s=0}^{t-1}\eta(s)/\tilde{\beta}(s)}{\sum_{s=0}^{t-1}\eta(s)}\Big) - \gamma_1^{(m)}\Big(\frac{\sum_{s=0}^{t-1}\eta(s)\|\tilde{a}(s)\|_1}{\sum_{s=0}^{t-1}\eta(s)}\Big).\end{aligned}$$

Thus, using the fact that $\|\tilde{a}(s)\|_1 \le \|a(s)\| = \beta(s)$, and that $\tilde{\beta}(s) \ge 1$, it follows

$$\frac{\sum_{s=0}^{t-1} \eta(s)\beta(s)}{\sum_{s=0}^{t-1} \eta(s)} \ge \alpha - \frac{\log n}{\gamma_1^{(m)}} - S_\alpha(t).$$

As a consequence

$$\sum_{s=0}^{t-1} \frac{\beta(s)}{\sqrt{s+1}} \gtrsim \sqrt{t+1}\left(\alpha - \frac{\alpha\log(\alpha)+\log(t)}{\sqrt{t+1}-1}\right)$$

Taking for instance $\alpha = \sqrt{t}$ shows that $\sum_{s=0}^{t-1} \frac{\beta(s)}{\sqrt{s+1}} \gtrsim t - \log(t)$ and thus $\beta(t) \to \infty$. By Lemma E.3 then $\beta(t)$ is increasing for $t \ge t_0$ and grows to ∞ at a super-polynomial rate and the conclusion follows. □

We now prove the asymptotic rate of growth of the norm of the iterates.

Lemma E.3. *If $\eta(t) \asymp 1/\sqrt{t+1}$ and $\beta(t) \to \infty$, then $\beta(t)$ is increasing for t large enough and*

$$\log(\beta(t)) \gtrsim \min\{1, \gamma_1^{(m)}\}\sqrt{t}.$$

Proof. We have for all t,

$$\frac{\beta(t+1)}{\beta(t)} = 1 + \eta(t)\nabla S(Za(t))^\top Z\bar{a}(t) + O(1/(t+1)).$$

By Eq. (15) (which holds irrespective of this lemma), we know that $\beta(t) \to \infty$ implies $\bar{a}(t) \to \bar{a}^*$ where $\bar{a}^*$ is the ℓ_1-max-margin solution. Since $\nabla S(Za(t)) \in \Delta^{n-1}$, it holds for t large enough

$$\frac{\beta(t+1)}{\beta(t)} \ge 1 + \frac{1}{2}\gamma_1^{(m)}\eta(t) + O(1/(t+1)).$$

Taking the logarithm and summing, we get

$$\log(\beta(t)) - \log(\beta(0)) \ge \sum_{s=0}^{t-1}\left(\frac{1}{2}\gamma_1^{(m)}\eta(s) + O(1/s)\right) = \frac{1}{2}\gamma_1^{(m)}\sum_{s=0}^{t-1}\eta(s) + O(\log(t)).$$

The result follows since $\sum_{s=0}^{t-1}(t+1)^{-1/2} \ge 2(\sqrt{t-1}-1)$. □

F Appendix to Section 5

Let us recall Proposition 5.1 and prove it.

Proposition F.1. *Let $a(t) = r(t)/m$, $\beta(t) = \max\{1, \max_{0\le s\le t}\sqrt{m}\|a(t)\|_2\}$ and $\bar{a}(t) = a(t)/\beta(t)$ and assume that $\gamma_2^{(m)}$ is positive. For the step-sizes $\eta(t) = \beta(t)\sqrt{2}/(\|z\|_\infty\sqrt{t+1})$ and initialization $r(0) = 0$, it holds*

$$\max_{0\le s\le t-1}\min_{i\in[n]} z_i^\top \bar{a}(s) \ge \gamma_2^{(m)} - \frac{\|z\|_\infty}{\sqrt{t}}\left(2\sqrt{2} + \frac{\sqrt{3}\log n}{\gamma_2^{(m)}}\right).$$

Proof. Using the fact that $a(t) = r(t)/m$ and $m\nabla F(r) = \nabla G(r/m)$ we have

$$a(t+1) = a(t) + \frac{\eta(t)}{m}\nabla G(a(t)).$$

It follows that

$$\frac{a(t+1)}{\beta(t)} = \bar{a}(t) + \frac{\eta(t)}{m\beta(t)}\nabla G_{\beta(t)}(\bar{a}(t)) =: b(t+1).$$

and thus

$$\bar{a}(t+1) = \frac{\beta(t)}{\beta(t+1)}\frac{a(t+1)}{\beta(t)} = \frac{\beta(t)}{\beta(t+1)}b(t+1).$$

Finally, since $\beta(t)\max\{1, \sqrt{m}\|b(t+1)\|_2\} = \max\{\beta(t), \sqrt{m}\|a(t+1)\|_2\} = \beta(t+1)$ it follows that $\bar{a}(t+1) = b(t+1)/\max\{1, \sqrt{m}\|b(t+1)\|_2\}$. Thus $\bar{a}(t)$ follows the iterations $\bar{a}(0) = 0$ and

$$\begin{cases} b(t+1) = \bar{a}(t) + \dfrac{\eta(t)}{m\beta(t)}\nabla G_{\beta(t)}(\bar{a}(t)) \\ \bar{a}(t+1) = b(t+1)/\max\{1, \sqrt{m}\|b(t+1)\|_2\}. \end{cases}$$

