# Analysis of Gradient Descent on Wide Two-Layer ReLU Neural Networks

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# Supervised learning with neural networks

## Prediction/classification task

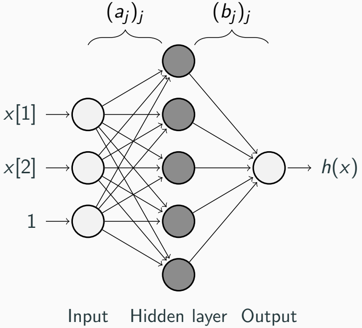
- Couple of random variables $(X, Y)$ on $\mathbb{R}^d \times \mathbb{R}$
- Given $n$ i.i.d. samples $(x_i, y_i)_{i=1}^n$, build $h$ s.t. $h(X) \approx Y$

## Wide 2-layer ReLU neural network

For a *width* $m \gg 1$, predictor $h$ given by

$$h((w_j)_j, x) := \frac{1}{m} \sum_{j=1}^{m} \phi(w_j, x)$$

where $\begin{cases} \phi(w, x) := b\,(a^\top [x; 1])_+ \\ w := (a, b) \in \mathbb{R}^{d+1} \times \mathbb{R} \end{cases}.$




$\rightsquigarrow$ $\phi$ is 2-homogeneous in $w$, i.e. $\phi(rw, x) = r^2 \phi(w, x), \forall r > 0$

# Gradient flow of the empirical risk

Convex smooth loss $\ell$: $\begin{cases} \ell(p,y) = \log(1+\exp(-yp)) & \text{(logistic)} \\ \ell(p,y) = (y-p)^2 & \text{(square)} \end{cases}$

**Empirical risk with weight decay ($\lambda \geq 0$)**

$$F_m((w_j)_j) := \underbrace{\frac{1}{n}\sum_{i=1}^{n} \ell(h((w_j)_j, x_i), y_i)}_{\text{empirical risk}} \quad + \quad \underbrace{\frac{\lambda}{m}\sum_{j=1}^{m} \|w_j\|_2^2}_{\text{(optional) regularization}}$$

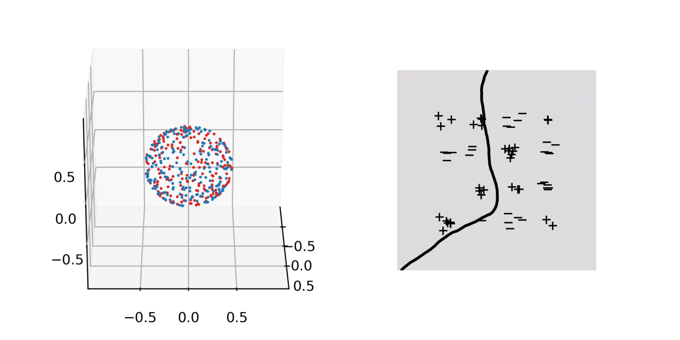
**Gradient-based learning**

- Initialize $w_1(0), \dots, w_m(0) \overset{\text{i.i.d}}{\sim} \mu_0 \in \mathcal{P}_2(\mathbb{R}^{d+1} \times \mathbb{R})$
- Decrease the non-convex objective via gradient flow, for $t \geq 0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}(w_j(t))_j = -m\nabla F_m((w_j(t))_j)$$

$\rightsquigarrow$ in practice, discretized with variants of gradient descent

# Illustration




## Space of parameters

- plot $|b| \cdot a$
- color depends on sign of $b$
- tanh radial scale

## Space of predictors

- $(+/-)$ training set
- color shows $h((w_j(t))_j, \cdot)$
- line shows 0 level set

**Main question**

What is performance of the learnt predictor $h((w_j(\infty))_j, \cdot)$ ?

# Motivations

- Understanding 2-layer networks
  - ⇝ role of initialization $\mu_0$, loss, regularization, data structure, etc.
- Understanding representation learning via back-propagation
  - ⇝ not captured by current theories for deeper models who study perturbative regimes around the initialization (e.g. NTK)
- Natural next theoretical step after linear models
  - ⇝ we can't understand the deep if we don't understand the shallow

# Outline

Global convergence in the infinite width limit

Generalization with regularization

Unregularized case: implicit bias

# Global convergence in the infinite width limit

# Dynamics in the infinite width limit

- Parameterize with a probability measure $\mu \in \mathcal{P}_2(\mathbb{R}^{d+2})$

$$h(\mu, x) = \int \phi(w, x)\,\mathrm{d}\mu(w)$$

- Objective on the space of probability measures

$$F(\mu) := \frac{1}{n}\sum_{i=1}^{n} \ell(h(\mu, x_i), y_i) + \lambda \int \|w\|_2^2\,\mathrm{d}\mu(w)$$

**Theorem (dynamical infinite width limit, adapted to ReLU)**

Assume that

$$\mathrm{spt}(\mu_0) \subset \{(a, b) \in \mathbb{R}^{d+1} \times \mathbb{R}\ ;\ \|a\|_2 = |b|\}.$$

As $m \to \infty$, $\mu_{t,m} = \frac{1}{m}\sum_{j=1}^{m} \delta_{w_j(t)}$ converges in $\mathcal{P}_2(\mathbb{R}^{d+2})$ to $\mu_t$, the unique Wasserstein gradient flow of $F$ starting from $\mu_0$.

Ambrosio, Gigli, Savaré (2008). *Gradient flows: in metric spaces and in the space of probability measures.*

# Global convergence

**Theorem (C. & Bach, '18, adapted to ReLU)**

*Assume that* $\mu_0 = \mathcal{U}_{\mathbb{S}^d} \otimes \mathcal{U}_{\{-1,1\}}$ *and technical conditions. If* $\mu_t$ *converges to* $\mu_\infty$ *in* $\mathcal{P}_2(\mathbb{R}^{d+2})$*, then* $\mu_\infty$ *is a global minimizer of* $F$*.*

- Initialization matters: the key assumption on $\mu_0$ is *diversity*
- Corollary: $\lim_{m,t\to\infty} F(\mu_{m,t}) = \min F$
- Open question: convergence of $\mu_t$

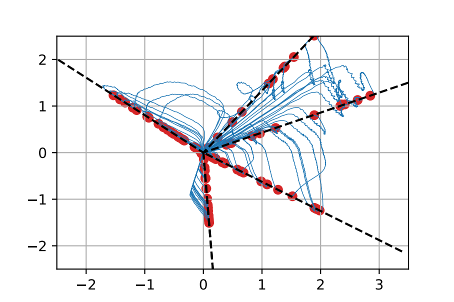
**Performance of the learnt predictor?**

Depends on the objective $F$ and the data! If $F$ is the ...

- **regularized empirical risk**: "just" statistics (this talk)
- **unregularized empirical risk**: need implicit bias (this talk)
- **population risk**: need convergence speed (open question)

Chizat, Bach (2018). *On the Global Convergence of Gradient Descent for Over-parameterized Models [...].*

# Illustration of global convergence (population risk)




Stochastic gradient descent on expected square loss ($m = 100$, $d = 1$)
Teacher-student setting: $X \sim \mathcal{U}_{\mathbb{S}^d}$ and $Y = f^*(X)$ where $f^*$ is a ReLU neural network with 5 units (dashed lines).

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**[Related work studying infinite width limits]:**

Nitanda, Suzuki (2017). *Stochastic particle gradient descent for infinite ensembles.*

Mei, Montanari, Nguyen (2018). *A Mean Field View of the Landscape of Two-Layers Neural Networks.*

Rotskoff, Vanden-Eijndem (2018). *Parameters as Interacting Particles [...].*

Sirignano, Spiliopoulos (2018). *Mean Field Analysis of Neural Networks.*

Wojtowytsch (2020). *On the Convergence of Gradient Descent Training for Two-layer ReLU-networks [...]*

# Generalization with regularization

# Variation norm

## Definition (Variation norm)

For a predictor $h : \mathbb{R}^d \to \mathbb{R}$, its variation norm is

$$\|h\|_{\mathcal{F}_1} := \min_{\mu \in \mathcal{P}_2(\mathbb{R}^{d+2})} \left\{ \frac{1}{2} \int \|w\|_2^2 \, \mathrm{d}\mu(w) \; ; \; h(x) = \int \phi(w, x) \, \mathrm{d}\mu(w) \right\}$$
$$= \min_{\nu \in \mathcal{M}(\mathbb{S}^d)} \left\{ \|\nu\|_{TV} \; ; \; h(x) = \int (a^\top [x; 1])_+ \, \mathrm{d}\nu(a) \right\}$$