These are *online projected gradient ascent* iterations on the set $\{a \in \mathbb{R}^m \ ; \ \sqrt{m}\|a\|_2 \le 1\}$ and for the sequence of functions $G_{\beta(t)}$, with step-size $\eta(t)/(m\beta(t))$. Using the fact that the Lipschitz constant of G_β if upper bounded by $\max_{i\in[n]}\|z_i\|_2 \le \sqrt{m}\|z\|_\infty$ and the diameter of the constraint set is $2/\sqrt{m}$, we have the classical bound, with the step-size $\eta(t)/(m\beta(t)) = \sqrt{2}/(m\|z\|_\infty\sqrt{t+1})$,

$$\frac{1}{t}\sum_{s=0}^{t-1}\left(G_{\beta(s)}(\bar{a}^*) - G_{\beta(s)}(\bar{a}(s))\right) \le \frac{1}{t}DL\sqrt{2t} = \frac{2\sqrt{2}\|z\|_\infty}{\sqrt{t}}.$$

Now using the bound of Eq. (14), it follows

$$\max_{0\le s\le t-1}\min_{i\in[n]} z_i^\top \bar{a}(s) \ge \gamma_2^{(m)} - \frac{\log n}{t}\sum_{s=0}^{t-1}\frac{1}{\beta(s)} - \frac{2\sqrt{2}\|z\|_\infty}{\sqrt{t}}.$$

Let us now look at the evolution of $\beta(t)$. Let $\bar{a}^*$ be a max ℓ_2-margin solution and remark that

$$a(t+1)^\top\bar{a}^* - a(t)^\top\bar{a}^* = \eta(t)\nabla G(a(t))^\top\bar{a}^* \ge \eta(t)\gamma_2^{(m)}$$

since $\nabla G(a(t)) \in \Delta^{m-1}$. It follows that $\beta(t) \ge \sqrt{m}\|a(t)\|_2 \ge m\gamma_2^{(m)}\sum_{s=0}^{s-1}\eta(s)$. Using the fact that $\beta(t) \ge C\sum_{s=0}^{s-1}\beta(s)/\sqrt{s+1}$ with $C = \gamma_2^{(m)}\sqrt{2}/\|z\|_\infty$ and the bound $\sum_{s=0}^{s-1}1/\sqrt{s+1} \ge 2(\sqrt{t-1}-1)$, it follows that $\beta(t) \ge 2C\sqrt{t+1}/\sqrt{6}$ and thus

$$\sum_{s=0}^{t-1}\frac{1}{\beta(s)} \le \frac{\sqrt{6}}{2C}\sum_{s=0}^{t-1}\frac{1}{\sqrt{s+1}} \le \frac{\sqrt{6t}}{C}.$$

Plugging into the previous bound gives the conclusion. Note that we did not attempt to make the lower bound on $\beta(t)$ tight. □

G Appendix to Section 6

Lemma G.1. *Assume that $\|x_i\|_2 \le R$ for $i \in [n]$. For any $\epsilon \in (0,1)$ and $r \in [d]$, there exists $C(r), C_\epsilon(r) > 0$ such that*

$$\gamma_2 \ge \min\left\{C(d), C_\epsilon(d)\left(\frac{\Delta_d(S_n)}{R}\right)^{\frac{d+3}{2-\epsilon}}\right\} \quad \text{and} \quad \gamma_1 \ge \min_{r\in[d]}\min\left\{C(r), C_\epsilon(r)\left(\frac{\Delta_r(S_n)}{R}\right)^{\frac{r+3}{2-\epsilon}}\right\}.$$

Proof. Let $\mathrm{dist}_{\mathcal{S}}$ be the distance function to a set $\mathcal{S}$, i.e. $\mathrm{dist}_{\mathcal{S}}(x) = \inf_{\tilde{x}\in\mathcal{S}} \|x - \tilde{x}\|_2$, which is 1-Lipschitz, and let $D_\pm = \{x_i \,;\, y_i = \pm 1\}$. For P_r a projection that achieves the supremum in Eq. (10) (which exists by compactness of Grassmannians and continuity of the objective), we consider the following function

$$f_r(x) = 2\max\left(0, 1 - \frac{2\,\mathrm{dist}_{P_r(D_+)}(P_r(x))}{\Delta_r(S_n)}\right) - 2\max\left(0, 1 - \frac{2\,\mathrm{dist}_{P_r(D_-)}(P_r(x))}{\Delta_r(S_n)}\right).$$