## Proposition

*If $\mu^* \in \mathcal{P}_2(\mathbb{R}^{d+2})$ minimizes $F$ then $h(\mu^*, \cdot)$ minimizes*

$$\frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), y_i) + 2\lambda \|h\|_{\mathcal{F}_1}.$$


Barron (1993). *Universal approximation bounds for superpositions of a sigmoidal function.*
Kurkova, Sanguineti (2001). *Bounds on rates of variable-basis and neural-network approximation.*
Neyshabur, Tomioka, Srebro (2015). *Norm-Based Capacity Control in Neural Networks.*

# Generalization with variation norm regularization

## Regression of a Lipschitz function

Assume that $X$ is bounded and $Y = f^*(X)$ where $f^*$ is 1-Lipschitz.
Error bound on $\mathbf{E}\left[(h(X) - f^*(X))^2\right]$ for any estimator $h$?

$\rightsquigarrow$ in general $\succeq n^{-1/d}$ unavoidable (curse of dimensionality)

**Anisotropy assumption:**

What if moreover $f^*(x) = g(\pi_r(x))$ for some rank $r$ projection $\pi_r$?

## Theorem (Bach '14, reformulated)

*For a suitable choice of regularization $\lambda(n) > 0$, the minimizer of $F$ with square loss enjoys an error bound in $\tilde{O}(n^{-1/(r+3)})$.*

- methods with fixed features (e.g. kernels) remain $\sim n^{-1/d}$
- no need to bound the number $m$ of units

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Bach (2014). *Breaking the curse of dimensionality with convex neural networks.*

# Fixing hidden layer and conjugate RKHS

What if we only train the output layer?

$\rightsquigarrow$ Let $\mathcal{S} := \{\mu \in \mathcal{P}_2(\mathbb{R}^{d+2})$ with marginal $\mathcal{U}_{\mathbb{S}^d}$ on input weights$\}$

**Definition (Conjugate RKHS)**

For a predictor $h : \mathbb{R}^d \to \mathbb{R}$, its conjugate RKHS norm is

$$\|h\|^2_{\mathcal{F}_2} := \min \left\{ \int |b|_2^2 \, \mathrm{d}\mu(a, b) \; ; \; h = \int \phi(w, \cdot) \, \mathrm{d}\mu(w), \; \mu \in \mathcal{S} \right\}$$

**Proposition (Kernel ridge regression)**

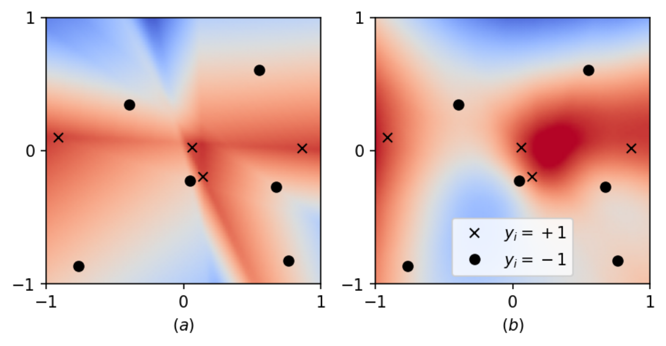
*All else unchanged, fixing the hidden layer leads to minimizing*

$$\frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), y_i) + \lambda \|h\|^2_{\mathcal{F}_2}.$$

- Solving: $\mathcal{F}_2$ random features, convex optim. / $\mathcal{F}_1$ difficult
- Priors: $\mathcal{F}_2$ isotropic smoothness / $\mathcal{F}_1$ anisotropic smoothness

# Illustration of the predictor

Predictor learnt via gradient descent (square loss & weight decay)




(a) Training both layers ($\mathcal{F}_1$-norm) (b) Training output layer ($\mathcal{F}_2$-norm)

# Unregularized case: implicit bias

# Preliminary: linear classification and exponential loss

## Classification task

- $Y \in \{-1, 1\}$ and the prediction is $\text{sign}(h(X))$
- $\ell(p, y) = \exp(-py)$ or logistic $\ell(p, y) = \log(1 + \exp(-py))$
- no regularization ($\lambda = 0$)

## Theorem (SHNGS 2018, reformulated)

*Consider $h(w, x) = w^\intercal x$ and a linearly separable training set. For any $w(0)$, the normalized gradient flow $\bar{w}(t) = w(t)/\|w(t)\|_2$ converges to a $\|\cdot\|_2$-max-margin classifier, i.e. a solution to*

$$\max_{\|w\|_2 \leq 1} \min_{i \in [n]} y_i \cdot w^\intercal x_i.$$

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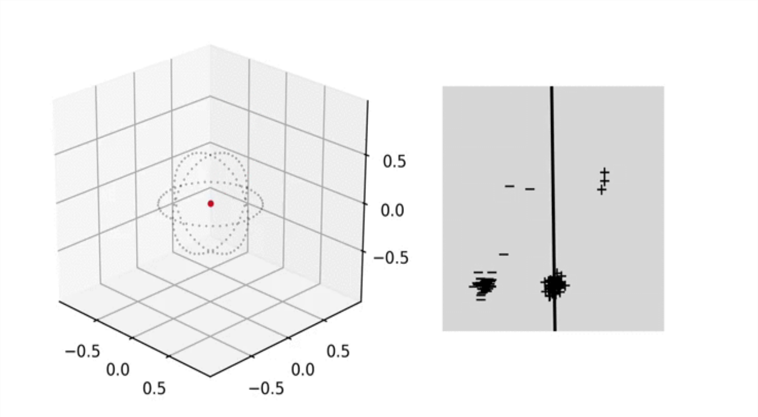
Telgarsky (2013). *Margins, shrinkage, and boosting.*

Soudry, Hoffer, Nacson, Gunasekar, Srebro (2018). *The Implicit Bias of Gradient Descent on Separable Data.*

# Implicit bias for linear classification: illustration




Implicit bias of gradient descent for classification ($d = 2$)

# Implicit bias for two-layer neural networks

Let us go back to wide two-layer ReLU neural networks.

**Theorem (C. & Bach, 2020)**

*Assume that* $\mu_0 = \mathcal{U}_{\mathbb{S}^d} \otimes \mathcal{U}_{\{-1,1\}}$, *that the training set is consistant* ( $[x_i = x_j] \Rightarrow [y_i = y_j]$) *and other technical conditions. Then* $h(\mu_t, \cdot)/\|h(\mu_t, \cdot)\|_{\mathcal{F}_1}$ *converges to the* $\mathcal{F}_1$*-max-margin classifier, i.e. it solves*

$$\max_{\|h\|_{\mathcal{F}_1} \leq 1} \min_{i \in [n]} y_i h(x_i).$$

- no efficient algorithm is known to solve this problem
- fixing the hidden layer leads to the $\mathcal{F}_2$-max-margin classifier
- well also prove convergence speed bounds in simpler settings

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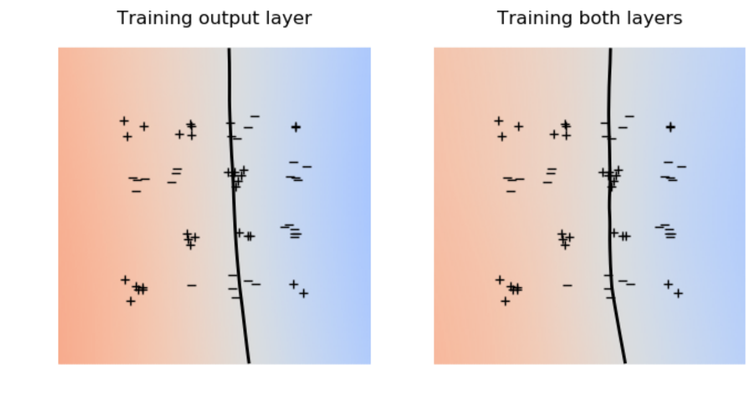
Chizat, Bach (2020). *Implicit Bias of Gradient Descent for Wide Two-layer Neural Networks [...].*

# Illustration



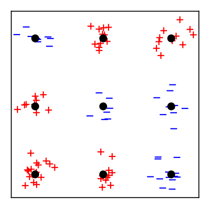

$h(\mu_t, \cdot)$ for the exponential loss, $\lambda = 0$ ($d = 2$)