This function is $4/\Delta_r(S_n)$-Lipschitz continuous, satisfies $\|f\|_\infty \leq 2$ and $y_i f(x_i) = 2$ for all $i \in [n]$. Let us first consider the case $r = d$. Using the approximation results of Lipschitz functions in $\mathcal{F}_2$ from Bach (2017a, Prop. 6), we know that if $N > 0$ is larger than a constant independent of $\Delta_d(S_n)$ and satisfies

$$C(d)\eta(N/\eta)^{-2/(d+1)}\log(N/\eta) \leq 1$$

where $\eta = \max\{2, 4R/\Delta_d(S_n)\} = 4R/\Delta_d(S_n)$, then there exists $\hat{f}$ such that $\|\hat{f}\|_{\mathcal{F}_2} \leq N$ and $\sup_{\|x\|_2\leq R} |\hat{f}(x) - f_d(x)| \leq 1$. Since $\hat{f}/N$ is feasible for the $\mathcal{F}_2$-max-margin problem Eq. (6), this shows that $\gamma_2 \leq 1/N$ and it remains to estimate how large N must be. In the next computations, the dimension dependent constant $C(d)$ might change from line to line. Using the bound $\log(u) \leq C(\epsilon, d)u^{\epsilon/(d+1)}$ for $\epsilon > 0$, we obtain the stronger condition on N:

$$C(\epsilon,d)\eta(N/\eta)^{(\epsilon-2)/(d+1)} \leq 1 \quad \Leftrightarrow \quad N \geq C(\epsilon,d)\eta^{(d+3-\epsilon)/(2-\epsilon)} \leq C(\epsilon,d)\left(\frac{\Delta_d(S_n)}{R}\right)^{(d+3)/(2-\epsilon)}.$$

This gives the bound on γ_2. For the bound on γ_1, it follows from the fact that for all $r \in [d]$, $\mathcal{F}_1$ contains the functions of the form $f \circ P_r$ where f belongs to the space $\mathcal{F}_2$ over $\mathbb{R}^r$ and $\|f \circ P_r\|_{\mathcal{F}_1} \leq \|f\|_{\mathcal{F}_2}$, see arguments and details in Bach (2017a, Section 4.5). □

Theorem G.2 (Generalization bound)**.** *For any $\epsilon \in (0,1)$ and $r \in [d]$, there exist $C(r), C_\epsilon(r) > 0$ such that the following holds. If $(x,y) \sim \mathbb{P}$ is such that for some $R > 0$ and $0 < \Delta_r(\mathbb{P}) \leq C(r)$, it holds $\Delta_r(S_n) \leq \Delta_r(\mathbb{P})$ and $\|x\|_2 \leq R$ almost surely, then for f the $\mathcal{F}_1$-max-margin classifier, it holds with probability at least $1-\delta$ over the choice of i.i.d. samples $S_n = (x_i, y_i)_{i=1}^n$,*

$$\mathbb{P}[yf(x) < 0] \leq \frac{C_\epsilon(r)}{\sqrt{n}}\left(\frac{R}{\Delta_r(\mathbb{P})}\right)^{\frac{r+3}{2-\epsilon}} + \sqrt{\frac{\log(B)}{n}} + \sqrt{\frac{\log(1/\delta)}{2n}}.$$

where $B = \log_2(4(R+1)C_2(r)) + (r+2)\log_2(R/\Delta_r(\mathbb{P}))$. The same bound holds for the $\mathcal{F}_2$-max-margin classifier for $r = d$.

Proof. This is a direct application of the margin-based generalization bounds of Theorem G.3, using that for any $f \in \mathcal{F}_1$ with $\|f\|_{\mathcal{F}_1} \leq 1$,

$$\sup_{\|x\|_2\leq R} f(x) \leq \sup_{\|x\|_2\leq R, \theta\in\mathbb{S}^{p-1}} \phi(\theta, x) \leq R + 1$$

and the same holds in $\mathcal{F}_2$ since for $g \in \mathcal{F}_2$ it holds $g \in \mathcal{F}_1$ and $\|g\|_{\mathcal{F}_1} \leq \|g\|_{\mathcal{F}_2}$ by Jensen's inequality. We also use the Rademacher complexity bound $\mathrm{Rad}_n(B_2) \leq \mathrm{Rad}_n(B_1) \leq \frac{1}{\sqrt{n}}$. where B_i is the unit ball in $\mathcal{F}_i$. This can be found for instance in Bach (2017a, Prop. 7). □

In the next theorem, $\mathcal{F}$ refers to a hypothesis class, $\mathrm{Rad}_n(\mathcal{F})$ to its Rademacher complexity and γ to its margin over the training set (see the cited reference for definitions).

Theorem G.3 (Koltchinskii and Panchenko (2002))**.** *Assume that $\forall f \in \mathcal{F}$ we have $\sup_x |f(x)| \leq C$. Then, with probability at least $1-\delta$ over the sample, for all margins $\gamma > 0$ and all $f \in \mathcal{F}$ we have*

$$\mathbb{P}[yf(x) < 0] \leq 4\frac{\mathrm{Rad}_n(\mathcal{F})}{\gamma} + \sqrt{\frac{\log(\log_2 \frac{4C}{\gamma})}{n}} + \sqrt{\frac{\log(1/\delta)}{2n}}.$$