# Numerical experiments

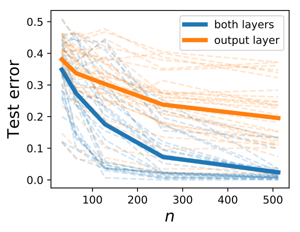
## Setting

Two-class classification in dimension $d = 15$:

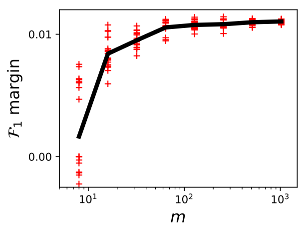
- two first coordinates as shown on the right
- all other coordinates uniformly at random



Coordinates 1 & 2




**(a)** Test error vs. $n$




**(b)** Margin vs. $m$ ($n = 256$)

# Statistical efficiency

Assume that $\|X\|_2 \leq D$ a.s. and that, for some $r \leq d$, it holds a.s.

$$\Delta(r) \leq \sup_{\pi} \left\{ \inf_{y_i \neq y_{i'}} \|\pi(x_i) - \pi(x_{i'})\|_2 \; ; \; \pi \text{ is a rank } r \text{ projection} \right\}.$$

**Theorem (C. & Bach, 2020)**

*The $\mathcal{F}_1$-max-margin classifier $h^*$ admits the risk bound, with probability $1-\delta$ (over the random training set),*

$$\underbrace{\mathbf{P}(Y\, h^*(X) < 0)}_{\text{proportion of mistakes}} \lesssim \frac{1}{\sqrt{n}}\left[\left(\frac{D}{\Delta(r)}\right)^{\frac{r}{2}+2} + \sqrt{\log(1/\delta)}\right].$$

- this is a strong *dimension independent* non-asymptotic bound
- for learning in $\mathcal{F}_2$ the bound with $r = d$ is true
- this task is *asymptotically* easy (the rate $n^{-1/2}$ is suboptimal)

**[Refs]:**

Chizat, Bach (2020). *Implicit Bias of Gradient Descent for Wide Two-layer Neural Networks [...].*

# Two implicit biases in one dynamics (I)

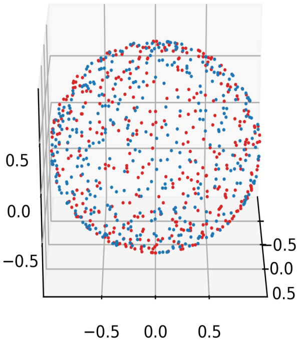
**Lazy training (informal)**

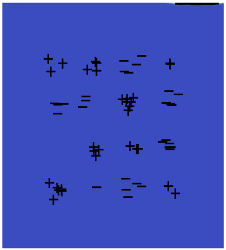
All other things equal, if the variance at initialization is large and the step-size is small then the model behaves like its first order expansion over a significant time.

- Each neuron hardly moves but the total change in $h(\mu_t, \cdot)$ is significant
- Here the linearization converges to a max-margin classifier in the tangent RKHS (similar to $\mathcal{F}_2$)
- Eventually converges to $\mathcal{F}_1$-max-margin

Jacot, Gabriel, Hongler (2018). *Neural Tangent Kernel: Convergence and Generalization in Neural Networks.*
Chizat, Oyallon, Bach (2018). *On Lazy Training in Differentiable Programming.*
Woodworth et al. (2019). *Kernel and deep regimes in overparametrized models.*

# Two implicit biases in one dynamics (II)



**Space of parameters** **Space of predictors**

See also: Moroshko, Gunasekar, Woodworth, Lee, Srebro, Soudry (2020). *Implicit Bias in Deep Linear Classification: Initialization Scale vs Training Accuracy*.

## Perspectives

- **Quantitative bounds for optimization**
- **More complex architectures**

[Papers :]

- Chizat, Bach (2018). On the Global Convergence of Over-parameterized Models using Optimal Transport
- Chizat, Oyallon, Bach (2019). On Lazy Training in Differentiable Programming
- Chizat (2019). Sparse Optimization on Measures with Over-parameterized Gradient Descent
- Chizat, Bach (2020). Implicit Bias of Gradient Descent for Wide Two-layer Neural Networks Trained with the Logistic Loss

[Blog post :]

- https://francisbach.com/